Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:43 PM UTC

PDB ID	:	8WM6 / pdb_00008wm6
EMDB ID	:	EMD-37642
Title	:	The structure of PSI-CAC(L-14)of R.salina at 2.7 angstroms resolution
Authors	:	Zhang, S.M.; Si, L.; Li, M.
Deposited on	:	2023-10-03
Resolution	:	2.70 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:

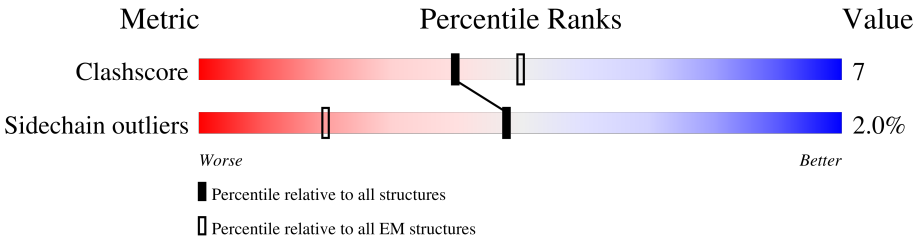
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

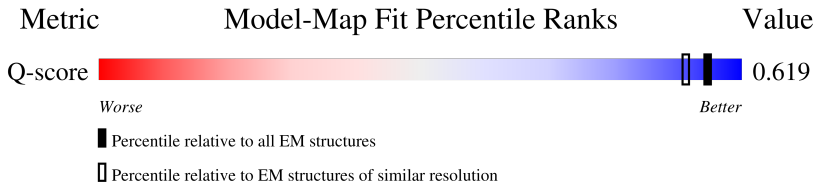
1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	A	752	87% 11%
2	B	734	87% 12%
3	C	81	81% 17%
4	D	141	81% 17%
5	E	64	84% 9% 6%

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Mol	Chain	Length	Quality of chain
6	F	188	76% 10% 14%
7	I	36	81% 14% 6%
8	J	42	88% 12%
9	L	153	87% 11%
10	M	30	90% 10%
11	O	146	5% 53% 16% 29%
12	K	87	61% 18% 21%
13	s	269	50% 7% 43%
14	c	216	68% 10% 21%
15	a	216	71% 9% 19%
16	b	223	70% 17% 13%
17	h	225	65% 6% 28%
18	f	212	68% 13% 18%
18	j	212	68% 12% 19%
18	m	212	69% 13% 18%
19	e	203	74% 8% 17%
20	l	238	65% 9% 26%
21	k	241	9% 60% 14% 25%
22	i	218	18% 70% 11% 20%
23	d	213	21% 46% 14% 39%
24	g	255	8% 73% 12% 14%
25	R	129	64% 6% 30%
26	n	219	8% 68% 14% 17%
27	Q	234	59% 59% 16% 24%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	A	801	X	-	-	-
28	CLA	A	802	X	-	-	-
28	CLA	A	803	X	-	-	-
28	CLA	A	804	X	-	-	-
28	CLA	A	805	X	-	-	-
28	CLA	A	806	X	-	-	-
28	CLA	A	807	X	-	-	-
28	CLA	A	808	X	-	-	-
28	CLA	A	809	X	-	-	-
28	CLA	A	810	X	-	-	-
28	CLA	A	812	X	-	-	-
28	CLA	A	813	X	-	-	-
28	CLA	A	815	X	-	-	-
28	CLA	A	816	X	-	-	-
28	CLA	A	817	X	-	-	-
28	CLA	A	818	X	-	-	-
28	CLA	A	819	X	-	-	-
28	CLA	A	820	X	-	-	-
28	CLA	A	822	X	-	-	-
28	CLA	A	824	X	-	-	-
28	CLA	A	826	X	-	-	-
28	CLA	A	827	X	-	-	-
28	CLA	A	829	X	-	-	-
28	CLA	A	831	X	-	-	-
28	CLA	A	832	X	-	-	-
28	CLA	A	833	X	-	-	-
28	CLA	A	834	X	-	-	-
28	CLA	A	835	X	-	-	-
28	CLA	A	837	X	-	-	-
28	CLA	A	838	X	-	-	-
28	CLA	A	839	X	-	-	-
28	CLA	A	840	X	-	-	-
28	CLA	A	841	X	-	-	-
28	CLA	A	851	X	-	-	-
28	CLA	A	852	X	-	-	-
28	CLA	A	854	X	-	-	-
28	CLA	A	855	X	-	-	-
28	CLA	B	801	X	-	-	-
28	CLA	B	802	X	-	-	-
28	CLA	B	803	X	-	-	-
28	CLA	B	804	X	-	-	-
28	CLA	B	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	B	806	X	-	-	-
28	CLA	B	807	X	-	-	-
28	CLA	B	808	X	-	-	-
28	CLA	B	809	X	-	-	-
28	CLA	B	810	X	-	-	-
28	CLA	B	811	X	-	-	-
28	CLA	B	812	X	-	-	-
28	CLA	B	813	X	-	-	-
28	CLA	B	815	X	-	-	-
28	CLA	B	817	X	-	-	-
28	CLA	B	820	X	-	-	-
28	CLA	B	821	X	-	-	-
28	CLA	B	823	X	-	-	-
28	CLA	B	824	X	-	-	-
28	CLA	B	825	X	-	-	-
28	CLA	B	826	X	-	-	-
28	CLA	B	828	X	-	-	-
28	CLA	B	830	X	-	-	-
28	CLA	B	831	X	-	-	-
28	CLA	B	832	X	-	-	-
28	CLA	B	833	X	-	-	-
28	CLA	B	834	X	-	-	-
28	CLA	B	835	X	-	-	-
28	CLA	B	836	X	-	-	-
28	CLA	B	837	X	-	-	-
28	CLA	B	838	X	-	-	-
28	CLA	B	839	X	-	-	-
28	CLA	B	840	X	-	-	-
28	CLA	F	201	X	-	-	-
28	CLA	F	202	X	-	-	-
28	CLA	J	103	X	-	-	-
28	CLA	K	101	X	-	-	-
28	CLA	K	103	X	-	-	-
28	CLA	L	202	X	-	-	-
28	CLA	L	207	X	-	-	-
28	CLA	O	201	X	-	-	-
28	CLA	O	202	X	-	-	-
28	CLA	O	206	X	-	-	-
28	CLA	Q	302	X	-	-	-
28	CLA	Q	303	X	-	-	-
28	CLA	R	203	X	-	-	-
28	CLA	a	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	a	304	X	-	-	-
28	CLA	a	305	X	-	-	-
28	CLA	a	306	X	-	-	-
28	CLA	a	307	X	-	-	-
28	CLA	a	308	X	-	-	-
28	CLA	a	309	X	-	-	-
28	CLA	a	310	X	-	-	-
28	CLA	a	311	X	-	-	-
28	CLA	a	312	X	-	-	-
28	CLA	b	601	X	-	-	-
28	CLA	b	602	X	-	-	-
28	CLA	b	603	X	-	-	-
28	CLA	b	605	X	-	-	-
28	CLA	b	606	X	-	-	-
28	CLA	b	607	X	-	-	-
28	CLA	b	608	X	-	-	-
28	CLA	b	609	X	-	-	-
28	CLA	b	610	X	-	-	-
28	CLA	b	611	X	-	-	-
28	CLA	b	612	X	-	-	-
28	CLA	c	601	X	-	-	-
28	CLA	c	602	X	-	-	-
28	CLA	c	603	X	-	-	-
28	CLA	c	605	X	-	-	-
28	CLA	c	607	X	-	-	-
28	CLA	c	608	X	-	-	-
28	CLA	c	609	X	-	-	-
28	CLA	c	612	X	-	-	-
28	CLA	d	301	X	-	-	-
28	CLA	d	302	X	-	-	-
28	CLA	d	303	X	-	-	-
28	CLA	d	304	X	-	-	-
28	CLA	d	305	X	-	-	-
28	CLA	d	306	X	-	-	-
28	CLA	d	307	X	-	-	-
28	CLA	d	308	X	-	-	-
28	CLA	d	309	X	-	-	-
28	CLA	e	601	X	-	-	-
28	CLA	e	603	X	-	-	-
28	CLA	e	606	X	-	-	-
28	CLA	e	607	X	-	-	-
28	CLA	e	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	e	610	X	-	-	-
28	CLA	e	611	X	-	-	-
28	CLA	f	601	X	-	-	-
28	CLA	f	602	X	-	-	-
28	CLA	f	603	X	-	-	-
28	CLA	f	604	X	-	-	-
28	CLA	f	608	X	-	-	-
28	CLA	f	609	X	-	-	-
28	CLA	f	610	X	-	-	-
28	CLA	f	612	X	-	-	-
28	CLA	f	613	X	-	-	-
28	CLA	g	302	X	-	-	-
28	CLA	g	303	X	-	-	-
28	CLA	g	304	X	-	-	-
28	CLA	g	306	X	-	-	-
28	CLA	g	307	X	-	-	-
28	CLA	g	308	X	-	-	-
28	CLA	g	309	X	-	-	-
28	CLA	g	310	X	-	-	-
28	CLA	g	311	X	-	-	-
28	CLA	g	315	X	-	-	-
28	CLA	g	322	X	-	-	-
28	CLA	h	302	X	-	-	-
28	CLA	h	303	X	-	-	-
28	CLA	h	304	X	-	-	-
28	CLA	h	305	X	-	-	-
28	CLA	h	306	X	-	-	-
28	CLA	h	307	X	-	-	-
28	CLA	h	308	X	-	-	-
28	CLA	h	313	X	-	-	-
28	CLA	i	302	X	-	-	-
28	CLA	i	303	X	-	-	-
28	CLA	i	304	X	-	-	-
28	CLA	i	306	X	-	-	-
28	CLA	i	307	X	-	-	-
28	CLA	i	308	X	-	-	-
28	CLA	i	309	X	-	-	-
28	CLA	i	311	X	-	-	-
28	CLA	i	312	X	-	-	-
28	CLA	j	601	X	-	-	-
28	CLA	j	602	X	-	-	-
28	CLA	j	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	j	605	X	-	-	-
28	CLA	j	606	X	-	-	-
28	CLA	j	607	X	-	-	-
28	CLA	j	608	X	-	-	-
28	CLA	j	609	X	-	-	-
28	CLA	j	610	X	-	-	-
28	CLA	j	612	X	-	-	-
28	CLA	j	613	X	-	-	-
28	CLA	k	602	X	-	-	-
28	CLA	k	603	X	-	-	-
28	CLA	k	604	X	-	-	-
28	CLA	k	605	X	-	-	-
28	CLA	k	607	X	-	-	-
28	CLA	k	608	X	-	-	-
28	CLA	k	609	X	-	-	-
28	CLA	k	610	X	-	-	-
28	CLA	k	614	X	-	-	-
28	CLA	l	302	X	-	-	-
28	CLA	l	303	X	-	-	-
28	CLA	l	304	X	-	-	-
28	CLA	l	305	X	-	-	-
28	CLA	l	306	X	-	-	-
28	CLA	l	307	X	-	-	-
28	CLA	l	308	X	-	-	-
28	CLA	l	309	X	-	-	-
28	CLA	l	311	X	-	-	-
28	CLA	m	601	X	-	-	-
28	CLA	m	602	X	-	-	-
28	CLA	m	603	X	-	-	-
28	CLA	m	606	X	-	-	-
28	CLA	m	607	X	-	-	-
28	CLA	m	608	X	-	-	-
28	CLA	m	609	X	-	-	-
28	CLA	m	610	X	-	-	-
28	CLA	m	612	X	-	-	-
28	CLA	m	613	X	-	-	-
28	CLA	n	601	X	-	-	-
28	CLA	n	603	X	-	-	-
28	CLA	n	604	X	-	-	-
28	CLA	n	605	X	-	-	-
28	CLA	n	606	X	-	-	-
28	CLA	n	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	n	608	X	-	-	-
28	CLA	n	609	X	-	-	-
28	CLA	n	610	X	-	-	-
28	CLA	n	613	X	-	-	-
28	CLA	s	202	X	-	-	-
28	CLA	s	206	X	-	-	-
28	CLA	s	208	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 61164 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	742	5825	3802	994	1001	28	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5826	3844	982	985	15	1	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	592	361	103	116	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	139	1084	692	186	203	3	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	60	484	309	84	91	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1254	814	212	226	2	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			264	182	35	45	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	S	0	0
			351	240	49	59	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	151	Total	C	N	O	S	0	0
			1146	753	182	208	3		

- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			232	155	38	38	1		

- Molecule 11 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	104	Total	C	N	O	S	0	0
			773	515	117	138	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	69	Total	C	N	O	S	0	0
			488	319	80	87	2		

- Molecule 13 is a protein called chain s.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	154	Total	C	N	O	S	0	0
			1140	719	195	217	9		

- Molecule 14 is a protein called cac-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	170	Total	C	N	O	S	0	0
			1357	897	221	236	3		

- Molecule 15 is a protein called cac-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	175	Total	C	N	O	S	0	0
			1361	889	217	245	10		

- Molecule 16 is a protein called cac-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	194	Total	C	N	O	S	0	0
			1439	916	251	258	14		

- Molecule 17 is a protein called cac-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	162	Total	C	N	O	S	0	0
			1200	778	202	214	6		

- Molecule 18 is a protein called cac-f.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	174	Total	C	N	O	S	0	0
			1309	846	214	241	8		
18	f	174	Total	C	N	O	S	0	0
			1302	842	212	240	8		
18	j	172	Total	C	N	O	S	0	0
			1293	834	212	239	8		

- Molecule 19 is a protein called cac-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	169	Total	C	N	O	S	0	0
			1286	843	207	228	8		

- Molecule 20 is a protein called cac-l.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	175	Total	C	N	O	S	0	0
			1344	869	230	238	7		

- Molecule 21 is a protein called cac-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	180	Total	C	N	O	S	0	0
			1346	872	223	239	12		

- Molecule 22 is a protein called cac-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	175	Total	C	N	O	S	0	0
			1324	849	227	237	11		

- Molecule 23 is a protein called cac-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	129	Total	C	N	O	S	0	0
			974	624	169	171	10		

- Molecule 24 is a protein called cac-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	219	Total	C	N	O	S	0	0
			1630	1060	267	292	11		

- Molecule 25 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	90	Total	C	N	O	S	0	0
			664	434	105	124	1		

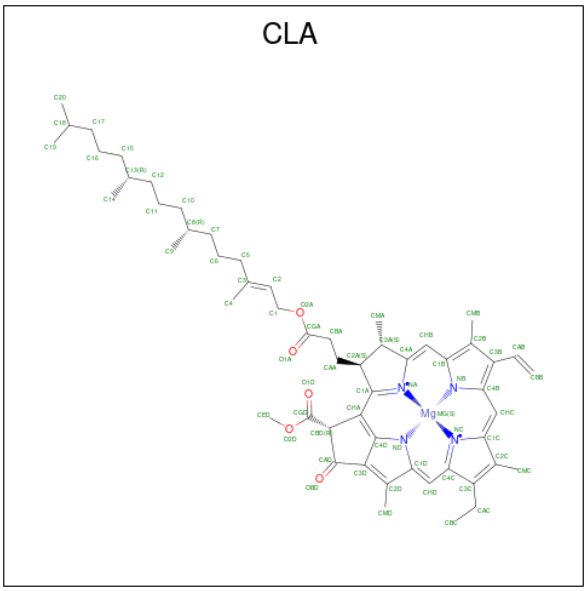
- Molecule 26 is a protein called cac-n.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	181	Total	C	N	O	S	0	0
			1350	870	228	242	10		

- Molecule 27 is a protein called PsaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	179	Total	C	N	O	S	0	0
			1294	814	222	252	6		

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
28	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	A	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
28	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	s	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	m	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
28	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	k	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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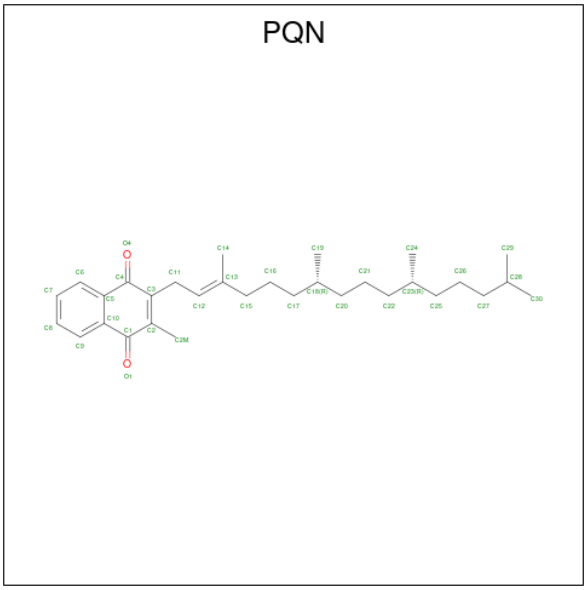
Mol	Chain	Residues	Atoms					AltConf
28	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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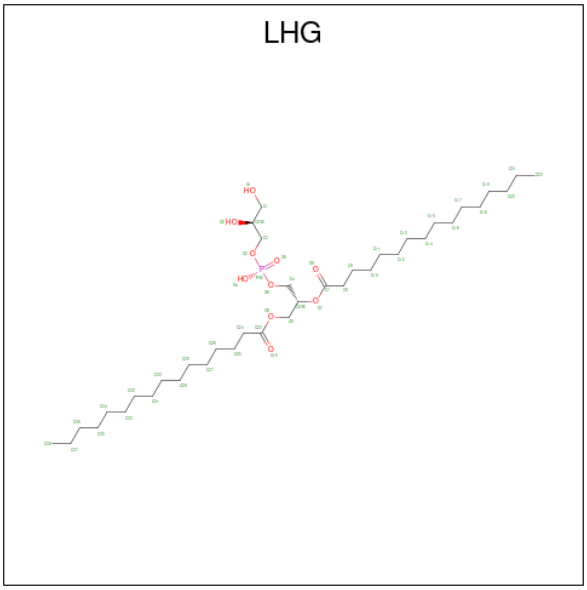
Mol	Chain	Residues	Atoms					AltConf
28	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total 33	C 31	O 2	0
29	B	1	Total 33	C 31	O 2	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



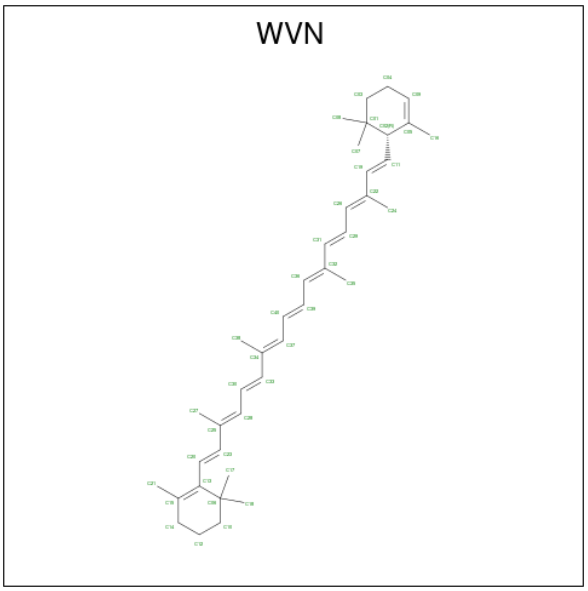
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total 48	C 37	O 10	P 1	0
30	A	1	Total 27	C 16	O 10	P 1	0
30	A	1	Total 38	C 27	O 10	P 1	0
30	J	1	Total 49	C 38	O 10	P 1	0
30	L	1	Total 49	C 38	O 10	P 1	0
30	c	1	Total 37	C 26	O 10	P 1	0
30	c	1	Total 37	C 26	O 10	P 1	0
30	a	1	Total 49	C 38	O 10	P 1	0
30	a	1	Total 49	C 38	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			31	20	10	1	
30	m	1	Total	C	O	P	0
			37	26	10	1	
30	e	1	Total	C	O	P	0
			37	26	10	1	
30	l	1	Total	C	O	P	0
			32	21	10	1	
30	k	1	Total	C	O	P	0
			37	26	10	1	
30	f	1	Total	C	O	P	0
			49	38	10	1	
30	i	1	Total	C	O	P	0
			37	26	10	1	
30	j	1	Total	C	O	P	0
			30	19	10	1	
30	d	1	Total	C	O	P	0
			37	26	10	1	
30	g	1	Total	C	O	P	0
			37	26	10	1	
30	g	1	Total	C	O	P	0
			37	26	10	1	
30	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 31 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: $C_{40}H_{56}$).



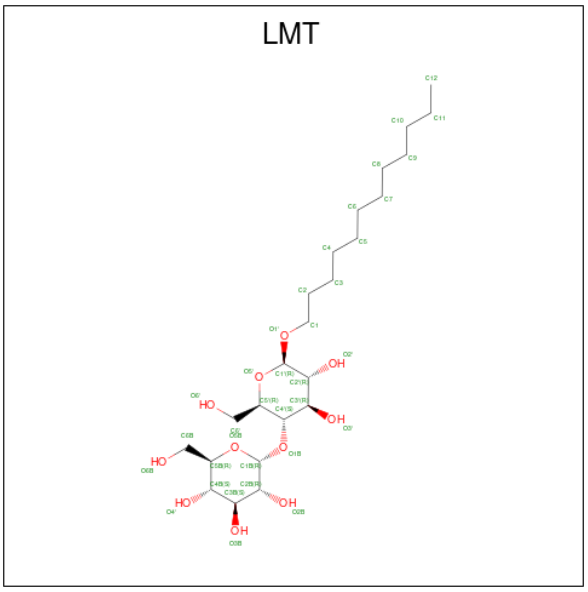
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	F	1	Total C 40 40	0
31	F	1	Total C 40 40	0
31	I	1	Total C 40 40	0
31	J	1	Total C 40 40	0
31	J	1	Total C 40 40	0

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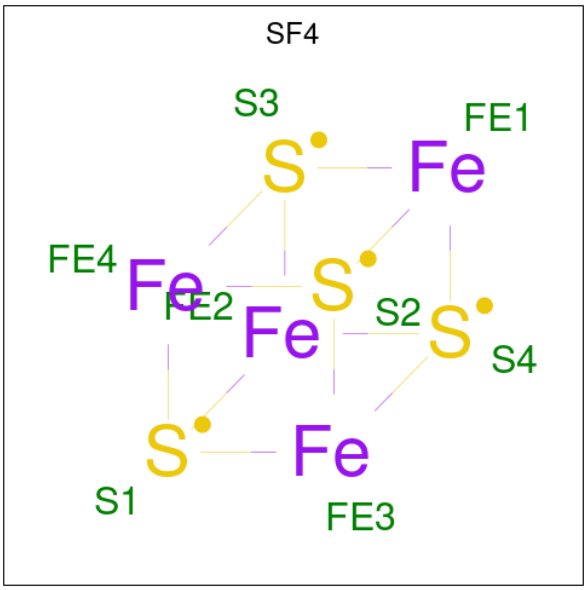
Mol	Chain	Residues	Atoms	AltConf
31	L	1	Total C 40 40	0
31	L	1	Total C 40 40	0
31	L	1	Total C 40 40	0
31	M	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	e	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	i	1	Total C 40 40	0
31	R	1	Total C 40 40	0
31	R	1	Total C 40 40	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



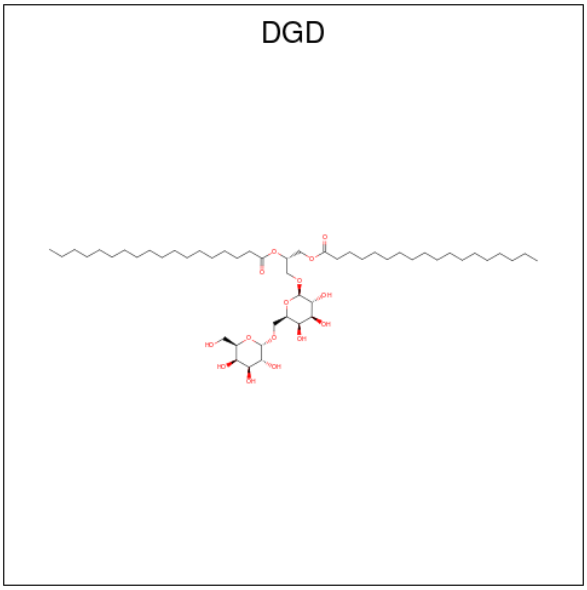
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 35 24 11	0
32	a	1	Total C O 24 18 6	0
32	a	1	Total C O 35 24 11	0
32	b	1	Total C O 24 18 6	0

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



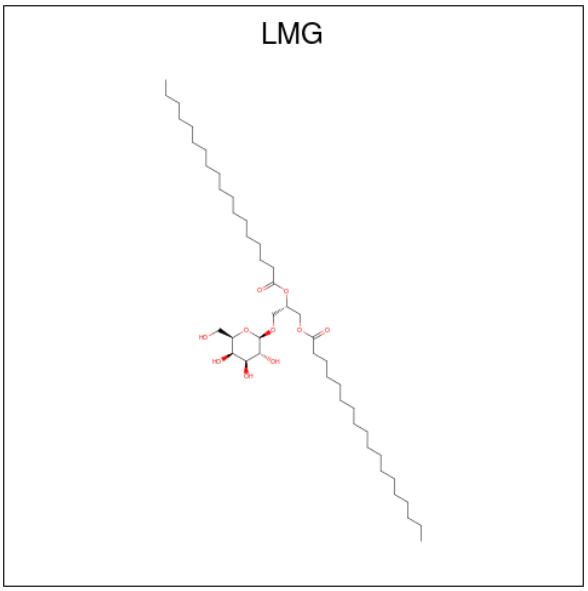
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total 8	Fe 4	S 4	0
33	C	1	Total 8	Fe 4	S 4	0
33	C	1	Total 8	Fe 4	S 4	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



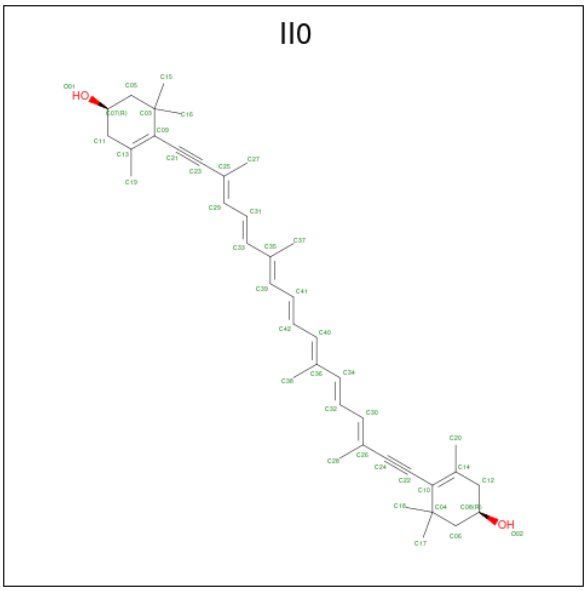
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total 60	C 45	O 15	0

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
35	F	1	Total C O 48 38 10	0
35	J	1	Total C O 55 45 10	0
35	L	1	Total C O 55 45 10	0
35	O	1	Total C O 26 16 10	0
35	c	1	Total C O 55 45 10	0
35	b	1	Total C O 49 39 10	0
35	n	1	Total C O 55 45 10	0
35	Q	1	Total C O 38 28 10	0

- Molecule 36 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	J	1	Total	C	O	0
			42	40	2	
36	O	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	c	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	h	1	Total	C	O	0
			28	27	1	

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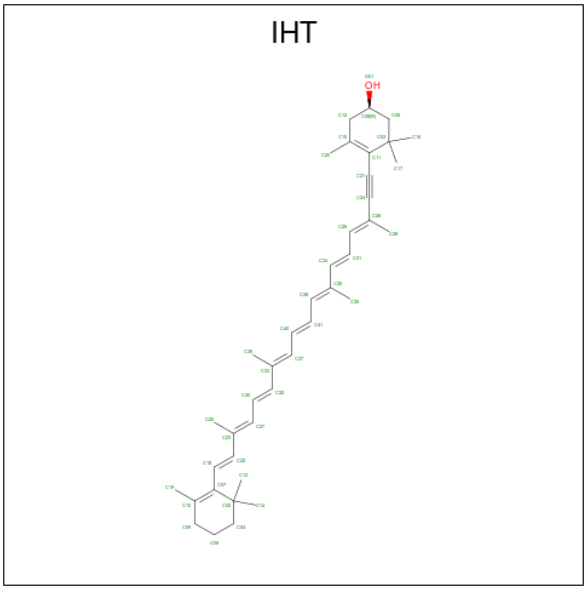
Mol	Chain	Residues	Atoms			AltConf
36	h	1	Total	C	O	0
			42	40	2	
36	h	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	m	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	e	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	l	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	k	1	Total	C	O	0
			42	40	2	
36	f	1	Total	C	O	0
			42	40	2	
36	f	1	Total	C	O	0
			42	40	2	

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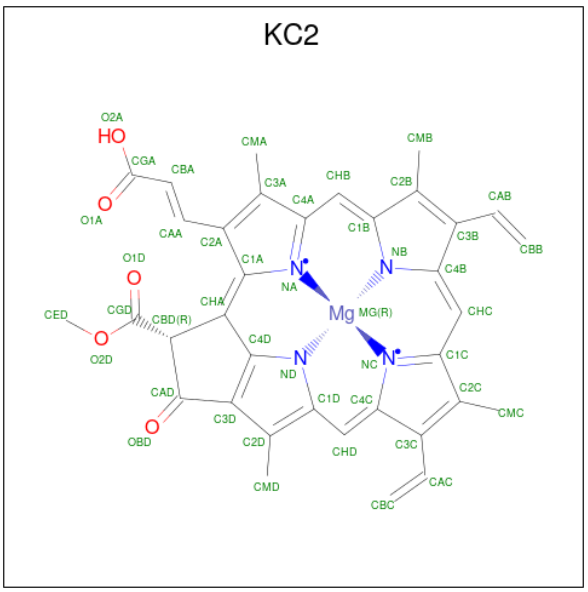
Mol	Chain	Residues	Atoms			AltConf
36	f	1	Total	C	O	0
			42	40	2	
36	f	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	i	1	Total	C	O	0
			42	40	2	
36	j	1	Total	C	O	0
			42	40	2	
36	j	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	d	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	

- Molecule 37 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
37	O	1	Total	C	O	0
			41	40	1	
37	c	1	Total	C	O	0
			41	40	1	
37	a	1	Total	C	O	0
			41	40	1	
37	b	1	Total	C	O	0
			41	40	1	
37	b	1	Total	C	O	0
			41	40	1	
37	m	1	Total	C	O	0
			41	40	1	
37	k	1	Total	C	O	0
			41	40	1	
37	f	1	Total	C	O	0
			41	40	1	
37	j	1	Total	C	O	0
			41	40	1	
37	g	1	Total	C	O	0
			41	40	1	
37	R	1	Total	C	O	0
			41	40	1	
37	n	1	Total	C	O	0
			41	40	1	

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



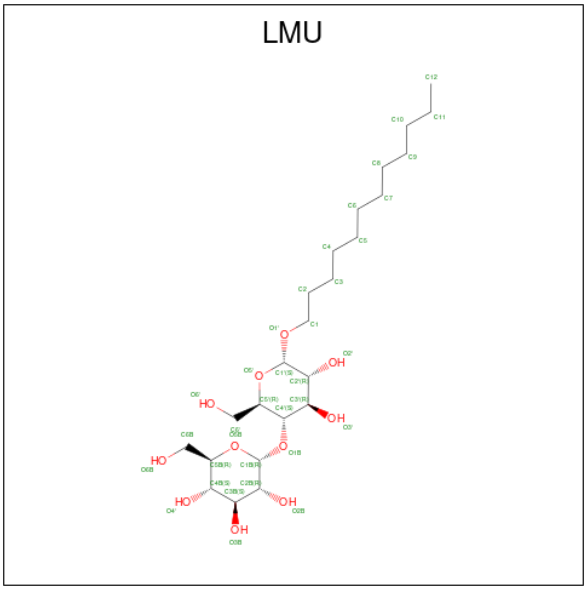
Mol	Chain	Residues	Atoms					AltConf
38	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
38	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
39	i	1	Total	C	O	0
			35	24	11	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	50	Total	O	0
			50	50	

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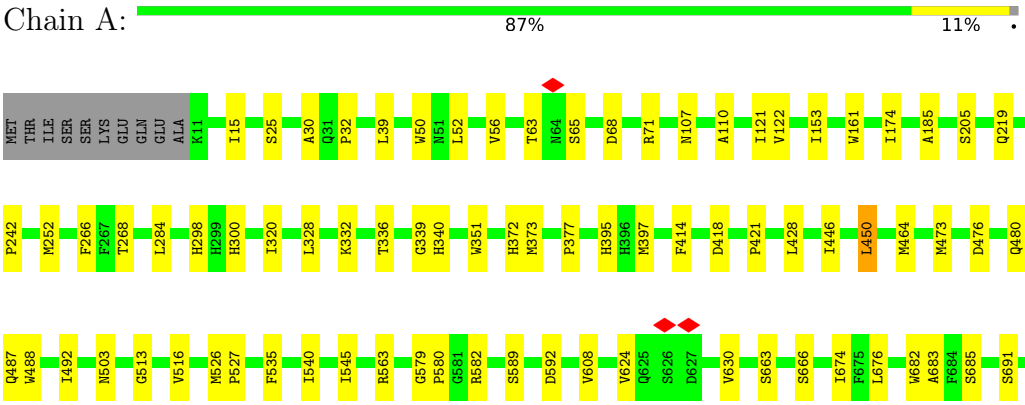
Mol	Chain	Residues	Atoms	AltConf
40	B	57	Total O 57 57	0
40	C	8	Total O 8 8	0
40	D	1	Total O 1 1	0
40	F	2	Total O 2 2	0
40	I	1	Total O 1 1	0
40	J	1	Total O 1 1	0
40	L	1	Total O 1 1	0
40	O	1	Total O 1 1	0
40	K	1	Total O 1 1	0
40	a	3	Total O 3 3	0
40	b	2	Total O 2 2	0
40	h	1	Total O 1 1	0
40	m	1	Total O 1 1	0
40	e	4	Total O 4 4	0
40	R	1	Total O 1 1	0
40	n	3	Total O 3 3	0
40	Q	1	Total O 1 1	0

3 Residue-property plots (i)

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

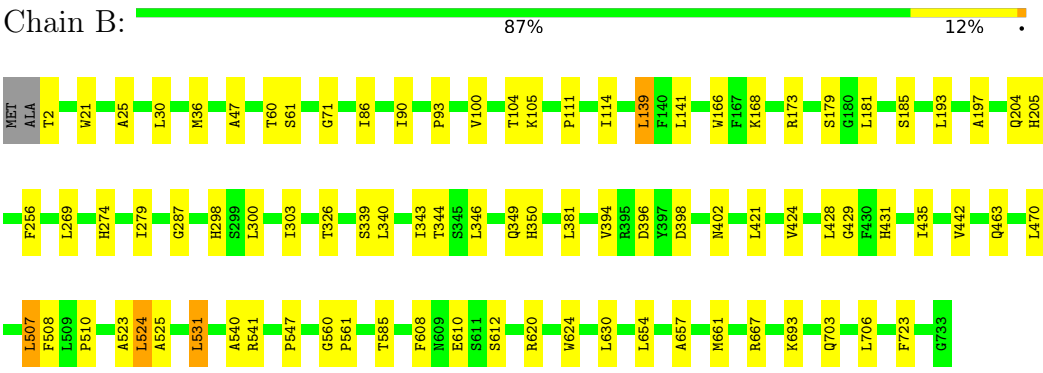
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



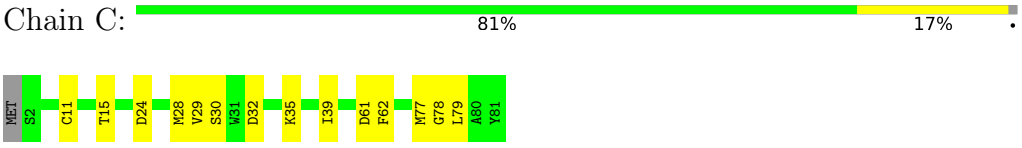
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



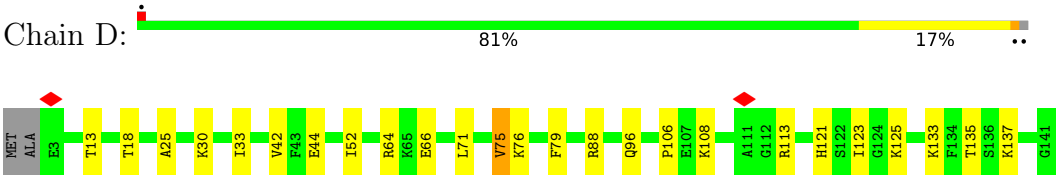
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



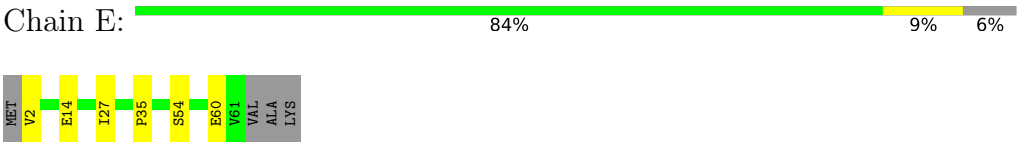
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



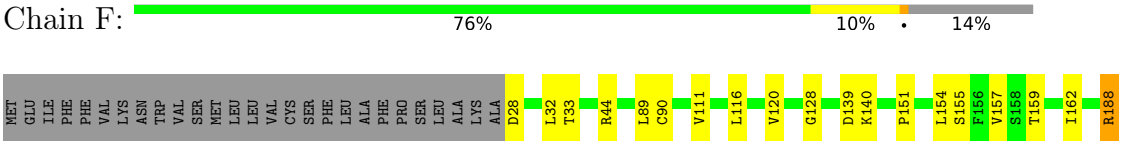
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



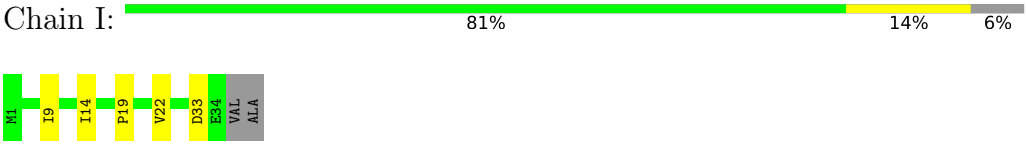
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



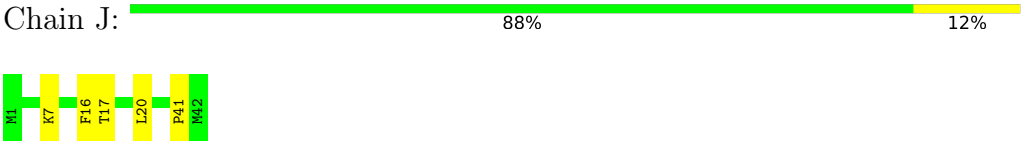
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



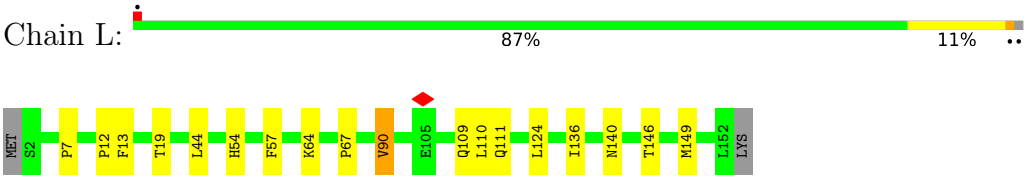
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



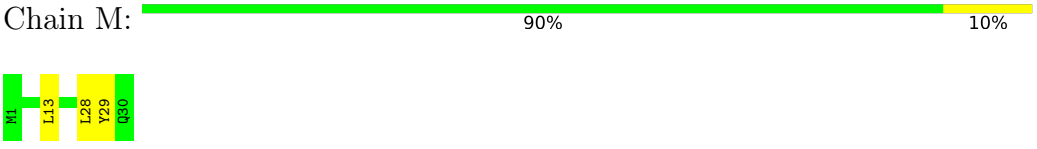
• Molecule 9: Photosystem I reaction center subunit XI

Chain L:

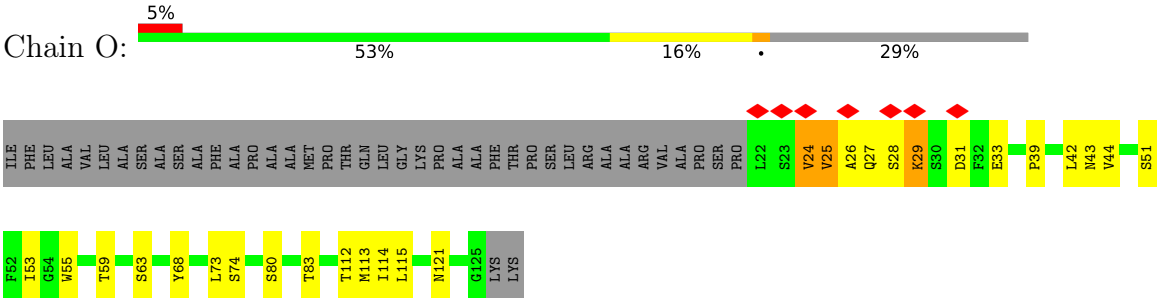


• Molecule 10: Photosystem I reaction center subunit XII

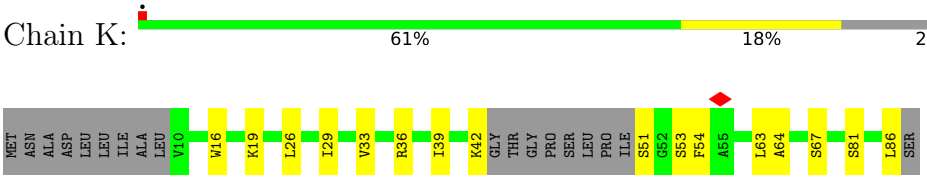
Chain M:



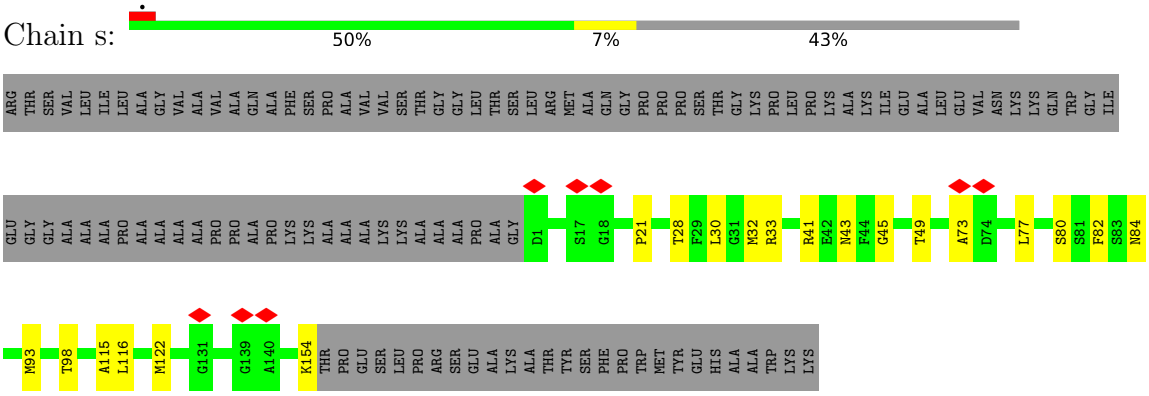
• Molecule 11: PsaO



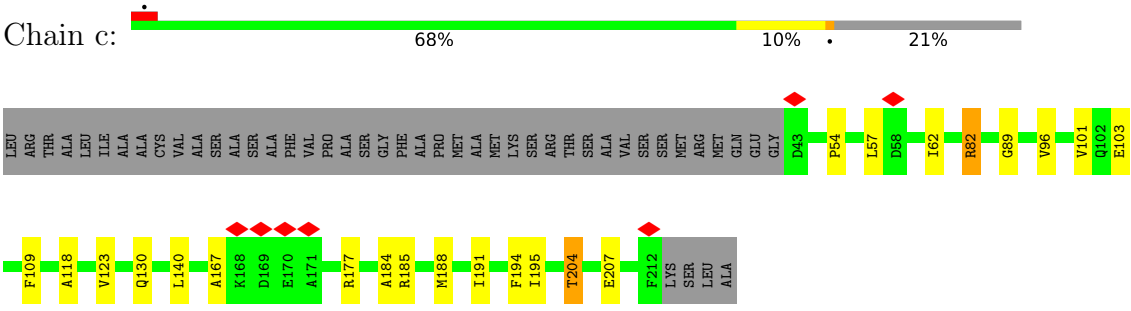
• Molecule 12: Photosystem I reaction center subunit PsaK



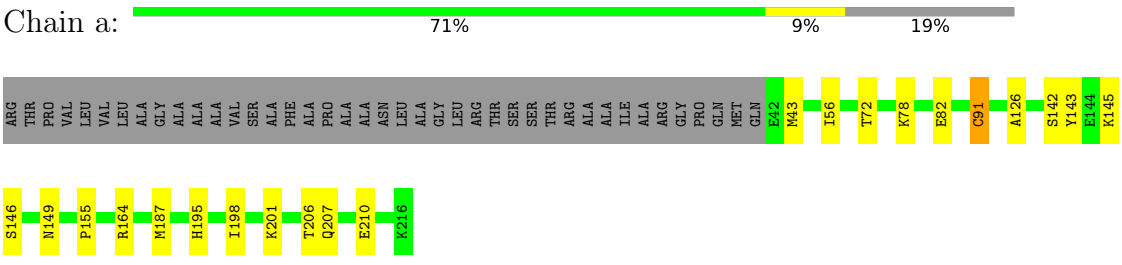
• Molecule 13: chain s



• Molecule 14: cac-c

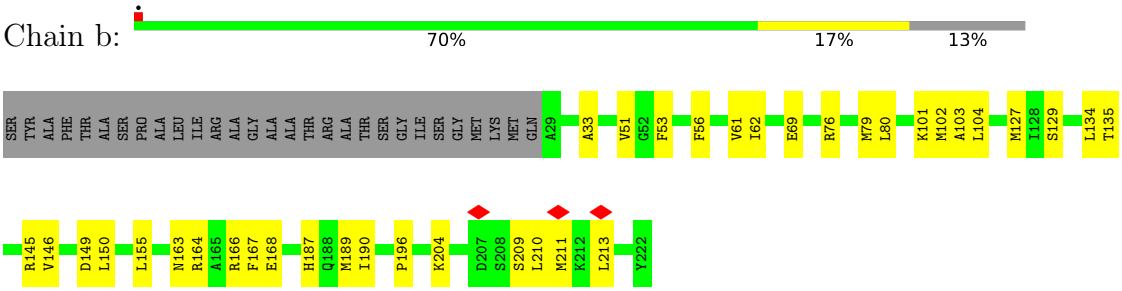


• Molecule 15: cac-a



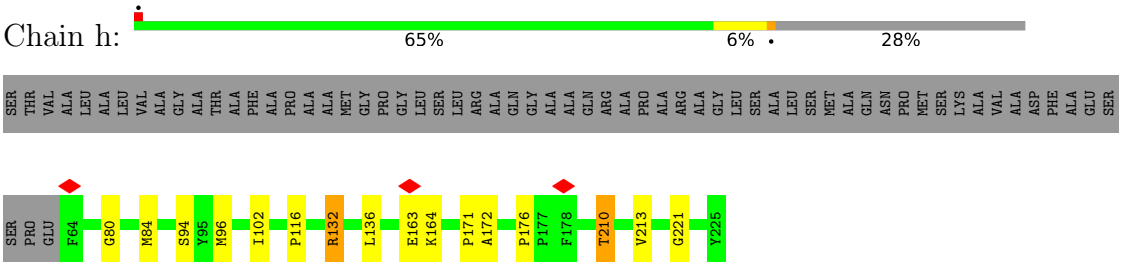
• Molecule 16: cac-b

Chain b:



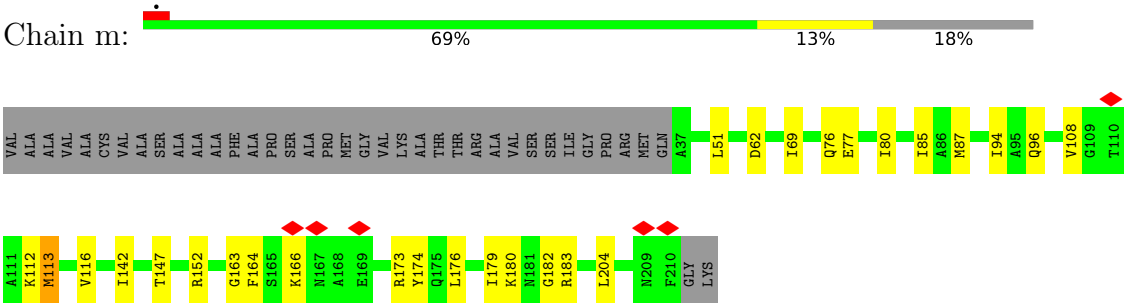
• Molecule 17: cac-h

Chain h:



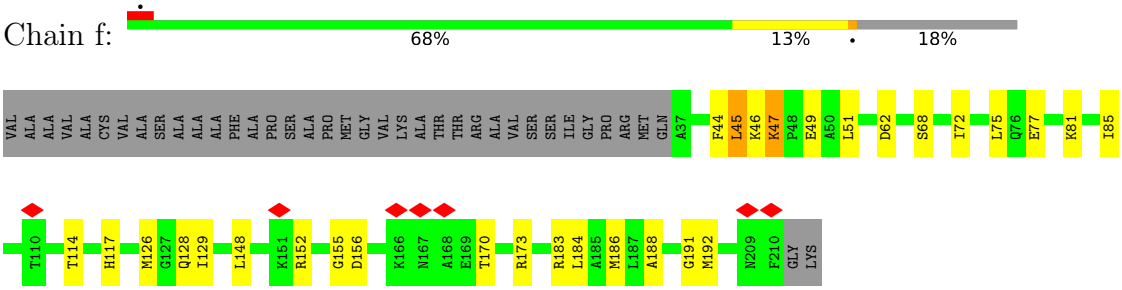
• Molecule 18: cac-f

Chain m:



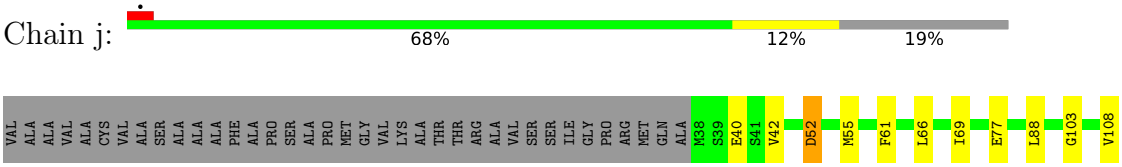
• Molecule 18: cac-f

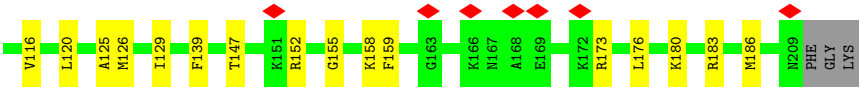
Chain f:



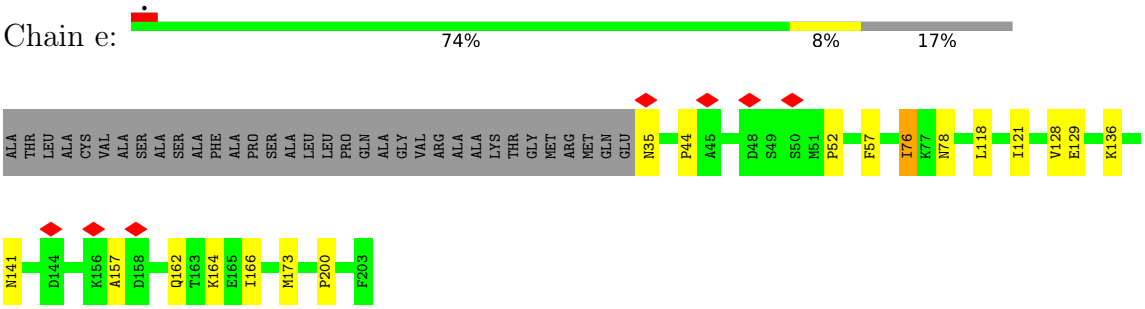
• Molecule 18: cac-f

Chain j:

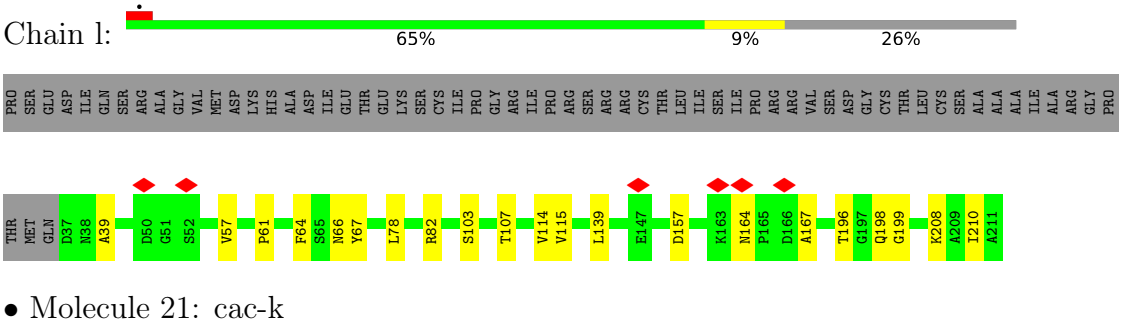




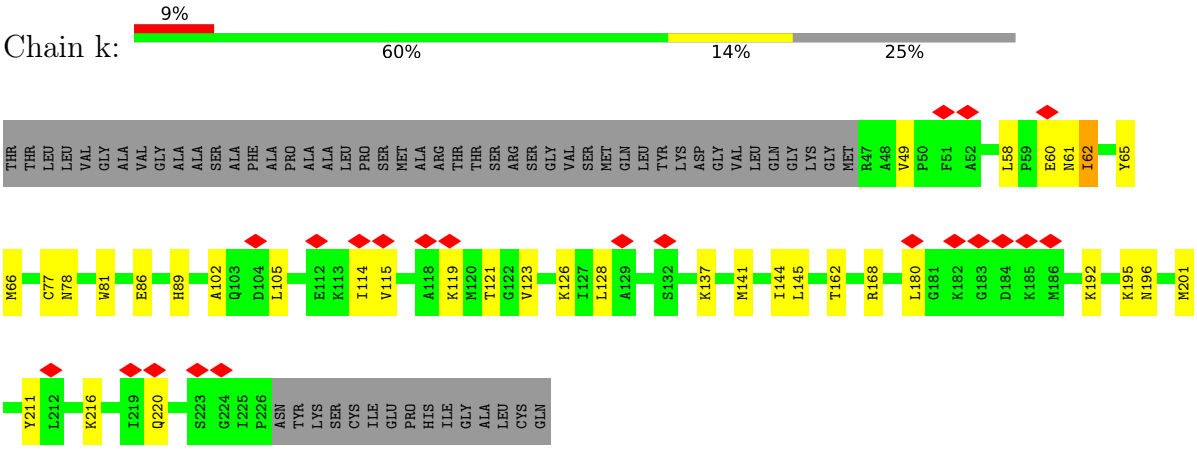
• Molecule 19: cac-e



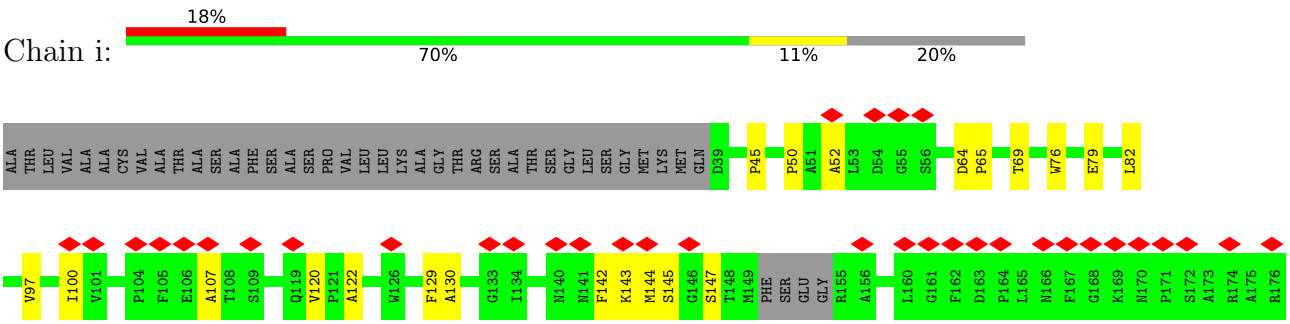
• Molecule 20: cac-l

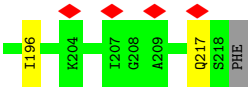


• Molecule 21: cac-k



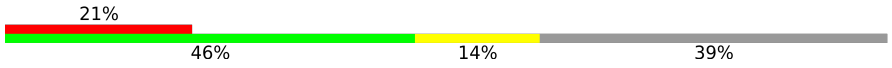
• Molecule 22: cac-i

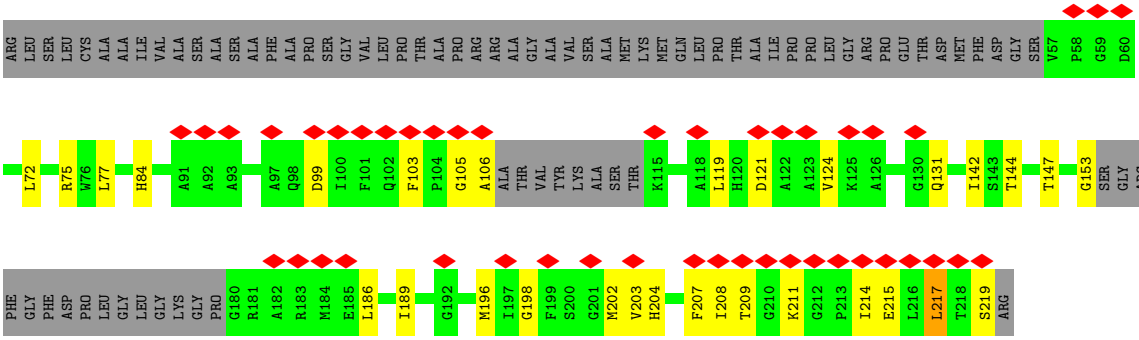




• Molecule 23: cac-d

Chain d:

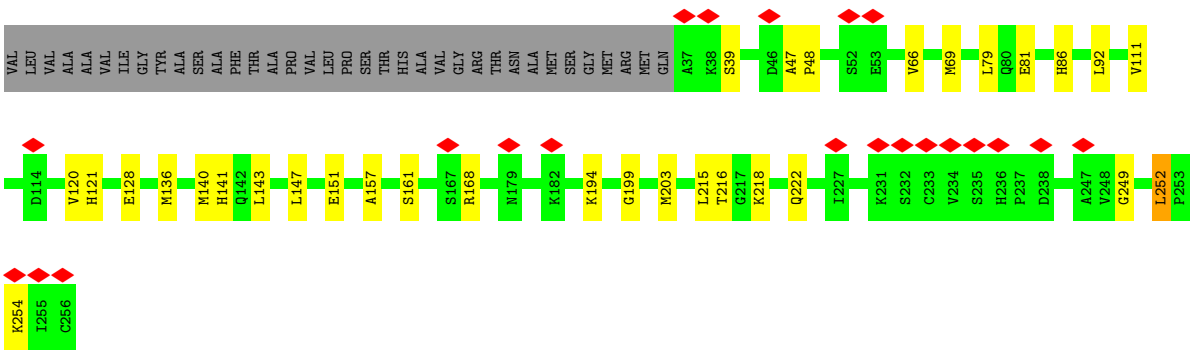




• Molecule 24: cac-g

Chain g:





• Molecule 25: PsaR

Chain R:

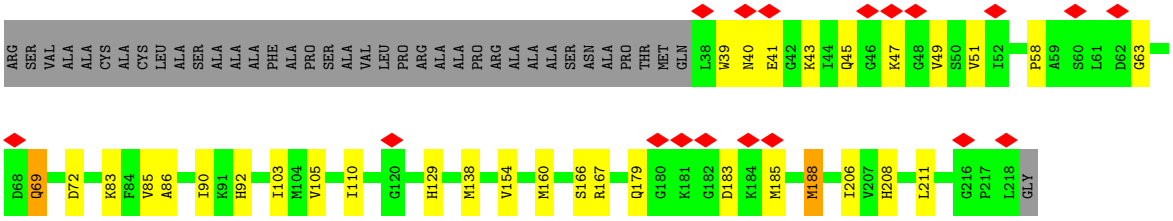




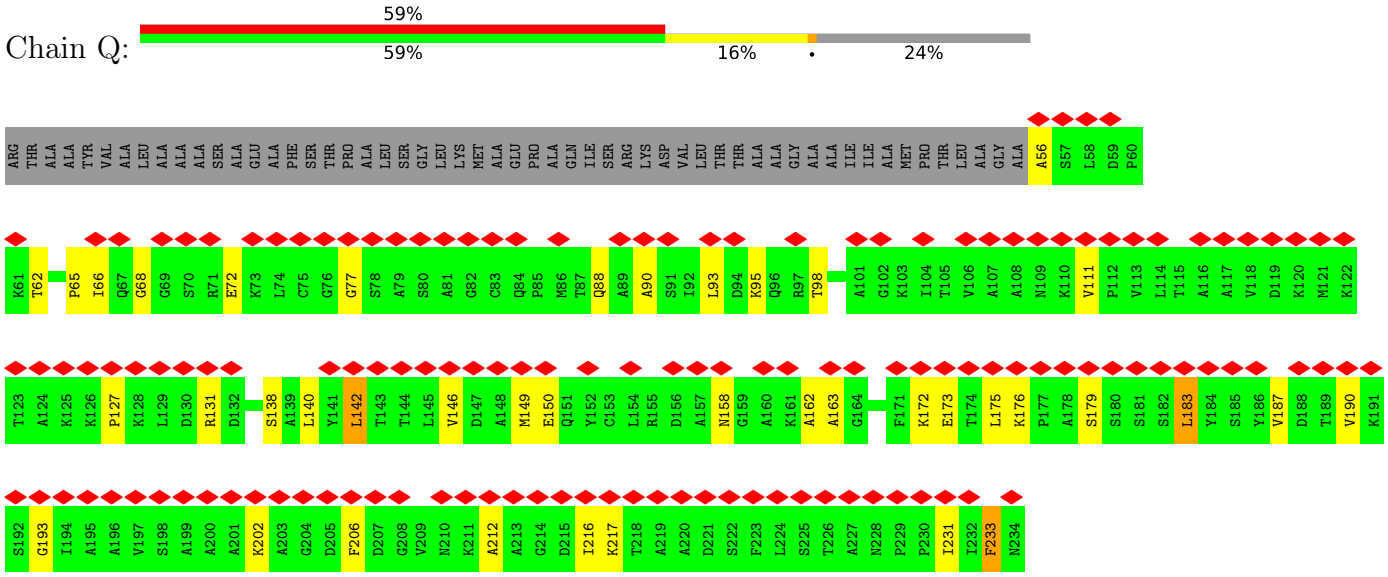
• Molecule 26: cac-n

Chain n:





• Molecule 27: PsaQ



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86231	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.296	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, LHG, IHT, II0, DGD, SF4, LMG, CLA, KC2, PQN, LMU, WVN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.41	0/6019	0.60	0/8204
2	B	0.41	0/6045	0.62	1/8254 (0.0%)
3	C	0.38	0/601	0.71	2/813 (0.2%)
4	D	0.35	0/1109	0.55	0/1500
5	E	0.41	0/492	0.59	0/666
6	F	0.40	0/1287	0.61	0/1747
7	I	0.42	0/271	0.65	0/370
8	J	0.40	0/364	0.64	0/495
9	L	0.33	0/1175	0.63	0/1599
10	M	0.30	0/233	0.68	2/315 (0.6%)
11	O	0.56	0/799	0.80	0/1094
12	K	0.32	0/495	0.64	0/672
13	s	0.33	0/1170	0.64	2/1580 (0.1%)
14	c	0.38	0/1396	0.68	0/1889
15	a	0.41	0/1406	0.72	0/1903
16	b	0.43	0/1469	0.71	1/1983 (0.1%)
17	h	0.37	0/1226	0.66	0/1667
18	f	0.37	0/1328	0.68	2/1790 (0.1%)
18	j	0.41	0/1318	0.73	0/1775
18	m	0.35	0/1335	0.63	1/1798 (0.1%)
19	e	0.35	0/1324	0.65	0/1795
20	l	0.32	0/1379	0.56	0/1863
21	k	0.37	0/1380	0.67	0/1869
22	i	0.40	0/1359	0.70	0/1835
23	d	0.43	0/993	0.70	0/1335
24	g	0.39	0/1673	0.66	0/2264
25	R	0.32	0/686	0.56	0/940
26	n	0.38	0/1383	0.67	0/1867
27	Q	0.42	0/1313	0.78	0/1775
All	All	0.39	0/41028	0.65	11/55657 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	f	191	GLY	CA-C-N	5.90	130.56	120.71
18	f	191	GLY	C-N-CA	5.90	130.56	120.71
2	B	667	ARG	N-CA-C	5.72	118.25	111.33
3	C	61	ASP	CA-C-N	-5.67	114.72	122.93
3	C	61	ASP	C-N-CA	-5.67	114.72	122.93
10	M	29	TYR	CA-C-N	5.66	131.88	121.70
10	M	29	TYR	C-N-CA	5.66	131.88	121.70
16	b	209	SER	N-CA-C	-5.62	106.19	113.16
18	m	113	MET	CB-CA-C	-5.62	110.08	116.54
13	s	115	ALA	CA-C-N	5.11	131.30	121.54
13	s	115	ALA	C-N-CA	5.11	131.30	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5677	64	0
2	B	5826	0	5640	65	0
3	C	592	0	567	7	0
4	D	1084	0	1080	15	0
5	E	484	0	486	4	0
6	F	1254	0	1264	18	0
7	I	264	0	276	4	0
8	J	351	0	344	6	0
9	L	1146	0	1160	13	0
10	M	232	0	265	2	0
11	O	773	0	765	36	0
12	K	488	0	516	9	0
13	s	1140	0	1099	15	0
14	c	1357	0	1337	16	0
15	a	1361	0	1305	11	0
16	b	1439	0	1456	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	h	1200	0	1228	12	0
18	f	1302	0	1320	30	0
18	j	1293	0	1321	20	0
18	m	1309	0	1335	19	0
19	e	1286	0	1262	11	0
20	l	1344	0	1315	14	0
21	k	1346	0	1349	20	0
22	i	1324	0	1298	24	0
23	d	974	0	978	22	0
24	g	1630	0	1644	20	0
25	R	664	0	647	5	0
26	n	1350	0	1348	22	0
27	Q	1294	0	1333	23	0
28	A	2706	0	2777	92	0
28	B	2454	0	2485	76	0
28	F	117	0	115	6	0
28	J	42	0	31	2	0
28	K	93	0	72	0	0
28	L	215	0	191	11	0
28	O	182	0	187	13	0
28	Q	110	0	105	7	0
28	R	51	0	41	1	0
28	a	619	0	588	10	0
28	b	724	0	737	28	0
28	c	586	0	520	14	0
28	d	498	0	407	17	0
28	e	582	0	578	20	0
28	f	700	0	695	21	0
28	g	661	0	611	21	0
28	h	505	0	470	14	0
28	i	528	0	451	14	0
28	j	637	0	556	11	0
28	k	596	0	534	13	0
28	l	535	0	538	10	0
28	m	651	0	606	17	0
28	n	605	0	552	16	0
28	s	246	0	257	5	0
29	A	33	0	46	1	0
29	B	33	0	46	1	0
30	A	113	0	142	3	0
30	J	49	0	74	6	0
30	L	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	98	0	148	3	0
30	b	80	0	106	2	0
30	c	74	0	88	1	0
30	d	37	0	44	0	0
30	e	37	0	44	0	0
30	f	49	0	74	2	0
30	g	74	0	88	2	0
30	i	37	0	44	2	0
30	j	30	0	30	2	0
30	k	37	0	44	0	0
30	l	32	0	34	1	0
30	m	37	0	44	2	0
30	n	43	0	59	1	0
31	A	160	0	0	5	0
31	B	200	0	0	2	0
31	F	80	0	0	0	0
31	I	40	0	0	2	0
31	J	80	0	0	1	0
31	K	80	0	0	1	0
31	L	120	0	0	1	0
31	M	40	0	0	0	0
31	R	80	0	0	7	0
31	e	40	0	0	0	0
31	h	40	0	0	0	0
31	i	40	0	0	0	0
31	l	80	0	0	0	0
31	s	80	0	0	0	0
32	A	35	0	45	1	0
32	a	59	0	78	0	0
32	b	24	0	34	2	0
33	A	8	0	0	0	0
33	C	16	0	0	0	0
34	B	60	0	81	2	0
35	F	48	0	69	4	0
35	J	55	0	86	4	0
35	L	55	0	86	7	0
35	O	26	0	22	0	0
35	Q	38	0	46	4	0
35	b	49	0	71	3	0
35	c	55	0	86	3	0
35	n	55	0	86	3	0
36	J	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	O	42	0	0	0	0
36	a	168	0	0	0	0
36	b	126	0	0	0	0
36	c	168	0	0	0	0
36	d	168	0	0	2	0
36	e	168	0	0	0	0
36	f	168	0	0	1	0
36	g	168	0	0	0	0
36	h	112	0	0	0	0
36	i	210	0	0	1	0
36	j	84	0	0	0	0
36	k	210	0	0	1	0
36	l	168	0	0	1	0
36	m	168	0	0	1	0
36	n	168	0	0	1	0
37	O	41	0	0	0	0
37	R	41	0	0	0	0
37	a	41	0	0	0	0
37	b	82	0	0	1	0
37	c	41	0	0	0	0
37	f	41	0	0	1	0
37	g	41	0	0	0	0
37	j	41	0	0	1	0
37	k	41	0	0	0	0
37	m	41	0	0	0	0
37	n	41	0	0	2	0
38	c	45	0	0	0	0
38	d	90	0	0	0	0
38	e	45	0	0	0	0
38	f	45	0	0	1	0
38	g	135	0	0	3	0
38	i	90	0	0	10	0
38	j	45	0	0	0	0
38	k	135	0	0	0	0
38	l	45	0	0	0	0
38	m	45	0	0	0	0
38	n	90	0	0	0	0
38	s	90	0	0	1	0
39	i	35	0	46	2	0
40	A	50	0	0	0	0
40	B	57	0	0	0	0
40	C	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	D	1	0	0	0	0
40	F	2	0	0	0	0
40	I	1	0	0	0	0
40	J	1	0	0	0	0
40	K	1	0	0	0	0
40	L	1	0	0	0	0
40	O	1	0	0	0	0
40	Q	1	0	0	0	0
40	R	1	0	0	0	0
40	a	3	0	0	0	0
40	b	2	0	0	0	0
40	e	4	0	0	0	0
40	h	1	0	0	0	0
40	m	1	0	0	2	0
40	n	3	0	0	0	0
All	All	61164	0	55784	828	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 7.

All (828) 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)
28:B:813:CLA:H61	31:R:202:WVN:C17	1.71	1.21
28:B:813:CLA:H8	31:R:202:WVN:C14	1.78	1.13
11:O:24:VAL:HG22	11:O:44:VAL:HG11	1.15	1.08
28:B:813:CLA:C6	31:R:202:WVN:C17	2.42	0.97
11:O:24:VAL:HG22	11:O:44:VAL:CG1	2.01	0.91
11:O:27:GLN:HE21	18:f:148:LEU:CD1	1.85	0.90
22:i:142:PHE:HB3	38:i:319:KC2:CMC	2.06	0.86
2:B:339:SER:HB3	28:B:821:CLA:H42	1.58	0.84
28:A:822:CLA:HBB2	28:A:836:CLA:H18	1.63	0.80
22:i:129:PHE:HE2	38:i:319:KC2:O1A	1.69	0.76
11:O:24:VAL:CG2	11:O:44:VAL:HG11	2.08	0.75
11:O:28:SER:CB	18:f:148:LEU:O	2.34	0.75
28:A:814:CLA:H12	28:A:814:CLA:HBD	1.70	0.74
11:O:27:GLN:HE21	18:f:148:LEU:HD13	1.51	0.73
11:O:28:SER:HB3	18:f:148:LEU:O	1.88	0.73
28:b:612:CLA:H3A	30:b:620:LHG:HC62	1.70	0.71
22:i:144:MET:H	22:i:147:SER:HB2	1.55	0.71
28:B:813:CLA:C8	31:R:202:WVN:C14	2.64	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:76:ARG:HB3	28:b:607:CLA:HBC3	1.74	0.70
31:A:847:WVN:C21	28:O:206:CLA:H93	2.22	0.70
22:i:50:PRO:HG2	22:i:64:ASP:HB3	1.74	0.70
28:m:612:CLA:ND	40:m:701:HOH:O	2.25	0.69
9:L:90:VAL:HG21	9:L:124:LEU:HB2	1.75	0.69
21:k:66:MET:HE1	21:k:195:LYS:HD3	1.74	0.69
11:O:27:GLN:NE2	18:f:148:LEU:CD1	2.55	0.68
28:A:851:CLA:H91	28:B:803:CLA:H101	1.76	0.68
28:l:306:CLA:H102	28:l:306:CLA:HMA3	1.75	0.68
17:h:210:THR:HG23	27:Q:68:GLY:HA3	1.75	0.67
18:m:147:THR:OG1	18:m:152:ARG:NH1	2.28	0.66
28:A:855:CLA:HMA1	35:c:619:LMG:HC92	1.78	0.66
23:d:119:LEU:HD21	28:d:303:CLA:HED3	1.78	0.66
11:O:27:GLN:HE21	18:f:148:LEU:HD12	1.60	0.66
30:g:301:LHG:H101	30:g:301:LHG:H292	1.78	0.66
1:A:50:TRP:HE1	28:A:840:CLA:HBB1	1.61	0.66
11:O:27:GLN:NE2	18:f:148:LEU:HD13	2.10	0.66
16:b:155:LEU:HD13	35:b:621:LMG:H131	1.78	0.65
1:A:513:GLY:HA2	1:A:527:PRO:HB3	1.79	0.65
4:D:64:ARG:NH2	4:D:66:GLU:OE1	2.30	0.65
11:O:27:GLN:NE2	11:O:27:GLN:H	1.94	0.65
21:k:114:ILE:HG23	21:k:115:VAL:HG23	1.79	0.65
4:D:121:HIS:HB2	4:D:125:LYS:HD2	1.78	0.65
1:A:205:SER:HB3	28:A:819:CLA:HBC3	1.78	0.64
13:s:28:THR:HG23	13:s:41:ARG:HH11	1.62	0.64
11:O:53:ILE:HG13	28:f:608:CLA:HMB3	1.80	0.64
3:C:29:VAL:HG12	4:D:113:ARG:HB3	1.78	0.64
14:c:89:GLY:HA3	14:c:184:ALA:HB1	1.79	0.64
21:k:216:LYS:HD2	21:k:220:GLN:HB3	1.78	0.64
30:g:301:LHG:H312	30:g:301:LHG:H121	1.80	0.64
4:D:25:ALA:HB1	4:D:30:LYS:HG3	1.80	0.63
22:i:142:PHE:CD1	38:i:319:KC2:CAC	2.81	0.63
28:B:806:CLA:H12	7:I:14:ILE:HG13	1.80	0.63
14:c:54:PRO:HG2	14:c:57:LEU:HD22	1.79	0.63
28:e:606:CLA:H2A	28:e:606:CLA:HED2	1.81	0.63
18:j:147:THR:OG1	18:j:152:ARG:NH1	2.29	0.62
28:A:807:CLA:H12	31:J:101:WVN:C24	2.29	0.62
16:b:127:MET:HA	16:b:134:LEU:HD21	1.81	0.62
11:O:28:SER:HB2	18:f:148:LEU:O	1.98	0.62
19:e:35:ASN:HB2	19:e:44:PRO:HD2	1.80	0.62
16:b:189:MET:HE2	16:b:196:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:852:CLA:HAA2	28:B:828:CLA:HMB1	1.82	0.62
28:B:809:CLA:HBA2	39:i:301:LMU:H41	1.81	0.62
11:O:29:LYS:O	11:O:29:LYS:HG3	1.99	0.61
24:g:66:VAL:HG11	28:g:303:CLA:H2	1.82	0.61
6:F:159:THR:HG22	16:b:135:THR:HB	1.82	0.61
2:B:610:GLU:OE2	6:F:44:ARG:NH2	2.33	0.61
28:i:307:CLA:HBB2	38:i:319:KC2:CED	2.30	0.61
6:F:151:PRO:HG3	16:b:61:VAL:HG13	1.83	0.61
27:Q:158:ASN:HD21	27:Q:162:ALA:HB2	1.65	0.61
14:c:62:ILE:HD13	14:c:177:ARG:HD2	1.82	0.61
27:Q:138:SER:HA	27:Q:142:LEU:HB2	1.81	0.61
18:f:114:THR:HB	37:f:617:IHT:C05	2.31	0.61
13:s:73:ALA:O	20:l:208:LYS:NZ	2.32	0.61
22:i:107:ALA:HB1	22:i:120:VAL:HA	1.83	0.60
22:i:142:PHE:CE1	38:i:319:KC2:CAC	2.84	0.60
6:F:120:VAL:HG13	28:F:201:CLA:HAA1	1.82	0.60
11:O:27:GLN:OE1	11:O:43:ASN:HA	2.02	0.60
28:n:603:CLA:HBB2	37:n:617:IHT:C41	2.32	0.60
28:A:831:CLA:HBA1	28:A:854:CLA:H42	1.84	0.59
4:D:42:VAL:HG22	4:D:52:ILE:HG12	1.85	0.59
18:j:129:ILE:HB	28:j:607:CLA:HBC1	1.84	0.59
14:c:167:ALA:HB2	28:c:608:CLA:HBA1	1.84	0.59
24:g:151:GLU:HG2	28:g:309:CLA:NB	2.17	0.59
11:O:24:VAL:HG13	11:O:44:VAL:HB	1.84	0.59
1:A:535:PHE:HA	28:A:835:CLA:HED1	1.85	0.59
28:n:603:CLA:HBC1	35:n:620:LMG:H192	1.83	0.59
22:i:69:THR:HG23	28:i:303:CLA:HBA1	1.83	0.59
22:i:122:ALA:HB3	27:Q:95:LYS:HZ2	1.66	0.59
28:B:817:CLA:H142	28:B:823:CLA:H3A	1.85	0.58
6:F:28:ASP:N	6:F:32:LEU:O	2.36	0.58
24:g:111:VAL:HG11	24:g:136:MET:HE2	1.85	0.58
21:k:144:ILE:HB	28:k:607:CLA:HBC1	1.84	0.58
24:g:215:LEU:HD12	24:g:216:THR:HG23	1.86	0.58
18:f:183:ARG:HA	18:f:186:MET:HE3	1.84	0.58
24:g:249:GLY:HA2	24:g:254:LYS:HB2	1.85	0.58
28:B:835:CLA:H162	28:B:836:CLA:H111	1.84	0.58
21:k:114:ILE:O	21:k:126:LYS:NZ	2.36	0.58
28:m:602:CLA:H93	28:m:603:CLA:H61	1.86	0.58
14:c:185:ARG:HB3	28:c:602:CLA:HBC2	1.86	0.58
38:g:312:KC2:CAA	38:g:312:KC2:CGD	2.82	0.58
2:B:204:GLN:NE2	2:B:205:HIS:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:835:CLA:HBB2	29:B:842:PQN:H141	1.86	0.57
11:O:55:TRP:HB2	11:O:112:THR:HG21	1.86	0.57
21:k:180:LEU:HD11	28:k:609:CLA:H11	1.86	0.57
13:s:82:PHE:HB3	13:s:98:THR:HG21	1.86	0.57
2:B:398:ASP:O	2:B:402:ASN:ND2	2.31	0.57
6:F:32:LEU:HB2	6:F:89:LEU:HD23	1.86	0.57
28:F:201:CLA:HBC2	8:J:20:LEU:HD11	1.86	0.57
23:d:77:LEU:HD13	28:d:301:CLA:HBA2	1.87	0.57
28:A:852:CLA:HBB2	6:F:128:GLY:HA3	1.87	0.57
11:O:27:GLN:OE1	11:O:43:ASN:CA	2.52	0.57
11:O:80:SER:HA	11:O:83:THR:HG22	1.85	0.57
23:d:106:ALA:HB1	28:d:303:CLA:HED2	1.86	0.57
1:A:268:THR:HB	12:K:16:TRP:HB2	1.86	0.57
19:e:136:LYS:HD2	19:e:141:ASN:HB3	1.85	0.57
28:O:202:CLA:HHB	28:O:202:CLA:H42	1.85	0.57
2:B:100:VAL:O	2:B:104:THR:OG1	2.22	0.56
18:j:61:PHE:HE1	28:j:601:CLA:HBC3	1.70	0.56
25:R:51:LYS:HD2	25:R:63:ASP:HB3	1.87	0.56
28:A:839:CLA:H2	28:L:203:CLA:H43	1.88	0.56
16:b:80:LEU:HD13	28:b:604:CLA:H102	1.87	0.56
23:d:209:THR:HB	23:d:211:LYS:HD2	1.87	0.56
35:L:209:LMG:H452	28:g:309:CLA:HAA1	1.87	0.56
12:K:63:LEU:O	12:K:67:SER:OG	2.21	0.56
18:f:85:ILE:HD12	28:f:608:CLA:HMD3	1.86	0.56
28:f:608:CLA:H92	28:f:608:CLA:HAA1	1.88	0.56
19:e:128:VAL:HG21	28:e:604:CLA:H18	1.87	0.56
20:l:115:VAL:HG21	28:l:305:CLA:H2A	1.88	0.56
23:d:75:ARG:NH1	23:d:153:GLY:O	2.39	0.56
11:O:113:MET:SD	28:O:206:CLA:HAB	2.45	0.56
21:k:89:HIS:HB3	21:k:201:MET:HE3	1.87	0.56
28:A:830:CLA:HMA2	9:L:19:THR:HG21	1.88	0.55
28:B:833:CLA:H201	6:F:111:VAL:HA	1.88	0.55
20:l:164:ASN:HB3	20:l:167:ALA:HB3	1.88	0.55
1:A:32:PRO:HB3	28:A:841:CLA:HAC1	1.88	0.55
28:O:206:CLA:HBD	28:O:206:CLA:HBA1	1.87	0.55
28:L:202:CLA:H41	28:g:308:CLA:H142	1.89	0.55
14:c:103:GLU:HG2	14:c:204:THR:HG21	1.88	0.55
22:i:129:PHE:CE2	38:i:319:KC2:O1A	2.56	0.55
1:A:624:VAL:HG22	1:A:630:VAL:HG22	1.88	0.55
20:l:107:THR:HG22	20:l:199:GLY:H	1.72	0.55
28:A:802:CLA:HBA2	2:B:524:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:25:VAL:HG23	11:O:42:LEU:HB2	1.88	0.55
18:m:164:PHE:HB3	18:m:174:TYR:HE2	1.71	0.55
18:f:128:GLN:NE2	28:f:606:CLA:NA	2.55	0.55
26:n:45:GLN:H	26:n:49:VAL:HG11	1.72	0.55
1:A:153:ILE:HD13	28:A:813:CLA:HED3	1.89	0.54
4:D:135:THR:HG22	4:D:137:LYS:H	1.72	0.54
35:L:209:LMG:H291	28:g:308:CLA:H2	1.88	0.54
18:f:51:LEU:HD21	28:f:602:CLA:HAA2	1.89	0.54
22:i:142:PHE:CD1	38:i:319:KC2:C3C	2.90	0.54
28:A:802:CLA:HBA1	28:B:801:CLA:HBB2	1.88	0.54
28:A:804:CLA:H52	31:A:846:WVN:C17	2.38	0.54
18:j:176:LEU:HD11	18:j:180:LYS:HE3	1.89	0.54
1:A:63:THR:HG21	1:A:68:ASP:HB2	1.90	0.54
28:m:606:CLA:HBA2	28:l:311:CLA:HBD	1.89	0.54
1:A:284:LEU:HD21	1:A:377:PRO:HD2	1.89	0.54
2:B:93:PRO:HA	17:h:116:PRO:HB2	1.89	0.54
18:m:183:ARG:HB3	28:m:602:CLA:HBC2	1.90	0.54
18:f:77:GLU:OE1	18:f:155:GLY:N	2.32	0.54
22:i:217:GLN:O	36:i:320:II0:O02	2.26	0.54
31:I:101:WVN:C19	31:I:101:WVN:C16	2.85	0.54
26:n:40:ASN:HB3	26:n:43:LYS:HB2	1.90	0.54
16:b:102:MET:HE2	16:b:104:LEU:HB2	1.89	0.53
26:n:39:TRP:HB3	26:n:41:GLU:HG3	1.90	0.53
27:Q:149:MET:HB3	27:Q:187:VAL:HG22	1.90	0.53
17:h:221:GLY:HA3	28:h:308:CLA:H2A	1.90	0.53
23:d:208:ILE:HG22	23:d:209:THR:HG23	1.90	0.53
30:A:849:LHG:HC31	28:B:801:CLA:H51	1.90	0.53
28:b:611:CLA:H2	28:b:611:CLA:H102	1.89	0.53
28:e:604:CLA:H151	28:e:607:CLA:HBC1	1.89	0.53
2:B:394:VAL:HG23	2:B:540:ALA:HB1	1.90	0.53
35:F:205:LMG:H232	28:b:606:CLA:HBB2	1.90	0.53
17:h:172:ALA:HB1	17:h:176:PRO:HG3	1.89	0.53
28:m:612:CLA:C4D	40:m:701:HOH:O	2.55	0.53
22:i:143:LYS:HD2	22:i:147:SER:HB3	1.91	0.53
31:R:202:WVN:C23	31:R:202:WVN:C18	2.86	0.53
27:Q:93:LEU:HD13	27:Q:163:ALA:HB2	1.90	0.53
28:A:837:CLA:H101	8:J:17:THR:HG23	1.91	0.53
28:b:608:CLA:H3A	30:n:619:LHG:O9	2.09	0.53
23:d:103:PHE:CE2	28:d:303:CLA:H42	2.44	0.53
31:A:847:WVN:C17	31:A:847:WVN:C23	2.87	0.53
23:d:204:HIS:HA	23:d:207:PHE:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:846:WVN:C17	31:B:846:WVN:C23	2.86	0.53
28:d:302:CLA:HMD3	28:d:307:CLA:HBA2	1.91	0.53
28:g:322:CLA:H3A	28:g:322:CLA:H171	1.89	0.53
28:k:608:CLA:H2A	28:k:608:CLA:HED2	1.91	0.52
28:B:807:CLA:H203	28:B:824:CLA:H172	1.91	0.52
6:F:116:LEU:HD23	30:J:106:LHG:H151	1.91	0.52
14:c:185:ARG:HA	14:c:188:MET:HE3	1.91	0.52
1:A:71:ARG:HG2	1:A:185:ALA:HB1	1.92	0.52
30:A:849:LHG:HC12	28:B:801:CLA:H71	1.92	0.52
28:F:201:CLA:H72	28:b:606:CLA:H11	1.91	0.52
24:g:128:GLU:OE2	24:g:141:HIS:ND1	2.41	0.52
28:B:837:CLA:H2A	28:B:837:CLA:HED2	1.92	0.52
4:D:75:VAL:HA	4:D:79:PHE:HD2	1.75	0.52
26:n:208:HIS:HA	26:n:211:LEU:HD12	1.92	0.52
1:A:589:SER:OG	1:A:592:ASP:OD2	2.27	0.52
28:B:817:CLA:H162	28:B:830:CLA:H43	1.91	0.52
1:A:15:ILE:HD13	28:A:809:CLA:HAA2	1.91	0.52
18:m:96:GLN:NE2	36:m:615:II0:O02	2.36	0.52
28:m:604:CLA:H202	28:l:311:CLA:H13	1.91	0.52
24:g:218:LYS:HB3	24:g:222:GLN:HB2	1.92	0.52
1:A:476:ASP:HA	1:A:480:GLN:HG3	1.92	0.51
18:f:62:ASP:OD1	36:f:615:II0:O01	2.28	0.51
1:A:351:TRP:HB3	28:A:804:CLA:HAC1	1.93	0.51
2:B:256:PHE:CD2	28:B:815:CLA:HBB1	2.46	0.51
19:e:200:PRO:HA	28:e:610:CLA:HED2	1.91	0.51
24:g:252:LEU:HD13	28:g:315:CLA:H43	1.92	0.51
28:A:809:CLA:H2	28:A:811:CLA:HBC2	1.92	0.51
30:J:106:LHG:H201	30:J:106:LHG:H141	1.92	0.51
8:J:41:PRO:HG2	28:b:612:CLA:HMD3	1.92	0.51
17:h:80:GLY:O	17:h:84:MET:HG3	2.10	0.51
28:f:610:CLA:H51	38:f:611:KC2:CMD	2.41	0.51
24:g:194:LYS:NZ	38:g:312:KC2:O1D	2.27	0.51
11:O:28:SER:HB3	18:f:148:LEU:C	2.34	0.51
28:k:601:CLA:H43	28:k:610:CLA:HBB2	1.93	0.51
23:d:144:THR:HA	23:d:147:THR:HG22	1.93	0.51
2:B:396:ASP:OD1	4:D:133:LYS:NZ	2.39	0.51
28:A:823:CLA:H2	28:A:836:CLA:H121	1.92	0.51
26:n:51:VAL:HG13	26:n:69:GLN:HB2	1.92	0.51
6:F:162:ILE:HD12	35:F:205:LMG:H111	1.93	0.51
9:L:140:ASN:HB3	28:g:308:CLA:HAA2	1.92	0.51
14:c:96:VAL:HG23	14:c:194:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:607:CLA:H3A	28:e:607:CLA:H2	1.93	0.51
28:i:302:CLA:HAB	18:j:159:PHE:HD1	1.76	0.51
28:A:818:CLA:HBC2	28:A:828:CLA:H121	1.93	0.50
16:b:33:ALA:HB2	16:b:51:VAL:HG13	1.92	0.50
1:A:545:ILE:HD11	28:A:834:CLA:HBB1	1.94	0.50
28:i:307:CLA:CBB	38:i:319:KC2:CED	2.89	0.50
28:B:822:CLA:H52	28:B:841:CLA:H201	1.93	0.50
18:m:94:ILE:HG23	18:m:204:LEU:HD21	1.93	0.50
28:A:827:CLA:H92	30:A:849:LHG:H223	1.94	0.50
28:B:804:CLA:H93	28:B:811:CLA:H2	1.93	0.50
31:A:848:WVN:C17	31:A:848:WVN:C14	2.85	0.50
15:a:82:GLU:OE2	15:a:145:LYS:NZ	2.37	0.50
26:n:103:ILE:HG21	26:n:206:ILE:HG21	1.94	0.50
1:A:56:VAL:HG21	28:A:803:CLA:C2D	2.41	0.50
2:B:100:VAL:HG13	2:B:111:PRO:HG3	1.93	0.50
2:B:706:LEU:HD23	34:B:843:DGD:HA21	1.94	0.50
28:B:814:CLA:C1D	28:B:815:CLA:HBB2	2.42	0.50
23:d:198:GLY:O	23:d:202:MET:HG3	2.12	0.49
1:A:373:MET:HE3	28:A:818:CLA:HBA1	1.95	0.49
28:A:840:CLA:HAA1	28:A:841:CLA:H52	1.94	0.49
12:K:26:LEU:HD21	28:e:606:CLA:H121	1.94	0.49
13:s:33:ARG:NH2	16:b:149:ASP:OD2	2.44	0.49
21:k:77:CYS:SG	21:k:78:ASN:N	2.86	0.49
1:A:332:LYS:HB3	1:A:339:GLY:HA3	1.94	0.49
35:b:621:LMG:H332	28:m:608:CLA:HBA1	1.94	0.49
26:n:83:LYS:HB3	26:n:160:MET:SD	2.51	0.49
1:A:225:PRO:HD3	1:A:252:MET:HE1	1.95	0.49
1:A:421:PRO:HG3	4:D:44:GLU:HB2	1.93	0.49
28:A:838:CLA:HHC	28:A:838:CLA:HBB1	1.93	0.49
15:a:56:ILE:HG23	15:a:72:THR:HG21	1.94	0.49
27:Q:190:VAL:HG13	27:Q:216:ILE:HG23	1.93	0.49
16:b:53:PHE:HE1	28:b:601:CLA:HBC3	1.77	0.49
24:g:81:GLU:HG3	28:g:309:CLA:HED1	1.93	0.49
28:B:839:CLA:HBB1	28:B:839:CLA:HHC	1.94	0.49
13:s:116:LEU:HD21	28:b:605:CLA:H92	1.95	0.49
18:j:173:ARG:HG3	28:j:610:CLA:HED1	1.93	0.49
2:B:2:THR:HB	7:I:33:ASP:HA	1.94	0.49
28:n:602:CLA:H2	28:n:603:CLA:H43	1.95	0.49
1:A:482:LYS:HE3	1:A:487:GLN:HE22	1.77	0.49
28:B:827:CLA:HAB	28:B:834:CLA:HBB2	1.95	0.49
18:m:85:ILE:HD12	28:m:608:CLA:HMD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:117:HIS:HD2	18:f:126:MET:HE2	1.78	0.49
22:i:97:VAL:HA	22:i:100:ILE:HG12	1.94	0.49
28:A:821:CLA:HMB1	28:A:822:CLA:H12	1.94	0.48
2:B:428:LEU:HD11	28:B:833:CLA:HMB2	1.94	0.48
28:B:807:CLA:H102	28:B:807:CLA:H62	1.56	0.48
12:K:81:SER:HA	12:K:86:LEU:HD23	1.95	0.48
23:d:119:LEU:HD21	28:d:303:CLA:CED	2.43	0.48
23:d:121:ASP:HA	23:d:124:VAL:HG22	1.95	0.48
2:B:193:LEU:HA	2:B:197:ALA:HB3	1.93	0.48
5:E:35:PRO:HD2	5:E:54:SER:HA	1.95	0.48
18:f:188:ALA:O	18:f:192:MET:HG3	2.13	0.48
28:A:806:CLA:H18	35:J:105:LMG:H211	1.96	0.48
24:g:79:LEU:HD13	28:g:303:CLA:HBA2	1.96	0.48
28:B:813:CLA:H62	31:R:202:WVN:C17	2.37	0.48
11:O:27:GLN:NE2	11:O:27:GLN:N	2.60	0.48
11:O:27:GLN:H	18:f:148:LEU:HD13	1.78	0.48
28:e:610:CLA:H161	28:e:610:CLA:H121	1.65	0.48
21:k:128:LEU:HG	21:k:141:MET:HG3	1.96	0.48
21:k:162:THR:HG22	21:k:168:ARG:HG3	1.95	0.48
18:j:52:ASP:H	18:j:55:MET:HE2	1.76	0.48
1:A:563:ARG:NH2	4:D:18:THR:O	2.45	0.48
28:B:830:CLA:H61	28:B:830:CLA:H2	1.55	0.48
28:J:103:CLA:HMA2	28:b:611:CLA:H13	1.94	0.48
12:K:51:SER:HB3	12:K:54:PHE:HB3	1.96	0.48
27:Q:131:ARG:HD2	27:Q:202:LYS:HD3	1.94	0.48
1:A:397:MET:HE2	1:A:608:VAL:HG11	1.95	0.48
28:i:306:CLA:H3A	28:i:306:CLA:HBA2	1.49	0.48
1:A:372:HIS:ND1	28:A:817:CLA:OBD	2.40	0.48
28:A:811:CLA:HHC	28:A:811:CLA:HBB1	1.96	0.48
30:J:106:LHG:O3	30:J:106:LHG:O1	2.27	0.48
28:b:608:CLA:H43	26:n:154:VAL:HG11	1.95	0.48
26:n:129:HIS:HD2	26:n:138:MET:HE3	1.78	0.48
28:d:302:CLA:HBB2	36:d:315:II0:C41	2.44	0.48
1:A:503:ASN:HB2	28:A:838:CLA:HED2	1.96	0.48
1:A:579:GLY:HA2	2:B:561:PRO:HD3	1.95	0.48
28:A:820:CLA:HBC3	28:A:826:CLA:H171	1.96	0.48
2:B:25:ALA:HB2	34:B:843:DGD:HA62	1.96	0.48
28:B:801:CLA:O1A	28:B:801:CLA:H3A	2.13	0.48
11:O:33:GLU:HA	11:O:39:PRO:HA	1.95	0.48
19:e:52:PRO:HB3	19:e:162:GLN:HB3	1.96	0.48
30:i:318:LHG:HC61	30:i:318:LHG:H112	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:27:GLN:OE1	11:O:43:ASN:HB3	2.14	0.48
28:h:301:CLA:H52	28:h:301:CLA:H8	1.64	0.48
2:B:541:ARG:HB2	6:F:188:ARG:HG2	1.95	0.47
28:B:810:CLA:HHC	28:B:810:CLA:HBB1	1.95	0.47
15:a:72:THR:HG23	28:a:304:CLA:HBA1	1.96	0.47
28:f:602:CLA:HBA2	28:f:602:CLA:H3A	1.49	0.47
28:i:306:CLA:HBA1	27:Q:77:GLY:O	2.14	0.47
26:n:208:HIS:HE1	37:n:617:IHT:C38	2.27	0.47
28:A:821:CLA:HBB1	28:O:202:CLA:H71	1.96	0.47
18:m:51:LEU:HD21	28:m:602:CLA:HAA2	1.96	0.47
28:e:611:CLA:H161	28:e:611:CLA:H121	1.50	0.47
28:A:836:CLA:H191	11:O:114:ILE:HG21	1.96	0.47
28:B:802:CLA:H62	28:B:802:CLA:H2	1.63	0.47
4:D:108:LYS:O	4:D:113:ARG:NH1	2.46	0.47
30:m:619:LHG:H272	30:m:619:LHG:H301	1.67	0.47
18:j:120:LEU:HB3	18:j:125:ALA:HB3	1.95	0.47
1:A:63:THR:HG22	1:A:65:SER:H	1.80	0.47
28:B:839:CLA:HBA2	9:L:67:PRO:HG3	1.95	0.47
28:b:602:CLA:H3A	28:b:602:CLA:HBA2	1.47	0.47
17:h:96:MET:HG3	17:h:102:ILE:HG13	1.96	0.47
28:B:832:CLA:HMB2	28:B:834:CLA:HED1	1.97	0.47
28:O:202:CLA:HBB2	28:O:202:CLA:H202	1.95	0.47
28:a:304:CLA:H3A	28:a:304:CLA:HBA2	1.50	0.47
16:b:76:ARG:HA	16:b:79:MET:HE3	1.96	0.47
11:O:26:ALA:HB1	18:f:148:LEU:HD22	1.96	0.47
28:c:601:CLA:HBC2	23:d:142:ILE:HG21	1.97	0.47
28:c:606:CLA:HBA1	35:c:619:LMG:H441	1.96	0.47
18:m:176:LEU:HD11	18:m:180:LYS:HE3	1.97	0.47
30:l:317:LHG:H241	30:l:317:LHG:H271	1.50	0.47
22:i:130:ALA:HA	38:i:319:KC2:CED	2.45	0.47
18:j:108:VAL:HG11	18:j:116:VAL:HG12	1.96	0.47
2:B:139:LEU:HD22	10:M:13:LEU:HD12	1.96	0.47
9:L:44:LEU:HD21	28:g:309:CLA:H202	1.96	0.47
11:O:68:TYR:CZ	11:O:73:LEU:HB2	2.50	0.47
28:s:202:CLA:H61	28:s:202:CLA:H142	1.96	0.47
28:a:308:CLA:H151	28:a:308:CLA:H111	1.38	0.47
28:b:610:CLA:H112	28:b:610:CLA:H72	1.78	0.47
28:l:303:CLA:H3A	28:l:303:CLA:HBA2	1.54	0.47
28:f:602:CLA:H41	28:f:602:CLA:H62	1.70	0.47
26:n:85:VAL:HG22	28:n:602:CLA:HHB	1.97	0.47
28:A:854:CLA:H61	28:A:854:CLA:H41	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:839:CLA:H141	28:B:839:CLA:H162	1.74	0.47
28:a:303:CLA:H3A	28:a:303:CLA:HBA2	1.51	0.47
11:O:51:SER:HB3	11:O:112:THR:HG23	1.97	0.47
28:b:604:CLA:H2	28:b:604:CLA:H61	1.60	0.47
28:d:303:CLA:H3A	28:d:303:CLA:HBA2	1.50	0.47
2:B:179:SER:HB3	2:B:287:GLY:HA3	1.96	0.47
2:B:547:PRO:HB2	5:E:14:GLU:HG2	1.97	0.47
20:l:78:LEU:HD23	20:l:82:ARG:NH2	2.29	0.47
21:k:62:ILE:HG12	21:k:65:TYR:HB2	1.97	0.47
28:j:601:CLA:H52	30:j:617:LHG:H132	1.96	0.47
23:d:99:ASP:HB2	23:d:214:ILE:HD11	1.97	0.47
28:B:819:CLA:HBC2	28:B:820:CLA:HBA1	1.96	0.46
28:L:204:CLA:H2	28:L:207:CLA:H2	1.97	0.46
19:e:118:LEU:HD23	19:e:121:ILE:HD12	1.97	0.46
28:i:311:CLA:H3A	28:i:311:CLA:HBA2	1.52	0.46
26:n:105:VAL:HG21	28:n:604:CLA:HBC3	1.97	0.46
35:Q:301:LMG:H322	35:Q:301:LMG:H292	1.59	0.46
2:B:496:TRP:CE3	28:B:815:CLA:H11	2.50	0.46
15:a:78:LYS:HG3	15:a:155:PRO:HG3	1.96	0.46
28:m:603:CLA:HMA1	28:m:603:CLA:H2	1.97	0.46
28:d:303:CLA:H152	28:d:308:CLA:HBC1	1.97	0.46
1:A:540:ILE:HG23	28:A:801:CLA:H193	1.98	0.46
28:A:851:CLA:H2	2:B:654:LEU:HD22	1.98	0.46
28:A:820:CLA:H2	28:A:820:CLA:H62	1.59	0.46
28:A:821:CLA:HMD1	31:K:102:WVN:C19	2.46	0.46
28:A:839:CLA:H41	28:A:839:CLA:H61	1.62	0.46
2:B:523:ALA:HB2	28:B:833:CLA:HMA1	1.96	0.46
28:B:837:CLA:H52	28:B:837:CLA:H11	1.72	0.46
31:I:101:WVN:C07	31:I:101:WVN:C09	2.91	0.46
35:L:209:LMG:H452	28:g:309:CLA:CAA	2.45	0.46
28:s:202:CLA:H72	28:s:202:CLA:H112	1.68	0.46
28:e:606:CLA:H202	28:e:606:CLA:H161	1.80	0.46
20:l:139:LEU:HD22	28:l:307:CLA:HMA1	1.98	0.46
28:i:305:CLA:H2	28:i:305:CLA:H61	1.78	0.46
1:A:298:HIS:HB3	28:A:817:CLA:HMB2	1.96	0.46
2:B:349:GLN:HG3	28:B:822:CLA:HED1	1.97	0.46
35:J:105:LMG:H312	32:b:618:LMT:H41	1.96	0.46
12:K:33:VAL:HG21	28:e:606:CLA:H43	1.97	0.46
14:c:140:LEU:HD23	16:b:56:PHE:HZ	1.80	0.46
28:m:603:CLA:HBA1	28:m:603:CLA:H3A	1.77	0.46
28:f:608:CLA:H202	28:f:608:CLA:H161	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:88:LEU:HB3	28:j:604:CLA:HAB	1.98	0.46
1:A:219:GLN:HE22	1:A:300:HIS:HD1	1.62	0.46
28:F:202:CLA:HBA1	28:F:202:CLA:H3A	1.43	0.46
28:m:603:CLA:H62	28:m:603:CLA:H92	1.80	0.46
18:f:170:THR:HA	18:f:173:ARG:HE	1.81	0.46
26:n:47:LYS:HG3	26:n:63:GLY:HA3	1.97	0.46
28:B:801:CLA:H61	28:B:801:CLA:H41	1.65	0.46
28:c:601:CLA:H12	28:c:601:CLA:NA	2.29	0.46
19:e:76:ILE:HD13	19:e:166:ILE:HD11	1.97	0.46
28:k:608:CLA:H162	28:k:608:CLA:H122	1.56	0.46
18:f:129:ILE:HB	28:f:607:CLA:HBC1	1.98	0.46
26:n:179:GLN:HG3	28:n:609:CLA:H2	1.98	0.46
27:Q:150:GLU:HG2	27:Q:187:VAL:HG11	1.98	0.46
9:L:146:THR:HB	9:L:149:MET:HB2	1.96	0.46
15:a:142:SER:O	15:a:146:SER:OG	2.33	0.46
28:g:308:CLA:H151	28:g:322:CLA:HBC3	1.98	0.46
2:B:21:TRP:CG	2:B:703:GLN:HE22	2.34	0.46
28:B:817:CLA:HMB2	28:B:821:CLA:HMA3	1.97	0.46
9:L:110:LEU:HD23	9:L:110:LEU:HA	1.78	0.46
28:L:207:CLA:H12	35:L:209:LMG:H273	1.96	0.46
11:O:27:GLN:N	11:O:27:GLN:CD	2.74	0.46
14:c:82:ARG:HA	14:c:82:ARG:HD3	1.69	0.46
28:f:608:CLA:H2A	28:f:608:CLA:HED2	1.98	0.46
2:B:181:LEU:O	2:B:185:SER:OG	2.32	0.46
2:B:344:THR:HG21	2:B:381:LEU:HD12	1.96	0.46
16:b:163:ASN:OD1	16:b:166:ARG:NH2	2.49	0.46
22:i:45:PRO:HB2	18:j:158:LYS:HB2	1.98	0.46
28:h:301:CLA:H93	28:h:301:CLA:H111	1.82	0.45
19:e:157:ALA:HB2	28:e:607:CLA:HBA2	1.98	0.45
24:g:66:VAL:HA	24:g:69:MET:HG3	1.97	0.45
35:Q:301:LMG:HC92	28:Q:302:CLA:HMD2	1.98	0.45
28:B:835:CLA:H162	28:B:835:CLA:H121	1.65	0.45
28:F:201:CLA:H102	28:b:606:CLA:HBB1	1.99	0.45
16:b:69:GLU:OE2	16:b:145:ARG:NH1	2.44	0.45
17:h:96:MET:HG2	28:h:304:CLA:H52	1.98	0.45
27:Q:56:ALA:HA	27:Q:231:ILE:HG21	1.98	0.45
1:A:582:ARG:HG2	3:C:78:GLY:HA3	1.98	0.45
7:I:19:PRO:HA	7:I:22:VAL:HG22	1.98	0.45
13:s:122:MET:HE1	28:m:607:CLA:H2A	1.99	0.45
28:a:312:CLA:H102	28:a:312:CLA:H61	1.68	0.45
16:b:213:LEU:HD11	37:b:615:IHT:C22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:621:LMG:H142	28:m:603:CLA:H12	1.98	0.45
18:f:44:PHE:HD1	24:g:157:ALA:HB2	1.82	0.45
3:C:62:PHE:HD2	4:D:123:ILE:HG21	1.80	0.45
1:A:480:GLN:HG2	1:A:482:LYS:HD3	1.97	0.45
18:m:173:ARG:HG3	28:m:610:CLA:HED1	1.98	0.45
19:e:129:GLU:HG3	28:e:606:CLA:NB	2.31	0.45
28:k:602:CLA:H3A	28:k:602:CLA:HBA2	1.47	0.45
18:j:66:LEU:HA	18:j:69:ILE:HD12	1.99	0.45
3:C:11:CYS:HB3	3:C:39:ILE:HG13	1.98	0.45
28:O:206:CLA:H122	28:O:206:CLA:H162	1.47	0.45
26:n:105:VAL:HG13	26:n:110:ILE:HB	1.99	0.45
1:A:674:ILE:HG23	28:A:807:CLA:H171	1.99	0.45
28:A:836:CLA:H52	28:O:206:CLA:H141	1.99	0.45
31:A:847:WVN:C21	28:O:206:CLA:C9	2.92	0.45
28:A:854:CLA:H13	28:A:854:CLA:H101	1.70	0.45
2:B:300:LEU:HD13	28:B:821:CLA:HAC2	1.97	0.45
9:L:136:ILE:HG23	30:L:208:LHG:H122	1.99	0.45
28:c:612:CLA:H91	28:c:612:CLA:H142	1.99	0.45
16:b:134:LEU:HD22	28:b:606:CLA:HMA1	1.98	0.45
28:m:610:CLA:H51	28:m:610:CLA:H12	1.73	0.45
28:f:610:CLA:H41	28:f:610:CLA:H61	1.53	0.45
23:d:106:ALA:HB1	28:d:303:CLA:CED	2.47	0.45
28:A:816:CLA:H122	28:A:816:CLA:H8	1.90	0.45
28:A:824:CLA:H102	28:A:824:CLA:H62	1.76	0.45
28:A:839:CLA:H13	28:L:203:CLA:HAA2	1.99	0.45
9:L:7:PRO:HB3	9:L:12:PRO:HA	1.98	0.45
11:O:59:THR:HG22	11:O:74:SER:H	1.81	0.45
30:c:620:LHG:H291	28:b:610:CLA:H93	1.99	0.45
16:b:129:SER:HB2	16:b:150:LEU:HD23	1.98	0.45
20:l:157:ASP:OD1	36:l:312:II0:O01	2.34	0.45
28:Q:302:CLA:H72	28:Q:302:CLA:H112	1.57	0.45
1:A:580:PRO:HD3	2:B:560:GLY:HA2	1.99	0.45
28:A:838:CLA:H111	28:A:838:CLA:H151	1.68	0.45
2:B:298:HIS:HB3	2:B:303:ILE:HD11	1.99	0.45
13:s:98:THR:HG22	28:s:202:CLA:HMA3	1.98	0.45
28:f:601:CLA:H3A	28:f:601:CLA:HBA2	1.65	0.45
28:j:610:CLA:H51	28:j:610:CLA:H12	1.72	0.45
28:g:322:CLA:H62	28:g:322:CLA:H101	1.60	0.45
2:B:168:LYS:NZ	25:R:42:SER:OG	2.40	0.45
2:B:463:GLN:HG2	2:B:508:PHE:CD1	2.52	0.45
28:B:805:CLA:H101	28:B:805:CLA:H62	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:k:609:CLA:H162	28:k:609:CLA:H122	1.65	0.45
18:f:117:HIS:CD2	18:f:126:MET:HE2	2.52	0.45
28:f:607:CLA:H202	28:f:607:CLA:H161	1.78	0.45
28:f:613:CLA:HBD	28:f:613:CLA:H61	1.99	0.45
22:i:79:GLU:HG3	28:i:307:CLA:HED2	1.99	0.45
28:A:817:CLA:H3A	28:A:817:CLA:HBA2	1.68	0.44
28:A:837:CLA:HBA2	28:A:837:CLA:H3A	1.59	0.44
28:B:827:CLA:H3A	28:B:827:CLA:HBA2	1.66	0.44
28:B:840:CLA:H62	28:B:840:CLA:H2	1.72	0.44
13:s:43:ASN:HB3	20:l:67:TYR:HE1	1.82	0.44
16:b:145:ARG:NH1	16:b:146:VAL:O	2.50	0.44
16:b:167:PHE:HZ	18:m:69:ILE:HD12	1.81	0.44
28:b:603:CLA:H202	28:b:603:CLA:H161	1.77	0.44
17:h:136:LEU:HD21	28:h:301:CLA:H102	1.98	0.44
28:h:306:CLA:H62	28:h:306:CLA:H2	1.80	0.44
18:j:183:ARG:HA	18:j:186:MET:HE3	1.98	0.44
1:A:485:PHE:HB3	28:A:834:CLA:H12	1.98	0.44
28:A:839:CLA:H52	28:L:203:CLA:H12	1.99	0.44
2:B:421:LEU:HB3	2:B:531:LEU:HG	1.99	0.44
28:B:836:CLA:H62	28:B:836:CLA:H41	1.54	0.44
6:F:188:ARG:HA	6:F:188:ARG:HD2	1.50	0.44
28:c:608:CLA:H3A	28:c:608:CLA:HBA2	1.38	0.44
18:m:80:ILE:HG12	18:m:179:ILE:HD11	1.99	0.44
28:n:608:CLA:HBA2	28:n:608:CLA:H3A	1.66	0.44
28:A:820:CLA:H111	28:A:820:CLA:H152	1.81	0.44
2:B:209:ASP:HA	28:Q:302:CLA:HMD3	2.00	0.44
1:A:482:LYS:HA	1:A:482:LYS:HD2	1.73	0.44
2:B:225:PHE:O	28:j:607:CLA:H2A	2.17	0.44
28:b:610:CLA:H152	28:b:610:CLA:H18	1.67	0.44
28:l:308:CLA:HBA2	28:l:308:CLA:H3A	1.49	0.44
28:f:607:CLA:H3A	28:f:607:CLA:HBA2	1.51	0.44
24:g:86:HIS:HB3	24:g:203:MET:SD	2.58	0.44
28:n:609:CLA:H62	28:n:609:CLA:H41	1.65	0.44
28:A:802:CLA:H111	28:A:802:CLA:H91	1.66	0.44
2:B:30:LEU:HB3	2:B:36:MET:HE3	1.99	0.44
2:B:661:MET:HB2	28:B:803:CLA:C1C	2.47	0.44
28:B:805:CLA:H151	28:B:825:CLA:HBB2	1.98	0.44
31:B:846:WVN:C12	28:i:312:CLA:CGA	2.96	0.44
30:f:619:LHG:H152	30:f:619:LHG:H121	1.56	0.44
28:i:302:CLA:HBA2	28:i:302:CLA:H3A	1.43	0.44
28:Q:302:CLA:H162	28:Q:302:CLA:H122	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:835:CLA:H141	28:A:835:CLA:H161	1.77	0.44
2:B:693:LYS:HE3	2:B:693:LYS:HB3	1.81	0.44
28:B:836:CLA:H92	28:B:836:CLA:H61	1.78	0.44
13:s:30:LEU:H	13:s:49:THR:HG21	1.83	0.44
28:h:306:CLA:H192	28:h:306:CLA:H161	1.82	0.44
27:Q:142:LEU:HD12	27:Q:142:LEU:HA	1.85	0.44
1:A:516:VAL:HG22	1:A:526:MET:HB2	2.00	0.44
30:L:208:LHG:H121	30:L:208:LHG:HC92	1.89	0.44
13:s:21:PRO:HG3	15:a:43:MET:HE2	1.98	0.44
28:a:305:CLA:HMD2	28:a:308:CLA:H52	2.00	0.44
28:b:606:CLA:H112	28:b:606:CLA:H91	1.75	0.44
28:l:306:CLA:HBA1	28:l:306:CLA:H11	1.69	0.44
28:f:610:CLA:H3A	28:f:610:CLA:HBA2	1.57	0.44
1:A:107:ASN:HB3	1:A:110:ALA:HB3	2.00	0.44
1:A:222:VAL:HG13	1:A:242:PRO:HB3	1.99	0.44
28:A:818:CLA:CAD	28:A:828:CLA:H41	2.48	0.44
2:B:340:LEU:O	2:B:344:THR:HG22	2.18	0.44
28:B:813:CLA:H62	28:B:813:CLA:H41	1.72	0.44
28:F:201:CLA:H101	28:F:201:CLA:H61	1.61	0.44
12:K:36:ARG:NE	12:K:53:SER:HA	2.32	0.44
35:c:619:LMG:H371	35:c:619:LMG:H401	1.73	0.44
13:s:154:LYS:HD3	14:c:109:PHE:HA	1.99	0.44
14:c:101:VAL:HG11	28:c:604:CLA:HAC2	2.00	0.44
14:c:118:ALA:HB2	28:c:604:CLA:HED2	1.99	0.44
15:a:91:CYS:SG	15:a:187:MET:HA	2.58	0.44
28:b:608:CLA:H122	28:b:608:CLA:H162	1.53	0.44
28:l:305:CLA:H11	28:l:305:CLA:C4D	2.47	0.44
28:A:839:CLA:H151	28:A:839:CLA:H112	1.67	0.43
13:s:80:SER:OG	13:s:84:ASN:OD1	2.31	0.43
37:j:616:IHT:C06	30:j:617:LHG:H102	2.48	0.43
23:d:103:PHE:HE2	28:d:303:CLA:H42	1.83	0.43
28:g:310:CLA:CGA	28:g:310:CLA:H3A	2.48	0.43
1:A:336:THR:HB	1:A:428:LEU:HD21	2.01	0.43
28:c:602:CLA:HBA2	28:c:602:CLA:H3A	1.41	0.43
28:b:607:CLA:H143	28:b:607:CLA:H162	1.86	0.43
28:e:611:CLA:HBA1	28:e:611:CLA:H12	1.74	0.43
18:f:47:LYS:HE3	18:f:47:LYS:HB3	1.61	0.43
22:i:144:MET:N	22:i:147:SER:HB2	2.28	0.43
23:d:105:GLY:HA3	28:d:304:CLA:C1D	2.48	0.43
28:d:301:CLA:C5	28:d:302:CLA:H3A	2.48	0.43
35:n:620:LMG:H332	35:n:620:LMG:H361	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Q:88:GLN:HG3	27:Q:90:ALA:H	1.83	0.43
27:Q:183:LEU:H	27:Q:183:LEU:HG	1.66	0.43
2:B:431:HIS:O	2:B:435:ILE:HG12	2.18	0.43
28:B:832:CLA:H51	28:B:832:CLA:H11	1.71	0.43
28:h:307:CLA:HBB2	28:h:308:CLA:HBB2	2.01	0.43
21:k:58:LEU:HD11	28:k:602:CLA:HAA2	2.00	0.43
21:k:81:TRP:CZ2	28:k:608:CLA:HAA2	2.54	0.43
23:d:186:LEU:HA	23:d:189:ILE:HG22	1.99	0.43
28:d:303:CLA:H61	28:d:303:CLA:H41	1.52	0.43
27:Q:95:LYS:HA	27:Q:98:THR:HG22	2.01	0.43
28:A:831:CLA:HAA2	31:L:206:WVN:C37	2.49	0.43
28:B:808:CLA:H3A	28:B:808:CLA:HBA1	1.67	0.43
38:s:201:KC2:C1C	30:a:319:LHG:H331	2.48	0.43
23:d:214:ILE:HA	23:d:217:LEU:HB3	2.00	0.43
1:A:663:SER:O	1:A:666:SER:OG	2.28	0.43
28:A:802:CLA:H3A	28:A:802:CLA:H11	2.01	0.43
28:A:826:CLA:H2	28:A:826:CLA:H61	1.59	0.43
28:B:803:CLA:H112	28:B:803:CLA:H72	1.76	0.43
11:O:115:LEU:HD12	28:O:202:CLA:HBB1	2.00	0.43
13:s:77:LEU:HD13	20:l:210:ILE:HG23	2.01	0.43
19:e:57:PHE:HE1	28:e:601:CLA:HAC2	1.83	0.43
20:l:196:THR:HB	20:l:198:GLN:HG2	1.99	0.43
36:k:621:II0:O01	18:j:183:ARG:NH2	2.51	0.43
30:f:619:LHG:H311	30:f:619:LHG:H281	1.76	0.43
28:i:303:CLA:H3A	28:i:303:CLA:HBA2	1.32	0.43
1:A:450:LEU:HD12	1:A:450:LEU:HA	1.88	0.43
2:B:90:ILE:HB	2:B:111:PRO:HB2	2.00	0.43
5:E:2:VAL:HG12	5:E:60:GLU:HG3	1.99	0.43
28:L:202:CLA:HHC	28:L:202:CLA:HBB1	2.01	0.43
28:h:306:CLA:H101	28:h:306:CLA:H61	1.55	0.43
19:e:78:ASN:HB3	19:e:173:MET:HE3	2.00	0.43
38:g:312:KC2:CHD	38:g:312:KC2:CBC	2.97	0.43
26:n:86:ALA:O	26:n:90:ILE:HG13	2.17	0.43
28:n:604:CLA:H12	36:n:618:II0:C40	2.49	0.43
27:Q:127:PRO:HB2	27:Q:206:PHE:CZ	2.52	0.43
1:A:266:PHE:HE1	28:A:816:CLA:HBB1	1.84	0.43
28:A:823:CLA:H41	28:A:823:CLA:H61	1.81	0.43
28:A:837:CLA:H93	8:J:17:THR:HA	2.01	0.43
2:B:470:LEU:HD21	2:B:510:PRO:HB3	2.00	0.43
28:a:311:CLA:H11	28:a:311:CLA:HBA1	1.76	0.43
28:b:601:CLA:H51	28:b:601:CLA:H11	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:82:LEU:HA	22:i:82:LEU:HD23	1.83	0.43
24:g:161:SER:HB2	24:g:168:ARG:HH21	1.83	0.43
25:R:118:TRP:CD1	25:R:121:HIS:HE1	2.37	0.43
31:R:202:WVN:C17	31:R:202:WVN:C14	2.95	0.43
1:A:121:ILE:HG13	1:A:122:VAL:HG13	1.99	0.43
28:A:835:CLA:H191	28:L:203:CLA:H72	2.00	0.43
28:a:309:CLA:HBB1	28:a:311:CLA:HAA1	2.01	0.43
18:m:142:ILE:HD13	20:l:61:PRO:HB2	2.01	0.43
28:e:605:CLA:H161	28:e:605:CLA:H121	1.92	0.43
22:i:196:ILE:HD12	22:i:196:ILE:HA	1.92	0.43
28:d:306:CLA:HBA1	28:d:306:CLA:H3A	1.67	0.43
26:n:160:MET:HB2	26:n:167:ARG:HE	1.84	0.43
28:n:607:CLA:H151	28:n:607:CLA:H111	1.44	0.43
35:Q:301:LMG:H122	28:Q:302:CLA:ND	2.33	0.43
28:B:832:CLA:H12	28:B:833:CLA:O1A	2.19	0.43
28:B:839:CLA:H112	28:h:301:CLA:HAB	2.00	0.43
11:O:63:SER:HB3	11:O:68:TYR:CD2	2.54	0.43
18:m:163:GLY:HA3	18:m:166:LYS:NZ	2.34	0.43
26:n:188:MET:HB3	26:n:188:MET:HE2	1.77	0.43
28:n:609:CLA:H143	28:n:609:CLA:H111	1.80	0.43
28:n:610:CLA:H3A	28:n:610:CLA:HBA2	1.49	0.43
28:B:813:CLA:O1D	28:B:813:CLA:H2A	2.18	0.43
4:D:88:ARG:HB3	4:D:96:GLN:HB3	2.01	0.43
28:e:605:CLA:H18	28:e:605:CLA:H151	1.74	0.43
28:k:606:CLA:H2A	28:k:606:CLA:HED3	2.01	0.43
18:j:126:MET:HE3	28:j:607:CLA:HBC3	2.00	0.43
28:j:610:CLA:HBA2	28:j:610:CLA:H3A	1.64	0.43
2:B:630:LEU:HD22	2:B:723:PHE:HA	2.01	0.42
28:B:822:CLA:H61	28:B:822:CLA:H101	1.73	0.42
12:K:39:ILE:O	12:K:42:LYS:NZ	2.49	0.42
16:b:187:HIS:HA	16:b:190:ILE:HD12	2.01	0.42
28:h:304:CLA:HHC	28:h:304:CLA:HAB	1.88	0.42
18:f:72:ILE:HA	18:f:75:LEU:HD12	2.01	0.42
22:i:65:PRO:HG3	18:j:139:PHE:HE1	1.84	0.42
2:B:71:GLY:HA2	2:B:86:ILE:CG2	2.50	0.42
35:J:105:LMG:H452	35:J:105:LMG:H421	1.83	0.42
9:L:64:LYS:HD2	9:L:64:LYS:HA	1.76	0.42
28:L:204:CLA:H11	35:L:209:LMG:H191	2.00	0.42
35:L:209:LMG:H142	35:L:209:LMG:H172	1.85	0.42
11:O:43:ASN:ND2	11:O:121:ASN:OD1	2.43	0.42
28:a:303:CLA:H41	28:a:303:CLA:H61	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:618:LMT:H52	32:b:618:LMT:H82	1.82	0.42
17:h:163:GLU:O	17:h:164:LYS:HB2	2.19	0.42
30:m:619:LHG:H132	30:m:619:LHG:H292	2.01	0.42
28:g:308:CLA:HAB	28:g:308:CLA:HHC	1.86	0.42
35:n:620:LMG:H391	35:n:620:LMG:H362	1.87	0.42
28:s:202:CLA:H201	28:s:208:CLA:HBB2	2.00	0.42
18:m:76:GLN:O	18:m:80:ILE:HG13	2.18	0.42
28:e:601:CLA:H3A	28:e:601:CLA:HBA2	1.38	0.42
28:l:306:CLA:H143	28:l:306:CLA:H161	1.84	0.42
22:i:76:TRP:CZ3	22:i:145:SER:HA	2.55	0.42
27:Q:212:ALA:O	27:Q:216:ILE:HG12	2.20	0.42
1:A:25:SER:OG	32:A:850:LMT:O6’	2.37	0.42
1:A:682:TRP:O	1:A:685:SER:OG	2.29	0.42
2:B:525:ALA:HB1	2:B:585:THR:HB	2.01	0.42
35:F:205:LMG:H142	35:F:205:LMG:H171	1.87	0.42
28:O:206:CLA:H91	28:O:206:CLA:H112	1.87	0.42
28:m:609:CLA:HBA2	28:m:609:CLA:H3A	1.59	0.42
28:f:613:CLA:H112	28:f:613:CLA:C4D	2.50	0.42
30:i:318:LHG:H112	30:i:318:LHG:H242	2.01	0.42
28:g:322:CLA:H91	28:g:322:CLA:H112	1.77	0.42
28:n:605:CLA:HBA1	28:n:605:CLA:H3A	1.75	0.42
1:A:174:ILE:HD12	1:A:174:ILE:HA	1.91	0.42
1:A:683:ALA:HB3	28:A:802:CLA:HBB2	2.01	0.42
28:A:801:CLA:HED2	28:A:801:CLA:HBD	1.71	0.42
28:A:802:CLA:HBA1	28:A:802:CLA:H11	1.62	0.42
2:B:60:THR:HB	2:B:141:LEU:HD13	2.00	0.42
2:B:269:LEU:HD23	2:B:269:LEU:HA	1.88	0.42
13:s:93:MET:HE1	28:s:202:CLA:HAB	2.01	0.42
15:a:195:HIS:HA	15:a:198:ILE:HD12	2.02	0.42
20:l:39:ALA:HB2	20:l:57:VAL:HG23	2.02	0.42
21:k:119:LYS:O	21:k:123:VAL:HG23	2.19	0.42
21:k:145:LEU:HD13	28:k:607:CLA:H41	2.02	0.42
18:f:184:LEU:HD13	28:f:610:CLA:HBC1	2.02	0.42
2:B:343:ILE:CG1	28:B:821:CLA:H43	2.49	0.42
35:J:105:LMG:H332	16:b:62:ILE:HD11	2.01	0.42
28:e:604:CLA:H102	28:e:604:CLA:H13	1.51	0.42
28:f:608:CLA:H93	28:f:608:CLA:H61	1.77	0.42
24:g:92:LEU:HB3	28:g:305:CLA:HAB	2.02	0.42
2:B:61:SER:HB3	2:B:141:LEU:HB2	2.02	0.42
2:B:326:THR:HG21	25:R:44:VAL:HG13	2.01	0.42
28:B:837:CLA:H51	28:B:837:CLA:H8	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:F:205:LMG:H222	35:F:205:LMG:H252	1.85	0.42
28:e:606:CLA:H93	28:e:606:CLA:H62	1.88	0.42
20:l:64:PHE:C	20:l:66:ASN:H	2.27	0.42
18:j:77:GLU:OE1	18:j:155:GLY:N	2.38	0.42
1:A:446:ILE:HD13	1:A:446:ILE:HA	1.92	0.42
28:A:803:CLA:H12	28:A:803:CLA:H52	1.87	0.42
2:B:173:ARG:HB2	28:B:811:CLA:HBC2	2.01	0.42
28:B:815:CLA:H62	28:B:815:CLA:H102	1.68	0.42
6:F:139:ASP:OD1	6:F:140:LYS:N	2.51	0.42
30:J:106:LHG:H141	30:J:106:LHG:H171	1.87	0.42
28:f:607:CLA:H161	28:f:607:CLA:H141	1.92	0.42
28:A:829:CLA:H102	28:A:829:CLA:H62	1.80	0.42
2:B:421:LEU:HD13	2:B:531:LEU:HA	2.01	0.42
2:B:657:ALA:HB3	28:B:803:CLA:HBB2	2.02	0.42
28:L:204:CLA:H3A	28:L:204:CLA:HBA2	1.70	0.42
16:b:164:ARG:O	16:b:168:GLU:HG3	2.20	0.42
17:h:94:SER:HA	17:h:213:VAL:HG13	2.02	0.42
18:m:113:MET:O	18:m:116:VAL:HG22	2.19	0.42
21:k:102:ALA:HA	21:k:105:LEU:HG	2.02	0.42
28:k:610:CLA:HBA2	28:k:610:CLA:H3A	1.60	0.42
28:i:302:CLA:HAB	18:j:159:PHE:CD1	2.55	0.42
2:B:274:HIS:HB3	28:B:815:CLA:HMB2	2.01	0.41
28:B:830:CLA:C4C	28:B:831:CLA:HAB	2.50	0.41
5:E:2:VAL:HG23	5:E:27:ILE:HD11	2.02	0.41
21:k:86:GLU:OE1	28:k:602:CLA:NA	2.52	0.41
22:i:142:PHE:HD1	38:i:319:KC2:C3C	2.32	0.41
27:Q:190:VAL:HG13	27:Q:216:ILE:HD12	2.02	0.41
28:A:801:CLA:H162	28:A:801:CLA:H122	1.80	0.41
28:A:802:CLA:H12	2:B:429:GLY:HA3	2.01	0.41
28:A:818:CLA:H3A	28:A:818:CLA:HBA2	1.75	0.41
28:A:841:CLA:HBA1	28:A:841:CLA:H11	1.84	0.41
9:L:109:GLN:HG3	9:L:111:GLN:H	1.85	0.41
14:c:204:THR:HG22	14:c:207:GLU:HB2	2.02	0.41
28:g:310:CLA:H11	28:g:310:CLA:HBA1	1.84	0.41
27:Q:65:PRO:HA	27:Q:231:ILE:HD11	2.02	0.41
28:c:612:CLA:H62	28:c:612:CLA:H2	1.75	0.41
15:a:126:ALA:HB3	28:a:307:CLA:HED2	2.03	0.41
23:d:84:HIS:HB3	23:d:196:MET:SD	2.60	0.41
28:d:304:CLA:HBA2	28:d:304:CLA:H3A	1.82	0.41
26:n:166:SER:O	26:n:166:SER:OG	2.35	0.41
1:A:414:PHE:CD1	1:A:418:ASP:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:817:CLA:HAC1	28:B:821:CLA:H192	2.03	0.41
11:O:27:GLN:OE1	11:O:43:ASN:CB	2.69	0.41
16:b:104:LEU:HD23	16:b:104:LEU:HA	1.93	0.41
16:b:164:ARG:NH2	28:b:607:CLA:O1D	2.53	0.41
17:h:171:PRO:HB2	28:h:302:CLA:HED3	2.01	0.41
18:m:87:MET:HG3	18:m:182:GLY:HA2	2.02	0.41
18:f:81:LYS:HE3	18:f:81:LYS:HB2	1.82	0.41
28:g:322:CLA:H172	28:g:322:CLA:H13	1.77	0.41
25:R:112:LEU:O	25:R:117:SER:OG	2.36	0.41
26:n:58:PRO:HG3	26:n:72:ASP:HB3	2.02	0.41
1:A:328:LEU:O	1:A:340:HIS:HB2	2.21	0.41
28:A:816:CLA:CHD	28:A:817:CLA:HBB2	2.51	0.41
28:B:813:CLA:H62	28:B:813:CLA:H92	1.80	0.41
28:B:824:CLA:H111	28:B:824:CLA:H72	1.92	0.41
6:F:154:LEU:HA	6:F:157:VAL:HG22	2.02	0.41
28:c:603:CLA:HBA1	28:c:603:CLA:H3A	1.71	0.41
28:b:607:CLA:HHD	28:b:607:CLA:HAC1	1.76	0.41
18:f:152:ARG:NE	18:f:156:ASP:O	2.49	0.41
26:n:92:HIS:NE2	28:n:603:CLA:NC	2.69	0.41
27:Q:193:GLY:HA3	27:Q:216:ILE:HD11	2.01	0.41
27:Q:231:ILE:HD12	27:Q:231:ILE:HA	1.93	0.41
28:A:854:CLA:H111	28:B:835:CLA:H62	2.02	0.41
4:D:33:ILE:HD13	4:D:71:LEU:HD23	2.03	0.41
6:F:33:THR:O	6:F:90:CYS:N	2.44	0.41
21:k:119:LYS:HB2	21:k:211:TYR:CE1	2.55	0.41
24:g:199:GLY:O	24:g:203:MET:HG3	2.20	0.41
1:A:30:ALA:HB1	8:J:7:LYS:HG2	2.01	0.41
1:A:161:TRP:CE2	28:A:815:CLA:HAA2	2.56	0.41
1:A:747:LEU:HD23	1:A:747:LEU:HA	1.81	0.41
28:A:810:CLA:H122	28:A:810:CLA:H162	1.81	0.41
29:A:842:PQN:H162	29:A:842:PQN:H192	1.75	0.41
28:B:805:CLA:H2	28:B:805:CLA:H61	1.81	0.41
28:L:202:CLA:H3A	28:L:202:CLA:HBA2	1.62	0.41
27:Q:65:PRO:HB3	27:Q:233:PHE:HD2	1.85	0.41
1:A:395:HIS:HE2	28:A:828:CLA:C1B	2.33	0.41
1:A:736:LEU:HD21	28:A:829:CLA:H193	2.02	0.41
28:A:852:CLA:H172	6:F:128:GLY:HA2	2.02	0.41
2:B:496:TRP:CH2	2:B:507:LEU:HD21	2.56	0.41
3:C:77:MET:HB3	3:C:79:LEU:HG	2.03	0.41
35:L:209:LMG:H141	35:L:209:LMG:H111	1.82	0.41
15:a:145:LYS:HA	15:a:149:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:603:CLA:H41	28:b:603:CLA:H61	1.57	0.41
28:b:604:CLA:H93	28:b:604:CLA:H111	1.87	0.41
1:A:320:ILE:HD13	12:K:64:ALA:HB2	2.02	0.41
1:A:488:TRP:CE2	1:A:492:ILE:HD11	2.55	0.41
28:A:824:CLA:H13	28:A:824:CLA:H172	1.74	0.41
2:B:346:LEU:HD22	2:B:350:HIS:CE1	2.56	0.41
2:B:421:LEU:HA	2:B:424:VAL:HG12	2.03	0.41
28:B:825:CLA:H3A	28:B:825:CLA:HBA2	1.88	0.41
28:B:840:CLA:H152	28:B:840:CLA:H112	1.89	0.41
6:F:155:SER:O	6:F:159:THR:HG23	2.20	0.41
13:s:28:THR:HG22	13:s:45:GLY:HA2	2.02	0.41
14:c:123:VAL:HG22	28:c:606:CLA:C2D	2.51	0.41
28:h:306:CLA:H91	28:h:306:CLA:H111	1.75	0.41
20:l:103:SER:HB3	20:l:114:VAL:HB	2.03	0.41
21:k:128:LEU:HA	21:k:128:LEU:HD23	1.81	0.41
22:i:52:ALA:HB3	22:i:69:THR:HB	2.02	0.41
18:j:40:GLU:HB3	28:j:601:CLA:HED1	2.02	0.41
23:d:203:VAL:HG12	23:d:207:PHE:HE2	1.86	0.41
28:n:610:CLA:H111	28:n:610:CLA:H72	1.68	0.41
1:A:464:MET:HB2	1:A:473:MET:HG2	2.02	0.41
2:B:105:LYS:HE2	2:B:114:ILE:HG12	2.02	0.41
28:B:822:CLA:H143	28:B:822:CLA:H111	1.81	0.41
3:C:24:ASP:OD1	4:D:106:PRO:HG3	2.21	0.41
28:J:103:CLA:C4D	30:b:619:LHG:H102	2.51	0.41
28:O:201:CLA:H62	28:O:201:CLA:H41	1.87	0.41
30:a:301:LHG:H191	30:a:301:LHG:H162	1.84	0.41
28:h:303:CLA:H12	28:h:303:CLA:HBA1	1.88	0.41
18:m:164:PHE:HB3	18:m:174:TYR:CE2	2.54	0.41
1:A:219:GLN:HA	1:A:223:SER:HB2	2.03	0.40
1:A:450:LEU:HD21	28:A:835:CLA:HMB2	2.02	0.40
28:A:824:CLA:HBA1	28:A:828:CLA:H193	2.04	0.40
28:A:826:CLA:H61	28:A:826:CLA:H101	1.92	0.40
28:A:836:CLA:C4D	28:O:206:CLA:H161	2.51	0.40
28:A:854:CLA:H41	28:A:854:CLA:H112	2.03	0.40
2:B:209:ASP:HA	28:Q:302:CLA:C2D	2.51	0.40
2:B:620:ARG:HA	2:B:624:TRP:HB3	2.03	0.40
30:J:106:LHG:H252	30:J:106:LHG:H332	2.03	0.40
15:a:143:TYR:CD1	28:R:203:CLA:HBA2	2.55	0.40
28:e:611:CLA:H112	28:e:611:CLA:H72	1.71	0.40
18:f:45:LEU:HD22	18:f:45:LEU:HA	1.97	0.40
26:n:185:MET:H	26:n:185:MET:HG2	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ALA:HB3	10:M:28:LEU:HD21	2.02	0.40
6:F:116:LEU:HG	30:J:106:LHG:H132	2.03	0.40
24:g:143:LEU:O	24:g:147:LEU:HB2	2.21	0.40
1:A:676:LEU:HD23	1:A:676:LEU:HA	1.95	0.40
2:B:608:PHE:O	2:B:612:SER:OG	2.37	0.40
28:B:835:CLA:H202	28:B:835:CLA:H161	1.93	0.40
7:I:9:ILE:HD11	17:h:132:ARG:HH12	1.87	0.40
9:L:12:PRO:HG2	9:L:13:PHE:CE2	2.57	0.40
9:L:54:HIS:HA	9:L:57:PHE:CE2	2.56	0.40
30:a:319:LHG:H361	30:a:319:LHG:H332	1.82	0.40
16:b:103:ALA:HB3	16:b:189:MET:HE1	2.03	0.40
23:d:72:LEU:HD23	23:d:77:LEU:HD21	2.04	0.40
24:g:121:HIS:HD2	24:g:140:MET:HE2	1.87	0.40
28:g:309:CLA:H3A	28:g:309:CLA:HBA1	1.82	0.40
27:Q:111:VAL:HG11	27:Q:217:LYS:HB2	2.02	0.40
1:A:39:LEU:HD13	1:A:52:LEU:HA	2.04	0.40
28:A:841:CLA:H93	8:J:16:PHE:HE1	1.85	0.40
3:C:15:THR:HG22	3:C:28:MET:HE2	2.01	0.40
14:c:130:GLN:HG3	28:c:605:CLA:C4D	2.51	0.40
21:k:192:LYS:O	21:k:196:ASN:ND2	2.48	0.40
28:i:308:CLA:CGA	28:i:308:CLA:H3A	2.52	0.40
28:d:303:CLA:H171	36:d:316:II0:C29	2.51	0.40
28:A:806:CLA:H141	28:A:806:CLA:H161	1.79	0.40
2:B:166:TRP:CD1	39:i:301:LMU:H6'1	2.57	0.40
28:B:815:CLA:HAA2	28:B:823:CLA:HBB2	2.03	0.40
18:m:51:LEU:HD11	18:m:62:ASP:HB2	2.02	0.40
18:m:112:LYS:HB2	18:m:112:LYS:HE3	1.79	0.40
18:j:103:GLY:HA3	28:j:605:CLA:NA	2.36	0.40
24:g:47:ALA:HA	24:g:48:PRO:HD3	1.92	0.40
28:n:613:CLA:HBA1	28:n:613:CLA:HBD	2.04	0.40
35:Q:301:LMG:H112	28:Q:302:CLA:H42	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	607/616 (98%)	604 (100%)	3 (0%)	81 92
2	B	593/593 (100%)	586 (99%)	7 (1%)	63 84
3	C	67/68 (98%)	64 (96%)	3 (4%)	24 52
4	D	116/117 (99%)	113 (97%)	3 (3%)	40 70
5	E	54/58 (93%)	54 (100%)	0	100 100
6	F	133/157 (85%)	132 (99%)	1 (1%)	73 88
7	I	28/29 (97%)	28 (100%)	0	100 100
8	J	39/39 (100%)	39 (100%)	0	100 100
9	L	124/126 (98%)	123 (99%)	1 (1%)	73 88
10	M	25/25 (100%)	25 (100%)	0	100 100
11	O	81/110 (74%)	77 (95%)	4 (5%)	22 49
12	K	52/66 (79%)	50 (96%)	2 (4%)	29 58
13	s	116/195 (60%)	115 (99%)	1 (1%)	70 87
14	c	138/171 (81%)	134 (97%)	4 (3%)	37 67
15	a	139/165 (84%)	133 (96%)	6 (4%)	26 54
16	b	149/168 (89%)	145 (97%)	4 (3%)	39 69
17	h	123/162 (76%)	121 (98%)	2 (2%)	55 80
18	f	135/161 (84%)	130 (96%)	5 (4%)	30 59
18	j	136/161 (84%)	134 (98%)	2 (2%)	57 81
18	m	137/161 (85%)	135 (98%)	2 (2%)	57 81
19	e	130/155 (84%)	128 (98%)	2 (2%)	57 81
20	l	137/191 (72%)	137 (100%)	0	100 100
21	k	138/186 (74%)	132 (96%)	6 (4%)	26 54
22	i	138/168 (82%)	138 (100%)	0	100 100
23	d	97/157 (62%)	93 (96%)	4 (4%)	27 56
24	g	171/199 (86%)	168 (98%)	3 (2%)	51 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	R	69/98 (70%)	69 (100%)	0	100 100
26	n	140/163 (86%)	137 (98%)	3 (2%)	47 75
27	Q	134/168 (80%)	121 (90%)	13 (10%)	8 20
All	All	4146/4833 (86%)	4065 (98%)	81 (2%)	48 76

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	LEU
1	A	691	SER
1	A	736	LEU
2	B	139	LEU
2	B	279	ILE
2	B	442	VAL
2	B	491	ILE
2	B	507	LEU
2	B	524	LEU
2	B	531	LEU
3	C	30	SER
3	C	32	ASP
3	C	35	LYS
4	D	13	THR
4	D	75	VAL
4	D	76	LYS
6	F	188	ARG
9	L	90	VAL
11	O	24	VAL
11	O	25	VAL
11	O	29	LYS
11	O	31	ASP
12	K	19	LYS
12	K	29	ILE
13	s	32	MET
14	c	82	ARG
14	c	191	ILE
14	c	195	ILE
14	c	204	THR
15	a	91	CYS
15	a	164	ARG
15	a	201	LYS
15	a	206	THR

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Mol	Chain	Res	Type
15	a	207	GLN
15	a	210	GLU
16	b	101	LYS
16	b	204	LYS
16	b	210	LEU
16	b	211	MET
17	h	132	ARG
17	h	210	THR
18	m	77	GLU
18	m	108	VAL
19	e	76	ILE
19	e	164	LYS
21	k	49	VAL
21	k	60	GLU
21	k	61	ASN
21	k	62	ILE
21	k	121	THR
21	k	137	LYS
18	f	45	LEU
18	f	46	LYS
18	f	47	LYS
18	f	49	GLU
18	f	68	SER
18	j	42	VAL
18	j	52	ASP
23	d	131	GLN
23	d	215	GLU
23	d	217	LEU
23	d	219	SER
24	g	39	SER
24	g	120	VAL
24	g	252	LEU
26	n	69	GLN
26	n	183	ASP
26	n	188	MET
27	Q	62	THR
27	Q	66	ILE
27	Q	72	GLU
27	Q	140	LEU
27	Q	142	LEU
27	Q	146	VAL
27	Q	172	LYS

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Mol	Chain	Res	Type
27	Q	173	GLU
27	Q	175	LEU
27	Q	176	LYS
27	Q	179	SER
27	Q	183	LEU
27	Q	233	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	420	ASN
1	A	444	ASN
1	A	717	GLN
2	B	75	GLN
2	B	113	ASN
2	B	401	GLN
2	B	632	ASN
2	B	635	ASN
3	C	38	GLN
4	D	140	ASN
8	J	31	ASN
9	L	9	ASN
9	L	109	GLN
16	b	100	GLN
16	b	194	GLN
18	m	76	GLN
18	m	123	GLN
18	m	128	GLN
21	k	103	GLN
18	f	175	GLN
24	g	80	GLN
24	g	100	GLN
24	g	121	HIS
26	n	81	ASN
26	n	162	ASN
26	n	189	GLN
26	n	195	ASN

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

415 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	II0	g	317	-	39,43,43	6.75	23 (58%)	48,60,60	2.08	13 (27%)
28	CLA	A	851	-	69,73,73	1.21	9 (13%)	82,113,113	1.27	7 (8%)
28	CLA	c	603	-	55,59,73	1.25	8 (14%)	64,96,113	1.39	7 (10%)
36	II0	m	618	-	39,43,43	6.81	22 (56%)	48,60,60	3.16	17 (35%)
28	CLA	l	303	20	69,73,73	1.15	8 (11%)	82,113,113	1.38	8 (9%)
30	LHG	i	318	28	36,36,48	1.12	2 (5%)	39,42,54	1.29	6 (15%)
28	CLA	b	605	40,28	69,73,73	1.13	6 (8%)	82,113,113	1.38	7 (8%)
28	CLA	s	206	40	69,73,73	1.16	7 (10%)	82,113,113	1.34	9 (10%)
28	CLA	A	835	-	69,73,73	1.12	6 (8%)	82,113,113	1.24	4 (4%)
28	CLA	j	612	-	55,59,73	1.45	7 (12%)	64,96,113	1.51	11 (17%)
28	CLA	A	837	-	69,73,73	1.12	6 (8%)	82,113,113	1.26	9 (10%)
28	CLA	B	824	-	69,73,73	1.12	8 (11%)	82,113,113	1.41	8 (9%)
28	CLA	A	830	-	54,58,73	1.28	8 (14%)	64,95,113	1.47	8 (12%)
36	II0	k	615	-	39,43,43	6.72	23 (58%)	48,60,60	2.02	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	WVN	R	201	-	40,41,41	1.74	10 (25%)	51,56,56	2.14	14 (27%)
36	II0	n	618	-	39,43,43	6.76	21 (53%)	48,60,60	1.92	15 (31%)
31	WVN	B	848	-	40,41,41	1.79	12 (30%)	51,56,56	2.17	18 (35%)
30	LHG	L	208	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
28	CLA	b	606	16	65,69,73	1.19	9 (13%)	77,108,113	1.42	9 (11%)
28	CLA	B	808	2	69,73,73	1.18	8 (11%)	82,113,113	1.46	10 (12%)
31	WVN	L	206	-	40,41,41	1.65	10 (25%)	51,56,56	2.56	22 (43%)
36	II0	m	615	-	39,43,43	6.61	24 (61%)	48,60,60	1.96	17 (35%)
37	IHT	g	319	-	40,42,42	6.33	26 (65%)	52,58,58	3.07	20 (38%)
28	CLA	B	840	-	69,73,73	1.15	7 (10%)	82,113,113	1.27	10 (12%)
30	LHG	m	619	28	36,36,48	1.08	2 (5%)	39,42,54	1.13	3 (7%)
28	CLA	m	609	18	55,59,73	1.27	7 (12%)	64,96,113	1.34	9 (14%)
28	CLA	h	303	17	54,58,73	1.29	8 (14%)	64,95,113	1.41	7 (10%)
28	CLA	g	322	35	69,73,73	1.15	6 (8%)	82,113,113	1.28	7 (8%)
31	WVN	I	101	-	40,41,41	1.69	9 (22%)	51,56,56	1.84	13 (25%)
35	LMG	b	621	-	49,49,55	0.97	3 (6%)	57,57,63	1.21	5 (8%)
28	CLA	h	308	17	55,59,73	1.32	6 (10%)	64,96,113	1.56	9 (14%)
31	WVN	F	204	-	40,41,41	1.78	10 (25%)	51,56,56	2.97	19 (37%)
37	IHT	b	616	-	40,42,42	6.34	26 (65%)	52,58,58	2.84	16 (30%)
36	II0	i	314	-	39,43,43	6.70	22 (56%)	48,60,60	1.75	14 (29%)
28	CLA	A	822	-	55,59,73	1.29	9 (16%)	64,96,113	1.36	6 (9%)
36	II0	i	315	-	39,43,43	6.73	20 (51%)	48,60,60	1.90	12 (25%)
28	CLA	b	608	30	69,73,73	1.16	7 (10%)	82,113,113	1.23	9 (10%)
28	CLA	d	304	23	55,59,73	1.31	6 (10%)	64,96,113	1.44	6 (9%)
28	CLA	B	817	40	69,73,73	1.17	9 (13%)	82,113,113	1.28	10 (12%)
30	LHG	g	321	28	36,36,48	1.07	2 (5%)	39,42,54	1.44	8 (20%)
28	CLA	B	821	40	69,73,73	1.23	10 (14%)	82,113,113	1.85	18 (21%)
28	CLA	i	303	22	54,58,73	1.28	7 (12%)	64,95,113	1.51	8 (12%)
28	CLA	g	303	24	54,58,73	1.25	7 (12%)	64,95,113	1.42	11 (17%)
33	SF4	C	101	3	0,12,12	-	-	-		
28	CLA	m	602	18	60,64,73	1.24	8 (13%)	71,102,113	1.32	10 (14%)
31	WVN	h	309	-	40,41,41	1.70	9 (22%)	51,56,56	2.49	23 (45%)
28	CLA	A	817	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	10 (12%)
36	II0	a	318	-	39,43,43	6.90	21 (53%)	48,60,60	2.66	13 (27%)
28	CLA	B	823	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	f	602	18	69,73,73	1.15	7 (10%)	82,113,113	1.29	9 (10%)
36	II0	e	616	-	39,43,43	6.69	22 (56%)	48,60,60	1.87	15 (31%)
28	CLA	Q	303	27	49,53,73	1.43	10 (20%)	58,89,113	1.56	8 (13%)
28	CLA	h	305	17	55,59,73	1.26	7 (12%)	64,96,113	1.32	7 (10%)
31	WVN	J	101	-	40,41,41	1.82	10 (25%)	51,56,56	3.49	22 (43%)
28	CLA	h	306	17	69,73,73	1.18	7 (10%)	82,113,113	1.16	9 (10%)
28	CLA	A	814	-	54,58,73	1.28	6 (11%)	64,95,113	1.37	8 (12%)
28	CLA	A	812	-	69,73,73	1.15	6 (8%)	82,113,113	1.47	11 (13%)
28	CLA	B	804	-	69,73,73	1.11	6 (8%)	82,113,113	1.40	8 (9%)
28	CLA	c	601	14	55,59,73	1.29	6 (10%)	64,96,113	1.31	5 (7%)
34	DGD	B	843	-	61,61,67	0.91	2 (3%)	75,75,81	1.10	4 (5%)
28	CLA	m	607	-	55,59,73	1.33	7 (12%)	64,96,113	1.35	10 (15%)
28	CLA	n	610	40	69,73,73	1.17	6 (8%)	82,113,113	1.20	5 (6%)
28	CLA	a	306	40	69,73,73	1.11	7 (10%)	82,113,113	1.24	7 (8%)
28	CLA	j	605	18	49,53,73	1.46	8 (16%)	58,89,113	1.51	6 (10%)
36	II0	a	315	-	39,43,43	6.59	23 (58%)	48,60,60	2.10	16 (33%)
36	II0	i	320	-	39,43,43	6.65	21 (53%)	48,60,60	1.75	10 (20%)
36	II0	l	316	-	39,43,43	6.74	23 (58%)	48,60,60	1.71	15 (31%)
28	CLA	j	607	-	55,59,73	1.27	6 (10%)	64,96,113	1.32	5 (7%)
28	CLA	i	305	22	69,73,73	1.15	5 (7%)	82,113,113	1.25	7 (8%)
28	CLA	i	308	22	55,59,73	1.30	7 (12%)	64,96,113	1.40	6 (9%)
32	LMT	a	320	-	36,36,36	1.22	6 (16%)	47,47,47	1.30	7 (14%)
28	CLA	A	805	1	69,73,73	1.15	9 (13%)	82,113,113	1.35	9 (10%)
28	CLA	A	806	-	69,73,73	1.15	7 (10%)	82,113,113	1.23	9 (10%)
30	LHG	j	617	28	29,29,48	1.19	2 (6%)	32,35,54	1.36	6 (18%)
28	CLA	O	202	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	9 (10%)
28	CLA	B	811	-	69,73,73	1.16	8 (11%)	82,113,113	1.43	14 (17%)
28	CLA	B	828	-	53,57,73	1.27	8 (15%)	61,93,113	1.43	10 (16%)
28	CLA	m	612	40	55,59,73	1.27	8 (14%)	64,96,113	1.40	8 (12%)
28	CLA	d	307	23	50,54,73	1.35	5 (10%)	59,90,113	1.30	4 (6%)
28	CLA	g	310	24	55,59,73	1.28	7 (12%)	64,96,113	1.39	9 (14%)
31	WVN	B	847	-	40,41,41	1.62	13 (32%)	51,56,56	2.31	15 (29%)
28	CLA	O	206	-	69,73,73	1.18	10 (14%)	82,113,113	1.55	15 (18%)
28	CLA	j	613	-	69,73,73	1.14	5 (7%)	82,113,113	1.25	6 (7%)
28	CLA	f	604	18	69,73,73	1.13	5 (7%)	82,113,113	1.18	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	c	609	30	49,53,73	1.38	6 (12%)	58,89,113	1.21	5 (8%)
28	CLA	b	601	16	55,59,73	1.28	6 (10%)	64,96,113	1.52	7 (10%)
28	CLA	j	609	18	55,59,73	1.27	7 (12%)	64,96,113	1.30	6 (9%)
28	CLA	a	304	15	54,58,73	1.30	7 (12%)	64,95,113	1.39	8 (12%)
36	II0	k	619	-	39,43,43	6.68	21 (53%)	48,60,60	2.08	17 (35%)
30	LHG	k	620	28	36,36,48	1.15	2 (5%)	39,42,54	1.09	3 (7%)
33	SF4	A	853	2,1	0,12,12	-	-	-		
28	CLA	n	602	26	54,58,73	1.28	8 (14%)	64,95,113	1.35	10 (15%)
28	CLA	h	302	17	54,58,73	1.27	7 (12%)	64,95,113	1.38	5 (7%)
28	CLA	B	825	-	69,73,73	1.14	7 (10%)	82,113,113	1.17	6 (7%)
28	CLA	e	607	19	69,73,73	1.15	7 (10%)	82,113,113	1.21	5 (6%)
28	CLA	B	806	-	69,73,73	1.09	6 (8%)	82,113,113	1.37	7 (8%)
28	CLA	h	313	40	69,73,73	1.14	7 (10%)	82,113,113	1.21	9 (10%)
28	CLA	L	207	40	55,59,73	1.28	7 (12%)	64,96,113	1.30	5 (7%)
36	II0	c	614	-	39,43,43	6.69	21 (53%)	48,60,60	2.08	17 (35%)
28	CLA	d	312	-	55,59,73	1.28	6 (10%)	64,96,113	1.40	11 (17%)
30	LHG	e	617	28	36,36,48	1.09	2 (5%)	39,42,54	1.33	5 (12%)
28	CLA	B	820	-	57,61,73	1.25	8 (14%)	67,98,113	1.28	8 (11%)
28	CLA	A	803	28	59,63,73	1.23	7 (11%)	70,101,113	1.40	8 (11%)
36	II0	b	617	-	39,43,43	6.61	20 (51%)	48,60,60	2.11	17 (35%)
28	CLA	k	606	21	55,59,73	1.29	8 (14%)	64,96,113	1.34	6 (9%)
28	CLA	B	810	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	6 (8%)
28	CLA	A	855	30	45,49,73	1.47	5 (11%)	54,84,113	2.03	7 (12%)
36	II0	l	314	-	39,43,43	6.74	21 (53%)	48,60,60	1.96	16 (33%)
38	KC2	g	313	38	49,53,53	2.76	20 (40%)	60,89,89	3.69	33 (55%)
38	KC2	d	311	-	49,53,53	2.77	19 (38%)	60,89,89	3.59	32 (53%)
38	KC2	f	611	18	49,53,53	2.73	19 (38%)	60,89,89	3.73	32 (53%)
28	CLA	b	611	-	69,73,73	1.14	6 (8%)	82,113,113	1.15	6 (7%)
28	CLA	k	608	21	69,73,73	1.16	7 (10%)	82,113,113	1.28	8 (9%)
30	LHG	a	319	28	48,48,48	0.90	2 (4%)	51,54,54	1.10	4 (7%)
36	II0	e	614	-	39,43,43	6.83	22 (56%)	48,60,60	1.97	14 (29%)
28	CLA	c	602	14	54,58,73	1.25	9 (16%)	64,95,113	1.57	11 (17%)
30	LHG	c	620	28	36,36,48	1.06	2 (5%)	39,42,54	1.26	4 (10%)
28	CLA	n	601	26	49,53,73	1.38	9 (18%)	58,89,113	1.29	5 (8%)
29	PQN	A	842	-	34,34,34	1.87	5 (14%)	43,45,45	1.35	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMT	b	618	-	24,24,36	1.10	3 (12%)	29,29,47	1.08	0
28	CLA	k	605	21	49,53,73	1.38	6 (12%)	58,89,113	1.51	9 (15%)
36	II0	f	616	-	39,43,43	6.67	21 (53%)	48,60,60	1.87	12 (25%)
36	II0	n	616	-	39,43,43	6.79	22 (56%)	48,60,60	1.81	13 (27%)
28	CLA	i	302	22	55,59,73	1.30	6 (10%)	64,96,113	1.34	7 (10%)
36	II0	k	621	-	39,43,43	6.68	22 (56%)	48,60,60	2.11	12 (25%)
38	KC2	k	613	-	49,53,53	2.77	20 (40%)	60,89,89	3.70	32 (53%)
35	LMG	c	619	-	55,55,55	0.97	2 (3%)	63,63,63	1.48	11 (17%)
36	II0	a	314	-	39,43,43	6.61	24 (61%)	48,60,60	1.93	17 (35%)
28	CLA	j	603	-	55,59,73	1.29	8 (14%)	64,96,113	1.40	8 (12%)
37	IHT	m	617	-	40,42,42	6.17	26 (65%)	52,58,58	2.40	16 (30%)
28	CLA	A	818	-	69,73,73	1.17	9 (13%)	82,113,113	1.48	12 (14%)
28	CLA	L	202	9	53,57,73	1.29	8 (15%)	61,93,113	1.38	7 (11%)
36	II0	h	312	-	39,43,43	6.77	20 (51%)	48,60,60	1.95	14 (29%)
31	WVN	A	845	-	40,41,41	1.72	10 (25%)	51,56,56	2.01	13 (25%)
28	CLA	b	612	30	55,59,73	1.32	10 (18%)	64,96,113	1.63	10 (15%)
28	CLA	B	809	-	58,62,73	1.32	7 (12%)	71,100,113	1.27	7 (9%)
28	CLA	m	601	18	46,50,73	1.40	8 (17%)	53,85,113	1.29	5 (9%)
28	CLA	g	308	-	69,73,73	1.14	6 (8%)	82,113,113	1.38	8 (9%)
31	WVN	s	207	-	40,41,41	1.76	10 (25%)	51,56,56	2.23	12 (23%)
28	CLA	F	202	6	56,60,73	1.28	7 (12%)	65,97,113	1.46	5 (7%)
31	WVN	B	846	-	40,41,41	1.71	10 (25%)	51,56,56	2.10	15 (29%)
38	KC2	c	610	-	49,53,53	2.70	20 (40%)	60,89,89	3.76	33 (55%)
28	CLA	l	304	-	55,59,73	1.30	7 (12%)	64,96,113	1.34	7 (10%)
28	CLA	B	839	-	69,73,73	1.17	7 (10%)	82,113,113	1.36	9 (10%)
28	CLA	J	103	8	46,50,73	1.36	8 (17%)	53,85,113	1.32	5 (9%)
28	CLA	k	603	-	55,59,73	1.27	7 (12%)	64,96,113	1.51	9 (14%)
36	II0	m	616	-	39,43,43	6.65	22 (56%)	48,60,60	1.97	15 (31%)
36	II0	f	614	-	39,43,43	6.73	22 (56%)	48,60,60	1.94	12 (25%)
30	LHG	c	618	28	36,36,48	1.11	2 (5%)	39,42,54	1.20	3 (7%)
37	IHT	j	616	-	40,42,42	6.22	26 (65%)	52,58,58	2.27	15 (28%)
38	KC2	k	612	-	49,53,53	2.81	21 (42%)	60,89,89	3.68	33 (55%)
28	CLA	L	204	40	54,58,73	1.31	8 (14%)	64,95,113	1.37	9 (14%)
30	LHG	a	301	28	48,48,48	0.92	2 (4%)	51,54,54	1.17	4 (7%)
28	CLA	f	612	18	55,59,73	1.29	8 (14%)	64,96,113	1.34	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	A	825	40	69,73,73	1.13	8 (11%)	82,113,113	1.19	6 (7%)
36	II0	n	615	-	39,43,43	6.68	22 (56%)	48,60,60	1.88	14 (29%)
30	LHG	n	619	-	42,42,48	0.99	2 (4%)	45,48,54	1.14	4 (8%)
28	CLA	f	608	18	69,73,73	1.22	7 (10%)	82,113,113	1.34	11 (13%)
28	CLA	B	831	40	49,53,73	1.38	8 (16%)	58,89,113	1.37	5 (8%)
28	CLA	a	303	15	56,60,73	1.31	6 (10%)	65,97,113	1.44	7 (10%)
38	KC2	e	609	19	49,53,53	2.74	20 (40%)	60,89,89	3.77	33 (55%)
38	KC2	k	611	21	49,53,53	2.74	20 (40%)	60,89,89	3.86	34 (56%)
28	CLA	n	613	-	55,59,73	1.29	6 (10%)	64,96,113	1.20	3 (4%)
28	CLA	l	307	20	69,73,73	1.14	6 (8%)	82,113,113	1.30	9 (10%)
28	CLA	B	836	-	69,73,73	1.14	7 (10%)	82,113,113	1.42	10 (12%)
28	CLA	d	308	23	45,49,73	1.38	7 (15%)	54,84,113	1.40	9 (16%)
28	CLA	g	305	24	69,73,73	1.18	5 (7%)	82,113,113	1.29	6 (7%)
31	WVN	s	205	-	40,41,41	1.62	10 (25%)	51,56,56	2.42	22 (43%)
28	CLA	d	303	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	6 (7%)
35	LMG	Q	301	-	38,38,55	1.04	2 (5%)	46,46,63	1.18	2 (4%)
36	II0	d	316	-	39,43,43	6.84	22 (56%)	48,60,60	1.93	14 (29%)
28	CLA	f	613	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	5 (6%)
28	CLA	h	301	40	69,73,73	1.21	9 (13%)	82,113,113	1.27	9 (10%)
36	II0	k	616	-	39,43,43	6.74	22 (56%)	48,60,60	2.06	16 (33%)
28	CLA	b	604	-	69,73,73	1.17	8 (11%)	82,113,113	1.14	6 (7%)
28	CLA	c	608	14	69,73,73	1.14	8 (11%)	82,113,113	1.32	11 (13%)
36	II0	e	612	-	39,43,43	6.74	22 (56%)	48,60,60	1.83	12 (25%)
28	CLA	n	607	-	69,73,73	1.14	5 (7%)	82,113,113	1.32	8 (9%)
32	LMT	a	302	-	24,24,36	1.05	2 (8%)	29,29,47	0.81	0
28	CLA	A	826	-	69,73,73	1.16	6 (8%)	82,113,113	1.45	9 (10%)
28	CLA	l	306	20	69,73,73	1.21	6 (8%)	82,113,113	1.42	9 (10%)
28	CLA	j	602	18	54,58,73	1.26	8 (14%)	64,95,113	1.39	7 (10%)
38	KC2	s	204	-	49,53,53	2.71	21 (42%)	60,89,89	3.73	36 (60%)
35	LMG	L	209	28	55,55,55	0.84	2 (3%)	63,63,63	1.43	10 (15%)
28	CLA	c	605	14	55,59,73	1.30	6 (10%)	64,96,113	1.55	7 (10%)
28	CLA	d	302	-	55,59,73	1.27	7 (12%)	64,96,113	1.44	10 (15%)
28	CLA	a	305	-	55,59,73	1.28	9 (16%)	64,96,113	1.41	8 (12%)
28	CLA	e	601	19	49,53,73	1.36	8 (16%)	58,89,113	1.47	5 (8%)
28	CLA	i	309	30	50,54,73	1.34	6 (12%)	59,90,113	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	e	604	40	69,73,73	1.15	7 (10%)	82,113,113	1.43	9 (10%)
28	CLA	B	813	-	63,67,73	1.14	6 (9%)	74,105,113	1.49	8 (10%)
28	CLA	d	306	-	55,59,73	1.32	6 (10%)	64,96,113	1.31	5 (7%)
28	CLA	l	309	30	65,69,73	1.19	7 (10%)	77,108,113	1.36	5 (6%)
28	CLA	B	816	-	61,65,73	1.20	7 (11%)	72,103,113	1.29	9 (12%)
31	WVN	e	615	-	40,41,41	1.77	10 (25%)	51,56,56	2.10	15 (29%)
28	CLA	A	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.40	6 (7%)
36	II0	n	614	-	39,43,43	6.79	21 (53%)	48,60,60	2.01	11 (22%)
28	CLA	n	606	26	55,59,73	1.32	6 (10%)	64,96,113	1.38	7 (10%)
28	CLA	B	832	-	62,66,73	1.22	8 (12%)	73,104,113	1.40	12 (16%)
30	LHG	b	620	-	30,30,48	1.13	2 (6%)	33,36,54	1.19	3 (9%)
31	WVN	J	102	-	40,41,41	1.75	10 (25%)	51,56,56	1.99	16 (31%)
28	CLA	f	605	18	49,53,73	1.39	7 (14%)	58,89,113	1.40	5 (8%)
36	II0	l	312	-	39,43,43	6.73	23 (58%)	48,60,60	1.91	13 (27%)
28	CLA	B	807	-	69,73,73	1.16	7 (10%)	82,113,113	1.20	9 (10%)
33	SF4	C	102	3	0,12,12	-	-	-		
28	CLA	B	833	-	69,73,73	1.12	8 (11%)	82,113,113	1.33	9 (10%)
28	CLA	A	810	28	66,70,73	1.14	7 (10%)	78,109,113	1.19	6 (7%)
28	CLA	n	608	26	55,59,73	1.33	8 (14%)	64,96,113	1.34	6 (9%)
30	LHG	b	619	28	48,48,48	0.91	2 (4%)	51,54,54	1.13	5 (9%)
31	WVN	K	104	-	40,41,41	1.73	10 (25%)	51,56,56	2.13	16 (31%)
28	CLA	B	801	40	69,73,73	1.14	9 (13%)	82,113,113	1.39	9 (10%)
28	CLA	f	601	18	51,55,73	1.37	7 (13%)	60,91,113	1.48	8 (13%)
28	CLA	l	302	20	51,55,73	1.32	7 (13%)	60,91,113	1.29	5 (8%)
31	WVN	l	315	-	40,41,41	1.78	10 (25%)	51,56,56	2.34	18 (35%)
28	CLA	A	819	-	49,53,73	1.38	6 (12%)	58,89,113	1.65	9 (15%)
28	CLA	K	101	40	55,59,73	1.27	6 (10%)	64,96,113	1.63	11 (17%)
31	WVN	B	844	-	40,41,41	1.68	11 (27%)	51,56,56	2.58	18 (35%)
35	LMG	n	620	-	55,55,55	0.89	2 (3%)	63,63,63	0.91	2 (3%)
36	II0	d	315	-	39,43,43	6.81	22 (56%)	48,60,60	2.16	18 (37%)
30	LHG	J	106	28	48,48,48	0.93	2 (4%)	51,54,54	1.11	4 (7%)
36	II0	m	614	-	39,43,43	6.81	22 (56%)	48,60,60	1.72	13 (27%)
28	CLA	A	811	-	58,62,73	1.27	6 (10%)	68,99,113	1.37	8 (11%)
28	CLA	A	828	-	69,73,73	1.14	8 (11%)	82,113,113	1.39	9 (10%)
28	CLA	A	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LHG	f	619	-	48,48,48	0.91	2 (4%)	51,54,54	1.04	3 (5%)
31	WVN	L	201	-	40,41,41	1.71	13 (32%)	51,56,56	2.54	19 (37%)
31	WVN	A	848	-	40,41,41	1.69	10 (25%)	51,56,56	2.79	17 (33%)
28	CLA	K	103	-	46,50,73	1.40	7 (15%)	53,85,113	1.42	8 (15%)
28	CLA	m	608	18	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
32	LMT	A	850	-	36,36,36	1.16	6 (16%)	47,47,47	1.42	6 (12%)
28	CLA	Q	302	40	69,73,73	1.18	7 (10%)	82,113,113	1.26	8 (9%)
28	CLA	A	809	-	60,64,73	1.18	6 (10%)	71,102,113	1.24	4 (5%)
31	WVN	F	203	-	40,41,41	1.71	10 (25%)	51,56,56	2.62	21 (41%)
28	CLA	L	203	-	69,73,73	1.12	8 (11%)	82,113,113	1.21	8 (9%)
38	KC2	n	612	-	49,53,53	2.72	20 (40%)	60,89,89	3.75	32 (53%)
28	CLA	a	313	-	52,56,73	1.32	6 (11%)	61,92,113	1.26	6 (9%)
35	LMG	F	205	-	48,48,55	0.97	2 (4%)	56,56,63	1.24	5 (8%)
28	CLA	A	808	1	69,73,73	1.13	7 (10%)	82,113,113	1.37	11 (13%)
28	CLA	n	604	26	64,68,73	1.20	5 (7%)	76,107,113	1.36	8 (10%)
36	II0	c	617	-	39,43,43	6.61	21 (53%)	48,60,60	2.02	13 (27%)
36	II0	a	316	-	39,43,43	6.62	20 (51%)	48,60,60	2.13	14 (29%)
31	WVN	A	847	-	40,41,41	1.71	11 (27%)	51,56,56	2.16	20 (39%)
36	II0	h	310	-	26,28,43	6.06	13 (50%)	30,37,60	2.09	9 (30%)
28	CLA	F	201	40	69,73,73	1.19	8 (11%)	82,113,113	1.19	6 (7%)
28	CLA	A	852	-	69,73,73	1.12	8 (11%)	82,113,113	1.34	12 (14%)
35	LMG	J	105	-	55,55,55	0.85	2 (3%)	63,63,63	0.92	6 (9%)
38	KC2	n	611	26	49,53,53	2.68	20 (40%)	60,89,89	3.78	32 (53%)
28	CLA	h	304	-	55,59,73	1.28	7 (12%)	64,96,113	1.43	9 (14%)
28	CLA	d	305	23	55,59,73	1.48	6 (10%)	64,96,113	1.45	8 (12%)
36	II0	O	203	-	39,43,43	6.67	21 (53%)	48,60,60	2.00	14 (29%)
36	II0	d	313	-	39,43,43	6.66	21 (53%)	48,60,60	2.00	13 (27%)
28	CLA	B	827	-	54,58,73	1.25	5 (9%)	64,95,113	1.32	9 (14%)
28	CLA	a	310	30	52,56,73	1.28	6 (11%)	61,92,113	1.29	6 (9%)
28	CLA	A	838	1	69,73,73	1.18	7 (10%)	82,113,113	1.31	8 (9%)
30	LHG	A	849	-	37,37,48	1.03	2 (5%)	40,43,54	1.15	4 (10%)
28	CLA	A	813	-	49,53,73	1.33	6 (12%)	58,89,113	1.50	9 (15%)
37	IHT	R	204	-	40,42,42	6.26	26 (65%)	52,58,58	2.28	15 (28%)
28	CLA	A	815	40	49,53,73	1.38	7 (14%)	58,89,113	1.66	11 (18%)
28	CLA	B	838	-	61,65,73	1.20	5 (8%)	72,103,113	1.27	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LHG	A	843	-	47,47,48	0.95	2 (4%)	50,53,54	1.09	3 (6%)
28	CLA	i	304	-	55,59,73	1.31	6 (10%)	64,96,113	1.32	8 (12%)
28	CLA	i	306	-	55,59,73	1.29	7 (12%)	64,96,113	1.38	3 (4%)
36	II0	f	618	-	39,43,43	6.73	22 (56%)	48,60,60	2.21	14 (29%)
36	II0	h	311	-	39,43,43	6.64	20 (51%)	48,60,60	1.96	17 (35%)
28	CLA	n	609	26	69,73,73	1.13	8 (11%)	82,113,113	1.36	11 (13%)
38	KC2	g	314	38	49,53,53	2.76	19 (38%)	60,89,89	3.82	32 (53%)
38	KC2	m	611	18	49,53,53	2.70	20 (40%)	60,89,89	3.80	34 (56%)
36	II0	g	320	-	39,43,43	6.75	22 (56%)	48,60,60	2.12	17 (35%)
28	CLA	d	309	30	45,49,73	1.39	6 (13%)	54,84,113	1.37	6 (11%)
31	WVN	A	846	-	40,41,41	1.73	12 (30%)	51,56,56	3.13	20 (39%)
31	WVN	R	202	-	40,41,41	1.68	10 (25%)	51,56,56	2.30	20 (39%)
28	CLA	b	610	16	69,73,73	1.14	6 (8%)	82,113,113	1.27	4 (4%)
28	CLA	m	605	18	46,50,73	1.39	7 (15%)	53,85,113	1.51	5 (9%)
28	CLA	c	606	-	56,60,73	1.31	10 (17%)	65,97,113	1.46	10 (15%)
28	CLA	e	611	-	69,73,73	1.17	6 (8%)	82,113,113	1.28	6 (7%)
28	CLA	f	609	18	69,73,73	1.15	7 (10%)	82,113,113	1.27	10 (12%)
37	IHT	n	617	-	40,42,42	6.19	26 (65%)	52,58,58	2.27	16 (30%)
37	IHT	O	204	-	40,42,42	6.26	26 (65%)	52,58,58	2.37	16 (30%)
36	II0	i	313	-	39,43,43	6.67	22 (56%)	48,60,60	2.20	17 (35%)
28	CLA	a	312	-	69,73,73	1.14	6 (8%)	82,113,113	1.34	7 (8%)
36	II0	g	316	-	39,43,43	6.76	22 (56%)	48,60,60	1.99	12 (25%)
28	CLA	c	611	14	49,53,73	1.50	8 (16%)	58,89,113	1.53	7 (12%)
28	CLA	A	832	-	69,73,73	1.13	6 (8%)	82,113,113	1.57	13 (15%)
28	CLA	B	830	40	69,73,73	1.14	4 (5%)	82,113,113	1.25	7 (8%)
28	CLA	k	604	21	69,73,73	1.17	7 (10%)	82,113,113	1.25	9 (10%)
28	CLA	j	606	18	55,59,73	1.31	9 (16%)	64,96,113	1.41	6 (9%)
28	CLA	A	827	-	66,70,73	1.15	7 (10%)	78,109,113	1.23	8 (10%)
28	CLA	A	840	40	69,73,73	1.14	6 (8%)	82,113,113	1.22	10 (12%)
28	CLA	h	307	17	61,65,73	1.25	6 (9%)	72,103,113	1.15	4 (5%)
38	KC2	i	319	-	49,53,53	2.72	20 (40%)	60,89,89	3.85	35 (58%)
36	II0	e	613	-	39,43,43	6.74	22 (56%)	48,60,60	1.94	16 (33%)
28	CLA	g	311	30	58,62,73	1.31	8 (13%)	68,99,113	1.24	6 (8%)
28	CLA	s	208	-	55,59,73	1.29	7 (12%)	64,96,113	1.35	7 (10%)
28	CLA	e	610	40	69,73,73	1.16	7 (10%)	82,113,113	1.24	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	a	307	15	49,53,73	1.36	7 (14%)	58,89,113	1.56	7 (12%)
28	CLA	j	608	18	49,53,73	1.37	6 (12%)	58,89,113	1.40	7 (12%)
28	CLA	b	603	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	9 (10%)
28	CLA	R	203	-	55,59,73	1.26	6 (10%)	64,96,113	1.59	9 (14%)
28	CLA	k	607	-	55,59,73	1.31	6 (10%)	64,96,113	1.44	9 (14%)
28	CLA	i	307	22	65,69,73	1.18	6 (9%)	77,108,113	1.24	7 (9%)
28	CLA	B	815	-	63,67,73	1.17	8 (12%)	74,105,113	1.23	7 (9%)
38	KC2	g	312	24	49,53,53	2.74	20 (40%)	60,89,89	3.81	33 (55%)
38	KC2	s	201	13	49,53,53	2.66	20 (40%)	60,89,89	3.73	35 (58%)
31	WVN	i	316	-	40,41,41	1.78	10 (25%)	51,56,56	2.34	18 (35%)
36	II0	b	614	-	39,43,43	6.74	23 (58%)	48,60,60	1.70	10 (20%)
28	CLA	O	201	30	56,60,73	1.25	6 (10%)	65,97,113	1.40	9 (13%)
28	CLA	m	610	30	59,63,73	1.26	6 (10%)	70,101,113	1.35	8 (11%)
36	II0	l	313	-	39,43,43	6.83	21 (53%)	48,60,60	2.34	13 (27%)
29	PQN	B	842	-	34,34,34	1.78	5 (14%)	43,45,45	1.37	6 (13%)
30	LHG	A	844	28	26,26,48	1.25	2 (7%)	29,32,54	1.37	5 (17%)
28	CLA	f	607	-	69,73,73	1.15	6 (8%)	82,113,113	1.23	7 (8%)
28	CLA	A	836	-	69,73,73	1.14	5 (7%)	82,113,113	1.46	10 (12%)
28	CLA	m	604	18	69,73,73	1.18	7 (10%)	82,113,113	1.31	6 (7%)
28	CLA	A	821	-	53,57,73	1.26	8 (15%)	61,93,113	1.40	9 (14%)
28	CLA	f	610	30	69,73,73	1.14	8 (11%)	82,113,113	1.19	8 (9%)
28	CLA	a	309	15	69,73,73	1.15	8 (11%)	82,113,113	1.54	10 (12%)
31	WVN	l	301	-	40,41,41	1.68	10 (25%)	51,56,56	2.30	19 (37%)
28	CLA	j	604	18	69,73,73	1.15	6 (8%)	82,113,113	1.24	8 (9%)
28	CLA	B	837	-	69,73,73	1.09	5 (7%)	82,113,113	1.36	8 (9%)
28	CLA	A	833	-	54,58,73	1.25	4 (7%)	64,95,113	1.30	4 (6%)
36	II0	J	104	-	39,43,43	6.60	22 (56%)	48,60,60	1.93	11 (22%)
28	CLA	B	802	-	69,73,73	1.14	6 (8%)	82,113,113	1.28	10 (12%)
37	IHT	a	317	-	40,42,42	6.31	26 (65%)	52,58,58	2.06	14 (26%)
28	CLA	A	820	40	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
28	CLA	A	841	-	69,73,73	1.15	6 (8%)	82,113,113	1.41	10 (12%)
35	LMG	O	205	-	26,26,55	1.27	2 (7%)	34,34,63	1.17	4 (11%)
36	II0	b	613	-	39,43,43	6.74	22 (56%)	48,60,60	2.09	15 (31%)
28	CLA	A	802	-	69,73,73	1.11	7 (10%)	82,113,113	1.52	13 (15%)
28	CLA	B	829	-	54,58,73	1.31	7 (12%)	64,95,113	1.26	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	A	823	-	59,63,73	1.23	7 (11%)	70,101,113	1.26	4 (5%)
28	CLA	B	841	30	69,73,73	1.15	7 (10%)	82,113,113	1.30	9 (10%)
28	CLA	k	601	21	55,59,73	1.32	7 (12%)	64,96,113	1.50	8 (12%)
28	CLA	e	605	19	69,73,73	1.16	9 (13%)	82,113,113	1.22	7 (8%)
38	KC2	j	611	18	49,53,53	2.70	21 (42%)	60,89,89	3.83	34 (56%)
28	CLA	g	302	24	46,50,73	1.40	7 (15%)	53,85,113	1.48	6 (11%)
30	LHG	d	317	28	36,36,48	1.11	2 (5%)	39,42,54	1.04	2 (5%)
28	CLA	l	305	20	69,73,73	1.13	6 (8%)	82,113,113	1.37	9 (10%)
28	CLA	A	816	-	69,73,73	1.09	4 (5%)	82,113,113	1.43	13 (15%)
28	CLA	e	606	19	69,73,73	1.16	6 (8%)	82,113,113	1.27	5 (6%)
28	CLA	B	835	40	69,73,73	1.18	7 (10%)	82,113,113	1.14	5 (6%)
28	CLA	l	308	20	55,59,73	1.28	8 (14%)	64,96,113	1.37	9 (14%)
28	CLA	f	603	-	55,59,73	1.27	8 (14%)	64,96,113	1.40	7 (10%)
31	WVN	L	205	-	40,41,41	1.76	10 (25%)	51,56,56	2.15	15 (29%)
28	CLA	n	603	-	55,59,73	1.29	8 (14%)	64,96,113	1.36	6 (9%)
28	CLA	g	304	-	55,59,73	1.30	6 (10%)	64,96,113	1.38	6 (9%)
28	CLA	A	807	1	69,73,73	1.10	4 (5%)	82,113,113	1.31	8 (9%)
28	CLA	a	308	15	69,73,73	1.15	7 (10%)	82,113,113	1.29	8 (9%)
28	CLA	f	606	18	55,59,73	1.31	6 (10%)	64,96,113	1.33	7 (10%)
36	II0	c	615	-	39,43,43	6.73	21 (53%)	48,60,60	2.11	15 (31%)
28	CLA	B	822	40	68,72,73	1.16	9 (13%)	80,111,113	1.37	8 (10%)
30	LHG	l	317	28	31,31,48	1.15	2 (6%)	34,37,54	1.20	4 (11%)
28	CLA	k	609	21	69,73,73	1.15	7 (10%)	82,113,113	1.44	9 (10%)
28	CLA	i	312	-	55,59,73	1.27	6 (10%)	64,96,113	1.35	9 (14%)
28	CLA	j	601	18	55,59,73	1.30	6 (10%)	64,96,113	1.26	5 (7%)
28	CLA	B	834	-	51,55,73	1.31	8 (15%)	60,91,113	1.50	6 (10%)
28	CLA	A	801	-	69,73,73	1.15	5 (7%)	82,113,113	1.20	8 (9%)
28	CLA	B	818	-	50,54,73	1.29	6 (12%)	59,90,113	1.40	9 (15%)
38	KC2	i	310	22	49,53,53	2.74	20 (40%)	60,89,89	3.63	33 (55%)
36	II0	f	615	-	39,43,43	6.70	23 (58%)	48,60,60	2.04	15 (31%)
28	CLA	a	311	15	69,73,73	1.15	8 (11%)	82,113,113	1.34	10 (12%)
37	IHT	f	617	-	40,42,42	6.24	26 (65%)	52,58,58	2.14	13 (25%)
28	CLA	m	603	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	8 (9%)
37	IHT	b	615	-	40,42,42	6.22	26 (65%)	52,58,58	2.45	15 (28%)
28	CLA	k	614	-	55,59,73	1.31	7 (12%)	64,96,113	1.32	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	c	604	14	69,73,73	1.16	6 (8%)	82,113,113	1.31	7 (8%)
28	CLA	A	854	40	69,73,73	1.21	9 (13%)	82,113,113	1.43	10 (12%)
28	CLA	B	819	-	59,63,73	1.24	7 (11%)	70,101,113	1.20	4 (5%)
28	CLA	m	606	-	69,73,73	1.16	6 (8%)	82,113,113	1.19	5 (6%)
28	CLA	A	834	-	55,59,73	1.31	8 (14%)	64,96,113	1.53	11 (17%)
28	CLA	s	202	13	69,73,73	1.20	8 (11%)	82,113,113	1.36	11 (13%)
28	CLA	m	613	-	47,51,73	1.35	7 (14%)	55,86,113	1.54	12 (21%)
36	II0	k	617	-	39,43,43	6.79	20 (51%)	48,60,60	2.03	18 (37%)
31	WVN	M	101	-	40,41,41	1.73	12 (30%)	51,56,56	2.27	19 (37%)
38	KC2	d	310	23	49,53,53	2.76	21 (42%)	60,89,89	3.80	33 (55%)
28	CLA	i	311	-	55,59,73	1.36	8 (14%)	64,96,113	1.26	7 (10%)
28	CLA	l	311	20	69,73,73	1.16	6 (8%)	82,113,113	1.17	7 (8%)
28	CLA	c	607	14	50,54,73	1.36	6 (12%)	59,90,113	1.24	6 (10%)
28	CLA	A	824	40	69,73,73	1.15	10 (14%)	82,113,113	1.32	8 (9%)
28	CLA	k	610	30	55,59,73	1.27	6 (10%)	64,96,113	1.42	4 (6%)
36	II0	d	314	-	39,43,43	6.78	20 (51%)	48,60,60	1.99	10 (20%)
36	II0	j	615	-	39,43,43	6.75	22 (56%)	48,60,60	1.92	16 (33%)
38	KC2	l	310	20	49,53,53	2.70	20 (40%)	60,89,89	3.88	33 (55%)
30	LHG	g	301	28	36,36,48	1.10	2 (5%)	39,42,54	1.23	3 (7%)
36	II0	g	318	-	39,43,43	6.78	21 (53%)	48,60,60	1.85	13 (27%)
28	CLA	j	610	30	65,69,73	1.20	6 (9%)	77,108,113	1.26	6 (7%)
28	CLA	b	602	16	59,63,73	1.21	7 (11%)	70,101,113	1.42	11 (15%)
28	CLA	g	315	-	55,59,73	1.31	8 (14%)	64,96,113	1.29	5 (7%)
28	CLA	A	829	-	69,73,73	1.19	7 (10%)	82,113,113	1.33	7 (8%)
28	CLA	g	306	24	55,59,73	1.33	8 (14%)	64,96,113	1.33	5 (7%)
28	CLA	B	803	-	69,73,73	1.15	10 (14%)	82,113,113	1.64	11 (13%)
28	CLA	c	612	-	69,73,73	1.13	6 (8%)	82,113,113	1.21	6 (7%)
36	II0	i	317	-	39,43,43	6.81	20 (51%)	48,60,60	1.89	13 (27%)
28	CLA	B	826	-	55,59,73	1.31	6 (10%)	64,96,113	1.47	8 (12%)
28	CLA	e	602	19	54,58,73	1.31	7 (12%)	64,95,113	1.35	11 (17%)
28	CLA	b	609	-	55,59,73	1.20	7 (12%)	64,96,113	1.70	9 (14%)
28	CLA	g	307	24	55,59,73	1.28	7 (12%)	64,96,113	1.29	8 (12%)
36	II0	c	613	-	39,43,43	6.71	22 (56%)	48,60,60	2.02	15 (31%)
28	CLA	A	839	-	69,73,73	1.12	6 (8%)	82,113,113	1.25	5 (6%)
28	CLA	B	814	-	59,63,73	1.19	6 (10%)	70,101,113	1.30	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	WVN	B	845	-	40,41,41	1.60	10 (25%)	51,56,56	2.25	13 (25%)
28	CLA	e	603	19	55,59,73	1.32	5 (9%)	64,96,113	1.37	6 (9%)
28	CLA	e	608	30	50,54,73	1.32	7 (14%)	59,90,113	1.48	6 (10%)
28	CLA	g	309	24	69,73,73	1.18	8 (11%)	82,113,113	1.23	7 (8%)
28	CLA	b	607	16	69,73,73	1.14	6 (8%)	82,113,113	1.50	11 (13%)
37	IHT	c	616	-	40,42,42	6.27	26 (65%)	52,58,58	2.25	13 (25%)
28	CLA	B	812	-	64,68,73	1.24	7 (10%)	76,107,113	1.28	10 (13%)
31	WVN	K	102	-	40,41,41	1.65	11 (27%)	51,56,56	2.39	16 (31%)
28	CLA	n	605	26	55,59,73	1.33	7 (12%)	64,96,113	1.41	8 (12%)
28	CLA	B	805	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	7 (8%)
36	II0	j	614	-	39,43,43	6.72	21 (53%)	48,60,60	2.11	14 (29%)
28	CLA	k	602	21	54,58,73	1.31	5 (9%)	64,95,113	1.46	11 (17%)
28	CLA	d	301	23	54,58,73	1.32	5 (9%)	64,95,113	1.40	9 (14%)
37	IHT	k	618	-	40,42,42	6.23	26 (65%)	52,58,58	2.39	17 (32%)
28	CLA	s	203	13,28	69,73,73	1.16	6 (8%)	82,113,113	1.36	6 (7%)
39	LMU	i	301	-	36,36,36	1.18	4 (11%)	47,47,47	1.18	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	II0	g	317	-	-	5/21/67/67	0/2/2/2
28	CLA	A	851	-	1/1/15/20	4/39/115/115	-
28	CLA	c	603	-	1/1/12/20	2/23/99/115	-
36	II0	m	618	-	-	6/21/67/67	0/2/2/2
28	CLA	l	303	20	1/1/15/20	21/39/115/115	-
30	LHG	i	318	28	-	13/41/41/53	-
28	CLA	b	605	40,28	1/1/15/20	11/39/115/115	-
28	CLA	s	206	40	1/1/15/20	12/39/115/115	-
28	CLA	A	835	-	1/1/15/20	12/39/115/115	-
28	CLA	j	612	-	1/1/12/20	8/23/99/115	-
28	CLA	A	837	-	1/1/15/20	9/39/115/115	-
28	CLA	B	824	-	1/1/15/20	9/39/115/115	-
28	CLA	A	830	-	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	II0	k	615	-	-	6/21/67/67	0/2/2/2
31	WVN	R	201	-	-	6/29/63/63	0/2/2/2
36	II0	n	618	-	-	6/21/67/67	0/2/2/2
31	WVN	B	848	-	-	6/29/63/63	0/2/2/2
30	LHG	L	208	-	-	21/53/53/53	-
28	CLA	b	606	16	1/1/14/20	14/35/111/115	-
28	CLA	B	808	2	1/1/15/20	12/39/115/115	-
31	WVN	L	206	-	-	3/29/63/63	0/2/2/2
36	II0	m	615	-	-	7/21/67/67	0/2/2/2
37	IHT	g	319	-	-	8/25/65/65	0/2/2/2
28	CLA	B	840	-	1/1/15/20	10/39/115/115	-
30	LHG	m	619	28	-	18/41/41/53	-
28	CLA	m	609	18	1/1/12/20	7/23/99/115	-
28	CLA	h	303	17	1/1/12/20	8/21/97/115	-
28	CLA	g	322	35	1/1/15/20	18/39/115/115	-
31	WVN	I	101	-	-	8/29/63/63	0/2/2/2
35	LMG	b	621	-	-	17/44/64/70	0/1/1/1
28	CLA	h	308	17	1/1/12/20	9/23/99/115	-
31	WVN	F	204	-	-	12/29/63/63	0/2/2/2
37	IHT	b	616	-	-	8/25/65/65	0/2/2/2
36	II0	i	314	-	-	4/21/67/67	0/2/2/2
28	CLA	A	822	-	1/1/12/20	8/23/99/115	-
36	II0	i	315	-	-	4/21/67/67	0/2/2/2
28	CLA	b	608	30	1/1/15/20	10/39/115/115	-
28	CLA	d	304	23	1/1/12/20	6/23/99/115	-
28	CLA	B	817	40	1/1/15/20	11/39/115/115	-
30	LHG	g	321	28	-	12/41/41/53	-
28	CLA	B	821	40	1/1/15/20	8/39/115/115	-
28	CLA	i	303	22	1/1/12/20	9/21/97/115	-
28	CLA	g	303	24	1/1/12/20	2/21/97/115	-
33	SF4	C	101	3	-	-	0/6/5/5
28	CLA	m	602	18	1/1/13/20	10/29/105/115	-
31	WVN	h	309	-	-	8/29/63/63	0/2/2/2
28	CLA	A	817	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	II0	a	318	-	-	7/21/67/67	0/2/2/2
28	CLA	B	823	-	1/1/15/20	2/39/115/115	-
28	CLA	f	602	18	1/1/15/20	16/39/115/115	-
36	II0	e	616	-	-	5/21/67/67	0/2/2/2
28	CLA	Q	303	27	1/1/11/20	8/15/91/115	-
28	CLA	h	305	17	1/1/12/20	6/23/99/115	-
31	WVN	J	101	-	-	11/29/63/63	0/2/2/2
28	CLA	h	306	17	1/1/15/20	19/39/115/115	-
28	CLA	A	814	-	-	8/21/97/115	-
28	CLA	A	812	-	1/1/15/20	20/39/115/115	-
28	CLA	B	804	-	1/1/15/20	15/39/115/115	-
28	CLA	c	601	14	1/1/12/20	8/23/99/115	-
34	DGD	B	843	-	-	5/49/89/95	0/2/2/2
28	CLA	m	607	-	1/1/12/20	6/23/99/115	-
28	CLA	n	610	40	1/1/15/20	15/39/115/115	-
28	CLA	a	306	40	1/1/15/20	13/39/115/115	-
28	CLA	j	605	18	1/1/11/20	6/15/91/115	-
36	II0	a	315	-	-	2/21/67/67	0/2/2/2
36	II0	i	320	-	-	7/21/67/67	0/2/2/2
36	II0	l	316	-	-	6/21/67/67	0/2/2/2
28	CLA	j	607	-	1/1/12/20	7/23/99/115	-
28	CLA	i	305	22	-	9/39/115/115	-
28	CLA	i	308	22	1/1/12/20	2/23/99/115	-
32	LMT	a	320	-	-	10/21/61/61	0/2/2/2
28	CLA	A	805	1	1/1/15/20	7/39/115/115	-
28	CLA	A	806	-	1/1/15/20	9/39/115/115	-
30	LHG	j	617	28	-	5/34/34/53	-
28	CLA	O	202	-	1/1/15/20	13/39/115/115	-
28	CLA	B	811	-	1/1/15/20	14/39/115/115	-
28	CLA	B	828	-	1/1/11/20	5/20/96/115	-
28	CLA	m	612	40	1/1/12/20	10/23/99/115	-
28	CLA	d	307	23	1/1/11/20	5/17/93/115	-
28	CLA	g	310	24	1/1/12/20	7/23/99/115	-
31	WVN	B	847	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	O	206	-	1/1/15/20	17/39/115/115	-
28	CLA	j	613	-	1/1/15/20	16/39/115/115	-
28	CLA	f	604	18	1/1/15/20	8/39/115/115	-
28	CLA	c	609	30	1/1/11/20	4/15/91/115	-
28	CLA	b	601	16	1/1/12/20	10/23/99/115	-
28	CLA	j	609	18	1/1/12/20	2/23/99/115	-
28	CLA	a	304	15	1/1/12/20	7/21/97/115	-
36	II0	k	619	-	-	5/21/67/67	0/2/2/2
30	LHG	k	620	28	-	18/41/41/53	-
33	SF4	A	853	2,1	-	-	0/6/5/5
28	CLA	n	602	26	-	4/21/97/115	-
28	CLA	h	302	17	1/1/12/20	6/21/97/115	-
28	CLA	B	825	-	1/1/15/20	7/39/115/115	-
28	CLA	e	607	19	1/1/15/20	21/39/115/115	-
28	CLA	B	806	-	1/1/15/20	10/39/115/115	-
28	CLA	h	313	40	1/1/15/20	6/39/115/115	-
28	CLA	L	207	40	1/1/12/20	6/23/99/115	-
36	II0	c	614	-	-	1/21/67/67	0/2/2/2
28	CLA	d	312	-	-	6/23/99/115	-
30	LHG	e	617	28	-	26/41/41/53	-
28	CLA	B	820	-	1/1/12/20	6/25/101/115	-
28	CLA	A	803	28	1/1/13/20	6/27/103/115	-
36	II0	b	617	-	-	0/21/67/67	0/2/2/2
28	CLA	k	606	21	-	12/23/99/115	-
28	CLA	B	810	-	1/1/13/20	6/27/103/115	-
28	CLA	A	855	30	1/1/10/20	4/10/86/115	-
36	II0	l	314	-	-	4/21/67/67	0/2/2/2
38	KC2	g	313	38	-	2/15/71/71	-
38	KC2	d	311	-	-	5/15/71/71	-
38	KC2	f	611	18	-	7/15/71/71	-
28	CLA	b	611	-	1/1/15/20	21/39/115/115	-
28	CLA	k	608	21	1/1/15/20	16/39/115/115	-
30	LHG	a	319	28	-	15/53/53/53	-
36	II0	e	614	-	-	3/21/67/67	0/2/2/2
28	CLA	c	602	14	1/1/12/20	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	c	620	28	-	25/41/41/53	-
28	CLA	n	601	26	1/1/11/20	6/15/91/115	-
29	PQN	A	842	-	-	9/23/43/43	0/2/2/2
32	LMT	b	618	-	-	9/15/35/61	0/1/1/2
28	CLA	k	605	21	1/1/11/20	5/15/91/115	-
36	II0	f	616	-	-	3/21/67/67	0/2/2/2
36	II0	n	616	-	-	4/21/67/67	0/2/2/2
28	CLA	i	302	22	1/1/12/20	9/23/99/115	-
36	II0	k	621	-	-	8/21/67/67	0/2/2/2
38	KC2	k	613	-	-	6/15/71/71	-
35	LMG	c	619	-	-	21/50/70/70	0/1/1/1
36	II0	a	314	-	-	4/21/67/67	0/2/2/2
28	CLA	j	603	-	1/1/12/20	5/23/99/115	-
37	IHT	m	617	-	-	8/25/65/65	0/2/2/2
28	CLA	A	818	-	1/1/15/20	17/39/115/115	-
28	CLA	L	202	9	1/1/11/20	8/20/96/115	-
36	II0	h	312	-	-	7/21/67/67	0/2/2/2
31	WVN	A	845	-	-	7/29/63/63	0/2/2/2
28	CLA	b	612	30	1/1/12/20	9/23/99/115	-
28	CLA	B	809	-	1/1/13/20	4/25/101/115	-
28	CLA	m	601	18	1/1/10/20	2/12/88/115	-
28	CLA	g	308	-	1/1/15/20	18/39/115/115	-
31	WVN	s	207	-	-	7/29/63/63	0/2/2/2
28	CLA	F	202	6	1/1/12/20	10/24/100/115	-
31	WVN	B	846	-	-	5/29/63/63	0/2/2/2
38	KC2	c	610	-	-	8/15/71/71	-
28	CLA	l	304	-	1/1/12/20	4/23/99/115	-
28	CLA	B	839	-	1/1/15/20	12/39/115/115	-
28	CLA	J	103	8	1/1/10/20	4/12/88/115	-
28	CLA	k	603	-	1/1/12/20	2/23/99/115	-
36	II0	m	616	-	-	3/21/67/67	0/2/2/2
36	II0	f	614	-	-	3/21/67/67	0/2/2/2
30	LHG	c	618	28	-	14/41/41/53	-
37	IHT	j	616	-	-	5/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC2	k	612	-	-	5/15/71/71	-
28	CLA	L	204	40	-	5/21/97/115	-
30	LHG	a	301	28	-	14/53/53/53	-
28	CLA	f	612	18	1/1/12/20	8/23/99/115	-
28	CLA	A	825	40	-	10/39/115/115	-
36	II0	n	615	-	-	4/21/67/67	0/2/2/2
30	LHG	n	619	-	-	16/47/47/53	-
28	CLA	f	608	18	1/1/15/20	15/39/115/115	-
28	CLA	B	831	40	1/1/11/20	6/15/91/115	-
28	CLA	a	303	15	1/1/12/20	12/24/100/115	-
38	KC2	e	609	19	-	8/15/71/71	-
38	KC2	k	611	21	-	6/15/71/71	-
28	CLA	n	613	-	1/1/12/20	9/23/99/115	-
28	CLA	l	307	20	1/1/15/20	12/39/115/115	-
28	CLA	B	836	-	1/1/15/20	27/39/115/115	-
28	CLA	d	308	23	1/1/10/20	2/10/86/115	-
28	CLA	g	305	24	-	10/39/115/115	-
31	WVN	s	205	-	-	4/29/63/63	0/2/2/2
28	CLA	d	303	-	1/1/15/20	17/39/115/115	-
35	LMG	Q	301	-	-	22/33/53/70	0/1/1/1
36	II0	d	316	-	-	7/21/67/67	0/2/2/2
28	CLA	f	613	-	1/1/15/20	22/39/115/115	-
28	CLA	h	301	40	-	15/39/115/115	-
36	II0	k	616	-	-	8/21/67/67	0/2/2/2
28	CLA	b	604	-	-	17/39/115/115	-
28	CLA	c	608	14	1/1/15/20	15/39/115/115	-
36	II0	e	612	-	-	5/21/67/67	0/2/2/2
28	CLA	n	607	-	1/1/15/20	13/39/115/115	-
32	LMT	a	302	-	-	4/15/35/61	0/1/1/2
28	CLA	A	826	-	1/1/15/20	7/39/115/115	-
28	CLA	l	306	20	1/1/15/20	19/39/115/115	-
28	CLA	j	602	18	1/1/12/20	6/21/97/115	-
38	KC2	s	204	-	-	6/15/71/71	-
35	LMG	L	209	28	-	19/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	c	605	14	1/1/12/20	9/23/99/115	-
28	CLA	d	302	-	1/1/12/20	6/23/99/115	-
28	CLA	a	305	-	1/1/12/20	6/23/99/115	-
28	CLA	e	601	19	1/1/11/20	4/15/91/115	-
28	CLA	i	309	30	1/1/11/20	4/17/93/115	-
28	CLA	e	604	40	-	20/39/115/115	-
28	CLA	B	813	-	1/1/13/20	13/32/108/115	-
28	CLA	d	306	-	1/1/12/20	9/23/99/115	-
28	CLA	l	309	30	1/1/14/20	14/35/111/115	-
28	CLA	B	816	-	-	9/30/106/115	-
31	WVN	e	615	-	-	11/29/63/63	0/2/2/2
28	CLA	A	804	-	1/1/15/20	6/39/115/115	-
36	II0	n	614	-	-	1/21/67/67	0/2/2/2
28	CLA	n	606	26	1/1/12/20	6/23/99/115	-
28	CLA	B	832	-	1/1/13/20	4/31/107/115	-
30	LHG	b	620	-	-	15/35/35/53	-
31	WVN	J	102	-	-	10/29/63/63	0/2/2/2
28	CLA	f	605	18	-	6/15/91/115	-
36	II0	l	312	-	-	4/21/67/67	0/2/2/2
28	CLA	B	807	-	1/1/15/20	13/39/115/115	-
33	SF4	C	102	3	-	-	0/6/5/5
28	CLA	B	833	-	1/1/15/20	8/39/115/115	-
28	CLA	A	810	28	1/1/14/20	10/36/112/115	-
28	CLA	n	608	26	1/1/12/20	7/23/99/115	-
30	LHG	b	619	28	-	21/53/53/53	-
31	WVN	K	104	-	-	5/29/63/63	0/2/2/2
28	CLA	B	801	40	1/1/15/20	11/39/115/115	-
28	CLA	f	601	18	1/1/11/20	10/18/94/115	-
28	CLA	l	302	20	1/1/11/20	6/18/94/115	-
31	WVN	l	315	-	-	9/29/63/63	0/2/2/2
28	CLA	A	819	-	1/1/11/20	4/15/91/115	-
28	CLA	K	101	40	1/1/12/20	3/23/99/115	-
31	WVN	B	844	-	-	7/29/63/63	0/2/2/2
35	LMG	n	620	-	-	13/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	II0	d	315	-	-	5/21/67/67	0/2/2/2
30	LHG	J	106	28	-	27/53/53/53	-
36	II0	m	614	-	-	3/21/67/67	0/2/2/2
28	CLA	A	831	-	1/1/15/20	10/39/115/115	-
28	CLA	A	811	-	-	5/26/102/115	-
28	CLA	A	828	-	-	9/39/115/115	-
30	LHG	f	619	-	-	36/53/53/53	-
31	WVN	L	201	-	-	8/29/63/63	0/2/2/2
31	WVN	A	848	-	-	9/29/63/63	0/2/2/2
28	CLA	K	103	-	1/1/10/20	5/12/88/115	-
28	CLA	m	608	18	1/1/15/20	21/39/115/115	-
32	LMT	A	850	-	-	12/21/61/61	0/2/2/2
28	CLA	Q	302	40	1/1/15/20	18/39/115/115	-
28	CLA	A	809	-	1/1/13/20	10/29/105/115	-
31	WVN	F	203	-	-	8/29/63/63	0/2/2/2
28	CLA	L	203	-	-	14/39/115/115	-
38	KC2	n	612	-	-	7/15/71/71	-
28	CLA	a	313	-	-	9/19/95/115	-
35	LMG	F	205	-	-	11/43/63/70	0/1/1/1
28	CLA	A	808	1	1/1/15/20	8/39/115/115	-
28	CLA	n	604	26	1/1/14/20	11/33/109/115	-
36	II0	c	617	-	-	3/21/67/67	0/2/2/2
36	II0	a	316	-	-	2/21/67/67	0/2/2/2
31	WVN	A	847	-	-	6/29/63/63	0/2/2/2
36	II0	h	310	-	-	3/17/40/67	0/1/1/2
28	CLA	F	201	40	1/1/15/20	14/39/115/115	-
28	CLA	A	852	-	1/1/15/20	11/39/115/115	-
35	LMG	J	105	-	-	13/50/70/70	0/1/1/1
38	KC2	n	611	26	-	7/15/71/71	-
28	CLA	h	304	-	1/1/12/20	6/23/99/115	-
28	CLA	d	305	23	1/1/12/20	9/23/99/115	-
36	II0	O	203	-	-	3/21/67/67	0/2/2/2
36	II0	d	313	-	-	5/21/67/67	0/2/2/2
28	CLA	B	827	-	-	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	a	310	30	1/1/11/20	8/19/95/115	-
28	CLA	A	838	1	1/1/15/20	12/39/115/115	-
30	LHG	A	849	-	-	16/42/42/53	-
28	CLA	A	813	-	1/1/11/20	5/15/91/115	-
37	IHT	R	204	-	-	3/25/65/65	0/2/2/2
28	CLA	A	815	40	1/1/11/20	3/15/91/115	-
28	CLA	B	838	-	1/1/13/20	10/30/106/115	-
30	LHG	A	843	-	-	4/52/52/53	-
28	CLA	i	304	-	1/1/12/20	5/23/99/115	-
28	CLA	i	306	-	1/1/12/20	11/23/99/115	-
36	II0	f	618	-	-	7/21/67/67	0/2/2/2
36	II0	h	311	-	-	7/21/67/67	0/2/2/2
28	CLA	n	609	26	1/1/15/20	10/39/115/115	-
38	KC2	g	314	38	-	5/15/71/71	-
38	KC2	m	611	18	-	6/15/71/71	-
36	II0	g	320	-	-	4/21/67/67	0/2/2/2
28	CLA	d	309	30	1/1/10/20	2/10/86/115	-
31	WVN	A	846	-	-	10/29/63/63	0/2/2/2
31	WVN	R	202	-	-	6/29/63/63	0/2/2/2
28	CLA	b	610	16	1/1/15/20	21/39/115/115	-
28	CLA	m	605	18	-	4/12/88/115	-
28	CLA	c	606	-	-	11/24/100/115	-
28	CLA	e	611	-	1/1/15/20	19/39/115/115	-
28	CLA	f	609	18	1/1/15/20	12/39/115/115	-
37	IHT	n	617	-	-	8/25/65/65	0/2/2/2
37	IHT	O	204	-	-	8/25/65/65	0/2/2/2
36	II0	i	313	-	-	7/21/67/67	0/2/2/2
28	CLA	a	312	-	1/1/15/20	18/39/115/115	-
36	II0	g	316	-	-	5/21/67/67	0/2/2/2
28	CLA	c	611	14	-	5/15/91/115	-
28	CLA	A	832	-	1/1/15/20	14/39/115/115	-
28	CLA	B	830	40	1/1/15/20	13/39/115/115	-
28	CLA	k	604	21	1/1/15/20	13/39/115/115	-
28	CLA	j	606	18	1/1/12/20	9/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	827	-	1/1/14/20	8/36/112/115	-
28	CLA	A	840	40	1/1/15/20	19/39/115/115	-
28	CLA	h	307	17	1/1/13/20	12/30/106/115	-
38	KC2	i	319	-	-	6/15/71/71	-
36	II0	e	613	-	-	4/21/67/67	0/2/2/2
28	CLA	g	311	30	1/1/12/20	4/26/102/115	-
28	CLA	s	208	-	1/1/12/20	8/23/99/115	-
28	CLA	e	610	40	1/1/15/20	15/39/115/115	-
28	CLA	a	307	15	1/1/11/20	4/15/91/115	-
28	CLA	j	608	18	1/1/11/20	6/15/91/115	-
28	CLA	b	603	-	1/1/15/20	18/39/115/115	-
28	CLA	R	203	-	1/1/12/20	6/23/99/115	-
28	CLA	k	607	-	1/1/12/20	10/23/99/115	-
28	CLA	i	307	22	1/1/14/20	10/35/111/115	-
28	CLA	B	815	-	1/1/13/20	8/32/108/115	-
38	KC2	g	312	24	-	7/15/71/71	-
38	KC2	s	201	13	-	9/15/71/71	-
31	WVN	i	316	-	-	9/29/63/63	0/2/2/2
36	II0	b	614	-	-	7/21/67/67	0/2/2/2
28	CLA	O	201	30	1/1/12/20	5/24/100/115	-
28	CLA	m	610	30	1/1/13/20	11/27/103/115	-
36	II0	l	313	-	-	5/21/67/67	0/2/2/2
29	PQN	B	842	-	-	5/23/43/43	0/2/2/2
30	LHG	A	844	28	-	5/31/31/53	-
28	CLA	f	607	-	-	22/39/115/115	-
28	CLA	A	836	-	-	8/39/115/115	-
28	CLA	m	604	18	-	10/39/115/115	-
28	CLA	A	821	-	-	7/20/96/115	-
28	CLA	f	610	30	1/1/15/20	15/39/115/115	-
28	CLA	a	309	15	1/1/15/20	10/39/115/115	-
31	WVN	l	301	-	-	4/29/63/63	0/2/2/2
28	CLA	j	604	18	-	11/39/115/115	-
28	CLA	B	837	-	1/1/15/20	12/39/115/115	-
28	CLA	A	833	-	1/1/12/20	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	II0	J	104	-	-	6/21/67/67	0/2/2/2
28	CLA	B	802	-	1/1/15/20	19/39/115/115	-
37	IHT	a	317	-	-	8/25/65/65	0/2/2/2
28	CLA	A	820	40	1/1/15/20	3/39/115/115	-
28	CLA	A	841	-	1/1/15/20	21/39/115/115	-
35	LMG	O	205	-	-	7/21/41/70	0/1/1/1
36	II0	b	613	-	-	2/21/67/67	0/2/2/2
28	CLA	A	802	-	1/1/15/20	16/39/115/115	-
28	CLA	B	829	-	-	6/21/97/115	-
28	CLA	A	823	-	-	6/27/103/115	-
28	CLA	B	841	30	-	4/39/115/115	-
28	CLA	k	601	21	-	12/23/99/115	-
28	CLA	e	605	19	-	17/39/115/115	-
38	KC2	j	611	18	-	6/15/71/71	-
28	CLA	g	302	24	1/1/10/20	4/12/88/115	-
30	LHG	d	317	28	-	14/41/41/53	-
28	CLA	l	305	20	1/1/15/20	13/39/115/115	-
28	CLA	A	816	-	1/1/15/20	14/39/115/115	-
28	CLA	e	606	19	1/1/15/20	20/39/115/115	-
28	CLA	B	835	40	1/1/15/20	15/39/115/115	-
28	CLA	l	308	20	1/1/12/20	6/23/99/115	-
28	CLA	f	603	-	1/1/12/20	7/23/99/115	-
31	WVN	L	205	-	-	6/29/63/63	0/2/2/2
28	CLA	n	603	-	1/1/12/20	10/23/99/115	-
28	CLA	g	304	-	1/1/12/20	2/23/99/115	-
28	CLA	A	807	1	1/1/15/20	9/39/115/115	-
28	CLA	a	308	15	1/1/15/20	20/39/115/115	-
28	CLA	f	606	18	-	4/23/99/115	-
36	II0	c	615	-	-	2/21/67/67	0/2/2/2
28	CLA	B	822	40	-	9/38/114/115	-
30	LHG	l	317	28	-	14/36/36/53	-
28	CLA	k	609	21	1/1/15/20	12/39/115/115	-
28	CLA	i	312	-	1/1/12/20	5/23/99/115	-
28	CLA	j	601	18	1/1/12/20	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	834	-	1/1/11/20	4/18/94/115	-
28	CLA	A	801	-	1/1/15/20	11/39/115/115	-
28	CLA	B	818	-	-	2/17/93/115	-
38	KC2	i	310	22	-	7/15/71/71	-
36	II0	f	615	-	-	4/21/67/67	0/2/2/2
28	CLA	a	311	15	1/1/15/20	12/39/115/115	-
37	IHT	f	617	-	-	6/25/65/65	0/2/2/2
28	CLA	m	603	-	1/1/15/20	12/39/115/115	-
37	IHT	b	615	-	-	6/25/65/65	0/2/2/2
28	CLA	k	614	-	1/1/12/20	10/23/99/115	-
28	CLA	c	604	14	-	3/39/115/115	-
28	CLA	A	854	40	1/1/15/20	15/39/115/115	-
28	CLA	B	819	-	-	9/27/103/115	-
28	CLA	m	606	-	1/1/15/20	12/39/115/115	-
28	CLA	A	834	-	1/1/12/20	3/23/99/115	-
28	CLA	s	202	13	1/1/15/20	18/39/115/115	-
28	CLA	m	613	-	1/1/10/20	8/13/89/115	-
36	II0	k	617	-	-	1/21/67/67	0/2/2/2
31	WVN	M	101	-	-	7/29/63/63	0/2/2/2
38	KC2	d	310	23	-	6/15/71/71	-
28	CLA	i	311	-	1/1/12/20	7/23/99/115	-
28	CLA	l	311	20	1/1/15/20	13/39/115/115	-
28	CLA	c	607	14	1/1/11/20	3/17/93/115	-
28	CLA	A	824	40	1/1/15/20	8/39/115/115	-
28	CLA	k	610	30	1/1/12/20	12/23/99/115	-
36	II0	d	314	-	-	1/21/67/67	0/2/2/2
36	II0	j	615	-	-	2/21/67/67	0/2/2/2
38	KC2	l	310	20	-	6/15/71/71	-
30	LHG	g	301	28	-	20/41/41/53	-
36	II0	g	318	-	-	2/21/67/67	0/2/2/2
28	CLA	j	610	30	1/1/14/20	16/35/111/115	-
28	CLA	b	602	16	1/1/13/20	10/27/103/115	-
28	CLA	g	315	-	1/1/12/20	10/23/99/115	-
28	CLA	A	829	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	g	306	24	1/1/12/20	10/23/99/115	-
28	CLA	B	803	-	1/1/15/20	9/39/115/115	-
28	CLA	c	612	-	1/1/15/20	13/39/115/115	-
36	II0	i	317	-	-	7/21/67/67	0/2/2/2
28	CLA	B	826	-	1/1/12/20	5/23/99/115	-
28	CLA	e	602	19	-	9/21/97/115	-
28	CLA	b	609	-	1/1/12/20	5/23/99/115	-
28	CLA	g	307	24	1/1/12/20	8/23/99/115	-
36	II0	c	613	-	-	3/21/67/67	0/2/2/2
28	CLA	A	839	-	1/1/15/20	16/39/115/115	-
28	CLA	B	814	-	-	9/27/103/115	-
31	WVN	B	845	-	-	0/29/63/63	0/2/2/2
28	CLA	e	603	19	1/1/12/20	4/23/99/115	-
28	CLA	e	608	30	1/1/11/20	4/17/93/115	-
28	CLA	g	309	24	1/1/15/20	11/39/115/115	-
28	CLA	b	607	16	1/1/15/20	17/39/115/115	-
37	IHT	c	616	-	-	10/25/65/65	0/2/2/2
28	CLA	B	812	-	1/1/14/20	13/33/109/115	-
31	WVN	K	102	-	-	6/29/63/63	0/2/2/2
28	CLA	n	605	26	1/1/12/20	6/23/99/115	-
28	CLA	B	805	-	1/1/15/20	13/39/115/115	-
36	II0	j	614	-	-	6/21/67/67	0/2/2/2
28	CLA	k	602	21	1/1/12/20	8/21/97/115	-
28	CLA	d	301	23	1/1/12/20	4/21/97/115	-
37	IHT	k	618	-	-	11/25/65/65	0/2/2/2
28	CLA	s	203	13,28	-	18/39/115/115	-
39	LMU	i	301	-	-	8/21/61/61	0/2/2/2

All (4109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	616	IHT	C15-C11	25.69	1.63	1.35
37	g	319	IHT	C15-C11	25.58	1.63	1.35
37	a	317	IHT	C15-C11	25.42	1.63	1.35
37	R	204	IHT	C15-C11	25.28	1.63	1.35
37	O	204	IHT	C15-C11	25.23	1.63	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	615	IHT	C15-C11	25.16	1.62	1.35
37	c	616	IHT	C15-C11	25.10	1.62	1.35
37	j	616	IHT	C15-C11	24.89	1.62	1.35
37	k	618	IHT	C15-C11	24.88	1.62	1.35
37	f	617	IHT	C15-C11	24.70	1.62	1.35
37	m	617	IHT	C15-C11	24.61	1.62	1.35
37	n	617	IHT	C15-C11	24.58	1.62	1.35
36	a	318	II0	C14-C10	24.31	1.61	1.35
36	b	613	II0	C14-C10	23.83	1.61	1.35
36	g	318	II0	C14-C10	23.82	1.61	1.35
36	d	316	II0	C14-C10	23.69	1.61	1.35
36	c	615	II0	C14-C10	23.62	1.61	1.35
36	n	614	II0	C14-C10	23.56	1.61	1.35
36	i	317	II0	C13-C09	23.55	1.61	1.35
36	e	614	II0	C13-C09	23.50	1.61	1.35
36	e	612	II0	C14-C10	23.43	1.61	1.35
36	k	617	II0	C14-C10	23.42	1.60	1.35
36	h	312	II0	C13-C09	23.40	1.60	1.35
36	e	613	II0	C14-C10	23.40	1.60	1.35
36	n	616	II0	C13-C09	23.38	1.60	1.35
36	n	618	II0	C13-C09	23.34	1.60	1.35
36	i	314	II0	C14-C10	23.34	1.60	1.35
36	g	316	II0	C13-C09	23.33	1.60	1.35
36	k	615	II0	C14-C10	23.32	1.60	1.35
36	l	313	II0	C14-C10	23.32	1.60	1.35
36	d	314	II0	C14-C10	23.32	1.60	1.35
36	d	315	II0	C14-C10	23.30	1.60	1.35
36	c	617	II0	C13-C09	23.29	1.60	1.35
36	b	614	II0	C13-C09	23.28	1.60	1.35
36	e	614	II0	C14-C10	23.28	1.60	1.35
36	k	621	II0	C14-C10	23.28	1.60	1.35
36	m	614	II0	C14-C10	23.27	1.60	1.35
36	l	313	II0	C13-C09	23.23	1.60	1.35
36	m	618	II0	C13-C09	23.22	1.60	1.35
36	b	617	II0	C13-C09	23.22	1.60	1.35
36	a	318	II0	C13-C09	23.21	1.60	1.35
36	c	613	II0	C13-C09	23.21	1.60	1.35
36	j	615	II0	C14-C10	23.19	1.60	1.35
36	f	618	II0	C14-C10	23.18	1.60	1.35
36	j	614	II0	C14-C10	23.14	1.60	1.35
36	J	104	II0	C14-C10	23.10	1.60	1.35
36	h	312	II0	C14-C10	23.10	1.60	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	j	614	II0	C13-C09	23.09	1.60	1.35
36	m	614	II0	C13-C09	23.07	1.60	1.35
36	d	316	II0	C13-C09	23.06	1.60	1.35
36	c	614	II0	C14-C10	23.04	1.60	1.35
36	f	614	II0	C14-C10	23.03	1.60	1.35
36	l	314	II0	C13-C09	23.02	1.60	1.35
36	k	616	II0	C14-C10	23.02	1.60	1.35
36	f	615	II0	C13-C09	22.98	1.60	1.35
36	a	315	II0	C14-C10	22.98	1.60	1.35
36	l	316	II0	C14-C10	22.98	1.60	1.35
36	n	615	II0	C13-C09	22.98	1.60	1.35
36	j	615	II0	C13-C09	22.97	1.60	1.35
36	f	616	II0	C13-C09	22.95	1.60	1.35
36	l	312	II0	C13-C09	22.93	1.60	1.35
36	e	616	II0	C14-C10	22.89	1.60	1.35
36	i	315	II0	C14-C10	22.88	1.60	1.35
36	l	312	II0	C14-C10	22.88	1.60	1.35
36	g	317	II0	C13-C09	22.86	1.60	1.35
36	k	617	II0	C13-C09	22.86	1.60	1.35
36	b	614	II0	C14-C10	22.84	1.60	1.35
36	f	614	II0	C13-C09	22.84	1.60	1.35
36	d	315	II0	C13-C09	22.84	1.60	1.35
36	a	314	II0	C14-C10	22.84	1.60	1.35
36	g	320	II0	C14-C10	22.83	1.60	1.35
36	g	320	II0	C13-C09	22.83	1.60	1.35
36	i	313	II0	C13-C09	22.82	1.60	1.35
36	h	310	II0	C13-C09	22.80	1.60	1.35
36	g	316	II0	C14-C10	22.80	1.60	1.35
36	n	618	II0	C14-C10	22.79	1.60	1.35
36	h	311	II0	C13-C09	22.79	1.60	1.35
36	d	313	II0	C14-C10	22.78	1.60	1.35
36	m	616	II0	C14-C10	22.77	1.60	1.35
36	i	317	II0	C14-C10	22.77	1.60	1.35
36	d	314	II0	C13-C09	22.76	1.60	1.35
36	O	203	II0	C13-C09	22.75	1.60	1.35
36	i	313	II0	C14-C10	22.73	1.60	1.35
36	k	616	II0	C13-C09	22.72	1.60	1.35
36	n	614	II0	C13-C09	22.70	1.60	1.35
36	k	619	II0	C14-C10	22.66	1.60	1.35
36	l	316	II0	C13-C09	22.65	1.60	1.35
36	f	618	II0	C13-C09	22.64	1.60	1.35
36	f	615	II0	C14-C10	22.63	1.60	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	i	315	II0	C13-C09	22.62	1.60	1.35
36	O	203	II0	C14-C10	22.61	1.60	1.35
36	i	320	II0	C13-C09	22.60	1.60	1.35
36	n	615	II0	C14-C10	22.58	1.60	1.35
36	e	616	II0	C13-C09	22.57	1.60	1.35
36	c	614	II0	C13-C09	22.57	1.60	1.35
36	m	618	II0	C14-C10	22.54	1.60	1.35
36	g	318	II0	C13-C09	22.54	1.60	1.35
36	m	615	II0	C13-C09	22.54	1.60	1.35
36	b	613	II0	C13-C09	22.54	1.60	1.35
36	a	316	II0	C13-C09	22.53	1.60	1.35
36	l	314	II0	C14-C10	22.47	1.59	1.35
36	n	616	II0	C14-C10	22.45	1.59	1.35
36	a	316	II0	C14-C10	22.45	1.59	1.35
36	m	616	II0	C13-C09	22.42	1.59	1.35
36	c	613	II0	C14-C10	22.41	1.59	1.35
36	e	613	II0	C13-C09	22.40	1.59	1.35
36	k	619	II0	C13-C09	22.39	1.59	1.35
36	m	615	II0	C14-C10	22.37	1.59	1.35
36	f	616	II0	C14-C10	22.33	1.59	1.35
36	i	314	II0	C13-C09	22.31	1.59	1.35
36	i	320	II0	C14-C10	22.31	1.59	1.35
36	g	317	II0	C14-C10	22.25	1.59	1.35
36	e	612	II0	C13-C09	22.25	1.59	1.35
36	c	615	II0	C13-C09	22.24	1.59	1.35
36	k	615	II0	C13-C09	22.13	1.59	1.35
36	h	311	II0	C14-C10	22.06	1.59	1.35
36	a	314	II0	C13-C09	22.01	1.59	1.35
36	k	621	II0	C13-C09	21.98	1.59	1.35
36	J	104	II0	C13-C09	21.98	1.59	1.35
36	b	617	II0	C14-C10	21.89	1.59	1.35
36	d	313	II0	C13-C09	21.84	1.59	1.35
36	a	315	II0	C13-C09	21.74	1.59	1.35
36	c	617	II0	C14-C10	21.43	1.58	1.35
37	b	616	IHT	C10-C07	15.76	1.60	1.34
37	g	319	IHT	C10-C07	15.72	1.60	1.34
37	a	317	IHT	C10-C07	15.51	1.60	1.34
37	c	616	IHT	C10-C07	15.48	1.60	1.34
37	k	618	IHT	C10-C07	15.31	1.60	1.34
37	b	615	IHT	C10-C07	15.28	1.60	1.34
37	f	617	IHT	C10-C07	15.25	1.60	1.34
37	R	204	IHT	C10-C07	15.19	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	j	616	IHT	C10-C07	15.12	1.59	1.34
37	m	617	IHT	C10-C07	15.12	1.59	1.34
37	n	617	IHT	C10-C07	15.04	1.59	1.34
37	O	204	IHT	C10-C07	14.98	1.59	1.34
36	a	318	II0	C05-C07	-11.91	1.35	1.52
36	a	315	II0	C05-C07	-11.83	1.35	1.52
36	l	313	II0	C05-C07	-11.76	1.35	1.52
37	g	319	IHT	C05-C08	-11.73	1.35	1.52
36	c	615	II0	C05-C07	-11.70	1.35	1.52
36	l	314	II0	C05-C07	-11.66	1.35	1.52
37	j	616	IHT	C05-C08	-11.65	1.35	1.52
36	g	320	II0	C05-C07	-11.63	1.35	1.52
37	a	317	IHT	C05-C08	-11.62	1.35	1.52
36	f	615	II0	C05-C07	-11.62	1.35	1.52
36	e	613	II0	C05-C07	-11.59	1.35	1.52
36	b	614	II0	C05-C07	-11.57	1.35	1.52
37	b	616	IHT	C05-C08	-11.56	1.35	1.52
37	O	204	IHT	C05-C08	-11.55	1.35	1.52
36	i	315	II0	C05-C07	-11.53	1.36	1.52
36	k	617	II0	C05-C07	-11.52	1.36	1.52
36	c	617	II0	C05-C07	-11.52	1.36	1.52
36	j	614	II0	C05-C07	-11.49	1.36	1.52
36	b	617	II0	C05-C07	-11.48	1.36	1.52
36	m	614	II0	C05-C07	-11.47	1.36	1.52
36	J	104	II0	C05-C07	-11.47	1.36	1.52
37	c	616	IHT	C05-C08	-11.45	1.36	1.52
36	a	314	II0	C05-C07	-11.45	1.36	1.52
37	b	615	IHT	C05-C08	-11.45	1.36	1.52
36	c	614	II0	C05-C07	-11.44	1.36	1.52
36	f	614	II0	C05-C07	-11.41	1.36	1.52
37	R	204	IHT	C05-C08	-11.40	1.36	1.52
36	g	316	II0	C05-C07	-11.40	1.36	1.52
36	a	316	II0	C05-C07	-11.38	1.36	1.52
36	k	615	II0	C05-C07	-11.37	1.36	1.52
36	O	203	II0	C05-C07	-11.36	1.36	1.52
36	m	618	II0	C05-C07	-11.35	1.36	1.52
36	k	621	II0	C05-C07	-11.34	1.36	1.52
36	l	312	II0	C05-C07	-11.34	1.36	1.52
37	f	617	IHT	C05-C08	-11.33	1.36	1.52
36	c	613	II0	C05-C07	-11.32	1.36	1.52
36	i	313	II0	C05-C07	-11.31	1.36	1.52
36	n	618	II0	C05-C07	-11.29	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	617	IHT	C05-C08	-11.29	1.36	1.52
36	n	615	II0	C05-C07	-11.27	1.36	1.52
36	n	614	II0	C05-C07	-11.24	1.36	1.52
36	m	615	II0	C05-C07	-11.23	1.36	1.52
37	k	618	IHT	C05-C08	-11.22	1.36	1.52
36	f	616	II0	C05-C07	-11.22	1.36	1.52
36	h	310	II0	C05-C07	-11.22	1.36	1.52
36	n	616	II0	C05-C07	-11.22	1.36	1.52
36	e	614	II0	C05-C07	-11.21	1.36	1.52
37	f	617	IHT	C12-C08	11.20	1.71	1.52
37	m	617	IHT	C05-C08	-11.17	1.36	1.52
36	i	320	II0	C05-C07	-11.16	1.36	1.52
36	k	619	II0	C11-C07	11.15	1.71	1.52
36	j	615	II0	C05-C07	-11.15	1.36	1.52
36	h	312	II0	C05-C07	-11.15	1.36	1.52
36	m	618	II0	C06-C08	-11.15	1.36	1.52
36	d	314	II0	C05-C07	-11.12	1.36	1.52
36	h	311	II0	C05-C07	-11.11	1.36	1.52
36	g	318	II0	C05-C07	-11.09	1.36	1.52
36	e	616	II0	C11-C07	11.08	1.71	1.52
36	g	317	II0	C11-C07	11.08	1.71	1.52
36	k	616	II0	C05-C07	-11.07	1.36	1.52
36	c	614	II0	C06-C08	-11.04	1.36	1.52
36	d	316	II0	C11-C07	11.03	1.71	1.52
36	g	317	II0	C05-C07	-11.03	1.36	1.52
36	l	316	II0	C05-C07	-11.02	1.36	1.52
36	b	613	II0	C05-C07	-11.02	1.36	1.52
36	m	616	II0	C11-C07	11.01	1.71	1.52
36	d	315	II0	C11-C07	11.01	1.71	1.52
36	i	320	II0	C11-C07	11.01	1.71	1.52
36	j	615	II0	C06-C08	-11.00	1.36	1.52
36	k	619	II0	C05-C07	-11.00	1.36	1.52
36	l	313	II0	C06-C08	-10.97	1.36	1.52
37	n	617	IHT	C12-C08	10.96	1.71	1.52
37	m	617	IHT	C12-C08	10.96	1.71	1.52
36	a	315	II0	C06-C08	-10.95	1.36	1.52
37	a	317	IHT	C12-C08	10.92	1.71	1.52
36	g	318	II0	C11-C07	10.90	1.71	1.52
37	k	618	IHT	C12-C08	10.89	1.71	1.52
36	g	320	II0	C06-C08	-10.88	1.36	1.52
37	R	204	IHT	C12-C08	10.88	1.71	1.52
36	d	315	II0	C06-C08	-10.87	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	i	315	II0	C11-C07	10.87	1.71	1.52
36	m	616	II0	C05-C07	-10.86	1.36	1.52
36	i	314	II0	C05-C07	-10.83	1.37	1.52
37	g	319	IHT	C12-C08	10.82	1.71	1.52
36	n	616	II0	C11-C07	10.81	1.71	1.52
37	c	616	IHT	C12-C08	10.81	1.71	1.52
36	a	314	II0	C06-C08	-10.80	1.37	1.52
36	b	614	II0	C06-C08	-10.80	1.37	1.52
36	d	313	II0	C05-C07	-10.80	1.37	1.52
37	b	616	IHT	C12-C08	10.79	1.71	1.52
37	O	204	IHT	C12-C08	10.78	1.71	1.52
36	e	612	II0	C11-C07	10.76	1.71	1.52
36	i	317	II0	C11-C07	10.76	1.71	1.52
36	l	316	II0	C11-C07	10.75	1.71	1.52
36	k	616	II0	C06-C08	-10.75	1.37	1.52
36	b	617	II0	C11-C07	10.72	1.71	1.52
36	e	612	II0	C06-C08	-10.71	1.37	1.52
36	k	621	II0	C11-C07	10.71	1.71	1.52
37	b	615	IHT	C12-C08	10.70	1.71	1.52
36	d	313	II0	C11-C07	10.68	1.71	1.52
36	i	314	II0	C06-C08	-10.68	1.37	1.52
36	e	614	II0	C11-C07	10.66	1.71	1.52
36	i	314	II0	C11-C07	10.66	1.71	1.52
36	h	312	II0	C11-C07	10.65	1.70	1.52
36	f	615	II0	C06-C08	-10.65	1.37	1.52
36	c	617	II0	C11-C07	10.64	1.70	1.52
36	m	614	II0	C06-C08	-10.64	1.37	1.52
36	i	317	II0	C05-C07	-10.63	1.37	1.52
36	f	618	II0	C11-C07	10.62	1.70	1.52
36	f	618	II0	C06-C08	-10.62	1.37	1.52
36	f	614	II0	C06-C08	-10.61	1.37	1.52
36	l	312	II0	C06-C08	-10.60	1.37	1.52
36	d	314	II0	C11-C07	10.59	1.70	1.52
37	j	616	IHT	C12-C08	10.59	1.70	1.52
36	c	613	II0	C11-C07	10.59	1.70	1.52
36	f	618	II0	C05-C07	-10.58	1.37	1.52
36	l	312	II0	C11-C07	10.57	1.70	1.52
36	m	614	II0	C11-C07	10.57	1.70	1.52
36	a	316	II0	C11-C07	10.56	1.70	1.52
36	l	314	II0	C11-C07	10.56	1.70	1.52
36	J	104	II0	C06-C08	-10.56	1.37	1.52
36	O	203	II0	C06-C08	-10.55	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	n	618	II0	C11-C07	10.54	1.70	1.52
36	i	313	II0	C11-C07	10.54	1.70	1.52
36	g	320	II0	C11-C07	10.53	1.70	1.52
36	g	317	II0	C06-C08	-10.53	1.37	1.52
36	n	614	II0	C11-C07	10.50	1.70	1.52
36	k	616	II0	C11-C07	10.49	1.70	1.52
36	a	318	II0	C11-C07	10.46	1.70	1.52
36	a	316	II0	C06-C08	-10.46	1.37	1.52
36	m	615	II0	C06-C08	-10.45	1.37	1.52
36	k	615	II0	C06-C08	-10.45	1.37	1.52
36	h	310	II0	C11-C07	10.43	1.70	1.52
36	k	615	II0	C11-C07	10.42	1.70	1.52
36	c	613	II0	C06-C08	-10.41	1.37	1.52
36	h	311	II0	C11-C07	10.41	1.70	1.52
36	g	316	II0	C11-C07	10.41	1.70	1.52
36	O	203	II0	C11-C07	10.40	1.70	1.52
36	j	614	II0	C11-C07	10.40	1.70	1.52
36	h	311	II0	C06-C08	-10.38	1.37	1.52
36	e	613	II0	C11-C07	10.36	1.70	1.52
36	d	316	II0	C05-C07	-10.36	1.37	1.52
36	c	614	II0	C11-C07	10.34	1.70	1.52
36	k	621	II0	C06-C08	-10.34	1.37	1.52
36	m	615	II0	C11-C07	10.34	1.70	1.52
36	i	317	II0	C06-C08	-10.33	1.37	1.52
36	m	618	II0	C11-C07	10.33	1.70	1.52
36	n	616	II0	C06-C08	-10.31	1.37	1.52
36	b	613	II0	C11-C07	10.31	1.70	1.52
36	m	616	II0	C06-C08	-10.29	1.37	1.52
36	e	612	II0	C05-C07	-10.28	1.37	1.52
36	j	615	II0	C11-C07	10.28	1.70	1.52
36	f	614	II0	C11-C07	10.24	1.70	1.52
36	k	617	II0	C06-C08	-10.21	1.37	1.52
36	b	613	II0	C06-C08	-10.21	1.37	1.52
36	e	616	II0	C05-C07	-10.19	1.37	1.52
36	n	615	II0	C11-C07	10.16	1.70	1.52
36	e	613	II0	C06-C08	-10.16	1.37	1.52
36	e	614	II0	C06-C08	-10.16	1.37	1.52
36	f	616	II0	C11-C07	10.15	1.70	1.52
36	k	617	II0	C11-C07	10.13	1.70	1.52
36	h	312	II0	C06-C08	-10.12	1.38	1.52
36	l	313	II0	C11-C07	10.12	1.70	1.52
36	k	619	II0	C06-C08	-10.10	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	316	II0	C06-C08	-10.08	1.38	1.52
36	f	615	II0	C11-C07	10.06	1.69	1.52
36	j	614	II0	C06-C08	-10.04	1.38	1.52
36	e	616	II0	C06-C08	-10.04	1.38	1.52
36	J	104	II0	C11-C07	10.04	1.69	1.52
36	l	316	II0	C06-C08	-10.02	1.38	1.52
36	i	315	II0	C06-C08	-10.01	1.38	1.52
36	d	313	II0	C06-C08	-10.00	1.38	1.52
36	c	617	II0	C06-C08	-9.98	1.38	1.52
36	d	316	II0	C06-C08	-9.98	1.38	1.52
36	a	315	II0	C11-C07	9.94	1.69	1.52
36	c	615	II0	C11-C07	9.93	1.69	1.52
36	l	314	II0	C06-C08	-9.90	1.38	1.52
36	i	320	II0	C06-C08	-9.87	1.38	1.52
36	i	313	II0	C06-C08	-9.87	1.38	1.52
36	n	615	II0	C06-C08	-9.86	1.38	1.52
36	b	617	II0	C06-C08	-9.85	1.38	1.52
36	g	318	II0	C06-C08	-9.82	1.38	1.52
36	a	314	II0	C11-C07	9.77	1.69	1.52
36	n	614	II0	C06-C08	-9.74	1.38	1.52
36	d	314	II0	C06-C08	-9.67	1.38	1.52
36	d	315	II0	C05-C07	-9.63	1.38	1.52
36	c	615	II0	C06-C08	-9.57	1.38	1.52
36	b	614	II0	C11-C07	9.57	1.69	1.52
36	a	318	II0	C06-C08	-9.50	1.38	1.52
36	n	618	II0	C06-C08	-9.50	1.38	1.52
36	f	616	II0	C06-C08	-9.37	1.39	1.52
36	n	618	II0	C12-C08	9.10	1.68	1.52
36	f	616	II0	C12-C08	8.89	1.67	1.52
36	m	618	II0	C12-C08	8.87	1.67	1.52
36	n	614	II0	C12-C08	8.85	1.67	1.52
36	d	313	II0	C12-C08	8.81	1.67	1.52
36	d	314	II0	C12-C08	8.78	1.67	1.52
36	g	316	II0	C12-C08	8.77	1.67	1.52
36	l	313	II0	C12-C08	8.72	1.67	1.52
36	e	613	II0	C12-C08	8.72	1.67	1.52
36	i	315	II0	C12-C08	8.70	1.67	1.52
36	i	320	II0	C12-C08	8.68	1.67	1.52
36	c	615	II0	C12-C08	8.67	1.67	1.52
36	d	315	II0	C12-C08	8.64	1.67	1.52
36	f	615	II0	C12-C08	8.57	1.67	1.52
36	a	316	II0	C12-C08	8.56	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	615	II0	C12-C08	8.54	1.67	1.52
36	i	317	II0	C12-C08	8.54	1.67	1.52
36	e	616	II0	C12-C08	8.51	1.67	1.52
36	l	314	II0	C12-C08	8.50	1.67	1.52
36	g	318	II0	C12-C08	8.47	1.67	1.52
36	k	617	II0	C12-C08	8.47	1.67	1.52
36	J	104	II0	C12-C08	8.45	1.67	1.52
36	b	617	II0	C12-C08	8.42	1.67	1.52
36	l	316	II0	C12-C08	8.42	1.67	1.52
36	f	618	II0	C12-C08	8.41	1.67	1.52
36	j	615	II0	C12-C08	8.38	1.66	1.52
36	k	616	II0	C12-C08	8.38	1.66	1.52
36	m	614	II0	C12-C08	8.36	1.66	1.52
36	l	312	II0	C12-C08	8.36	1.66	1.52
36	e	614	II0	C12-C08	8.36	1.66	1.52
36	c	617	II0	C12-C08	8.34	1.66	1.52
36	m	616	II0	C12-C08	8.33	1.66	1.52
36	n	616	II0	C12-C08	8.33	1.66	1.52
36	c	613	II0	C12-C08	8.33	1.66	1.52
36	g	320	II0	C12-C08	8.32	1.66	1.52
36	a	315	II0	C12-C08	8.30	1.66	1.52
36	k	621	II0	C12-C08	8.28	1.66	1.52
36	e	612	II0	C12-C08	8.27	1.66	1.52
36	d	316	II0	C12-C08	8.26	1.66	1.52
36	c	614	II0	C12-C08	8.25	1.66	1.52
36	g	317	II0	C12-C08	8.20	1.66	1.52
36	O	203	II0	C12-C08	8.18	1.66	1.52
36	i	313	II0	C12-C08	8.12	1.66	1.52
36	j	614	II0	C12-C08	8.04	1.66	1.52
36	b	613	II0	C12-C08	8.04	1.66	1.52
36	a	318	II0	C12-C08	8.03	1.66	1.52
36	n	615	II0	C12-C08	8.02	1.66	1.52
36	m	615	II0	C12-C08	8.02	1.66	1.52
36	h	312	II0	C12-C08	8.00	1.66	1.52
36	d	313	II0	C22-C10	7.90	1.57	1.42
36	f	614	II0	C12-C08	7.88	1.66	1.52
36	k	619	II0	C12-C08	7.86	1.66	1.52
36	d	314	II0	C22-C10	7.86	1.57	1.42
36	h	311	II0	C12-C08	7.83	1.66	1.52
36	a	318	II0	C22-C10	7.81	1.57	1.42
36	a	314	II0	C12-C08	7.77	1.65	1.52
36	n	616	II0	C21-C09	7.76	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	614	II0	C12-C08	7.76	1.65	1.52
36	k	617	II0	C22-C10	7.74	1.57	1.42
36	i	317	II0	C21-C09	7.72	1.57	1.42
36	k	615	II0	C22-C10	7.72	1.57	1.42
36	d	316	II0	C21-C09	7.68	1.57	1.42
36	l	316	II0	C22-C10	7.68	1.57	1.42
36	n	618	II0	C21-C09	7.64	1.56	1.42
36	m	618	II0	C21-C09	7.63	1.56	1.42
36	f	616	II0	C21-C09	7.62	1.56	1.42
36	e	612	II0	C21-C09	7.58	1.56	1.42
36	d	316	II0	C22-C10	7.57	1.56	1.42
36	n	614	II0	C21-C09	7.57	1.56	1.42
36	d	315	II0	C22-C10	7.54	1.56	1.42
36	i	317	II0	C22-C10	7.53	1.56	1.42
36	i	315	II0	C21-C09	7.52	1.56	1.42
36	l	316	II0	C21-C09	7.50	1.56	1.42
36	i	320	II0	C21-C09	7.44	1.56	1.42
36	l	313	II0	C22-C10	7.44	1.56	1.42
38	k	612	KC2	C4C-NC	7.42	1.49	1.37
29	A	842	PQN	C3-C2	7.42	1.48	1.35
36	l	314	II0	C21-C09	7.42	1.56	1.42
36	i	315	II0	C22-C10	7.41	1.56	1.42
36	d	315	II0	C21-C09	7.40	1.56	1.42
36	d	314	II0	C21-C09	7.40	1.56	1.42
36	g	316	II0	C21-C09	7.40	1.56	1.42
36	i	314	II0	C22-C10	7.40	1.56	1.42
37	g	319	IHT	C04-C06	-7.40	1.35	1.52
36	n	614	II0	C22-C10	7.39	1.56	1.42
36	g	318	II0	C21-C09	7.39	1.56	1.42
36	i	314	II0	C12-C08	7.38	1.65	1.52
36	k	619	II0	C21-C09	7.38	1.56	1.42
37	b	616	IHT	C04-C06	-7.37	1.35	1.52
36	k	619	II0	C22-C10	7.37	1.56	1.42
36	k	621	II0	C22-C10	7.37	1.56	1.42
36	e	616	II0	C22-C10	7.35	1.56	1.42
36	e	616	II0	C21-C09	7.33	1.56	1.42
36	k	616	II0	C22-C10	7.32	1.56	1.42
36	g	320	II0	C22-C10	7.32	1.56	1.42
36	f	616	II0	C22-C10	7.31	1.56	1.42
36	c	615	II0	C22-C10	7.31	1.56	1.42
36	c	615	II0	C21-C09	7.31	1.56	1.42
36	l	314	II0	C22-C10	7.29	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	842	PQN	C3-C2	7.29	1.48	1.35
36	f	618	II0	C22-C10	7.28	1.56	1.42
36	k	617	II0	C21-C09	7.28	1.56	1.42
36	g	316	II0	C22-C10	7.27	1.56	1.42
37	k	618	IHT	C04-C06	-7.26	1.35	1.52
36	n	618	II0	C22-C10	7.26	1.56	1.42
36	h	312	II0	C22-C10	7.24	1.56	1.42
36	d	313	II0	C21-C09	7.24	1.56	1.42
38	g	313	KC2	C4C-NC	7.24	1.49	1.37
36	g	318	II0	C22-C10	7.23	1.56	1.42
36	l	313	II0	C21-C09	7.22	1.56	1.42
36	f	618	II0	C21-C09	7.22	1.56	1.42
37	c	616	IHT	C04-C06	-7.20	1.35	1.52
37	j	616	IHT	C04-C06	-7.19	1.35	1.52
36	e	612	II0	C22-C10	7.19	1.56	1.42
36	f	614	II0	C21-C09	7.19	1.56	1.42
36	k	615	II0	C21-C09	7.18	1.56	1.42
37	b	615	IHT	C04-C06	-7.18	1.35	1.52
36	e	614	II0	C22-C10	7.18	1.56	1.42
36	b	613	II0	C21-C09	7.17	1.56	1.42
36	n	616	II0	C22-C10	7.16	1.56	1.42
36	c	617	II0	C21-C09	7.15	1.56	1.42
36	m	614	II0	C21-C09	7.14	1.56	1.42
36	h	311	II0	C21-C09	7.13	1.55	1.42
36	m	616	II0	C22-C10	7.13	1.55	1.42
37	f	617	IHT	C04-C06	-7.12	1.35	1.52
38	i	319	KC2	C4C-NC	7.12	1.49	1.37
36	n	615	II0	C21-C09	7.12	1.55	1.42
36	m	618	II0	C22-C10	7.11	1.55	1.42
36	c	617	II0	C22-C10	7.10	1.55	1.42
36	g	317	II0	C22-C10	7.10	1.55	1.42
36	c	613	II0	C21-C09	7.09	1.55	1.42
36	e	614	II0	C21-C09	7.09	1.55	1.42
37	R	204	IHT	C04-C06	-7.08	1.35	1.52
37	O	204	IHT	C04-C06	-7.08	1.35	1.52
36	h	310	II0	C21-C09	7.08	1.55	1.42
36	b	617	II0	C21-C09	7.07	1.55	1.42
36	l	312	II0	C22-C10	7.07	1.55	1.42
38	e	609	KC2	C4C-NC	7.07	1.49	1.37
37	a	317	IHT	C04-C06	-7.06	1.35	1.52
38	d	310	KC2	C4C-NC	7.06	1.49	1.37
37	n	617	IHT	C04-C06	-7.05	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	318	II0	C21-C09	7.04	1.55	1.42
36	k	616	II0	C21-C09	7.04	1.55	1.42
38	n	612	KC2	C4C-NC	7.03	1.49	1.37
36	a	316	II0	C22-C10	7.03	1.55	1.42
36	e	613	II0	C22-C10	7.02	1.55	1.42
36	g	320	II0	C21-C09	7.02	1.55	1.42
38	s	201	KC2	C4C-NC	7.02	1.49	1.37
37	m	617	IHT	C04-C06	-7.02	1.36	1.52
36	m	614	II0	C22-C10	7.01	1.55	1.42
36	i	314	II0	C21-C09	7.01	1.55	1.42
37	a	317	IHT	C21-C11	7.00	1.55	1.42
38	k	611	KC2	C4C-NC	7.00	1.49	1.37
36	j	615	II0	C22-C10	6.99	1.55	1.42
36	c	613	II0	C22-C10	6.98	1.55	1.42
38	d	311	KC2	C4C-NC	6.98	1.49	1.37
36	n	615	II0	C22-C10	6.98	1.55	1.42
36	l	312	II0	C21-C09	6.97	1.55	1.42
38	f	611	KC2	C4C-NC	6.97	1.49	1.37
38	g	314	KC2	C4C-NC	6.97	1.49	1.37
38	k	613	KC2	C4C-NC	6.97	1.49	1.37
36	h	312	II0	C21-C09	6.96	1.55	1.42
38	g	312	KC2	C4C-NC	6.96	1.49	1.37
37	f	617	IHT	C21-C11	6.96	1.55	1.42
37	R	204	IHT	C02-C07	-6.96	1.44	1.53
36	f	614	II0	C22-C10	6.96	1.55	1.42
36	m	616	II0	C21-C09	6.95	1.55	1.42
37	O	204	IHT	C02-C07	-6.95	1.44	1.53
38	s	204	KC2	C4C-NC	6.95	1.49	1.37
37	g	319	IHT	C21-C11	6.94	1.55	1.42
36	k	621	II0	C21-C09	6.93	1.55	1.42
36	m	615	II0	C21-C09	6.92	1.55	1.42
36	g	317	II0	C21-C09	6.91	1.55	1.42
38	m	611	KC2	C4C-NC	6.90	1.49	1.37
38	j	611	KC2	C4C-NC	6.90	1.48	1.37
36	j	614	II0	C22-C10	6.90	1.55	1.42
36	O	203	II0	C22-C10	6.89	1.55	1.42
37	b	616	IHT	C21-C11	6.89	1.55	1.42
36	b	614	II0	C21-C09	6.88	1.55	1.42
36	j	615	II0	C21-C09	6.87	1.55	1.42
36	c	614	II0	C21-C09	6.87	1.55	1.42
36	i	313	II0	C21-C09	6.86	1.55	1.42
37	O	204	IHT	C21-C11	6.85	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	j	616	IHT	C02-C07	-6.85	1.45	1.53
36	e	613	II0	C21-C09	6.85	1.55	1.42
38	n	611	KC2	C4C-NC	6.85	1.48	1.37
36	j	614	II0	C21-C09	6.84	1.55	1.42
36	O	203	II0	C21-C09	6.84	1.55	1.42
36	b	614	II0	C22-C10	6.80	1.55	1.42
38	l	310	KC2	C4C-NC	6.78	1.48	1.37
36	a	316	II0	C21-C09	6.78	1.55	1.42
37	f	617	IHT	C02-C07	-6.77	1.45	1.53
38	c	610	KC2	C4C-NC	6.76	1.48	1.37
37	n	617	IHT	C21-C11	6.76	1.55	1.42
36	h	311	II0	C22-C10	6.75	1.55	1.42
36	f	615	II0	C21-C09	6.74	1.55	1.42
36	b	613	II0	C22-C10	6.74	1.55	1.42
36	b	617	II0	C22-C10	6.70	1.55	1.42
37	R	204	IHT	C21-C11	6.70	1.55	1.42
37	j	616	IHT	C21-C11	6.69	1.55	1.42
38	i	310	KC2	C4C-NC	6.65	1.48	1.37
37	m	617	IHT	C21-C11	6.65	1.55	1.42
37	n	617	IHT	C02-C07	-6.65	1.45	1.53
36	a	314	II0	C21-C09	6.64	1.55	1.42
37	k	618	IHT	C21-C11	6.63	1.55	1.42
36	a	314	II0	C22-C10	6.63	1.55	1.42
36	c	614	II0	C22-C10	6.62	1.55	1.42
36	a	315	II0	C22-C10	6.61	1.54	1.42
37	c	616	IHT	C21-C11	6.61	1.54	1.42
37	b	615	IHT	C21-C11	6.50	1.54	1.42
37	b	615	IHT	C02-C07	-6.50	1.45	1.53
37	k	618	IHT	C02-C07	-6.49	1.45	1.53
36	J	104	II0	C22-C10	6.48	1.54	1.42
37	m	617	IHT	C02-C07	-6.46	1.45	1.53
36	i	313	II0	C22-C10	6.42	1.54	1.42
36	J	104	II0	C21-C09	6.42	1.54	1.42
36	f	615	II0	C22-C10	6.39	1.54	1.42
36	m	615	II0	C22-C10	6.35	1.54	1.42
36	i	320	II0	C22-C10	6.29	1.54	1.42
37	a	317	IHT	C02-C07	-6.29	1.45	1.53
37	b	616	IHT	C02-C07	-6.29	1.45	1.53
37	c	616	IHT	C02-C07	-6.27	1.45	1.53
36	g	317	II0	C28-C26	6.23	1.55	1.50
36	a	314	II0	C11-C13	-6.21	1.41	1.51
36	e	613	II0	C11-C13	-6.16	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	614	II0	C11-C13	-6.11	1.41	1.51
37	k	618	IHT	C12-C15	-6.09	1.41	1.51
37	j	616	IHT	C12-C15	-6.06	1.41	1.51
37	g	319	IHT	C22-C23	6.03	1.58	1.46
37	c	616	IHT	C22-C23	6.02	1.58	1.46
37	b	615	IHT	C12-C15	-6.02	1.41	1.51
37	f	617	IHT	C22-C23	6.00	1.58	1.46
37	n	617	IHT	C22-C23	5.99	1.58	1.46
37	a	317	IHT	C22-C23	5.99	1.58	1.46
37	k	618	IHT	C22-C23	5.95	1.58	1.46
37	R	204	IHT	C22-C23	5.90	1.58	1.46
36	k	616	II0	C11-C13	-5.88	1.41	1.51
37	n	617	IHT	C12-C15	-5.87	1.41	1.51
37	c	616	IHT	C12-C15	-5.85	1.41	1.51
38	k	612	KC2	C2A-C3A	5.85	1.49	1.37
36	a	315	II0	C21-C09	5.84	1.53	1.42
37	j	616	IHT	C22-C23	5.82	1.58	1.46
38	g	313	KC2	C2A-C3A	5.80	1.48	1.37
38	d	311	KC2	C2A-C3A	5.80	1.48	1.37
37	m	617	IHT	C12-C15	-5.78	1.42	1.51
36	f	615	II0	C11-C13	-5.75	1.42	1.51
37	b	616	IHT	C22-C23	5.75	1.58	1.46
36	f	616	II0	C11-C13	-5.74	1.42	1.51
37	m	617	IHT	C22-C23	5.74	1.58	1.46
36	e	614	II0	C27-C25	5.74	1.54	1.50
36	h	311	II0	C27-C25	5.74	1.54	1.50
37	O	204	IHT	C22-C23	5.73	1.58	1.46
38	i	310	KC2	C2A-C3A	5.72	1.48	1.37
36	n	615	II0	C11-C13	-5.70	1.42	1.51
37	O	204	IHT	C12-C15	-5.69	1.42	1.51
38	l	310	KC2	C2A-C3A	5.69	1.48	1.37
37	f	617	IHT	C12-C15	-5.67	1.42	1.51
37	g	319	IHT	C02-C07	-5.66	1.46	1.53
38	f	611	KC2	C2A-C3A	5.65	1.48	1.37
36	g	320	II0	C11-C13	-5.62	1.42	1.51
38	n	612	KC2	C2A-C3A	5.62	1.48	1.37
37	b	615	IHT	C22-C23	5.61	1.58	1.46
37	b	616	IHT	C12-C15	-5.61	1.42	1.51
36	i	313	II0	C11-C13	-5.60	1.42	1.51
36	b	613	II0	C11-C13	-5.59	1.42	1.51
38	g	314	KC2	C2A-C3A	5.59	1.48	1.37
38	g	312	KC2	C2A-C3A	5.58	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	310	KC2	C2A-C3A	5.58	1.48	1.37
36	h	310	II0	C11-C13	-5.58	1.42	1.51
36	j	615	II0	C11-C13	-5.57	1.42	1.51
36	k	617	II0	C11-C13	-5.57	1.42	1.51
38	k	612	KC2	CHD-C4C	5.56	1.49	1.38
37	R	204	IHT	C12-C15	-5.54	1.42	1.51
37	b	616	IHT	C34-C35	5.54	1.57	1.46
38	i	310	KC2	C3C-C2C	5.53	1.48	1.37
38	i	319	KC2	C2A-C3A	5.52	1.48	1.37
36	f	614	II0	C11-C13	-5.51	1.42	1.51
36	k	615	II0	C11-C13	-5.50	1.42	1.51
37	g	319	IHT	C12-C15	-5.49	1.42	1.51
36	l	313	II0	C11-C13	-5.47	1.42	1.51
36	J	104	II0	C11-C13	-5.47	1.42	1.51
36	c	614	II0	C11-C13	-5.46	1.42	1.51
37	f	617	IHT	C34-C35	5.46	1.57	1.46
36	n	614	II0	C11-C13	-5.46	1.42	1.51
36	h	311	II0	C11-C13	-5.45	1.42	1.51
38	k	611	KC2	C2A-C3A	5.45	1.48	1.37
36	i	314	II0	C11-C13	-5.42	1.42	1.51
38	c	610	KC2	C2A-C3A	5.42	1.48	1.37
36	m	618	II0	C11-C13	-5.42	1.42	1.51
38	e	609	KC2	C2A-C3A	5.41	1.48	1.37
38	k	613	KC2	C2A-C3A	5.41	1.48	1.37
37	a	317	IHT	C12-C15	-5.40	1.42	1.51
36	l	314	II0	C27-C25	5.39	1.54	1.50
36	m	614	II0	C11-C13	-5.37	1.42	1.51
38	k	613	KC2	CHD-C4C	5.36	1.49	1.38
38	g	312	KC2	CHD-C4C	5.36	1.49	1.38
36	m	615	II0	C11-C13	-5.36	1.42	1.51
37	O	204	IHT	C34-C35	5.36	1.57	1.46
36	c	613	II0	C11-C13	-5.36	1.42	1.51
38	s	201	KC2	CHD-C4C	5.36	1.49	1.38
37	g	319	IHT	C34-C35	5.35	1.57	1.46
36	d	315	II0	C11-C13	-5.34	1.42	1.51
36	k	621	II0	C11-C13	-5.34	1.42	1.51
37	n	617	IHT	C34-C35	5.34	1.57	1.46
38	g	314	KC2	C3C-C2C	5.32	1.48	1.37
36	a	315	II0	C11-C13	-5.32	1.42	1.51
38	d	310	KC2	CHD-C4C	5.32	1.49	1.38
36	l	312	II0	C11-C13	-5.32	1.42	1.51
36	a	318	II0	C11-C13	-5.30	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	j	611	KC2	C2A-C3A	5.29	1.47	1.37
37	c	616	IHT	C34-C35	5.29	1.57	1.46
37	m	617	IHT	C34-C35	5.29	1.57	1.46
37	b	615	IHT	C04-C02	5.28	1.66	1.54
36	d	313	II0	C11-C13	-5.27	1.42	1.51
36	a	316	II0	C11-C13	-5.27	1.42	1.51
38	s	204	KC2	CHD-C4C	5.27	1.49	1.38
36	h	312	II0	C11-C13	-5.27	1.42	1.51
38	d	311	KC2	C3C-C2C	5.26	1.47	1.37
37	a	317	IHT	C34-C35	5.26	1.57	1.46
37	j	616	IHT	C34-C35	5.26	1.57	1.46
38	d	310	KC2	C3C-C2C	5.25	1.47	1.37
38	k	611	KC2	C3C-C2C	5.25	1.47	1.37
36	i	313	II0	C27-C25	5.25	1.54	1.50
36	g	318	II0	C11-C13	-5.25	1.42	1.51
38	e	609	KC2	CHD-C4C	5.24	1.49	1.38
36	c	615	II0	C11-C13	-5.24	1.42	1.51
36	f	618	II0	C11-C13	-5.24	1.42	1.51
36	i	317	II0	C11-C13	-5.23	1.42	1.51
36	j	614	II0	C11-C13	-5.23	1.42	1.51
36	e	616	II0	C11-C13	-5.22	1.42	1.51
36	O	203	II0	C11-C13	-5.22	1.42	1.51
37	R	204	IHT	C34-C35	5.22	1.57	1.46
38	c	610	KC2	CHD-C4C	5.22	1.48	1.38
38	e	609	KC2	C3C-C2C	5.20	1.47	1.37
38	s	204	KC2	C2A-C3A	5.19	1.47	1.37
38	k	611	KC2	CHD-C4C	5.19	1.48	1.38
37	m	617	IHT	C04-C02	5.19	1.66	1.54
38	m	611	KC2	C2A-C3A	5.18	1.47	1.37
38	i	310	KC2	CHD-C4C	5.17	1.48	1.38
38	n	611	KC2	C2A-C3A	5.17	1.47	1.37
38	j	611	KC2	C3C-C2C	5.17	1.47	1.37
36	e	612	II0	C11-C13	-5.17	1.43	1.51
36	l	314	II0	C11-C13	-5.17	1.43	1.51
37	g	319	IHT	C04-C02	5.17	1.65	1.54
38	m	611	KC2	C3C-C2C	5.16	1.47	1.37
37	c	616	IHT	C04-C02	5.16	1.65	1.54
38	g	312	KC2	C3C-C2C	5.16	1.47	1.37
38	g	314	KC2	CHD-C4C	5.15	1.48	1.38
38	k	613	KC2	C3C-C2C	5.15	1.47	1.37
38	i	319	KC2	CHD-C4C	5.15	1.48	1.38
38	j	611	KC2	CHD-C4C	5.15	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	617	II0	C11-C13	-5.15	1.43	1.51
37	n	617	IHT	C04-C02	5.14	1.65	1.54
38	l	310	KC2	C3C-C2C	5.14	1.47	1.37
36	i	315	II0	C11-C13	-5.14	1.43	1.51
36	d	314	II0	C11-C13	-5.13	1.43	1.51
37	k	618	IHT	C04-C02	5.13	1.65	1.54
37	k	618	IHT	C34-C35	5.12	1.56	1.46
37	O	204	IHT	C04-C02	5.12	1.65	1.54
38	m	611	KC2	CHD-C4C	5.10	1.48	1.38
38	g	313	KC2	CHD-C4C	5.10	1.48	1.38
36	m	614	II0	C27-C25	5.10	1.54	1.50
36	m	616	II0	C11-C13	-5.09	1.43	1.51
38	k	611	KC2	C3B-C2B	5.09	1.47	1.37
38	g	313	KC2	C3B-C2B	5.09	1.47	1.37
38	n	612	KC2	CHD-C4C	5.09	1.48	1.38
37	f	617	IHT	C04-C02	5.09	1.65	1.54
38	n	611	KC2	C3C-C2C	5.08	1.47	1.37
38	d	311	KC2	C3B-C2B	5.08	1.47	1.37
38	f	611	KC2	CHD-C4C	5.07	1.48	1.38
38	f	611	KC2	C3B-C2B	5.07	1.47	1.37
36	l	316	II0	C11-C13	-5.07	1.43	1.51
38	n	612	KC2	C3B-C2B	5.06	1.47	1.37
38	i	319	KC2	C3C-C2C	5.06	1.47	1.37
38	s	201	KC2	C3C-C2C	5.05	1.47	1.37
38	f	611	KC2	C3C-C2C	5.05	1.47	1.37
38	m	611	KC2	C1A-NA	5.05	1.48	1.38
36	g	317	II0	C11-C13	-5.05	1.43	1.51
38	c	610	KC2	C3B-C2B	5.04	1.47	1.37
37	R	204	IHT	C04-C02	5.04	1.65	1.54
38	c	610	KC2	C3C-C2C	5.03	1.47	1.37
38	g	313	KC2	C3C-C2C	5.03	1.47	1.37
37	a	317	IHT	C04-C02	5.03	1.65	1.54
38	e	609	KC2	C3B-C2B	5.03	1.47	1.37
38	l	310	KC2	CHD-C4C	5.02	1.48	1.38
37	b	615	IHT	C34-C35	5.01	1.56	1.46
36	n	618	II0	C11-C13	-5.01	1.43	1.51
38	g	314	KC2	C3B-C2B	5.01	1.47	1.37
36	m	618	II0	C27-C25	4.99	1.54	1.50
38	n	611	KC2	CHD-C4C	4.98	1.48	1.38
37	j	616	IHT	C04-C02	4.98	1.65	1.54
37	b	616	IHT	C04-C02	4.98	1.65	1.54
38	d	310	KC2	C3B-C2B	4.97	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	n	611	KC2	C1A-NA	4.97	1.48	1.38
38	m	611	KC2	C3B-C2B	4.97	1.47	1.37
38	g	314	KC2	C1A-NA	4.96	1.48	1.38
38	k	613	KC2	C3B-C2B	4.95	1.47	1.37
36	n	616	II0	C11-C13	-4.94	1.43	1.51
38	s	204	KC2	C3B-C2B	4.93	1.47	1.37
38	i	319	KC2	C1A-NA	4.93	1.48	1.38
36	d	316	II0	C11-C13	-4.93	1.43	1.51
36	b	617	II0	C11-C13	-4.93	1.43	1.51
36	g	316	II0	C11-C13	-4.93	1.43	1.51
38	k	612	KC2	C3C-C2C	4.92	1.47	1.37
36	k	619	II0	C11-C13	-4.92	1.43	1.51
38	s	204	KC2	C3C-C2C	4.90	1.47	1.37
38	k	612	KC2	C3B-C2B	4.90	1.47	1.37
38	d	311	KC2	CHD-C4C	4.90	1.48	1.38
38	l	310	KC2	C3B-C2B	4.90	1.47	1.37
38	j	611	KC2	C3B-C2B	4.90	1.47	1.37
38	l	310	KC2	C1A-NA	4.90	1.48	1.38
36	e	614	II0	C11-C13	-4.89	1.43	1.51
38	e	609	KC2	C1A-NA	4.88	1.48	1.38
38	k	613	KC2	C1A-NA	4.88	1.48	1.38
38	d	311	KC2	C1A-NA	4.87	1.48	1.38
38	f	611	KC2	C1A-NA	4.83	1.48	1.38
38	i	310	KC2	C1A-NA	4.83	1.48	1.38
38	n	611	KC2	C3B-C2B	4.83	1.47	1.37
38	i	310	KC2	C3B-C2B	4.83	1.47	1.37
38	j	611	KC2	C1A-NA	4.82	1.48	1.38
38	g	312	KC2	C3B-C2B	4.81	1.46	1.37
38	n	612	KC2	C1A-NA	4.80	1.48	1.38
38	g	313	KC2	C1A-NA	4.79	1.48	1.38
38	c	610	KC2	C1A-NA	4.79	1.48	1.38
36	i	320	II0	C11-C13	-4.79	1.43	1.51
38	k	611	KC2	C1A-NA	4.79	1.48	1.38
38	k	612	KC2	C1A-NA	4.79	1.48	1.38
38	s	204	KC2	C1A-NA	4.77	1.47	1.38
37	R	204	IHT	C06-C09	4.77	1.67	1.52
38	d	310	KC2	C1A-NA	4.76	1.47	1.38
38	n	612	KC2	C3C-C2C	4.76	1.46	1.37
36	n	616	II0	C27-C25	4.75	1.54	1.50
36	b	613	II0	C27-C25	4.75	1.54	1.50
38	s	201	KC2	C2A-C3A	4.74	1.46	1.37
37	n	617	IHT	C06-C09	4.73	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	611	KC2	O2D-CGD	4.73	1.44	1.33
38	i	319	KC2	C3B-C2B	4.72	1.46	1.37
37	a	317	IHT	C06-C09	4.72	1.67	1.52
37	m	617	IHT	C06-C09	4.70	1.67	1.52
37	f	617	IHT	C06-C09	4.69	1.67	1.52
36	d	316	II0	C31-C29	4.69	1.57	1.43
35	c	619	LMG	O7-C10	4.69	1.47	1.34
37	g	319	IHT	C30-C27	4.68	1.57	1.43
37	a	317	IHT	C30-C27	4.67	1.57	1.43
37	c	616	IHT	C06-C09	4.67	1.67	1.52
36	i	320	II0	C27-C25	4.67	1.54	1.50
38	g	312	KC2	C1A-NA	4.67	1.47	1.38
36	d	313	II0	C27-C25	4.67	1.54	1.50
37	j	616	IHT	C06-C09	4.66	1.67	1.52
37	O	204	IHT	C06-C09	4.66	1.67	1.52
36	d	315	II0	C42-C40	4.66	1.57	1.43
36	d	314	II0	C27-C25	4.64	1.54	1.50
36	a	318	II0	C42-C40	4.63	1.57	1.43
28	d	305	CLA	C4B-NB	4.63	1.43	1.37
36	d	315	II0	C27-C25	4.63	1.54	1.50
38	g	312	KC2	O2D-CGD	4.63	1.44	1.33
36	i	314	II0	C27-C25	4.62	1.54	1.50
38	e	609	KC2	O2D-CGD	4.61	1.44	1.33
36	g	317	II0	C27-C25	4.61	1.54	1.50
36	m	618	II0	C31-C29	4.60	1.57	1.43
37	k	618	IHT	C06-C09	4.60	1.66	1.52
37	b	616	IHT	C06-C09	4.59	1.66	1.52
36	k	617	II0	C27-C25	4.59	1.53	1.50
37	c	616	IHT	C30-C27	4.58	1.57	1.43
38	s	201	KC2	C3B-C2B	4.58	1.46	1.37
36	e	612	II0	C27-C25	4.57	1.53	1.50
37	f	617	IHT	C30-C27	4.56	1.57	1.43
38	g	314	KC2	O2D-CGD	4.56	1.44	1.33
30	k	620	LHG	O7-C7	4.56	1.47	1.34
37	b	615	IHT	C06-C09	4.55	1.66	1.52
38	k	613	KC2	O2D-CGD	4.55	1.44	1.33
37	n	617	IHT	C30-C27	4.55	1.57	1.43
38	i	319	KC2	O2D-CGD	4.55	1.44	1.33
38	i	310	KC2	O2D-CGD	4.54	1.44	1.33
36	n	616	II0	C31-C29	4.54	1.57	1.43
38	d	310	KC2	O2D-CGD	4.54	1.44	1.33
38	m	611	KC2	O2D-CGD	4.54	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	612	KC2	O2D-CGD	4.53	1.44	1.33
37	k	618	IHT	C30-C27	4.53	1.57	1.43
36	k	616	II0	C27-C25	4.52	1.53	1.50
29	A	842	PQN	C10-C1	4.52	1.56	1.48
38	n	612	KC2	O2D-CGD	4.52	1.44	1.33
36	n	618	II0	C27-C25	4.51	1.53	1.50
38	d	311	KC2	O2D-CGD	4.51	1.44	1.33
38	j	611	KC2	O2D-CGD	4.51	1.44	1.33
36	e	612	II0	C31-C29	4.51	1.57	1.43
36	c	614	II0	C27-C25	4.50	1.53	1.50
37	b	616	IHT	C30-C27	4.50	1.57	1.43
30	i	318	LHG	O8-C23	4.49	1.46	1.33
36	d	315	II0	C32-C30	4.49	1.57	1.43
36	i	317	II0	C31-C29	4.49	1.57	1.43
37	j	616	IHT	C30-C27	4.49	1.57	1.43
38	n	611	KC2	O2D-CGD	4.48	1.44	1.33
37	R	204	IHT	C30-C27	4.46	1.57	1.43
36	k	619	II0	C06-C04	4.46	1.68	1.54
38	l	310	KC2	O2D-CGD	4.46	1.44	1.33
36	d	316	II0	C42-C40	4.46	1.57	1.43
30	k	620	LHG	O8-C23	4.45	1.46	1.33
36	d	314	II0	C42-C40	4.45	1.57	1.43
36	f	614	II0	C27-C25	4.45	1.53	1.50
36	O	203	II0	C27-C25	4.45	1.53	1.50
30	g	301	LHG	O7-C7	4.44	1.46	1.34
30	d	317	LHG	O7-C7	4.44	1.46	1.34
37	g	319	IHT	C06-C09	4.44	1.66	1.52
36	b	614	II0	C27-C25	4.43	1.53	1.50
37	O	204	IHT	C30-C27	4.42	1.56	1.43
38	s	201	KC2	C1A-NA	4.42	1.47	1.38
36	k	619	II0	C31-C29	4.42	1.56	1.43
37	m	617	IHT	C30-C27	4.41	1.56	1.43
36	l	316	II0	C42-C40	4.41	1.56	1.43
36	i	317	II0	C32-C30	4.40	1.56	1.43
36	e	612	II0	C32-C30	4.40	1.56	1.43
36	c	615	II0	C06-C04	4.39	1.68	1.54
36	g	320	II0	C32-C30	4.39	1.56	1.43
36	i	317	II0	C42-C40	4.39	1.56	1.43
36	j	615	II0	C27-C25	4.39	1.53	1.50
36	d	314	II0	C32-C30	4.39	1.56	1.43
38	f	611	KC2	O2D-CGD	4.38	1.44	1.33
36	l	316	II0	C31-C29	4.37	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	c	610	KC2	O2D-CGD	4.37	1.44	1.33
30	c	618	LHG	O8-C23	4.37	1.46	1.33
34	B	843	DGD	O2G-C1B	4.37	1.46	1.34
36	a	316	II0	C27-C25	4.37	1.53	1.50
36	i	320	II0	C42-C40	4.36	1.56	1.43
36	j	614	II0	C06-C04	4.36	1.67	1.54
36	c	613	II0	C27-C25	4.36	1.53	1.50
30	e	617	LHG	O7-C7	4.35	1.46	1.34
36	h	310	II0	C42-C40	4.35	1.56	1.43
36	c	617	II0	C06-C04	4.35	1.67	1.54
36	e	613	II0	C27-C25	4.34	1.53	1.50
36	n	614	II0	C32-C30	4.34	1.56	1.43
36	a	318	II0	C31-C29	4.34	1.56	1.43
38	d	311	KC2	CBC-CAC	4.34	1.51	1.30
36	n	614	II0	C42-C40	4.33	1.56	1.43
36	m	615	II0	C12-C14	-4.33	1.44	1.51
30	A	843	LHG	O8-C23	4.33	1.46	1.33
36	g	316	II0	C27-C25	4.33	1.53	1.50
35	Q	301	LMG	O7-C10	4.32	1.46	1.34
37	b	615	IHT	C30-C27	4.32	1.56	1.43
36	f	616	II0	C27-C25	4.32	1.53	1.50
38	g	313	KC2	O2D-CGD	4.32	1.43	1.33
36	d	315	II0	C31-C29	4.32	1.56	1.43
36	k	615	II0	C42-C40	4.32	1.56	1.43
36	k	615	II0	C27-C25	4.32	1.53	1.50
36	n	618	II0	C31-C29	4.31	1.56	1.43
35	F	205	LMG	O8-C28	4.31	1.45	1.33
36	a	318	II0	C32-C30	4.31	1.56	1.43
36	n	614	II0	C31-C29	4.31	1.56	1.43
36	d	313	II0	C32-C30	4.31	1.56	1.43
36	c	617	II0	C31-C29	4.31	1.56	1.43
36	e	616	II0	C31-C29	4.31	1.56	1.43
36	k	615	II0	C32-C30	4.30	1.56	1.43
36	l	316	II0	C32-C30	4.30	1.56	1.43
36	a	318	II0	C06-C04	4.30	1.67	1.54
36	d	314	II0	C06-C04	4.29	1.67	1.54
36	b	617	II0	C06-C04	4.29	1.67	1.54
36	e	616	II0	C42-C40	4.29	1.56	1.43
36	f	615	II0	C27-C25	4.28	1.53	1.50
38	i	319	KC2	CBC-CAC	4.28	1.51	1.30
36	e	616	II0	C06-C04	4.28	1.67	1.54
36	d	316	II0	C32-C30	4.28	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	842	PQN	C5-C4	4.27	1.56	1.48
30	L	208	LHG	O8-C23	4.27	1.45	1.33
30	d	317	LHG	O8-C23	4.27	1.45	1.33
36	g	318	II0	C27-C25	4.27	1.53	1.50
28	d	305	CLA	C1D-ND	4.26	1.43	1.37
38	g	312	KC2	CBC-CAC	4.26	1.50	1.30
36	f	616	II0	C42-C40	4.26	1.56	1.43
36	e	616	II0	C32-C30	4.26	1.56	1.43
36	k	617	II0	C32-C30	4.26	1.56	1.43
36	n	615	II0	C06-C04	4.26	1.67	1.54
36	d	316	II0	C06-C04	4.26	1.67	1.54
30	J	106	LHG	O8-C23	4.26	1.45	1.33
36	e	614	II0	C06-C04	4.26	1.67	1.54
36	c	615	II0	C27-C25	4.25	1.53	1.50
36	c	615	II0	C31-C29	4.25	1.56	1.43
38	f	611	KC2	CBC-CAC	4.25	1.50	1.30
38	k	613	KC2	CBC-CAC	4.25	1.50	1.30
36	n	616	II0	C42-C40	4.25	1.56	1.43
35	b	621	LMG	O7-C10	4.24	1.46	1.34
36	m	615	II0	C31-C29	4.24	1.56	1.43
36	e	614	II0	C32-C30	4.24	1.56	1.43
38	s	204	KC2	CHD-C1D	4.24	1.48	1.39
38	s	201	KC2	O2D-CGD	4.24	1.43	1.33
36	l	316	II0	C06-C04	4.24	1.67	1.54
38	i	310	KC2	CHC-C4B	4.24	1.46	1.38
36	c	615	II0	C42-C40	4.24	1.56	1.43
36	n	614	II0	C06-C04	4.24	1.67	1.54
36	f	616	II0	C06-C04	4.23	1.67	1.54
35	n	620	LMG	O8-C28	4.23	1.45	1.33
36	l	314	II0	C06-C04	4.23	1.67	1.54
36	i	317	II0	C06-C04	4.23	1.67	1.54
36	k	621	II0	C27-C25	4.23	1.53	1.50
38	k	613	KC2	CHB-C1B	4.23	1.46	1.38
36	k	619	II0	C27-C25	4.23	1.53	1.50
38	k	611	KC2	CBC-CAC	4.23	1.50	1.30
36	i	320	II0	C31-C29	4.23	1.56	1.43
36	i	315	II0	C42-C40	4.23	1.56	1.43
38	d	311	KC2	OBD-CAD	4.22	1.29	1.22
34	B	843	DGD	O1G-C1A	4.22	1.45	1.33
36	d	313	II0	C42-C40	4.22	1.56	1.43
30	j	617	LHG	O8-C23	4.22	1.45	1.33
36	d	314	II0	C31-C29	4.22	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	f	614	II0	C06-C04	4.22	1.67	1.54
38	e	609	KC2	CBC-CAC	4.22	1.50	1.30
38	d	311	KC2	CHB-C1B	4.22	1.46	1.38
36	d	313	II0	C31-C29	4.22	1.56	1.43
36	l	313	II0	C31-C29	4.21	1.56	1.43
36	f	618	II0	C31-C29	4.21	1.56	1.43
38	i	310	KC2	CBC-CAC	4.21	1.50	1.30
30	g	321	LHG	O7-C7	4.21	1.46	1.34
36	J	104	II0	C42-C40	4.21	1.56	1.43
36	f	618	II0	C06-C04	4.21	1.67	1.54
36	g	317	II0	C32-C30	4.21	1.56	1.43
36	m	614	II0	C42-C40	4.21	1.56	1.43
36	a	314	II0	C27-C25	4.20	1.53	1.50
30	m	619	LHG	O7-C7	4.20	1.46	1.34
36	f	614	II0	C42-C40	4.20	1.56	1.43
38	n	612	KC2	CHB-C1B	4.20	1.46	1.38
36	i	315	II0	C06-C04	4.20	1.67	1.54
36	g	316	II0	C31-C29	4.20	1.56	1.43
35	O	205	LMG	O8-C28	4.20	1.45	1.33
38	g	313	KC2	CBC-CAC	4.20	1.50	1.30
36	h	311	II0	C42-C40	4.20	1.56	1.43
36	n	615	II0	C31-C29	4.20	1.56	1.43
38	d	310	KC2	CBC-CAC	4.19	1.50	1.30
30	i	318	LHG	O7-C7	4.19	1.46	1.34
38	g	314	KC2	CBC-CAC	4.18	1.50	1.30
30	c	620	LHG	O8-C23	4.18	1.45	1.33
36	e	612	II0	C42-C40	4.18	1.56	1.43
38	s	201	KC2	CBC-CAC	4.18	1.50	1.30
38	s	204	KC2	CBC-CAC	4.18	1.50	1.30
36	O	203	II0	C42-C40	4.18	1.56	1.43
36	n	618	II0	C32-C30	4.17	1.56	1.43
38	n	611	KC2	OBD-CAD	4.17	1.29	1.22
36	c	615	II0	C32-C30	4.17	1.56	1.43
38	i	310	KC2	CHB-C1B	4.17	1.46	1.38
36	l	313	II0	C32-C30	4.17	1.56	1.43
36	f	618	II0	C32-C30	4.17	1.56	1.43
38	i	319	KC2	OBD-CAD	4.17	1.29	1.22
38	n	611	KC2	CBC-CAC	4.17	1.50	1.30
38	k	612	KC2	CBC-CAC	4.16	1.50	1.30
38	n	612	KC2	OBD-CAD	4.16	1.29	1.22
36	d	313	II0	C06-C04	4.16	1.67	1.54
36	h	312	II0	C06-C04	4.16	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	m	611	KC2	CBC-CAC	4.16	1.50	1.30
36	g	318	II0	C06-C04	4.16	1.67	1.54
30	A	849	LHG	O8-C23	4.16	1.45	1.33
38	s	204	KC2	O2D-CGD	4.16	1.43	1.33
36	k	617	II0	C06-C04	4.16	1.67	1.54
36	k	617	II0	C31-C29	4.16	1.56	1.43
38	k	613	KC2	OBD-CAD	4.16	1.29	1.22
36	g	318	II0	C31-C29	4.15	1.56	1.43
30	n	619	LHG	O8-C23	4.15	1.45	1.33
36	n	615	II0	C42-C40	4.15	1.56	1.43
36	i	315	II0	C32-C30	4.15	1.56	1.43
30	a	301	LHG	O7-C7	4.15	1.46	1.34
37	b	615	IHT	C09-C10	-4.15	1.43	1.51
36	b	614	II0	C31-C29	4.15	1.56	1.43
36	m	616	II0	C06-C04	4.15	1.67	1.54
38	f	611	KC2	CHB-C1B	4.14	1.46	1.38
36	b	614	II0	C42-C40	4.14	1.56	1.43
36	a	318	II0	C41-C39	4.14	1.56	1.43
36	l	314	II0	C42-C40	4.14	1.56	1.43
36	k	621	II0	C42-C40	4.14	1.56	1.43
30	c	618	LHG	O7-C7	4.14	1.46	1.34
37	g	319	IHT	C09-C10	-4.14	1.43	1.51
36	k	619	II0	C42-C40	4.14	1.56	1.43
38	j	611	KC2	CBC-CAC	4.14	1.50	1.30
36	h	311	II0	C06-C04	4.13	1.67	1.54
36	e	614	II0	C42-C40	4.13	1.56	1.43
28	j	612	CLA	C1D-ND	4.13	1.43	1.37
38	i	310	KC2	CHD-C1D	4.13	1.48	1.39
36	l	312	II0	C42-C40	4.13	1.56	1.43
38	j	611	KC2	OBD-CAD	4.13	1.29	1.22
36	e	613	II0	C31-C29	4.13	1.56	1.43
36	i	314	II0	C31-C29	4.13	1.56	1.43
30	g	301	LHG	O8-C23	4.12	1.45	1.33
36	g	318	II0	C32-C30	4.12	1.56	1.43
36	h	312	II0	C31-C29	4.12	1.56	1.43
38	g	312	KC2	OBD-CAD	4.12	1.29	1.22
36	g	318	II0	C42-C40	4.12	1.56	1.43
36	f	618	II0	C42-C40	4.12	1.56	1.43
36	l	312	II0	C31-C29	4.12	1.56	1.43
36	k	617	II0	C42-C40	4.12	1.55	1.43
30	e	617	LHG	O8-C23	4.12	1.45	1.33
30	j	617	LHG	O7-C7	4.12	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	844	LHG	O8-C23	4.11	1.45	1.33
36	d	316	II0	C41-C39	4.11	1.55	1.43
36	n	618	II0	C06-C04	4.11	1.67	1.54
38	l	310	KC2	CBC-CAC	4.11	1.50	1.30
36	g	316	II0	C06-C04	4.11	1.67	1.54
38	g	313	KC2	CHB-C1B	4.11	1.46	1.38
36	g	316	II0	C32-C30	4.11	1.55	1.43
36	d	315	II0	C06-C04	4.11	1.67	1.54
36	g	317	II0	C42-C40	4.11	1.55	1.43
36	l	314	II0	C31-C29	4.11	1.55	1.43
36	m	616	II0	C32-C30	4.11	1.55	1.43
36	f	614	II0	C31-C29	4.11	1.55	1.43
36	h	311	II0	C31-C29	4.10	1.55	1.43
38	g	314	KC2	CHB-C1B	4.10	1.46	1.38
37	m	617	IHT	C09-C10	-4.10	1.43	1.51
36	l	312	II0	C32-C30	4.10	1.55	1.43
38	n	612	KC2	CBC-CAC	4.10	1.50	1.30
36	m	614	II0	C32-C30	4.10	1.55	1.43
36	k	621	II0	C06-C04	4.10	1.67	1.54
30	L	208	LHG	O7-C7	4.10	1.45	1.34
36	k	619	II0	C32-C30	4.10	1.55	1.43
29	B	842	PQN	C10-C1	4.09	1.56	1.48
36	m	618	II0	C42-C40	4.09	1.55	1.43
36	j	614	II0	C27-C25	4.09	1.53	1.50
30	f	619	LHG	O8-C23	4.09	1.45	1.33
36	l	314	II0	C32-C30	4.08	1.55	1.43
36	b	614	II0	C06-C04	4.08	1.67	1.54
36	g	320	II0	C06-C04	4.08	1.67	1.54
37	c	616	IHT	C09-C10	-4.08	1.43	1.51
36	c	613	II0	C06-C04	4.08	1.67	1.54
36	d	315	II0	C41-C39	4.08	1.55	1.43
36	k	616	II0	C31-C29	4.08	1.55	1.43
36	i	315	II0	C31-C29	4.08	1.55	1.43
36	i	313	II0	C06-C04	4.08	1.67	1.54
30	l	317	LHG	O8-C23	4.08	1.45	1.33
38	k	612	KC2	OBD-CAD	4.08	1.29	1.22
30	m	619	LHG	O8-C23	4.07	1.45	1.33
36	n	616	II0	C32-C30	4.07	1.55	1.43
38	d	310	KC2	OBD-CAD	4.07	1.29	1.22
38	k	612	KC2	CHB-C1B	4.07	1.46	1.38
35	J	105	LMG	O8-C28	4.07	1.45	1.33
36	m	615	II0	C06-C04	4.07	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e	613	II0	C42-C40	4.07	1.55	1.43
35	F	205	LMG	O7-C10	4.07	1.45	1.34
30	n	619	LHG	O7-C7	4.06	1.45	1.34
38	k	611	KC2	OBD-CAD	4.06	1.29	1.22
36	j	614	II0	C42-C40	4.06	1.55	1.43
30	A	844	LHG	O7-C7	4.06	1.45	1.34
36	f	614	II0	C32-C30	4.06	1.55	1.43
36	i	314	II0	C32-C30	4.06	1.55	1.43
30	l	317	LHG	O7-C7	4.06	1.45	1.34
36	g	317	II0	C06-C04	4.05	1.67	1.54
38	g	312	KC2	CHB-C1B	4.05	1.46	1.38
37	m	617	IHT	C05-C03	4.05	1.67	1.54
36	i	314	II0	C42-C40	4.05	1.55	1.43
36	c	617	II0	C42-C40	4.05	1.55	1.43
36	j	614	II0	C31-C29	4.05	1.55	1.43
36	n	618	II0	C42-C40	4.05	1.55	1.43
36	n	615	II0	C32-C30	4.04	1.55	1.43
35	O	205	LMG	O7-C10	4.04	1.45	1.34
36	n	614	II0	C27-C25	4.04	1.53	1.50
30	b	620	LHG	O8-C23	4.04	1.45	1.33
36	h	312	II0	C27-C25	4.04	1.53	1.50
36	g	320	II0	C31-C29	4.04	1.55	1.43
36	b	613	II0	C06-C04	4.04	1.66	1.54
36	b	617	II0	C31-C29	4.04	1.55	1.43
30	A	843	LHG	O7-C7	4.04	1.45	1.34
38	d	310	KC2	CHD-C1D	4.03	1.48	1.39
36	J	104	II0	C31-C29	4.03	1.55	1.43
36	k	621	II0	C32-C30	4.03	1.55	1.43
36	n	616	II0	C06-C04	4.03	1.66	1.54
36	O	203	II0	C06-C04	4.03	1.66	1.54
38	c	610	KC2	CBC-CAC	4.03	1.49	1.30
37	k	618	IHT	C05-C03	4.03	1.66	1.54
36	k	616	II0	C42-C40	4.03	1.55	1.43
36	h	310	II0	C31-C29	4.03	1.55	1.43
36	a	314	II0	C06-C04	4.03	1.66	1.54
37	b	616	IHT	C09-C10	-4.03	1.43	1.51
38	g	312	KC2	CHD-C1D	4.02	1.48	1.39
36	f	616	II0	C31-C29	4.02	1.55	1.43
30	a	319	LHG	O8-C23	4.02	1.45	1.33
36	i	313	II0	C42-C40	4.02	1.55	1.43
36	g	320	II0	C42-C40	4.02	1.55	1.43
37	k	618	IHT	C09-C10	-4.02	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	617	IHT	C05-C03	4.02	1.66	1.54
38	g	314	KC2	OBD-CAD	4.02	1.29	1.22
36	n	616	II0	C41-C39	4.02	1.55	1.43
36	c	613	II0	C32-C30	4.01	1.55	1.43
38	s	204	KC2	OBD-CAD	4.01	1.29	1.22
36	i	314	II0	C12-C14	-4.01	1.44	1.51
37	b	616	IHT	C41-C38	4.01	1.55	1.43
36	c	613	II0	C31-C29	4.01	1.55	1.43
36	c	614	II0	C31-C29	4.01	1.55	1.43
36	h	312	II0	C42-C40	4.01	1.55	1.43
37	O	204	IHT	C09-C10	-4.01	1.43	1.51
36	h	311	II0	C32-C30	4.00	1.55	1.43
36	f	616	II0	C32-C30	4.00	1.55	1.43
36	g	316	II0	C42-C40	4.00	1.55	1.43
37	j	616	IHT	C05-C03	4.00	1.66	1.54
36	e	614	II0	C31-C29	4.00	1.55	1.43
30	a	301	LHG	O8-C23	4.00	1.45	1.33
35	b	621	LMG	O8-C28	4.00	1.45	1.33
38	k	612	KC2	CHD-C1D	4.00	1.48	1.39
36	m	616	II0	C42-C40	4.00	1.55	1.43
37	O	204	IHT	C05-C03	4.00	1.66	1.54
38	e	609	KC2	CHB-C1B	4.00	1.46	1.38
36	O	203	II0	C32-C30	4.00	1.55	1.43
38	d	310	KC2	CHB-C1B	4.00	1.46	1.38
36	l	312	II0	C06-C04	4.00	1.66	1.54
36	i	317	II0	C41-C39	3.99	1.55	1.43
37	c	616	IHT	C05-C03	3.99	1.66	1.54
36	k	616	II0	C32-C30	3.99	1.55	1.43
36	n	615	II0	C27-C25	3.99	1.53	1.50
38	n	612	KC2	CHC-C4B	3.99	1.46	1.38
38	g	312	KC2	CHC-C4B	3.99	1.46	1.38
38	k	611	KC2	CHB-C1B	3.99	1.46	1.38
36	a	314	II0	C31-C29	3.99	1.55	1.43
37	g	319	IHT	C41-C38	3.98	1.55	1.43
37	b	615	IHT	C05-C03	3.98	1.66	1.54
38	k	611	KC2	CHC-C4B	3.98	1.46	1.38
30	g	321	LHG	O8-C23	3.98	1.45	1.33
36	m	616	II0	C31-C29	3.98	1.55	1.43
36	b	613	II0	C31-C29	3.98	1.55	1.43
38	k	613	KC2	CHC-C4B	3.98	1.46	1.38
37	f	617	IHT	C41-C38	3.98	1.55	1.43
38	c	610	KC2	OBD-CAD	3.98	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	104	II0	C32-C30	3.98	1.55	1.43
36	k	615	II0	C31-C29	3.98	1.55	1.43
35	c	619	LMG	O8-C28	3.97	1.44	1.33
36	k	621	II0	C31-C29	3.97	1.55	1.43
38	n	611	KC2	CHC-C4B	3.97	1.46	1.38
37	j	616	IHT	C09-C10	-3.97	1.43	1.51
36	g	317	II0	C31-C29	3.97	1.55	1.43
36	a	316	II0	C32-C30	3.97	1.55	1.43
38	c	610	KC2	CHB-C1B	3.97	1.46	1.38
36	i	320	II0	C41-C39	3.96	1.55	1.43
36	m	614	II0	C31-C29	3.96	1.55	1.43
36	b	613	II0	C32-C30	3.96	1.55	1.43
36	e	612	II0	C06-C04	3.96	1.66	1.54
38	g	314	KC2	CHC-C4B	3.96	1.46	1.38
36	l	312	II0	C27-C25	3.96	1.53	1.50
36	b	613	II0	C42-C40	3.96	1.55	1.43
38	m	611	KC2	OBD-CAD	3.95	1.29	1.22
36	h	312	II0	C12-C14	-3.95	1.44	1.51
37	n	617	IHT	C09-C10	-3.95	1.43	1.51
36	O	203	II0	C31-C29	3.95	1.55	1.43
37	a	317	IHT	C05-C03	3.95	1.66	1.54
38	i	310	KC2	OBD-CAD	3.95	1.29	1.22
38	s	201	KC2	CHD-C1D	3.95	1.48	1.39
38	i	319	KC2	CHD-C1D	3.95	1.48	1.39
37	g	319	IHT	C05-C03	3.94	1.66	1.54
36	e	613	II0	C32-C30	3.94	1.55	1.43
36	c	617	II0	C32-C30	3.94	1.55	1.43
38	s	201	KC2	CHC-C4B	3.94	1.46	1.38
38	k	613	KC2	CHD-C1D	3.94	1.48	1.39
37	R	204	IHT	C05-C03	3.94	1.66	1.54
36	d	315	II0	C34-C36	3.94	1.54	1.46
36	d	314	II0	C41-C39	3.94	1.55	1.43
38	g	313	KC2	CHC-C4B	3.94	1.46	1.38
37	a	317	IHT	C09-C10	-3.94	1.43	1.51
36	e	613	II0	C06-C04	3.93	1.66	1.54
36	h	312	II0	C32-C30	3.93	1.55	1.43
36	k	616	II0	C06-C04	3.93	1.66	1.54
36	a	316	II0	C06-C04	3.93	1.66	1.54
36	b	617	II0	C12-C14	-3.93	1.44	1.51
36	f	615	II0	C31-C29	3.93	1.55	1.43
38	e	609	KC2	OBD-CAD	3.93	1.29	1.22
36	m	614	II0	C41-C39	3.93	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	m	618	II0	C32-C30	3.92	1.55	1.43
37	f	617	IHT	C09-C10	-3.92	1.43	1.51
36	i	313	II0	C32-C30	3.92	1.55	1.43
38	s	204	KC2	CHC-C4B	3.92	1.46	1.38
30	c	620	LHG	O7-C7	3.92	1.45	1.34
36	i	313	II0	C31-C29	3.92	1.55	1.43
38	e	609	KC2	CHC-C4B	3.92	1.46	1.38
37	b	616	IHT	C05-C03	3.91	1.66	1.54
36	l	313	II0	C42-C40	3.91	1.55	1.43
36	a	316	II0	C31-C29	3.91	1.55	1.43
36	a	315	II0	C27-C25	3.91	1.53	1.50
38	d	310	KC2	CHC-C4B	3.90	1.46	1.38
38	j	611	KC2	CHB-C1B	3.90	1.46	1.38
31	J	101	WVN	C31-C32	3.90	1.54	1.46
36	b	617	II0	C42-C40	3.90	1.55	1.43
36	l	316	II0	C41-C39	3.90	1.55	1.43
36	i	320	II0	C32-C30	3.90	1.55	1.43
30	a	319	LHG	O7-C7	3.89	1.45	1.34
30	J	106	LHG	O7-C7	3.89	1.45	1.34
37	c	616	IHT	C41-C38	3.89	1.55	1.43
38	c	610	KC2	CHC-C4B	3.89	1.46	1.38
30	f	619	LHG	O7-C7	3.89	1.45	1.34
36	a	315	II0	C06-C04	3.89	1.66	1.54
36	k	615	II0	C06-C04	3.89	1.66	1.54
28	c	611	CLA	C4B-NB	3.89	1.43	1.37
36	a	314	II0	C32-C30	3.89	1.55	1.43
36	j	615	II0	C42-C40	3.89	1.55	1.43
36	J	104	II0	C06-C04	3.89	1.66	1.54
37	R	204	IHT	C09-C10	-3.89	1.43	1.51
36	i	320	II0	C12-C14	-3.89	1.45	1.51
38	n	611	KC2	CHB-C1B	3.89	1.46	1.38
36	h	310	II0	C41-C39	3.89	1.55	1.43
38	g	313	KC2	OBD-CAD	3.88	1.29	1.22
38	s	204	KC2	CHB-C1B	3.88	1.46	1.38
35	n	620	LMG	O7-C10	3.88	1.45	1.34
36	m	615	II0	C42-C40	3.88	1.55	1.43
37	a	317	IHT	C41-C38	3.88	1.55	1.43
36	c	614	II0	C42-C40	3.88	1.55	1.43
36	e	612	II0	C41-C39	3.88	1.55	1.43
36	j	615	II0	C31-C29	3.87	1.55	1.43
36	b	614	II0	C32-C30	3.87	1.55	1.43
38	g	314	KC2	CHD-C1D	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	m	614	II0	C06-C04	3.87	1.66	1.54
36	e	616	II0	C41-C39	3.87	1.55	1.43
36	b	617	II0	C32-C30	3.87	1.55	1.43
36	a	316	II0	C42-C40	3.87	1.55	1.43
30	A	849	LHG	O7-C7	3.87	1.45	1.34
36	l	313	II0	C41-C39	3.86	1.55	1.43
36	f	618	II0	C41-C39	3.86	1.55	1.43
36	h	310	II0	C27-C25	3.86	1.53	1.50
38	e	609	KC2	CHD-C1D	3.86	1.48	1.39
37	m	617	IHT	C41-C38	3.86	1.55	1.43
36	c	613	II0	C12-C14	-3.86	1.45	1.51
38	c	610	KC2	CHD-C1D	3.86	1.48	1.39
36	c	613	II0	C42-C40	3.86	1.55	1.43
36	h	311	II0	C41-C39	3.86	1.55	1.43
36	n	615	II0	C41-C39	3.86	1.55	1.43
38	l	310	KC2	CHB-C1B	3.86	1.45	1.38
28	f	608	CLA	C1D-ND	3.86	1.42	1.37
36	f	614	II0	C41-C39	3.85	1.55	1.43
38	s	201	KC2	OBD-CAD	3.85	1.29	1.22
36	k	615	II0	C41-C39	3.85	1.55	1.43
37	k	618	IHT	C41-C38	3.85	1.55	1.43
36	l	313	II0	C34-C36	3.85	1.54	1.46
28	j	612	CLA	C4B-NB	3.85	1.42	1.37
36	d	313	II0	C05-C03	3.84	1.66	1.54
36	g	320	II0	C27-C25	3.84	1.53	1.50
38	i	319	KC2	CHB-C1B	3.84	1.45	1.38
37	O	204	IHT	C41-C38	3.84	1.55	1.43
36	g	318	II0	C41-C39	3.84	1.55	1.43
37	j	616	IHT	C41-C38	3.84	1.55	1.43
36	h	310	II0	C34-C36	3.83	1.54	1.46
36	i	315	II0	C41-C39	3.83	1.55	1.43
37	f	617	IHT	C05-C03	3.83	1.66	1.54
37	g	319	IHT	C40-C37	3.83	1.55	1.43
35	L	209	LMG	O7-C10	3.82	1.45	1.34
36	n	618	II0	C41-C39	3.82	1.55	1.43
30	b	620	LHG	O7-C7	3.82	1.45	1.34
36	f	615	II0	C42-C40	3.82	1.55	1.43
38	g	313	KC2	CHD-C1D	3.82	1.48	1.39
36	i	315	II0	C27-C25	3.82	1.53	1.50
28	c	611	CLA	C1D-ND	3.82	1.42	1.37
36	i	314	II0	C06-C04	3.82	1.66	1.54
36	l	313	II0	C06-C04	3.82	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	315	II0	C05-C03	3.82	1.66	1.54
36	d	313	II0	C41-C39	3.81	1.55	1.43
30	b	619	LHG	O8-C23	3.81	1.44	1.33
36	b	613	II0	C05-C03	3.81	1.66	1.54
38	m	611	KC2	CHB-C1B	3.81	1.45	1.38
36	d	314	II0	C34-C36	3.81	1.54	1.46
38	j	611	KC2	CHC-C4B	3.81	1.45	1.38
38	m	611	KC2	CHD-C1D	3.81	1.48	1.39
38	l	310	KC2	OBD-CAD	3.81	1.29	1.22
38	f	611	KC2	OBD-CAD	3.81	1.29	1.22
37	R	204	IHT	C41-C38	3.80	1.55	1.43
36	a	314	II0	C42-C40	3.80	1.55	1.43
28	e	603	CLA	C1D-ND	3.80	1.42	1.37
36	g	316	II0	C41-C39	3.80	1.55	1.43
37	f	617	IHT	C40-C37	3.80	1.55	1.43
36	e	612	II0	C05-C03	3.80	1.66	1.54
38	i	319	KC2	CHC-C4B	3.80	1.45	1.38
37	c	616	IHT	C40-C37	3.80	1.55	1.43
37	n	617	IHT	C41-C38	3.80	1.55	1.43
28	j	605	CLA	C1D-ND	3.79	1.42	1.37
38	k	612	KC2	CHC-C4B	3.79	1.45	1.38
36	i	317	II0	C27-C25	3.79	1.53	1.50
38	f	611	KC2	CHC-C4B	3.79	1.45	1.38
36	n	614	II0	C41-C39	3.78	1.54	1.43
37	a	317	IHT	C40-C37	3.78	1.54	1.43
36	l	316	II0	C34-C36	3.78	1.54	1.46
36	j	614	II0	C32-C30	3.78	1.54	1.43
37	b	616	IHT	C40-C37	3.78	1.54	1.43
36	j	615	II0	C32-C30	3.78	1.54	1.43
36	c	617	II0	C41-C39	3.77	1.54	1.43
38	j	611	KC2	CHD-C1D	3.77	1.47	1.39
38	k	611	KC2	CHD-C1D	3.77	1.47	1.39
36	i	317	II0	C05-C03	3.77	1.66	1.54
36	a	315	II0	C32-C30	3.77	1.54	1.43
36	b	614	II0	C12-C14	-3.76	1.45	1.51
36	l	314	II0	C41-C39	3.76	1.54	1.43
36	f	615	II0	C32-C30	3.76	1.54	1.43
36	a	314	II0	C12-C14	-3.76	1.45	1.51
36	l	316	II0	C27-C25	3.76	1.53	1.50
36	a	315	II0	C12-C14	-3.75	1.45	1.51
36	b	614	II0	C41-C39	3.75	1.54	1.43
38	l	310	KC2	CHD-C1D	3.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	l	310	KC2	CHC-C4B	3.74	1.45	1.38
36	f	615	II0	C06-C04	3.74	1.66	1.54
36	n	616	II0	C05-C03	3.74	1.66	1.54
36	J	104	II0	C41-C39	3.74	1.54	1.43
37	a	317	IHT	C14-C02	3.74	1.60	1.53
28	j	612	CLA	MG-NA	3.74	2.15	2.06
36	d	316	II0	C27-C25	3.74	1.53	1.50
36	e	616	II0	C05-C03	3.74	1.66	1.54
28	n	608	CLA	C1D-ND	3.73	1.42	1.37
36	c	615	II0	C34-C36	3.73	1.53	1.46
38	f	611	KC2	CHD-C1D	3.73	1.47	1.39
36	l	312	II0	C41-C39	3.73	1.54	1.43
36	e	612	II0	C34-C36	3.73	1.53	1.46
31	B	844	WVN	C19-C22	3.73	1.53	1.46
28	n	605	CLA	C1D-ND	3.73	1.42	1.37
36	i	317	II0	C34-C36	3.72	1.53	1.46
36	n	614	II0	C05-C03	3.72	1.66	1.54
36	k	617	II0	C41-C39	3.72	1.54	1.43
36	a	315	II0	C42-C40	3.72	1.54	1.43
37	c	616	IHT	C14-C02	3.72	1.60	1.53
36	m	615	II0	C27-C25	3.72	1.53	1.50
36	m	615	II0	C32-C30	3.71	1.54	1.43
36	c	615	II0	C41-C39	3.71	1.54	1.43
36	m	618	II0	C06-C04	3.71	1.65	1.54
28	l	306	CLA	C1D-ND	3.71	1.42	1.37
28	n	604	CLA	C1D-ND	3.71	1.42	1.37
36	f	614	II0	C05-C03	3.71	1.65	1.54
36	d	316	II0	C33-C35	3.70	1.53	1.46
36	O	203	II0	C41-C39	3.70	1.54	1.43
36	k	616	II0	C41-C39	3.70	1.54	1.43
35	L	209	LMG	O8-C28	3.70	1.44	1.33
30	b	619	LHG	O7-C7	3.70	1.44	1.34
28	g	309	CLA	C1D-ND	3.70	1.42	1.37
37	b	615	IHT	C41-C38	3.70	1.54	1.43
36	i	313	II0	C41-C39	3.70	1.54	1.43
37	m	617	IHT	C14-C02	3.70	1.60	1.53
36	f	616	II0	C41-C39	3.70	1.54	1.43
36	m	615	II0	C05-C03	3.70	1.65	1.54
28	d	306	CLA	C1D-ND	3.70	1.42	1.37
37	R	204	IHT	C14-C02	3.69	1.60	1.53
36	i	314	II0	C05-C03	3.69	1.65	1.54
28	k	608	CLA	C1D-ND	3.69	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	f	615	II0	C12-C14	-3.69	1.45	1.51
36	k	615	II0	C34-C36	3.69	1.53	1.46
36	e	614	II0	C41-C39	3.69	1.54	1.43
37	b	616	IHT	C14-C02	3.69	1.60	1.53
38	m	611	KC2	CHC-C4B	3.69	1.45	1.38
37	m	617	IHT	C40-C37	3.68	1.54	1.43
36	i	314	II0	C41-C39	3.68	1.54	1.43
31	J	102	WVN	C23-C25	3.68	1.53	1.46
36	m	616	II0	C12-C14	-3.68	1.45	1.51
38	d	311	KC2	CHB-C4A	3.67	1.47	1.39
36	e	614	II0	C34-C36	3.67	1.53	1.46
37	n	617	IHT	C40-C37	3.67	1.54	1.43
38	n	612	KC2	CHD-C1D	3.67	1.47	1.39
36	f	618	II0	C27-C25	3.66	1.53	1.50
36	c	614	II0	C32-C30	3.66	1.54	1.43
37	k	618	IHT	C40-C37	3.66	1.54	1.43
36	d	316	II0	C05-C03	3.66	1.65	1.54
37	j	616	IHT	C40-C37	3.66	1.54	1.43
36	h	311	II0	C12-C14	-3.66	1.45	1.51
28	d	301	CLA	C1D-ND	3.65	1.42	1.37
36	n	616	II0	C34-C36	3.65	1.53	1.46
36	k	619	II0	C41-C39	3.65	1.54	1.43
38	d	311	KC2	CHC-C4B	3.65	1.45	1.38
36	n	616	II0	C33-C35	3.65	1.53	1.46
36	c	614	II0	C06-C04	3.65	1.65	1.54
36	j	615	II0	C41-C39	3.65	1.54	1.43
28	k	604	CLA	C1D-ND	3.65	1.42	1.37
36	m	614	II0	C05-C03	3.65	1.65	1.54
36	m	615	II0	C41-C39	3.64	1.54	1.43
28	K	103	CLA	C1D-ND	3.64	1.42	1.37
28	j	608	CLA	C1D-ND	3.64	1.42	1.37
36	j	615	II0	C05-C03	3.64	1.65	1.54
36	k	619	II0	C12-C14	-3.64	1.45	1.51
37	O	204	IHT	C40-C37	3.64	1.54	1.43
36	d	316	II0	C34-C36	3.64	1.53	1.46
37	k	618	IHT	C14-C02	3.64	1.60	1.53
28	l	305	CLA	C1D-ND	3.63	1.42	1.37
36	f	618	II0	C05-C03	3.63	1.65	1.54
36	e	614	II0	C05-C03	3.63	1.65	1.54
28	n	606	CLA	C1D-ND	3.63	1.42	1.37
36	m	616	II0	C41-C39	3.63	1.54	1.43
36	n	614	II0	C34-C36	3.63	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	614	II0	C12-C14	-3.63	1.45	1.51
36	j	615	II0	C06-C04	3.63	1.65	1.54
36	f	616	II0	C05-C03	3.63	1.65	1.54
36	n	615	II0	C12-C14	-3.63	1.45	1.51
37	f	617	IHT	C28-C26	3.63	1.53	1.50
36	f	618	II0	C34-C36	3.62	1.53	1.46
28	i	311	CLA	C4B-NB	3.62	1.42	1.37
36	e	613	II0	C05-C03	3.62	1.65	1.54
36	l	316	II0	C05-C03	3.62	1.65	1.54
36	i	315	II0	C34-C36	3.62	1.53	1.46
36	i	313	II0	C12-C14	-3.62	1.45	1.51
36	g	318	II0	C34-C36	3.62	1.53	1.46
35	J	105	LMG	O7-C10	3.62	1.44	1.34
39	i	301	LMU	O5B-C1B	3.61	1.51	1.41
36	j	614	II0	C41-C39	3.61	1.54	1.43
28	n	613	CLA	C1D-ND	3.61	1.42	1.37
29	B	842	PQN	C5-C4	3.61	1.55	1.48
37	g	319	IHT	C14-C02	3.61	1.60	1.53
36	a	314	II0	C41-C39	3.61	1.54	1.43
37	b	616	IHT	C31-C29	3.61	1.54	1.43
37	j	616	IHT	C14-C02	3.61	1.60	1.53
36	l	312	II0	C12-C14	-3.60	1.45	1.51
28	i	309	CLA	C1D-ND	3.60	1.42	1.37
36	d	314	II0	C05-C03	3.60	1.65	1.54
28	g	304	CLA	C1D-ND	3.60	1.42	1.37
37	O	204	IHT	C14-C02	3.60	1.60	1.53
38	d	311	KC2	CHD-C1D	3.60	1.47	1.39
28	B	808	CLA	CMB-C2B	-3.60	1.43	1.50
37	a	317	IHT	C28-C26	3.59	1.53	1.50
37	k	618	IHT	C28-C26	3.59	1.53	1.50
37	R	204	IHT	C40-C37	3.59	1.54	1.43
31	J	101	WVN	C29-C26	3.59	1.54	1.43
37	f	617	IHT	C14-C02	3.59	1.60	1.53
28	c	607	CLA	C1D-ND	3.59	1.42	1.37
28	k	605	CLA	C1D-ND	3.59	1.42	1.37
36	a	318	II0	C34-C36	3.59	1.53	1.46
36	g	318	II0	C05-C03	3.59	1.65	1.54
31	B	848	WVN	C23-C25	3.59	1.53	1.46
36	m	618	II0	C12-C14	-3.59	1.45	1.51
36	l	313	II0	C27-C25	3.59	1.53	1.50
36	c	614	II0	C41-C39	3.59	1.54	1.43
36	e	616	II0	C34-C36	3.59	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	n	615	II0	C05-C03	3.58	1.65	1.54
28	c	609	CLA	C1D-ND	3.58	1.42	1.37
37	g	319	IHT	C32-C33	3.58	1.53	1.46
37	b	615	IHT	C14-C02	3.58	1.60	1.53
31	L	206	WVN	C33-C34	3.58	1.53	1.46
37	f	617	IHT	C31-C29	3.58	1.54	1.43
28	k	601	CLA	C1D-ND	3.58	1.42	1.37
36	a	315	II0	C31-C29	3.58	1.54	1.43
36	m	618	II0	C41-C39	3.57	1.54	1.43
36	m	618	II0	C05-C03	3.57	1.65	1.54
36	k	621	II0	C41-C39	3.57	1.54	1.43
36	g	320	II0	C12-C14	-3.57	1.45	1.51
36	i	320	II0	C06-C04	3.57	1.65	1.54
36	O	203	II0	C05-C03	3.57	1.65	1.54
37	O	204	IHT	C28-C26	3.57	1.53	1.50
28	g	305	CLA	C1D-ND	3.57	1.42	1.37
36	h	312	II0	C41-C39	3.57	1.54	1.43
36	i	320	II0	C05-C03	3.57	1.65	1.54
36	m	616	II0	C05-C03	3.56	1.65	1.54
36	h	311	II0	C05-C03	3.56	1.65	1.54
38	n	611	KC2	CHD-C1D	3.56	1.47	1.39
28	m	604	CLA	C1D-ND	3.56	1.42	1.37
37	a	317	IHT	C31-C29	3.56	1.54	1.43
36	h	310	II0	C05-C03	3.56	1.65	1.54
28	A	811	CLA	C1D-ND	3.56	1.42	1.37
36	c	614	II0	C05-C03	3.55	1.65	1.54
36	m	618	II0	C33-C35	3.55	1.53	1.46
36	k	619	II0	C34-C36	3.55	1.53	1.46
36	e	613	II0	C41-C39	3.55	1.54	1.43
36	m	616	II0	C27-C25	3.54	1.53	1.50
37	O	204	IHT	C31-C29	3.54	1.54	1.43
37	a	317	IHT	C32-C33	3.54	1.53	1.46
38	s	201	KC2	C1B-NB	-3.54	1.33	1.37
28	A	814	CLA	C1D-ND	3.54	1.42	1.37
36	d	313	II0	C34-C36	3.54	1.53	1.46
31	l	315	WVN	C31-C32	3.54	1.53	1.46
36	f	615	II0	C41-C39	3.53	1.54	1.43
31	B	848	WVN	C19-C22	3.53	1.53	1.46
28	A	826	CLA	C1D-ND	3.53	1.42	1.37
36	k	617	II0	C34-C36	3.53	1.53	1.46
35	Q	301	LMG	O8-C28	3.53	1.43	1.33
36	i	320	II0	C34-C36	3.53	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	207	CLA	C1D-ND	3.53	1.42	1.37
36	c	613	II0	C41-C39	3.53	1.54	1.43
36	l	312	II0	C34-C36	3.53	1.53	1.46
36	n	616	II0	C12-C14	-3.53	1.45	1.51
37	b	615	IHT	C40-C37	3.53	1.54	1.43
36	g	320	II0	C41-C39	3.53	1.54	1.43
28	i	305	CLA	C1D-ND	3.52	1.42	1.37
36	a	315	II0	C05-C03	3.52	1.65	1.54
28	l	308	CLA	C1D-ND	3.52	1.42	1.37
36	k	621	II0	C34-C36	3.51	1.53	1.46
36	f	616	II0	C34-C36	3.51	1.53	1.46
36	b	613	II0	C12-C14	-3.51	1.45	1.51
28	e	606	CLA	C1D-ND	3.51	1.42	1.37
28	m	610	CLA	C1D-ND	3.51	1.42	1.37
36	h	312	II0	C34-C36	3.51	1.53	1.46
38	s	201	KC2	CHB-C1B	3.51	1.45	1.38
36	m	614	II0	C34-C36	3.51	1.53	1.46
37	c	616	IHT	C28-C26	3.51	1.53	1.50
28	k	607	CLA	C1D-ND	3.51	1.42	1.37
36	a	316	II0	C05-C03	3.51	1.65	1.54
36	i	313	II0	C34-C36	3.50	1.53	1.46
37	g	319	IHT	C31-C29	3.50	1.54	1.43
36	h	312	II0	C05-C03	3.50	1.65	1.54
28	i	304	CLA	C1D-ND	3.50	1.42	1.37
28	b	608	CLA	C1D-ND	3.50	1.42	1.37
28	g	302	CLA	C1D-ND	3.50	1.42	1.37
36	l	312	II0	C05-C03	3.49	1.65	1.54
37	n	617	IHT	C14-C02	3.49	1.60	1.53
28	h	307	CLA	C1D-ND	3.49	1.42	1.37
28	e	610	CLA	C1D-ND	3.49	1.42	1.37
28	d	307	CLA	C1D-ND	3.49	1.42	1.37
36	b	617	II0	C41-C39	3.49	1.54	1.43
37	c	616	IHT	C31-C29	3.49	1.54	1.43
28	b	601	CLA	C1D-ND	3.49	1.42	1.37
28	k	610	CLA	C1D-ND	3.49	1.42	1.37
28	i	307	CLA	C1D-ND	3.49	1.42	1.37
38	f	611	KC2	CHB-C4A	3.49	1.47	1.39
36	a	318	II0	C12-C14	-3.49	1.45	1.51
36	k	615	II0	C05-C03	3.48	1.65	1.54
36	f	618	II0	C12-C14	-3.48	1.45	1.51
36	k	619	II0	C05-C03	3.48	1.65	1.54
28	e	601	CLA	C1D-ND	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	803	CLA	C1D-ND	3.48	1.42	1.37
28	j	606	CLA	C1D-ND	3.48	1.42	1.37
36	l	314	II0	C34-C36	3.48	1.53	1.46
31	L	205	WVN	C23-C25	3.48	1.53	1.46
36	n	615	II0	C34-C36	3.48	1.53	1.46
36	c	617	II0	C05-C03	3.48	1.65	1.54
36	f	615	II0	C05-C03	3.47	1.65	1.54
36	k	617	II0	C05-C03	3.47	1.65	1.54
31	l	315	WVN	C29-C26	3.47	1.53	1.43
28	A	819	CLA	C1D-ND	3.47	1.42	1.37
37	m	617	IHT	C28-C26	3.47	1.53	1.50
39	i	301	LMU	O5'-C1'	3.47	1.50	1.41
36	l	314	II0	C05-C03	3.46	1.65	1.54
28	k	603	CLA	C1D-ND	3.46	1.42	1.37
36	c	617	II0	C34-C36	3.46	1.53	1.46
36	c	615	II0	C05-C03	3.46	1.65	1.54
37	R	204	IHT	C28-C26	3.46	1.53	1.50
37	n	617	IHT	C31-C29	3.45	1.53	1.43
37	f	617	IHT	C32-C33	3.45	1.53	1.46
37	j	616	IHT	C31-C29	3.45	1.53	1.43
31	A	847	WVN	C33-C34	3.45	1.53	1.46
28	a	311	CLA	C1D-ND	3.45	1.42	1.37
28	f	605	CLA	C1D-ND	3.45	1.42	1.37
36	k	621	II0	C05-C03	3.45	1.65	1.54
36	a	318	II0	C27-C25	3.45	1.53	1.50
36	g	316	II0	C05-C03	3.44	1.65	1.54
28	j	610	CLA	C1D-ND	3.44	1.42	1.37
36	O	203	II0	C12-C14	-3.44	1.45	1.51
36	l	314	II0	C12-C14	-3.44	1.45	1.51
36	g	316	II0	C34-C36	3.44	1.53	1.46
28	s	203	CLA	C1D-ND	3.44	1.42	1.37
36	k	616	II0	C05-C03	3.44	1.65	1.54
36	g	320	II0	C05-C03	3.44	1.65	1.54
36	a	316	II0	C41-C39	3.44	1.53	1.43
28	A	812	CLA	C1D-ND	3.44	1.42	1.37
31	i	316	WVN	C33-C34	3.44	1.53	1.46
28	B	811	CLA	C1D-ND	3.44	1.42	1.37
36	b	613	II0	C41-C39	3.43	1.53	1.43
38	k	613	KC2	CHB-C4A	3.43	1.47	1.39
28	A	829	CLA	CMB-C2B	-3.43	1.43	1.50
28	h	302	CLA	C1D-ND	3.43	1.42	1.37
36	f	614	II0	C12-C14	-3.43	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	317	II0	C05-C03	3.43	1.65	1.54
28	i	306	CLA	C1D-ND	3.43	1.42	1.37
28	i	312	CLA	C1D-ND	3.42	1.42	1.37
28	h	308	CLA	C1D-ND	3.42	1.42	1.37
28	B	832	CLA	C1D-ND	3.42	1.42	1.37
36	J	104	II0	C34-C36	3.42	1.53	1.46
36	i	313	II0	C05-C03	3.42	1.65	1.54
36	j	614	II0	C12-C14	-3.42	1.45	1.51
28	m	601	CLA	C1D-ND	3.42	1.42	1.37
28	n	607	CLA	C1D-ND	3.41	1.42	1.37
36	d	313	II0	C33-C35	3.41	1.53	1.46
31	I	101	WVN	C31-C32	3.41	1.53	1.46
37	m	617	IHT	C31-C29	3.41	1.53	1.43
28	d	303	CLA	C1D-ND	3.41	1.42	1.37
31	J	102	WVN	C19-C22	3.41	1.53	1.46
36	n	618	II0	C34-C36	3.41	1.53	1.46
28	a	310	CLA	C1D-ND	3.41	1.42	1.37
36	e	616	II0	C12-C14	-3.41	1.45	1.51
28	m	609	CLA	C1D-ND	3.41	1.42	1.37
28	l	304	CLA	C1D-ND	3.41	1.42	1.37
28	g	308	CLA	C1D-ND	3.41	1.42	1.37
31	F	204	WVN	C33-C34	3.41	1.53	1.46
28	f	606	CLA	C1D-ND	3.40	1.42	1.37
28	n	608	CLA	C4B-NB	3.40	1.42	1.37
37	k	618	IHT	C31-C29	3.40	1.53	1.43
36	g	317	II0	C41-C39	3.40	1.53	1.43
37	j	616	IHT	C28-C26	3.40	1.53	1.50
28	e	611	CLA	C1D-ND	3.39	1.42	1.37
28	k	614	CLA	C1D-ND	3.39	1.42	1.37
36	a	314	II0	C05-C03	3.39	1.65	1.54
28	j	609	CLA	C1D-ND	3.39	1.42	1.37
31	i	316	WVN	C30-C28	3.39	1.53	1.43
28	s	206	CLA	C1D-ND	3.39	1.42	1.37
31	h	309	WVN	C31-C32	3.39	1.53	1.46
28	j	613	CLA	C1D-ND	3.39	1.42	1.37
36	i	315	II0	C05-C03	3.39	1.64	1.54
28	i	302	CLA	C4B-NB	3.39	1.42	1.37
28	A	826	CLA	CMC-C2C	-3.39	1.43	1.50
28	k	602	CLA	C1D-ND	3.39	1.42	1.37
31	J	101	WVN	C19-C22	3.39	1.53	1.46
31	J	102	WVN	C31-C32	3.38	1.53	1.46
28	f	601	CLA	C1D-ND	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	307	CLA	C4B-NB	3.38	1.42	1.37
36	f	618	II0	C33-C35	3.38	1.53	1.46
28	e	604	CLA	C1D-ND	3.38	1.42	1.37
28	g	315	CLA	C1D-ND	3.38	1.42	1.37
37	R	204	IHT	C31-C29	3.38	1.53	1.43
37	n	617	IHT	C28-C26	3.38	1.53	1.50
28	B	839	CLA	C1D-ND	3.37	1.42	1.37
31	J	101	WVN	C33-C34	3.37	1.53	1.46
36	h	311	II0	C34-C36	3.37	1.53	1.46
36	k	616	II0	C34-C36	3.37	1.53	1.46
38	k	612	KC2	C3C-C4C	3.37	1.51	1.44
28	b	610	CLA	C1D-ND	3.37	1.42	1.37
36	l	316	II0	C33-C35	3.37	1.53	1.46
28	a	309	CLA	C1D-ND	3.36	1.42	1.37
28	l	302	CLA	C1D-ND	3.36	1.42	1.37
28	i	311	CLA	C1D-ND	3.36	1.42	1.37
36	l	313	II0	C05-C03	3.36	1.64	1.54
31	l	315	WVN	C33-C34	3.36	1.53	1.46
28	b	604	CLA	C1D-ND	3.36	1.42	1.37
28	m	605	CLA	C1D-ND	3.36	1.42	1.37
38	g	313	KC2	CHB-C4A	3.36	1.46	1.39
28	L	202	CLA	C1D-ND	3.36	1.42	1.37
28	a	308	CLA	C1D-ND	3.36	1.42	1.37
36	n	618	II0	C33-C35	3.36	1.53	1.46
38	n	612	KC2	CHB-C4A	3.36	1.46	1.39
36	n	618	II0	C05-C03	3.36	1.64	1.54
36	k	616	II0	C12-C14	-3.35	1.45	1.51
28	A	822	CLA	C1D-ND	3.35	1.42	1.37
28	A	801	CLA	C1D-ND	3.35	1.42	1.37
28	B	812	CLA	C1D-ND	3.35	1.42	1.37
28	n	601	CLA	C1D-ND	3.35	1.42	1.37
37	n	617	IHT	C32-C33	3.35	1.53	1.46
28	f	608	CLA	C4B-NB	3.35	1.42	1.37
36	a	315	II0	C41-C39	3.35	1.53	1.43
36	e	613	II0	C34-C36	3.34	1.53	1.46
37	b	615	IHT	C31-C29	3.34	1.53	1.43
28	A	808	CLA	C1D-ND	3.34	1.42	1.37
28	J	103	CLA	C1D-ND	3.34	1.42	1.37
36	k	619	II0	C33-C35	3.34	1.53	1.46
31	F	204	WVN	C23-C25	3.34	1.53	1.46
28	i	302	CLA	C1D-ND	3.34	1.42	1.37
28	g	311	CLA	C1D-ND	3.34	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	604	CLA	C1D-ND	3.34	1.42	1.37
36	f	614	II0	C34-C36	3.34	1.53	1.46
28	A	835	CLA	C1D-ND	3.34	1.42	1.37
28	m	607	CLA	C1D-ND	3.34	1.42	1.37
36	c	613	II0	C05-C03	3.33	1.64	1.54
28	j	605	CLA	C4B-NB	3.33	1.42	1.37
36	a	318	II0	C05-C03	3.33	1.64	1.54
28	a	313	CLA	C1D-ND	3.33	1.42	1.37
36	e	616	II0	C27-C25	3.33	1.53	1.50
36	j	615	II0	C12-C14	-3.33	1.45	1.51
28	B	810	CLA	C1D-ND	3.33	1.42	1.37
37	k	618	IHT	C32-C33	3.33	1.53	1.46
28	B	819	CLA	C1D-ND	3.33	1.42	1.37
37	c	616	IHT	C32-C33	3.33	1.53	1.46
28	B	810	CLA	C4B-NB	3.33	1.42	1.37
28	j	604	CLA	C1D-ND	3.33	1.42	1.37
31	e	615	WVN	C33-C34	3.33	1.53	1.46
36	i	314	II0	C34-C36	3.33	1.53	1.46
28	O	202	CLA	C1D-ND	3.33	1.42	1.37
28	h	306	CLA	C1D-ND	3.33	1.42	1.37
36	j	614	II0	C05-C03	3.33	1.64	1.54
31	F	204	WVN	C30-C28	3.32	1.53	1.43
36	d	315	II0	C33-C35	3.32	1.53	1.46
28	f	603	CLA	C1D-ND	3.32	1.42	1.37
36	e	612	II0	C33-C35	3.32	1.53	1.46
28	B	821	CLA	C1D-ND	3.32	1.42	1.37
28	n	609	CLA	C1D-ND	3.32	1.42	1.37
28	l	311	CLA	C1D-ND	3.32	1.42	1.37
31	A	848	WVN	C33-C34	3.32	1.53	1.46
28	g	311	CLA	C4B-NB	3.32	1.42	1.37
36	O	203	II0	C34-C36	3.32	1.53	1.46
28	B	809	CLA	C1D-ND	3.32	1.42	1.37
28	e	608	CLA	C1D-ND	3.32	1.42	1.37
28	f	613	CLA	C4B-NB	3.32	1.42	1.37
36	a	318	II0	C33-C35	3.32	1.53	1.46
28	F	202	CLA	C1D-ND	3.31	1.42	1.37
28	f	604	CLA	C1D-ND	3.31	1.42	1.37
28	b	602	CLA	C1D-ND	3.31	1.42	1.37
36	h	311	II0	C33-C35	3.31	1.53	1.46
37	j	616	IHT	C32-C33	3.31	1.53	1.46
36	i	320	II0	C33-C35	3.31	1.53	1.46
28	f	612	CLA	C4B-NB	3.31	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	g	312	KC2	CHC-C1C	3.31	1.46	1.39
31	s	207	WVN	C31-C32	3.31	1.53	1.46
28	B	835	CLA	C1D-ND	3.31	1.42	1.37
28	A	855	CLA	C1D-ND	3.30	1.42	1.37
28	g	310	CLA	C1D-ND	3.30	1.42	1.37
28	f	606	CLA	C4B-NB	3.30	1.42	1.37
28	h	313	CLA	C1D-ND	3.30	1.42	1.37
36	m	618	II0	C34-C36	3.30	1.53	1.46
28	f	613	CLA	C1D-ND	3.30	1.42	1.37
37	b	615	IHT	C28-C26	3.30	1.53	1.50
28	A	836	CLA	C1D-ND	3.30	1.42	1.37
31	e	615	WVN	C30-C28	3.30	1.53	1.43
31	L	205	WVN	C33-C34	3.30	1.53	1.46
28	B	807	CLA	C4B-NB	3.30	1.42	1.37
38	k	612	KC2	CHB-C4A	3.29	1.46	1.39
36	b	614	II0	C05-C03	3.29	1.64	1.54
36	l	316	II0	C12-C14	-3.29	1.45	1.51
28	a	304	CLA	C1D-ND	3.29	1.42	1.37
28	d	304	CLA	C1D-ND	3.29	1.42	1.37
28	n	610	CLA	C1D-ND	3.29	1.42	1.37
28	d	312	CLA	C1D-ND	3.29	1.42	1.37
28	d	309	CLA	C1D-ND	3.29	1.42	1.37
28	m	606	CLA	C1D-ND	3.29	1.42	1.37
28	A	832	CLA	C1D-ND	3.29	1.42	1.37
36	g	317	II0	C34-C36	3.29	1.53	1.46
28	k	607	CLA	C4B-NB	3.29	1.42	1.37
31	A	846	WVN	C33-C34	3.29	1.53	1.46
28	A	806	CLA	C4B-NB	3.29	1.42	1.37
28	B	822	CLA	CMD-C2D	-3.29	1.44	1.50
31	s	207	WVN	C33-C34	3.28	1.53	1.46
37	R	204	IHT	C32-C33	3.28	1.53	1.46
31	e	615	WVN	C23-C25	3.28	1.53	1.46
28	j	601	CLA	C1D-ND	3.28	1.42	1.37
28	m	601	CLA	C4B-NB	3.28	1.42	1.37
28	j	607	CLA	C1D-ND	3.28	1.42	1.37
28	s	208	CLA	C1D-ND	3.28	1.42	1.37
28	f	602	CLA	C1D-ND	3.28	1.42	1.37
28	c	612	CLA	C1D-ND	3.28	1.42	1.37
28	R	203	CLA	C1D-ND	3.28	1.42	1.37
28	j	602	CLA	C1D-ND	3.28	1.42	1.37
28	h	305	CLA	C1D-ND	3.28	1.42	1.37
38	s	204	KC2	CHB-C4A	3.28	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	306	CLA	C1D-ND	3.28	1.42	1.37
28	e	607	CLA	C1D-ND	3.28	1.42	1.37
28	A	816	CLA	C1D-ND	3.28	1.42	1.37
28	A	806	CLA	C1D-ND	3.27	1.42	1.37
28	d	308	CLA	C1D-ND	3.27	1.42	1.37
28	d	305	CLA	MG-NC	3.27	2.14	2.06
31	i	316	WVN	C23-C25	3.27	1.53	1.46
36	j	615	II0	C34-C36	3.27	1.53	1.46
36	b	614	II0	C34-C36	3.27	1.53	1.46
28	d	303	CLA	C4B-NB	3.27	1.42	1.37
36	c	613	II0	C34-C36	3.27	1.52	1.46
28	B	838	CLA	C1D-ND	3.27	1.42	1.37
28	g	306	CLA	C1D-ND	3.27	1.42	1.37
28	h	307	CLA	C4B-NB	3.27	1.42	1.37
36	g	317	II0	C12-C14	-3.27	1.45	1.51
36	d	314	II0	C33-C35	3.27	1.52	1.46
38	s	201	KC2	CHC-C1C	3.27	1.46	1.39
37	g	319	IHT	C28-C26	3.26	1.53	1.50
28	B	823	CLA	C1D-ND	3.26	1.42	1.37
28	d	309	CLA	C4B-NB	3.26	1.42	1.37
28	n	610	CLA	C4B-NB	3.26	1.42	1.37
28	d	306	CLA	C4B-NB	3.26	1.42	1.37
28	A	811	CLA	C4B-NB	3.26	1.42	1.37
28	n	603	CLA	C1D-ND	3.26	1.42	1.37
36	i	317	II0	C33-C35	3.26	1.52	1.46
31	J	102	WVN	C40-C37	3.26	1.53	1.43
28	i	308	CLA	C1D-ND	3.26	1.42	1.37
38	e	609	KC2	CHB-C4A	3.26	1.46	1.39
31	l	315	WVN	C19-C22	3.25	1.52	1.46
28	A	841	CLA	C1D-ND	3.25	1.42	1.37
31	F	204	WVN	C40-C37	3.25	1.53	1.43
36	m	614	II0	C12-C14	-3.25	1.46	1.51
31	l	301	WVN	C33-C34	3.25	1.52	1.46
28	O	206	CLA	C1D-ND	3.25	1.42	1.37
36	b	617	II0	C05-C03	3.25	1.64	1.54
28	f	607	CLA	C1D-ND	3.25	1.42	1.37
36	e	616	II0	C33-C35	3.25	1.52	1.46
31	K	104	WVN	C33-C34	3.25	1.52	1.46
31	F	204	WVN	C31-C32	3.25	1.52	1.46
28	j	603	CLA	C1D-ND	3.25	1.42	1.37
28	g	306	CLA	C4B-NB	3.25	1.42	1.37
31	R	201	WVN	C33-C34	3.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	g	314	KC2	CHB-C4A	3.25	1.46	1.39
37	b	616	IHT	C32-C33	3.24	1.52	1.46
31	s	207	WVN	C30-C28	3.24	1.53	1.43
31	l	315	WVN	C39-C36	3.24	1.53	1.43
36	d	313	II0	C12-C14	-3.24	1.46	1.51
28	O	201	CLA	C1D-ND	3.24	1.42	1.37
28	l	309	CLA	C1D-ND	3.24	1.42	1.37
28	L	204	CLA	C1D-ND	3.24	1.42	1.37
37	b	616	IHT	C28-C26	3.24	1.53	1.50
36	f	615	II0	C34-C36	3.23	1.52	1.46
28	A	854	CLA	C4B-NB	3.23	1.42	1.37
28	B	829	CLA	C4B-NB	3.23	1.42	1.37
36	c	617	II0	C12-C14	-3.23	1.46	1.51
31	e	615	WVN	C39-C36	3.23	1.53	1.43
36	g	320	II0	C34-C36	3.23	1.52	1.46
28	n	602	CLA	C1D-ND	3.23	1.42	1.37
28	A	831	CLA	C1D-ND	3.23	1.42	1.37
28	c	601	CLA	C4B-NB	3.23	1.42	1.37
28	c	606	CLA	C1D-ND	3.23	1.42	1.37
28	a	305	CLA	C1D-ND	3.23	1.42	1.37
31	R	201	WVN	C40-C37	3.23	1.53	1.43
31	l	315	WVN	C30-C28	3.23	1.53	1.43
28	k	606	CLA	C1D-ND	3.22	1.42	1.37
28	j	610	CLA	C4B-NB	3.22	1.42	1.37
31	h	309	WVN	C29-C26	3.22	1.53	1.43
36	i	315	II0	C12-C14	-3.22	1.46	1.51
28	b	607	CLA	C4B-NB	3.22	1.42	1.37
38	c	610	KC2	CHB-C4A	3.22	1.46	1.39
28	l	304	CLA	C4B-NB	3.22	1.42	1.37
36	f	616	II0	C12-C14	-3.22	1.46	1.51
31	L	205	WVN	C30-C28	3.22	1.53	1.43
28	m	613	CLA	C1D-ND	3.21	1.42	1.37
38	l	310	KC2	CHB-C4A	3.21	1.46	1.39
28	d	312	CLA	C4B-NB	3.21	1.42	1.37
28	A	838	CLA	C4B-NB	3.21	1.42	1.37
28	F	201	CLA	C4B-NB	3.21	1.42	1.37
28	d	308	CLA	C4B-NB	3.21	1.42	1.37
31	s	207	WVN	C29-C26	3.21	1.53	1.43
36	n	614	II0	C12-C14	-3.21	1.46	1.51
37	O	204	IHT	C32-C33	3.21	1.52	1.46
28	B	803	CLA	CMC-C2C	-3.21	1.44	1.50
28	A	834	CLA	C1D-ND	3.21	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	316	II0	C12-C14	-3.21	1.46	1.51
31	A	847	WVN	C30-C28	3.21	1.53	1.43
37	m	617	IHT	C32-C33	3.20	1.52	1.46
31	l	315	WVN	C40-C37	3.20	1.53	1.43
31	i	316	WVN	C40-C37	3.20	1.53	1.43
38	e	609	KC2	CHC-C1C	3.20	1.46	1.39
28	A	815	CLA	C1D-ND	3.20	1.42	1.37
31	e	615	WVN	C40-C37	3.20	1.53	1.43
31	B	846	WVN	C40-C37	3.20	1.53	1.43
28	f	605	CLA	C4B-NB	3.20	1.42	1.37
28	B	826	CLA	CMD-C2D	-3.20	1.44	1.50
31	e	615	WVN	C31-C32	3.20	1.52	1.46
28	B	805	CLA	C1D-ND	3.20	1.42	1.37
28	f	601	CLA	C4B-NB	3.20	1.42	1.37
31	R	201	WVN	C31-C32	3.20	1.52	1.46
28	A	805	CLA	C1D-ND	3.20	1.42	1.37
28	l	311	CLA	C4B-NB	3.20	1.42	1.37
28	j	601	CLA	C4B-NB	3.20	1.42	1.37
36	J	104	II0	C05-C03	3.20	1.64	1.54
31	i	316	WVN	C39-C36	3.20	1.53	1.43
38	j	611	KC2	CHB-C4A	3.19	1.46	1.39
36	b	617	II0	C34-C36	3.19	1.52	1.46
36	e	612	II0	C12-C14	-3.19	1.46	1.51
31	A	846	WVN	C39-C36	3.19	1.53	1.43
28	B	820	CLA	C1D-ND	3.19	1.42	1.37
36	e	614	II0	C12-C14	-3.19	1.46	1.51
28	A	804	CLA	C1D-ND	3.19	1.42	1.37
28	f	610	CLA	C4B-NB	3.19	1.42	1.37
28	g	305	CLA	C4B-NB	3.19	1.42	1.37
28	A	823	CLA	C1D-ND	3.19	1.42	1.37
36	m	616	II0	C34-C36	3.19	1.52	1.46
28	e	605	CLA	C1D-ND	3.18	1.42	1.37
31	i	316	WVN	C29-C26	3.18	1.53	1.43
38	n	611	KC2	CHB-C4A	3.18	1.46	1.39
28	e	602	CLA	C4B-NB	3.18	1.42	1.37
38	n	612	KC2	CHC-C1C	3.18	1.46	1.39
28	a	313	CLA	C4B-NB	3.18	1.42	1.37
31	K	102	WVN	C31-C32	3.18	1.52	1.46
28	Q	303	CLA	C4B-NB	3.18	1.42	1.37
28	k	614	CLA	C4B-NB	3.17	1.42	1.37
28	n	601	CLA	C4B-NB	3.17	1.42	1.37
28	d	302	CLA	C1D-ND	3.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	h	309	WVN	C33-C34	3.17	1.52	1.46
38	g	312	KC2	CHB-C4A	3.17	1.46	1.39
31	s	207	WVN	C19-C22	3.17	1.52	1.46
31	A	845	WVN	C31-C32	3.17	1.52	1.46
28	A	851	CLA	C4B-NB	3.17	1.42	1.37
36	i	317	II0	C12-C14	-3.17	1.46	1.51
31	s	207	WVN	C23-C25	3.16	1.52	1.46
38	m	611	KC2	CHB-C4A	3.16	1.46	1.39
28	g	309	CLA	C4B-NB	3.16	1.42	1.37
31	s	207	WVN	C39-C36	3.16	1.53	1.43
38	d	310	KC2	CHB-C4A	3.16	1.46	1.39
28	h	304	CLA	C1D-ND	3.16	1.42	1.37
28	e	611	CLA	C4B-NB	3.16	1.42	1.37
31	R	201	WVN	C39-C36	3.16	1.53	1.43
28	m	608	CLA	C1D-ND	3.16	1.42	1.37
36	k	617	II0	C33-C35	3.16	1.52	1.46
38	k	613	KC2	CHC-C1C	3.16	1.46	1.39
28	B	834	CLA	C1D-ND	3.16	1.42	1.37
31	h	309	WVN	C30-C28	3.16	1.53	1.43
28	O	201	CLA	CMD-C2D	-3.16	1.44	1.50
31	R	201	WVN	C30-C28	3.16	1.53	1.43
28	A	854	CLA	CMB-C2B	-3.15	1.44	1.50
28	c	608	CLA	C1D-ND	3.15	1.42	1.37
38	k	611	KC2	CHC-C1C	3.15	1.46	1.39
31	L	201	WVN	C23-C25	3.15	1.52	1.46
28	a	312	CLA	C1D-ND	3.15	1.42	1.37
38	d	310	KC2	CHC-C1C	3.15	1.46	1.39
36	g	316	II0	C12-C14	-3.15	1.46	1.51
28	k	604	CLA	C4B-NB	3.15	1.42	1.37
38	m	611	KC2	C1B-NB	-3.15	1.33	1.37
36	d	315	II0	C12-C14	-3.15	1.46	1.51
36	m	615	II0	C34-C36	3.15	1.52	1.46
28	A	817	CLA	C1D-ND	3.15	1.42	1.37
31	A	846	WVN	C29-C26	3.15	1.52	1.43
28	g	307	CLA	C1D-ND	3.15	1.42	1.37
31	h	309	WVN	C23-C25	3.15	1.52	1.46
28	A	824	CLA	C1D-ND	3.15	1.42	1.37
36	n	615	II0	C33-C35	3.14	1.52	1.46
28	d	305	CLA	C1B-C2B	3.14	1.50	1.43
28	k	609	CLA	C1D-ND	3.14	1.42	1.37
38	g	314	KC2	CHC-C1C	3.14	1.46	1.39
38	k	611	KC2	CHB-C4A	3.14	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	838	CLA	C1D-ND	3.14	1.42	1.37
28	B	809	CLA	C4B-NB	3.14	1.42	1.37
28	b	611	CLA	C4B-NB	3.14	1.42	1.37
28	k	608	CLA	C4B-NB	3.13	1.42	1.37
28	i	304	CLA	C4B-NB	3.13	1.42	1.37
38	i	310	KC2	CHB-C4A	3.13	1.46	1.39
31	K	104	WVN	C30-C28	3.13	1.52	1.43
28	B	841	CLA	C1D-ND	3.13	1.42	1.37
28	B	804	CLA	C1D-ND	3.13	1.42	1.37
36	h	312	II0	C33-C35	3.13	1.52	1.46
31	B	847	WVN	C23-C25	3.12	1.52	1.46
28	B	813	CLA	C1D-ND	3.12	1.42	1.37
28	e	605	CLA	C4B-NB	3.12	1.42	1.37
31	e	615	WVN	C29-C26	3.12	1.52	1.43
28	F	201	CLA	C1D-ND	3.12	1.42	1.37
28	e	607	CLA	C4B-NB	3.12	1.42	1.37
28	f	602	CLA	C4B-NB	3.12	1.42	1.37
38	s	204	KC2	CHC-C1C	3.12	1.46	1.39
28	c	609	CLA	C4B-NB	3.12	1.42	1.37
28	k	606	CLA	C4B-NB	3.12	1.42	1.37
31	B	846	WVN	C30-C28	3.12	1.52	1.43
31	J	102	WVN	C33-C34	3.12	1.52	1.46
31	L	205	WVN	C29-C26	3.11	1.52	1.43
38	i	319	KC2	CHB-C4A	3.11	1.46	1.39
28	s	202	CLA	C1D-ND	3.11	1.42	1.37
38	n	611	KC2	CHC-C1C	3.11	1.46	1.39
28	b	606	CLA	C1D-ND	3.11	1.42	1.37
28	A	854	CLA	C1D-ND	3.11	1.41	1.37
28	B	834	CLA	C4B-NB	3.11	1.41	1.37
28	B	818	CLA	C1D-ND	3.11	1.41	1.37
28	B	826	CLA	C4B-NB	3.11	1.41	1.37
28	b	603	CLA	C1D-ND	3.11	1.41	1.37
38	c	610	KC2	CHC-C1C	3.11	1.46	1.39
28	A	818	CLA	C4B-NB	3.11	1.41	1.37
28	A	855	CLA	C4B-NB	3.11	1.41	1.37
28	i	303	CLA	C1D-ND	3.11	1.41	1.37
36	c	615	II0	C33-C35	3.11	1.52	1.46
36	O	203	II0	C33-C35	3.11	1.52	1.46
31	I	101	WVN	C29-C26	3.11	1.52	1.43
36	f	614	II0	C33-C35	3.11	1.52	1.46
28	B	830	CLA	C1D-ND	3.11	1.41	1.37
31	L	206	WVN	C40-C37	3.11	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	607	CLA	C4B-NB	3.11	1.41	1.37
28	j	612	CLA	C1B-C2B	3.11	1.50	1.43
28	A	825	CLA	CMD-C2D	-3.10	1.44	1.50
28	m	612	CLA	C1D-ND	3.10	1.41	1.37
36	a	314	II0	C34-C36	3.10	1.52	1.46
28	A	810	CLA	C4B-NB	3.10	1.41	1.37
28	g	322	CLA	C4B-NB	3.10	1.41	1.37
28	A	829	CLA	C1D-ND	3.10	1.41	1.37
28	Q	302	CLA	C4B-NB	3.10	1.41	1.37
31	R	201	WVN	C29-C26	3.10	1.52	1.43
36	J	104	II0	C12-C14	-3.10	1.46	1.51
31	A	847	WVN	C23-C25	3.10	1.52	1.46
31	s	207	WVN	C40-C37	3.09	1.52	1.43
28	e	602	CLA	C1D-ND	3.09	1.41	1.37
28	h	306	CLA	C4B-NB	3.09	1.41	1.37
36	g	318	II0	C33-C35	3.09	1.52	1.46
28	i	311	CLA	C1B-C2B	3.09	1.50	1.43
36	e	613	II0	C12-C14	-3.09	1.46	1.51
28	h	301	CLA	C1D-ND	3.09	1.41	1.37
31	l	301	WVN	C30-C28	3.08	1.52	1.43
28	B	802	CLA	C1D-ND	3.08	1.41	1.37
28	b	605	CLA	C1D-ND	3.08	1.41	1.37
28	c	607	CLA	C4B-NB	3.08	1.41	1.37
28	Q	302	CLA	CMD-C2D	-3.08	1.44	1.50
28	B	828	CLA	C1D-ND	3.08	1.41	1.37
31	B	846	WVN	C33-C34	3.08	1.52	1.46
28	c	611	CLA	C1B-C2B	3.08	1.50	1.43
28	A	813	CLA	C1D-ND	3.08	1.41	1.37
38	i	319	KC2	CHC-C1C	3.08	1.46	1.39
28	m	608	CLA	C4B-NB	3.08	1.41	1.37
28	l	307	CLA	C1D-ND	3.08	1.41	1.37
31	h	309	WVN	C39-C36	3.08	1.52	1.43
28	i	306	CLA	C4B-NB	3.08	1.41	1.37
28	B	829	CLA	C1D-ND	3.07	1.41	1.37
28	h	313	CLA	C4B-NB	3.07	1.41	1.37
38	j	611	KC2	CHC-C1C	3.07	1.46	1.39
28	a	307	CLA	C1D-ND	3.07	1.41	1.37
28	B	809	CLA	CAB-C3B	-3.07	1.44	1.50
28	L	202	CLA	C4B-NB	3.07	1.41	1.37
28	A	839	CLA	C1D-ND	3.07	1.41	1.37
28	m	605	CLA	C4B-NB	3.07	1.41	1.37
36	i	314	II0	C33-C35	3.07	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	612	CLA	C1D-ND	3.06	1.41	1.37
38	k	612	KC2	CHC-C1C	3.06	1.46	1.39
31	J	101	WVN	C30-C28	3.06	1.52	1.43
28	B	815	CLA	C1D-ND	3.06	1.41	1.37
28	B	833	CLA	C1D-ND	3.06	1.41	1.37
28	b	608	CLA	C4B-NB	3.06	1.41	1.37
31	L	205	WVN	C31-C32	3.06	1.52	1.46
28	m	610	CLA	C4B-NB	3.06	1.41	1.37
31	B	848	WVN	C30-C28	3.06	1.52	1.43
36	c	617	II0	C33-C35	3.06	1.52	1.46
31	B	846	WVN	C39-C36	3.06	1.52	1.43
28	B	831	CLA	C1D-ND	3.06	1.41	1.37
36	l	313	II0	C12-C14	-3.06	1.46	1.51
28	l	306	CLA	C4B-NB	3.06	1.41	1.37
31	s	205	WVN	C39-C36	3.06	1.52	1.43
28	B	831	CLA	C4B-NB	3.05	1.41	1.37
28	f	612	CLA	C1D-ND	3.05	1.41	1.37
37	b	615	IHT	C32-C33	3.05	1.52	1.46
28	a	303	CLA	C4B-NB	3.05	1.41	1.37
31	h	309	WVN	C40-C37	3.05	1.52	1.43
36	e	614	II0	C33-C35	3.05	1.52	1.46
28	c	604	CLA	C4B-NB	3.05	1.41	1.37
36	h	310	II0	C33-C35	3.04	1.52	1.46
36	J	104	II0	C33-C35	3.04	1.52	1.46
28	f	609	CLA	C1D-ND	3.04	1.41	1.37
28	i	307	CLA	C4B-NB	3.04	1.41	1.37
31	I	101	WVN	C23-C25	3.04	1.52	1.46
31	A	845	WVN	C29-C26	3.04	1.52	1.43
28	n	606	CLA	C4B-NB	3.04	1.41	1.37
31	J	102	WVN	C29-C26	3.04	1.52	1.43
31	A	848	WVN	C39-C36	3.04	1.52	1.43
28	B	836	CLA	C1D-ND	3.04	1.41	1.37
38	g	313	KC2	CHC-C1C	3.04	1.46	1.39
31	F	204	WVN	C29-C26	3.04	1.52	1.43
31	B	845	WVN	C39-C36	3.03	1.52	1.43
28	A	852	CLA	C1D-ND	3.03	1.41	1.37
28	A	818	CLA	C1D-ND	3.03	1.41	1.37
28	A	837	CLA	C1D-ND	3.03	1.41	1.37
28	B	816	CLA	C1D-ND	3.03	1.41	1.37
28	K	101	CLA	C1D-ND	3.03	1.41	1.37
38	s	204	KC2	C1B-NB	-3.03	1.33	1.37
28	A	833	CLA	C1D-ND	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	n	614	II0	C33-C35	3.03	1.52	1.46
31	K	104	WVN	C19-C22	3.03	1.52	1.46
28	g	315	CLA	C4B-NB	3.03	1.41	1.37
31	K	104	WVN	C39-C36	3.03	1.52	1.43
38	f	611	KC2	CHC-C1C	3.03	1.46	1.39
38	d	311	KC2	C1B-NB	-3.03	1.33	1.37
28	B	801	CLA	C4B-NB	3.02	1.41	1.37
36	l	313	II0	C33-C35	3.02	1.52	1.46
31	L	206	WVN	C39-C36	3.02	1.52	1.43
31	J	101	WVN	C40-C37	3.02	1.52	1.43
31	A	845	WVN	C40-C37	3.02	1.52	1.43
36	a	316	II0	C34-C36	3.02	1.52	1.46
28	m	607	CLA	CMD-C2D	-3.02	1.44	1.50
31	i	316	WVN	C19-C22	3.02	1.52	1.46
31	K	104	WVN	C40-C37	3.02	1.52	1.43
28	k	610	CLA	C4B-NB	3.02	1.41	1.37
28	i	308	CLA	C4B-NB	3.02	1.41	1.37
38	m	611	KC2	CHC-C1C	3.02	1.46	1.39
28	B	837	CLA	C1D-ND	3.02	1.41	1.37
36	i	313	II0	C33-C35	3.02	1.52	1.46
36	c	617	II0	C27-C25	3.02	1.52	1.50
31	l	301	WVN	C40-C37	3.02	1.52	1.43
36	a	315	II0	C34-C36	3.02	1.52	1.46
28	c	606	CLA	C4B-NB	3.02	1.41	1.37
28	k	605	CLA	C4B-NB	3.02	1.41	1.37
38	l	310	KC2	C1B-NB	-3.02	1.33	1.37
31	l	315	WVN	C23-C25	3.02	1.52	1.46
31	i	316	WVN	C31-C32	3.01	1.52	1.46
31	J	102	WVN	C30-C28	3.01	1.52	1.43
28	s	208	CLA	C4B-NB	3.01	1.41	1.37
28	b	611	CLA	C1D-ND	3.01	1.41	1.37
36	d	314	II0	C12-C14	-3.01	1.46	1.51
38	d	311	KC2	CHC-C1C	3.01	1.46	1.39
31	A	848	WVN	C40-C37	3.01	1.52	1.43
28	n	604	CLA	C4B-NB	3.01	1.41	1.37
28	A	851	CLA	CMB-C2B	-3.01	1.44	1.50
31	A	846	WVN	C31-C32	3.01	1.52	1.46
28	A	827	CLA	C1D-ND	3.01	1.41	1.37
31	L	205	WVN	C39-C36	3.01	1.52	1.43
38	i	319	KC2	C1B-NB	-3.01	1.33	1.37
31	B	844	WVN	C39-C36	3.01	1.52	1.43
31	B	845	WVN	C40-C37	3.01	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	l	303	CLA	C4B-NB	3.00	1.41	1.37
38	f	611	KC2	C1B-NB	-3.00	1.33	1.37
31	L	205	WVN	C19-C22	3.00	1.52	1.46
31	R	201	WVN	C19-C22	3.00	1.52	1.46
31	A	845	WVN	C39-C36	3.00	1.52	1.43
38	c	610	KC2	C1B-NB	-3.00	1.33	1.37
36	c	613	II0	C33-C35	3.00	1.52	1.46
31	B	845	WVN	C33-C34	3.00	1.52	1.46
28	j	608	CLA	C4B-NB	3.00	1.41	1.37
28	B	839	CLA	C4B-NB	3.00	1.41	1.37
31	A	848	WVN	C29-C26	3.00	1.52	1.43
28	g	302	CLA	C4B-NB	3.00	1.41	1.37
36	g	316	II0	C33-C35	2.99	1.52	1.46
31	K	102	WVN	C33-C34	2.99	1.52	1.46
36	b	617	II0	C33-C35	2.99	1.52	1.46
36	k	621	II0	C12-C14	-2.99	1.46	1.51
28	l	302	CLA	C4B-NB	2.99	1.41	1.37
31	K	102	WVN	C40-C37	2.99	1.52	1.43
28	e	610	CLA	C4B-NB	2.99	1.41	1.37
28	n	613	CLA	C4B-NB	2.99	1.41	1.37
31	J	101	WVN	C02-C11	2.99	1.54	1.50
31	F	204	WVN	C39-C36	2.99	1.52	1.43
31	A	847	WVN	C19-C22	2.99	1.52	1.46
28	A	807	CLA	C1D-ND	2.99	1.41	1.37
28	c	605	CLA	C1D-ND	2.99	1.41	1.37
31	I	101	WVN	C39-C36	2.99	1.52	1.43
28	b	606	CLA	C4B-NB	2.99	1.41	1.37
38	n	611	KC2	C1B-NB	-2.99	1.33	1.37
28	h	301	CLA	C4B-NB	2.99	1.41	1.37
28	d	304	CLA	C4B-NB	2.99	1.41	1.37
31	B	846	WVN	C19-C22	2.98	1.52	1.46
28	a	303	CLA	C1D-ND	2.98	1.41	1.37
28	B	806	CLA	C1D-ND	2.98	1.41	1.37
28	k	602	CLA	C4B-NB	2.98	1.41	1.37
28	B	821	CLA	C4B-NB	2.98	1.41	1.37
28	s	202	CLA	C4B-NB	2.98	1.41	1.37
28	c	612	CLA	C4B-NB	2.98	1.41	1.37
31	B	844	WVN	C40-C37	2.98	1.52	1.43
32	a	320	LMT	O3'-C3'	-2.98	1.35	1.43
31	L	201	WVN	C30-C28	2.98	1.52	1.43
31	K	102	WVN	C23-C25	2.98	1.52	1.46
31	e	615	WVN	C19-C22	2.98	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	605	CLA	C4B-NB	2.98	1.41	1.37
28	c	601	CLA	C1D-ND	2.98	1.41	1.37
36	b	617	II0	C27-C25	2.97	1.52	1.50
31	K	102	WVN	C30-C28	2.97	1.52	1.43
28	g	304	CLA	C4B-NB	2.97	1.41	1.37
28	Q	303	CLA	CMB-C2B	-2.97	1.44	1.50
28	B	817	CLA	C4B-NB	2.97	1.41	1.37
28	L	207	CLA	C4B-NB	2.97	1.41	1.37
36	j	614	II0	C33-C35	2.97	1.52	1.46
31	M	101	WVN	C40-C37	2.97	1.52	1.43
31	J	101	WVN	C39-C36	2.96	1.52	1.43
36	b	614	II0	C33-C35	2.96	1.52	1.46
28	i	305	CLA	C4B-NB	2.96	1.41	1.37
36	l	314	II0	C33-C35	2.96	1.52	1.46
28	B	807	CLA	C1D-ND	2.96	1.41	1.37
28	A	813	CLA	C4B-NB	2.96	1.41	1.37
31	B	848	WVN	C40-C37	2.96	1.52	1.43
28	B	817	CLA	C1D-ND	2.96	1.41	1.37
31	B	845	WVN	C30-C28	2.96	1.52	1.43
36	k	617	II0	C12-C14	-2.96	1.46	1.51
28	B	802	CLA	C1B-C2B	2.96	1.50	1.43
31	R	202	WVN	C40-C37	2.95	1.52	1.43
31	s	205	WVN	C29-C26	2.95	1.52	1.43
36	g	318	II0	C12-C14	-2.95	1.46	1.51
28	b	604	CLA	C4B-NB	2.95	1.41	1.37
31	A	848	WVN	C30-C28	2.95	1.52	1.43
31	B	848	WVN	C33-C34	2.95	1.52	1.46
31	L	206	WVN	C30-C28	2.95	1.52	1.43
36	a	314	II0	C33-C35	2.94	1.52	1.46
28	A	801	CLA	C4B-NB	2.94	1.41	1.37
28	f	609	CLA	C4B-NB	2.94	1.41	1.37
38	j	611	KC2	C1B-NB	-2.94	1.34	1.37
31	K	102	WVN	C39-C36	2.94	1.52	1.43
31	l	301	WVN	C19-C22	2.94	1.52	1.46
28	m	607	CLA	C4B-NB	2.94	1.41	1.37
31	R	202	WVN	C30-C28	2.94	1.52	1.43
31	B	846	WVN	C23-C25	2.93	1.52	1.46
36	a	316	II0	C12-C14	-2.93	1.46	1.51
31	A	848	WVN	C19-C22	2.93	1.52	1.46
28	g	307	CLA	C4B-NB	2.93	1.41	1.37
31	M	101	WVN	C30-C28	2.93	1.52	1.43
31	J	101	WVN	C23-C25	2.93	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	835	CLA	C4B-NB	2.93	1.41	1.37
28	F	202	CLA	C4B-NB	2.93	1.41	1.37
28	j	604	CLA	C4B-NB	2.92	1.41	1.37
28	b	602	CLA	C4B-NB	2.92	1.41	1.37
28	h	302	CLA	C4B-NB	2.92	1.41	1.37
31	s	205	WVN	C31-C32	2.92	1.52	1.46
31	B	846	WVN	C31-C32	2.92	1.52	1.46
31	A	845	WVN	C19-C22	2.92	1.52	1.46
28	f	610	CLA	C1D-ND	2.92	1.41	1.37
38	l	310	KC2	CHC-C1C	2.92	1.45	1.39
28	A	801	CLA	C1B-C2B	2.92	1.50	1.43
31	l	301	WVN	C29-C26	2.92	1.52	1.43
28	B	831	CLA	CMB-C2B	-2.92	1.44	1.50
36	b	613	II0	C34-C36	2.92	1.52	1.46
28	j	605	CLA	C1B-C2B	2.92	1.50	1.43
31	B	847	WVN	C39-C36	2.91	1.52	1.43
31	s	205	WVN	C40-C37	2.91	1.52	1.43
31	M	101	WVN	C33-C34	2.91	1.52	1.46
28	d	301	CLA	C4B-NB	2.91	1.41	1.37
28	B	825	CLA	C1D-ND	2.91	1.41	1.37
36	c	615	II0	C12-C14	-2.91	1.46	1.51
31	B	848	WVN	C29-C26	2.91	1.52	1.43
31	K	104	WVN	C31-C32	2.90	1.52	1.46
28	i	311	CLA	MG-NA	2.90	2.13	2.06
38	k	612	KC2	C1B-NB	-2.90	1.34	1.37
28	B	820	CLA	C4B-NB	2.90	1.41	1.37
28	a	306	CLA	C4B-NB	2.90	1.41	1.37
31	J	102	WVN	C39-C36	2.90	1.52	1.43
28	Q	303	CLA	C1D-ND	2.90	1.41	1.37
28	B	840	CLA	C4B-NB	2.90	1.41	1.37
28	B	814	CLA	C1D-ND	2.90	1.41	1.37
31	B	848	WVN	C31-C32	2.90	1.52	1.46
36	m	614	II0	C33-C35	2.90	1.52	1.46
36	m	616	II0	C33-C35	2.90	1.52	1.46
28	c	605	CLA	C4B-NB	2.90	1.41	1.37
36	g	317	II0	C30-C26	-2.90	1.31	1.37
36	b	613	II0	C33-C35	2.90	1.52	1.46
31	B	845	WVN	C23-C25	2.90	1.52	1.46
38	k	611	KC2	C1B-NB	-2.90	1.34	1.37
36	i	315	II0	C33-C35	2.90	1.52	1.46
31	B	848	WVN	C39-C36	2.89	1.52	1.43
28	B	812	CLA	C4B-NB	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	308	CLA	C4B-NB	2.89	1.41	1.37
31	B	847	WVN	C31-C32	2.89	1.52	1.46
28	d	301	CLA	C1B-C2B	2.89	1.49	1.43
28	m	606	CLA	C4B-NB	2.89	1.41	1.37
31	M	101	WVN	C39-C36	2.89	1.52	1.43
36	k	621	II0	C33-C35	2.89	1.52	1.46
28	B	836	CLA	C4B-NB	2.89	1.41	1.37
28	k	609	CLA	C4B-NB	2.89	1.41	1.37
36	m	615	II0	C33-C35	2.89	1.52	1.46
31	B	844	WVN	C30-C28	2.89	1.52	1.43
31	I	101	WVN	C19-C22	2.89	1.52	1.46
28	b	607	CLA	C1D-ND	2.89	1.41	1.37
28	A	815	CLA	CMB-C2B	-2.89	1.44	1.50
31	B	844	WVN	C33-C34	2.89	1.52	1.46
31	L	201	WVN	C39-C36	2.88	1.52	1.43
28	g	306	CLA	C1B-C2B	2.88	1.49	1.43
28	f	603	CLA	C4B-NB	2.88	1.41	1.37
31	F	203	WVN	C39-C36	2.88	1.52	1.43
36	d	316	II0	C28-C26	2.88	1.52	1.50
31	R	202	WVN	C33-C34	2.88	1.52	1.46
28	A	840	CLA	C1D-ND	2.88	1.41	1.37
36	e	613	II0	C33-C35	2.88	1.52	1.46
28	B	826	CLA	C1D-ND	2.88	1.41	1.37
28	b	610	CLA	C4B-NB	2.88	1.41	1.37
28	e	601	CLA	C4B-NB	2.88	1.41	1.37
28	L	204	CLA	C4B-NB	2.88	1.41	1.37
28	A	835	CLA	C4B-NB	2.87	1.41	1.37
28	R	203	CLA	C4B-NB	2.87	1.41	1.37
36	c	614	II0	C34-C36	2.87	1.52	1.46
28	B	825	CLA	CMD-C2D	-2.87	1.44	1.50
31	s	205	WVN	C33-C34	2.87	1.52	1.46
28	m	603	CLA	C1D-ND	2.87	1.41	1.37
28	l	303	CLA	C1D-ND	2.87	1.41	1.37
28	k	601	CLA	C4B-NB	2.87	1.41	1.37
28	j	607	CLA	CMD-C2D	-2.87	1.44	1.50
28	A	819	CLA	C4B-NB	2.87	1.41	1.37
28	e	606	CLA	C1B-C2B	2.87	1.49	1.43
28	b	610	CLA	C1B-C2B	2.87	1.49	1.43
28	b	612	CLA	CMD-C2D	-2.87	1.44	1.50
31	F	203	WVN	C40-C37	2.87	1.52	1.43
28	B	830	CLA	C4B-NB	2.87	1.41	1.37
28	A	829	CLA	C4B-NB	2.87	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	101	WVN	C33-C34	2.87	1.52	1.46
38	g	313	KC2	C1B-NB	-2.87	1.34	1.37
38	i	310	KC2	CHC-C1C	2.87	1.45	1.39
31	L	205	WVN	C40-C37	2.86	1.52	1.43
38	g	314	KC2	C1B-NB	-2.86	1.34	1.37
28	n	609	CLA	C1B-C2B	2.86	1.49	1.43
38	i	310	KC2	C3C-C4C	2.86	1.50	1.44
28	h	303	CLA	C1D-ND	2.86	1.41	1.37
28	O	202	CLA	C4B-NB	2.86	1.41	1.37
31	M	101	WVN	C31-C32	2.86	1.52	1.46
31	I	101	WVN	C40-C37	2.86	1.52	1.43
28	A	820	CLA	C1D-ND	2.86	1.41	1.37
28	c	603	CLA	C4B-NB	2.86	1.41	1.37
28	b	601	CLA	C4B-NB	2.86	1.41	1.37
28	e	608	CLA	C4B-NB	2.86	1.41	1.37
28	d	304	CLA	CMC-C2C	-2.86	1.44	1.50
28	h	303	CLA	C4B-NB	2.85	1.41	1.37
28	K	101	CLA	C4B-NB	2.85	1.41	1.37
31	l	301	WVN	C31-C32	2.85	1.52	1.46
31	M	101	WVN	C29-C26	2.85	1.52	1.43
36	l	312	II0	C33-C35	2.85	1.52	1.46
28	A	802	CLA	C4B-NB	2.85	1.41	1.37
28	j	603	CLA	C4B-NB	2.85	1.41	1.37
31	l	301	WVN	C39-C36	2.85	1.52	1.43
36	k	616	II0	C33-C35	2.85	1.52	1.46
28	B	816	CLA	C4B-NB	2.85	1.41	1.37
31	B	847	WVN	C30-C28	2.85	1.52	1.43
36	k	615	II0	C12-C14	-2.85	1.46	1.51
28	e	604	CLA	C1B-C2B	2.84	1.49	1.43
28	B	810	CLA	C3B-C4B	2.84	1.51	1.42
31	e	615	WVN	C02-C11	2.84	1.54	1.50
28	A	809	CLA	C1D-ND	2.84	1.41	1.37
28	f	604	CLA	C4B-NB	2.84	1.41	1.37
31	A	845	WVN	C33-C34	2.84	1.52	1.46
31	F	204	WVN	C19-C22	2.84	1.52	1.46
31	B	848	WVN	C02-C11	2.84	1.54	1.50
31	s	205	WVN	C30-C28	2.84	1.52	1.43
28	j	613	CLA	C4B-NB	2.84	1.41	1.37
28	B	841	CLA	C4B-NB	2.84	1.41	1.37
28	f	605	CLA	C1B-C2B	2.84	1.49	1.43
36	c	614	II0	C33-C35	2.84	1.52	1.46
31	A	846	WVN	C30-C28	2.83	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	824	CLA	C1D-ND	2.83	1.41	1.37
28	j	602	CLA	C4B-NB	2.83	1.41	1.37
28	l	308	CLA	C4B-NB	2.83	1.41	1.37
31	K	104	WVN	C29-C26	2.83	1.52	1.43
28	A	811	CLA	C3B-C4B	2.83	1.51	1.42
28	a	305	CLA	C4B-NB	2.83	1.41	1.37
31	A	846	WVN	C19-C22	2.83	1.52	1.46
28	s	206	CLA	C4B-NB	2.83	1.41	1.37
31	R	201	WVN	C02-C11	2.83	1.54	1.50
28	A	822	CLA	CMD-C2D	-2.83	1.45	1.50
31	K	104	WVN	C20-C13	2.83	1.54	1.45
31	F	203	WVN	C29-C26	2.83	1.51	1.43
28	i	312	CLA	C4B-NB	2.83	1.41	1.37
31	A	847	WVN	C40-C37	2.83	1.51	1.43
28	A	851	CLA	C1D-ND	2.83	1.41	1.37
28	A	804	CLA	CMC-C2C	-2.82	1.45	1.50
28	n	609	CLA	C4B-NB	2.82	1.41	1.37
28	B	823	CLA	C4B-NB	2.82	1.41	1.37
28	a	311	CLA	C4B-NB	2.82	1.41	1.37
28	Q	302	CLA	C1D-ND	2.82	1.41	1.37
31	F	203	WVN	C31-C32	2.82	1.52	1.46
28	A	838	CLA	C3B-C4B	2.82	1.50	1.42
31	B	847	WVN	C40-C37	2.81	1.51	1.43
28	h	304	CLA	C4B-NB	2.81	1.41	1.37
38	g	313	KC2	C3C-C4C	2.81	1.50	1.44
28	A	803	CLA	C4B-NB	2.81	1.41	1.37
31	B	846	WVN	C29-C26	2.81	1.51	1.43
28	m	602	CLA	C1D-ND	2.81	1.41	1.37
28	j	607	CLA	C4B-NB	2.81	1.41	1.37
31	F	203	WVN	C33-C34	2.80	1.52	1.46
28	K	103	CLA	C1B-C2B	2.80	1.49	1.43
28	B	837	CLA	C4B-NB	2.80	1.41	1.37
28	e	606	CLA	C4B-NB	2.80	1.41	1.37
28	m	604	CLA	C4B-NB	2.80	1.41	1.37
28	A	809	CLA	C4B-NB	2.80	1.41	1.37
31	A	847	WVN	C39-C36	2.80	1.51	1.43
38	n	612	KC2	C1B-NB	-2.80	1.34	1.37
36	g	320	II0	C33-C35	2.80	1.51	1.46
28	j	609	CLA	C4B-NB	2.80	1.41	1.37
31	L	201	WVN	C29-C26	2.80	1.51	1.43
28	l	307	CLA	CMD-C2D	-2.79	1.45	1.50
28	A	821	CLA	C4B-NB	2.79	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	810	CLA	C1D-ND	2.79	1.41	1.37
28	i	303	CLA	C4B-NB	2.79	1.41	1.37
28	m	610	CLA	C1B-C2B	2.79	1.49	1.43
31	s	205	WVN	C19-C22	2.79	1.51	1.46
36	f	616	II0	C33-C35	2.78	1.51	1.46
31	R	202	WVN	C31-C32	2.78	1.51	1.46
38	e	609	KC2	C1B-NB	-2.78	1.34	1.37
28	e	603	CLA	C4B-NB	2.78	1.41	1.37
31	L	201	WVN	C33-C34	2.78	1.51	1.46
36	e	612	II0	C16-C03	2.78	1.59	1.53
36	j	614	II0	C34-C36	2.78	1.51	1.46
31	K	104	WVN	C23-C25	2.78	1.51	1.46
36	k	615	II0	C33-C35	2.78	1.51	1.46
31	A	846	WVN	C40-C37	2.78	1.51	1.43
36	n	618	II0	C12-C14	-2.77	1.46	1.51
28	m	612	CLA	C4B-NB	2.77	1.41	1.37
38	i	310	KC2	C1A-CHA	2.77	1.47	1.40
28	a	307	CLA	C4B-NB	2.77	1.41	1.37
31	L	206	WVN	C31-C32	2.77	1.51	1.46
31	A	845	WVN	C30-C28	2.77	1.51	1.43
28	A	818	CLA	CMB-C2B	-2.77	1.45	1.50
38	d	310	KC2	C1B-NB	-2.76	1.34	1.37
31	I	101	WVN	C30-C28	2.76	1.51	1.43
28	a	312	CLA	C4B-NB	2.76	1.41	1.37
28	i	309	CLA	C4B-NB	2.76	1.41	1.37
36	f	615	II0	C33-C35	2.76	1.51	1.46
28	c	602	CLA	C4B-NB	2.76	1.41	1.37
28	g	322	CLA	C1B-C2B	2.76	1.49	1.43
31	F	203	WVN	C19-C22	2.76	1.51	1.46
31	L	201	WVN	C19-C22	2.76	1.51	1.46
28	h	307	CLA	C1B-C2B	2.76	1.49	1.43
28	l	307	CLA	C1B-C2B	2.75	1.49	1.43
28	A	837	CLA	C1B-C2B	2.75	1.49	1.43
31	A	847	WVN	C31-C32	2.75	1.51	1.46
37	a	317	IHT	C18-C07	2.75	1.54	1.45
28	n	613	CLA	C1B-C2B	2.75	1.49	1.43
31	R	202	WVN	C39-C36	2.75	1.51	1.43
28	Q	302	CLA	C1B-C2B	2.75	1.49	1.43
28	i	303	CLA	CMD-C2D	-2.75	1.45	1.50
28	A	840	CLA	C4B-NB	2.75	1.41	1.37
28	m	605	CLA	C1B-C2B	2.75	1.49	1.43
28	B	827	CLA	C1D-ND	2.75	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	803	CLA	C4B-NB	2.74	1.41	1.37
31	L	201	WVN	C40-C37	2.74	1.51	1.43
31	K	102	WVN	C29-C26	2.74	1.51	1.43
28	b	609	CLA	C1D-ND	2.74	1.41	1.37
28	k	603	CLA	C4B-NB	2.73	1.41	1.37
28	l	309	CLA	C4B-NB	2.73	1.41	1.37
28	B	821	CLA	C4-C3	-2.73	1.44	1.50
28	k	605	CLA	C1B-C2B	2.73	1.49	1.43
28	j	610	CLA	C1B-C2B	2.73	1.49	1.43
28	l	305	CLA	C4B-NB	2.73	1.41	1.37
31	F	204	WVN	C02-C11	2.73	1.54	1.50
28	B	808	CLA	C1D-ND	2.73	1.41	1.37
28	A	830	CLA	CMD-C2D	-2.73	1.45	1.50
28	A	823	CLA	C4B-NB	2.73	1.41	1.37
28	B	835	CLA	CMD-C2D	-2.73	1.45	1.50
28	A	814	CLA	C4B-NB	2.73	1.41	1.37
31	R	202	WVN	C29-C26	2.72	1.51	1.43
28	f	609	CLA	CMC-C2C	-2.72	1.45	1.50
28	f	601	CLA	C3B-C4B	2.72	1.50	1.42
28	A	821	CLA	C1D-ND	2.72	1.41	1.37
28	A	823	CLA	C1B-C2B	2.72	1.49	1.43
28	B	827	CLA	C4B-NB	2.72	1.41	1.37
28	A	855	CLA	CMB-C2B	-2.72	1.45	1.50
28	A	804	CLA	C4B-NB	2.72	1.41	1.37
28	L	203	CLA	C4B-NB	2.72	1.41	1.37
28	h	302	CLA	CMC-C2C	-2.72	1.45	1.50
31	l	315	WVN	C02-C11	2.71	1.54	1.50
31	R	202	WVN	C23-C25	2.71	1.51	1.46
28	l	302	CLA	C1B-C2B	2.71	1.49	1.43
28	B	819	CLA	CMD-C2D	-2.71	1.45	1.50
28	c	606	CLA	CMB-C2B	-2.71	1.45	1.50
38	s	201	KC2	CHB-C4A	2.71	1.45	1.39
28	m	602	CLA	C4B-NB	2.71	1.41	1.37
37	c	616	IHT	C25-C23	2.71	1.56	1.50
29	A	842	PQN	O4-C4	-2.71	1.17	1.23
28	m	603	CLA	C4B-NB	2.71	1.41	1.37
28	m	609	CLA	C4B-NB	2.71	1.41	1.37
28	B	825	CLA	C4B-NB	2.71	1.41	1.37
28	n	603	CLA	C4B-NB	2.71	1.41	1.37
28	n	602	CLA	C4B-NB	2.70	1.41	1.37
31	A	848	WVN	C31-C32	2.70	1.51	1.46
28	n	610	CLA	C3B-C4B	2.70	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	207	CLA	C1B-C2B	2.70	1.49	1.43
31	B	844	WVN	C29-C26	2.70	1.51	1.43
28	B	814	CLA	C4B-NB	2.70	1.41	1.37
38	g	312	KC2	C1B-NB	-2.70	1.34	1.37
31	e	615	WVN	C20-C13	2.70	1.54	1.45
28	c	608	CLA	C4B-NB	2.70	1.41	1.37
31	L	206	WVN	C29-C26	2.70	1.51	1.43
28	m	606	CLA	C1B-C2B	2.70	1.49	1.43
28	B	839	CLA	C3B-C4B	2.69	1.50	1.42
28	a	310	CLA	C1B-C2B	2.69	1.49	1.43
28	B	818	CLA	C4B-NB	2.69	1.41	1.37
28	A	820	CLA	CMB-C2B	-2.69	1.45	1.50
28	k	601	CLA	C1B-C2B	2.69	1.49	1.43
37	k	618	IHT	C18-C07	2.69	1.54	1.45
28	g	303	CLA	CMD-C2D	-2.69	1.45	1.50
31	J	102	WVN	C02-C11	2.69	1.54	1.50
38	d	311	KC2	C1A-CHA	2.69	1.47	1.40
28	l	306	CLA	C1B-C2B	2.69	1.49	1.43
28	f	608	CLA	CMC-C2C	-2.69	1.45	1.50
28	f	613	CLA	C3B-C4B	2.69	1.50	1.42
31	M	101	WVN	C19-C22	2.69	1.51	1.46
38	s	201	KC2	C1A-CHA	2.68	1.47	1.40
28	B	802	CLA	CMD-C2D	-2.68	1.45	1.50
36	j	615	II0	C33-C35	2.68	1.51	1.46
28	h	308	CLA	C4B-NB	2.68	1.41	1.37
28	f	603	CLA	C1B-C2B	2.68	1.49	1.43
37	k	618	IHT	C25-C23	2.68	1.56	1.50
38	m	611	KC2	C1A-CHA	2.68	1.47	1.40
28	A	839	CLA	C1B-C2B	2.67	1.49	1.43
28	g	308	CLA	C1B-C2B	2.67	1.49	1.43
31	R	202	WVN	C19-C22	2.67	1.51	1.46
28	m	601	CLA	C1B-C2B	2.67	1.49	1.43
31	B	845	WVN	C29-C26	2.67	1.51	1.43
28	F	202	CLA	C1B-C2B	2.67	1.49	1.43
37	c	616	IHT	C18-C07	2.67	1.54	1.45
28	h	304	CLA	C1B-C2B	2.67	1.49	1.43
28	s	203	CLA	C4B-NB	2.67	1.41	1.37
28	g	309	CLA	C1B-C2B	2.67	1.49	1.43
37	m	617	IHT	C25-C23	2.67	1.56	1.50
31	F	203	WVN	C28-C25	-2.67	1.29	1.35
28	j	612	CLA	C3B-C4B	2.67	1.50	1.42
28	A	817	CLA	C4B-NB	2.67	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	m	607	CLA	C3B-C4B	2.67	1.50	1.42
28	e	608	CLA	C1B-C2B	2.67	1.49	1.43
28	b	606	CLA	C1B-C2B	2.66	1.49	1.43
38	k	613	KC2	C1B-NB	-2.66	1.34	1.37
28	s	203	CLA	C1B-C2B	2.66	1.49	1.43
28	L	203	CLA	C1D-ND	2.66	1.41	1.37
28	A	824	CLA	C4B-NB	2.66	1.41	1.37
31	F	203	WVN	C30-C28	2.66	1.51	1.43
28	f	608	CLA	CHC-C1C	2.66	1.43	1.38
38	d	310	KC2	C1A-CHA	2.65	1.47	1.40
28	A	830	CLA	C4B-NB	2.65	1.41	1.37
28	m	613	CLA	C4B-NB	2.65	1.41	1.37
37	b	616	IHT	C25-C23	2.65	1.56	1.50
28	j	601	CLA	C1B-C2B	2.65	1.49	1.43
28	B	826	CLA	CMB-C2B	-2.65	1.45	1.50
37	b	615	IHT	C25-C23	2.65	1.56	1.50
28	c	608	CLA	C1B-C2B	2.65	1.49	1.43
28	c	609	CLA	C1B-C2B	2.65	1.49	1.43
28	g	303	CLA	C1D-ND	2.65	1.41	1.37
31	B	844	WVN	C31-C32	2.65	1.51	1.46
36	d	313	II0	C16-C03	2.65	1.58	1.53
28	K	103	CLA	C4B-NB	2.65	1.41	1.37
28	k	607	CLA	C1B-C2B	2.65	1.49	1.43
37	j	616	IHT	C25-C23	2.65	1.56	1.50
28	a	309	CLA	MG-NB	-2.64	2.00	2.05
28	f	606	CLA	C3B-C4B	2.64	1.50	1.42
31	L	205	WVN	C20-C13	2.64	1.54	1.45
37	O	204	IHT	C25-C23	2.64	1.56	1.50
28	A	822	CLA	C4B-NB	2.64	1.41	1.37
28	s	208	CLA	C1B-C2B	2.64	1.49	1.43
28	A	831	CLA	C1B-C2B	2.64	1.49	1.43
28	l	304	CLA	C1B-C2B	2.64	1.49	1.43
28	e	601	CLA	C3B-C4B	2.64	1.50	1.42
31	M	101	WVN	C23-C25	2.64	1.51	1.46
31	R	201	WVN	C23-C25	2.64	1.51	1.46
28	h	308	CLA	C1B-C2B	2.64	1.49	1.43
28	L	202	CLA	C3B-C4B	2.64	1.50	1.42
28	B	809	CLA	C1B-C2B	2.63	1.49	1.43
28	A	827	CLA	C4B-NB	2.63	1.41	1.37
37	g	319	IHT	C25-C23	2.63	1.56	1.50
28	A	819	CLA	C1B-C2B	2.63	1.49	1.43
38	f	611	KC2	C1A-CHA	2.63	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	802	CLA	C4B-NB	2.63	1.41	1.37
28	b	611	CLA	C1B-C2B	2.63	1.49	1.43
28	B	830	CLA	C1B-C2B	2.63	1.49	1.43
28	A	835	CLA	C1B-C2B	2.63	1.49	1.43
28	A	808	CLA	C1B-C2B	2.63	1.49	1.43
28	A	828	CLA	C1D-ND	2.62	1.41	1.37
28	B	817	CLA	C3B-C4B	2.62	1.50	1.42
28	l	305	CLA	C1B-C2B	2.62	1.49	1.43
28	A	810	CLA	C1B-C2B	2.62	1.49	1.43
32	b	618	LMT	O3'-C3'	-2.62	1.36	1.43
28	j	606	CLA	C1B-C2B	2.62	1.49	1.43
28	d	312	CLA	C1B-C2B	2.62	1.49	1.43
36	g	317	II0	C16-C03	2.62	1.58	1.53
28	i	309	CLA	C1B-C2B	2.62	1.49	1.43
28	m	612	CLA	C1B-C2B	2.62	1.49	1.43
28	J	103	CLA	C1B-C2B	2.62	1.49	1.43
28	O	206	CLA	C4B-NB	2.62	1.41	1.37
28	A	820	CLA	C4B-NB	2.62	1.41	1.37
28	h	301	CLA	CMB-C2B	-2.62	1.45	1.50
28	B	819	CLA	C4B-NB	2.62	1.41	1.37
28	A	837	CLA	C4B-NB	2.61	1.41	1.37
36	g	317	II0	C33-C35	2.61	1.51	1.46
28	B	838	CLA	C4B-NB	2.61	1.41	1.37
37	f	617	IHT	C18-C07	2.61	1.54	1.45
28	c	611	CLA	C3B-C4B	2.61	1.50	1.42
37	b	616	IHT	C18-C07	2.61	1.54	1.45
28	B	812	CLA	CMD-C2D	-2.61	1.45	1.50
28	j	609	CLA	C1B-C2B	2.61	1.49	1.43
28	i	307	CLA	C1B-C2B	2.61	1.49	1.43
28	a	308	CLA	C3B-C4B	2.61	1.50	1.42
31	L	206	WVN	C23-C25	2.61	1.51	1.46
29	B	842	PQN	O4-C4	-2.61	1.17	1.23
28	B	821	CLA	CMC-C2C	-2.61	1.45	1.50
28	Q	303	CLA	CMD-C2D	-2.61	1.45	1.50
28	A	806	CLA	C3B-C4B	2.61	1.50	1.42
28	B	833	CLA	C4B-NB	2.61	1.41	1.37
28	e	604	CLA	C4B-NB	2.61	1.41	1.37
28	A	840	CLA	C1B-C2B	2.61	1.49	1.43
28	l	303	CLA	C1B-C2B	2.61	1.49	1.43
28	f	609	CLA	C3B-C4B	2.60	1.50	1.42
28	A	815	CLA	MG-NB	-2.60	2.00	2.05
28	i	304	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	304	CLA	C1B-C2B	2.60	1.49	1.43
36	i	320	II0	C16-C03	2.60	1.58	1.53
32	A	850	LMT	O3'-C3'	-2.60	1.36	1.43
28	B	806	CLA	C1B-C2B	2.60	1.49	1.43
28	g	322	CLA	CMD-C2D	-2.60	1.45	1.50
28	A	831	CLA	C4B-NB	2.60	1.41	1.37
28	c	603	CLA	C1D-ND	2.60	1.41	1.37
31	B	848	WVN	C20-C13	2.60	1.54	1.45
38	k	613	KC2	C1A-CHA	2.60	1.47	1.40
28	e	602	CLA	C3B-C4B	2.60	1.50	1.42
28	L	204	CLA	CMD-C2D	-2.60	1.45	1.50
28	m	607	CLA	CMC-C2C	-2.60	1.45	1.50
28	f	612	CLA	C1B-C2B	2.59	1.49	1.43
28	A	841	CLA	C1B-C2B	2.59	1.49	1.43
28	g	310	CLA	C4B-NB	2.59	1.41	1.37
28	A	834	CLA	CMD-C2D	-2.59	1.45	1.50
31	s	207	WVN	C20-C13	2.59	1.53	1.45
28	c	612	CLA	C1B-C2B	2.59	1.49	1.43
31	B	847	WVN	C33-C34	2.59	1.51	1.46
37	n	617	IHT	C18-C07	2.59	1.53	1.45
28	s	202	CLA	CMB-C2B	-2.59	1.45	1.50
28	n	607	CLA	C4B-NB	2.59	1.41	1.37
28	A	839	CLA	C4B-NB	2.59	1.41	1.37
28	i	305	CLA	C1B-C2B	2.59	1.49	1.43
28	g	322	CLA	C1D-ND	2.58	1.41	1.37
28	c	601	CLA	C1B-C2B	2.58	1.49	1.43
28	a	304	CLA	C4B-NB	2.58	1.41	1.37
32	a	302	LMT	O3'-C3'	-2.58	1.36	1.43
28	A	855	CLA	C1B-C2B	2.58	1.49	1.43
28	n	601	CLA	C1B-C2B	2.58	1.49	1.43
37	g	319	IHT	C18-C07	2.58	1.53	1.45
28	j	606	CLA	C4B-NB	2.58	1.41	1.37
28	f	608	CLA	C3B-C4B	2.58	1.50	1.42
28	c	608	CLA	CMC-C2C	-2.58	1.45	1.50
37	f	617	IHT	C25-C23	2.58	1.56	1.50
28	f	609	CLA	CHC-C1C	2.58	1.43	1.38
38	g	313	KC2	C1A-CHA	2.57	1.46	1.40
28	i	302	CLA	C1B-C2B	2.57	1.49	1.43
28	A	832	CLA	C4B-NB	2.57	1.41	1.37
28	B	828	CLA	C4B-NB	2.57	1.41	1.37
28	h	303	CLA	CMB-C2B	-2.57	1.45	1.50
37	n	617	IHT	C25-C23	2.57	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	k	610	CLA	C1B-C2B	2.57	1.49	1.43
28	b	601	CLA	C1B-C2B	2.57	1.49	1.43
31	B	845	WVN	C31-C32	2.57	1.51	1.46
31	R	201	WVN	C20-C13	2.57	1.53	1.45
28	B	829	CLA	C1B-C2B	2.56	1.49	1.43
28	n	605	CLA	C1B-C2B	2.56	1.49	1.43
28	a	309	CLA	C1B-C2B	2.56	1.49	1.43
28	n	610	CLA	C1B-C2B	2.56	1.49	1.43
28	A	828	CLA	C4B-NB	2.56	1.41	1.37
36	d	314	II0	C18-C04	2.56	1.58	1.53
28	A	812	CLA	C4B-NB	2.56	1.41	1.37
38	d	311	KC2	C3C-C4C	2.56	1.49	1.44
36	a	316	II0	C33-C35	2.56	1.51	1.46
31	I	101	WVN	C20-C13	2.56	1.53	1.45
28	A	855	CLA	CMD-C2D	-2.56	1.45	1.50
38	k	612	KC2	C1A-CHA	2.56	1.46	1.40
28	d	302	CLA	C4B-NB	2.56	1.41	1.37
28	g	304	CLA	C1B-C2B	2.56	1.49	1.43
28	g	311	CLA	C1B-C2B	2.55	1.49	1.43
28	B	808	CLA	C4B-NB	2.55	1.41	1.37
28	b	604	CLA	C1B-C2B	2.55	1.49	1.43
28	A	841	CLA	C4B-NB	2.55	1.41	1.37
28	A	816	CLA	C1B-C2B	2.55	1.49	1.43
28	B	801	CLA	C1D-ND	2.55	1.41	1.37
38	k	613	KC2	C3C-C4C	2.55	1.49	1.44
28	A	828	CLA	CMD-C2D	-2.55	1.45	1.50
28	B	829	CLA	CMB-C2B	-2.55	1.45	1.50
28	i	306	CLA	C1B-C2B	2.55	1.49	1.43
28	e	603	CLA	C1B-C2B	2.55	1.49	1.43
28	e	607	CLA	C1B-C2B	2.55	1.49	1.43
28	B	825	CLA	C1B-C2B	2.55	1.49	1.43
28	i	302	CLA	C3B-C4B	2.55	1.50	1.42
31	B	844	WVN	C23-C25	2.54	1.51	1.46
31	A	847	WVN	C29-C26	2.54	1.51	1.43
36	d	315	II0	C16-C03	2.54	1.58	1.53
28	b	603	CLA	C4B-NB	2.54	1.41	1.37
28	n	606	CLA	C1B-C2B	2.54	1.49	1.43
28	A	807	CLA	C4B-NB	2.54	1.41	1.37
28	g	308	CLA	C4B-NB	2.54	1.41	1.37
28	l	309	CLA	C1B-C2B	2.54	1.49	1.43
28	l	307	CLA	C4B-NB	2.54	1.41	1.37
37	m	617	IHT	C18-C07	2.54	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	h	308	CLA	CMD-C2D	-2.54	1.45	1.50
28	s	203	CLA	CMD-C2D	-2.53	1.45	1.50
28	j	604	CLA	CMD-C2D	-2.53	1.45	1.50
28	m	608	CLA	C1B-C2B	2.53	1.49	1.43
28	d	309	CLA	C1B-C2B	2.53	1.49	1.43
28	e	611	CLA	C1B-C2B	2.53	1.49	1.43
28	c	604	CLA	CMB-C2B	-2.53	1.45	1.50
28	m	603	CLA	CMD-C2D	-2.53	1.45	1.50
31	A	846	WVN	C23-C25	2.53	1.51	1.46
38	s	201	KC2	C3C-C4C	2.53	1.49	1.44
38	l	310	KC2	C1A-CHA	2.53	1.46	1.40
28	d	307	CLA	C3B-C4B	2.52	1.50	1.42
28	d	307	CLA	C1B-C2B	2.52	1.49	1.43
28	F	201	CLA	C3B-C4B	2.52	1.50	1.42
28	a	303	CLA	CMD-C2D	-2.52	1.45	1.50
29	A	842	PQN	O1-C1	-2.52	1.18	1.23
28	g	311	CLA	C3B-C4B	2.52	1.50	1.42
28	n	608	CLA	CMD-C2D	-2.52	1.45	1.50
28	f	602	CLA	C1B-C2B	2.52	1.49	1.43
28	j	612	CLA	MG-NC	2.52	2.12	2.06
28	A	825	CLA	C1D-ND	2.52	1.41	1.37
28	i	311	CLA	C3B-C4B	2.52	1.50	1.42
28	K	101	CLA	C1B-C2B	2.52	1.49	1.43
28	B	813	CLA	C4B-NB	2.52	1.41	1.37
28	d	305	CLA	C3B-C4B	2.52	1.50	1.42
36	c	614	II0	C16-C03	2.51	1.58	1.53
37	m	617	IHT	C39-C35	2.51	1.55	1.50
28	d	308	CLA	C3B-C4B	2.51	1.50	1.42
31	i	316	WVN	C20-C13	2.51	1.53	1.45
28	A	833	CLA	C1B-C2B	2.51	1.49	1.43
28	l	303	CLA	CMD-C2D	-2.51	1.45	1.50
28	J	103	CLA	CMD-C2D	-2.51	1.45	1.50
28	A	833	CLA	CMB-C2B	-2.51	1.45	1.50
38	g	314	KC2	C3C-C4C	2.51	1.49	1.44
28	s	206	CLA	C1B-C2B	2.51	1.49	1.43
28	g	302	CLA	C1B-C2B	2.51	1.49	1.43
36	a	315	II0	C16-C03	2.51	1.58	1.53
29	B	842	PQN	O1-C1	-2.51	1.18	1.23
28	B	838	CLA	C1B-C2B	2.51	1.49	1.43
28	F	201	CLA	CMC-C2C	-2.51	1.45	1.50
37	a	317	IHT	C25-C23	2.51	1.55	1.50
28	B	807	CLA	CMD-C2D	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	613	CLA	C1B-C2B	2.51	1.49	1.43
28	B	804	CLA	C1B-C2B	2.51	1.49	1.43
28	O	206	CLA	CMB-C2B	-2.51	1.45	1.50
31	A	848	WVN	C02-C11	2.51	1.54	1.50
31	L	201	WVN	C31-C32	2.51	1.51	1.46
28	d	303	CLA	C1B-C2B	2.51	1.49	1.43
28	B	836	CLA	C1B-C2B	2.51	1.49	1.43
28	a	303	CLA	C1B-C2B	2.50	1.49	1.43
28	m	602	CLA	CMC-C2C	-2.50	1.45	1.50
28	b	606	CLA	CMC-C2C	-2.50	1.45	1.50
28	h	306	CLA	C3B-C4B	2.50	1.50	1.42
28	A	852	CLA	MG-NB	-2.50	2.00	2.05
38	c	610	KC2	C1A-CHA	2.50	1.46	1.40
28	i	308	CLA	C1B-C2B	2.50	1.49	1.43
28	B	814	CLA	CMC-C2C	-2.50	1.45	1.50
28	B	822	CLA	C1D-ND	2.50	1.41	1.37
28	k	614	CLA	C1B-C2B	2.50	1.49	1.43
28	f	607	CLA	C3B-C4B	2.50	1.50	1.42
38	g	312	KC2	C4A-C3A	2.50	1.49	1.44
36	a	318	II0	C16-C03	2.50	1.58	1.53
28	k	604	CLA	C1B-C2B	2.50	1.49	1.43
28	h	306	CLA	CHC-C1C	2.49	1.43	1.38
28	k	606	CLA	C1B-C2B	2.49	1.49	1.43
28	a	305	CLA	CMD-C2D	-2.49	1.45	1.50
36	g	320	II0	C16-C03	2.49	1.58	1.53
28	B	807	CLA	C3B-C4B	2.49	1.50	1.42
38	n	612	KC2	C4A-C3A	2.49	1.49	1.44
28	B	812	CLA	C3B-C4B	2.49	1.50	1.42
28	b	607	CLA	C1B-C2B	2.49	1.49	1.43
28	g	305	CLA	C1B-C2B	2.49	1.49	1.43
28	B	807	CLA	CMB-C2B	-2.49	1.45	1.50
28	L	204	CLA	C1B-C2B	2.49	1.49	1.43
28	c	608	CLA	CMA-C3A	-2.48	1.47	1.53
28	c	607	CLA	C3B-C4B	2.48	1.50	1.42
38	i	319	KC2	C3C-C4C	2.48	1.49	1.44
28	A	830	CLA	C1D-ND	2.48	1.41	1.37
28	A	833	CLA	C4B-NB	2.48	1.41	1.37
37	R	204	IHT	C18-C07	2.48	1.53	1.45
28	B	827	CLA	C1B-C2B	2.48	1.49	1.43
38	d	310	KC2	C3C-C4C	2.48	1.49	1.44
28	a	303	CLA	CMB-C2B	-2.48	1.45	1.50
28	A	802	CLA	C1B-NB	-2.48	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	g	311	CLA	C4-C3	-2.48	1.44	1.50
37	O	204	IHT	C39-C35	2.48	1.55	1.50
31	h	309	WVN	C19-C22	2.48	1.51	1.46
28	A	825	CLA	C1B-C2B	2.48	1.48	1.43
28	e	604	CLA	CMD-C2D	-2.48	1.45	1.50
28	h	313	CLA	CMD-C2D	-2.48	1.45	1.50
28	b	608	CLA	C1B-C2B	2.48	1.48	1.43
28	a	304	CLA	C1B-C2B	2.48	1.48	1.43
28	B	801	CLA	CHC-C1C	2.48	1.43	1.38
37	b	615	IHT	C18-C07	2.48	1.53	1.45
37	k	618	IHT	C39-C35	2.48	1.55	1.50
31	L	201	WVN	C20-C13	2.47	1.53	1.45
36	b	613	II0	C16-C03	2.47	1.58	1.53
36	i	313	II0	C16-C03	2.47	1.58	1.53
36	i	315	II0	C18-C04	2.47	1.58	1.53
38	e	609	KC2	C3C-C4C	2.47	1.49	1.44
38	g	314	KC2	C1A-CHA	2.47	1.46	1.40
28	f	604	CLA	C1B-C2B	2.47	1.48	1.43
28	A	817	CLA	CMC-C2C	-2.47	1.45	1.50
28	h	306	CLA	C1B-C2B	2.47	1.48	1.43
28	A	809	CLA	CMC-C2C	-2.47	1.45	1.50
28	B	828	CLA	C3B-C4B	2.47	1.49	1.42
28	A	803	CLA	C1B-C2B	2.46	1.48	1.43
28	O	202	CLA	C1B-C2B	2.46	1.48	1.43
28	j	604	CLA	C1B-C2B	2.46	1.48	1.43
28	A	852	CLA	CHC-C1C	2.46	1.43	1.38
28	m	609	CLA	C3B-C4B	2.46	1.49	1.42
28	B	805	CLA	C4B-NB	2.46	1.41	1.37
28	d	306	CLA	C1B-C2B	2.46	1.48	1.43
38	s	201	KC2	CBD-CAD	-2.46	1.45	1.56
28	A	830	CLA	CMB-C2B	-2.46	1.45	1.50
28	A	809	CLA	C1B-C2B	2.46	1.48	1.43
37	j	616	IHT	C18-C07	2.46	1.53	1.45
28	B	808	CLA	MG-NB	-2.46	2.00	2.05
38	j	611	KC2	C1A-CHA	2.46	1.46	1.40
36	l	313	II0	C16-C03	2.46	1.58	1.53
37	R	204	IHT	C39-C35	2.46	1.55	1.50
28	A	814	CLA	C1B-C2B	2.46	1.48	1.43
28	A	840	CLA	CMD-C2D	-2.46	1.45	1.50
38	n	612	KC2	C1A-CHA	2.46	1.46	1.40
36	m	618	II0	C16-C03	2.45	1.58	1.53
28	j	601	CLA	C3B-C4B	2.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	811	CLA	CMC-C2C	-2.45	1.45	1.50
28	a	312	CLA	C1B-C2B	2.45	1.48	1.43
28	h	302	CLA	C3B-C4B	2.45	1.49	1.42
28	c	601	CLA	C3B-C4B	2.45	1.49	1.42
28	F	201	CLA	C1B-C2B	2.45	1.48	1.43
38	k	613	KC2	C4A-C3A	2.45	1.49	1.44
38	l	310	KC2	CBD-CAD	-2.45	1.45	1.56
28	A	817	CLA	CMB-C2B	-2.45	1.45	1.50
31	A	846	WVN	C28-C25	-2.45	1.30	1.35
28	B	813	CLA	CMC-C2C	-2.45	1.45	1.50
28	f	606	CLA	C1B-C2B	2.45	1.48	1.43
28	m	603	CLA	C3B-C4B	2.45	1.49	1.42
28	g	315	CLA	C1B-C2B	2.45	1.48	1.43
28	B	811	CLA	C1B-C2B	2.45	1.48	1.43
28	A	805	CLA	C1B-C2B	2.44	1.48	1.43
28	e	603	CLA	CMD-C2D	-2.44	1.45	1.50
36	n	618	II0	C16-C03	2.44	1.58	1.53
38	e	609	KC2	C1A-CHA	2.44	1.46	1.40
28	n	603	CLA	C3B-C4B	2.44	1.49	1.42
36	a	315	II0	C28-C26	2.44	1.52	1.50
37	O	204	IHT	C20-C15	2.44	1.54	1.50
38	i	319	KC2	C1A-CHA	2.44	1.46	1.40
37	R	204	IHT	C25-C23	2.44	1.55	1.50
28	d	308	CLA	C1B-C2B	2.44	1.48	1.43
31	i	316	WVN	C02-C11	2.44	1.54	1.50
28	A	803	CLA	CHC-C1C	2.44	1.43	1.38
28	i	312	CLA	C1B-C2B	2.44	1.48	1.43
28	c	603	CLA	C1B-C2B	2.44	1.48	1.43
28	A	803	CLA	C3B-C4B	2.44	1.49	1.42
28	c	602	CLA	C1D-ND	2.44	1.41	1.37
28	A	824	CLA	C1B-C2B	2.43	1.48	1.43
28	j	603	CLA	C3B-C4B	2.43	1.49	1.42
28	A	825	CLA	C4B-NB	2.43	1.41	1.37
31	M	101	WVN	C20-C13	2.43	1.53	1.45
38	i	310	KC2	C1B-NB	-2.43	1.34	1.37
28	g	302	CLA	C3B-C4B	2.43	1.49	1.42
28	B	834	CLA	C3B-C4B	2.43	1.49	1.42
28	l	311	CLA	C1B-C2B	2.43	1.48	1.43
38	s	204	KC2	CBD-CAD	-2.43	1.45	1.56
28	B	824	CLA	C4B-NB	2.43	1.41	1.37
28	i	306	CLA	CMD-C2D	-2.43	1.45	1.50
28	h	307	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	320	LMT	O2'-C2'	-2.43	1.36	1.43
28	B	817	CLA	CMD-C2D	-2.43	1.45	1.50
37	c	616	IHT	C39-C35	2.43	1.55	1.50
28	A	827	CLA	C1B-C2B	2.43	1.48	1.43
38	k	611	KC2	C3C-C4C	2.43	1.49	1.44
28	i	303	CLA	C1B-C2B	2.43	1.48	1.43
28	B	801	CLA	C3B-C4B	2.42	1.49	1.42
28	B	835	CLA	C3B-C4B	2.42	1.49	1.42
31	B	847	WVN	C19-C22	2.42	1.51	1.46
28	f	601	CLA	C1B-C2B	2.42	1.48	1.43
28	c	605	CLA	C1B-C2B	2.42	1.48	1.43
31	B	844	WVN	C20-C13	2.42	1.53	1.45
37	j	616	IHT	C20-C15	2.42	1.54	1.50
28	f	604	CLA	C3B-C4B	2.42	1.49	1.42
28	B	819	CLA	C1B-C2B	2.42	1.48	1.43
37	b	616	IHT	C20-C15	2.42	1.54	1.50
28	k	609	CLA	C3B-C4B	2.42	1.49	1.42
28	b	603	CLA	CMD-C2D	-2.42	1.45	1.50
38	g	313	KC2	CBD-CAD	-2.42	1.45	1.56
28	k	602	CLA	C1B-C2B	2.42	1.48	1.43
28	i	308	CLA	C3B-C4B	2.42	1.49	1.42
28	B	840	CLA	C1D-ND	2.42	1.41	1.37
28	c	607	CLA	C1B-C2B	2.42	1.48	1.43
37	c	616	IHT	C20-C15	2.42	1.54	1.50
28	c	602	CLA	CMD-C2D	-2.41	1.45	1.50
28	n	606	CLA	C3B-C4B	2.41	1.49	1.42
28	A	830	CLA	MG-NB	-2.41	2.01	2.05
36	l	316	II0	C16-C03	2.41	1.58	1.53
28	d	304	CLA	C3B-C4B	2.41	1.49	1.42
28	B	834	CLA	C1B-C2B	2.41	1.48	1.43
37	O	204	IHT	C18-C07	2.41	1.53	1.45
28	k	602	CLA	C3B-C4B	2.41	1.49	1.42
37	R	204	IHT	C20-C15	2.41	1.54	1.50
28	e	610	CLA	C1B-C2B	2.41	1.48	1.43
28	K	103	CLA	CMC-C2C	-2.41	1.45	1.50
28	b	602	CLA	C1B-C2B	2.41	1.48	1.43
31	F	203	WVN	C23-C25	2.41	1.51	1.46
36	b	614	II0	C16-C03	2.41	1.58	1.53
28	c	611	CLA	MG-NA	2.41	2.12	2.06
28	A	834	CLA	C4B-NB	2.41	1.41	1.37
28	h	305	CLA	C4B-NB	2.41	1.41	1.37
38	s	204	KC2	C1A-CHA	2.41	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	n	611	KC2	C1A-CHA	2.41	1.46	1.40
28	n	608	CLA	C1B-C2B	2.41	1.48	1.43
36	m	615	II0	C18-C04	2.41	1.58	1.53
28	A	812	CLA	C3B-C4B	2.41	1.49	1.42
28	A	854	CLA	C3B-C4B	2.41	1.49	1.42
28	B	817	CLA	CMB-C2B	-2.40	1.45	1.50
28	B	832	CLA	C4B-NB	2.40	1.41	1.37
31	J	101	WVN	C20-C13	2.40	1.53	1.45
28	A	812	CLA	CMC-C2C	-2.40	1.45	1.50
36	j	615	II0	C18-C04	2.40	1.58	1.53
28	g	310	CLA	C1B-C2B	2.40	1.48	1.43
28	n	604	CLA	C1B-C2B	2.40	1.48	1.43
37	n	617	IHT	C39-C35	2.40	1.55	1.50
31	B	847	WVN	C29-C26	2.40	1.50	1.43
28	k	609	CLA	C1B-C2B	2.40	1.48	1.43
28	B	820	CLA	CMC-C2C	-2.40	1.45	1.50
37	j	616	IHT	C39-C35	2.40	1.55	1.50
28	A	805	CLA	C4B-NB	2.40	1.41	1.37
28	e	605	CLA	C1B-C2B	2.40	1.48	1.43
28	h	306	CLA	CMD-C2D	-2.40	1.45	1.50
31	B	846	WVN	C20-C13	2.40	1.53	1.45
28	A	827	CLA	C3B-C4B	2.40	1.49	1.42
28	B	836	CLA	CMB-C2B	-2.40	1.45	1.50
28	e	611	CLA	C3B-C4B	2.40	1.49	1.42
28	B	804	CLA	C4B-NB	2.40	1.41	1.37
28	g	308	CLA	CMD-C2D	-2.40	1.45	1.50
38	e	609	KC2	C4A-C3A	2.40	1.49	1.44
28	m	602	CLA	CMD-C2D	-2.39	1.45	1.50
28	b	605	CLA	C1B-C2B	2.39	1.48	1.43
28	B	820	CLA	C1B-C2B	2.39	1.48	1.43
28	h	301	CLA	CMA-C3A	-2.39	1.48	1.53
38	g	314	KC2	C4A-C3A	2.39	1.49	1.44
28	B	822	CLA	MG-NB	-2.39	2.01	2.05
28	c	606	CLA	CMD-C2D	-2.39	1.45	1.50
38	f	611	KC2	CBD-CAD	-2.39	1.45	1.56
37	k	618	IHT	C20-C15	2.39	1.54	1.50
36	e	616	II0	C16-C03	2.39	1.58	1.53
28	B	829	CLA	CMD-C2D	-2.39	1.45	1.50
28	R	203	CLA	C3B-C4B	2.39	1.49	1.42
28	B	837	CLA	C1B-C2B	2.39	1.48	1.43
28	e	601	CLA	C1B-C2B	2.39	1.48	1.43
28	f	613	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	840	CLA	C1B-C2B	2.39	1.48	1.43
38	s	201	KC2	C1D-C2D	2.39	1.48	1.43
28	O	201	CLA	C1B-C2B	2.39	1.48	1.43
31	l	301	WVN	C23-C25	2.39	1.51	1.46
28	A	828	CLA	MG-NB	-2.39	2.01	2.05
28	B	824	CLA	MG-NB	-2.38	2.01	2.05
28	f	610	CLA	C1B-C2B	2.38	1.48	1.43
28	j	602	CLA	C1B-C2B	2.38	1.48	1.43
28	A	826	CLA	C3B-C4B	2.38	1.49	1.42
36	n	616	II0	C16-C03	2.38	1.58	1.53
28	B	841	CLA	C1B-C2B	2.38	1.48	1.43
28	k	606	CLA	CMD-C2D	-2.38	1.45	1.50
28	B	806	CLA	C4B-NB	2.38	1.41	1.37
28	A	813	CLA	C1B-C2B	2.38	1.48	1.43
28	g	307	CLA	C1B-C2B	2.38	1.48	1.43
28	g	310	CLA	CMD-C2D	-2.38	1.45	1.50
28	A	836	CLA	C1B-C2B	2.38	1.48	1.43
28	A	804	CLA	C1B-C2B	2.38	1.48	1.43
37	f	617	IHT	C20-C15	2.38	1.54	1.50
28	A	812	CLA	C1B-C2B	2.38	1.48	1.43
28	B	811	CLA	C4B-NB	2.38	1.41	1.37
28	B	808	CLA	C1B-NB	-2.38	1.34	1.37
38	d	311	KC2	C4A-C3A	2.38	1.49	1.44
28	A	826	CLA	C1B-C2B	2.38	1.48	1.43
37	f	617	IHT	C39-C35	2.38	1.55	1.50
28	c	606	CLA	CMC-C2C	-2.37	1.45	1.50
28	c	611	CLA	CMD-C2D	-2.37	1.45	1.50
31	A	847	WVN	C20-C13	2.37	1.53	1.45
28	R	203	CLA	C1B-C2B	2.37	1.48	1.43
28	a	305	CLA	C1B-C2B	2.37	1.48	1.43
28	A	805	CLA	CMD-C2D	-2.37	1.45	1.50
28	a	312	CLA	CMD-C2D	-2.37	1.45	1.50
36	f	615	II0	C18-C04	2.37	1.58	1.53
31	l	315	WVN	C20-C13	2.37	1.53	1.45
28	m	603	CLA	MG-NB	-2.37	2.01	2.05
36	a	315	II0	C30-C26	-2.37	1.32	1.37
38	m	611	KC2	C3C-C4C	2.37	1.49	1.44
28	c	602	CLA	CMC-C2C	-2.37	1.45	1.50
28	A	815	CLA	C1B-NB	-2.37	1.34	1.37
37	g	319	IHT	C20-C15	2.37	1.54	1.50
28	A	817	CLA	C3B-C4B	2.37	1.49	1.42
36	n	614	II0	C16-C03	2.37	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	612	CLA	MG-NA	2.37	2.11	2.06
28	h	303	CLA	C1B-C2B	2.37	1.48	1.43
38	g	312	KC2	C1D-C2D	2.37	1.48	1.43
28	B	803	CLA	C1B-NB	-2.37	1.34	1.37
28	i	311	CLA	MG-NC	2.37	2.11	2.06
28	j	603	CLA	C1B-C2B	2.36	1.48	1.43
28	n	603	CLA	C1B-C2B	2.36	1.48	1.43
28	A	841	CLA	CMD-C2D	-2.36	1.45	1.50
28	i	308	CLA	CHC-C1C	2.36	1.43	1.38
28	b	612	CLA	MG-NB	-2.36	2.01	2.05
28	a	309	CLA	CMC-C2C	-2.36	1.45	1.50
28	c	605	CLA	CMB-C2B	-2.36	1.45	1.50
28	j	609	CLA	C3B-C4B	2.36	1.49	1.42
28	B	832	CLA	C3B-C4B	2.36	1.49	1.42
28	O	206	CLA	CMD-C2D	-2.36	1.45	1.50
28	m	601	CLA	C3B-C4B	2.36	1.49	1.42
28	k	604	CLA	C3B-C4B	2.36	1.49	1.42
28	d	309	CLA	C3B-C4B	2.36	1.49	1.42
38	g	312	KC2	C3C-C4C	2.36	1.49	1.44
28	A	822	CLA	C1B-C2B	2.36	1.48	1.43
28	c	605	CLA	CMD-C2D	-2.36	1.45	1.50
38	m	611	KC2	CBD-CAD	-2.36	1.46	1.56
28	n	605	CLA	CMD-C2D	-2.36	1.45	1.50
38	n	611	KC2	CBD-CAD	-2.36	1.46	1.56
28	B	813	CLA	C3B-C4B	2.36	1.49	1.42
28	B	805	CLA	C1B-C2B	2.36	1.48	1.43
36	c	613	II0	C16-C03	2.36	1.58	1.53
28	c	601	CLA	CMD-C2D	-2.35	1.45	1.50
28	k	603	CLA	C1B-C2B	2.35	1.48	1.43
28	k	608	CLA	C3B-C4B	2.35	1.49	1.42
28	a	304	CLA	CMD-C2D	-2.35	1.45	1.50
36	k	616	II0	C18-C04	2.35	1.58	1.53
38	g	313	KC2	C4A-C3A	2.35	1.49	1.44
28	i	307	CLA	C3B-C4B	2.35	1.49	1.42
37	b	615	IHT	C39-C35	2.35	1.55	1.50
38	k	611	KC2	C4A-C3A	2.35	1.49	1.44
28	A	840	CLA	CMB-C2B	-2.35	1.46	1.50
28	e	602	CLA	CHC-C1C	2.35	1.43	1.38
28	B	830	CLA	CMD-C2D	-2.35	1.46	1.50
28	i	304	CLA	C3B-C4B	2.35	1.49	1.42
28	m	602	CLA	MG-NB	-2.35	2.01	2.05
28	B	810	CLA	CMC-C2C	-2.35	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	312	II0	C16-C03	2.35	1.58	1.53
28	B	809	CLA	C4B-C3B	2.35	1.48	1.43
28	a	311	CLA	C1B-C2B	2.35	1.48	1.43
28	h	305	CLA	C1B-C2B	2.35	1.48	1.43
31	h	309	WVN	C20-C13	2.35	1.53	1.45
28	Q	303	CLA	MG-NB	-2.35	2.01	2.05
28	n	607	CLA	C1B-C2B	2.34	1.48	1.43
36	n	615	II0	C16-C03	2.34	1.58	1.53
28	Q	303	CLA	MG-NA	2.34	2.11	2.06
28	i	303	CLA	C3B-C4B	2.34	1.49	1.42
28	A	829	CLA	C1B-NB	-2.34	1.34	1.37
28	c	602	CLA	CHC-C1C	2.34	1.43	1.38
36	j	614	II0	C16-C03	2.34	1.58	1.53
28	L	204	CLA	CMC-C2C	-2.34	1.46	1.50
38	s	201	KC2	C4B-NB	-2.34	1.34	1.37
38	k	611	KC2	C1A-CHA	2.34	1.46	1.40
32	A	850	LMT	O2B-C2B	-2.34	1.37	1.43
28	h	302	CLA	C1B-C2B	2.34	1.48	1.43
28	i	307	CLA	CMC-C2C	-2.34	1.46	1.50
28	B	822	CLA	C4B-NB	2.34	1.40	1.37
28	A	817	CLA	MG-NB	-2.34	2.01	2.05
28	B	824	CLA	CMC-C2C	-2.34	1.46	1.50
28	B	823	CLA	C3B-C4B	2.34	1.49	1.42
28	F	202	CLA	C3B-C4B	2.34	1.49	1.42
36	f	614	II0	C16-C03	2.34	1.58	1.53
38	c	610	KC2	CBD-CAD	-2.34	1.46	1.56
32	A	850	LMT	O4'-C4B	-2.34	1.37	1.43
36	k	617	II0	C18-C04	2.34	1.58	1.53
32	a	320	LMT	O1'-C1'	-2.34	1.36	1.40
28	d	306	CLA	C3B-C4B	2.34	1.49	1.42
28	B	801	CLA	MG-ND	-2.34	2.01	2.05
38	j	611	KC2	C3C-C4C	2.34	1.49	1.44
28	B	832	CLA	CMD-C2D	-2.34	1.46	1.50
28	s	202	CLA	CMD-C2D	-2.34	1.46	1.50
28	n	608	CLA	CHC-C1C	2.34	1.43	1.38
28	a	313	CLA	C1B-C2B	2.34	1.48	1.43
28	B	818	CLA	C1B-C2B	2.34	1.48	1.43
28	d	303	CLA	C3B-C4B	2.34	1.49	1.42
38	f	611	KC2	C3C-C4C	2.33	1.49	1.44
36	k	615	II0	C16-C03	2.33	1.58	1.53
28	b	611	CLA	C3B-C4B	2.33	1.49	1.42
28	e	603	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	m	603	CLA	CHC-C1C	2.33	1.43	1.38
28	b	605	CLA	MG-NB	-2.33	2.01	2.05
28	A	836	CLA	C4B-NB	2.33	1.40	1.37
31	J	102	WVN	C20-C13	2.33	1.53	1.45
28	f	609	CLA	C1B-C2B	2.33	1.48	1.43
28	m	607	CLA	CMB-C2B	-2.33	1.46	1.50
28	A	818	CLA	C3B-C4B	2.33	1.49	1.42
37	b	616	IHT	C39-C35	2.33	1.55	1.50
28	g	306	CLA	CMC-C2C	-2.33	1.46	1.50
31	A	848	WVN	C23-C25	2.33	1.50	1.46
28	l	308	CLA	C1B-C2B	2.33	1.48	1.43
28	m	613	CLA	C3C-C2C	2.33	1.41	1.36
28	B	841	CLA	C3B-C4B	2.33	1.49	1.42
28	B	836	CLA	C3B-C4B	2.33	1.49	1.42
36	a	318	II0	C18-C04	2.33	1.58	1.53
28	A	854	CLA	CMD-C2D	-2.33	1.46	1.50
36	f	615	II0	C30-C26	-2.33	1.32	1.37
28	B	815	CLA	C4B-NB	2.33	1.40	1.37
28	j	605	CLA	CMB-C2B	-2.33	1.46	1.50
28	k	609	CLA	CMC-C2C	-2.33	1.46	1.50
36	J	104	II0	C16-C03	2.33	1.58	1.53
28	a	310	CLA	C4B-NB	2.33	1.40	1.37
28	b	605	CLA	C4B-NB	2.33	1.40	1.37
31	B	847	WVN	C26-C22	-2.33	1.30	1.35
38	j	611	KC2	CBD-CAD	-2.33	1.46	1.56
36	g	316	II0	C16-C03	2.33	1.58	1.53
28	g	303	CLA	C4B-NB	2.32	1.40	1.37
28	B	824	CLA	CMD-C2D	-2.32	1.46	1.50
28	m	608	CLA	CMB-C2B	-2.32	1.46	1.50
28	B	822	CLA	C1B-C2B	2.32	1.48	1.43
28	b	612	CLA	C4B-NB	2.32	1.40	1.37
28	m	613	CLA	C3B-C4B	2.32	1.49	1.42
28	a	310	CLA	CMD-C2D	-2.32	1.46	1.50
36	c	613	II0	C18-C04	2.32	1.58	1.53
28	B	817	CLA	MG-NB	-2.32	2.01	2.05
32	a	320	LMT	O3B-C3B	-2.32	1.37	1.43
28	B	803	CLA	MG-NB	-2.32	2.01	2.05
28	A	821	CLA	C1B-C2B	2.32	1.48	1.43
38	k	611	KC2	CBD-CAD	-2.32	1.46	1.56
28	A	819	CLA	CMB-C2B	-2.32	1.46	1.50
36	l	314	II0	C18-C04	2.32	1.58	1.53
36	j	615	II0	C16-C03	2.32	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	820	CLA	CMD-C2D	-2.32	1.46	1.50
28	B	816	CLA	CMB-C2B	-2.32	1.46	1.50
36	a	315	II0	C33-C35	2.32	1.50	1.46
28	e	610	CLA	C3B-C4B	2.32	1.49	1.42
38	s	204	KC2	C3C-C4C	2.32	1.49	1.44
28	l	311	CLA	C3B-C4B	2.32	1.49	1.42
28	B	803	CLA	C3B-C4B	2.32	1.49	1.42
28	A	828	CLA	C1B-C2B	2.32	1.48	1.43
28	A	827	CLA	CHC-C1C	2.32	1.43	1.38
28	A	835	CLA	C3B-C4B	2.32	1.49	1.42
28	m	602	CLA	CMB-C2B	-2.32	1.46	1.50
28	B	801	CLA	CMD-C2D	-2.32	1.46	1.50
36	d	315	II0	C18-C04	2.32	1.58	1.53
28	j	606	CLA	CHC-C4B	-2.31	1.34	1.39
28	a	306	CLA	C1B-C2B	2.31	1.48	1.43
36	e	613	II0	C16-C03	2.31	1.58	1.53
28	d	304	CLA	CHC-C1C	2.31	1.43	1.38
37	g	319	IHT	C39-C35	2.31	1.55	1.50
28	O	206	CLA	C1B-NB	-2.31	1.34	1.37
28	A	802	CLA	CMD-C2D	-2.31	1.46	1.50
28	l	309	CLA	C3B-C4B	2.31	1.49	1.42
28	n	601	CLA	C3B-C4B	2.31	1.49	1.42
31	L	206	WVN	C19-C22	2.31	1.50	1.46
28	j	608	CLA	C1B-C2B	2.31	1.48	1.43
28	A	820	CLA	CMC-C2C	-2.31	1.46	1.50
31	F	203	WVN	C20-C13	2.31	1.53	1.45
28	k	614	CLA	C3B-C4B	2.31	1.49	1.42
28	A	852	CLA	C4B-NB	2.31	1.40	1.37
28	a	308	CLA	C1B-C2B	2.31	1.48	1.43
36	n	615	II0	C18-C04	2.31	1.58	1.53
36	i	314	II0	C16-C03	2.31	1.58	1.53
28	A	802	CLA	C3B-C4B	2.31	1.49	1.42
28	j	604	CLA	C3B-C4B	2.31	1.49	1.42
28	n	608	CLA	C3B-C4B	2.31	1.49	1.42
36	f	618	II0	C16-C03	2.31	1.58	1.53
28	B	813	CLA	C1B-C2B	2.31	1.48	1.43
28	f	605	CLA	CMB-C2B	-2.30	1.46	1.50
38	k	612	KC2	CBD-CAD	-2.30	1.46	1.56
28	B	812	CLA	CHC-C1C	2.30	1.43	1.38
28	B	833	CLA	C1B-C2B	2.30	1.48	1.43
31	B	845	WVN	C20-C13	2.30	1.52	1.45
28	A	804	CLA	CMD-C2D	-2.30	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	601	CLA	CMD-C2D	-2.30	1.46	1.50
28	A	821	CLA	MG-NB	-2.30	2.01	2.05
28	B	812	CLA	C1B-C2B	2.30	1.48	1.43
36	f	615	II0	C16-C03	2.30	1.58	1.53
28	e	605	CLA	C3B-C4B	2.30	1.49	1.42
28	B	834	CLA	CMD-C2D	-2.30	1.46	1.50
28	a	306	CLA	C3B-C4B	2.30	1.49	1.42
28	j	607	CLA	C1B-C2B	2.30	1.48	1.43
28	i	312	CLA	C3B-C4B	2.30	1.49	1.42
28	A	804	CLA	C3B-C4B	2.30	1.49	1.42
28	b	608	CLA	C3B-C4B	2.30	1.49	1.42
28	B	822	CLA	MG-ND	-2.30	2.01	2.05
38	i	310	KC2	CBD-CAD	-2.30	1.46	1.56
28	A	810	CLA	C3B-C4B	2.30	1.49	1.42
28	j	603	CLA	CHC-C1C	2.30	1.43	1.38
28	g	310	CLA	CMC-C2C	-2.30	1.46	1.50
28	L	203	CLA	C1B-C2B	2.30	1.48	1.43
28	B	803	CLA	CMD-C2D	-2.29	1.46	1.50
28	c	602	CLA	C3B-C4B	2.29	1.49	1.42
28	B	823	CLA	C1B-C2B	2.29	1.48	1.43
28	a	304	CLA	CMA-C3A	-2.29	1.48	1.53
28	A	811	CLA	C1B-C2B	2.29	1.48	1.43
31	R	202	WVN	C26-C22	-2.29	1.30	1.35
28	B	821	CLA	C1B-C2B	2.29	1.48	1.43
28	l	304	CLA	C3B-C4B	2.29	1.49	1.42
28	B	824	CLA	C1B-C2B	2.29	1.48	1.43
28	k	606	CLA	C3B-C4B	2.29	1.49	1.42
37	b	615	IHT	C20-C15	2.29	1.54	1.50
31	s	205	WVN	C20-C13	2.29	1.52	1.45
28	A	817	CLA	CMD-C2D	-2.29	1.46	1.50
28	g	315	CLA	C3B-C4B	2.29	1.49	1.42
28	Q	303	CLA	CHC-C1C	2.29	1.43	1.38
28	A	803	CLA	CMC-C2C	-2.29	1.46	1.50
28	b	609	CLA	CMC-C2C	-2.29	1.46	1.50
28	B	841	CLA	CHC-C1C	2.29	1.43	1.38
28	g	310	CLA	C3B-C4B	2.29	1.49	1.42
38	e	609	KC2	CBD-CAD	-2.29	1.46	1.56
37	n	617	IHT	C20-C15	2.29	1.54	1.50
28	A	819	CLA	C3B-C4B	2.29	1.49	1.42
28	A	806	CLA	C1B-C2B	2.29	1.48	1.43
28	A	836	CLA	CMD-C2D	-2.29	1.46	1.50
28	h	313	CLA	C1B-C2B	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	314	II0	C18-C04	2.28	1.58	1.53
28	j	606	CLA	CMC-C2C	-2.28	1.46	1.50
28	h	304	CLA	CMD-C2D	-2.28	1.46	1.50
28	A	840	CLA	MG-NB	-2.28	2.01	2.05
28	c	607	CLA	CHC-C1C	2.28	1.43	1.38
36	c	615	II0	C28-C26	2.28	1.52	1.50
31	M	101	WVN	C02-C11	2.28	1.53	1.50
28	m	602	CLA	C1B-C2B	2.28	1.48	1.43
36	k	616	II0	C16-C03	2.28	1.58	1.53
28	A	801	CLA	CMD-C2D	-2.28	1.46	1.50
28	d	308	CLA	CHC-C1C	2.28	1.43	1.38
28	m	606	CLA	C3B-C4B	2.28	1.49	1.42
28	b	609	CLA	CMD-C2D	-2.28	1.46	1.50
28	i	311	CLA	CMD-C2D	-2.28	1.46	1.50
28	B	810	CLA	C1B-C2B	2.28	1.48	1.43
31	A	848	WVN	C28-C25	-2.28	1.30	1.35
28	B	811	CLA	C3B-C4B	2.28	1.49	1.42
28	a	311	CLA	C3B-C4B	2.28	1.49	1.42
28	n	601	CLA	CHC-C1C	2.28	1.43	1.38
38	d	310	KC2	C4A-C3A	2.28	1.49	1.44
28	B	814	CLA	C1B-C2B	2.28	1.48	1.43
28	c	608	CLA	C3B-C4B	2.28	1.49	1.42
28	B	822	CLA	CAC-C3C	-2.28	1.45	1.51
28	k	601	CLA	CMD-C2D	-2.28	1.46	1.50
28	A	814	CLA	CMC-C2C	-2.28	1.46	1.50
28	n	602	CLA	CMD-C2D	-2.28	1.46	1.50
28	B	832	CLA	CHC-C1C	2.27	1.43	1.38
28	B	837	CLA	CMD-C2D	-2.27	1.46	1.50
28	s	206	CLA	C3B-C4B	2.27	1.49	1.42
31	B	848	WVN	C26-C22	-2.27	1.30	1.35
28	a	312	CLA	C3B-C4B	2.27	1.49	1.42
36	a	315	II0	C18-C04	2.27	1.58	1.53
36	b	614	II0	C18-C04	2.27	1.58	1.53
28	g	303	CLA	C3B-C4B	2.27	1.49	1.42
31	K	102	WVN	C20-C13	2.27	1.52	1.45
28	A	807	CLA	C1B-C2B	2.27	1.48	1.43
28	n	605	CLA	C3B-C4B	2.27	1.49	1.42
36	n	614	II0	C20-C14	2.27	1.54	1.50
36	k	619	II0	C18-C04	2.27	1.58	1.53
28	c	611	CLA	CMC-C2C	-2.27	1.46	1.50
28	a	311	CLA	CMC-C2C	-2.27	1.46	1.50
28	B	839	CLA	C1B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	603	CLA	C3B-C4B	2.27	1.49	1.42
28	b	602	CLA	C3B-C4B	2.27	1.49	1.42
28	k	608	CLA	C1B-C2B	2.27	1.48	1.43
28	m	609	CLA	CHC-C1C	2.27	1.43	1.38
28	f	612	CLA	C3B-C4B	2.27	1.49	1.42
28	A	831	CLA	CMB-C2B	-2.27	1.46	1.50
38	k	613	KC2	CBD-CAD	-2.27	1.46	1.56
28	F	201	CLA	CMB-C2B	-2.27	1.46	1.50
28	B	802	CLA	CMC-C2C	-2.27	1.46	1.50
28	b	610	CLA	CMC-C2C	-2.27	1.46	1.50
28	e	606	CLA	C3B-C4B	2.27	1.49	1.42
28	g	309	CLA	C3B-C4B	2.27	1.49	1.42
28	m	613	CLA	CMD-C2D	-2.26	1.46	1.50
28	A	817	CLA	MG-ND	-2.26	2.01	2.05
31	F	204	WVN	C20-C13	2.26	1.52	1.45
28	c	604	CLA	C1B-C2B	2.26	1.48	1.43
28	e	602	CLA	C1B-C2B	2.26	1.48	1.43
36	e	612	II0	C18-C04	2.26	1.58	1.53
28	m	603	CLA	C1B-C2B	2.26	1.48	1.43
28	B	801	CLA	CMC-C2C	-2.26	1.46	1.50
31	R	202	WVN	C20-C13	2.26	1.52	1.45
36	h	312	II0	C16-C03	2.26	1.58	1.53
28	B	836	CLA	CMD-C2D	-2.26	1.46	1.50
28	A	826	CLA	C4B-NB	2.26	1.40	1.37
28	c	609	CLA	C3B-C4B	2.26	1.49	1.42
28	f	607	CLA	C1B-C2B	2.26	1.48	1.43
28	h	303	CLA	C3B-C4B	2.26	1.49	1.42
28	l	305	CLA	CMC-C2C	-2.26	1.46	1.50
28	b	609	CLA	MG-NB	-2.26	2.01	2.05
28	A	851	CLA	CMD-C2D	-2.26	1.46	1.50
28	f	601	CLA	CMD-C2D	-2.26	1.46	1.50
28	A	825	CLA	MG-NB	-2.26	2.01	2.05
28	A	816	CLA	C4B-NB	2.26	1.40	1.37
28	f	603	CLA	CMD-C2D	-2.26	1.46	1.50
28	B	821	CLA	C3B-C4B	2.26	1.49	1.42
28	s	202	CLA	MG-NB	-2.26	2.01	2.05
28	L	204	CLA	CHC-C1C	2.26	1.43	1.38
28	B	816	CLA	MG-NB	-2.25	2.01	2.05
28	d	302	CLA	CMD-C2D	-2.25	1.46	1.50
28	B	823	CLA	CMC-C2C	-2.25	1.46	1.50
28	m	605	CLA	CMB-C2B	-2.25	1.46	1.50
28	A	813	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	610	CLA	C3B-C4B	2.25	1.49	1.42
28	B	820	CLA	C3B-C4B	2.25	1.49	1.42
28	B	832	CLA	CMC-C2C	-2.25	1.46	1.50
28	b	604	CLA	CMD-C2D	-2.25	1.46	1.50
28	d	308	CLA	CMC-C2C	-2.25	1.46	1.50
28	c	606	CLA	C3B-C4B	2.25	1.49	1.42
28	a	307	CLA	C1B-C2B	2.25	1.48	1.43
28	a	309	CLA	CHC-C1C	2.25	1.43	1.38
28	B	831	CLA	MG-NB	-2.25	2.01	2.05
37	a	317	IHT	C39-C35	2.25	1.55	1.50
28	j	612	CLA	CMD-C2D	-2.25	1.46	1.50
28	A	837	CLA	CMD-C2D	-2.25	1.46	1.50
28	L	202	CLA	C1B-C2B	2.25	1.48	1.43
28	c	612	CLA	C3B-C4B	2.25	1.49	1.42
28	B	821	CLA	CMB-C2B	-2.25	1.46	1.50
36	f	616	II0	C18-C04	2.25	1.58	1.53
28	B	814	CLA	C3B-C4B	2.25	1.49	1.42
28	m	604	CLA	C3B-C4B	2.25	1.49	1.42
28	i	308	CLA	CMC-C2C	-2.25	1.46	1.50
28	g	304	CLA	C3B-C4B	2.25	1.49	1.42
28	k	609	CLA	CHC-C1C	2.25	1.43	1.38
28	B	817	CLA	CMC-C2C	-2.25	1.46	1.50
31	K	102	WVN	C19-C22	2.25	1.50	1.46
28	A	802	CLA	CMC-C2C	-2.25	1.46	1.50
36	l	314	II0	C16-C03	2.25	1.58	1.53
28	g	305	CLA	C3B-C4B	2.25	1.49	1.42
28	A	851	CLA	MG-NB	-2.25	2.01	2.05
28	n	602	CLA	C1B-C2B	2.25	1.48	1.43
28	A	827	CLA	CMD-C2D	-2.25	1.46	1.50
28	A	830	CLA	MG-ND	-2.24	2.01	2.05
31	B	847	WVN	C20-C13	2.24	1.52	1.45
28	d	302	CLA	MG-NB	-2.24	2.01	2.05
28	l	308	CLA	C3B-C4B	2.24	1.49	1.42
28	m	603	CLA	CAA-C2A	-2.24	1.50	1.54
28	j	609	CLA	CHC-C1C	2.24	1.43	1.38
28	B	809	CLA	CMB-C2B	-2.24	1.46	1.50
28	B	816	CLA	C1B-C2B	2.24	1.48	1.43
28	a	305	CLA	C3B-C4B	2.24	1.49	1.42
28	a	309	CLA	C3B-C4B	2.24	1.49	1.42
28	A	824	CLA	CMD-C2D	-2.24	1.46	1.50
38	i	319	KC2	CBD-CAD	-2.24	1.46	1.56
28	l	306	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	603	CLA	MG-NB	-2.24	2.01	2.05
28	B	837	CLA	C3B-C4B	2.24	1.49	1.42
28	k	604	CLA	CMD-C2D	-2.24	1.46	1.50
28	j	602	CLA	C3B-C4B	2.24	1.49	1.42
28	A	810	CLA	CMD-C2D	-2.24	1.46	1.50
28	B	804	CLA	CMD-C2D	-2.24	1.46	1.50
38	n	612	KC2	CBD-CAD	-2.24	1.46	1.56
28	Q	303	CLA	C3B-C4B	2.24	1.49	1.42
28	L	204	CLA	C3B-C4B	2.24	1.49	1.42
28	j	608	CLA	C3B-C4B	2.24	1.49	1.42
38	l	310	KC2	C3C-C4C	2.24	1.49	1.44
38	d	310	KC2	CBD-CAD	-2.24	1.46	1.56
28	m	604	CLA	CMA-C3A	-2.24	1.48	1.53
28	g	303	CLA	C1B-C2B	2.24	1.48	1.43
28	j	610	CLA	CMB-C2B	-2.24	1.46	1.50
28	l	303	CLA	C3B-C4B	2.24	1.49	1.42
32	A	850	LMT	O3B-C3B	-2.23	1.37	1.43
28	L	207	CLA	C3B-C4B	2.23	1.49	1.42
38	g	314	KC2	CBD-CAD	-2.23	1.46	1.56
28	O	201	CLA	C4B-NB	2.23	1.40	1.37
28	A	806	CLA	CMB-C2B	-2.23	1.46	1.50
28	e	611	CLA	CHC-C1C	2.23	1.43	1.38
28	g	315	CLA	CMD-C2D	-2.23	1.46	1.50
38	l	310	KC2	C4A-C3A	2.23	1.49	1.44
28	h	301	CLA	CMD-C2D	-2.23	1.46	1.50
28	i	309	CLA	C3B-C4B	2.23	1.49	1.42
28	B	826	CLA	C3B-C4B	2.23	1.49	1.42
31	A	846	WVN	C20-C13	2.23	1.52	1.45
31	B	846	WVN	C26-C22	-2.23	1.30	1.35
28	a	307	CLA	MG-NB	-2.23	2.01	2.05
28	A	821	CLA	C3B-C4B	2.23	1.49	1.42
28	g	309	CLA	CMC-C2C	-2.23	1.46	1.50
28	n	603	CLA	CMD-C2D	-2.23	1.46	1.50
28	s	202	CLA	C3B-C4B	2.23	1.49	1.42
28	i	305	CLA	C3B-C4B	2.23	1.49	1.42
28	A	815	CLA	MG-ND	-2.23	2.01	2.05
28	O	206	CLA	MG-ND	-2.23	2.01	2.05
28	O	206	CLA	CMC-C2C	-2.23	1.46	1.50
28	d	312	CLA	C3B-C4B	2.23	1.49	1.42
36	g	318	II0	C20-C14	2.23	1.54	1.50
31	A	845	WVN	C28-C25	-2.23	1.30	1.35
36	d	313	II0	C15-C03	2.22	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	839	CLA	CMD-C2D	-2.22	1.46	1.50
28	c	604	CLA	C3B-C4B	2.22	1.49	1.42
28	c	611	CLA	MG-NC	2.22	2.11	2.06
28	l	305	CLA	C3B-C4B	2.22	1.49	1.42
28	f	602	CLA	C3B-C4B	2.22	1.49	1.42
28	A	851	CLA	MG-ND	-2.22	2.01	2.05
28	A	851	CLA	CHC-C1C	2.22	1.42	1.38
28	c	603	CLA	C3B-C4B	2.22	1.49	1.42
36	k	621	II0	C16-C03	2.22	1.58	1.53
37	a	317	IHT	C20-C15	2.22	1.54	1.50
28	b	603	CLA	CHC-C1C	2.22	1.42	1.38
28	m	604	CLA	CMB-C2B	-2.22	1.46	1.50
36	a	314	II0	C30-C26	-2.22	1.32	1.37
28	a	313	CLA	CMD-C2D	-2.22	1.46	1.50
28	n	609	CLA	CMC-C2C	-2.22	1.46	1.50
28	h	302	CLA	CHC-C1C	2.22	1.42	1.38
28	d	301	CLA	C3B-C4B	2.22	1.49	1.42
28	k	607	CLA	C3B-C4B	2.22	1.49	1.42
28	n	607	CLA	CMD-C2D	-2.22	1.46	1.50
36	g	318	II0	C28-C26	2.22	1.52	1.50
28	A	824	CLA	C3B-C4B	2.22	1.49	1.42
28	l	311	CLA	CMD-C2D	-2.22	1.46	1.50
36	k	615	II0	C18-C04	2.22	1.57	1.53
28	m	601	CLA	CMD-C2D	-2.22	1.46	1.50
28	b	602	CLA	CHC-C1C	2.22	1.42	1.38
36	l	313	II0	C18-C04	2.22	1.57	1.53
28	n	602	CLA	MG-NB	-2.21	2.01	2.05
31	L	206	WVN	C20-C13	2.21	1.52	1.45
28	A	851	CLA	C3B-C4B	2.21	1.49	1.42
28	B	818	CLA	C3B-C4B	2.21	1.49	1.42
28	h	303	CLA	CMD-C2D	-2.21	1.46	1.50
38	n	611	KC2	C3C-C4C	2.21	1.49	1.44
28	f	607	CLA	CMD-C2D	-2.21	1.46	1.50
28	d	302	CLA	C3B-C4B	2.21	1.49	1.42
32	a	302	LMT	O2'-C2'	-2.21	1.37	1.43
28	b	603	CLA	CMC-C2C	-2.21	1.46	1.50
28	L	203	CLA	C3B-C4B	2.21	1.49	1.42
28	A	801	CLA	CMB-C2B	-2.21	1.46	1.50
28	m	609	CLA	C1B-C2B	2.21	1.48	1.43
28	l	302	CLA	CMD-C2D	-2.21	1.46	1.50
28	n	613	CLA	CMD-C2D	-2.21	1.46	1.50
36	m	616	II0	C16-C03	2.21	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	606	CLA	CHC-C1C	2.21	1.42	1.38
28	n	608	CLA	CMC-C2C	-2.21	1.46	1.50
28	A	830	CLA	C3B-C4B	2.21	1.49	1.42
28	b	606	CLA	C3B-C4B	2.21	1.49	1.42
28	b	601	CLA	C3B-C4B	2.21	1.49	1.42
28	A	815	CLA	CMD-C2D	-2.21	1.46	1.50
28	g	306	CLA	C3B-C4B	2.20	1.49	1.42
36	a	316	II0	C18-C04	2.20	1.57	1.53
28	F	201	CLA	CMD-C2D	-2.20	1.46	1.50
28	j	606	CLA	CMD-C2D	-2.20	1.46	1.50
38	k	612	KC2	C4A-C3A	2.20	1.49	1.44
28	A	820	CLA	C1B-NB	-2.20	1.35	1.37
28	B	832	CLA	MG-NB	-2.20	2.01	2.05
36	J	104	II0	C18-C04	2.20	1.57	1.53
36	J	104	II0	C27-C25	2.20	1.52	1.50
28	A	839	CLA	CMB-C2B	-2.20	1.46	1.50
28	d	301	CLA	CMD-C2D	-2.20	1.46	1.50
31	B	845	WVN	C26-C22	-2.20	1.30	1.35
31	l	301	WVN	C02-C11	2.20	1.53	1.50
36	i	314	II0	C18-C04	2.20	1.57	1.53
36	g	320	II0	C18-C04	2.20	1.57	1.53
28	h	303	CLA	MG-NB	-2.20	2.01	2.05
28	B	819	CLA	CMB-C2B	-2.20	1.46	1.50
28	k	603	CLA	C3B-C4B	2.20	1.49	1.42
38	k	613	KC2	C1D-C2D	2.20	1.48	1.43
28	c	603	CLA	CHC-C1C	2.20	1.42	1.38
28	B	805	CLA	MG-NB	-2.20	2.01	2.05
28	A	818	CLA	C1B-NB	-2.20	1.35	1.37
28	B	835	CLA	C1B-C2B	2.20	1.48	1.43
28	m	606	CLA	CMD-C2D	-2.20	1.46	1.50
28	R	203	CLA	CHC-C1C	2.20	1.42	1.38
28	a	307	CLA	C3B-C4B	2.20	1.49	1.42
32	a	320	LMT	O4'-C4B	-2.20	1.37	1.43
28	d	306	CLA	CMD-C2D	-2.20	1.46	1.50
36	j	614	II0	C15-C03	2.20	1.57	1.53
36	b	613	II0	C18-C04	2.20	1.57	1.53
38	g	312	KC2	CBD-CAD	-2.19	1.46	1.56
28	b	612	CLA	C1B-C2B	2.19	1.48	1.43
28	c	606	CLA	MG-NB	-2.19	2.01	2.05
38	c	610	KC2	C3C-C4C	2.19	1.49	1.44
28	a	313	CLA	C3B-C4B	2.19	1.49	1.42
28	j	607	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	814	CLA	CMD-C2D	-2.19	1.46	1.50
28	c	607	CLA	CMD-C2D	-2.19	1.46	1.50
31	l	301	WVN	C20-C13	2.19	1.52	1.45
28	B	817	CLA	C1B-NB	-2.19	1.35	1.37
36	l	316	II0	C18-C04	2.19	1.57	1.53
36	h	311	II0	C18-C04	2.19	1.57	1.53
28	j	605	CLA	C3B-C4B	2.19	1.49	1.42
28	g	306	CLA	CMD-C2D	-2.19	1.46	1.50
28	L	202	CLA	CMB-C2B	-2.19	1.46	1.50
36	e	613	II0	C20-C14	2.19	1.54	1.50
32	A	850	LMT	O1'-C1'	-2.19	1.36	1.40
36	c	615	II0	C18-C04	2.19	1.57	1.53
36	m	615	II0	C16-C03	2.19	1.57	1.53
28	b	607	CLA	CMB-C2B	-2.19	1.46	1.50
28	m	612	CLA	CMD-C2D	-2.19	1.46	1.50
28	m	613	CLA	C1B-C2B	2.19	1.48	1.43
28	f	607	CLA	CMB-C2B	-2.19	1.46	1.50
37	m	617	IHT	C20-C15	2.19	1.54	1.50
28	m	609	CLA	CMD-C2D	-2.19	1.46	1.50
28	j	606	CLA	CMB-C2B	-2.19	1.46	1.50
36	e	613	II0	C15-C03	2.19	1.57	1.53
28	A	803	CLA	CMD-C2D	-2.19	1.46	1.50
31	K	102	WVN	C15-C13	-2.19	1.30	1.34
32	b	618	LMT	O2'-C2'	-2.19	1.37	1.43
28	A	829	CLA	CMD-C2D	-2.19	1.46	1.50
31	A	845	WVN	C37-C34	-2.18	1.30	1.35
28	A	838	CLA	CMD-C2D	-2.18	1.46	1.50
31	K	104	WVN	C02-C11	2.18	1.53	1.50
36	h	310	II0	C16-C03	2.18	1.57	1.53
38	s	204	KC2	C4B-NB	-2.18	1.35	1.37
28	B	828	CLA	CHC-C1C	2.18	1.42	1.38
28	L	207	CLA	CMC-C2C	-2.18	1.46	1.50
28	b	609	CLA	C1B-C2B	2.18	1.48	1.43
28	i	309	CLA	CMD-C2D	-2.18	1.46	1.50
28	g	306	CLA	CMB-C2B	-2.18	1.46	1.50
28	A	852	CLA	C3B-C4B	2.18	1.49	1.42
38	k	612	KC2	C1D-C2D	2.18	1.48	1.43
28	b	604	CLA	C3B-C4B	2.18	1.49	1.42
28	K	103	CLA	CMD-C2D	-2.18	1.46	1.50
28	A	838	CLA	C1B-C2B	2.18	1.48	1.43
28	a	306	CLA	CMD-C2D	-2.18	1.46	1.50
36	l	312	II0	C18-C04	2.18	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Q	302	CLA	CMB-C2B	-2.18	1.46	1.50
36	m	614	II0	C18-C04	2.18	1.57	1.53
37	m	617	IHT	C13-C02	2.18	1.57	1.53
28	k	605	CLA	CMC-C2C	-2.18	1.46	1.50
28	A	832	CLA	C3B-C4B	2.18	1.49	1.42
36	f	614	II0	C18-C04	2.18	1.57	1.53
28	A	812	CLA	CMD-C2D	-2.18	1.46	1.50
28	A	851	CLA	CMC-C2C	-2.18	1.46	1.50
28	A	854	CLA	MG-NB	-2.18	2.01	2.05
28	f	601	CLA	CMB-C2B	-2.18	1.46	1.50
28	A	813	CLA	MG-NB	-2.18	2.01	2.05
28	i	308	CLA	CMD-C2D	-2.18	1.46	1.50
28	i	304	CLA	CHC-C1C	2.18	1.42	1.38
28	i	307	CLA	CHC-C1C	2.18	1.42	1.38
38	c	610	KC2	C1D-C2D	2.18	1.48	1.43
28	n	607	CLA	C3B-C4B	2.18	1.49	1.42
28	k	608	CLA	CHC-C1C	2.18	1.42	1.38
36	a	314	II0	C16-C03	2.18	1.57	1.53
28	A	836	CLA	MG-NB	-2.18	2.01	2.05
28	R	203	CLA	CMC-C2C	-2.18	1.46	1.50
28	A	822	CLA	CHC-C1C	2.18	1.42	1.38
38	l	310	KC2	C4B-NB	-2.18	1.35	1.37
28	d	302	CLA	CHC-C1C	2.18	1.42	1.38
28	l	309	CLA	CMD-C2D	-2.17	1.46	1.50
28	O	206	CLA	C1B-C2B	2.17	1.48	1.43
28	B	833	CLA	C3B-C4B	2.17	1.49	1.42
28	n	603	CLA	CMC-C2C	-2.17	1.46	1.50
36	k	616	II0	C15-C03	2.17	1.57	1.53
28	m	608	CLA	CMD-C2D	-2.17	1.46	1.50
28	b	610	CLA	CMD-C2D	-2.17	1.46	1.50
28	g	302	CLA	CMD-C2D	-2.17	1.46	1.50
28	A	822	CLA	C3B-C4B	2.17	1.49	1.42
28	K	103	CLA	CMB-C2B	-2.17	1.46	1.50
28	A	804	CLA	CHC-C1C	2.17	1.42	1.38
28	O	202	CLA	CMD-C2D	-2.17	1.46	1.50
38	i	319	KC2	C4A-C3A	2.17	1.48	1.44
36	m	615	II0	C30-C26	-2.17	1.32	1.37
28	a	310	CLA	CMC-C2C	-2.17	1.46	1.50
28	m	604	CLA	CMD-C2D	-2.17	1.46	1.50
36	g	317	II0	C15-C03	2.17	1.57	1.53
28	m	604	CLA	C1B-C2B	2.17	1.48	1.43
28	b	608	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e	616	II0	C18-C04	2.17	1.57	1.53
28	a	311	CLA	CMD-C2D	-2.17	1.46	1.50
28	e	606	CLA	CMC-C2C	-2.17	1.46	1.50
28	A	809	CLA	C3B-C4B	2.17	1.49	1.42
28	B	823	CLA	CHC-C1C	2.17	1.42	1.38
36	k	619	II0	C15-C03	2.17	1.57	1.53
28	j	606	CLA	C3B-C4B	2.17	1.49	1.42
28	B	838	CLA	C3B-C4B	2.17	1.49	1.42
28	s	208	CLA	CMB-C2B	-2.17	1.46	1.50
37	a	317	IHT	C13-C02	2.17	1.57	1.53
28	K	101	CLA	C3B-C4B	2.17	1.49	1.42
28	d	303	CLA	CMD-C2D	-2.17	1.46	1.50
28	i	306	CLA	C3B-C4B	2.17	1.49	1.42
28	A	852	CLA	CMC-C2C	-2.17	1.46	1.50
28	B	841	CLA	CMD-C2D	-2.17	1.46	1.50
28	n	602	CLA	C3B-C4B	2.17	1.49	1.42
28	h	306	CLA	CMC-C2C	-2.17	1.46	1.50
28	B	801	CLA	C1B-C2B	2.16	1.48	1.43
28	h	301	CLA	C3B-C4B	2.16	1.49	1.42
28	B	801	CLA	MG-NB	-2.16	2.01	2.05
28	A	813	CLA	C3B-C4B	2.16	1.49	1.42
38	g	312	KC2	C1A-CHA	2.16	1.45	1.40
28	b	611	CLA	CMB-C2B	-2.16	1.46	1.50
28	A	834	CLA	MG-NB	-2.16	2.01	2.05
28	h	302	CLA	CMD-C2D	-2.16	1.46	1.50
28	n	613	CLA	C3B-C4B	2.16	1.49	1.42
31	B	847	WVN	C28-C25	-2.16	1.30	1.35
28	g	303	CLA	MG-ND	-2.16	2.01	2.05
28	B	805	CLA	CMD-C2D	-2.16	1.46	1.50
28	A	821	CLA	CMB-C2B	-2.16	1.46	1.50
28	B	818	CLA	CMD-C2D	-2.16	1.46	1.50
28	h	305	CLA	CMD-C2D	-2.16	1.46	1.50
28	A	835	CLA	CMB-C2B	-2.16	1.46	1.50
32	A	850	LMT	O2'-C2'	-2.16	1.37	1.43
28	n	609	CLA	C3B-C4B	2.16	1.49	1.42
32	a	320	LMT	O2B-C2B	-2.16	1.37	1.43
28	a	307	CLA	CMB-C2B	-2.16	1.46	1.50
28	b	601	CLA	CMD-C2D	-2.16	1.46	1.50
28	A	815	CLA	C4B-NB	2.16	1.40	1.37
31	M	101	WVN	C26-C22	-2.16	1.30	1.35
28	A	838	CLA	CMB-C2B	-2.16	1.46	1.50
28	B	835	CLA	CMB-C2B	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	g	302	CLA	MG-NB	-2.16	2.01	2.05
28	d	312	CLA	CMC-C2C	-2.16	1.46	1.50
28	j	610	CLA	CMD-C2D	-2.16	1.46	1.50
28	m	608	CLA	C3B-C4B	2.16	1.49	1.42
28	F	202	CLA	O2A-CGA	2.16	1.39	1.33
28	A	832	CLA	C1B-C2B	2.16	1.48	1.43
28	s	206	CLA	CMD-C2D	-2.15	1.46	1.50
28	B	806	CLA	CMD-C2D	-2.15	1.46	1.50
28	m	609	CLA	CMC-C2C	-2.15	1.46	1.50
28	B	813	CLA	CMD-C2D	-2.15	1.46	1.50
28	O	206	CLA	C3B-C4B	2.15	1.49	1.42
28	c	604	CLA	CMD-C2D	-2.15	1.46	1.50
36	g	316	II0	C18-C04	2.15	1.57	1.53
28	B	834	CLA	MG-NB	-2.15	2.01	2.05
28	B	821	CLA	CMD-C2D	-2.15	1.46	1.50
28	B	827	CLA	CMB-C2B	-2.15	1.46	1.50
28	k	607	CLA	CMD-C2D	-2.15	1.46	1.50
38	s	204	KC2	C1D-C2D	2.15	1.48	1.43
28	k	605	CLA	C3B-C4B	2.15	1.49	1.42
28	a	304	CLA	C3B-C4B	2.15	1.49	1.42
38	k	612	KC2	C4B-NB	-2.15	1.35	1.37
28	A	810	CLA	CMC-C2C	-2.15	1.46	1.50
28	A	823	CLA	CMB-C2B	-2.15	1.46	1.50
28	k	614	CLA	CMD-C2D	-2.15	1.46	1.50
28	A	808	CLA	MG-NB	-2.15	2.01	2.05
28	g	322	CLA	C3B-C4B	2.15	1.49	1.42
28	A	808	CLA	CMD-C2D	-2.15	1.46	1.50
36	d	316	II0	C20-C14	2.15	1.54	1.50
28	A	807	CLA	CMD-C2D	-2.15	1.46	1.50
28	B	831	CLA	C3B-C4B	2.15	1.49	1.42
28	O	202	CLA	C3B-C4B	2.15	1.49	1.42
36	O	203	II0	C18-C04	2.15	1.57	1.53
31	B	847	WVN	C36-C32	-2.15	1.30	1.35
28	B	815	CLA	C1B-C2B	2.15	1.48	1.43
38	e	609	KC2	C1D-C2D	2.14	1.48	1.43
28	f	603	CLA	C3B-C4B	2.14	1.49	1.42
28	B	803	CLA	C1D-ND	2.14	1.40	1.37
35	b	621	LMG	O1-C1	2.14	1.43	1.40
28	i	305	CLA	CHC-C1C	2.14	1.42	1.38
28	B	815	CLA	MG-NB	-2.14	2.01	2.05
28	A	819	CLA	CMD-C2D	-2.14	1.46	1.50
28	B	811	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	k	608	CLA	CMB-C2B	-2.14	1.46	1.50
36	g	320	II0	C20-C14	2.14	1.54	1.50
28	l	304	CLA	CHC-C1C	2.14	1.42	1.38
28	e	607	CLA	CMB-C2B	-2.14	1.46	1.50
28	B	819	CLA	C3B-C4B	2.14	1.49	1.42
28	g	303	CLA	MG-NB	-2.14	2.01	2.05
28	B	820	CLA	CMD-C2D	-2.14	1.46	1.50
28	s	208	CLA	CMD-C2D	-2.14	1.46	1.50
28	n	604	CLA	C3B-C4B	2.14	1.49	1.42
28	B	821	CLA	CHC-C1C	2.14	1.42	1.38
28	B	808	CLA	CMD-C2D	-2.14	1.46	1.50
28	A	820	CLA	MG-NB	-2.14	2.01	2.05
28	B	820	CLA	CMB-C2B	-2.14	1.46	1.50
28	O	202	CLA	CMC-C2C	-2.14	1.46	1.50
28	j	602	CLA	CMD-C2D	-2.14	1.46	1.50
36	c	617	II0	C16-C03	2.14	1.57	1.53
28	B	807	CLA	C1B-C2B	2.14	1.48	1.43
28	b	608	CLA	CMB-C2B	-2.14	1.46	1.50
28	A	823	CLA	C3B-C4B	2.14	1.49	1.42
28	B	824	CLA	C3B-C4B	2.14	1.49	1.42
28	e	606	CLA	CMD-C2D	-2.14	1.46	1.50
28	b	612	CLA	C3B-C4B	2.14	1.49	1.42
38	m	611	KC2	C4A-C3A	2.14	1.48	1.44
28	A	828	CLA	CMC-C2C	-2.14	1.46	1.50
28	B	828	CLA	CMB-C2B	-2.14	1.46	1.50
28	F	202	CLA	CMD-C2D	-2.14	1.46	1.50
28	b	606	CLA	CMB-C2B	-2.14	1.46	1.50
28	f	613	CLA	CHC-C1C	2.14	1.42	1.38
38	j	611	KC2	C4A-C3A	2.14	1.48	1.44
28	j	602	CLA	CMC-C2C	-2.14	1.46	1.50
36	f	616	II0	C16-C03	2.14	1.57	1.53
36	n	616	II0	C15-C03	2.14	1.57	1.53
28	f	608	CLA	CMD-C2D	-2.13	1.46	1.50
28	e	607	CLA	CMD-C2D	-2.13	1.46	1.50
28	h	301	CLA	C1B-C2B	2.13	1.48	1.43
28	c	609	CLA	CMD-C2D	-2.13	1.46	1.50
28	e	602	CLA	CMD-C2D	-2.13	1.46	1.50
31	B	847	WVN	C37-C34	-2.13	1.30	1.35
28	j	610	CLA	C3B-C4B	2.13	1.49	1.42
28	B	815	CLA	CMD-C2D	-2.13	1.46	1.50
38	d	311	KC2	CBD-CAD	-2.13	1.46	1.56
28	B	811	CLA	MG-NB	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	608	CLA	CMD-C2D	-2.13	1.46	1.50
28	g	311	CLA	CMD-C2D	-2.13	1.46	1.50
28	b	612	CLA	CHC-C1C	2.13	1.42	1.38
36	m	616	II0	C18-C04	2.13	1.57	1.53
28	B	834	CLA	CMB-C2B	-2.13	1.46	1.50
28	f	608	CLA	CMB-C2B	-2.13	1.46	1.50
28	f	604	CLA	CMD-C2D	-2.13	1.46	1.50
28	b	604	CLA	CHC-C1C	2.13	1.42	1.38
28	b	608	CLA	CHC-C1C	2.13	1.42	1.38
28	B	818	CLA	CHC-C1C	2.13	1.42	1.38
28	m	612	CLA	C3B-C4B	2.13	1.48	1.42
28	j	605	CLA	CMD-C2D	-2.13	1.46	1.50
28	a	303	CLA	MG-NB	-2.13	2.01	2.05
36	l	316	II0	C20-C14	2.13	1.54	1.50
28	B	838	CLA	CMD-C2D	-2.13	1.46	1.50
28	A	820	CLA	C3B-C4B	2.13	1.48	1.42
28	g	302	CLA	CHC-C1C	2.13	1.42	1.38
36	e	614	II0	C16-C03	2.13	1.57	1.53
28	A	854	CLA	CMC-C2C	-2.13	1.46	1.50
38	k	611	KC2	C4B-NB	-2.12	1.35	1.37
31	L	201	WVN	C26-C22	-2.12	1.30	1.35
28	d	302	CLA	C1B-C2B	2.12	1.48	1.43
28	b	606	CLA	CMD-C2D	-2.12	1.46	1.50
38	s	204	KC2	C4A-C3A	2.12	1.48	1.44
28	A	825	CLA	MG-ND	-2.12	2.01	2.05
31	L	201	WVN	C28-C25	-2.12	1.30	1.35
28	J	103	CLA	C4B-NB	2.12	1.40	1.37
28	s	202	CLA	C1B-C2B	2.12	1.48	1.43
28	a	306	CLA	CHC-C1C	2.12	1.42	1.38
28	L	202	CLA	CMD-C2D	-2.12	1.46	1.50
28	a	308	CLA	CMB-C2B	-2.12	1.46	1.50
28	m	605	CLA	CMD-C2D	-2.12	1.46	1.50
28	B	835	CLA	CMC-C2C	-2.12	1.46	1.50
28	F	202	CLA	CMB-C2B	-2.12	1.46	1.50
38	d	310	KC2	C1D-C2D	2.12	1.48	1.43
28	n	610	CLA	CMB-C2B	-2.12	1.46	1.50
28	g	308	CLA	CMB-C2B	-2.12	1.46	1.50
36	i	320	II0	C15-C03	2.12	1.57	1.53
28	B	825	CLA	MG-NB	-2.12	2.01	2.05
28	g	307	CLA	C3B-C4B	2.12	1.48	1.42
28	a	305	CLA	CHC-C1C	2.12	1.42	1.38
28	A	811	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	e	610	CLA	CMD-C2D	-2.12	1.46	1.50
28	n	606	CLA	CMD-C2D	-2.12	1.46	1.50
36	d	316	II0	C18-C04	2.12	1.57	1.53
28	h	301	CLA	MG-NB	-2.12	2.01	2.05
28	h	313	CLA	C3B-C4B	2.12	1.48	1.42
28	k	601	CLA	C3B-C4B	2.12	1.48	1.42
28	m	612	CLA	CMB-C2B	-2.12	1.46	1.50
28	k	606	CLA	CMB-C2B	-2.12	1.46	1.50
28	B	826	CLA	CMC-C2C	-2.12	1.46	1.50
36	f	614	II0	C15-C03	2.12	1.57	1.53
28	l	307	CLA	MG-ND	-2.12	2.01	2.05
28	h	313	CLA	CMB-C2B	-2.12	1.46	1.50
28	b	612	CLA	MG-ND	-2.12	2.01	2.05
28	L	207	CLA	CMD-C2D	-2.12	1.46	1.50
28	l	308	CLA	CMD-C2D	-2.12	1.46	1.50
28	A	831	CLA	CMD-C2D	-2.12	1.46	1.50
28	m	603	CLA	CMC-C2C	-2.12	1.46	1.50
28	O	201	CLA	MG-NB	-2.12	2.01	2.05
28	Q	302	CLA	C3B-C4B	2.12	1.48	1.42
28	A	816	CLA	CMC-C2C	-2.12	1.46	1.50
28	l	308	CLA	CMB-C2B	-2.12	1.46	1.50
28	A	834	CLA	C1B-C2B	2.12	1.48	1.43
36	O	203	II0	C20-C14	2.12	1.54	1.50
36	n	615	II0	C15-C03	2.12	1.57	1.53
28	B	839	CLA	CMB-C2B	-2.12	1.46	1.50
38	j	611	KC2	C4B-NB	-2.12	1.35	1.37
28	A	854	CLA	O2A-CGA	2.12	1.39	1.33
28	c	606	CLA	MG-ND	-2.12	2.01	2.05
28	B	822	CLA	C1B-NB	-2.11	1.35	1.37
28	O	202	CLA	CMB-C2B	-2.11	1.46	1.50
28	l	305	CLA	CMD-C2D	-2.11	1.46	1.50
28	A	837	CLA	MG-NB	-2.11	2.01	2.05
28	f	602	CLA	CHC-C1C	2.11	1.42	1.38
31	A	846	WVN	C37-C34	-2.11	1.30	1.35
28	A	811	CLA	CMD-C2D	-2.11	1.46	1.50
28	b	605	CLA	CMD-C2D	-2.11	1.46	1.50
28	j	608	CLA	CHC-C1C	2.11	1.42	1.38
36	n	616	II0	C18-C04	2.11	1.57	1.53
37	n	617	IHT	C13-C02	2.11	1.57	1.53
28	A	837	CLA	CMC-C2C	-2.11	1.46	1.50
28	A	814	CLA	C3B-C4B	2.11	1.48	1.42
28	B	803	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	602	CLA	CHC-C1C	2.11	1.42	1.38
28	e	611	CLA	CMD-C2D	-2.11	1.46	1.50
28	f	613	CLA	CMB-C2B	-2.11	1.46	1.50
28	c	609	CLA	CHC-C1C	2.11	1.42	1.38
28	b	611	CLA	CMD-C2D	-2.11	1.46	1.50
28	l	307	CLA	MG-NB	-2.11	2.01	2.05
31	L	205	WVN	C02-C11	2.11	1.53	1.50
28	L	203	CLA	CMD-C2D	-2.11	1.46	1.50
28	B	804	CLA	C3B-C4B	2.11	1.48	1.42
28	A	818	CLA	CMD-C2D	-2.11	1.46	1.50
28	f	612	CLA	CMC-C2C	-2.11	1.46	1.50
28	B	828	CLA	CMD-C2D	-2.11	1.46	1.50
28	h	305	CLA	CMB-C2B	-2.11	1.46	1.50
28	f	610	CLA	CMB-C2B	-2.11	1.46	1.50
28	b	603	CLA	MG-ND	-2.11	2.01	2.05
38	n	612	KC2	C3C-C4C	2.11	1.49	1.44
36	m	614	II0	C15-C03	2.11	1.57	1.53
28	A	818	CLA	MG-NB	-2.11	2.01	2.05
28	B	803	CLA	MG-ND	-2.11	2.01	2.05
28	j	613	CLA	C3B-C4B	2.11	1.48	1.42
28	B	828	CLA	MG-NB	-2.11	2.01	2.05
28	c	605	CLA	MG-NB	-2.11	2.01	2.05
36	f	618	II0	C18-C04	2.11	1.57	1.53
36	c	613	II0	C15-C03	2.11	1.57	1.53
28	c	612	CLA	CMD-C2D	-2.10	1.46	1.50
28	b	610	CLA	CMB-C2B	-2.10	1.46	1.50
31	B	844	WVN	C26-C22	-2.10	1.30	1.35
28	j	601	CLA	CMB-C2B	-2.10	1.46	1.50
31	A	845	WVN	C23-C25	2.10	1.50	1.46
28	b	601	CLA	CMB-C2B	-2.10	1.46	1.50
28	A	834	CLA	C3B-C4B	2.10	1.48	1.42
28	m	610	CLA	CMD-C2D	-2.10	1.46	1.50
28	e	601	CLA	CMD-C2D	-2.10	1.46	1.50
28	n	610	CLA	CMD-C2D	-2.10	1.46	1.50
28	a	307	CLA	CHC-C1C	2.10	1.42	1.38
28	B	809	CLA	CMD-C2D	-2.10	1.46	1.50
28	B	806	CLA	MG-NB	-2.10	2.01	2.05
28	g	307	CLA	CMD-C2D	-2.10	1.46	1.50
28	e	607	CLA	C3B-C4B	2.10	1.48	1.42
28	A	830	CLA	C1B-NB	-2.10	1.35	1.37
28	B	834	CLA	CHC-C1C	2.10	1.42	1.38
28	O	202	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	303	CLA	CHC-C1C	2.10	1.42	1.38
36	c	614	II0	C15-C03	2.10	1.57	1.53
37	c	616	IHT	C13-C02	2.10	1.57	1.53
28	k	606	CLA	CHC-C1C	2.10	1.42	1.38
28	j	605	CLA	CHC-C1C	2.10	1.42	1.38
31	B	845	WVN	C19-C22	2.10	1.50	1.46
28	k	605	CLA	CMD-C2D	-2.10	1.46	1.50
28	f	609	CLA	CMD-C2D	-2.10	1.46	1.50
31	B	844	WVN	C28-C25	-2.10	1.30	1.35
31	L	201	WVN	C36-C32	-2.10	1.30	1.35
28	J	103	CLA	C3B-C4B	2.10	1.48	1.42
28	c	602	CLA	C1B-C2B	2.10	1.48	1.43
28	B	841	CLA	MG-NB	-2.10	2.01	2.05
31	L	206	WVN	C26-C22	-2.10	1.31	1.35
28	i	302	CLA	CMD-C2D	-2.10	1.46	1.50
28	g	304	CLA	CMD-C2D	-2.10	1.46	1.50
28	B	840	CLA	CMB-C2B	-2.09	1.46	1.50
28	f	602	CLA	CMC-C2C	-2.09	1.46	1.50
28	f	606	CLA	CMD-C2D	-2.09	1.46	1.50
28	n	606	CLA	CMB-C2B	-2.09	1.46	1.50
28	h	313	CLA	CHC-C1C	2.09	1.42	1.38
28	B	812	CLA	CMC-C2C	-2.09	1.46	1.50
28	B	829	CLA	MG-ND	-2.09	2.01	2.05
36	b	614	II0	C15-C03	2.09	1.57	1.53
28	j	613	CLA	CMD-C2D	-2.09	1.46	1.50
28	s	208	CLA	C3B-C4B	2.09	1.48	1.42
28	h	305	CLA	CMC-C2C	-2.09	1.46	1.50
28	l	303	CLA	CHC-C1C	2.09	1.42	1.38
28	m	612	CLA	MG-ND	-2.09	2.01	2.05
28	k	610	CLA	CMB-C2B	-2.09	1.46	1.50
28	A	825	CLA	C3B-C4B	2.09	1.48	1.42
28	b	604	CLA	MG-NB	-2.09	2.01	2.05
28	Q	302	CLA	CMC-C2C	-2.09	1.46	1.50
28	A	802	CLA	MG-NB	-2.09	2.01	2.05
28	e	605	CLA	CMB-C2B	-2.09	1.46	1.50
28	i	306	CLA	CMB-C2B	-2.09	1.46	1.50
28	l	302	CLA	C3B-C4B	2.09	1.48	1.42
28	Q	303	CLA	C1B-NB	-2.09	1.35	1.37
38	i	319	KC2	C1D-C2D	2.09	1.48	1.43
28	A	839	CLA	CMD-C2D	-2.09	1.46	1.50
28	B	823	CLA	CMD-C2D	-2.09	1.46	1.50
28	g	305	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	i	317	II0	C16-C03	2.09	1.57	1.53
37	k	618	IHT	C13-C02	2.09	1.57	1.53
28	n	613	CLA	CHC-C1C	2.09	1.42	1.38
28	l	309	CLA	CMB-C2B	-2.09	1.46	1.50
28	d	307	CLA	CMD-C2D	-2.09	1.46	1.50
28	g	307	CLA	CHC-C1C	2.09	1.42	1.38
36	k	621	II0	C20-C14	2.09	1.54	1.50
36	m	618	II0	C15-C03	2.09	1.57	1.53
28	A	823	CLA	CMC-C2C	-2.09	1.46	1.50
28	B	814	CLA	CMD-C2D	-2.09	1.46	1.50
28	e	605	CLA	CMD-C2D	-2.09	1.46	1.50
28	m	610	CLA	CMB-C2B	-2.08	1.46	1.50
28	f	605	CLA	CMD-C2D	-2.08	1.46	1.50
28	a	305	CLA	CMC-C2C	-2.08	1.46	1.50
28	m	606	CLA	CMB-C2B	-2.08	1.46	1.50
38	i	310	KC2	C4A-C3A	2.08	1.48	1.44
36	b	613	II0	C15-C03	2.08	1.57	1.53
28	A	802	CLA	CHC-C1C	2.08	1.42	1.38
28	B	824	CLA	CMB-C2B	-2.08	1.46	1.50
28	b	602	CLA	CMD-C2D	-2.08	1.46	1.50
28	b	612	CLA	CMB-C2B	-2.08	1.46	1.50
28	k	609	CLA	CMD-C2D	-2.08	1.46	1.50
28	n	603	CLA	CMB-C2B	-2.08	1.46	1.50
28	l	308	CLA	CMC-C2C	-2.08	1.46	1.50
28	b	609	CLA	CMB-C2B	-2.08	1.46	1.50
28	A	829	CLA	MG-NB	-2.08	2.01	2.05
28	A	805	CLA	MG-NB	-2.08	2.01	2.05
28	h	308	CLA	C3B-C4B	2.08	1.48	1.42
28	L	203	CLA	CMB-C2B	-2.08	1.46	1.50
28	m	601	CLA	CMB-C2B	-2.08	1.46	1.50
28	B	805	CLA	CMC-C2C	-2.08	1.46	1.50
28	i	304	CLA	CMD-C2D	-2.08	1.46	1.50
28	s	203	CLA	MG-NB	-2.08	2.01	2.05
28	k	601	CLA	MG-NB	-2.08	2.01	2.05
28	a	309	CLA	C4B-NB	2.08	1.40	1.37
37	b	616	IHT	C13-C02	2.08	1.57	1.53
28	d	308	CLA	CMD-C2D	-2.08	1.46	1.50
28	s	206	CLA	CHC-C1C	2.08	1.42	1.38
28	A	805	CLA	C3B-C4B	2.08	1.48	1.42
28	i	312	CLA	CMD-C2D	-2.08	1.46	1.50
28	f	613	CLA	CMD-C2D	-2.08	1.46	1.50
28	n	604	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	312	II0	C15-C03	2.08	1.57	1.53
28	B	803	CLA	C1B-C2B	2.08	1.48	1.43
28	g	322	CLA	CHC-C1C	2.08	1.42	1.38
28	g	311	CLA	CMB-C2B	-2.08	1.46	1.50
31	M	101	WVN	C21-C15	2.08	1.54	1.50
37	O	204	IHT	C13-C02	2.08	1.57	1.53
28	B	805	CLA	C3B-C4B	2.08	1.48	1.42
28	b	604	CLA	CMC-C2C	-2.08	1.46	1.50
28	A	808	CLA	C4B-NB	2.08	1.40	1.37
28	B	840	CLA	MG-NB	-2.07	2.01	2.05
28	g	309	CLA	CMB-C2B	-2.07	1.46	1.50
28	B	810	CLA	CMB-C2B	-2.07	1.46	1.50
28	O	206	CLA	CHC-C4B	-2.07	1.34	1.39
28	A	832	CLA	CMD-C2D	-2.07	1.46	1.50
28	c	601	CLA	CMB-C2B	-2.07	1.46	1.50
28	h	307	CLA	CMD-C2D	-2.07	1.46	1.50
28	O	201	CLA	CMC-C2C	-2.07	1.46	1.50
28	l	303	CLA	CMC-C2C	-2.07	1.46	1.50
28	B	817	CLA	MG-ND	-2.07	2.01	2.05
28	B	832	CLA	MG-ND	-2.07	2.01	2.05
28	B	840	CLA	C3B-C4B	2.07	1.48	1.42
36	b	617	II0	C16-C03	2.07	1.57	1.53
37	j	616	IHT	C13-C02	2.07	1.57	1.53
28	B	811	CLA	CMD-C2D	-2.07	1.46	1.50
28	f	606	CLA	CMB-C2B	-2.07	1.46	1.50
28	B	810	CLA	CMD-C2D	-2.07	1.46	1.50
28	m	608	CLA	CHC-C1C	2.07	1.42	1.38
28	A	822	CLA	CMB-C2B	-2.07	1.46	1.50
28	i	303	CLA	CMC-C2C	-2.07	1.46	1.50
28	A	821	CLA	CHC-C1C	2.07	1.42	1.38
28	b	607	CLA	C3B-C4B	2.07	1.48	1.42
28	B	807	CLA	CMC-C2C	-2.07	1.46	1.50
28	d	306	CLA	CHC-C1C	2.07	1.42	1.38
31	A	846	WVN	C36-C32	-2.07	1.31	1.35
28	A	828	CLA	MG-ND	-2.07	2.01	2.05
28	B	816	CLA	CMD-C2D	-2.07	1.46	1.50
28	A	806	CLA	CHC-C1C	2.07	1.42	1.38
28	g	315	CLA	CHC-C1C	2.07	1.42	1.38
28	h	305	CLA	C3B-C4B	2.07	1.48	1.42
36	c	617	II0	C30-C26	-2.07	1.32	1.37
28	O	202	CLA	MG-NB	-2.07	2.01	2.05
28	F	201	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	g	304	CLA	CHC-C1C	2.07	1.42	1.38
28	a	310	CLA	CMB-C2B	-2.07	1.46	1.50
28	e	610	CLA	CMB-C2B	-2.07	1.46	1.50
28	n	601	CLA	CMB-C2B	-2.07	1.46	1.50
28	L	203	CLA	CHC-C1C	2.07	1.42	1.38
28	A	831	CLA	MG-NB	-2.07	2.01	2.05
32	b	618	LMT	O5'-C5'	-2.06	1.39	1.44
28	m	612	CLA	CMC-C2C	-2.06	1.46	1.50
28	f	610	CLA	CMD-C2D	-2.06	1.46	1.50
28	d	305	CLA	CMD-C2D	-2.06	1.46	1.50
36	d	315	II0	C15-C03	2.06	1.57	1.53
28	c	612	CLA	CHC-C1C	2.06	1.42	1.38
28	l	304	CLA	CMB-C2B	-2.06	1.46	1.50
28	c	606	CLA	C1B-C2B	2.06	1.48	1.43
28	B	833	CLA	CHC-C1C	2.06	1.42	1.38
28	n	608	CLA	CMB-C2B	-2.06	1.46	1.50
28	m	601	CLA	CHC-C1C	2.06	1.42	1.38
28	a	306	CLA	CMC-C2C	-2.06	1.46	1.50
28	g	307	CLA	CMB-C2B	-2.06	1.46	1.50
28	e	604	CLA	MG-NB	-2.06	2.01	2.05
36	k	615	II0	C15-C03	2.06	1.57	1.53
28	A	841	CLA	CMC-C2C	-2.06	1.46	1.50
28	c	603	CLA	CMC-C2C	-2.06	1.46	1.50
31	s	205	WVN	C28-C25	-2.06	1.31	1.35
28	B	806	CLA	C3B-C4B	2.06	1.48	1.42
36	m	614	II0	C16-C03	2.06	1.57	1.53
28	h	304	CLA	CMB-C2B	-2.06	1.46	1.50
28	k	610	CLA	CMC-C2C	-2.06	1.46	1.50
28	l	302	CLA	CMC-C2C	-2.06	1.46	1.50
28	l	306	CLA	C2A-C1A	2.06	1.56	1.52
28	d	309	CLA	CMD-C2D	-2.06	1.46	1.50
28	a	304	CLA	CHC-C1C	2.06	1.42	1.38
28	g	306	CLA	CHC-C1C	2.06	1.42	1.38
28	K	103	CLA	CHC-C4B	-2.06	1.34	1.39
28	a	309	CLA	CMD-C2D	-2.06	1.46	1.50
28	A	818	CLA	C3C-C2C	2.06	1.41	1.36
28	A	808	CLA	CMC-C2C	-2.06	1.46	1.50
28	k	603	CLA	MG-NB	-2.06	2.01	2.05
28	i	311	CLA	CHC-C1C	2.06	1.42	1.38
28	h	307	CLA	CMB-C2B	-2.06	1.46	1.50
28	A	809	CLA	CMD-C2D	-2.06	1.46	1.50
28	A	810	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	802	CLA	CMB-C2B	-2.06	1.46	1.50
28	B	831	CLA	CMD-C2D	-2.06	1.46	1.50
28	L	204	CLA	CMB-C2B	-2.06	1.46	1.50
36	e	616	II0	C20-C14	2.06	1.54	1.50
28	f	603	CLA	CMC-C2C	-2.06	1.46	1.50
28	k	602	CLA	CMD-C2D	-2.06	1.46	1.50
38	j	611	KC2	C1D-C2D	2.06	1.48	1.43
28	b	603	CLA	C1B-NB	-2.06	1.35	1.37
36	f	615	II0	C20-C14	2.06	1.54	1.50
28	A	828	CLA	C3B-C4B	2.06	1.48	1.42
36	i	313	II0	C15-C03	2.06	1.57	1.53
28	b	609	CLA	C3B-C4B	2.05	1.48	1.42
28	A	805	CLA	MG-ND	-2.05	2.01	2.05
28	g	309	CLA	CMD-C2D	-2.05	1.46	1.50
28	e	601	CLA	CMB-C2B	-2.05	1.46	1.50
28	e	605	CLA	CMC-C2C	-2.05	1.46	1.50
28	A	831	CLA	MG-ND	-2.05	2.01	2.05
28	A	821	CLA	CMD-C2D	-2.05	1.46	1.50
28	A	832	CLA	CMB-C2B	-2.05	1.46	1.50
28	e	608	CLA	C3B-C4B	2.05	1.48	1.42
38	i	310	KC2	C1D-C2D	2.05	1.47	1.43
36	m	618	II0	C20-C14	2.05	1.54	1.50
28	g	315	CLA	CMC-C2C	-2.05	1.46	1.50
36	l	316	II0	C15-C03	2.05	1.57	1.53
28	K	101	CLA	CMC-C2C	-2.05	1.46	1.50
28	f	602	CLA	CMD-C2D	-2.05	1.46	1.50
28	A	838	CLA	CMC-C2C	-2.05	1.46	1.50
28	h	301	CLA	CMC-C2C	-2.05	1.46	1.50
28	k	603	CLA	CMD-C2D	-2.05	1.46	1.50
28	j	603	CLA	CMC-C2C	-2.05	1.46	1.50
28	n	601	CLA	CMC-C2C	-2.05	1.46	1.50
28	n	609	CLA	CMB-C2B	-2.05	1.46	1.50
28	B	831	CLA	C1B-C2B	2.05	1.47	1.43
28	A	852	CLA	CMD-C2D	-2.05	1.46	1.50
28	A	826	CLA	CHC-C1C	2.05	1.42	1.38
28	B	815	CLA	CHC-C1C	2.05	1.42	1.38
28	n	605	CLA	CMB-C2B	-2.05	1.46	1.50
28	s	208	CLA	MG-NB	-2.05	2.01	2.05
28	h	308	CLA	MG-NB	-2.05	2.01	2.05
28	A	804	CLA	CMB-C2B	-2.05	1.46	1.50
28	f	601	CLA	MG-ND	-2.05	2.01	2.05
28	a	313	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	821	CLA	C1B-NB	-2.05	1.35	1.37
28	A	805	CLA	CMC-C2C	-2.05	1.46	1.50
28	B	831	CLA	CMC-C2C	-2.05	1.46	1.50
28	B	836	CLA	CMC-C2C	-2.05	1.46	1.50
28	n	601	CLA	CMD-C2D	-2.05	1.46	1.50
28	c	603	CLA	MG-NB	-2.05	2.01	2.05
28	B	808	CLA	CHC-C4B	-2.05	1.34	1.39
28	k	607	CLA	CMB-C2B	-2.05	1.46	1.50
31	s	205	WVN	C02-C11	2.05	1.53	1.50
28	B	808	CLA	CMC-C2C	-2.05	1.46	1.50
36	k	615	II0	C20-C14	2.05	1.54	1.50
28	A	831	CLA	CMC-C2C	-2.05	1.46	1.50
28	f	603	CLA	CHC-C1C	2.05	1.42	1.38
38	c	610	KC2	C4B-NB	-2.05	1.35	1.37
28	b	602	CLA	CMC-C2C	-2.05	1.46	1.50
38	n	612	KC2	C1D-C2D	2.05	1.47	1.43
28	m	601	CLA	CMC-C2C	-2.05	1.46	1.50
28	B	840	CLA	CHC-C1C	2.05	1.42	1.38
28	d	312	CLA	CMB-C2B	-2.05	1.46	1.50
28	m	605	CLA	MG-NB	-2.04	2.01	2.05
28	A	839	CLA	MG-NB	-2.04	2.01	2.05
28	B	822	CLA	CMB-C2B	-2.04	1.46	1.50
28	k	604	CLA	CMB-C2B	-2.04	1.46	1.50
28	B	820	CLA	CHC-C1C	2.04	1.42	1.38
28	a	311	CLA	CHC-C1C	2.04	1.42	1.38
28	g	310	CLA	CHC-C1C	2.04	1.42	1.38
36	a	314	II0	C15-C03	2.04	1.57	1.53
37	b	615	IHT	C13-C02	2.04	1.57	1.53
28	b	612	CLA	CMC-C2C	-2.04	1.46	1.50
28	f	605	CLA	CMC-C2C	-2.04	1.46	1.50
36	a	314	II0	C20-C14	2.04	1.54	1.50
28	B	833	CLA	MG-NB	-2.04	2.01	2.05
28	L	202	CLA	MG-NB	-2.04	2.01	2.05
28	s	202	CLA	MG-ND	-2.04	2.01	2.05
28	B	815	CLA	CMC-C2C	-2.04	1.46	1.50
28	B	833	CLA	CMC-C2C	-2.04	1.46	1.50
28	s	203	CLA	CMB-C2B	-2.04	1.46	1.50
28	Q	303	CLA	CMC-C2C	-2.04	1.46	1.50
28	A	806	CLA	CMC-C2C	-2.04	1.46	1.50
28	n	605	CLA	CMC-C2C	-2.04	1.46	1.50
36	k	621	II0	C18-C04	2.04	1.57	1.53
28	l	303	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	l	311	CLA	CMB-C2B	-2.04	1.46	1.50
28	k	606	CLA	CMC-C2C	-2.04	1.46	1.50
28	A	818	CLA	C1B-C2B	2.04	1.47	1.43
36	j	615	II0	C20-C14	2.04	1.54	1.50
31	A	847	WVN	C26-C22	-2.04	1.31	1.35
28	m	602	CLA	MG-ND	-2.04	2.01	2.05
36	e	614	II0	C18-C04	2.04	1.57	1.53
28	l	309	CLA	CHC-C1C	2.04	1.42	1.38
28	d	303	CLA	CMB-C2B	-2.04	1.46	1.50
28	b	606	CLA	MG-NB	-2.04	2.01	2.05
28	a	312	CLA	CMB-C2B	-2.04	1.46	1.50
28	f	605	CLA	C3B-C4B	2.04	1.48	1.42
28	B	815	CLA	CMB-C2B	-2.04	1.46	1.50
28	B	805	CLA	MG-ND	-2.04	2.01	2.05
28	f	612	CLA	MG-NC	2.04	2.11	2.06
28	k	614	CLA	CHC-C1C	2.03	1.42	1.38
28	A	827	CLA	CMC-C2C	-2.03	1.46	1.50
28	l	304	CLA	CMD-C2D	-2.03	1.46	1.50
28	g	309	CLA	CHC-C1C	2.03	1.42	1.38
28	c	603	CLA	CMD-C2D	-2.03	1.46	1.50
28	b	607	CLA	CMC-C2C	-2.03	1.46	1.50
28	k	614	CLA	CMB-C2B	-2.03	1.46	1.50
28	i	312	CLA	CMC-C2C	-2.03	1.46	1.50
28	j	602	CLA	CHC-C1C	2.03	1.42	1.38
37	f	617	IHT	C13-C02	2.03	1.57	1.53
28	n	603	CLA	MG-NB	-2.03	2.01	2.05
28	A	852	CLA	C1B-C2B	2.03	1.47	1.43
36	J	104	II0	C20-C14	2.03	1.54	1.50
28	L	207	CLA	CHC-C1C	2.03	1.42	1.38
36	m	616	II0	C15-C03	2.03	1.57	1.53
28	B	833	CLA	CMD-C2D	-2.03	1.46	1.50
28	i	309	CLA	CMB-C2B	-2.03	1.46	1.50
28	j	607	CLA	CMB-C2B	-2.03	1.46	1.50
31	K	102	WVN	C36-C32	-2.03	1.31	1.35
28	e	607	CLA	CMC-C2C	-2.03	1.46	1.50
28	l	308	CLA	CHC-C1C	2.03	1.42	1.38
28	A	829	CLA	CHC-C4B	-2.03	1.34	1.39
28	A	824	CLA	MG-NB	-2.03	2.01	2.05
36	l	312	II0	C20-C14	2.03	1.54	1.50
28	f	612	CLA	CMD-C2D	-2.03	1.46	1.50
28	d	309	CLA	CMB-C2B	-2.03	1.46	1.50
28	m	607	CLA	C1B-C2B	2.03	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	602	CLA	MG-NB	-2.03	2.01	2.05
39	i	301	LMU	O5'-C5'	2.03	1.49	1.44
28	s	206	CLA	CMC-C2C	-2.03	1.46	1.50
28	m	610	CLA	C3B-C4B	2.03	1.48	1.42
28	k	610	CLA	C3B-C4B	2.03	1.48	1.42
28	k	603	CLA	CHC-C1C	2.03	1.42	1.38
28	c	606	CLA	CAC-C3C	-2.03	1.45	1.51
31	s	207	WVN	C02-C11	2.03	1.53	1.50
36	m	615	II0	C20-C14	2.03	1.54	1.50
28	J	103	CLA	CHC-C4B	-2.03	1.34	1.39
28	A	822	CLA	MG-NB	-2.03	2.01	2.05
28	g	308	CLA	CAC-C3C	-2.03	1.45	1.51
28	m	608	CLA	CMC-C2C	-2.03	1.46	1.50
28	a	305	CLA	MG-NB	-2.03	2.01	2.05
28	a	308	CLA	CMD-C2D	-2.03	1.46	1.50
28	A	854	CLA	C1B-C2B	2.03	1.47	1.43
28	b	603	CLA	C1B-C2B	2.03	1.47	1.43
28	J	103	CLA	MG-NB	-2.03	2.01	2.05
28	A	824	CLA	CMB-C2B	-2.03	1.46	1.50
28	A	841	CLA	CMB-C2B	-2.03	1.46	1.50
28	i	302	CLA	CMB-C2B	-2.03	1.46	1.50
28	e	608	CLA	CMB-C2B	-2.02	1.46	1.50
28	k	604	CLA	MG-NC	2.02	2.11	2.06
28	j	609	CLA	CMD-C2D	-2.02	1.46	1.50
28	B	825	CLA	C3B-C4B	2.02	1.48	1.42
28	A	835	CLA	CMC-C2C	-2.02	1.46	1.50
28	b	605	CLA	CMC-C2C	-2.02	1.46	1.50
28	A	834	CLA	C1B-NB	-2.02	1.35	1.37
38	f	611	KC2	C4B-NB	-2.02	1.35	1.37
31	L	201	WVN	C40-C39	-2.02	1.30	1.36
36	m	615	II0	C15-C03	2.02	1.57	1.53
36	g	316	II0	C15-C03	2.02	1.57	1.53
28	h	303	CLA	CMC-C2C	-2.02	1.46	1.50
28	B	839	CLA	CMC-C2C	-2.02	1.46	1.50
28	e	610	CLA	CMC-C2C	-2.02	1.46	1.50
28	k	601	CLA	CMB-C2B	-2.02	1.46	1.50
28	f	610	CLA	MG-NB	-2.02	2.01	2.05
28	L	203	CLA	CMC-C2C	-2.02	1.46	1.50
28	A	805	CLA	CMB-C2B	-2.02	1.46	1.50
28	B	828	CLA	CMC-C2C	-2.02	1.46	1.50
28	c	608	CLA	CHC-C1C	2.02	1.42	1.38
28	n	601	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	608	CLA	CMD-C2D	-2.02	1.46	1.50
28	l	306	CLA	CMB-C2B	-2.02	1.46	1.50
28	A	825	CLA	CHC-C1C	2.02	1.42	1.38
38	g	313	KC2	C1D-C2D	2.02	1.47	1.43
28	n	609	CLA	CMD-C2D	-2.02	1.46	1.50
28	B	819	CLA	CMC-C2C	-2.02	1.46	1.50
28	l	302	CLA	CMB-C2B	-2.02	1.46	1.50
28	h	304	CLA	MG-NB	-2.02	2.01	2.05
38	d	310	KC2	C4B-NB	-2.02	1.35	1.37
28	i	306	CLA	CMC-C2C	-2.02	1.46	1.50
31	B	848	WVN	C36-C32	-2.02	1.31	1.35
28	g	315	CLA	CMB-C2B	-2.02	1.46	1.50
28	k	608	CLA	CMD-C2D	-2.01	1.46	1.50
37	g	319	IHT	C13-C02	2.01	1.57	1.53
28	c	602	CLA	MG-NB	-2.01	2.01	2.05
28	m	605	CLA	C3B-C4B	2.01	1.48	1.42
28	n	609	CLA	CHC-C1C	2.01	1.42	1.38
28	a	305	CLA	CMB-C2B	-2.01	1.46	1.50
28	e	601	CLA	O2A-CGA	2.01	1.37	1.30
28	e	608	CLA	CHC-C1C	2.01	1.42	1.38
28	f	603	CLA	MG-NB	-2.01	2.01	2.05
36	i	314	II0	C15-C03	2.01	1.57	1.53
28	h	304	CLA	C3B-C4B	2.01	1.48	1.42
28	A	834	CLA	CMC-C2C	-2.01	1.46	1.50
28	e	601	CLA	CMC-C2C	-2.01	1.46	1.50
28	j	609	CLA	CMC-C2C	-2.01	1.46	1.50
28	e	605	CLA	CHC-C1C	2.01	1.42	1.38
28	B	829	CLA	C3B-C4B	2.01	1.48	1.42
38	n	611	KC2	C4A-C3A	2.01	1.48	1.44
28	J	103	CLA	MG-ND	-2.01	2.01	2.05
28	c	602	CLA	CMB-C2B	-2.01	1.46	1.50
39	i	301	LMU	O1'-C1'	-2.01	1.36	1.40
28	e	605	CLA	MG-NB	-2.01	2.01	2.05
28	a	311	CLA	CMB-C2B	-2.01	1.46	1.50
28	j	606	CLA	CAA-C2A	-2.01	1.50	1.54
36	f	618	II0	C20-C14	2.01	1.54	1.50
28	m	613	CLA	MG-ND	-2.01	2.01	2.05
28	B	825	CLA	CMB-C2B	-2.01	1.46	1.50
28	e	604	CLA	CMB-C2B	-2.01	1.46	1.50
28	A	824	CLA	CMC-C2C	-2.01	1.46	1.50
28	e	608	CLA	CMD-C2D	-2.01	1.46	1.50
36	e	614	II0	C20-C14	2.01	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	827	CLA	C3B-C4B	2.01	1.48	1.42
28	e	604	CLA	CMC-C2C	-2.01	1.46	1.50
28	B	805	CLA	CMB-C2B	-2.01	1.46	1.50
28	B	816	CLA	CMC-C2C	-2.01	1.46	1.50
28	e	602	CLA	CMB-C2B	-2.01	1.46	1.50
28	j	603	CLA	CMD-C2D	-2.01	1.46	1.50
28	a	308	CLA	CMC-C2C	-2.01	1.46	1.50
28	B	823	CLA	MG-NB	-2.01	2.01	2.05
28	j	604	CLA	CHC-C1C	2.01	1.42	1.38
28	A	823	CLA	CMD-C2D	-2.01	1.46	1.50
28	g	311	CLA	C2-C3	2.01	1.37	1.33
28	A	822	CLA	MG-ND	-2.01	2.01	2.05
28	i	303	CLA	CHC-C1C	2.01	1.42	1.38
36	e	612	II0	C15-C03	2.01	1.57	1.53
28	K	101	CLA	CMD-C2D	-2.01	1.46	1.50
37	R	204	IHT	C13-C02	2.01	1.57	1.53
36	n	618	II0	C20-C14	2.00	1.54	1.50
36	b	614	II0	C20-C14	2.00	1.54	1.50
28	A	824	CLA	CHC-C1C	2.00	1.42	1.38
28	A	808	CLA	MG-ND	-2.00	2.01	2.05
38	n	611	KC2	C4B-NB	-2.00	1.35	1.37
28	n	602	CLA	CMC-C2C	-2.00	1.46	1.50
28	B	804	CLA	CMB-C2B	-2.00	1.46	1.50
28	A	824	CLA	C1B-NB	-2.00	1.35	1.37
36	i	313	II0	C18-C04	2.00	1.57	1.53
28	j	605	CLA	CMC-C2C	-2.00	1.46	1.50
38	m	611	KC2	C4B-NB	-2.00	1.35	1.37
28	f	610	CLA	CHC-C1C	2.00	1.42	1.38
31	A	847	WVN	C36-C32	-2.00	1.31	1.35
28	L	202	CLA	CMC-C2C	-2.00	1.46	1.50

All (4325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	J	101	WVN	C29-C26-C22	13.57	146.31	127.28
38	g	312	KC2	C1A-NA-C4A	-12.09	101.16	106.68
38	i	319	KC2	C1A-NA-C4A	-11.97	101.22	106.68
38	l	310	KC2	C1A-NA-C4A	-11.93	101.24	106.68
36	m	618	II0	C42-C40-C36	-11.71	110.85	127.28
38	j	611	KC2	C1A-NA-C4A	-11.60	101.39	106.68
38	g	314	KC2	C1A-NA-C4A	-11.53	101.42	106.68
38	k	611	KC2	C1A-NA-C4A	-11.49	101.44	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	i	310	KC2	C1A-NA-C4A	-11.39	101.48	106.68
38	e	609	KC2	C1A-NA-C4A	-11.34	101.50	106.68
38	m	611	KC2	C1A-NA-C4A	-11.06	101.63	106.68
38	n	611	KC2	C1A-NA-C4A	-10.99	101.66	106.68
37	b	616	IHT	C40-C37-C33	-10.81	112.11	127.28
38	d	310	KC2	C1A-NA-C4A	-10.81	101.75	106.68
37	g	319	IHT	C18-C22-C23	-10.79	110.28	126.23
38	c	610	KC2	C1A-NA-C4A	-10.51	101.89	106.68
38	n	612	KC2	C1A-NA-C4A	-10.43	101.92	106.68
38	g	313	KC2	C1A-NA-C4A	-10.34	101.96	106.68
31	J	101	WVN	C19-C22-C26	10.29	135.19	119.01
38	s	201	KC2	C1A-NA-C4A	-10.28	101.99	106.68
38	k	613	KC2	C1A-NA-C4A	-10.20	102.03	106.68
38	s	204	KC2	C1A-NA-C4A	-10.18	102.03	106.68
38	k	612	KC2	C1A-NA-C4A	-10.14	102.06	106.68
37	b	616	IHT	C18-C22-C23	-9.67	111.92	126.23
38	n	612	KC2	CHD-C4C-NC	9.53	138.67	124.31
36	a	318	II0	C42-C40-C36	-9.28	114.26	127.28
28	A	855	CLA	C4A-NA-C1A	9.18	110.86	106.68
31	A	848	WVN	C20-C23-C25	-9.16	112.68	126.23
31	F	204	WVN	C20-C23-C25	-9.15	112.70	126.23
31	A	846	WVN	C39-C36-C32	-9.11	114.50	127.28
31	F	204	WVN	C30-C28-C25	-9.04	114.60	127.28
38	f	611	KC2	C1A-NA-C4A	-9.03	102.56	106.68
37	g	319	IHT	C40-C37-C33	-9.02	114.62	127.28
38	n	611	KC2	CHD-C4C-NC	9.01	137.87	124.31
38	f	611	KC2	CHD-C4C-NC	8.95	137.79	124.31
38	c	610	KC2	CHD-C4C-NC	8.92	137.74	124.31
38	k	611	KC2	CHD-C4C-NC	8.92	137.74	124.31
38	m	611	KC2	CHD-C4C-NC	8.86	137.65	124.31
38	j	611	KC2	CHD-C4C-NC	8.86	137.65	124.31
38	k	613	KC2	CHD-C4C-NC	8.84	137.63	124.31
38	d	310	KC2	CHD-C4C-NC	8.83	137.61	124.31
38	l	310	KC2	CHD-C4C-NC	8.81	137.58	124.31
38	g	312	KC2	CHD-C4C-NC	8.81	137.57	124.31
38	s	201	KC2	CHD-C4C-NC	8.78	137.54	124.31
38	e	609	KC2	CHD-C4C-NC	8.76	137.50	124.31
28	a	309	CLA	C4A-NA-C1A	8.75	110.67	106.68
36	l	313	II0	C41-C39-C35	-8.71	115.06	127.28
38	i	319	KC2	CHD-C4C-NC	8.70	137.41	124.31
31	B	847	WVN	C02-C11-C19	-8.57	111.25	124.58
28	b	609	CLA	C4A-NA-C1A	8.56	110.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	g	314	KC2	CHD-C4C-NC	8.56	137.21	124.31
38	g	313	KC2	CHD-C4C-NC	8.35	136.88	124.31
38	s	204	KC2	CHD-C4C-NC	8.33	136.85	124.31
36	d	315	II0	C41-C39-C35	-8.24	115.72	127.28
28	B	824	CLA	C4A-NA-C1A	8.23	110.43	106.68
36	i	313	II0	C42-C40-C36	-8.20	115.78	127.28
38	d	311	KC2	CHD-C4C-NC	8.13	136.55	124.31
36	m	618	II0	C41-C39-C35	8.05	138.56	127.28
31	s	207	WVN	C04-C09-C05	-8.02	117.17	124.83
28	B	834	CLA	C4A-NA-C1A	8.00	110.33	106.68
31	B	846	WVN	C21-C15-C13	-7.88	115.89	124.48
37	b	615	IHT	C30-C27-C23	-7.83	116.30	127.28
31	J	101	WVN	C24-C22-C26	-7.74	110.27	122.82
38	i	310	KC2	CHD-C4C-NC	7.71	135.93	124.31
31	F	204	WVN	C40-C37-C34	-7.69	116.49	127.28
31	K	102	WVN	C02-C11-C19	7.65	136.48	124.58
38	d	311	KC2	C1A-NA-C4A	-7.56	103.23	106.68
31	A	847	WVN	C20-C23-C25	-7.56	115.05	126.23
31	R	201	WVN	C02-C11-C19	-7.54	112.84	124.58
31	B	845	WVN	C02-C11-C19	-7.53	112.86	124.58
28	b	612	CLA	C4A-NA-C1A	7.47	110.09	106.68
31	B	844	WVN	C24-C22-C19	7.45	129.47	118.09
38	i	310	KC2	CHC-C4B-C3B	-7.44	112.66	125.21
38	f	611	KC2	CHC-C4B-C3B	-7.37	112.78	125.21
31	F	204	WVN	C40-C39-C36	-7.37	108.44	123.52
36	m	618	II0	C42-C41-C39	7.36	138.57	123.52
38	k	612	KC2	CHD-C4C-NC	7.33	135.35	124.31
36	f	618	II0	C41-C39-C35	-7.32	117.01	127.28
36	a	318	II0	C30-C32-C34	-7.31	102.01	123.20
31	A	846	WVN	C11-C19-C22	-7.30	110.63	126.32
38	l	310	KC2	CHC-C4B-C3B	-7.27	112.95	125.21
38	s	201	KC2	CHB-C4A-C3A	-7.25	113.59	125.03
36	k	616	II0	C41-C39-C35	-7.24	117.13	127.28
28	B	806	CLA	C4A-NA-C1A	7.22	109.97	106.68
38	i	319	KC2	CHB-C4A-C3A	-7.20	113.66	125.03
36	k	621	II0	C42-C40-C36	-7.19	117.19	127.28
38	d	311	KC2	C4C-C3C-C2C	-7.17	100.69	107.28
38	m	611	KC2	CHC-C4B-C3B	-7.17	113.12	125.21
36	l	313	II0	C42-C40-C36	-7.10	117.32	127.28
28	K	101	CLA	C4A-NA-C1A	7.08	109.91	106.68
38	i	310	KC2	CHC-C4B-NB	7.08	134.76	124.80
28	m	605	CLA	C4A-NA-C1A	7.03	109.89	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	e	601	CLA	C4A-NA-C1A	7.03	109.89	106.68
36	c	615	II0	C42-C40-C36	-7.02	117.43	127.28
38	j	611	KC2	CHC-C4B-C3B	-7.02	113.38	125.21
28	e	608	CLA	C4A-NA-C1A	7.01	109.88	106.68
38	k	612	KC2	CHC-C4B-C3B	-7.01	113.39	125.21
31	B	844	WVN	C04-C09-C05	-7.01	118.14	124.83
38	d	310	KC2	CHC-C4B-C3B	-7.00	113.40	125.21
38	k	613	KC2	CHC-C4B-C3B	-7.00	113.40	125.21
38	d	311	KC2	CHC-C4B-C3B	-7.00	113.40	125.21
38	g	314	KC2	CHC-C4B-C3B	-6.99	113.43	125.21
38	m	611	KC2	CHB-C4A-C3A	-6.98	114.00	125.03
28	A	819	CLA	C4A-NA-C1A	6.97	109.86	106.68
31	A	848	WVN	C29-C26-C22	-6.95	117.54	127.28
31	R	201	WVN	C30-C28-C25	-6.93	117.55	127.28
28	j	605	CLA	C4A-NA-C1A	6.91	109.83	106.68
38	e	609	KC2	CHC-C4B-C3B	-6.90	113.57	125.21
28	b	606	CLA	C4A-NA-C1A	6.89	109.82	106.68
31	J	101	WVN	C11-C19-C22	-6.89	111.51	126.32
38	l	310	KC2	CHB-C4A-C3A	-6.88	114.16	125.03
37	R	204	IHT	C40-C37-C33	-6.87	117.64	127.28
38	s	204	KC2	CHC-C4B-C3B	-6.86	113.64	125.21
38	n	612	KC2	CHC-C4B-C3B	-6.84	113.67	125.21
37	b	615	IHT	C40-C37-C33	-6.82	117.71	127.28
38	k	611	KC2	CHC-C4B-C3B	-6.79	113.76	125.21
31	A	846	WVN	C26-C29-C31	-6.79	103.53	123.20
31	A	845	WVN	C30-C28-C25	-6.78	117.76	127.28
28	F	202	CLA	C4A-NA-C1A	6.78	109.77	106.68
28	f	605	CLA	C4A-NA-C1A	6.77	109.77	106.68
38	c	610	KC2	C1A-C2A-C3A	-6.77	101.06	107.28
38	g	313	KC2	CHC-C4B-C3B	-6.77	113.80	125.21
38	f	611	KC2	CHC-C4B-NB	6.77	134.33	124.80
38	j	611	KC2	CHB-C4A-C3A	-6.76	114.35	125.03
28	h	308	CLA	C4A-NA-C1A	6.76	109.76	106.68
38	i	319	KC2	CHC-C4B-C3B	-6.75	113.82	125.21
36	m	618	II0	C41-C42-C40	6.73	137.29	123.52
38	d	310	KC2	CHB-C4A-C3A	-6.72	114.42	125.03
38	l	310	KC2	C2C-C1C-NC	6.71	118.75	110.45
28	B	803	CLA	C4A-NA-C1A	6.70	109.74	106.68
28	b	605	CLA	C4A-NA-C1A	6.69	109.73	106.68
38	n	611	KC2	CHB-C4A-C3A	-6.69	114.47	125.03
28	l	309	CLA	C4A-NA-C1A	6.68	109.73	106.68
36	g	320	II0	C42-C40-C36	-6.67	117.93	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	g	312	KC2	CHC-C4B-C3B	-6.66	113.97	125.21
36	n	614	II0	C42-C40-C36	-6.66	117.94	127.28
38	m	611	KC2	C2C-C1C-NC	6.63	118.66	110.45
38	c	610	KC2	CHC-C4B-C3B	-6.63	114.03	125.21
28	i	306	CLA	C4A-NA-C1A	6.62	109.70	106.68
36	d	314	II0	C41-C39-C35	-6.62	117.99	127.28
38	l	310	KC2	CHC-C4B-NB	6.62	134.12	124.80
38	s	204	KC2	C2C-C1C-NC	6.59	118.60	110.45
38	g	314	KC2	C2C-C1C-NC	6.58	118.60	110.45
38	k	611	KC2	CHB-C4A-C3A	-6.57	114.65	125.03
31	F	203	WVN	C39-C40-C37	-6.57	110.08	123.52
38	f	611	KC2	C1A-C2A-C3A	-6.57	101.25	107.28
28	g	308	CLA	C4A-NA-C1A	6.56	109.67	106.68
38	k	613	KC2	CHC-C4B-NB	6.55	134.03	124.80
38	g	313	KC2	C2C-C1C-NC	6.53	118.53	110.45
38	n	611	KC2	CHC-C4B-C3B	-6.52	114.22	125.21
38	i	319	KC2	C2C-C1C-NC	6.49	118.49	110.45
31	l	315	WVN	C29-C26-C22	-6.49	118.18	127.28
38	k	613	KC2	C2C-C1C-NC	6.48	118.48	110.45
38	j	611	KC2	C2C-C1C-NC	6.47	118.46	110.45
31	i	316	WVN	C29-C26-C22	-6.47	118.21	127.28
36	j	614	II0	C41-C39-C35	-6.47	118.21	127.28
38	j	611	KC2	CHC-C4B-NB	6.46	133.90	124.80
28	A	835	CLA	C4A-NA-C1A	6.46	109.63	106.68
28	g	306	CLA	C4A-NA-C1A	6.46	109.63	106.68
38	d	310	KC2	C2C-C1C-NC	6.46	118.44	110.45
36	c	613	II0	C41-C39-C35	-6.46	118.22	127.28
28	m	603	CLA	C4A-NA-C1A	6.46	109.62	106.68
38	g	314	KC2	CHC-C4B-NB	6.45	133.89	124.80
36	b	617	II0	C42-C40-C36	-6.45	118.24	127.28
38	n	611	KC2	OBD-CAD-C3D	-6.45	113.35	128.42
38	s	201	KC2	CHB-C1B-NB	6.45	133.88	124.80
38	n	612	KC2	CHC-C4B-NB	6.44	133.86	124.80
37	b	615	IHT	C41-C38-C35	-6.44	118.25	127.28
38	k	612	KC2	CHC-C4B-NB	6.43	133.86	124.80
31	A	846	WVN	C30-C28-C25	-6.43	118.26	127.28
38	g	314	KC2	CHB-C4A-C3A	-6.42	114.89	125.03
38	i	310	KC2	OBD-CAD-C3D	-6.42	113.40	128.42
38	k	612	KC2	C2C-C1C-NC	6.42	118.39	110.45
38	m	611	KC2	CHC-C4B-NB	6.42	133.84	124.80
38	e	609	KC2	CHC-C4B-NB	6.40	133.81	124.80
38	c	610	KC2	CHB-C4A-C3A	-6.40	114.93	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	f	614	II0	C41-C39-C35	-6.39	118.31	127.28
28	A	831	CLA	C4A-NA-C1A	6.39	109.59	106.68
28	A	836	CLA	C4A-NA-C1A	6.39	109.59	106.68
28	B	808	CLA	C4A-NA-C1A	6.39	109.59	106.68
38	g	314	KC2	C4C-C3C-C2C	-6.37	101.42	107.28
38	f	611	KC2	C2C-C1C-NC	6.37	118.33	110.45
28	e	606	CLA	C4A-NA-C1A	6.37	109.58	106.68
38	e	609	KC2	C2C-C1C-NC	6.36	118.32	110.45
38	k	611	KC2	OBD-CAD-C3D	-6.36	113.55	128.42
28	A	804	CLA	C4A-NA-C1A	6.35	109.58	106.68
38	d	310	KC2	CHC-C4B-NB	6.35	133.75	124.80
28	l	306	CLA	C4A-NA-C1A	6.35	109.58	106.68
38	e	609	KC2	CHB-C4A-C3A	-6.35	115.00	125.03
38	e	609	KC2	OBD-CAD-C3D	-6.35	113.58	128.42
36	h	310	II0	C42-C40-C36	-6.34	118.38	127.28
38	g	313	KC2	CHB-C4A-C3A	-6.34	115.03	125.03
38	k	612	KC2	CHB-C4A-C3A	-6.33	115.03	125.03
31	L	206	WVN	C02-C11-C19	-6.33	114.72	124.58
38	d	311	KC2	C2C-C1C-NC	6.33	118.29	110.45
38	g	313	KC2	CHC-C4B-NB	6.32	133.70	124.80
31	s	205	WVN	C02-C11-C19	-6.32	114.74	124.58
28	B	821	CLA	C4A-NA-C1A	6.32	109.56	106.68
28	A	826	CLA	C4A-NA-C1A	6.31	109.56	106.68
38	k	611	KC2	C2C-C1C-NC	6.31	118.26	110.45
28	A	807	CLA	C4A-NA-C1A	6.30	109.56	106.68
38	j	611	KC2	OBD-CAD-C3D	-6.30	113.70	128.42
38	d	311	KC2	CHC-C4B-NB	6.29	133.65	124.80
37	O	204	IHT	C30-C27-C23	-6.28	118.47	127.28
38	g	312	KC2	CHC-C4B-NB	6.28	133.64	124.80
38	k	611	KC2	CHC-C4B-NB	6.28	133.64	124.80
38	i	319	KC2	CHC-C4B-NB	6.28	133.64	124.80
38	g	313	KC2	C4C-C3C-C2C	-6.27	101.51	107.28
28	c	603	CLA	C4A-NA-C1A	6.27	109.54	106.68
28	e	604	CLA	C4A-NA-C1A	6.27	109.54	106.68
38	k	612	KC2	C4C-C3C-C2C	-6.26	101.53	107.28
38	n	612	KC2	C2C-C1C-NC	6.25	118.19	110.45
38	c	610	KC2	C2C-C1C-NC	6.24	118.18	110.45
38	g	312	KC2	CHB-C4A-C3A	-6.24	115.18	125.03
28	B	813	CLA	C4A-NA-C1A	6.24	109.52	106.68
38	l	310	KC2	C1A-C2A-C3A	-6.23	101.56	107.28
38	j	611	KC2	C1A-C2A-C3A	-6.23	101.56	107.28
38	s	204	KC2	CHC-C4B-NB	6.23	133.57	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	609	CLA	C4A-NA-C1A	6.22	109.52	106.68
38	g	314	KC2	OBD-CAD-C3D	-6.20	113.92	128.42
28	A	808	CLA	C4A-NA-C1A	6.20	109.51	106.68
37	k	618	IHT	C41-C38-C35	-6.19	118.59	127.28
36	g	316	II0	C41-C39-C35	-6.19	118.60	127.28
31	A	846	WVN	C21-C15-C13	-6.18	117.74	124.48
38	s	204	KC2	C1A-C2A-C3A	-6.17	101.61	107.28
28	b	610	CLA	C4A-NA-C1A	6.17	109.50	106.68
28	B	804	CLA	C4A-NA-C1A	6.17	109.49	106.68
38	k	611	KC2	C1A-C2A-C3A	-6.17	101.61	107.28
38	k	613	KC2	CHB-C4A-C3A	-6.16	115.30	125.03
38	g	312	KC2	C2C-C1C-NC	6.16	118.07	110.45
38	n	611	KC2	C2C-C1C-NC	6.16	118.07	110.45
28	k	601	CLA	C4A-NA-C1A	6.15	109.49	106.68
37	c	616	IHT	C40-C37-C33	-6.15	118.65	127.28
28	f	603	CLA	C4A-NA-C1A	6.15	109.49	106.68
38	d	311	KC2	OBD-CAD-C3D	-6.15	114.04	128.42
38	s	201	KC2	C2C-C1C-NC	6.15	118.06	110.45
31	L	201	WVN	C08-C01-C02	-6.14	100.24	109.55
36	b	613	II0	C42-C40-C36	-6.13	118.68	127.28
38	i	319	KC2	OBD-CAD-C3D	-6.12	114.11	128.42
36	k	617	II0	C42-C40-C36	-6.12	118.70	127.28
31	A	848	WVN	C02-C11-C19	-6.11	115.07	124.58
38	c	610	KC2	OBD-CAD-C3D	-6.11	114.14	128.42
36	m	616	II0	C42-C40-C36	-6.10	118.72	127.28
38	n	611	KC2	CHC-C4B-NB	6.10	133.39	124.80
31	L	206	WVN	C30-C28-C25	-6.09	118.73	127.28
28	s	203	CLA	C4A-NA-C1A	6.09	109.46	106.68
38	g	312	KC2	C1A-C2A-C3A	-6.09	101.68	107.28
38	s	201	KC2	CHC-C4B-C3B	-6.09	114.94	125.21
38	d	311	KC2	CMD-C2D-C1D	-6.09	116.15	125.42
38	s	204	KC2	CHB-C4A-C3A	-6.09	115.42	125.03
38	n	611	KC2	C1A-C2A-C3A	-6.08	101.69	107.28
37	g	319	IHT	C30-C32-C33	-6.08	109.69	126.36
38	f	611	KC2	C4C-C3C-C2C	-6.07	101.70	107.28
31	e	615	WVN	C30-C28-C25	-6.07	118.77	127.28
38	f	611	KC2	CHB-C4A-C3A	-6.06	115.46	125.03
28	g	302	CLA	C4A-NA-C1A	6.06	109.44	106.68
37	c	616	IHT	C30-C27-C23	-6.06	118.78	127.28
37	O	204	IHT	C18-C22-C23	-6.06	117.28	126.23
38	g	314	KC2	C1A-C2A-C3A	-6.05	101.72	107.28
37	a	317	IHT	C41-C38-C35	-6.05	118.79	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	601	CLA	C4A-NA-C1A	6.05	109.44	106.68
38	n	612	KC2	C1A-C2A-C3A	-6.04	101.73	107.28
31	K	102	WVN	C11-C19-C22	6.04	139.31	126.32
28	b	607	CLA	C4A-NA-C1A	6.03	109.43	106.68
38	n	612	KC2	CHB-C4A-C3A	-6.03	115.51	125.03
28	e	611	CLA	C4A-NA-C1A	6.03	109.43	106.68
36	g	317	II0	C41-C39-C35	-6.02	118.83	127.28
38	k	611	KC2	C4C-C3C-C2C	-6.02	101.75	107.28
28	c	611	CLA	C4A-NA-C1A	6.02	109.42	106.68
28	a	307	CLA	C4A-NA-C1A	6.02	109.42	106.68
38	c	610	KC2	CHC-C4B-NB	6.02	133.27	124.80
38	m	611	KC2	C4C-C3C-C2C	-6.02	101.75	107.28
28	A	841	CLA	C4A-NA-C1A	6.01	109.42	106.68
28	l	304	CLA	C4A-NA-C1A	5.97	109.40	106.68
38	s	201	KC2	C4C-C3C-C2C	-5.95	101.81	107.28
28	B	823	CLA	C4A-NA-C1A	5.95	109.39	106.68
38	d	310	KC2	OBD-CAD-C3D	-5.94	114.53	128.42
38	k	612	KC2	OBD-CAD-C3D	-5.93	114.56	128.42
28	d	304	CLA	C4A-NA-C1A	5.93	109.38	106.68
28	A	812	CLA	C4A-NA-C1A	5.93	109.38	106.68
28	k	609	CLA	C4A-NA-C1A	5.92	109.38	106.68
36	O	203	II0	C42-C40-C36	-5.91	118.98	127.28
28	l	305	CLA	C4A-NA-C1A	5.91	109.38	106.68
38	l	310	KC2	C4C-C3C-C2C	-5.89	101.86	107.28
36	i	315	II0	C41-C39-C35	-5.88	119.03	127.28
36	i	313	II0	C41-C39-C35	-5.88	119.03	127.28
28	A	813	CLA	C4A-NA-C1A	5.88	109.36	106.68
38	j	611	KC2	C4C-C3C-C2C	-5.88	101.88	107.28
28	k	603	CLA	C4A-NA-C1A	5.88	109.36	106.68
28	f	613	CLA	C4A-NA-C1A	5.87	109.36	106.68
28	Q	303	CLA	CMB-C2B-C1B	-5.87	116.48	125.42
38	e	609	KC2	C1A-C2A-C3A	-5.87	101.89	107.28
28	B	839	CLA	C4A-NA-C1A	5.87	109.36	106.68
38	g	313	KC2	C1A-C2A-C3A	-5.87	101.89	107.28
38	n	612	KC2	OBD-CAD-C3D	-5.86	114.71	128.42
38	n	611	KC2	C4C-C3C-C2C	-5.86	101.89	107.28
38	m	611	KC2	OBD-CAD-C3D	-5.86	114.72	128.42
28	c	604	CLA	C4A-NA-C1A	5.86	109.35	106.68
38	k	613	KC2	OBD-CAD-C3D	-5.85	114.73	128.42
38	s	204	KC2	OBD-CAD-C3D	-5.85	114.74	128.42
36	f	615	II0	C41-C39-C35	-5.85	119.07	127.28
38	e	609	KC2	C4C-C3C-C2C	-5.85	101.91	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	605	CLA	C4A-NA-C1A	5.84	109.34	106.68
38	s	201	KC2	CHC-C4B-NB	5.84	133.02	124.80
31	K	102	WVN	C39-C36-C32	-5.83	119.10	127.28
37	g	319	IHT	C19-C10-C07	-5.83	118.12	124.48
28	h	303	CLA	C4A-NA-C1A	5.83	109.34	106.68
36	n	616	II0	C41-C39-C35	-5.83	119.11	127.28
28	a	303	CLA	C4A-NA-C1A	5.82	109.33	106.68
36	a	316	II0	C20-C14-C10	-5.82	113.28	124.16
38	g	313	KC2	OBD-CAD-C3D	-5.82	114.81	128.42
38	f	611	KC2	CMD-C2D-C1D	-5.82	116.56	125.42
36	d	314	II0	C42-C40-C36	-5.81	119.13	127.28
37	m	617	IHT	C40-C37-C33	-5.80	119.14	127.28
38	i	319	KC2	C4C-C3C-C2C	-5.80	101.94	107.28
38	s	201	KC2	CHB-C1B-C2B	-5.80	113.42	125.49
38	k	613	KC2	C4C-C3C-C2C	-5.80	101.95	107.28
28	B	803	CLA	CAC-C3C-C4C	5.79	132.32	124.79
38	g	312	KC2	C4C-C3C-C2C	-5.78	101.96	107.28
37	k	618	IHT	C09-C10-C07	-5.78	114.89	122.70
38	k	612	KC2	C1A-C2A-C3A	-5.78	101.97	107.28
38	i	310	KC2	CHC-C1C-NC	-5.77	115.28	124.23
28	a	312	CLA	C4A-NA-C1A	5.77	109.31	106.68
28	A	815	CLA	CMB-C2B-C1B	-5.77	116.63	125.42
37	g	319	IHT	C22-C23-C27	5.77	128.08	119.01
28	A	809	CLA	C4A-NA-C1A	5.77	109.31	106.68
28	B	836	CLA	C4A-NA-C1A	5.76	109.31	106.68
38	d	310	KC2	C4C-C3C-C2C	-5.75	102.00	107.28
37	O	204	IHT	C41-C38-C35	-5.74	119.22	127.28
36	c	617	II0	C42-C40-C36	-5.74	119.23	127.28
28	a	305	CLA	C4A-NA-C1A	5.73	109.29	106.68
37	k	618	IHT	C40-C37-C33	-5.72	119.25	127.28
36	l	314	II0	C42-C40-C36	-5.70	119.28	127.28
28	O	202	CLA	C4A-NA-C1A	5.70	109.28	106.68
37	m	617	IHT	C18-C22-C23	-5.70	117.81	126.23
36	e	614	II0	C41-C39-C35	-5.69	119.30	127.28
36	a	316	II0	C42-C40-C36	-5.69	119.30	127.28
38	i	310	KC2	CHB-C1B-NB	5.69	132.81	124.80
31	A	848	WVN	C06-C13-C15	-5.68	114.88	122.64
28	B	837	CLA	C4A-NA-C1A	5.67	109.27	106.68
28	A	824	CLA	C4A-NA-C1A	5.67	109.27	106.68
37	b	616	IHT	C27-C30-C32	-5.67	106.78	123.20
37	j	616	IHT	C30-C27-C23	-5.67	119.33	127.28
28	A	803	CLA	C4A-NA-C1A	5.66	109.26	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	202	CLA	C4A-NA-C1A	5.66	109.26	106.68
37	c	616	IHT	C41-C38-C35	-5.66	119.34	127.28
31	A	848	WVN	C30-C28-C25	-5.66	119.34	127.28
31	L	206	WVN	C38-C34-C33	5.66	126.73	118.09
31	M	101	WVN	C01-C02-C11	-5.66	106.32	112.83
31	K	104	WVN	C02-C11-C19	-5.64	115.80	124.58
37	n	617	IHT	C40-C37-C33	-5.64	119.36	127.28
38	k	613	KC2	C1A-C2A-C3A	-5.64	102.09	107.28
38	n	611	KC2	CMD-C2D-C1D	-5.64	116.83	125.42
38	i	319	KC2	C1A-C2A-C3A	-5.63	102.10	107.28
37	n	617	IHT	C09-C10-C07	-5.63	115.09	122.70
31	s	205	WVN	C04-C09-C05	-5.63	119.45	124.83
28	B	810	CLA	C4A-NA-C1A	5.63	109.25	106.68
28	l	307	CLA	C4A-NA-C1A	5.63	109.25	106.68
28	A	838	CLA	C4A-NA-C1A	5.63	109.25	106.68
31	B	848	WVN	C02-C11-C19	-5.63	115.82	124.58
38	d	310	KC2	C1A-C2A-C3A	-5.62	102.11	107.28
31	F	203	WVN	C29-C26-C22	-5.62	119.39	127.28
38	s	201	KC2	OBD-CAD-C3D	-5.61	115.30	128.42
31	A	846	WVN	C19-C22-C26	5.61	127.83	119.01
36	d	316	II0	C41-C39-C35	-5.60	119.42	127.28
38	g	314	KC2	CMD-C2D-C1D	-5.60	116.89	125.42
28	L	204	CLA	C4A-NA-C1A	5.60	109.23	106.68
38	s	204	KC2	C4C-C3C-C2C	-5.59	102.14	107.28
31	L	201	WVN	C39-C36-C32	-5.59	119.44	127.28
36	j	614	II0	C42-C40-C36	-5.59	119.44	127.28
37	m	617	IHT	C30-C27-C23	-5.58	119.45	127.28
28	B	811	CLA	C4A-NA-C1A	5.58	109.22	106.68
37	f	617	IHT	C41-C38-C35	-5.58	119.46	127.28
37	m	617	IHT	C41-C38-C35	-5.57	119.46	127.28
31	L	205	WVN	C29-C26-C22	-5.57	119.47	127.28
31	i	316	WVN	C40-C37-C34	-5.57	119.47	127.28
28	A	839	CLA	C4A-NA-C1A	5.57	109.22	106.68
38	g	312	KC2	OBD-CAD-C3D	-5.57	115.41	128.42
36	n	618	II0	C41-C39-C35	-5.56	119.47	127.28
38	c	610	KC2	C4C-C3C-C2C	-5.56	102.17	107.28
38	m	611	KC2	C1A-C2A-C3A	-5.56	102.17	107.28
37	a	317	IHT	C30-C27-C23	-5.56	119.48	127.28
36	k	615	II0	C42-C40-C36	-5.56	119.49	127.28
36	k	615	II0	C41-C39-C35	-5.55	119.49	127.28
36	k	617	II0	C41-C39-C35	-5.55	119.49	127.28
28	g	322	CLA	C4A-NA-C1A	5.55	109.21	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	k	618	IHT	C30-C27-C23	-5.55	119.50	127.28
31	R	202	WVN	C02-C11-C19	-5.54	115.95	124.58
31	F	203	WVN	C02-C11-C19	-5.54	115.96	124.58
28	g	304	CLA	C4A-NA-C1A	5.53	109.20	106.68
36	l	312	II0	C41-C39-C35	-5.53	119.52	127.28
28	B	833	CLA	C4A-NA-C1A	5.53	109.20	106.68
36	f	618	II0	C41-C42-C40	-5.52	112.22	123.52
28	A	821	CLA	C4A-NA-C1A	5.51	109.19	106.68
36	a	318	II0	C34-C36-C40	5.51	127.67	119.01
28	A	832	CLA	C4A-NA-C1A	5.51	109.19	106.68
28	m	606	CLA	C4A-NA-C1A	5.50	109.19	106.68
31	i	316	WVN	C02-C11-C19	-5.50	116.02	124.58
38	f	611	KC2	OBD-CAD-C3D	-5.50	115.57	128.42
38	d	311	KC2	C1A-C2A-C3A	-5.49	102.23	107.28
31	L	201	WVN	C40-C37-C34	-5.49	119.57	127.28
28	b	601	CLA	C4A-NA-C1A	5.49	109.19	106.68
38	n	612	KC2	CHD-C4C-C3C	-5.49	107.43	125.91
28	m	608	CLA	C4A-NA-C1A	5.49	109.18	106.68
38	s	204	KC2	CMD-C2D-C1D	-5.49	117.06	125.42
35	Q	301	LMG	O7-C10-C11	5.48	123.34	111.48
31	B	844	WVN	C19-C22-C26	-5.48	110.39	119.01
36	g	317	II0	C42-C40-C36	-5.47	119.60	127.28
35	c	619	LMG	O7-C10-C11	5.46	123.28	111.48
28	k	610	CLA	C4A-NA-C1A	5.45	109.17	106.68
28	B	841	CLA	C4A-NA-C1A	5.44	109.16	106.68
36	n	615	II0	C41-C39-C35	-5.43	119.66	127.28
37	O	204	IHT	C40-C37-C33	-5.42	119.67	127.28
37	R	204	IHT	C30-C27-C23	-5.42	119.68	127.28
28	B	805	CLA	C4A-NA-C1A	5.41	109.14	106.68
28	B	840	CLA	C4A-NA-C1A	5.41	109.14	106.68
31	A	846	WVN	C31-C32-C36	5.41	127.51	119.01
38	n	612	KC2	C4C-C3C-C2C	-5.40	102.32	107.28
28	l	302	CLA	C4A-NA-C1A	5.39	109.14	106.68
28	B	802	CLA	C4A-NA-C1A	5.39	109.14	106.68
28	e	605	CLA	C4A-NA-C1A	5.39	109.14	106.68
28	e	610	CLA	C4A-NA-C1A	5.39	109.14	106.68
37	m	617	IHT	C09-C10-C07	-5.39	115.43	122.70
28	B	801	CLA	C4A-NA-C1A	5.38	109.13	106.68
28	A	823	CLA	C4A-NA-C1A	5.37	109.13	106.68
38	l	310	KC2	CMD-C2D-C1D	-5.37	117.25	125.42
31	K	104	WVN	C30-C28-C25	-5.36	119.76	127.28
31	l	315	WVN	C02-C11-C19	-5.36	116.24	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	845	WVN	C04-C09-C05	-5.35	119.72	124.83
38	l	310	KC2	OBD-CAD-C3D	-5.35	115.91	128.42
28	m	610	CLA	C4A-NA-C1A	5.35	109.12	106.68
38	i	310	KC2	C1D-ND-C4D	5.34	110.06	106.31
31	L	206	WVN	C04-C09-C05	-5.34	119.73	124.83
38	n	611	KC2	CHC-C1C-NC	-5.33	115.96	124.23
28	k	605	CLA	C4A-NA-C1A	5.33	109.11	106.68
36	h	312	II0	C41-C39-C35	-5.33	119.80	127.28
38	i	319	KC2	CHB-C1B-NB	5.32	132.29	124.80
38	d	311	KC2	CHB-C4A-C3A	-5.32	116.63	125.03
31	J	102	WVN	C04-C09-C05	-5.31	119.76	124.83
36	g	320	II0	C41-C39-C35	-5.31	119.83	127.28
28	A	833	CLA	C4A-NA-C1A	5.31	109.10	106.68
28	K	103	CLA	C4A-NA-C1A	5.31	109.10	106.68
31	A	848	WVN	C21-C15-C13	-5.31	118.69	124.48
31	h	309	WVN	C29-C26-C22	-5.31	119.84	127.28
31	L	201	WVN	C04-C09-C05	-5.30	119.77	124.83
31	R	202	WVN	C06-C13-C15	-5.30	115.39	122.64
31	l	301	WVN	C30-C28-C25	-5.30	119.84	127.28
36	J	104	II0	C42-C40-C36	-5.29	119.85	127.28
28	j	603	CLA	C4A-NA-C1A	5.29	109.09	106.68
31	M	101	WVN	C20-C23-C25	-5.29	118.42	126.23
36	c	614	II0	C42-C40-C36	-5.28	119.87	127.28
31	J	101	WVN	C04-C09-C05	-5.28	119.79	124.83
28	A	811	CLA	C4A-NA-C1A	5.28	109.09	106.68
38	n	611	KC2	CHD-C4C-C3C	-5.28	108.15	125.91
28	e	607	CLA	C4A-NA-C1A	5.28	109.09	106.68
38	k	612	KC2	C1D-ND-C4D	5.27	110.01	106.31
38	f	611	KC2	CHD-C4C-C3C	-5.27	108.17	125.91
38	n	612	KC2	CHC-C1C-NC	-5.26	116.07	124.23
28	A	820	CLA	C4A-NA-C1A	5.26	109.08	106.68
38	n	612	KC2	CHB-C1B-NB	5.25	132.20	124.80
31	h	309	WVN	C02-C11-C19	-5.25	116.41	124.58
38	l	310	KC2	CHD-C4C-C3C	-5.25	108.25	125.91
37	R	204	IHT	C18-C22-C23	-5.25	118.47	126.23
38	i	310	KC2	C2C-C1C-NC	5.25	116.94	110.45
37	f	617	IHT	C19-C10-C07	-5.25	118.76	124.48
28	h	304	CLA	C4A-NA-C1A	5.25	109.07	106.68
38	c	610	KC2	CHC-C1C-NC	-5.24	116.11	124.23
38	d	310	KC2	CHB-C1B-NB	5.24	132.17	124.80
31	h	309	WVN	C04-C09-C05	-5.23	119.83	124.83
28	d	305	CLA	C4A-NA-C1A	5.23	109.07	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	i	316	WVN	C21-C15-C13	-5.23	118.78	124.48
38	m	611	KC2	CHD-C4C-C3C	-5.22	108.33	125.91
31	B	847	WVN	C40-C37-C34	-5.22	119.96	127.28
38	k	611	KC2	CHD-C4C-C3C	-5.22	108.35	125.91
38	g	314	KC2	CHD-C4C-C3C	-5.21	108.37	125.91
38	n	611	KC2	CHB-C1B-NB	5.21	132.14	124.80
36	h	311	II0	C42-C40-C36	-5.21	119.97	127.28
31	F	203	WVN	C20-C23-C25	-5.21	118.53	126.23
38	d	311	KC2	C4B-CHC-C1C	-5.21	114.96	126.02
36	d	313	II0	C42-C40-C36	-5.20	119.99	127.28
38	k	611	KC2	CMD-C2D-C1D	-5.19	117.51	125.42
38	k	611	KC2	CHB-C1B-NB	5.19	132.11	124.80
28	i	305	CLA	C4A-NA-C1A	5.19	109.05	106.68
38	d	310	KC2	C1D-ND-C4D	5.19	109.95	106.31
36	l	312	II0	C42-C40-C36	-5.19	120.00	127.28
36	f	616	II0	C42-C40-C36	-5.19	120.01	127.28
38	j	611	KC2	CHD-C4C-C3C	-5.19	108.46	125.91
28	h	302	CLA	C4A-NA-C1A	5.18	109.04	106.68
28	n	603	CLA	C4A-NA-C1A	5.18	109.04	106.68
31	s	205	WVN	C21-C15-C13	-5.18	118.83	124.48
28	F	201	CLA	C4A-NA-C1A	5.18	109.04	106.68
38	k	611	KC2	CHC-C1C-NC	-5.17	116.22	124.23
36	i	317	II0	C41-C39-C35	-5.17	120.03	127.28
38	g	313	KC2	CHB-C1B-NB	5.17	132.08	124.80
28	j	612	CLA	C4A-NA-C1A	-5.17	104.32	106.68
37	j	616	IHT	C41-C38-C35	-5.17	120.03	127.28
38	k	613	KC2	CHB-C1B-NB	5.17	132.07	124.80
28	n	605	CLA	C4A-NA-C1A	5.16	109.03	106.68
36	c	615	II0	C41-C39-C35	-5.16	120.05	127.28
38	k	613	KC2	CHD-C4C-C3C	-5.15	108.57	125.91
31	F	203	WVN	C26-C29-C31	-5.15	108.28	123.20
38	m	611	KC2	CMD-C2D-C1D	-5.15	117.58	125.42
31	l	301	WVN	C02-C11-C19	-5.15	116.57	124.58
38	e	609	KC2	CHD-C4C-C3C	-5.14	108.60	125.91
38	s	204	KC2	C1D-ND-C4D	5.14	109.92	106.31
28	A	816	CLA	C4A-NA-C1A	5.14	109.02	106.68
38	k	612	KC2	CHB-C1B-NB	5.14	132.03	124.80
36	i	315	II0	C42-C40-C36	-5.13	120.09	127.28
38	c	610	KC2	CHD-C4C-C3C	-5.13	108.66	125.91
38	d	310	KC2	CHD-C4C-C3C	-5.12	108.67	125.91
31	F	204	WVN	C30-C33-C34	-5.12	112.31	126.36
38	g	314	KC2	CHB-C1B-NB	5.12	132.00	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	s	204	KC2	CHC-C1C-NC	-5.11	116.31	124.23
28	R	203	CLA	C4A-NA-C1A	5.10	109.01	106.68
38	g	312	KC2	CHD-C4C-C3C	-5.10	108.73	125.91
38	i	319	KC2	CHD-C4C-C3C	-5.10	108.75	125.91
36	d	313	II0	C19-C13-C11	5.10	123.80	114.42
28	A	802	CLA	CMB-C2B-C1B	-5.10	117.66	125.42
28	Q	302	CLA	C4A-NA-C1A	5.09	109.00	106.68
38	g	313	KC2	CHC-C1C-NC	-5.09	116.34	124.23
36	c	614	II0	C41-C39-C35	-5.09	120.14	127.28
38	i	310	KC2	CHB-C1B-C2B	-5.09	114.91	125.49
28	A	805	CLA	C4A-NA-C1A	5.09	109.00	106.68
28	A	830	CLA	C4A-NA-C1A	5.08	109.00	106.68
38	i	319	KC2	CHC-C1C-NC	-5.08	116.36	124.23
37	f	617	IHT	C30-C27-C23	-5.08	120.16	127.28
38	c	610	KC2	CHB-C1B-NB	5.07	131.95	124.80
28	a	306	CLA	C4A-NA-C1A	5.07	108.99	106.68
38	g	312	KC2	CHB-C1B-NB	5.07	131.94	124.80
28	g	305	CLA	C4A-NA-C1A	5.07	108.99	106.68
38	s	201	KC2	C3A-C4A-NA	5.07	116.72	110.45
36	e	614	II0	C42-C40-C36	-5.07	120.17	127.28
38	k	613	KC2	CHC-C1C-NC	-5.07	116.38	124.23
38	d	311	KC2	CHD-C4C-C3C	-5.06	108.90	125.91
38	n	612	KC2	C4B-CHC-C1C	-5.06	115.28	126.02
28	A	801	CLA	C4A-NA-C1A	5.05	108.98	106.68
36	e	612	II0	C19-C13-C09	-5.05	114.71	124.16
38	s	201	KC2	CHD-C4C-C3C	-5.05	108.91	125.91
28	a	310	CLA	C4A-NA-C1A	5.05	108.98	106.68
28	g	310	CLA	C4A-NA-C1A	5.05	108.98	106.68
36	e	613	II0	C41-C39-C35	-5.04	120.20	127.28
28	B	818	CLA	C4A-NA-C1A	5.04	108.98	106.68
28	L	203	CLA	C4A-NA-C1A	5.04	108.98	106.68
36	i	320	II0	C19-C13-C09	-5.04	114.74	124.16
28	A	855	CLA	CAA-C2A-C3A	-5.04	104.68	116.23
36	b	613	II0	C41-C39-C35	-5.04	120.21	127.28
28	i	308	CLA	C4A-NA-C1A	5.04	108.98	106.68
28	j	613	CLA	C4A-NA-C1A	5.04	108.98	106.68
30	e	617	LHG	O7-C7-C8	5.03	122.36	111.48
28	B	821	CLA	C4-C3-C2	-5.03	110.72	123.63
36	i	314	II0	C41-C39-C35	-5.02	120.24	127.28
28	i	304	CLA	C4A-NA-C1A	5.02	108.97	106.68
38	g	312	KC2	CHC-C1C-NC	-5.02	116.46	124.23
38	e	609	KC2	CHB-C1B-NB	5.01	131.86	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	k	619	II0	C42-C40-C36	-5.00	120.26	127.28
38	d	310	KC2	CMD-C2D-C1D	-5.00	117.81	125.42
28	O	206	CLA	C4A-NA-C1A	5.00	108.96	106.68
37	O	204	IHT	C19-C10-C07	-5.00	119.03	124.48
31	L	206	WVN	C20-C23-C25	-5.00	118.84	126.23
38	m	611	KC2	C4B-CHC-C1C	-5.00	115.40	126.02
38	l	310	KC2	CHC-C1C-NC	-5.00	116.48	124.23
28	s	206	CLA	C4A-NA-C1A	5.00	108.96	106.68
38	n	611	KC2	C4B-CHC-C1C	-5.00	115.40	126.02
38	i	319	KC2	C4B-CHC-C1C	-4.99	115.40	126.02
38	j	611	KC2	CHC-C1C-NC	-4.99	116.49	124.23
28	A	840	CLA	C4A-NA-C1A	4.99	108.96	106.68
38	d	310	KC2	CHC-C1C-NC	-4.99	116.50	124.23
38	j	611	KC2	CHB-C1B-NB	4.99	131.83	124.80
28	j	601	CLA	C4A-NA-C1A	4.98	108.95	106.68
31	A	846	WVN	C29-C26-C22	4.98	134.27	127.28
37	n	617	IHT	C41-C38-C35	-4.98	120.29	127.28
38	g	313	KC2	C1D-ND-C4D	4.98	109.81	106.31
36	m	615	II0	C41-C39-C35	-4.98	120.30	127.28
28	i	302	CLA	C4A-NA-C1A	4.98	108.95	106.68
31	l	301	WVN	C40-C37-C34	-4.98	120.30	127.28
28	d	301	CLA	C4A-NA-C1A	4.97	108.95	106.68
28	d	307	CLA	C4A-NA-C1A	4.97	108.95	106.68
38	g	313	KC2	CHD-C4C-C3C	-4.97	109.19	125.91
38	e	609	KC2	CHC-C1C-NC	-4.97	116.53	124.23
36	m	618	II0	C33-C35-C39	-4.97	111.20	119.01
28	s	208	CLA	C4A-NA-C1A	4.96	108.94	106.68
37	n	617	IHT	C19-C10-C07	-4.96	119.07	124.48
38	g	314	KC2	CHC-C1C-NC	-4.96	116.55	124.23
28	L	207	CLA	C4A-NA-C1A	4.95	108.94	106.68
38	m	611	KC2	CHC-C1C-NC	-4.95	116.56	124.23
38	i	319	KC2	C3A-C4A-NA	4.95	116.57	110.45
38	m	611	KC2	CHB-C1B-NB	4.94	131.76	124.80
38	l	310	KC2	C4B-CHC-C1C	-4.94	115.52	126.02
36	f	616	II0	C41-C39-C35	-4.94	120.35	127.28
37	j	616	IHT	C40-C37-C33	-4.94	120.35	127.28
38	s	204	KC2	CHB-C1B-NB	4.94	131.75	124.80
31	s	207	WVN	C40-C37-C34	-4.93	120.36	127.28
38	i	310	KC2	CHB-C4A-C3A	-4.93	117.24	125.03
38	n	612	KC2	CMD-C2D-C1D	-4.93	117.91	125.42
37	R	204	IHT	C09-C10-C07	-4.93	116.04	122.70
31	h	309	WVN	C39-C36-C32	-4.93	120.36	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	855	CLA	CMA-C3A-C2A	-4.93	104.93	116.23
31	L	201	WVN	C29-C26-C22	-4.93	120.37	127.28
28	B	838	CLA	C4A-NA-C1A	4.93	108.93	106.68
31	R	202	WVN	C14-C15-C13	-4.93	116.05	122.70
38	f	611	KC2	C4B-CHC-C1C	-4.92	115.56	126.02
38	s	201	KC2	CHC-C1C-NC	-4.92	116.60	124.23
38	j	611	KC2	C4B-CHC-C1C	-4.92	115.57	126.02
38	f	611	KC2	CHC-C1C-NC	-4.92	116.61	124.23
37	j	616	IHT	C18-C22-C23	-4.91	118.97	126.23
28	n	606	CLA	C4A-NA-C1A	4.91	108.92	106.68
28	n	610	CLA	C4A-NA-C1A	4.91	108.92	106.68
28	B	830	CLA	C4A-NA-C1A	4.91	108.92	106.68
36	g	318	II0	C41-C39-C35	-4.90	120.40	127.28
38	k	612	KC2	CMD-C2D-C1D	-4.90	117.96	125.42
38	s	204	KC2	CHD-C4C-C3C	-4.90	109.42	125.91
34	B	843	DGD	O2G-C1B-C2B	4.90	122.08	111.48
38	g	312	KC2	CHD-C1D-ND	-4.90	116.70	124.05
38	k	611	KC2	C4B-CHC-C1C	-4.89	115.63	126.02
38	g	314	KC2	C4B-CHC-C1C	-4.89	115.63	126.02
38	l	310	KC2	C3A-C4A-NA	4.89	116.50	110.45
31	h	309	WVN	C30-C28-C25	-4.88	120.43	127.28
31	F	203	WVN	C21-C15-C13	-4.88	119.16	124.48
36	g	316	II0	C42-C40-C36	-4.88	120.43	127.28
30	n	619	LHG	O7-C7-C8	4.88	122.04	111.48
28	A	828	CLA	C1-C2-C3	-4.88	118.20	126.20
38	c	610	KC2	CMD-C2D-C1D	-4.88	117.99	125.42
38	d	311	KC2	C1B-CHB-C4A	-4.88	115.65	126.02
31	I	101	WVN	C40-C37-C34	-4.87	120.44	127.28
38	s	201	KC2	C1B-CHB-C4A	-4.87	115.66	126.02
28	j	602	CLA	C4A-NA-C1A	4.87	108.90	106.68
38	j	611	KC2	CMD-C2D-C1D	-4.87	118.01	125.42
38	d	311	KC2	CHD-C1D-ND	-4.86	116.75	124.05
28	A	814	CLA	C4A-NA-C1A	4.86	108.90	106.68
38	s	201	KC2	C1D-ND-C4D	4.86	109.72	106.31
28	c	602	CLA	O2D-CGD-CBD	4.85	119.71	111.23
38	i	319	KC2	CHB-C1B-C2B	-4.85	115.41	125.49
38	k	613	KC2	CMD-C2D-C1D	-4.84	118.04	125.42
37	j	616	IHT	C09-C10-C07	-4.84	116.16	122.70
31	B	845	WVN	C20-C23-C25	-4.84	119.07	126.23
31	J	101	WVN	C26-C29-C31	4.84	137.23	123.20
28	d	303	CLA	C4A-NA-C1A	4.84	108.89	106.68
28	B	817	CLA	CMB-C2B-C1B	-4.84	118.05	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	d	310	KC2	C4B-CHC-C1C	-4.84	115.74	126.02
38	k	612	KC2	C4B-CHC-C1C	-4.84	115.74	126.02
31	F	203	WVN	C06-C13-C15	-4.83	116.03	122.64
28	A	837	CLA	C4A-NA-C1A	4.83	108.88	106.68
38	k	613	KC2	C1D-ND-C4D	4.82	109.69	106.31
31	K	102	WVN	C21-C15-C13	-4.82	119.23	124.48
31	J	101	WVN	C29-C31-C32	-4.82	113.15	126.36
36	m	618	II0	C31-C33-C35	-4.82	113.16	126.36
36	i	320	II0	C41-C39-C35	-4.82	120.52	127.28
38	l	310	KC2	CHB-C1B-NB	4.81	131.58	124.80
36	a	315	II0	C41-C39-C35	-4.81	120.53	127.28
30	g	301	LHG	O7-C7-C8	4.81	121.88	111.48
28	J	103	CLA	C4A-NA-C1A	4.80	108.87	106.68
28	A	817	CLA	C4A-NA-C1A	4.80	108.87	106.68
38	i	319	KC2	CMD-C2D-C1D	-4.80	118.11	125.42
31	R	202	WVN	C20-C23-C25	-4.80	119.14	126.23
36	m	616	II0	C41-C39-C35	-4.80	120.55	127.28
38	i	310	KC2	CHD-C4C-C3C	-4.80	109.77	125.91
28	B	809	CLA	C4A-NA-C1A	4.80	108.87	106.68
36	n	614	II0	C18-C04-C10	-4.79	101.93	110.52
36	a	318	II0	C31-C33-C35	-4.79	113.23	126.36
36	J	104	II0	C32-C34-C36	-4.79	113.23	126.36
36	i	317	II0	C41-C42-C40	-4.79	113.72	123.52
28	c	601	CLA	C4A-NA-C1A	4.79	108.86	106.68
38	s	201	KC2	CHD-C1D-ND	-4.77	116.89	124.05
28	B	831	CLA	C4A-NA-C1A	4.77	108.86	106.68
38	k	612	KC2	CHD-C1D-ND	-4.77	116.89	124.05
37	O	204	IHT	C09-C10-C07	-4.77	116.26	122.70
31	J	102	WVN	C39-C36-C32	-4.77	120.59	127.28
28	l	303	CLA	C4A-NA-C1A	4.77	108.86	106.68
38	g	312	KC2	C1B-CHB-C4A	-4.77	115.89	126.02
38	k	613	KC2	C4B-CHC-C1C	-4.77	115.89	126.02
36	c	617	II0	C20-C14-C12	4.76	123.18	114.42
28	m	604	CLA	C4A-NA-C1A	4.76	108.85	106.68
36	b	614	II0	C42-C40-C36	-4.76	120.61	127.28
38	c	610	KC2	C4B-CHC-C1C	-4.76	115.91	126.02
38	g	313	KC2	C4B-CHC-C1C	-4.76	115.91	126.02
38	e	609	KC2	C4B-CHC-C1C	-4.76	115.91	126.02
31	M	101	WVN	C39-C36-C32	-4.75	120.62	127.28
38	i	310	KC2	C1B-CHB-C4A	-4.75	115.93	126.02
38	n	611	KC2	CHB-C1B-C2B	-4.74	115.62	125.49
38	d	310	KC2	CHB-C1B-C2B	-4.74	115.63	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	207	WVN	C02-C11-C19	-4.74	117.21	124.58
28	c	606	CLA	C4A-NA-C1A	4.73	108.84	106.68
36	a	314	II0	C42-C40-C36	-4.73	120.64	127.28
38	i	310	KC2	CMD-C2D-C1D	-4.73	118.22	125.42
38	k	611	KC2	CHB-C1B-C2B	-4.73	115.66	125.49
28	j	609	CLA	C4A-NA-C1A	4.72	108.83	106.68
28	d	309	CLA	C4A-NA-C1A	4.72	108.83	106.68
31	B	844	WVN	C11-C19-C22	4.71	136.46	126.32
28	d	306	CLA	C4A-NA-C1A	4.71	108.83	106.68
38	g	313	KC2	CMD-C2D-C1D	-4.71	118.24	125.42
38	s	201	KC2	C4B-CHC-C1C	-4.71	116.01	126.02
28	B	836	CLA	CAC-C3C-C4C	4.70	130.91	124.79
36	d	313	II0	C41-C39-C35	-4.70	120.68	127.28
36	h	311	II0	C41-C39-C35	-4.70	120.68	127.28
28	A	822	CLA	C4A-NA-C1A	4.70	108.82	106.68
28	k	602	CLA	C4A-NA-C1A	4.70	108.82	106.68
30	c	618	LHG	O7-C7-C8	4.70	121.64	111.48
38	f	611	KC2	CHB-C1B-NB	4.69	131.40	124.80
28	B	816	CLA	C4A-NA-C1A	4.69	108.82	106.68
38	g	312	KC2	CMD-C2D-C1D	-4.69	118.28	125.42
28	f	608	CLA	CMB-C2B-C1B	-4.68	118.29	125.42
28	B	819	CLA	C4A-NA-C1A	4.68	108.81	106.68
28	i	303	CLA	O2D-CGD-CBD	4.67	119.40	111.23
28	A	829	CLA	CMB-C2B-C1B	-4.67	118.30	125.42
28	f	606	CLA	C4A-NA-C1A	4.67	108.81	106.68
36	c	617	II0	C32-C34-C36	-4.67	113.55	126.36
36	j	615	II0	C42-C40-C36	-4.67	120.73	127.28
38	e	609	KC2	CMD-C2D-C1D	-4.66	118.33	125.42
28	j	610	CLA	C4A-NA-C1A	4.66	108.80	106.68
36	k	619	II0	C31-C33-C35	-4.65	113.60	126.36
30	g	321	LHG	O7-C7-C8	4.65	121.53	111.48
38	s	204	KC2	CHD-C1D-ND	-4.65	117.08	124.05
28	l	303	CLA	O2D-CGD-CBD	4.64	119.34	111.23
38	m	611	KC2	C3A-C4A-NA	4.64	116.19	110.45
30	c	620	LHG	O7-C7-C8	4.64	121.52	111.48
28	R	203	CLA	CAA-C2A-C3A	-4.64	100.47	113.00
38	j	611	KC2	CHB-C1B-C2B	-4.63	115.85	125.49
38	c	610	KC2	CHB-C1B-C2B	-4.63	115.85	125.49
31	e	615	WVN	C39-C36-C32	-4.63	120.78	127.28
38	l	310	KC2	C1B-CHB-C4A	-4.63	116.17	126.02
38	m	611	KC2	CHB-C1B-C2B	-4.63	115.86	125.49
38	e	609	KC2	C1B-CHB-C4A	-4.62	116.19	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	O	203	II0	C31-C33-C35	-4.62	113.69	126.36
38	g	314	KC2	C3A-C4A-NA	4.62	116.17	110.45
38	k	612	KC2	CHB-C1B-C2B	-4.62	115.88	125.49
38	d	310	KC2	C3A-C4A-NA	4.62	116.16	110.45
28	A	802	CLA	C4A-NA-C1A	4.61	108.78	106.68
38	g	314	KC2	CHB-C1B-C2B	-4.61	115.90	125.49
28	A	832	CLA	O2D-CGD-O1D	-4.61	114.88	123.85
28	g	315	CLA	C4A-NA-C1A	4.61	108.78	106.68
38	i	319	KC2	C1B-CHB-C4A	-4.61	116.23	126.02
31	B	846	WVN	C02-C11-C19	-4.61	117.41	124.58
28	i	307	CLA	C4A-NA-C1A	4.61	108.78	106.68
38	g	312	KC2	C3A-C4A-NA	4.61	116.15	110.45
38	g	312	KC2	CHB-C1B-C2B	-4.60	115.92	125.49
36	m	614	II0	C41-C39-C35	-4.60	120.83	127.28
35	L	209	LMG	O7-C10-C11	4.60	121.42	111.48
38	g	312	KC2	C4B-CHC-C1C	-4.60	116.25	126.02
38	e	609	KC2	CHB-C1B-C2B	-4.59	115.93	125.49
31	L	205	WVN	C40-C37-C34	-4.59	120.84	127.28
28	c	612	CLA	C4A-NA-C1A	4.59	108.77	106.68
28	b	611	CLA	C4A-NA-C1A	4.59	108.77	106.68
28	b	603	CLA	C4A-NA-C1A	4.58	108.77	106.68
28	B	814	CLA	C4A-NA-C1A	4.58	108.77	106.68
38	n	612	KC2	CHB-C1B-C2B	-4.58	115.96	125.49
28	g	309	CLA	C4A-NA-C1A	4.58	108.77	106.68
28	b	607	CLA	CAC-C3C-C4C	-4.57	118.84	124.79
38	d	311	KC2	C4B-C3B-C2B	-4.57	102.85	106.81
28	f	602	CLA	C4A-NA-C1A	4.57	108.76	106.68
36	b	617	II0	C41-C39-C35	-4.57	120.87	127.28
37	b	616	IHT	C40-C41-C38	-4.57	114.17	123.52
31	B	848	WVN	C29-C26-C22	-4.56	120.88	127.28
38	c	610	KC2	CHD-C1D-ND	-4.56	117.20	124.05
28	m	601	CLA	C4A-NA-C1A	4.56	108.76	106.68
28	k	606	CLA	C4A-NA-C1A	4.56	108.76	106.68
37	b	616	IHT	C32-C33-C37	4.56	126.18	119.01
38	e	609	KC2	CHD-C1D-ND	-4.55	117.22	124.05
28	B	822	CLA	C4A-NA-C1A	4.55	108.76	106.68
36	c	617	II0	C20-C14-C10	-4.55	115.65	124.16
38	j	611	KC2	C1B-CHB-C4A	-4.55	116.35	126.02
31	L	201	WVN	C02-C11-C19	-4.55	117.50	124.58
31	A	845	WVN	C21-C15-C13	-4.54	119.53	124.48
36	a	315	II0	C41-C42-C40	-4.54	114.23	123.52
36	a	316	II0	C42-C41-C39	-4.54	114.24	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	616	IHT	C02-C07-C10	-4.53	116.44	122.64
31	A	846	WVN	C29-C31-C32	4.53	138.78	126.36
28	n	613	CLA	C4A-NA-C1A	4.53	108.74	106.68
38	s	204	KC2	C4B-CHC-C1C	-4.52	116.41	126.02
38	m	611	KC2	C1D-ND-C4D	4.52	109.48	106.31
38	i	310	KC2	C4B-CHC-C1C	-4.52	116.42	126.02
38	s	204	KC2	CHB-C1B-C2B	-4.51	116.10	125.49
28	B	821	CLA	C4-C3-C5	4.51	123.06	115.23
31	h	309	WVN	C30-C33-C34	-4.51	113.99	126.36
36	a	318	II0	C28-C26-C30	-4.51	115.42	124.18
38	j	611	KC2	C3A-C4A-NA	4.51	116.03	110.45
28	B	820	CLA	C4A-NA-C1A	4.51	108.74	106.68
36	c	615	II0	C19-C13-C09	-4.51	115.73	124.16
28	a	311	CLA	C4A-NA-C1A	4.50	108.73	106.68
38	s	204	KC2	C1B-CHB-C4A	-4.50	116.45	126.02
37	c	616	IHT	C09-C10-C07	-4.50	116.62	122.70
38	k	612	KC2	CHC-C1C-NC	-4.50	117.26	124.23
38	s	204	KC2	C4B-C3B-C2B	-4.50	102.92	106.81
38	g	313	KC2	CHB-C1B-C2B	-4.50	116.14	125.49
37	R	204	IHT	C02-C07-C10	-4.49	116.50	122.64
31	s	207	WVN	C30-C28-C25	-4.49	120.98	127.28
31	B	847	WVN	C04-C09-C05	-4.49	120.55	124.83
36	n	615	II0	C42-C40-C36	-4.49	120.99	127.28
38	f	611	KC2	C1D-ND-C4D	4.48	109.46	106.31
28	i	303	CLA	C4A-NA-C1A	4.48	108.72	106.68
28	n	604	CLA	C4A-NA-C1A	4.48	108.72	106.68
28	a	304	CLA	C4A-NA-C1A	4.48	108.72	106.68
37	k	618	IHT	C19-C10-C07	-4.48	119.60	124.48
28	c	608	CLA	C4A-NA-C1A	4.48	108.72	106.68
30	j	617	LHG	O7-C7-C8	4.48	121.17	111.48
38	g	314	KC2	C1B-CHB-C4A	-4.48	116.50	126.02
31	s	205	WVN	C39-C36-C32	-4.47	121.00	127.28
36	a	314	II0	C41-C39-C35	-4.47	121.00	127.28
38	l	310	KC2	CHB-C1B-C2B	-4.47	116.19	125.49
38	k	611	KC2	C3A-C4A-NA	4.46	115.97	110.45
31	l	315	WVN	C20-C23-C25	-4.46	119.63	126.23
38	k	612	KC2	C3A-C4A-NA	4.46	115.97	110.45
38	s	204	KC2	O2D-CGD-CBD	4.46	119.02	111.23
38	c	610	KC2	C1D-ND-C4D	4.46	109.44	106.31
31	e	615	WVN	C40-C37-C34	-4.46	121.03	127.28
36	n	614	II0	C42-C41-C39	-4.46	114.40	123.52
38	n	612	KC2	CHD-C1D-ND	-4.46	117.36	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	j	611	KC2	CHD-C1D-ND	-4.45	117.37	124.05
38	e	609	KC2	C3A-C4A-NA	4.45	115.95	110.45
28	B	826	CLA	CMB-C2B-C1B	-4.45	118.65	125.42
28	n	608	CLA	C4A-NA-C1A	4.45	108.71	106.68
31	s	205	WVN	C06-C13-C15	-4.45	116.56	122.64
31	L	205	WVN	C02-C11-C19	-4.44	117.67	124.58
36	d	314	II0	C19-C13-C09	-4.44	115.86	124.16
38	m	611	KC2	C1B-CHB-C4A	-4.44	116.59	126.02
38	f	611	KC2	O2D-CGD-CBD	4.43	118.98	111.23
37	m	617	IHT	C19-C10-C07	-4.43	119.65	124.48
36	d	313	II0	C20-C14-C12	4.43	122.57	114.42
28	s	203	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
31	l	315	WVN	C21-C15-C13	-4.43	119.65	124.48
31	l	301	WVN	C39-C36-C32	-4.43	121.07	127.28
38	d	310	KC2	C1B-CHB-C4A	-4.43	116.61	126.02
38	k	613	KC2	CHB-C1B-C2B	-4.42	116.29	125.49
28	b	602	CLA	C4A-NA-C1A	4.41	108.69	106.68
32	A	850	LMT	C3'-C4'-C5'	-4.41	101.14	110.93
28	a	308	CLA	C4A-NA-C1A	4.41	108.69	106.68
36	a	315	II0	C19-C13-C11	4.41	122.53	114.42
28	A	827	CLA	C4A-NA-C1A	4.40	108.69	106.68
36	J	104	II0	C19-C13-C09	-4.40	115.93	124.16
37	R	204	IHT	C19-C10-C07	-4.40	119.68	124.48
28	B	827	CLA	C4A-NA-C1A	4.40	108.69	106.68
28	B	829	CLA	C4A-NA-C1A	4.40	108.69	106.68
38	k	611	KC2	C1B-CHB-C4A	-4.39	116.68	126.02
38	i	319	KC2	C1D-ND-C4D	4.39	109.39	106.31
36	j	615	II0	C41-C39-C35	-4.39	121.12	127.28
38	d	311	KC2	C1D-ND-C4D	4.39	109.39	106.31
31	s	207	WVN	C39-C36-C32	-4.39	121.13	127.28
38	k	613	KC2	CHD-C1D-ND	-4.39	117.47	124.05
37	k	618	IHT	C02-C07-C10	-4.38	116.65	122.64
28	A	832	CLA	O2D-CGD-CBD	4.38	118.89	111.23
38	n	611	KC2	C1B-CHB-C4A	-4.38	116.71	126.02
28	B	821	CLA	C7-C6-C5	4.38	124.94	113.26
36	O	203	II0	C41-C39-C35	-4.38	121.13	127.28
36	f	618	II0	C31-C33-C35	-4.38	114.36	126.36
28	g	307	CLA	C4A-NA-C1A	4.38	108.68	106.68
28	B	839	CLA	CAA-C2A-C3A	-4.37	101.18	113.00
37	g	319	IHT	C04-C02-C07	4.37	116.79	110.44
38	g	313	KC2	C3A-C4A-NA	4.37	115.86	110.45
38	m	611	KC2	C4B-C3B-C2B	-4.37	103.03	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	101	WVN	C30-C28-C25	-4.37	121.15	127.28
28	b	602	CLA	O2D-CGD-CBD	4.36	118.85	111.23
28	d	312	CLA	C4A-NA-C1A	4.36	108.67	106.68
36	k	621	II0	C41-C39-C35	-4.35	121.17	127.28
38	s	201	KC2	C4B-C3B-C2B	-4.35	103.04	106.81
37	f	617	IHT	C02-C07-C10	-4.35	116.69	122.64
38	g	314	KC2	C1D-ND-C4D	4.35	109.36	106.31
28	b	604	CLA	C4A-NA-C1A	4.34	108.66	106.68
28	m	602	CLA	C4A-NA-C1A	4.34	108.66	106.68
37	g	319	IHT	C25-C23-C27	-4.34	115.79	122.82
38	d	310	KC2	O2D-CGD-CBD	4.33	118.81	111.23
38	l	310	KC2	CHD-C1D-ND	-4.33	117.55	124.05
28	h	307	CLA	C4A-NA-C1A	4.33	108.65	106.68
38	n	611	KC2	C3A-C4A-NA	4.32	115.80	110.45
38	k	611	KC2	C1D-ND-C4D	4.32	109.34	106.31
37	a	317	IHT	C09-C10-C07	-4.32	116.87	122.70
37	n	617	IHT	C30-C27-C23	-4.32	121.22	127.28
38	f	611	KC2	C4B-C3B-C2B	-4.32	103.07	106.81
36	e	616	II0	C42-C40-C36	-4.32	121.22	127.28
31	B	848	WVN	C04-C09-C05	-4.32	120.71	124.83
36	g	317	II0	C20-C14-C10	-4.32	116.09	124.16
28	B	803	CLA	CMB-C2B-C1B	-4.31	118.85	125.42
38	k	612	KC2	C1B-CHB-C4A	-4.31	116.85	126.02
36	l	314	II0	C41-C39-C35	-4.31	121.24	127.28
37	b	615	IHT	C19-C10-C07	-4.31	119.78	124.48
36	b	614	II0	C20-C14-C12	4.31	122.34	114.42
36	k	621	II0	C19-C13-C11	4.31	122.34	114.42
36	O	203	II0	C20-C14-C10	-4.31	116.11	124.16
38	k	612	KC2	CHD-C4C-C3C	-4.30	111.43	125.91
31	l	301	WVN	C04-C09-C05	-4.30	120.73	124.83
38	d	311	KC2	CHC-C1C-NC	-4.30	117.57	124.23
35	b	621	LMG	O7-C10-C11	4.29	120.77	111.48
28	a	312	CLA	CAA-C2A-C3A	-4.28	101.42	113.00
36	c	613	II0	C42-C40-C36	-4.28	121.28	127.28
31	K	104	WVN	C40-C37-C34	-4.28	121.28	127.28
28	i	303	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
38	k	611	KC2	CHD-C1D-ND	-4.28	117.64	124.05
31	K	104	WVN	C06-C13-C15	-4.27	116.80	122.64
37	f	617	IHT	C09-C10-C07	-4.27	116.93	122.70
28	k	607	CLA	C1-C2-C3	-4.27	119.20	126.20
38	d	310	KC2	CHD-C1D-ND	-4.26	117.65	124.05
38	n	612	KC2	O2D-CGD-CBD	4.26	118.68	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	k	611	KC2	O2D-CGD-CBD	4.26	118.67	111.23
37	n	617	IHT	C02-C07-C10	-4.25	116.82	122.64
36	b	613	II0	C42-C41-C39	-4.25	114.83	123.52
36	e	613	II0	C19-C13-C11	4.24	122.23	114.42
31	A	847	WVN	C02-C11-C19	-4.24	117.97	124.58
37	k	618	IHT	C31-C34-C35	-4.24	114.73	126.36
36	h	312	II0	C18-C04-C17	-4.24	96.49	108.63
36	e	612	II0	C42-C40-C36	-4.24	121.34	127.28
38	l	310	KC2	O2D-CGD-CBD	4.23	118.63	111.23
31	e	615	WVN	C11-C19-C22	-4.23	117.22	126.32
28	k	610	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
38	c	610	KC2	C4B-C3B-C2B	-4.23	103.14	106.81
38	i	310	KC2	CHD-C1D-ND	-4.23	117.70	124.05
31	l	315	WVN	C06-C13-C15	-4.23	116.86	122.64
28	f	609	CLA	C4A-NA-C1A	4.23	108.61	106.68
36	d	315	II0	C41-C42-C40	-4.23	114.86	123.52
36	J	104	II0	C20-C14-C10	-4.23	116.25	124.16
38	n	611	KC2	CHD-C1D-ND	-4.23	117.71	124.05
38	c	610	KC2	C1B-CHB-C4A	-4.23	117.04	126.02
36	m	615	II0	C19-C13-C11	4.22	122.17	114.42
28	A	805	CLA	CAA-C2A-C3A	-4.21	101.61	113.00
30	i	318	LHG	O7-C7-C8	4.21	120.59	111.48
36	n	616	II0	C42-C40-C36	-4.21	121.38	127.28
28	j	608	CLA	C4A-NA-C1A	4.21	108.60	106.68
38	d	310	KC2	C4B-C3B-C2B	-4.21	103.17	106.81
38	k	613	KC2	C1B-CHB-C4A	-4.20	117.08	126.02
28	l	303	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
29	B	842	PQN	C11-C12-C13	-4.20	119.60	126.83
28	B	832	CLA	CMB-C2B-C1B	-4.20	119.03	125.42
38	d	311	KC2	CHB-C1B-NB	4.19	130.71	124.80
28	c	602	CLA	O2D-CGD-O1D	-4.19	115.69	123.85
37	g	319	IHT	C41-C38-C35	-4.19	121.41	127.28
38	f	611	KC2	CHB-C1B-C2B	-4.18	116.80	125.49
28	e	604	CLA	O2D-CGD-O1D	-4.18	115.72	123.85
38	g	313	KC2	C1B-CHB-C4A	-4.18	117.14	126.02
38	f	611	KC2	CHD-C1D-ND	-4.17	117.79	124.05
35	F	205	LMG	C8-O7-C10	-4.17	107.81	117.80
36	k	619	II0	C19-C13-C11	4.17	122.09	114.42
36	n	614	II0	C19-C13-C09	-4.17	116.37	124.16
38	l	310	KC2	C4B-C3B-C2B	-4.17	103.20	106.81
38	i	319	KC2	CHD-C1D-ND	-4.16	117.80	124.05
38	g	314	KC2	CHD-C1D-ND	-4.16	117.80	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	616	IHT	C22-C23-C27	4.16	125.56	119.01
28	A	828	CLA	C4A-NA-C1A	4.16	108.58	106.68
38	n	612	KC2	C1B-CHB-C4A	-4.16	117.18	126.02
28	A	852	CLA	C4A-NA-C1A	4.16	108.58	106.68
38	g	313	KC2	C4B-C3B-C2B	-4.16	103.21	106.81
38	k	613	KC2	C3A-C4A-NA	4.16	115.59	110.45
28	A	818	CLA	C1-C2-C3	-4.15	119.39	126.20
31	B	845	WVN	C40-C37-C34	-4.15	121.46	127.28
35	F	205	LMG	O7-C10-C11	4.15	120.46	111.48
28	A	815	CLA	CMB-C2B-C3B	4.15	136.30	126.55
36	h	311	II0	C20-C14-C12	4.15	122.04	114.42
28	A	806	CLA	C4A-NA-C1A	4.14	108.57	106.68
38	m	611	KC2	CHD-C1D-ND	-4.14	117.83	124.05
38	n	612	KC2	C3A-C4A-NA	4.14	115.58	110.45
31	L	201	WVN	C07-C01-C02	4.14	115.81	109.55
31	l	301	WVN	C23-C20-C13	-4.13	115.96	127.00
36	m	615	II0	C42-C40-C36	-4.13	121.48	127.28
31	B	848	WVN	C40-C39-C36	-4.13	115.07	123.52
30	J	106	LHG	O7-C7-C8	4.13	120.41	111.48
31	B	848	WVN	C24-C22-C19	4.12	124.39	118.09
38	f	611	KC2	C1B-CHB-C4A	-4.12	117.27	126.02
28	B	807	CLA	C4A-NA-C1A	4.12	108.56	106.68
28	m	612	CLA	C4A-NA-C1A	4.12	108.56	106.68
36	e	616	II0	C41-C39-C35	-4.12	121.50	127.28
28	k	604	CLA	C4A-NA-C1A	4.12	108.56	106.68
38	n	612	KC2	C1D-ND-C4D	4.11	109.20	106.31
38	d	311	KC2	CMD-C2D-C3D	4.11	138.64	125.67
38	k	612	KC2	C4B-C3B-C2B	-4.11	103.25	106.81
38	k	611	KC2	C4B-C3B-C2B	-4.10	103.26	106.81
36	j	615	II0	C41-C42-C40	-4.10	115.13	123.52
30	A	843	LHG	O7-C7-C8	4.10	120.35	111.48
31	J	102	WVN	C02-C11-C19	-4.10	118.20	124.58
38	g	313	KC2	CHD-C1D-ND	-4.10	117.90	124.05
38	g	314	KC2	C4B-C3B-C2B	-4.10	103.26	106.81
38	c	610	KC2	O2D-CGD-CBD	4.10	118.39	111.23
36	a	318	II0	C15-C03-C09	-4.09	103.18	110.52
38	i	310	KC2	C4B-C3B-C2B	-4.09	103.27	106.81
31	J	101	WVN	C20-C23-C25	-4.09	120.18	126.23
28	B	802	CLA	O2D-CGD-O1D	-4.09	115.89	123.85
36	n	618	II0	C31-C33-C35	-4.08	115.17	126.36
28	A	818	CLA	CMB-C2B-C1B	-4.08	119.21	125.42
36	a	315	II0	C19-C13-C09	-4.08	116.54	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	202	WVN	C21-C15-C13	-4.08	120.04	124.48
28	A	834	CLA	CMB-C2B-C1B	-4.07	119.22	125.42
31	L	201	WVN	C30-C28-C25	-4.06	121.58	127.28
37	g	319	IHT	C30-C27-C23	4.06	132.97	127.28
31	L	205	WVN	C30-C28-C25	-4.06	121.59	127.28
36	g	316	II0	C19-C13-C09	-4.05	116.59	124.16
28	m	607	CLA	C4A-NA-C1A	4.05	108.53	106.68
28	m	609	CLA	C4A-NA-C1A	4.04	108.52	106.68
28	k	608	CLA	C4A-NA-C1A	4.04	108.52	106.68
28	k	609	CLA	CMA-C3A-C4A	-4.04	100.93	111.77
38	j	611	KC2	C1D-ND-C4D	4.03	109.14	106.31
37	k	618	IHT	C18-C22-C23	-4.03	120.27	126.23
38	i	319	KC2	C4B-C3B-C2B	-4.03	103.32	106.81
30	a	301	LHG	C5-O7-C7	-4.03	108.16	117.80
38	c	610	KC2	C3A-C4A-NA	4.03	115.43	110.45
31	A	846	WVN	C04-C09-C05	-4.03	120.99	124.83
28	A	834	CLA	C4A-NA-C1A	4.02	108.51	106.68
38	k	613	KC2	C4B-C3B-C2B	-4.02	103.33	106.81
31	A	848	WVN	C19-C22-C26	4.02	125.33	119.01
31	M	101	WVN	C11-C19-C22	-4.01	117.69	126.32
30	L	208	LHG	O7-C7-C8	4.01	120.16	111.48
28	B	825	CLA	C4A-NA-C1A	4.01	108.51	106.68
30	d	317	LHG	O7-C7-C8	4.01	120.16	111.48
31	I	101	WVN	C11-C19-C22	-4.01	117.70	126.32
31	L	201	WVN	C20-C23-C25	-4.01	120.31	126.23
38	g	312	KC2	C1D-ND-C4D	4.00	109.12	106.31
28	j	607	CLA	C4A-NA-C1A	4.00	108.51	106.68
28	h	301	CLA	C4A-NA-C1A	4.00	108.50	106.68
31	J	101	WVN	C21-C15-C13	-4.00	120.12	124.48
28	B	828	CLA	CMB-C2B-C1B	-4.00	119.33	125.42
28	O	201	CLA	C4A-NA-C1A	4.00	108.50	106.68
38	e	609	KC2	C4B-C3B-C2B	-4.00	103.35	106.81
37	j	616	IHT	C19-C10-C07	-4.00	120.12	124.48
36	J	104	II0	C31-C33-C35	-3.99	115.41	126.36
31	K	104	WVN	C04-C09-C05	-3.99	121.02	124.83
31	L	205	WVN	C14-C15-C13	-3.99	117.31	122.70
31	e	615	WVN	C21-C15-C13	-3.99	120.13	124.48
28	n	607	CLA	C4A-NA-C1A	3.98	108.50	106.68
36	k	617	II0	C19-C13-C09	-3.98	116.71	124.16
38	n	612	KC2	C4B-C3B-C2B	-3.98	103.36	106.81
36	l	314	II0	C20-C14-C12	3.98	121.74	114.42
37	a	317	IHT	C02-C07-C10	-3.98	117.20	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	e	609	KC2	C1D-ND-C4D	3.97	109.10	106.31
36	f	618	II0	C06-C04-C10	3.97	117.32	109.49
28	n	601	CLA	C4A-NA-C1A	3.97	108.49	106.68
36	c	617	II0	C41-C39-C35	-3.97	121.71	127.28
28	A	802	CLA	CMB-C2B-C3B	3.97	135.88	126.55
37	m	617	IHT	C02-C07-C10	-3.97	117.21	122.64
28	j	604	CLA	C4A-NA-C1A	3.97	108.49	106.68
31	s	205	WVN	C40-C37-C34	-3.97	121.72	127.28
28	s	202	CLA	CAA-CBA-CGA	-3.97	101.95	113.21
31	l	301	WVN	C21-C15-C13	-3.96	120.16	124.48
31	h	309	WVN	C21-C15-C13	-3.96	120.16	124.48
31	M	101	WVN	C14-C15-C13	-3.96	117.35	122.70
38	s	204	KC2	C3A-C4A-NA	3.96	115.35	110.45
28	F	202	CLA	C1-O2A-CGA	3.96	126.24	116.65
37	c	616	IHT	C18-C22-C23	-3.96	120.38	126.23
37	n	617	IHT	C30-C32-C33	-3.96	115.51	126.36
36	e	613	II0	C42-C40-C36	-3.96	121.73	127.28
31	A	845	WVN	C23-C20-C13	-3.95	116.44	127.00
36	g	320	II0	C32-C34-C36	-3.95	115.53	126.36
38	n	611	KC2	C4B-C3B-C2B	-3.95	103.39	106.81
31	B	845	WVN	C30-C28-C25	-3.94	121.75	127.28
36	m	614	II0	C42-C40-C36	-3.94	121.76	127.28
28	l	308	CLA	C4A-NA-C1A	3.93	108.47	106.68
31	B	845	WVN	C26-C29-C31	-3.93	111.82	123.20
28	A	836	CLA	CAA-CBA-CGA	-3.93	102.06	113.21
28	a	313	CLA	C4A-NA-C1A	3.93	108.47	106.68
28	A	811	CLA	C1-C2-C3	-3.92	119.77	126.20
31	h	309	WVN	C40-C37-C34	-3.92	121.78	127.28
38	n	611	KC2	C1D-ND-C4D	3.92	109.06	106.31
28	d	302	CLA	CMB-C2B-C1B	-3.92	119.45	125.42
28	B	822	CLA	CBC-CAC-C3C	-3.91	101.81	112.42
31	A	845	WVN	C02-C11-C19	-3.91	118.49	124.58
28	m	613	CLA	C4A-NA-C1A	3.91	108.46	106.68
28	h	313	CLA	C4A-NA-C1A	3.90	108.46	106.68
36	f	614	II0	C20-C14-C10	-3.90	116.87	124.16
28	j	606	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
38	d	311	KC2	O2D-CGD-CBD	3.90	118.05	111.23
37	c	616	IHT	C02-C07-C10	-3.90	117.31	122.64
38	f	611	KC2	CMD-C2D-C3D	3.90	137.97	125.67
28	l	311	CLA	C4A-NA-C1A	3.89	108.45	106.68
28	O	206	CLA	CAC-C3C-C4C	3.89	129.85	124.79
31	I	101	WVN	C21-C15-C13	-3.89	120.24	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	l	310	KC2	C1D-ND-C4D	3.89	109.04	106.31
31	K	102	WVN	C20-C23-C25	-3.88	120.49	126.23
36	a	316	II0	C41-C39-C35	-3.88	121.83	127.28
36	f	615	II0	C42-C40-C36	-3.88	121.83	127.28
31	J	102	WVN	C10-C06-C13	3.88	116.08	110.44
35	L	209	LMG	C4-C3-C2	3.88	117.64	110.83
38	j	611	KC2	C4B-C3B-C2B	-3.88	103.45	106.81
28	j	606	CLA	CBA-CAA-C2A	-3.87	102.27	113.79
28	A	852	CLA	C3B-C4B-NB	-3.87	107.08	110.53
37	g	319	IHT	C32-C33-C37	3.87	125.09	119.01
36	m	618	II0	C29-C31-C33	3.87	134.40	123.20
36	c	615	II0	C19-C13-C11	3.86	121.52	114.42
28	i	312	CLA	C4A-NA-C1A	3.86	108.44	106.68
37	c	616	IHT	C19-C10-C07	-3.86	120.27	124.48
28	n	602	CLA	C4A-NA-C1A	3.86	108.44	106.68
31	B	844	WVN	C07-C01-C02	3.86	115.39	109.55
36	g	316	II0	C41-C42-C40	-3.86	115.63	123.52
28	l	306	CLA	C2A-C1A-CHA	3.85	130.55	123.87
38	d	311	KC2	CHB-C1B-C2B	-3.85	117.48	125.49
31	M	101	WVN	C40-C37-C34	-3.84	121.89	127.28
36	k	621	II0	C20-C14-C10	-3.84	116.98	124.16
31	B	844	WVN	C28-C30-C33	-3.84	112.08	123.20
28	A	854	CLA	C4A-NA-C1A	3.83	108.43	106.68
38	g	312	KC2	C2A-C1A-NA	3.83	115.48	109.34
31	A	847	WVN	C21-C15-C13	-3.83	120.31	124.48
36	a	318	II0	C32-C34-C36	3.83	136.85	126.36
31	B	844	WVN	C02-C11-C19	3.83	130.53	124.58
28	k	602	CLA	C1-C2-C3	-3.82	120.58	126.76
28	h	306	CLA	C4A-NA-C1A	3.82	108.42	106.68
36	d	316	II0	C42-C40-C36	-3.82	121.92	127.28
36	a	318	II0	C38-C36-C34	-3.82	112.25	118.09
36	e	616	II0	C41-C42-C40	-3.82	115.71	123.52
31	J	102	WVN	C29-C26-C22	-3.81	121.94	127.28
36	g	317	II0	C41-C42-C40	-3.81	115.73	123.52
36	f	614	II0	C42-C40-C36	-3.81	121.94	127.28
28	l	305	CLA	O2D-CGD-O1D	-3.81	116.44	123.85
37	f	617	IHT	C40-C37-C33	-3.80	121.94	127.28
38	n	611	KC2	CMD-C2D-C3D	3.80	137.66	125.67
36	a	316	II0	C19-C13-C09	-3.80	117.05	124.16
31	M	101	WVN	C07-C01-C02	3.80	115.30	109.55
30	A	844	LHG	O7-C7-C8	3.80	119.70	111.48
36	k	615	II0	C19-C13-C11	3.80	121.40	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	R	204	IHT	C40-C41-C38	-3.79	115.76	123.52
28	A	825	CLA	C4A-NA-C1A	3.79	108.41	106.68
38	c	610	KC2	CBC-CAC-C3C	-3.78	108.62	127.53
38	g	312	KC2	C4B-C3B-C2B	-3.78	103.54	106.81
28	k	610	CLA	O2D-CGD-CBD	3.78	117.83	111.23
28	R	203	CLA	CMB-C2B-C1B	-3.77	119.68	125.42
31	K	102	WVN	C30-C28-C25	-3.76	122.00	127.28
28	B	821	CLA	CMB-C2B-C1B	-3.75	119.71	125.42
38	s	201	KC2	O2D-CGD-CBD	3.75	117.79	111.23
30	b	619	LHG	O7-C7-C8	3.75	119.59	111.48
38	i	319	KC2	O2D-CGD-CBD	3.75	117.78	111.23
28	Q	303	CLA	CMB-C2B-C3B	3.74	135.35	126.55
36	e	613	II0	C41-C42-C40	-3.74	115.86	123.52
36	g	318	II0	C19-C13-C11	3.74	121.30	114.42
36	j	614	II0	C32-C34-C36	-3.74	116.11	126.36
37	a	317	IHT	C40-C37-C33	-3.73	122.04	127.28
36	h	312	II0	C41-C42-C40	-3.73	115.88	123.52
28	k	608	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
30	l	317	LHG	O7-C7-C8	3.73	119.55	111.48
36	i	313	II0	C30-C32-C34	-3.73	112.40	123.20
31	K	104	WVN	C14-C15-C13	-3.73	117.67	122.70
36	h	311	II0	C19-C13-C11	3.73	121.27	114.42
29	A	842	PQN	C11-C12-C13	-3.72	120.42	126.83
36	f	614	II0	C19-C13-C11	3.72	121.26	114.42
28	f	610	CLA	C4A-NA-C1A	3.72	108.37	106.68
31	B	844	WVN	C26-C29-C31	-3.71	112.44	123.20
36	h	311	II0	C20-C14-C10	-3.71	117.22	124.16
36	h	310	II0	C42-C41-C39	-3.71	115.93	123.52
38	f	611	KC2	C3A-C4A-NA	3.70	115.03	110.45
31	A	846	WVN	C24-C22-C26	-3.70	116.82	122.82
28	B	821	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
36	l	312	II0	C19-C13-C09	-3.69	117.26	124.16
28	A	830	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
36	n	618	II0	C20-C14-C10	-3.69	117.26	124.16
28	n	602	CLA	CMB-C2B-C1B	-3.69	119.81	125.42
31	L	206	WVN	C26-C29-C31	-3.69	112.52	123.20
36	b	617	II0	C20-C14-C12	3.68	121.19	114.42
31	B	847	WVN	C02-C05-C09	-3.68	116.94	121.47
38	l	310	KC2	CMD-C2D-C3D	3.68	137.28	125.67
37	b	615	IHT	C09-C10-C07	-3.68	117.73	122.70
36	k	619	II0	C41-C39-C35	-3.68	122.12	127.28
28	A	820	CLA	CMB-C2B-C1B	-3.68	119.82	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	101	WVN	C29-C26-C22	-3.67	122.13	127.28
31	A	848	WVN	C10-C06-C13	-3.67	105.10	110.44
37	f	617	IHT	C20-C15-C12	3.67	121.17	114.42
28	n	610	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
28	B	826	CLA	C4A-NA-C1A	3.67	108.35	106.68
28	c	602	CLA	C4A-NA-C1A	3.67	108.35	106.68
28	B	837	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
28	f	604	CLA	CMB-C2B-C1B	-3.67	119.83	125.42
28	f	609	CLA	CMB-C2B-C1B	-3.67	119.84	125.42
36	h	312	II0	C42-C40-C36	-3.67	122.14	127.28
36	k	621	II0	C41-C42-C40	-3.67	116.02	123.52
38	g	314	KC2	CMD-C2D-C3D	3.67	137.23	125.67
36	b	614	II0	C29-C31-C33	-3.66	112.58	123.20
36	n	616	II0	C20-C14-C12	3.66	121.16	114.42
31	s	205	WVN	C23-C20-C13	-3.66	117.21	127.00
36	c	614	II0	C41-C42-C40	-3.66	116.03	123.52
31	L	205	WVN	C06-C13-C15	-3.66	117.64	122.64
36	d	315	II0	C42-C40-C36	-3.66	122.15	127.28
28	b	602	CLA	O2D-CGD-O1D	-3.66	116.73	123.85
38	s	201	KC2	CBC-CAC-C3C	-3.66	109.25	127.53
28	g	311	CLA	C4A-NA-C1A	3.66	108.35	106.68
28	c	602	CLA	CAC-C3C-C4C	3.66	129.55	124.79
37	b	616	IHT	C25-C23-C27	-3.66	116.89	122.82
28	O	206	CLA	CAA-C2A-C3A	-3.65	103.12	113.00
28	A	802	CLA	C1-C2-C3	-3.65	120.21	126.20
31	l	315	WVN	C39-C36-C32	-3.65	122.16	127.28
28	B	823	CLA	CMB-C2B-C1B	-3.65	119.86	125.42
28	c	605	CLA	C1-C2-C3	-3.65	120.22	126.20
28	j	606	CLA	O2D-CGD-CBD	3.65	117.61	111.23
36	n	615	II0	C31-C33-C35	-3.65	116.37	126.36
36	d	316	II0	C41-C42-C40	-3.63	116.08	123.52
28	k	609	CLA	CHB-C4A-NA	3.63	129.65	124.40
28	a	303	CLA	C1-C2-C3	-3.63	120.24	126.20
36	e	612	II0	C32-C34-C36	-3.63	116.41	126.36
28	f	602	CLA	CAA-CBA-CGA	-3.63	102.91	113.21
31	B	846	WVN	C04-C09-C05	-3.62	121.37	124.83
31	R	202	WVN	C01-C02-C11	-3.62	108.66	112.83
37	b	615	IHT	C18-C22-C23	-3.62	120.88	126.23
36	m	616	II0	C42-C41-C39	-3.62	116.11	123.52
28	B	828	CLA	C4A-NA-C1A	3.62	108.33	106.68
31	J	101	WVN	C39-C36-C32	-3.62	122.20	127.28
31	L	206	WVN	C21-C15-C13	-3.62	120.53	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	301	CLA	C1-C2-C3	-3.62	120.91	126.76
38	g	312	KC2	O2D-CGD-CBD	3.62	117.56	111.23
36	m	618	II0	C06-C04-C10	3.62	116.62	109.49
30	k	620	LHG	O7-C7-C8	3.62	119.31	111.48
30	f	619	LHG	O7-C7-C8	3.62	119.31	111.48
28	b	601	CLA	C1-C2-C3	-3.62	120.27	126.20
36	e	612	II0	C41-C39-C35	-3.62	122.21	127.28
31	B	844	WVN	C39-C40-C37	-3.61	116.14	123.52
28	B	808	CLA	CMB-C2B-C1B	-3.61	119.92	125.42
30	b	620	LHG	O7-C7-C8	3.61	119.28	111.48
35	c	619	LMG	C9-C8-C7	-3.60	103.38	111.78
30	A	849	LHG	O7-C7-C8	3.60	119.27	111.48
28	m	610	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
38	m	611	KC2	CHB-C4A-NA	3.60	129.81	124.23
31	B	847	WVN	C24-C22-C19	3.60	123.58	118.09
28	d	308	CLA	C4A-NA-C1A	3.59	108.32	106.68
37	b	616	IHT	C04-C02-C07	3.59	115.66	110.44
28	h	302	CLA	CMB-C2B-C1B	-3.59	119.95	125.42
38	s	204	KC2	CMD-C2D-C3D	3.59	137.00	125.67
36	c	614	II0	C19-C13-C11	3.59	121.02	114.42
36	c	613	II0	C41-C42-C40	-3.59	116.17	123.52
31	I	101	WVN	C29-C26-C22	-3.59	122.24	127.28
31	A	846	WVN	C20-C23-C25	-3.59	120.92	126.23
36	j	614	II0	C29-C31-C33	-3.59	112.80	123.20
36	J	104	II0	C41-C39-C35	-3.59	122.25	127.28
36	k	621	II0	C19-C13-C09	-3.59	117.45	124.16
28	f	612	CLA	CAC-C3C-C4C	3.59	129.46	124.79
38	g	314	KC2	O2D-CGD-O1D	-3.59	116.87	123.85
31	e	615	WVN	C04-C09-C05	-3.59	121.41	124.83
36	i	314	II0	C42-C41-C39	-3.58	116.19	123.52
28	A	851	CLA	CMB-C2B-C1B	-3.58	119.97	125.42
31	h	309	WVN	C20-C23-C25	-3.58	120.94	126.23
38	k	611	KC2	C2A-C1A-NA	3.57	115.07	109.34
28	c	606	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
38	n	612	KC2	CBC-CAC-C3C	-3.57	109.67	127.53
36	a	314	II0	C19-C13-C09	-3.57	117.48	124.16
38	i	319	KC2	CHB-C4A-NA	3.57	129.77	124.23
38	s	201	KC2	C1A-C2A-C3A	-3.57	104.00	107.28
28	f	604	CLA	C4A-NA-C1A	3.57	108.31	106.68
36	b	617	II0	C42-C41-C39	-3.56	116.23	123.52
28	B	801	CLA	CMB-C2B-C1B	-3.56	120.00	125.42
36	n	618	II0	C19-C13-C11	3.56	120.97	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	c	614	II0	C20-C14-C10	-3.56	117.50	124.16
37	a	317	IHT	C41-C40-C37	-3.56	116.23	123.52
37	R	204	IHT	C41-C38-C35	-3.56	122.29	127.28
38	g	312	KC2	CBC-CAC-C3C	-3.56	109.74	127.53
36	f	618	II0	C19-C13-C11	3.56	120.97	114.42
28	B	806	CLA	O2D-CGD-O1D	-3.56	116.93	123.85
36	l	313	II0	C19-C13-C11	3.56	120.96	114.42
28	A	854	CLA	O2D-CGD-CBD	3.55	117.44	111.23
30	a	319	LHG	O7-C7-C8	3.55	119.16	111.48
36	e	614	II0	C41-C42-C40	-3.55	116.25	123.52
28	a	308	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
28	f	602	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
38	m	611	KC2	CMD-C2D-C3D	3.55	136.86	125.67
38	n	611	KC2	CHB-C4A-NA	3.55	129.73	124.23
28	d	302	CLA	CMB-C2B-C3B	3.54	134.89	126.55
38	i	310	KC2	C1A-C2A-C3A	-3.54	104.02	107.28
28	f	607	CLA	C4A-NA-C1A	3.54	108.30	106.68
36	f	614	II0	C41-C42-C40	-3.54	116.28	123.52
28	b	601	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
28	m	609	CLA	CMB-C2B-C1B	-3.54	120.03	125.42
36	k	619	II0	C42-C41-C39	-3.54	116.28	123.52
29	A	842	PQN	C17-C16-C15	-3.54	103.84	113.26
38	d	311	KC2	C3A-C4A-NA	3.54	114.83	110.45
28	B	832	CLA	CMB-C2B-C3B	3.54	134.87	126.55
37	n	617	IHT	C18-C22-C23	-3.53	121.01	126.23
31	B	847	WVN	C20-C23-C25	-3.53	121.01	126.23
36	i	317	II0	C31-C33-C35	-3.53	116.68	126.36
31	F	203	WVN	C28-C30-C33	-3.53	112.97	123.20
36	h	311	II0	C42-C41-C39	-3.53	116.30	123.52
28	m	604	CLA	CMB-C2B-C1B	-3.53	120.04	125.42
36	d	315	II0	C20-C14-C10	-3.53	117.56	124.16
36	g	318	II0	C19-C13-C09	-3.53	117.56	124.16
28	B	817	CLA	C4A-NA-C1A	3.53	108.29	106.68
31	J	102	WVN	C30-C28-C25	-3.53	122.33	127.28
36	k	621	II0	C29-C31-C33	-3.53	112.98	123.20
28	A	810	CLA	C4A-NA-C1A	3.53	108.29	106.68
28	B	815	CLA	C4A-NA-C1A	3.52	108.29	106.68
28	g	303	CLA	C4A-NA-C1A	3.52	108.29	106.68
38	g	312	KC2	O2D-CGD-O1D	-3.52	116.99	123.85
38	k	611	KC2	CMD-C2D-C3D	3.52	136.78	125.67
36	b	614	II0	C42-C41-C39	-3.52	116.31	123.52
36	d	316	II0	C32-C34-C36	-3.52	116.71	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	n	612	KC2	CMD-C2D-C3D	3.52	136.77	125.67
38	l	310	KC2	C2A-C1A-NA	3.52	114.98	109.34
36	d	316	II0	C15-C03-C09	-3.52	104.21	110.52
38	s	201	KC2	CHB-C4A-NA	3.52	129.69	124.23
28	d	312	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
37	b	615	IHT	C30-C32-C33	-3.52	116.72	126.36
36	g	316	II0	C20-C14-C10	-3.52	117.58	124.16
37	a	317	IHT	C19-C10-C07	-3.52	120.65	124.48
38	i	310	KC2	C4C-C3C-C2C	-3.52	104.05	107.28
36	f	615	II0	C19-C13-C11	3.51	120.88	114.42
28	j	602	CLA	CMB-C2B-C1B	-3.51	120.07	125.42
38	k	611	KC2	O2D-CGD-O1D	-3.51	117.02	123.85
36	m	616	II0	C19-C13-C11	3.51	120.87	114.42
36	a	314	II0	C41-C42-C40	-3.50	116.36	123.52
36	c	613	II0	C38-C36-C34	3.50	123.43	118.09
36	i	317	II0	C20-C14-C10	-3.50	117.62	124.16
28	A	815	CLA	C4A-NA-C1A	3.50	108.27	106.68
36	a	315	II0	C31-C33-C35	-3.50	116.78	126.36
28	i	309	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
36	i	317	II0	C19-C13-C09	-3.49	117.63	124.16
30	a	301	LHG	O7-C7-C8	3.49	119.03	111.48
36	h	310	II0	C31-C33-C35	-3.49	116.79	126.36
31	B	845	WVN	C40-C39-C36	-3.49	116.38	123.52
38	c	610	KC2	CHB-C4A-NA	3.49	129.64	124.23
36	e	616	II0	C20-C14-C12	3.49	120.83	114.42
28	d	305	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
31	R	202	WVN	C29-C26-C22	-3.49	122.39	127.28
36	a	314	II0	C30-C32-C34	-3.49	113.10	123.20
36	f	615	II0	C41-C42-C40	-3.48	116.39	123.52
31	K	104	WVN	C39-C36-C32	-3.48	122.40	127.28
32	a	320	LMT	C8-C7-C6	-3.48	96.78	114.37
36	b	613	II0	C29-C31-C33	-3.48	113.13	123.20
38	j	611	KC2	CHB-C4A-NA	3.47	129.62	124.23
38	c	610	KC2	C2A-C1A-NA	3.47	114.91	109.34
28	i	303	CLA	CMB-C2B-C1B	-3.47	120.13	125.42
28	n	608	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
28	B	803	CLA	CMB-C2B-C3B	3.47	134.71	126.55
36	k	619	II0	C20-C14-C10	-3.47	117.67	124.16
38	j	611	KC2	CMD-C2D-C3D	3.47	136.60	125.67
38	d	310	KC2	CMD-C2D-C3D	3.47	136.60	125.67
36	i	313	II0	C38-C36-C34	3.47	123.38	118.09
28	A	822	CLA	C3B-C4B-NB	-3.46	107.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	616	IHT	C09-C10-C07	-3.46	118.02	122.70
31	i	316	WVN	C39-C36-C32	-3.46	122.42	127.28
31	A	847	WVN	C39-C40-C37	-3.46	116.44	123.52
38	j	611	KC2	C2A-C1A-NA	3.46	114.89	109.34
28	e	602	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
31	B	846	WVN	C20-C23-C25	-3.46	121.12	126.23
36	l	313	II0	C06-C04-C10	3.46	116.30	109.49
28	d	302	CLA	C4A-NA-C1A	3.46	108.26	106.68
28	l	309	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
38	g	314	KC2	C2A-C1A-NA	3.46	114.88	109.34
36	i	314	II0	C19-C13-C11	3.46	120.78	114.42
28	l	308	CLA	CMB-C2B-C1B	-3.45	120.16	125.42
28	s	202	CLA	C1-C2-C3	-3.45	120.54	126.20
31	F	204	WVN	C39-C40-C37	3.45	130.58	123.52
28	c	605	CLA	O2D-CGD-CBD	3.45	117.26	111.23
28	B	814	CLA	CMB-C2B-C1B	-3.45	120.17	125.42
37	b	615	IHT	C04-C02-C07	3.45	115.45	110.44
31	A	845	WVN	C39-C36-C32	-3.45	122.44	127.28
28	B	804	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
38	d	311	KC2	C1D-CHD-C4C	-3.44	118.15	126.25
28	B	821	CLA	O2A-C1-C2	-3.44	94.85	108.11
28	A	829	CLA	C4A-NA-C1A	3.44	108.25	106.68
31	R	201	WVN	C20-C23-C25	-3.44	121.14	126.23
36	l	313	II0	C31-C33-C35	-3.44	116.93	126.36
28	g	305	CLA	CMB-C2B-C1B	-3.44	120.18	125.42
28	A	834	CLA	CMB-C2B-C3B	3.44	134.64	126.55
28	B	835	CLA	C4A-NA-C1A	3.44	108.25	106.68
28	b	603	CLA	CMB-C2B-C1B	-3.44	120.19	125.42
37	m	617	IHT	C30-C32-C33	-3.44	116.94	126.36
38	i	310	KC2	CBC-CAC-C3C	-3.43	110.38	127.53
31	B	847	WVN	C40-C39-C36	-3.43	116.50	123.52
37	g	319	IHT	C09-C10-C07	-3.43	118.07	122.70
28	j	606	CLA	C4A-NA-C1A	3.43	108.24	106.68
36	l	316	II0	C20-C14-C10	-3.43	117.75	124.16
28	d	308	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
36	l	313	II0	C32-C34-C36	-3.43	116.97	126.36
31	B	846	WVN	C12-C14-C15	-3.42	107.95	114.06
31	B	847	WVN	C19-C22-C26	-3.42	113.63	119.01
36	i	320	II0	C31-C33-C35	-3.42	116.99	126.36
28	A	830	CLA	CMB-C2B-C1B	-3.42	120.21	125.42
31	B	847	WVN	C08-C01-C02	-3.42	104.37	109.55
36	e	614	II0	C19-C13-C11	3.41	120.70	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	818	CLA	CMB-C2B-C1B	-3.41	120.22	125.42
28	f	608	CLA	CMB-C2B-C3B	3.41	134.58	126.55
38	n	612	KC2	C2A-C1A-NA	3.41	114.81	109.34
30	i	318	LHG	O8-C23-C24	3.41	122.24	111.83
37	g	319	IHT	C36-C33-C37	-3.41	117.29	122.82
38	e	609	KC2	C2A-C1A-NA	3.41	114.81	109.34
30	A	843	LHG	O8-C23-C24	3.41	122.23	111.83
38	k	613	KC2	CMD-C2D-C3D	3.41	136.41	125.67
36	h	310	II0	C41-C39-C35	-3.41	122.50	127.28
28	k	606	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
38	f	611	KC2	CHB-C4A-NA	3.41	129.51	124.23
36	g	318	II0	C42-C40-C36	-3.40	122.50	127.28
38	c	610	KC2	CMD-C2D-C3D	3.40	136.40	125.67
28	e	602	CLA	C4A-NA-C1A	3.40	108.23	106.68
36	b	613	II0	C19-C13-C11	3.40	120.68	114.42
28	b	607	CLA	CAC-C3C-C2C	3.40	133.81	127.56
38	e	609	KC2	CMD-C2D-C3D	3.40	136.39	125.67
28	d	304	CLA	CMB-C2B-C1B	-3.40	120.24	125.42
28	l	307	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
31	B	846	WVN	C02-C05-C09	-3.40	117.29	121.47
28	B	817	CLA	CMB-C2B-C3B	3.40	134.54	126.55
36	c	613	II0	C19-C13-C09	-3.40	117.81	124.16
28	c	609	CLA	C4A-NA-C1A	3.40	108.23	106.68
28	A	829	CLA	O2D-CGD-CBD	3.39	117.16	111.23
28	A	816	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
36	k	616	II0	C19-C13-C11	3.39	120.66	114.42
28	i	308	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
31	J	101	WVN	C06-C13-C15	-3.39	118.01	122.64
36	a	318	II0	C19-C13-C09	-3.39	117.83	124.16
36	m	616	II0	C19-C13-C09	-3.39	117.83	124.16
36	O	203	II0	C42-C41-C39	-3.38	116.60	123.52
36	k	615	II0	C31-C33-C35	-3.38	117.10	126.36
31	L	201	WVN	C40-C39-C36	-3.38	116.61	123.52
31	R	201	WVN	C04-C09-C05	-3.38	121.61	124.83
31	R	201	WVN	C39-C36-C32	-3.38	122.54	127.28
37	b	615	IHT	C22-C18-C07	-3.38	117.98	127.00
28	i	306	CLA	CHB-C4A-NA	3.38	129.27	124.40
31	s	207	WVN	C30-C33-C34	-3.37	117.11	126.36
36	k	615	II0	C41-C42-C40	-3.37	116.61	123.52
28	b	608	CLA	C4A-NA-C1A	3.37	108.22	106.68
38	i	319	KC2	CBC-CAC-C3C	-3.37	110.67	127.53
28	a	311	CLA	CAA-C2A-C3A	-3.37	103.89	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	i	310	KC2	CMD-C2D-C3D	3.37	136.30	125.67
36	j	614	II0	C19-C13-C09	-3.37	117.86	124.16
38	i	319	KC2	CMD-C2D-C3D	3.37	136.29	125.67
31	B	848	WVN	C26-C29-C31	-3.37	113.44	123.20
28	A	837	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
28	B	832	CLA	C4A-NA-C1A	3.37	108.22	106.68
38	s	204	KC2	CBC-CAC-C3C	-3.37	110.71	127.53
31	i	316	WVN	C30-C28-C25	-3.36	122.56	127.28
28	A	812	CLA	CMB-C2B-C1B	-3.36	120.30	125.42
36	j	615	II0	C20-C14-C10	-3.36	117.87	124.16
36	k	616	II0	C41-C42-C40	-3.36	116.64	123.52
38	j	611	KC2	C3B-C2B-C1B	-3.36	103.87	107.05
37	n	617	IHT	C20-C15-C12	3.36	120.60	114.42
38	k	613	KC2	CBC-CAC-C3C	-3.36	110.74	127.53
31	B	844	WVN	C40-C37-C34	-3.36	122.57	127.28
38	k	612	KC2	CMD-C2D-C3D	3.36	136.25	125.67
28	B	813	CLA	CMB-C2B-C1B	-3.36	120.31	125.42
31	s	207	WVN	C21-C15-C13	-3.35	120.83	124.48
28	n	607	CLA	CMB-C2B-C1B	-3.35	120.32	125.42
38	g	313	KC2	O2D-CGD-CBD	3.35	117.08	111.23
38	g	313	KC2	CMD-C2D-C3D	3.35	136.23	125.67
36	f	614	II0	C31-C33-C35	-3.35	117.18	126.36
28	h	304	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
28	B	828	CLA	CMB-C2B-C3B	3.35	134.42	126.55
37	j	616	IHT	C19-C10-C09	3.35	120.73	113.60
39	i	301	LMU	O1B-C4'-C3'	3.35	115.73	107.23
31	A	847	WVN	C06-C13-C20	3.35	124.72	115.65
36	m	618	II0	C37-C35-C33	3.34	123.20	118.09
28	b	602	CLA	C1-C2-C3	-3.34	120.72	126.20
30	a	319	LHG	O8-C23-C24	3.34	122.03	111.83
28	a	304	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
38	d	310	KC2	CHB-C4A-NA	3.34	129.41	124.23
28	c	604	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
28	A	803	CLA	CAA-CBA-CGA	-3.34	103.73	113.21
28	i	307	CLA	CMB-C2B-C1B	-3.34	120.34	125.42
28	j	603	CLA	CMB-C2B-C1B	-3.34	120.34	125.42
28	c	612	CLA	CMB-C2B-C1B	-3.34	120.34	125.42
28	g	311	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
36	l	316	II0	C19-C13-C11	3.33	120.55	114.42
37	f	617	IHT	C22-C18-C07	-3.33	118.09	127.00
28	i	302	CLA	C1-C2-C3	-3.33	120.74	126.20
38	k	613	KC2	O2D-CGD-O1D	-3.33	117.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	g	318	II0	C20-C14-C10	-3.33	117.94	124.16
28	j	607	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
38	j	611	KC2	O2D-CGD-CBD	3.33	117.05	111.23
38	i	319	KC2	C2A-C1A-NA	3.33	114.67	109.34
36	l	314	II0	C42-C41-C39	-3.32	116.72	123.52
28	g	309	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
36	m	615	II0	C42-C41-C39	-3.32	116.72	123.52
38	f	611	KC2	CBC-CAC-C3C	-3.32	110.94	127.53
31	A	845	WVN	C04-C09-C05	-3.32	121.66	124.83
38	k	611	KC2	CHB-C4A-NA	3.32	129.37	124.23
31	i	316	WVN	C20-C23-C25	-3.32	121.33	126.23
36	f	616	II0	C20-C14-C12	3.32	120.52	114.42
28	e	603	CLA	CMB-C2B-C1B	-3.31	120.37	125.42
28	s	202	CLA	CMB-C2B-C1B	-3.31	120.38	125.42
28	s	206	CLA	CMB-C2B-C1B	-3.31	120.38	125.42
31	F	204	WVN	C20-C13-C15	-3.31	113.92	121.56
28	B	803	CLA	CAC-C3C-C2C	-3.31	121.48	127.56
36	m	616	II0	C20-C14-C12	3.31	120.51	114.42
38	d	311	KC2	O2D-CGD-O1D	-3.31	117.41	123.85
36	n	615	II0	C20-C14-C12	3.31	120.50	114.42
36	i	314	II0	C19-C13-C09	-3.31	117.98	124.16
28	A	839	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
28	A	829	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
28	K	101	CLA	CMB-C2B-C1B	-3.30	120.39	125.42
36	k	616	II0	C03-C05-C07	3.30	120.84	113.59
36	f	615	II0	C42-C41-C39	-3.30	116.76	123.52
28	B	824	CLA	CMB-C2B-C1B	-3.30	120.39	125.42
28	c	606	CLA	CAA-C2A-C3A	-3.30	104.07	113.00
31	l	315	WVN	C40-C37-C34	-3.30	122.65	127.28
38	i	310	KC2	C3A-C4A-NA	3.30	114.54	110.45
28	b	612	CLA	CHB-C4A-NA	3.30	129.16	124.40
28	A	822	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
31	i	316	WVN	C40-C39-C36	-3.30	116.77	123.52
28	B	812	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
31	F	204	WVN	C21-C15-C13	-3.30	120.88	124.48
28	B	841	CLA	CMB-C2B-C1B	-3.30	120.40	125.42
28	g	303	CLA	CMB-C2B-C1B	-3.30	120.40	125.42
28	A	818	CLA	C4A-NA-C1A	3.30	108.18	106.68
36	m	615	II0	C20-C14-C10	-3.30	117.99	124.16
28	b	609	CLA	CMB-C2B-C1B	-3.30	120.40	125.42
28	k	607	CLA	C4A-NA-C1A	3.30	108.18	106.68
36	m	614	II0	C20-C14-C10	-3.30	118.00	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	l	310	KC2	CHB-C4A-NA	3.29	129.34	124.23
28	A	804	CLA	CMB-C2B-C1B	-3.29	120.41	125.42
28	A	818	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
36	n	618	II0	C41-C42-C40	-3.29	116.78	123.52
28	s	208	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
28	m	603	CLA	CMB-C2B-C1B	-3.29	120.41	125.42
28	B	813	CLA	O2D-CGD-CBD	3.29	116.98	111.23
37	f	617	IHT	C18-C22-C23	-3.29	121.37	126.23
36	c	614	II0	C30-C32-C34	-3.29	113.67	123.20
28	A	852	CLA	C1-C2-C3	-3.29	120.81	126.20
36	c	614	II0	C18-C04-C10	-3.28	104.64	110.52
28	h	308	CLA	C2A-C1A-CHA	3.28	129.56	123.87
28	j	604	CLA	CMB-C2B-C1B	-3.28	120.42	125.42
28	B	829	CLA	O2D-CGD-CBD	3.28	116.97	111.23
31	i	316	WVN	C04-C09-C05	-3.28	121.70	124.83
28	k	603	CLA	CAA-C2A-C3A	-3.28	104.13	113.00
31	l	301	WVN	C26-C29-C31	-3.28	113.69	123.20
28	c	608	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
28	K	101	CLA	CHB-C4A-NA	3.28	129.13	124.40
31	L	206	WVN	C19-C22-C26	-3.28	113.86	119.01
28	e	604	CLA	C1-C2-C3	-3.28	120.83	126.20
31	A	847	WVN	C40-C37-C34	-3.28	122.68	127.28
28	B	801	CLA	O2D-CGD-CBD	3.27	116.95	111.23
28	b	612	CLA	C2A-C1A-CHA	3.27	129.55	123.87
31	L	205	WVN	C40-C39-C36	-3.27	116.82	123.52
31	I	101	WVN	C23-C20-C13	-3.27	118.26	127.00
28	B	801	CLA	CMB-C2B-C3B	3.27	134.24	126.55
28	B	801	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
37	O	204	IHT	C19-C10-C09	3.27	120.56	113.60
38	e	609	KC2	CBC-CAC-C3C	-3.27	111.21	127.53
28	g	310	CLA	CMB-C2B-C1B	-3.27	120.45	125.42
36	k	616	II0	C29-C31-C33	-3.26	113.74	123.20
36	a	315	II0	C42-C41-C39	-3.26	116.84	123.52
36	n	614	II0	C29-C31-C33	-3.26	113.75	123.20
28	a	306	CLA	CMB-C2B-C1B	-3.26	120.45	125.42
36	g	317	II0	C19-C13-C11	3.26	120.42	114.42
38	g	313	KC2	C2A-C1A-NA	3.26	114.56	109.34
28	d	305	CLA	C2C-C1C-NC	3.26	113.41	109.98
36	g	320	II0	C15-C03-C09	-3.26	104.68	110.52
38	m	611	KC2	CBC-CAC-C3C	-3.26	111.24	127.53
31	I	101	WVN	C06-C13-C15	-3.26	118.19	122.64
31	l	315	WVN	C14-C15-C13	-3.25	118.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	606	CLA	CBA-CAA-C2A	-3.25	104.11	113.79
31	L	205	WVN	C39-C36-C32	-3.25	122.72	127.28
31	B	847	WVN	C26-C29-C31	-3.25	113.78	123.20
28	K	101	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
28	m	608	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
28	n	608	CLA	O2D-CGD-CBD	3.25	116.91	111.23
36	b	617	II0	C06-C04-C10	3.25	115.89	109.49
38	g	312	KC2	CMD-C2D-C3D	3.25	135.91	125.67
36	f	618	II0	C11-C13-C09	-3.25	113.75	120.50
36	a	316	II0	C19-C13-C11	3.24	120.39	114.42
28	b	608	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
28	A	811	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
31	K	104	WVN	C26-C29-C31	-3.24	113.80	123.20
31	l	315	WVN	C04-C09-C05	-3.24	121.73	124.83
37	b	615	IHT	C19-C10-C09	3.24	120.51	113.60
28	l	303	CLA	C1-C2-C3	-3.24	120.89	126.20
38	n	611	KC2	CBC-CAC-C3C	-3.23	111.36	127.53
31	L	206	WVN	C30-C33-C34	3.23	135.23	126.36
28	B	837	CLA	C1-C2-C3	-3.23	120.90	126.20
36	i	315	II0	C19-C13-C09	-3.23	118.11	124.16
28	c	605	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
36	e	614	II0	C32-C34-C36	-3.23	117.50	126.36
28	f	608	CLA	C4A-NA-C1A	3.23	108.15	106.68
28	a	311	CLA	CMB-C2B-C1B	-3.23	120.50	125.42
28	l	306	CLA	CHB-C4A-NA	3.23	129.06	124.40
28	B	837	CLA	CMB-C2B-C1B	-3.23	120.50	125.42
28	A	817	CLA	C3B-C4B-NB	-3.23	107.65	110.53
36	n	614	II0	C05-C03-C09	3.23	115.84	109.49
38	s	204	KC2	C2A-C1A-NA	3.22	114.51	109.34
28	B	813	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
28	A	825	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
38	s	204	KC2	CHB-C4A-NA	3.22	129.22	124.23
31	F	203	WVN	C23-C20-C13	-3.22	118.40	127.00
28	A	828	CLA	CMB-C2B-C1B	-3.22	120.52	125.42
38	n	611	KC2	C2A-C1A-NA	3.22	114.50	109.34
28	A	831	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
38	l	310	KC2	CBC-CAC-C3C	-3.22	111.46	127.53
36	a	315	II0	C20-C14-C10	-3.21	118.15	124.16
36	i	313	II0	C19-C13-C09	-3.21	118.16	124.16
38	j	611	KC2	CBC-CAC-C3C	-3.21	111.48	127.53
36	i	313	II0	C20-C14-C12	3.21	120.32	114.42
28	B	803	CLA	CBC-CAC-C3C	3.21	121.12	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	k	618	IHT	C41-C40-C37	-3.21	116.95	123.52
36	g	320	II0	C20-C14-C10	-3.21	118.16	124.16
28	A	854	CLA	C4-C3-C5	3.21	120.79	115.23
28	A	854	CLA	C4-C3-C2	-3.20	115.40	123.63
28	B	809	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
28	m	612	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
28	g	304	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
28	A	818	CLA	CMC-C2C-C1C	-3.20	120.03	125.03
36	d	316	II0	C20-C14-C10	-3.20	118.17	124.16
28	B	828	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
28	a	304	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
28	B	827	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
38	e	609	KC2	O2D-CGD-CBD	3.20	116.82	111.23
36	l	312	II0	C20-C14-C10	-3.20	118.18	124.16
28	O	201	CLA	C1-C2-C3	-3.20	120.96	126.20
28	R	203	CLA	CMB-C2B-C3B	3.20	134.07	126.55
36	m	618	II0	C20-C14-C10	-3.20	118.19	124.16
36	h	312	II0	C20-C14-C10	-3.19	118.19	124.16
28	B	814	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
31	B	848	WVN	C24-C22-C26	-3.19	117.65	122.82
28	A	802	CLA	CAA-CBA-CGA	-3.19	104.15	113.21
36	l	314	II0	C19-C13-C09	-3.19	118.20	124.16
28	g	322	CLA	CAC-C3C-C4C	3.19	128.94	124.79
36	f	618	II0	C20-C14-C12	3.18	120.28	114.42
31	A	846	WVN	C35-C32-C36	-3.18	117.66	122.82
36	m	618	II0	C32-C34-C36	-3.18	117.64	126.36
38	d	310	KC2	C2A-C1A-NA	3.18	114.44	109.34
36	j	614	II0	C20-C14-C12	3.18	120.27	114.42
28	g	308	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
28	m	609	CLA	CMB-C2B-C3B	3.18	134.03	126.55
38	k	611	KC2	C3B-C2B-C1B	-3.18	104.04	107.05
28	J	103	CLA	CMB-C2B-C1B	-3.18	120.58	125.42
31	L	205	WVN	C01-C02-C11	-3.18	109.17	112.83
30	A	844	LHG	O8-C23-C24	3.17	120.79	111.15
28	j	608	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
32	A	850	LMT	O5B-C5B-C4B	3.17	115.41	109.70
28	k	607	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
31	B	848	WVN	C06-C13-C15	-3.17	118.31	122.64
28	A	832	CLA	CAA-CBA-CGA	-3.17	104.21	113.21
38	l	310	KC2	C3B-C2B-C1B	-3.17	104.05	107.05
28	Q	303	CLA	CHB-C1B-NB	3.17	128.80	124.05
28	O	206	CLA	CMB-C2B-C1B	-3.17	120.59	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	848	WVN	C39-C36-C32	-3.17	122.84	127.28
36	J	104	II0	C19-C13-C11	3.17	120.24	114.42
28	k	603	CLA	CMB-C2B-C1B	-3.17	120.60	125.42
36	k	615	II0	C20-C14-C12	3.17	120.24	114.42
28	A	830	CLA	O2D-CGD-CBD	3.17	116.76	111.23
31	s	205	WVN	C20-C23-C25	-3.17	121.55	126.23
31	L	206	WVN	C01-C02-C11	-3.17	109.19	112.83
38	k	612	KC2	CAC-C3C-C4C	3.16	138.38	124.39
37	g	319	IHT	C27-C30-C32	3.16	132.37	123.20
28	A	854	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
28	n	602	CLA	CMB-C2B-C3B	3.16	133.99	126.55
31	A	847	WVN	C06-C13-C15	-3.16	118.32	122.64
31	A	845	WVN	C40-C37-C34	-3.16	122.84	127.28
28	O	206	CLA	CAA-C2A-C1A	3.16	122.33	111.97
36	k	616	II0	C20-C14-C10	-3.16	118.25	124.16
37	g	319	IHT	C18-C07-C10	-3.16	114.28	121.56
28	B	833	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
31	B	846	WVN	C29-C26-C22	-3.16	122.85	127.28
38	f	611	KC2	C2A-C1A-NA	3.16	114.40	109.34
36	g	317	II0	C19-C13-C09	-3.16	118.25	124.16
28	c	603	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
28	B	806	CLA	O2D-CGD-CBD	3.16	116.75	111.23
28	A	826	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
28	O	202	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
28	j	612	CLA	C1D-ND-C4D	-3.16	104.10	106.31
28	B	808	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
28	O	201	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
36	g	320	II0	C42-C41-C39	-3.16	117.06	123.52
28	k	614	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
28	h	307	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
36	i	320	II0	C41-C42-C40	-3.15	117.06	123.52
28	g	308	CLA	CHB-C4A-NA	3.15	128.95	124.40
28	k	614	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
31	L	205	WVN	C20-C23-C25	-3.15	121.57	126.23
35	L	209	LMG	C3-C4-C5	3.15	115.95	110.23
31	h	309	WVN	C23-C20-C13	-3.15	118.58	127.00
38	e	609	KC2	C3B-C2B-C1B	-3.15	104.06	107.05
38	g	313	KC2	CHB-C4A-NA	3.15	129.12	124.23
28	k	601	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
38	k	612	KC2	C2A-C1A-NA	3.15	114.39	109.34
28	A	819	CLA	CAA-CBA-CGA	-3.15	104.09	112.49
37	c	616	IHT	C31-C34-C35	-3.15	117.73	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	f	614	II0	C32-C34-C36	-3.15	117.73	126.36
31	l	315	WVN	C12-C14-C15	-3.15	108.44	114.06
36	g	317	II0	C29-C31-C33	-3.15	114.08	123.20
37	O	204	IHT	C20-C15-C12	3.15	120.21	114.42
28	B	826	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
28	B	826	CLA	CMB-C2B-C3B	3.15	133.95	126.55
28	k	602	CLA	CMB-C2B-C1B	-3.14	120.63	125.42
28	h	301	CLA	C3B-C4B-NB	-3.14	107.72	110.53
38	k	613	KC2	CHB-C4A-NA	3.14	129.10	124.23
36	l	313	II0	C20-C14-C12	3.14	120.20	114.42
38	d	310	KC2	CBC-CAC-C3C	-3.14	111.83	127.53
28	h	305	CLA	CHB-C4A-NA	3.14	128.93	124.40
28	e	603	CLA	C4A-NA-C1A	3.14	108.11	106.68
30	m	619	LHG	O7-C7-C8	3.14	118.28	111.48
36	e	614	II0	C20-C14-C10	-3.14	118.29	124.16
36	i	317	II0	C18-C04-C10	-3.14	104.89	110.52
31	K	102	WVN	C14-C15-C13	-3.14	118.46	122.70
37	f	617	IHT	C30-C32-C33	-3.14	117.76	126.36
28	b	609	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
36	g	318	II0	C30-C32-C34	-3.14	114.11	123.20
28	j	602	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
28	B	804	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
38	e	609	KC2	O2D-CGD-O1D	-3.13	117.75	123.85
28	i	306	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
28	h	305	CLA	C4A-NA-C1A	3.13	108.11	106.68
28	d	307	CLA	CHB-C4A-NA	3.13	128.92	124.40
31	l	315	WVN	C19-C22-C26	3.13	123.94	119.01
28	g	303	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
38	k	613	KC2	C2A-C1A-NA	3.13	114.36	109.34
28	s	206	CLA	C11-C12-C13	-3.13	105.56	115.97
28	O	201	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
36	k	619	II0	C31-C29-C25	-3.13	117.86	126.61
28	B	836	CLA	CAC-C3C-C2C	-3.13	121.81	127.56
28	A	836	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
28	B	817	CLA	CHB-C1B-NB	3.13	128.74	124.05
28	e	606	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
36	h	312	II0	C20-C14-C12	3.13	120.17	114.42
36	b	613	II0	C20-C14-C12	3.13	120.17	114.42
36	b	617	II0	C30-C32-C34	-3.13	114.14	123.20
38	k	612	KC2	O2D-CGD-O1D	-3.13	117.76	123.85
36	l	316	II0	C41-C42-C40	-3.12	117.13	123.52
28	A	855	CLA	CHB-C4A-NA	3.12	128.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	J	104	II0	C42-C41-C39	-3.12	117.13	123.52
31	F	204	WVN	C04-C09-C05	-3.12	121.85	124.83
28	B	823	CLA	CMB-C2B-C3B	3.12	133.89	126.55
28	B	821	CLA	C11-C10-C8	-3.12	105.60	115.97
30	j	617	LHG	O8-C23-C24	3.12	121.34	111.83
28	B	821	CLA	O2D-CGD-CBD	3.12	116.68	111.23
36	f	615	II0	C38-C36-C34	3.11	122.85	118.09
36	d	316	II0	C19-C13-C11	3.11	120.15	114.42
28	h	303	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
36	g	320	II0	C06-C04-C10	3.11	115.62	109.49
36	n	615	II0	C20-C14-C10	-3.11	118.34	124.16
38	m	611	KC2	C3B-C2B-C1B	-3.11	104.10	107.05
38	g	312	KC2	C3B-C2B-C1B	-3.11	104.11	107.05
28	m	604	CLA	CHB-C4A-NA	3.11	128.88	124.40
28	B	812	CLA	CMB-C2B-C1B	-3.11	120.69	125.42
36	d	314	II0	C20-C14-C10	-3.11	118.35	124.16
28	m	613	CLA	CMC-C2C-C1C	-3.10	120.18	125.03
28	d	312	CLA	O2D-CGD-CBD	3.10	116.66	111.23
28	d	309	CLA	CAA-C2A-C3A	-3.10	109.11	116.23
38	e	609	KC2	CHB-C4A-NA	3.10	129.04	124.23
31	R	202	WVN	C30-C28-C25	-3.10	122.93	127.28
28	s	202	CLA	CAA-C2A-C3A	-3.10	104.61	113.00
31	F	203	WVN	C01-C02-C11	-3.10	109.26	112.83
28	A	803	CLA	CHB-C4A-NA	3.10	128.87	124.40
38	n	611	KC2	C3B-C2B-C1B	-3.10	104.12	107.05
28	A	841	CLA	O2D-CGD-CBD	3.10	116.64	111.23
36	a	315	II0	C42-C40-C36	-3.10	122.94	127.28
31	B	848	WVN	C08-C01-C02	-3.09	104.86	109.55
28	A	804	CLA	CHB-C4A-NA	3.09	128.87	124.40
30	b	620	LHG	C5-O7-C7	-3.09	110.39	117.80
38	k	611	KC2	CBC-CAC-C3C	-3.09	112.07	127.53
28	A	834	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
31	F	204	WVN	C29-C26-C22	-3.09	122.94	127.28
36	k	615	II0	C20-C14-C10	-3.09	118.38	124.16
38	k	612	KC2	C3B-C2B-C1B	-3.09	104.12	107.05
37	m	617	IHT	C31-C34-C35	-3.09	117.89	126.36
30	k	620	LHG	O8-C23-C24	3.09	121.25	111.83
38	c	610	KC2	C3B-C2B-C1B	-3.09	104.12	107.05
28	e	607	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
36	k	619	II0	C06-C04-C10	3.09	115.57	109.49
36	f	615	II0	C31-C33-C35	-3.09	117.90	126.36
28	b	601	CLA	O2D-CGD-CBD	3.08	116.62	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	e	615	WVN	C03-C04-C09	-3.08	106.89	112.07
36	j	614	II0	C06-C04-C10	3.08	115.56	109.49
28	B	817	CLA	C3B-C4B-NB	-3.08	107.78	110.53
28	j	608	CLA	CHB-C4A-NA	3.08	128.85	124.40
28	B	804	CLA	CHB-C4A-NA	3.08	128.85	124.40
31	A	848	WVN	C20-C13-C15	-3.08	114.46	121.56
38	g	314	KC2	C3B-C2B-C1B	-3.08	104.13	107.05
28	L	202	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
28	h	313	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
31	l	301	WVN	C06-C13-C15	-3.08	118.43	122.64
31	B	848	WVN	C01-C02-C11	-3.08	109.29	112.83
38	k	612	KC2	CHB-C4A-NA	3.08	129.00	124.23
28	B	830	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
31	L	205	WVN	C04-C09-C05	-3.08	121.89	124.83
28	l	308	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
28	a	303	CLA	CMB-C2B-C1B	-3.07	120.74	125.42
28	d	308	CLA	CMB-C2B-C1B	-3.07	120.74	125.42
37	a	317	IHT	C30-C32-C33	-3.07	117.94	126.36
28	j	612	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
28	h	305	CLA	C1-C2-C3	-3.07	121.16	126.20
31	F	204	WVN	C33-C34-C37	3.07	123.84	119.01
28	A	826	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
30	m	619	LHG	C5-O7-C7	-3.07	110.45	117.80
28	i	305	CLA	C1-C2-C3	-3.07	121.17	126.20
36	m	616	II0	C31-C33-C35	-3.07	117.95	126.36
28	j	605	CLA	C2A-C1A-CHA	3.07	129.19	123.87
28	b	612	CLA	C3B-C4B-NB	-3.07	107.79	110.53
28	A	854	CLA	O2A-CGA-O1A	-3.07	115.96	123.63
37	c	616	IHT	C31-C29-C26	-3.07	118.03	126.61
28	A	807	CLA	CHB-C4A-NA	3.06	128.82	124.40
28	e	608	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
28	A	823	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
28	m	602	CLA	C1-C2-C3	-3.06	121.18	126.20
37	a	317	IHT	C22-C18-C07	-3.06	118.82	127.00
28	f	609	CLA	CMB-C2B-C3B	3.06	133.75	126.55
28	k	604	CLA	CHB-C4A-NA	3.06	128.82	124.40
36	f	616	II0	C31-C29-C25	-3.06	118.05	126.61
28	b	605	CLA	CHB-C4A-NA	3.06	128.82	124.40
31	s	207	WVN	C23-C20-C13	-3.06	118.82	127.00
28	d	302	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
28	d	302	CLA	C3B-C4B-NB	-3.06	107.80	110.53
28	O	206	CLA	CHB-C4A-NA	3.06	128.82	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	611	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
28	B	840	CLA	CMB-C2B-C1B	-3.06	120.77	125.42
28	g	311	CLA	C6-C5-C3	-3.05	106.03	113.47
37	j	616	IHT	C22-C18-C07	-3.05	118.84	127.00
28	b	606	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
36	c	615	II0	C42-C41-C39	-3.05	117.27	123.52
35	L	209	LMG	O8-C28-C29	3.05	121.14	111.83
38	d	310	KC2	C3B-C2B-C1B	-3.05	104.16	107.05
36	e	613	II0	C05-C03-C09	3.05	115.50	109.49
28	d	301	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
37	m	617	IHT	C19-C10-C09	3.05	120.09	113.60
28	B	829	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
28	A	836	CLA	CMB-C2B-C1B	-3.05	120.78	125.42
31	L	206	WVN	C33-C34-C37	-3.05	114.22	119.01
36	b	613	II0	C05-C03-C09	3.04	115.49	109.49
28	B	822	CLA	CMB-C2B-C1B	-3.04	120.78	125.42
36	d	316	II0	C05-C03-C09	3.04	115.48	109.49
28	A	806	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
28	i	312	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
28	k	609	CLA	C1-C2-C3	-3.04	121.21	126.20
28	h	302	CLA	CMB-C2B-C3B	3.04	133.70	126.55
28	j	610	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
28	f	610	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
38	g	314	KC2	CHB-C4A-NA	3.04	128.94	124.23
28	a	309	CLA	CMB-C2B-C1B	-3.04	120.79	125.42
28	a	309	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
36	k	619	II0	C16-C03-C09	-3.04	105.08	110.52
36	d	315	II0	C19-C13-C11	3.04	120.00	114.42
28	b	607	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
36	i	315	II0	C20-C14-C10	-3.04	118.48	124.16
28	g	307	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
37	a	317	IHT	C29-C31-C34	-3.03	114.41	123.20
28	A	824	CLA	C2A-C1A-CHA	3.03	129.13	123.87
36	i	320	II0	C32-C34-C36	-3.03	118.05	126.36
28	h	303	CLA	C3B-C4B-NB	-3.03	107.82	110.53
28	B	821	CLA	C11-C12-C13	-3.03	105.89	115.97
28	e	601	CLA	CHB-C4A-NA	3.03	128.78	124.40
28	Q	303	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
28	K	103	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
28	j	601	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
38	i	319	KC2	C3B-C2B-C1B	-3.03	104.18	107.05
28	j	609	CLA	O2D-CGD-O1D	-3.03	117.95	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	607	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
28	e	602	CLA	CAA-CBA-CGA	-3.03	104.61	113.21
28	B	816	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
36	d	315	II0	C19-C13-C09	-3.03	118.50	124.16
36	f	616	II0	C41-C42-C40	-3.03	117.32	123.52
28	a	304	CLA	CHB-C4A-NA	3.03	128.77	124.40
31	l	315	WVN	C30-C28-C25	-3.03	123.03	127.28
28	A	809	CLA	CHB-C4A-NA	3.03	128.77	124.40
36	i	317	II0	C11-C13-C09	-3.03	114.20	120.50
31	A	846	WVN	C23-C20-C13	-3.02	118.92	127.00
31	K	104	WVN	C24-C22-C19	3.02	122.71	118.09
28	L	207	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
31	L	206	WVN	C28-C30-C33	3.02	131.96	123.20
36	i	317	II0	C06-C04-C10	3.02	115.44	109.49
31	B	844	WVN	C39-C36-C32	-3.02	123.04	127.28
36	m	614	II0	C41-C42-C40	-3.02	117.34	123.52
38	n	612	KC2	CHB-C4A-NA	3.02	128.91	124.23
28	f	601	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
28	n	608	CLA	C3B-C4B-NB	-3.02	107.83	110.53
36	j	614	II0	C18-C04-C10	-3.02	105.11	110.52
28	A	810	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
36	m	618	II0	C20-C14-C12	3.01	119.96	114.42
28	j	604	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
28	g	315	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
36	j	614	II0	C20-C14-C10	-3.01	118.53	124.16
28	m	612	CLA	CAA-C2A-C3A	-3.01	104.86	113.00
36	m	615	II0	C19-C13-C09	-3.01	118.53	124.16
28	B	813	CLA	CHB-C4A-NA	3.01	128.75	124.40
28	A	819	CLA	CHB-C4A-NA	3.01	128.75	124.40
36	l	316	II0	C19-C13-C09	-3.01	118.53	124.16
38	i	310	KC2	C1D-CHD-C4C	-3.01	119.17	126.25
36	e	616	II0	C19-C13-C11	3.01	119.95	114.42
28	i	303	CLA	CMB-C2B-C3B	3.01	133.62	126.55
36	h	310	II0	C31-C29-C25	-3.01	118.20	126.61
28	A	807	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
36	a	314	II0	C20-C14-C10	-3.00	118.55	124.16
28	A	833	CLA	CHB-C4A-NA	3.00	128.73	124.40
36	b	613	II0	C32-C34-C36	-3.00	118.13	126.36
28	A	824	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
31	L	201	WVN	C26-C29-C31	-3.00	114.51	123.20
37	c	616	IHT	C30-C32-C33	-3.00	118.14	126.36
36	d	315	II0	C20-C14-C12	3.00	119.94	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	316	II0	C29-C31-C33	-3.00	114.51	123.20
31	L	201	WVN	C21-C15-C13	-3.00	121.21	124.48
36	f	615	II0	C20-C14-C12	3.00	119.93	114.42
28	A	824	CLA	CMB-C2B-C1B	-3.00	120.86	125.42
37	g	319	IHT	C02-C07-C10	-3.00	118.54	122.64
37	j	616	IHT	C20-C15-C12	3.00	119.93	114.42
28	Q	302	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
36	f	615	II0	C30-C32-C34	-3.00	114.52	123.20
28	d	307	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
36	m	614	II0	C31-C33-C35	-2.99	118.15	126.36
28	B	814	CLA	CMB-C2B-C3B	2.99	133.59	126.55
38	s	201	KC2	CMD-C2D-C1D	-2.99	120.86	125.42
28	k	608	CLA	O2D-CGD-CBD	2.99	116.46	111.23
38	m	611	KC2	C2A-C1A-NA	2.99	114.13	109.34
28	A	855	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
28	m	603	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
28	A	815	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
38	f	611	KC2	CAB-C3B-C2B	2.99	138.14	128.43
28	B	805	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
28	A	814	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
28	n	607	CLA	O2A-CGA-O1A	-2.99	116.16	123.63
31	h	309	WVN	C11-C19-C22	-2.98	119.90	126.32
28	j	609	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
28	B	825	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
38	n	612	KC2	C3B-C2B-C1B	-2.98	104.22	107.05
28	b	603	CLA	CMB-C2B-C3B	2.98	133.56	126.55
28	i	311	CLA	C4A-NA-C1A	-2.98	105.32	106.68
36	i	315	II0	C05-C03-C09	2.98	115.36	109.49
28	F	202	CLA	CHB-C4A-NA	2.98	128.70	124.40
31	K	102	WVN	C21-C15-C14	2.98	119.95	113.60
31	B	845	WVN	C02-C05-C09	-2.98	117.80	121.47
35	L	209	LMG	C8-O7-C10	-2.98	110.67	117.80
28	a	304	CLA	CAA-CBA-CGA	-2.98	104.75	113.21
28	A	841	CLA	CAA-C2A-C3A	-2.98	104.95	113.00
30	b	619	LHG	O7-C7-O9	-2.98	116.74	123.70
28	A	803	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
28	B	815	CLA	C3B-C4B-NB	-2.98	107.87	110.53
28	i	305	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
31	I	101	WVN	C28-C30-C33	-2.97	114.58	123.20
28	f	607	CLA	C4-C3-C5	2.97	120.39	115.23
36	c	617	II0	C19-C13-C09	-2.97	118.60	124.16
35	F	205	LMG	C7-O1-C1	-2.97	107.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	821	CLA	CMB-C2B-C1B	-2.97	120.90	125.42
28	s	203	CLA	O2D-CGD-CBD	2.97	116.42	111.23
31	l	315	WVN	C07-C01-C02	2.97	114.04	109.55
36	g	317	II0	C22-C24-C26	-2.97	166.16	176.23
28	n	607	CLA	CMB-C2B-C3B	2.96	133.52	126.55
31	R	201	WVN	C30-C33-C34	-2.96	118.23	126.36
28	g	303	CLA	CMB-C2B-C3B	2.96	133.52	126.55
28	B	834	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
28	a	311	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
28	A	807	CLA	CMB-C2B-C1B	-2.96	120.91	125.42
28	e	608	CLA	CHB-C4A-NA	2.96	128.67	124.40
36	k	615	II0	C30-C32-C34	-2.96	114.63	123.20
31	l	315	WVN	C10-C12-C14	-2.96	104.78	111.28
36	a	315	II0	C34-C36-C40	-2.96	114.36	119.01
28	h	313	CLA	CMB-C2B-C1B	-2.96	120.92	125.42
28	B	836	CLA	CBC-CAC-C3C	2.96	120.43	112.42
28	m	609	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
28	A	831	CLA	C1-C2-C3	-2.95	121.36	126.20
28	k	605	CLA	CBC-CAC-C3C	2.95	120.43	112.42
37	b	616	IHT	C36-C33-C37	-2.95	118.03	122.82
36	c	613	II0	C42-C41-C39	-2.95	117.47	123.52
28	B	839	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
28	B	811	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
36	b	617	II0	C19-C13-C11	2.95	119.85	114.42
28	a	312	CLA	CHB-C4A-NA	2.95	128.66	124.40
28	m	613	CLA	CBC-CAC-C3C	2.95	120.42	112.42
38	i	310	KC2	O2D-CGD-CBD	2.95	116.39	111.23
28	k	607	CLA	CBC-CAC-C3C	-2.95	104.42	112.42
28	c	602	CLA	CMB-C2B-C1B	-2.95	120.92	125.42
36	a	318	II0	C18-C04-C17	-2.95	100.18	108.63
36	e	612	II0	C42-C41-C39	-2.95	117.48	123.52
28	m	602	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
36	a	316	II0	C30-C32-C34	-2.95	114.66	123.20
28	m	612	CLA	CHB-C4A-NA	2.95	128.65	124.40
28	O	206	CLA	C2A-C1A-CHA	2.95	128.98	123.87
28	f	607	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
31	K	102	WVN	C39-C40-C37	-2.95	117.49	123.52
31	h	309	WVN	C07-C01-C02	2.95	114.01	109.55
36	n	616	II0	C42-C41-C39	-2.95	117.49	123.52
28	h	308	CLA	CAA-C2A-C1A	2.95	121.63	111.97
36	i	314	II0	C38-C36-C34	2.95	122.59	118.09
28	f	606	CLA	O2D-CGD-O1D	-2.95	118.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	611	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
28	h	304	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
36	f	615	II0	C20-C14-C10	-2.94	118.66	124.16
28	b	605	CLA	C3B-C4B-NB	-2.94	107.90	110.53
35	n	620	LMG	O7-C10-C11	2.94	117.84	111.48
36	d	313	II0	C42-C41-C39	-2.94	117.50	123.52
31	K	102	WVN	C04-C09-C05	-2.94	122.02	124.83
36	O	203	II0	C19-C13-C09	-2.94	118.66	124.16
28	n	601	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
31	F	203	WVN	C14-C15-C13	-2.94	118.73	122.70
28	l	309	CLA	CHB-C4A-NA	2.94	128.64	124.40
28	f	612	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
31	B	847	WVN	C28-C30-C33	-2.94	114.69	123.20
28	s	202	CLA	C4A-NA-C1A	2.94	108.02	106.68
31	l	301	WVN	C20-C23-C25	-2.94	121.89	126.23
36	n	618	II0	C03-C05-C07	-2.94	107.15	113.59
28	f	604	CLA	CMB-C2B-C3B	2.93	133.45	126.55
28	A	801	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	e	616	II0	C32-C34-C36	-2.93	118.32	126.36
28	g	302	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
30	f	619	LHG	C5-O7-C7	-2.93	110.78	117.80
36	J	104	II0	C15-C03-C09	-2.93	105.27	110.52
28	B	819	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
28	B	804	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
30	c	620	LHG	C5-O7-C7	-2.93	110.79	117.80
28	m	613	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
28	b	604	CLA	C3B-C4B-NB	-2.93	107.92	110.53
36	m	614	II0	C19-C13-C09	-2.93	118.69	124.16
28	e	603	CLA	CHB-C4A-NA	2.93	128.62	124.40
28	j	606	CLA	CHB-C4A-NA	2.93	128.62	124.40
28	A	812	CLA	CMB-C2B-C3B	2.93	133.44	126.55
38	f	611	KC2	C3B-C2B-C1B	-2.93	104.28	107.05
28	n	604	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
36	i	320	II0	C20-C14-C10	-2.92	118.69	124.16
28	B	818	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
36	a	314	II0	C20-C14-C12	2.92	119.80	114.42
36	m	616	II0	C20-C14-C10	-2.92	118.69	124.16
31	A	847	WVN	C38-C34-C33	2.92	122.55	118.09
36	a	315	II0	C31-C29-C25	-2.92	118.44	126.61
38	i	310	KC2	C2A-C1A-NA	2.92	114.02	109.34
28	c	612	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	m	604	CLA	O2D-CGD-O1D	-2.92	118.16	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	309	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
38	f	611	KC2	O2D-CGD-O1D	-2.92	118.17	123.85
38	n	611	KC2	O2D-CGD-O1D	-2.92	118.17	123.85
28	F	202	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
36	n	614	II0	C06-C04-C10	2.92	115.24	109.49
28	A	825	CLA	CMB-C2B-C1B	-2.92	120.98	125.42
28	i	311	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
28	h	304	CLA	C2A-C1A-CHA	2.92	128.93	123.87
28	B	805	CLA	O1D-CGD-CBD	2.92	130.27	124.52
36	i	317	II0	C05-C03-C09	2.91	115.23	109.49
28	b	610	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
28	R	203	CLA	CHB-C4A-NA	2.91	128.61	124.40
28	n	602	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
28	k	609	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
32	A	850	LMT	C1B-O5B-C5B	2.91	119.40	113.72
28	B	826	CLA	C1-C2-C3	-2.91	121.43	126.20
36	a	318	II0	C32-C30-C26	2.91	134.76	126.61
36	l	316	II0	C42-C40-C36	-2.91	123.20	127.28
28	j	602	CLA	CMB-C2B-C3B	2.91	133.39	126.55
38	s	201	KC2	O2D-CGD-O1D	-2.91	118.18	123.85
28	b	601	CLA	C4-C3-C5	-2.91	112.70	116.13
31	i	316	WVN	C29-C31-C32	-2.91	118.39	126.36
31	F	203	WVN	C39-C36-C32	-2.91	123.20	127.28
28	a	310	CLA	CHB-C4A-NA	2.91	128.60	124.40
28	K	101	CLA	CMB-C2B-C3B	2.91	133.38	126.55
36	g	316	II0	C38-C36-C34	2.91	122.53	118.09
31	A	845	WVN	C39-C40-C37	-2.90	117.58	123.52
28	n	609	CLA	C1-C2-C3	-2.90	121.44	126.20
30	J	106	LHG	O8-C23-C24	2.90	120.69	111.83
30	g	321	LHG	C6-C5-C4	-2.90	105.02	111.78
36	i	320	II0	C20-C14-C12	2.90	119.76	114.42
28	A	805	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
36	c	615	II0	C31-C29-C25	-2.90	118.49	126.61
35	b	621	LMG	C4-C3-C2	2.90	115.93	110.83
28	B	818	CLA	CMB-C2B-C3B	2.90	133.38	126.55
28	A	812	CLA	CHB-C4A-NA	2.90	128.59	124.40
28	n	605	CLA	CHB-C4A-NA	2.90	128.59	124.40
28	i	307	CLA	CMB-C2B-C3B	2.90	133.37	126.55
28	i	308	CLA	CHB-C4A-NA	2.90	128.58	124.40
31	R	202	WVN	C08-C01-C07	2.90	112.09	107.87
36	d	314	II0	C31-C33-C35	-2.90	118.42	126.36
31	L	201	WVN	C10-C06-C13	2.90	114.65	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	201	CLA	C3B-C4B-NB	-2.90	107.94	110.53
28	n	604	CLA	CBA-CAA-C2A	2.89	122.40	113.79
28	k	605	CLA	CHB-C4A-NA	2.89	128.58	124.40
37	m	617	IHT	C20-C15-C11	-2.89	118.75	124.16
28	B	835	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
28	i	312	CLA	CHB-C4A-NA	2.89	128.57	124.40
35	J	105	LMG	O7-C10-C11	2.89	117.74	111.48
28	B	832	CLA	C3B-C4B-NB	-2.89	107.95	110.53
31	I	101	WVN	C39-C40-C37	-2.89	117.60	123.52
36	k	617	II0	C05-C03-C09	2.89	115.19	109.49
36	g	320	II0	C20-C14-C12	2.89	119.74	114.42
28	b	612	CLA	CAA-C2A-C1A	2.89	121.44	111.97
28	l	307	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
35	c	619	LMG	C7-O1-C1	-2.89	107.60	113.80
35	c	619	LMG	O6-C5-C4	2.89	114.90	109.70
28	A	841	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
38	g	313	KC2	C3B-C2B-C1B	-2.89	104.31	107.05
36	d	313	II0	C31-C33-C35	-2.89	118.45	126.36
28	R	203	CLA	C1-C2-C3	-2.89	121.47	126.20
36	j	614	II0	C37-C35-C33	2.88	122.49	118.09
28	f	605	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
28	d	304	CLA	CMB-C2B-C3B	2.88	133.33	126.55
36	m	615	II0	C38-C36-C34	2.88	122.49	118.09
28	a	306	CLA	CMB-C2B-C3B	2.88	133.33	126.55
28	k	610	CLA	CHB-C4A-NA	2.88	128.56	124.40
36	k	621	II0	C30-C32-C34	-2.88	114.85	123.20
31	i	316	WVN	C06-C13-C15	-2.88	118.70	122.64
28	g	308	CLA	O2D-CGD-CBD	2.88	116.27	111.23
28	m	602	CLA	CAA-CBA-CGA	-2.88	105.03	113.21
36	m	615	II0	C41-C42-C40	-2.88	117.63	123.52
28	B	831	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
28	m	606	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
37	j	616	IHT	C30-C32-C33	-2.88	118.47	126.36
28	m	607	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
36	g	317	II0	C30-C32-C34	-2.88	114.86	123.20
37	k	618	IHT	C31-C29-C26	-2.88	118.56	126.61
28	f	613	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
28	c	608	CLA	CAA-CBA-CGA	-2.88	105.04	113.21
31	K	102	WVN	C01-C02-C11	-2.87	109.52	112.83
36	g	316	II0	C29-C31-C33	-2.87	114.87	123.20
28	B	821	CLA	CMB-C2B-C3B	2.87	133.31	126.55
36	k	616	II0	C42-C40-C36	-2.87	123.25	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	315	CLA	CHB-C4A-NA	2.87	128.55	124.40
28	c	609	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
28	A	828	CLA	CMB-C2B-C3B	2.87	133.30	126.55
31	M	101	WVN	C39-C40-C37	-2.87	117.65	123.52
38	l	310	KC2	C1D-CHD-C4C	-2.87	119.50	126.25
36	k	617	II0	C20-C14-C10	-2.87	118.79	124.16
28	A	820	CLA	CHB-C4A-NA	2.87	128.54	124.40
28	a	312	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
28	h	308	CLA	CHB-C4A-NA	2.87	128.54	124.40
28	g	310	CLA	CMB-C2B-C3B	2.86	133.29	126.55
28	A	816	CLA	CBA-CAA-C2A	2.86	122.32	113.79
37	k	618	IHT	C12-C15-C11	-2.86	114.54	120.50
28	n	606	CLA	CHB-C4A-NA	2.86	128.53	124.40
38	g	312	KC2	CHB-C4A-NA	2.86	128.67	124.23
30	e	617	LHG	C6-C5-C4	-2.86	105.11	111.78
31	F	203	WVN	C21-C15-C14	2.86	119.69	113.60
36	b	613	II0	C37-C35-C33	2.86	122.46	118.09
28	B	813	CLA	CMB-C2B-C3B	2.86	133.28	126.55
28	A	827	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
28	l	304	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
29	B	842	PQN	C11-C3-C2	-2.86	119.99	124.89
36	f	616	II0	C31-C33-C35	-2.86	118.53	126.36
28	i	304	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
36	k	615	II0	C19-C13-C09	-2.86	118.82	124.16
28	K	101	CLA	C1-C2-C3	-2.86	121.52	126.20
36	f	618	II0	C05-C03-C09	2.86	115.12	109.49
38	j	611	KC2	O2D-CGD-O1D	-2.86	118.29	123.85
28	B	803	CLA	C3B-C4B-NB	-2.85	107.98	110.53
28	j	603	CLA	CMB-C2B-C3B	2.85	133.26	126.55
28	K	103	CLA	CHB-C4A-NA	2.85	128.52	124.40
28	A	802	CLA	C3B-C4B-NB	-2.85	107.98	110.53
36	j	615	II0	C30-C32-C34	-2.85	114.93	123.20
36	e	613	II0	C20-C14-C12	2.85	119.67	114.42
38	k	613	KC2	C3B-C2B-C1B	-2.85	104.35	107.05
28	O	201	CLA	CMB-C2B-C3B	2.85	133.25	126.55
28	d	312	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
28	A	816	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
28	j	612	CLA	C2B-C1B-NB	2.85	113.28	110.33
31	B	848	WVN	C27-C25-C23	2.85	122.44	118.09
36	e	614	II0	C06-C04-C10	2.85	115.10	109.49
28	n	607	CLA	CHB-C4A-NA	2.85	128.51	124.40
36	n	615	II0	C32-C30-C26	-2.85	118.65	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	838	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
28	s	202	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
28	A	841	CLA	CHB-C4A-NA	2.85	128.51	124.40
36	g	318	II0	C06-C04-C10	2.84	115.09	109.49
36	i	315	II0	C19-C13-C11	2.84	119.65	114.42
28	s	206	CLA	CAA-C2A-C3A	-2.84	105.31	113.00
28	B	815	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
28	a	307	CLA	C3B-C4B-NB	-2.84	107.99	110.53
28	i	302	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
28	B	806	CLA	CHB-C4A-NA	2.84	128.50	124.40
30	J	106	LHG	C5-O7-C7	-2.84	110.99	117.80
28	e	611	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
36	j	614	II0	C41-C42-C40	-2.84	117.71	123.52
28	A	830	CLA	CHB-C4A-NA	2.84	128.50	124.40
28	k	608	CLA	CHB-C4A-NA	2.84	128.50	124.40
28	B	841	CLA	CMB-C2B-C3B	2.84	133.23	126.55
28	a	304	CLA	CMB-C2B-C3B	2.84	133.23	126.55
36	n	615	II0	C06-C04-C10	2.84	115.08	109.49
28	i	312	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
28	f	610	CLA	C3B-C4B-NB	-2.84	108.00	110.53
28	B	841	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	k	603	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	f	609	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
28	A	817	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
28	i	308	CLA	CMB-C2B-C3B	2.84	133.22	126.55
28	j	607	CLA	CHB-C4A-NA	2.84	128.50	124.40
28	e	603	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
36	n	616	II0	C19-C13-C11	2.84	119.64	114.42
37	g	319	IHT	C31-C34-C35	-2.84	118.58	126.36
28	b	603	CLA	CHB-C4A-NA	2.84	128.49	124.40
28	f	601	CLA	CHB-C4A-NA	2.84	128.49	124.40
28	B	811	CLA	CBC-CAC-C3C	2.83	120.11	112.42
28	m	601	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
38	s	204	KC2	C3B-C2B-C1B	-2.83	104.36	107.05
28	e	603	CLA	CMB-C2B-C3B	2.83	133.22	126.55
31	F	204	WVN	C23-C25-C28	2.83	123.47	119.01
28	A	826	CLA	CMB-C2B-C3B	2.83	133.21	126.55
28	l	308	CLA	CMB-C2B-C3B	2.83	133.21	126.55
28	m	604	CLA	CMB-C2B-C3B	2.83	133.21	126.55
28	g	305	CLA	CMB-C2B-C3B	2.83	133.21	126.55
28	n	604	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
28	m	603	CLA	CMB-C2B-C3B	2.83	133.20	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	821	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
36	k	616	II0	C05-C03-C09	2.83	115.06	109.49
36	j	615	II0	C19-C13-C11	2.83	119.62	114.42
37	b	615	IHT	C41-C40-C37	-2.83	117.74	123.52
36	n	618	II0	C32-C30-C26	-2.82	118.71	126.61
28	O	202	CLA	C16-C15-C13	-2.82	106.58	115.97
28	g	304	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
28	A	812	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
36	j	615	II0	C31-C33-C35	-2.82	118.63	126.36
28	i	305	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
31	B	844	WVN	C06-C13-C15	-2.82	118.78	122.64
28	a	308	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
28	B	810	CLA	CHB-C4A-NA	2.82	128.47	124.40
28	L	204	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	c	601	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	g	302	CLA	C3B-C4B-NB	-2.82	108.01	110.53
28	B	810	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	i	309	CLA	C4A-NA-C1A	2.82	107.97	106.68
36	k	617	II0	C19-C13-C11	2.82	119.60	114.42
28	A	804	CLA	CMB-C2B-C3B	2.82	133.18	126.55
36	c	614	II0	C31-C33-C35	-2.82	118.64	126.36
28	k	607	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
37	n	617	IHT	C22-C18-C07	-2.82	119.47	127.00
28	B	834	CLA	C3B-C4B-NB	-2.82	108.02	110.53
28	L	203	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
28	h	308	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
36	i	315	II0	C31-C33-C35	-2.81	118.65	126.36
28	A	837	CLA	C16-C15-C13	-2.81	106.62	115.97
36	n	615	II0	C19-C13-C09	-2.81	118.90	124.16
31	A	847	WVN	C04-C09-C05	-2.81	122.15	124.83
36	g	318	II0	C29-C31-C33	-2.81	115.06	123.20
28	B	807	CLA	O2D-CGD-CBD	2.81	116.14	111.23
31	J	102	WVN	C27-C25-C23	2.81	122.38	118.09
36	O	203	II0	C19-C13-C11	2.81	119.59	114.42
28	B	837	CLA	O2D-CGD-CBD	2.81	116.14	111.23
35	O	205	LMG	O8-C28-C29	2.81	120.39	111.83
31	J	101	WVN	C35-C32-C36	-2.81	118.27	122.82
38	e	609	KC2	C1D-CHD-C4C	-2.81	119.65	126.25
36	h	312	II0	C19-C13-C11	2.81	119.58	114.42
31	B	844	WVN	C30-C28-C25	-2.81	123.34	127.28
28	c	608	CLA	CHB-C4A-NA	2.80	128.45	124.40
31	I	101	WVN	C01-C02-C11	-2.80	109.60	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J	103	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
36	b	617	II0	C20-C14-C10	-2.80	118.92	124.16
28	B	827	CLA	C3B-C4B-NB	-2.80	108.03	110.53
31	h	309	WVN	C06-C13-C15	-2.80	118.81	122.64
28	O	206	CLA	CBA-CAA-C2A	2.80	122.13	113.79
28	A	835	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
31	B	846	WVN	C26-C29-C31	-2.80	115.09	123.20
28	m	613	CLA	CMC-C2C-C3C	2.80	133.72	126.15
28	k	614	CLA	C4A-NA-C1A	2.80	107.96	106.68
28	f	608	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
36	l	313	II0	C38-C36-C40	-2.80	118.28	122.82
28	B	812	CLA	CMB-C2B-C3B	2.80	133.13	126.55
28	g	305	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
28	A	802	CLA	CAA-C2A-C1A	-2.80	102.81	111.97
28	d	305	CLA	CHB-C4A-NA	2.80	128.43	124.40
36	e	616	II0	C06-C04-C10	2.80	115.00	109.49
28	a	305	CLA	CAA-C2A-C3A	-2.80	105.45	113.00
36	a	315	II0	C38-C36-C34	2.79	122.36	118.09
31	B	844	WVN	C23-C20-C13	-2.79	119.53	127.00
36	g	318	II0	C38-C36-C34	2.79	122.36	118.09
36	f	616	II0	C20-C14-C10	-2.79	118.94	124.16
28	l	306	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
28	B	806	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
36	j	615	II0	C19-C13-C09	-2.79	118.94	124.16
28	c	608	CLA	CMA-C3A-C2A	-2.79	103.19	113.98
28	A	832	CLA	CMC-C2C-C1C	-2.79	120.67	125.03
28	d	303	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
28	h	306	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
31	A	848	WVN	C39-C40-C37	-2.79	117.81	123.52
28	A	818	CLA	CMC-C2C-C3C	2.79	133.69	126.15
36	O	203	II0	C32-C34-C36	-2.79	118.72	126.36
36	c	614	II0	C19-C13-C09	-2.79	118.95	124.16
31	J	102	WVN	C21-C15-C13	-2.79	121.44	124.48
36	n	618	II0	C20-C14-C12	2.79	119.55	114.42
38	m	611	KC2	CAB-C3B-C2B	2.79	137.49	128.43
37	n	617	IHT	C19-C10-C09	2.79	119.54	113.60
31	s	205	WVN	C28-C30-C33	-2.79	115.13	123.20
36	m	618	II0	C19-C13-C09	-2.78	118.95	124.16
28	b	606	CLA	C3B-C4B-NB	-2.78	108.04	110.53
28	B	807	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
28	B	820	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
31	M	101	WVN	C30-C33-C34	-2.78	118.73	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	i	304	CLA	C1-C2-C3	-2.78	121.64	126.20
28	A	835	CLA	CHB-C4A-NA	2.78	128.41	124.40
36	l	314	II0	C06-C04-C10	2.78	114.97	109.49
36	l	312	II0	C38-C36-C34	2.78	122.33	118.09
36	j	615	II0	C29-C31-C33	-2.78	115.15	123.20
38	d	311	KC2	CHB-C4A-NA	2.78	128.54	124.23
28	J	103	CLA	CHB-C4A-NA	2.78	128.41	124.40
28	m	608	CLA	CHB-C4A-NA	2.78	128.41	124.40
28	A	819	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
28	n	604	CLA	C1-C2-C3	-2.78	121.65	126.20
36	k	619	II0	C12-C14-C10	-2.78	114.72	120.50
28	g	310	CLA	CHB-C4A-NA	2.78	128.41	124.40
28	A	815	CLA	CHB-C1B-NB	2.78	128.22	124.05
36	b	614	II0	C32-C34-C36	-2.78	118.75	126.36
28	m	607	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
28	b	609	CLA	CMB-C2B-C3B	2.78	133.08	126.55
38	g	314	KC2	C1D-CHD-C4C	-2.77	119.72	126.25
28	d	306	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
28	n	607	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
28	c	612	CLA	CMB-C2B-C3B	2.77	133.07	126.55
28	a	307	CLA	CAC-C3C-C4C	2.77	128.40	124.79
36	l	312	II0	C31-C33-C35	-2.77	118.76	126.36
28	a	310	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
31	F	204	WVN	C26-C29-C31	-2.77	115.17	123.20
28	A	851	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
38	k	611	KC2	CAB-C3B-C2B	2.77	137.44	128.43
28	c	607	CLA	CMB-C2B-C3B	2.77	133.07	126.55
28	h	303	CLA	CHB-C4A-NA	2.77	128.40	124.40
36	i	320	II0	C34-C36-C40	-2.77	114.65	119.01
28	A	813	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
28	A	841	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
28	e	604	CLA	C7-C6-C5	-2.77	105.89	113.26
31	s	205	WVN	C02-C05-C09	-2.77	118.06	121.47
28	f	607	CLA	CAA-CBA-CGA	-2.77	105.35	113.21
36	f	618	II0	C20-C14-C10	-2.77	118.98	124.16
37	b	616	IHT	C20-C15-C12	2.77	119.51	114.42
28	A	822	CLA	CHB-C4A-NA	2.77	128.39	124.40
38	s	204	KC2	CAB-C3B-C2B	2.77	137.43	128.43
36	k	616	II0	C38-C36-C34	2.77	122.31	118.09
31	h	309	WVN	C24-C22-C19	-2.77	113.86	118.09
28	A	816	CLA	CHB-C4A-NA	2.77	128.39	124.40
31	B	848	WVN	C21-C15-C13	-2.77	121.47	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	l	301	WVN	C39-C40-C37	-2.76	117.86	123.52
36	e	612	II0	C06-C04-C10	2.76	114.94	109.49
28	A	828	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
28	a	305	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
28	A	818	CLA	C7-C6-C5	-2.76	105.90	113.26
28	g	311	CLA	CHB-C4A-NA	2.76	128.39	124.40
28	c	601	CLA	C1-C2-C3	-2.76	121.67	126.20
28	a	309	CLA	C1-C2-C3	-2.76	121.67	126.20
36	m	615	II0	C32-C34-C36	-2.76	118.79	126.36
28	A	803	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
36	b	617	II0	C31-C33-C35	-2.76	118.79	126.36
36	a	314	II0	C31-C29-C25	-2.76	118.89	126.61
28	B	810	CLA	CAC-C3C-C4C	2.76	128.38	124.79
28	A	826	CLA	CHB-C4A-NA	2.76	128.38	124.40
28	A	802	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
38	g	312	KC2	C1D-CHD-C4C	-2.76	119.76	126.25
28	n	606	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
28	a	308	CLA	CHB-C4A-NA	2.76	128.38	124.40
36	h	310	II0	C19-C13-C11	2.76	119.49	114.42
38	s	201	KC2	C3B-C2B-C1B	-2.76	104.44	107.05
36	l	314	II0	C31-C29-C25	-2.76	118.89	126.61
38	s	201	KC2	C2A-C3A-C4A	-2.76	104.34	106.41
36	l	316	II0	C20-C14-C12	2.76	119.49	114.42
28	g	303	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
36	e	614	II0	C16-C03-C09	-2.76	105.58	110.52
28	B	815	CLA	CHB-C4A-NA	2.76	128.38	124.40
28	b	612	CLA	CBA-CAA-C2A	-2.76	105.59	113.79
28	f	606	CLA	C3B-C4B-NB	-2.75	108.07	110.53
28	d	301	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
28	k	604	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
28	s	206	CLA	C1-C2-C3	-2.75	121.69	126.20
28	e	607	CLA	C11-C12-C13	-2.75	106.82	115.97
28	h	306	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
28	B	831	CLA	C3B-C4B-NB	-2.75	108.07	110.53
28	g	315	CLA	C1-C2-C3	-2.75	121.69	126.20
28	f	606	CLA	CHB-C4A-NA	2.75	128.37	124.40
36	k	617	II0	C31-C29-C25	-2.75	118.92	126.61
28	b	608	CLA	C11-C12-C13	-2.75	106.83	115.97
28	A	834	CLA	CAA-C2A-C3A	-2.75	105.57	113.00
28	g	302	CLA	CHB-C4A-NA	2.75	128.37	124.40
36	g	317	II0	C20-C14-C12	2.75	119.47	114.42
31	L	206	WVN	C23-C20-C13	-2.75	119.66	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	615	IHT	C20-C15-C12	2.75	119.47	114.42
36	b	617	II0	C31-C29-C25	-2.75	118.93	126.61
28	g	322	CLA	O2D-CGD-CBD	2.75	116.03	111.23
31	l	301	WVN	C08-C01-C02	-2.74	105.39	109.55
28	L	204	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
28	B	824	CLA	CMB-C2B-C3B	2.74	133.00	126.55
36	j	614	II0	C42-C41-C39	-2.74	117.91	123.52
28	m	609	CLA	CHB-C4A-NA	2.74	128.36	124.40
28	B	807	CLA	CBA-CAA-C2A	2.74	121.95	113.79
38	k	613	KC2	O2D-CGD-CBD	2.74	116.02	111.23
28	f	612	CLA	C4-C3-C5	2.74	119.35	116.13
28	j	604	CLA	CMB-C2B-C3B	2.74	133.00	126.55
28	k	604	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
38	n	612	KC2	C1D-CHD-C4C	-2.74	119.80	126.25
31	L	206	WVN	C40-C37-C34	-2.74	123.44	127.28
37	a	317	IHT	C20-C15-C12	2.74	119.46	114.42
36	a	315	II0	C29-C31-C33	-2.74	115.26	123.20
31	M	101	WVN	C06-C13-C15	-2.74	118.89	122.64
28	A	833	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
28	m	603	CLA	C3B-C4B-NB	-2.74	108.09	110.53
28	B	802	CLA	C1-C2-C3	-2.74	121.71	126.20
28	c	602	CLA	C3B-C4B-NB	-2.74	108.09	110.53
36	g	316	II0	C20-C14-C12	2.74	119.45	114.42
28	j	612	CLA	CMB-C2B-C1B	-2.73	121.25	125.42
28	B	804	CLA	CMB-C2B-C3B	2.73	132.98	126.55
38	g	313	KC2	CAB-C3B-C2B	2.73	137.32	128.43
28	s	206	CLA	CMB-C2B-C3B	2.73	132.98	126.55
36	l	316	II0	C32-C30-C26	-2.73	118.97	126.61
28	B	826	CLA	CAA-CBA-CGA	-2.73	105.45	113.21
36	l	312	II0	C29-C31-C33	-2.73	115.29	123.20
36	d	313	II0	C20-C14-C10	-2.73	119.06	124.16
28	A	808	CLA	CHB-C4A-NA	2.73	128.34	124.40
36	h	312	II0	C38-C36-C34	2.73	122.26	118.09
28	k	603	CLA	CMB-C2B-C3B	2.73	132.97	126.55
28	k	606	CLA	C1-C2-C3	-2.73	121.73	126.20
36	i	313	II0	C20-C14-C10	-2.73	119.06	124.16
31	s	205	WVN	C30-C28-C25	-2.73	123.46	127.28
36	n	616	II0	C19-C13-C09	-2.72	119.06	124.16
28	g	303	CLA	CHB-C4A-NA	2.72	128.33	124.40
39	i	301	LMU	C3'-C4'-C5'	-2.72	104.89	110.93
30	b	619	LHG	C5-O7-C7	-2.72	111.28	117.80
37	R	204	IHT	C22-C18-C07	-2.72	119.73	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	838	CLA	CHB-C4A-NA	2.72	128.33	124.40
28	a	308	CLA	O2D-CGD-CBD	2.72	115.99	111.23
28	d	308	CLA	CAA-C2A-C3A	-2.72	109.99	116.23
28	A	825	CLA	CMB-C2B-C3B	2.72	132.95	126.55
28	A	809	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
28	B	808	CLA	O2D-CGD-CBD	2.72	115.98	111.23
28	L	202	CLA	CHB-C4A-NA	2.72	128.32	124.40
36	c	615	II0	C20-C14-C10	-2.72	119.08	124.16
28	A	829	CLA	CMB-C2B-C3B	2.72	132.95	126.55
36	l	314	II0	C32-C34-C36	-2.72	118.91	126.36
28	A	813	CLA	CAA-CBA-CGA	-2.72	105.24	112.49
28	A	838	CLA	CHB-C4A-NA	2.72	128.32	124.40
28	n	609	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
35	F	205	LMG	O1-C1-C2	2.72	112.40	108.27
31	A	848	WVN	C21-C15-C14	2.72	119.39	113.60
28	b	603	CLA	CAA-C2A-C3A	-2.72	105.66	113.00
36	j	614	II0	C30-C32-C34	-2.72	115.33	123.20
29	A	842	PQN	C11-C3-C2	-2.72	120.23	124.89
28	B	811	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
28	J	103	CLA	CMB-C2B-C3B	2.72	132.94	126.55
30	c	618	LHG	O8-C23-C24	2.72	120.11	111.83
38	s	201	KC2	CHD-C1D-C2D	2.71	135.31	127.43
31	A	845	WVN	C02-C05-C09	-2.71	118.13	121.47
28	b	610	CLA	CHB-C4A-NA	2.71	128.32	124.40
28	A	835	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
35	L	209	LMG	O7-C10-O9	-2.71	117.36	123.70
38	d	311	KC2	C3B-C2B-C1B	-2.71	104.48	107.05
28	B	827	CLA	CHB-C4A-NA	2.71	128.31	124.40
28	e	610	CLA	CHB-C4A-NA	2.71	128.31	124.40
28	i	303	CLA	CHB-C4A-NA	2.71	128.31	124.40
36	i	315	II0	C12-C14-C10	-2.71	114.86	120.50
28	h	302	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
28	A	854	CLA	C1-O2A-CGA	2.71	123.21	116.65
28	B	839	CLA	CHB-C4A-NA	2.71	128.31	124.40
28	s	208	CLA	CHB-C4A-NA	2.71	128.31	124.40
28	e	607	CLA	CHB-C4A-NA	2.71	128.31	124.40
28	A	816	CLA	CMB-C2B-C3B	2.71	132.92	126.55
38	d	310	KC2	O2D-CGD-O1D	-2.71	118.58	123.85
28	b	609	CLA	CHB-C4A-NA	2.71	128.31	124.40
36	a	315	II0	C11-C13-C09	-2.71	114.87	120.50
36	i	314	II0	C20-C14-C10	-2.71	119.10	124.16
28	A	852	CLA	CMB-C2B-C3B	2.71	132.92	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	l	303	CLA	C3B-C4B-NB	-2.71	108.11	110.53
36	b	613	II0	C11-C13-C09	-2.71	114.87	120.50
36	g	316	II0	C30-C32-C34	-2.71	115.36	123.20
34	B	843	DGD	O1G-C1A-C2A	2.70	120.08	111.83
28	c	608	CLA	CMB-C2B-C1B	-2.70	121.30	125.42
28	a	312	CLA	C1-C2-C3	-2.70	121.77	126.20
28	a	311	CLA	CMB-C2B-C3B	2.70	132.91	126.55
36	c	615	II0	C29-C31-C33	-2.70	115.37	123.20
28	A	814	CLA	C1-C2-C3	-2.70	122.39	126.76
28	c	602	CLA	CAA-CBA-CGA	-2.70	105.54	113.21
28	m	607	CLA	C3B-C4B-NB	-2.70	108.12	110.53
31	R	201	WVN	C29-C26-C22	-2.70	123.49	127.28
28	b	602	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	c	603	CLA	CMB-C2B-C3B	2.70	132.90	126.55
38	m	611	KC2	O2D-CGD-CBD	2.70	115.95	111.23
28	c	602	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	a	309	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	m	605	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
38	d	310	KC2	CAB-C3B-C2B	2.70	137.21	128.43
31	B	848	WVN	C14-C15-C13	-2.70	119.06	122.70
28	s	203	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
28	a	305	CLA	CHB-C4A-NA	2.70	128.30	124.40
28	B	833	CLA	CHB-C4A-NA	2.70	128.29	124.40
28	K	101	CLA	CAA-C2A-C1A	2.70	120.82	111.97
32	a	320	LMT	C1'-O5'-C5'	2.70	118.99	113.72
28	k	601	CLA	CHB-C4A-NA	2.70	128.29	124.40
28	i	303	CLA	C1-C2-C3	-2.69	122.40	126.76
28	B	833	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
31	s	207	WVN	C29-C26-C22	-2.69	123.50	127.28
31	K	102	WVN	C35-C32-C36	-2.69	118.45	122.82
28	B	824	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
28	A	841	CLA	CAA-CBA-CGA	-2.69	105.56	113.21
28	b	608	CLA	C1-C2-C3	-2.69	121.78	126.20
28	a	307	CLA	CHB-C4A-NA	2.69	128.29	124.40
28	a	306	CLA	O2A-CGA-O1A	-2.69	116.89	123.63
28	l	306	CLA	CHA-C1A-NA	-2.69	120.29	126.39
28	A	830	CLA	CMB-C2B-C3B	2.69	132.88	126.55
36	g	320	II0	C41-C42-C40	-2.69	118.01	123.52
37	m	617	IHT	C22-C18-C07	-2.69	119.81	127.00
28	j	609	CLA	CMB-C2B-C3B	2.69	132.88	126.55
28	a	303	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
35	O	205	LMG	O7-C10-C11	2.69	120.81	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	846	WVN	C02-C05-C09	-2.69	118.16	121.47
28	d	301	CLA	CAA-CBA-CGA	-2.69	105.57	113.21
36	f	616	II0	C12-C14-C10	-2.69	114.91	120.50
32	a	320	LMT	O5'-C5'-C6'	2.69	113.10	106.44
28	A	838	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	k	603	CLA	CHB-C4A-NA	2.69	128.28	124.40
28	A	808	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
31	A	848	WVN	C24-C22-C26	-2.68	118.47	122.82
37	a	317	IHT	C19-C10-C09	2.68	119.31	113.60
31	h	309	WVN	C14-C15-C13	-2.68	119.08	122.70
36	d	313	II0	C31-C29-C25	-2.68	119.11	126.61
28	B	837	CLA	CMB-C2B-C3B	2.68	132.86	126.55
28	A	817	CLA	C1-C2-C3	-2.68	121.80	126.20
28	g	322	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
28	A	810	CLA	C1-C2-C3	-2.68	121.81	126.20
28	B	811	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
36	e	613	II0	C29-C31-C33	-2.68	115.44	123.20
28	A	811	CLA	C3B-C4B-NB	-2.68	108.14	110.53
28	l	307	CLA	CAA-CBA-CGA	-2.68	105.60	113.21
30	g	321	LHG	O4-P-O5	2.68	124.90	112.44
38	l	310	KC2	CAB-C3B-C2B	2.68	137.13	128.43
28	A	852	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
31	A	845	WVN	C20-C23-C25	-2.68	122.28	126.23
28	n	609	CLA	CHB-C4A-NA	2.68	128.26	124.40
28	e	610	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
28	d	306	CLA	CHB-C4A-NA	2.67	128.26	124.40
28	j	609	CLA	CHB-C4A-NA	2.67	128.26	124.40
28	d	306	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
28	c	611	CLA	CBC-CAC-C3C	2.67	119.67	112.42
31	l	301	WVN	C24-C22-C19	2.67	122.17	118.09
36	k	616	II0	C11-C13-C09	-2.67	114.94	120.50
28	d	303	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
36	k	617	II0	C42-C41-C39	-2.67	118.05	123.52
28	l	303	CLA	CAA-CBA-CGA	-2.67	105.62	113.21
28	m	613	CLA	CHB-C4A-NA	2.67	128.25	124.40
28	k	604	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
28	j	613	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
28	m	602	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
38	m	611	KC2	C1D-CHD-C4C	-2.67	119.97	126.25
31	J	101	WVN	C39-C40-C37	-2.67	118.06	123.52
28	b	602	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
28	B	823	CLA	C1-C2-C3	-2.67	121.83	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	n	616	II0	C05-C03-C09	2.67	114.75	109.49
28	A	814	CLA	CHB-C4A-NA	2.67	128.25	124.40
31	R	201	WVN	C40-C37-C34	-2.67	123.54	127.28
36	c	613	II0	C31-C33-C35	-2.67	119.05	126.36
28	B	825	CLA	C1-C2-C3	-2.67	121.83	126.20
28	A	851	CLA	C4A-NA-C1A	2.67	107.89	106.68
36	c	613	II0	C31-C29-C25	-2.67	119.16	126.61
28	A	818	CLA	CMB-C2B-C3B	2.66	132.82	126.55
36	m	615	II0	C34-C36-C40	-2.66	114.82	119.01
37	O	204	IHT	C41-C40-C37	-2.66	118.07	123.52
28	A	836	CLA	CMB-C2B-C3B	2.66	132.81	126.55
31	s	205	WVN	C03-C04-C09	-2.66	107.60	112.07
31	B	844	WVN	C20-C23-C25	-2.66	122.30	126.23
28	d	312	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
28	L	202	CLA	C3B-C4B-NB	-2.66	108.15	110.53
28	B	806	CLA	CMB-C2B-C3B	2.66	132.81	126.55
37	O	204	IHT	C22-C18-C07	-2.66	119.89	127.00
38	i	310	KC2	C3B-C2B-C1B	-2.66	104.53	107.05
28	A	820	CLA	CMB-C2B-C3B	2.66	132.81	126.55
28	B	823	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
31	R	201	WVN	C07-C01-C02	2.66	113.57	109.55
28	h	304	CLA	CAA-CBA-CGA	-2.66	105.66	113.21
36	e	616	II0	C31-C29-C25	-2.66	119.18	126.61
28	L	207	CLA	CMB-C2B-C3B	2.66	132.80	126.55
36	e	616	II0	C19-C13-C09	-2.66	119.19	124.16
36	e	612	II0	C20-C14-C12	2.66	119.31	114.42
36	g	320	II0	C19-C13-C09	-2.66	119.19	124.16
28	R	203	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
28	B	825	CLA	CMB-C2B-C3B	2.66	132.80	126.55
36	a	316	II0	C20-C14-C12	2.66	119.30	114.42
36	e	614	II0	C20-C14-C12	2.65	119.30	114.42
28	d	305	CLA	O2D-CGD-CBD	2.65	115.87	111.23
37	c	616	IHT	C22-C18-C07	-2.65	119.91	127.00
38	d	311	KC2	C2A-C1A-NA	2.65	113.59	109.34
30	l	317	LHG	C5-O7-C7	-2.65	111.45	117.80
28	e	606	CLA	CHB-C4A-NA	2.65	128.22	124.40
28	i	304	CLA	CHB-C4A-NA	2.65	128.22	124.40
31	F	203	WVN	C40-C39-C36	2.65	128.94	123.52
38	j	611	KC2	C1D-CHD-C4C	-2.65	120.02	126.25
28	B	836	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
28	A	807	CLA	CMB-C2B-C3B	2.65	132.78	126.55
28	B	839	CLA	C3B-C4B-NB	-2.65	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	314	II0	C32-C30-C26	-2.65	119.20	126.61
37	f	617	IHT	C19-C10-C09	2.65	119.24	113.60
36	m	618	II0	C17-C04-C10	-2.65	105.78	110.52
28	i	308	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
28	A	819	CLA	CMC-C2C-C3C	2.65	133.31	126.15
36	l	312	II0	C41-C42-C40	-2.65	118.11	123.52
36	k	616	II0	C42-C41-C39	-2.65	118.11	123.52
38	c	610	KC2	CAB-C3B-C2B	2.65	137.03	128.43
28	A	806	CLA	C1-C2-C3	-2.65	121.86	126.20
28	c	602	CLA	CMB-C2B-C3B	2.64	132.77	126.55
36	g	318	II0	C41-C42-C40	-2.64	118.11	123.52
36	k	616	II0	C20-C14-C12	2.64	119.28	114.42
28	m	603	CLA	CHB-C4A-NA	2.64	128.21	124.40
28	b	606	CLA	CHB-C4A-NA	2.64	128.21	124.40
28	A	836	CLA	C11-C12-C13	-2.64	107.19	115.97
28	A	832	CLA	CMC-C2C-C3C	2.64	133.29	126.15
36	h	312	II0	C31-C29-C25	-2.64	119.23	126.61
28	j	613	CLA	CHB-C4A-NA	2.64	128.21	124.40
31	A	848	WVN	C30-C33-C34	-2.64	119.13	126.36
36	n	615	II0	C41-C42-C40	-2.64	118.12	123.52
28	A	817	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
28	A	810	CLA	CHB-C4A-NA	2.63	128.20	124.40
28	B	824	CLA	CHB-C4A-NA	2.63	128.20	124.40
28	A	826	CLA	O2D-CGD-CBD	2.63	115.83	111.23
36	i	317	II0	C20-C14-C12	2.63	119.26	114.42
31	l	301	WVN	C21-C15-C14	2.63	119.21	113.60
36	m	614	II0	C30-C32-C34	-2.63	115.57	123.20
36	k	615	II0	C31-C29-C25	-2.63	119.25	126.61
30	c	620	LHG	O8-C23-C24	2.63	119.86	111.83
28	a	309	CLA	CMB-C2B-C3B	2.63	132.74	126.55
28	A	827	CLA	CMB-C2B-C3B	2.63	132.74	126.55
28	j	612	CLA	CMB-C2B-C3B	2.63	132.74	126.55
28	d	308	CLA	CMB-C2B-C3B	2.63	132.74	126.55
28	F	201	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
36	f	616	II0	C32-C34-C36	-2.63	119.15	126.36
31	B	846	WVN	C40-C37-C34	-2.63	123.59	127.28
28	A	805	CLA	C7-C6-C5	-2.63	106.26	113.26
28	A	804	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
28	n	604	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
28	h	304	CLA	CHB-C4A-NA	2.63	128.19	124.40
38	g	314	KC2	CBC-CAC-C3C	-2.63	114.40	127.53
31	i	316	WVN	C23-C20-C13	-2.63	119.98	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	l	302	CLA	CHB-C4A-NA	2.63	128.19	124.40
28	g	305	CLA	CHB-C4A-NA	2.63	128.19	124.40
28	l	311	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
28	j	612	CLA	CAA-C2A-C1A	2.62	120.57	111.97
36	f	616	II0	C29-C31-C33	-2.62	115.60	123.20
36	c	617	II0	C31-C29-C25	-2.62	119.28	126.61
38	j	611	KC2	CAB-C3B-C2B	2.62	136.96	128.43
36	b	614	II0	C12-C14-C10	-2.62	115.04	120.50
28	a	306	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
31	A	848	WVN	C12-C10-C06	-2.62	105.15	114.43
28	a	311	CLA	CHB-C4A-NA	2.62	128.18	124.40
32	a	320	LMT	O5'-C5'-C4'	2.62	115.14	109.72
31	L	206	WVN	C39-C36-C32	-2.62	123.60	127.28
28	c	602	CLA	CBC-CAC-C3C	2.62	119.52	112.42
36	e	613	II0	C11-C13-C09	-2.62	115.05	120.50
28	d	302	CLA	CHB-C4A-NA	2.62	128.18	124.40
28	L	207	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
28	n	603	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
28	n	604	CLA	CHB-C4A-NA	2.62	128.18	124.40
28	B	816	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
31	e	615	WVN	C07-C01-C02	2.62	113.51	109.55
36	f	614	II0	C05-C03-C09	2.62	114.65	109.49
28	A	840	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
38	f	611	KC2	C1D-CHD-C4C	-2.62	120.09	126.25
28	s	206	CLA	CHB-C4A-NA	2.62	128.18	124.40
36	e	614	II0	C31-C33-C35	-2.62	119.19	126.36
36	c	617	II0	C19-C13-C11	2.62	119.23	114.42
28	B	805	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
28	B	819	CLA	O2D-CGD-CBD	2.61	115.80	111.23
38	d	311	KC2	CAB-C3B-C2B	2.61	136.93	128.43
28	e	604	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
28	d	302	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
28	A	806	CLA	C3B-C4B-NB	-2.61	108.20	110.53
28	A	831	CLA	CHB-C4A-NA	2.61	128.17	124.40
35	L	209	LMG	C1-O6-C5	-2.61	108.62	113.72
36	l	314	II0	C19-C13-C11	2.61	119.22	114.42
28	A	852	CLA	CHB-C4A-NA	2.61	128.17	124.40
38	k	612	KC2	CAB-C3B-C2B	2.61	136.91	128.43
28	A	830	CLA	C3B-C4B-NB	-2.61	108.20	110.53
36	i	313	II0	C31-C33-C35	-2.61	119.21	126.36
28	k	602	CLA	CMB-C2B-C3B	2.61	132.68	126.55
28	m	607	CLA	CHB-C4A-NA	2.61	128.16	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	e	602	CLA	CHB-C4A-NA	2.61	128.16	124.40
28	A	851	CLA	CMB-C2B-C3B	2.61	132.68	126.55
30	e	617	LHG	O8-C23-C24	2.61	119.78	111.83
36	e	612	II0	C19-C13-C11	2.61	119.21	114.42
36	h	310	II0	C30-C32-C34	-2.61	120.04	125.28
36	f	616	II0	C27-C25-C29	-2.61	119.12	124.18
28	B	835	CLA	C3B-C4B-NB	-2.61	108.20	110.53
28	i	309	CLA	CHB-C4A-NA	2.60	128.16	124.40
31	R	202	WVN	C39-C40-C37	-2.60	118.19	123.52
38	k	612	KC2	O2D-CGD-CBD	2.60	115.78	111.23
28	B	808	CLA	C1-C2-C3	-2.60	121.93	126.20
28	c	605	CLA	O2A-CGA-O1A	-2.60	117.11	123.63
31	K	102	WVN	C06-C13-C15	-2.60	119.08	122.64
28	b	609	CLA	C3B-C4B-NB	-2.60	108.21	110.53
38	g	314	KC2	CAB-C3B-C2B	2.60	136.89	128.43
31	R	202	WVN	C21-C15-C14	2.60	119.14	113.60
28	l	302	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
37	n	617	IHT	C31-C34-C35	-2.60	119.24	126.36
37	b	615	IHT	C31-C34-C35	-2.60	119.24	126.36
28	l	304	CLA	CHB-C4A-NA	2.60	128.15	124.40
28	A	807	CLA	O2D-CGD-CBD	2.60	115.77	111.23
28	B	830	CLA	CHB-C4A-NA	2.60	128.15	124.40
38	s	201	KC2	C2B-C1B-NB	2.60	112.70	110.13
31	R	202	WVN	C40-C39-C36	-2.60	118.21	123.52
28	e	602	CLA	C3B-C4B-NB	-2.60	108.21	110.53
28	k	601	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
28	f	612	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
28	j	607	CLA	O2D-CGD-CBD	2.59	115.77	111.23
28	n	601	CLA	C3B-C4B-NB	-2.59	108.21	110.53
36	a	316	II0	C05-C03-C09	2.59	114.60	109.49
37	O	204	IHT	C30-C32-C33	-2.59	119.25	126.36
38	n	612	KC2	CAB-C3B-C2B	2.59	136.86	128.43
36	k	619	II0	C32-C34-C36	-2.59	119.25	126.36
28	b	607	CLA	CHB-C4A-NA	2.59	128.14	124.40
31	e	615	WVN	C39-C40-C37	-2.59	118.21	123.52
28	c	606	CLA	C2A-C1A-CHA	2.59	128.37	123.87
28	l	311	CLA	C3B-C4B-NB	-2.59	108.22	110.53
28	c	601	CLA	CHB-C4A-NA	2.59	128.14	124.40
28	g	322	CLA	CHB-C4A-NA	2.59	128.14	124.40
36	l	313	II0	C20-C14-C10	-2.59	119.32	124.16
28	A	803	CLA	CMB-C2B-C3B	2.59	132.64	126.55
36	c	614	II0	C31-C29-C25	-2.59	119.37	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	i	302	CLA	CHB-C4A-NA	2.59	128.14	124.40
32	a	320	LMT	O1'-C1'-C2'	2.59	112.20	108.27
28	A	836	CLA	CHB-C4A-NA	2.59	128.14	124.40
28	b	602	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
28	g	308	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
28	A	811	CLA	CHB-C4A-NA	2.59	128.13	124.40
37	R	204	IHT	C29-C31-C34	-2.59	115.70	123.20
37	n	617	IHT	C41-C40-C37	-2.59	118.22	123.52
28	f	603	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
36	e	613	II0	C20-C14-C10	-2.59	119.32	124.16
36	d	315	II0	C33-C35-C39	2.59	123.08	119.01
30	a	301	LHG	O8-C23-C24	2.59	119.72	111.83
31	J	102	WVN	C03-C04-C09	-2.59	107.73	112.07
28	A	818	CLA	CHB-C1B-NB	2.59	127.93	124.05
31	B	846	WVN	C28-C30-C33	-2.58	115.71	123.20
36	e	616	II0	C27-C25-C29	-2.58	119.16	124.18
37	j	616	IHT	C31-C34-C35	-2.58	119.28	126.36
36	g	320	II0	C29-C31-C33	-2.58	115.71	123.20
28	B	823	CLA	CHB-C4A-NA	2.58	128.13	124.40
28	e	605	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
28	n	605	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
28	h	301	CLA	CHD-C1D-ND	-2.58	121.17	124.80
36	c	613	II0	C12-C14-C10	-2.58	115.12	120.50
28	B	822	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
36	h	312	II0	C19-C13-C09	-2.58	119.33	124.16
28	n	613	CLA	CHB-C4A-NA	2.58	128.13	124.40
28	k	605	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
28	A	834	CLA	O2D-CGD-CBD	2.58	115.74	111.23
37	m	617	IHT	C31-C29-C26	-2.58	119.40	126.61
28	R	203	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
28	c	606	CLA	CHB-C4A-NA	2.58	128.12	124.40
36	a	315	II0	C30-C32-C34	-2.58	115.73	123.20
28	g	307	CLA	C3B-C4B-NB	-2.58	108.23	110.53
28	B	826	CLA	O2D-CGD-CBD	2.58	115.73	111.23
38	i	310	KC2	CHB-C4A-NA	2.58	128.23	124.23
28	A	814	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
36	b	613	II0	C19-C13-C09	-2.58	119.34	124.16
28	i	307	CLA	CHB-C4A-NA	2.57	128.12	124.40
28	Q	302	CLA	CHB-C4A-NA	2.57	128.12	124.40
35	n	620	LMG	O8-C28-C29	2.57	119.69	111.83
31	I	101	WVN	C14-C15-C13	-2.57	119.23	122.70
28	B	837	CLA	CHB-C4A-NA	2.57	128.11	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	309	CLA	CHB-C4A-NA	2.57	128.11	124.40
28	K	101	CLA	O2D-CGD-CBD	2.57	115.73	111.23
37	R	204	IHT	C19-C10-C09	2.57	119.08	113.60
28	B	832	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
28	A	821	CLA	CMB-C2B-C3B	2.57	132.60	126.55
28	n	613	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
28	B	821	CLA	C2A-C1A-CHA	2.57	128.33	123.87
36	i	315	II0	C41-C42-C40	-2.57	118.26	123.52
28	d	307	CLA	C3B-C4B-NB	-2.57	108.23	110.53
31	F	203	WVN	C40-C37-C34	-2.57	123.67	127.28
28	d	309	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
36	k	617	II0	C41-C42-C40	-2.57	118.26	123.52
28	B	812	CLA	C4A-NA-C1A	2.57	107.85	106.68
28	A	806	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
28	B	838	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
28	A	805	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
28	B	822	CLA	O1D-CGD-CBD	2.57	129.59	124.52
28	A	822	CLA	O2D-CGD-CBD	2.57	115.72	111.23
28	A	813	CLA	O2D-CGD-CBD	2.57	115.72	111.23
38	k	612	KC2	CAC-C3C-C2C	-2.57	120.08	128.43
28	f	606	CLA	C1-C2-C3	-2.57	121.99	126.20
38	i	319	KC2	C1D-CHD-C4C	-2.57	120.21	126.25
28	A	854	CLA	C3B-C4B-NB	-2.57	108.24	110.53
31	R	202	WVN	C17-C06-C13	-2.57	106.22	110.24
28	b	606	CLA	C1-C2-C3	-2.57	121.99	126.20
31	A	846	WVN	C30-C33-C34	-2.57	119.33	126.36
28	h	301	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
36	m	616	II0	C31-C29-C25	-2.57	119.44	126.61
28	A	824	CLA	CHB-C4A-NA	2.56	128.10	124.40
28	l	305	CLA	CHB-C4A-NA	2.56	128.10	124.40
38	k	612	KC2	CAA-CBA-CGA	-2.56	114.01	127.05
28	A	821	CLA	O2D-CGD-CBD	2.56	115.71	111.23
28	h	302	CLA	CHB-C4A-NA	2.56	128.10	124.40
28	A	824	CLA	CMB-C2B-C3B	2.56	132.57	126.55
38	c	610	KC2	O2D-CGD-O1D	-2.56	118.86	123.85
31	K	104	WVN	C30-C33-C34	-2.56	119.34	126.36
35	c	619	LMG	O6-C1-O1	2.56	116.09	110.04
28	A	832	CLA	CHB-C4A-NA	2.56	128.09	124.40
31	I	101	WVN	C35-C32-C31	2.56	122.00	118.09
28	d	309	CLA	CMB-C2B-C3B	2.56	132.57	126.55
28	A	817	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
28	A	816	CLA	C4-C3-C2	-2.56	117.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	320	LMT	C1-O1'-C1'	-2.56	109.31	113.68
36	e	613	II0	C30-C32-C34	-2.56	115.79	123.20
38	d	310	KC2	CAA-CBA-CGA	-2.56	114.05	127.05
28	h	313	CLA	O2D-CGD-CBD	2.56	115.70	111.23
30	b	619	LHG	O3-P-O5	-2.56	98.80	108.94
28	k	605	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
36	i	313	II0	C29-C31-C33	-2.56	115.80	123.20
31	F	203	WVN	C07-C01-C02	2.55	113.42	109.55
28	e	611	CLA	C1-C2-C3	-2.55	122.01	126.20
30	g	301	LHG	O8-C23-C24	2.55	119.62	111.83
28	e	605	CLA	C3B-C4B-NB	-2.55	108.25	110.53
28	l	306	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
28	i	312	CLA	CMB-C2B-C3B	2.55	132.56	126.55
28	a	309	CLA	CHB-C4A-NA	2.55	128.08	124.40
28	c	611	CLA	CHB-C4A-NA	2.55	128.08	124.40
28	h	303	CLA	C1-C2-C3	-2.55	122.64	126.76
36	e	616	II0	C20-C14-C10	-2.55	119.39	124.16
28	A	838	CLA	CAA-CBA-CGA	-2.55	105.97	113.21
36	a	314	II0	C19-C13-C11	2.55	119.11	114.42
36	g	320	II0	C31-C29-C25	-2.55	119.48	126.61
28	h	305	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
36	c	614	II0	C06-C04-C10	2.55	114.51	109.49
31	L	206	WVN	C24-C22-C19	2.55	121.98	118.09
36	c	614	II0	C05-C03-C09	2.55	114.51	109.49
28	e	605	CLA	CHB-C4A-NA	2.55	128.08	124.40
28	A	834	CLA	C1-C2-C3	-2.55	122.02	126.20
38	f	611	KC2	CAA-CBA-CGA	-2.55	114.09	127.05
36	f	615	II0	C31-C29-C25	-2.55	119.49	126.61
28	a	306	CLA	CHB-C4A-NA	2.55	128.07	124.40
28	e	601	CLA	C3B-C4B-NB	-2.55	108.26	110.53
28	k	607	CLA	CHB-C4A-NA	2.54	128.07	124.40
28	l	305	CLA	O1D-CGD-CBD	2.54	129.53	124.52
28	A	820	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
28	A	838	CLA	CHB-C1B-NB	2.54	127.86	124.05
28	k	606	CLA	C3B-C4B-NB	-2.54	108.26	110.53
36	m	614	II0	C05-C03-C09	2.54	114.50	109.49
28	B	812	CLA	CAA-C2A-C3A	-2.54	106.13	113.00
28	B	815	CLA	CMB-C2B-C3B	2.54	132.53	126.55
28	h	308	CLA	C3B-C4B-NB	-2.54	108.26	110.53
28	B	801	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
30	g	321	LHG	O8-C23-C24	2.54	119.58	111.83
28	k	602	CLA	CAA-CBA-CGA	-2.54	106.00	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	816	CLA	C4-C3-C5	2.54	119.64	115.23
28	O	206	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
28	m	610	CLA	C1-C2-C3	-2.54	122.04	126.20
36	l	312	II0	C05-C03-C09	2.54	114.49	109.49
38	g	314	KC2	O2D-CGD-CBD	2.54	115.66	111.23
28	B	817	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
28	e	601	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
31	J	102	WVN	C40-C37-C34	-2.53	123.72	127.28
36	i	313	II0	C42-C41-C39	-2.53	118.34	123.52
28	a	305	CLA	C3B-C4B-NB	-2.53	108.27	110.53
28	f	609	CLA	C3B-C4B-NB	-2.53	108.27	110.53
38	e	609	KC2	CAB-C3B-C2B	2.53	136.66	128.43
28	B	803	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
28	a	313	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
36	l	312	II0	C19-C13-C11	2.53	119.08	114.42
28	B	828	CLA	CHB-C4A-NA	2.53	128.05	124.40
36	f	615	II0	C34-C36-C40	-2.53	115.03	119.01
28	k	608	CLA	C3B-C4B-NB	-2.53	108.27	110.53
36	g	320	II0	C31-C33-C35	-2.53	119.43	126.36
36	k	615	II0	C38-C36-C34	2.53	121.95	118.09
28	j	604	CLA	C1-C2-C3	-2.53	122.05	126.20
32	a	320	LMT	O5'-C1'-C2'	2.53	115.56	110.37
38	f	611	KC2	CAB-C3B-C4B	-2.53	118.78	124.82
36	d	315	II0	C31-C29-C25	-2.53	119.54	126.61
36	m	618	II0	C34-C36-C40	2.53	122.98	119.01
36	f	615	II0	C29-C31-C33	-2.53	115.88	123.20
28	j	613	CLA	O1D-CGD-CBD	2.53	129.50	124.52
36	f	618	II0	C32-C30-C26	-2.53	119.55	126.61
31	L	206	WVN	C39-C40-C37	-2.53	118.35	123.52
28	f	607	CLA	CHB-C4A-NA	2.53	128.04	124.40
28	g	303	CLA	CMD-C2D-C1D	-2.53	120.28	124.73
31	L	206	WVN	C21-C15-C14	2.53	118.98	113.60
28	h	306	CLA	CMB-C2B-C3B	2.53	132.49	126.55
28	f	613	CLA	C3B-C4B-NB	-2.52	108.28	110.53
31	K	104	WVN	C29-C26-C22	-2.52	123.74	127.28
31	F	203	WVN	C12-C14-C15	-2.52	109.56	114.06
36	d	314	II0	C19-C13-C11	2.52	119.06	114.42
36	b	617	II0	C38-C36-C34	2.52	121.94	118.09
36	h	312	II0	C31-C33-C35	-2.52	119.45	126.36
28	A	827	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
28	L	203	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
36	k	616	II0	C31-C29-C25	-2.52	119.56	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	616	IHT	C02-C07-C10	-2.52	119.19	122.64
31	s	205	WVN	C29-C31-C32	-2.52	119.45	126.36
31	F	204	WVN	C35-C32-C31	2.52	121.94	118.09
28	B	823	CLA	CAA-CBA-CGA	-2.52	106.05	113.21
30	f	619	LHG	O8-C23-C24	2.52	119.52	111.83
37	O	204	IHT	C02-C07-C10	-2.52	119.19	122.64
28	c	608	CLA	CMB-C2B-C3B	2.52	132.47	126.55
38	k	613	KC2	CAB-C3B-C2B	2.52	136.62	128.43
28	m	612	CLA	CAC-C3C-C4C	2.52	128.07	124.79
28	i	311	CLA	C2B-C1B-NB	2.52	112.94	110.33
28	d	304	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
28	L	207	CLA	CHB-C4A-NA	2.52	128.03	124.40
28	f	603	CLA	CHB-C4A-NA	2.52	128.03	124.40
28	m	613	CLA	CAC-C3C-C2C	2.51	132.18	127.56
37	R	204	IHT	C20-C15-C11	-2.51	119.46	124.16
28	d	302	CLA	O2D-CGD-CBD	2.51	115.62	111.23
38	k	612	KC2	CHD-C1D-C2D	2.51	134.72	127.43
29	B	842	PQN	C14-C13-C15	2.51	119.59	115.23
28	B	833	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
28	K	101	CLA	C2A-C1A-CHA	2.51	128.23	123.87
28	A	813	CLA	C3B-C4B-NB	-2.51	108.29	110.53
28	c	603	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
28	B	829	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
28	b	603	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
36	l	316	II0	C31-C29-C25	-2.51	119.59	126.61
36	a	314	II0	C12-C14-C10	-2.51	115.28	120.50
36	c	614	II0	C42-C41-C39	-2.51	118.39	123.52
28	e	602	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
28	B	836	CLA	C1-C2-C3	-2.51	122.09	126.20
28	m	607	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
37	g	319	IHT	C20-C15-C12	2.50	119.03	114.42
28	h	304	CLA	CMB-C2B-C3B	2.50	132.44	126.55
36	n	615	II0	C17-C04-C10	-2.50	106.03	110.52
36	e	612	II0	C29-C31-C33	-2.50	115.94	123.20
28	s	203	CLA	CHB-C4A-NA	2.50	128.01	124.40
28	n	603	CLA	CHB-C4A-NA	2.50	128.01	124.40
28	k	602	CLA	CHB-C4A-NA	2.50	128.01	124.40
28	A	811	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
28	i	305	CLA	CMB-C2B-C3B	2.50	132.44	126.55
36	k	619	II0	C05-C03-C09	2.50	114.42	109.49
28	m	602	CLA	CAC-C3C-C4C	2.50	128.04	124.79
28	j	608	CLA	CMB-C2B-C1B	-2.50	121.61	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	m	605	CLA	CAA-C2A-C1A	2.50	117.68	112.14
36	O	203	II0	C37-C35-C33	2.50	121.91	118.09
28	k	602	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
28	g	306	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
36	d	313	II0	C28-C26-C30	-2.50	119.33	124.18
36	b	617	II0	C16-C03-C15	-2.50	101.48	108.63
32	A	850	LMT	C3B-C4B-C5B	-2.50	105.70	110.23
28	e	603	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
28	f	609	CLA	CHB-C4A-NA	2.50	128.00	124.40
38	k	611	KC2	C1D-CHD-C4C	-2.50	120.37	126.25
28	f	604	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
28	A	854	CLA	O2A-CGA-CBA	2.50	119.45	111.83
28	d	312	CLA	CHB-C4A-NA	2.50	128.00	124.40
38	s	204	KC2	CHD-C1D-C2D	2.50	134.67	127.43
35	b	621	LMG	C9-C8-C7	-2.50	105.97	111.78
38	n	612	KC2	O2D-CGD-O1D	-2.49	118.99	123.85
38	g	313	KC2	CAC-C3C-C4C	2.49	135.41	124.39
36	m	615	II0	C29-C31-C33	-2.49	115.98	123.20
28	L	203	CLA	C3B-C4B-NB	-2.49	108.31	110.53
28	B	820	CLA	CHB-C4A-NA	2.49	128.00	124.40
28	c	603	CLA	CHB-C4A-NA	2.49	127.99	124.40
28	k	606	CLA	CHB-C4A-NA	2.49	127.99	124.40
31	A	847	WVN	C19-C22-C26	-2.49	115.09	119.01
28	l	306	CLA	CMC-C2C-C1C	-2.49	121.14	125.03
35	F	205	LMG	O8-C28-C29	2.49	119.43	111.83
28	e	604	CLA	CHB-C4A-NA	2.49	127.99	124.40
28	k	601	CLA	C1-C2-C3	-2.49	122.12	126.20
28	B	833	CLA	CMB-C2B-C3B	2.49	132.40	126.55
37	f	617	IHT	C41-C40-C37	-2.49	118.43	123.52
28	B	822	CLA	CMB-C2B-C3B	2.49	132.40	126.55
28	A	855	CLA	C2A-C1A-CHA	2.49	128.17	123.86
28	i	307	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
28	A	841	CLA	CMB-C2B-C3B	2.49	132.40	126.55
28	i	311	CLA	CAA-CBA-CGA	-2.49	106.15	113.21
28	n	606	CLA	O2A-CGA-O1A	-2.48	117.41	123.63
28	B	807	CLA	C3B-C4B-NB	-2.48	108.31	110.53
37	k	618	IHT	C22-C18-C07	-2.48	120.36	127.00
28	j	605	CLA	CHA-C1A-NA	-2.48	120.77	126.39
31	J	101	WVN	C30-C28-C25	-2.48	123.80	127.28
28	d	305	CLA	CAC-C3C-C4C	2.48	128.02	124.79
38	g	312	KC2	CMB-C2B-C1B	2.48	129.10	124.73
31	M	101	WVN	C26-C29-C31	-2.48	116.00	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	821	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	g	309	CLA	O2D-CGD-CBD	2.48	115.57	111.23
28	n	608	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	n	607	CLA	C1-C2-C3	-2.48	122.13	126.20
38	g	312	KC2	CHD-C1D-C2D	2.48	134.63	127.43
28	B	814	CLA	CHB-C4A-NA	2.48	127.98	124.40
36	j	615	II0	C06-C04-C10	2.48	114.38	109.49
36	i	315	II0	C32-C34-C36	-2.48	119.57	126.36
30	d	317	LHG	O8-C23-C24	2.48	119.39	111.83
28	B	839	CLA	O1D-CGD-CBD	2.48	129.41	124.52
31	h	309	WVN	C03-C04-C09	-2.48	107.91	112.07
28	k	608	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
36	f	618	II0	C15-C03-C09	-2.48	106.08	110.52
28	b	611	CLA	C1-C2-C3	-2.48	122.14	126.20
28	B	840	CLA	CMB-C2B-C3B	2.48	132.38	126.55
38	s	204	KC2	O2D-CGD-O1D	-2.48	119.03	123.85
31	R	202	WVN	C26-C29-C31	-2.48	116.03	123.20
28	l	309	CLA	C3B-C4B-NB	-2.48	108.32	110.53
31	A	847	WVN	C01-C02-C11	-2.47	109.98	112.83
28	f	602	CLA	C3B-C4B-NB	-2.47	108.32	110.53
28	n	604	CLA	CMB-C2B-C3B	2.47	132.37	126.55
28	g	310	CLA	C1-C2-C3	-2.47	122.14	126.20
28	g	308	CLA	CMB-C2B-C3B	2.47	132.37	126.55
36	d	313	II0	C06-C04-C10	2.47	114.36	109.49
28	j	604	CLA	CHB-C4A-NA	2.47	127.97	124.40
28	k	609	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
28	j	608	CLA	CMB-C2B-C3B	2.47	132.37	126.55
28	B	810	CLA	C3B-C4B-NB	-2.47	108.32	110.53
38	n	611	KC2	O2D-CGD-CBD	2.47	115.55	111.23
28	A	803	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
28	B	807	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
28	l	305	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
30	c	618	LHG	O7-C7-O9	-2.47	117.93	123.70
28	d	312	CLA	CMB-C2B-C3B	2.47	132.36	126.55
28	a	313	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
28	c	605	CLA	CHB-C4A-NA	2.47	127.96	124.40
28	j	603	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
28	B	820	CLA	C3B-C4B-NB	-2.47	108.33	110.53
28	b	607	CLA	CHD-C1D-ND	-2.47	121.33	124.80
28	O	206	CLA	CMB-C2B-C3B	2.47	132.36	126.55
31	K	104	WVN	C39-C40-C37	-2.47	118.47	123.52
38	d	310	KC2	C1D-CHD-C4C	-2.47	120.44	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	811	CLA	O2D-CGD-CBD	2.47	115.54	111.23
28	A	837	CLA	CAA-CBA-CGA	-2.47	106.20	113.21
28	h	303	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
28	l	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
36	c	613	II0	C19-C13-C11	2.47	118.96	114.42
36	O	203	II0	C31-C29-C25	-2.47	119.71	126.61
28	f	612	CLA	CAA-CBA-CGA	-2.47	106.20	113.21
36	g	320	II0	C05-C03-C09	2.47	114.35	109.49
36	h	311	II0	C12-C14-C10	-2.47	115.37	120.50
36	k	616	II0	C34-C36-C40	-2.47	115.13	119.01
28	f	601	CLA	O2D-CGD-CBD	2.46	115.54	111.23
28	l	303	CLA	CHB-C4A-NA	2.46	127.96	124.40
36	l	316	II0	C38-C36-C34	2.46	121.85	118.09
36	g	317	II0	C31-C33-C35	-2.46	119.61	126.36
36	e	613	II0	C38-C36-C34	2.46	121.85	118.09
28	A	802	CLA	C11-C12-C13	-2.46	107.78	115.97
36	i	314	II0	C41-C42-C40	-2.46	118.48	123.52
38	l	310	KC2	O2D-CGD-O1D	-2.46	119.05	123.85
28	A	839	CLA	O2D-CGD-CBD	2.46	115.53	111.23
28	Q	303	CLA	O2D-CGD-CBD	2.46	115.53	111.23
31	h	309	WVN	C21-C15-C14	2.46	118.85	113.60
28	e	610	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
36	j	615	II0	C31-C29-C25	-2.46	119.72	126.61
36	h	312	II0	C30-C32-C34	-2.46	116.07	123.20
31	B	844	WVN	C01-C02-C11	-2.46	110.00	112.83
31	M	101	WVN	C21-C15-C13	-2.46	121.80	124.48
28	B	817	CLA	C1-C2-C3	-2.46	122.16	126.20
28	j	610	CLA	CMC-C2C-C3C	2.46	132.81	126.15
28	B	835	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	j	605	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	A	832	CLA	C7-C6-C5	-2.46	106.70	113.26
28	g	304	CLA	CMB-C2B-C3B	2.46	132.34	126.55
36	n	618	II0	C32-C34-C36	-2.46	119.62	126.36
31	B	847	WVN	C21-C15-C13	-2.46	121.80	124.48
28	c	607	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
28	g	304	CLA	CHB-C4A-NA	2.46	127.95	124.40
38	s	204	KC2	C1D-CHD-C4C	-2.46	120.47	126.25
31	B	845	WVN	C14-C15-C13	-2.46	119.38	122.70
36	j	615	II0	C42-C41-C39	-2.46	118.49	123.52
36	l	312	II0	C32-C34-C36	-2.46	119.63	126.36
28	A	839	CLA	CHB-C4A-NA	2.45	127.94	124.40
28	c	609	CLA	CHB-C4A-NA	2.45	127.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	i	311	CLA	CMB-C2B-C3B	2.45	132.32	126.55
28	B	812	CLA	C3B-C4B-NB	-2.45	108.34	110.53
28	k	604	CLA	CMB-C2B-C3B	2.45	132.32	126.55
36	b	613	II0	C32-C30-C26	-2.45	119.75	126.61
28	A	822	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
28	k	609	CLA	C3B-C4B-NB	-2.45	108.34	110.53
38	s	201	KC2	C2D-C1D-ND	-2.45	107.78	110.33
31	A	847	WVN	C31-C32-C36	-2.45	115.16	119.01
28	l	307	CLA	CMB-C2B-C3B	2.45	132.31	126.55
28	m	607	CLA	CHB-C1B-NB	2.45	127.72	124.05
28	f	605	CLA	CHB-C4A-NA	2.45	127.94	124.40
35	J	105	LMG	C8-O7-C10	-2.45	111.94	117.80
28	B	830	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
31	B	845	WVN	C11-C19-C22	-2.45	121.06	126.32
28	B	805	CLA	CHB-C4A-NA	2.45	127.93	124.40
28	O	201	CLA	C2D-C1D-ND	-2.45	107.71	110.13
28	A	854	CLA	CHB-C1B-NB	2.44	127.72	124.05
31	A	847	WVN	C20-C13-C15	-2.44	115.92	121.56
28	f	612	CLA	CHB-C4A-NA	2.44	127.93	124.40
28	h	313	CLA	CMB-C2B-C3B	2.44	132.30	126.55
36	c	613	II0	C34-C36-C40	-2.44	115.17	119.01
28	B	820	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
28	h	301	CLA	C6-C7-C8	-2.44	107.85	115.97
28	n	605	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
31	K	102	WVN	C26-C29-C31	-2.44	116.13	123.20
31	B	845	WVN	C23-C20-C13	-2.44	120.48	127.00
28	b	608	CLA	CHB-C4A-NA	2.44	127.92	124.40
28	A	802	CLA	CHB-C1B-NB	2.44	127.71	124.05
36	k	616	II0	C30-C32-C34	-2.44	116.13	123.20
28	A	808	CLA	CMB-C2B-C3B	2.44	132.29	126.55
28	B	802	CLA	O1D-CGD-CBD	2.44	129.33	124.52
28	d	301	CLA	CHB-C4A-NA	2.44	127.92	124.40
28	B	826	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
28	A	852	CLA	CBA-CAA-C2A	2.44	121.05	113.79
28	A	838	CLA	C12-C11-C10	2.44	124.20	113.28
28	B	836	CLA	CHB-C4A-NA	2.44	127.92	124.40
28	i	311	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
28	l	306	CLA	CMC-C2C-C3C	2.44	132.74	126.15
28	A	808	CLA	C1-C2-C3	-2.44	122.21	126.20
28	k	605	CLA	C2A-C1A-CHA	2.44	128.09	123.87
36	a	315	II0	C32-C34-C36	-2.44	119.69	126.36
28	A	837	CLA	O2D-CGD-CBD	2.44	115.49	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	831	CLA	CHB-C1B-NB	2.44	127.70	124.05
28	m	601	CLA	C3B-C4B-NB	-2.43	108.36	110.53
28	f	608	CLA	O2D-CGD-CBD	2.43	115.48	111.23
28	s	208	CLA	O2D-CGD-CBD	2.43	115.48	111.23
31	F	204	WVN	C07-C01-C02	2.43	113.23	109.55
36	l	314	II0	C31-C33-C35	-2.43	119.69	126.36
36	b	614	II0	C30-C32-C34	-2.43	116.15	123.20
36	m	615	II0	C05-C03-C09	2.43	114.28	109.49
28	B	822	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
28	c	611	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
36	d	313	II0	C30-C32-C34	-2.43	116.16	123.20
28	h	306	CLA	CHB-C4A-NA	2.43	127.91	124.40
36	n	618	II0	C19-C13-C09	-2.43	119.62	124.16
36	k	617	II0	C38-C36-C34	2.43	121.80	118.09
28	i	308	CLA	CAA-C2A-C1A	2.43	119.93	111.97
28	c	608	CLA	C1-C2-C3	-2.43	122.22	126.20
28	B	819	CLA	CHB-C4A-NA	2.43	127.90	124.40
28	j	605	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
28	m	608	CLA	C3B-C4B-NB	-2.43	108.36	110.53
28	m	613	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
28	L	203	CLA	CHD-C1D-ND	-2.43	121.39	124.80
28	i	311	CLA	CHB-C4A-NA	2.43	127.90	124.40
28	B	838	CLA	O2D-CGD-CBD	2.42	115.47	111.23
28	A	820	CLA	CAC-C3C-C4C	2.42	127.94	124.79
36	g	318	II0	C31-C33-C35	-2.42	119.72	126.36
28	B	824	CLA	O2D-CGD-CBD	2.42	115.47	111.23
28	a	309	CLA	O2D-CGD-CBD	2.42	115.47	111.23
31	A	848	WVN	C14-C15-C13	-2.42	119.43	122.70
28	i	307	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
36	e	612	II0	C20-C14-C10	-2.42	119.63	124.16
36	e	614	II0	C19-C13-C09	-2.42	119.63	124.16
36	c	617	II0	C29-C31-C33	-2.42	116.19	123.20
28	b	604	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
28	B	828	CLA	C3B-C4B-NB	-2.42	108.37	110.53
36	a	318	II0	C22-C24-C26	-2.42	168.01	176.23
28	O	202	CLA	CHB-C4A-NA	2.42	127.89	124.40
38	k	613	KC2	CAA-CBA-CGA	-2.42	114.75	127.05
28	A	827	CLA	CHB-C4A-NA	2.42	127.89	124.40
28	m	610	CLA	CHB-C4A-NA	2.42	127.89	124.40
28	d	303	CLA	CMB-C2B-C3B	2.42	132.24	126.55
36	O	203	II0	C11-C13-C09	-2.42	115.47	120.50
31	B	848	WVN	C35-C32-C31	2.42	121.78	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	i	312	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
36	f	615	II0	C12-C14-C10	-2.42	115.47	120.50
30	b	619	LHG	O4-P-O3	2.42	118.52	107.57
28	A	821	CLA	C3B-C4B-NB	-2.42	108.37	110.53
36	c	614	II0	C32-C34-C36	-2.41	119.74	126.36
31	B	846	WVN	C24-C22-C26	-2.41	118.90	122.82
28	k	603	CLA	C3A-C2A-C1A	2.41	104.95	101.34
36	k	617	II0	C12-C14-C10	-2.41	115.47	120.50
37	R	204	IHT	C30-C32-C33	-2.41	119.75	126.36
30	L	208	LHG	C5-O7-C7	-2.41	112.02	117.80
28	c	612	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	m	605	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	B	808	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	k	614	CLA	C3B-C4B-NB	-2.41	108.38	110.53
31	A	847	WVN	C26-C29-C31	-2.41	116.21	123.20
36	n	618	II0	C42-C40-C36	-2.41	123.90	127.28
28	A	812	CLA	C1-C2-C3	-2.41	122.25	126.20
36	e	616	II0	C32-C30-C26	-2.41	119.87	126.61
31	B	846	WVN	C40-C39-C36	-2.41	118.59	123.52
28	e	605	CLA	CMD-C2D-C3D	2.41	133.22	127.69
28	B	816	CLA	CMB-C2B-C3B	2.41	132.22	126.55
36	b	617	II0	C17-C04-C10	-2.41	106.20	110.52
28	k	608	CLA	C1-C2-C3	-2.41	122.25	126.20
28	e	611	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	j	610	CLA	CMC-C2C-C1C	-2.41	121.27	125.03
28	s	202	CLA	C2A-C1A-CHA	2.41	128.05	123.87
36	f	615	II0	C05-C03-C09	2.41	114.23	109.49
36	b	614	II0	C06-C04-C10	2.41	114.23	109.49
28	g	307	CLA	CHB-C4A-NA	2.41	127.87	124.40
28	A	840	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
28	B	817	CLA	CHB-C1B-C2B	-2.41	120.44	127.43
36	b	617	II0	C12-C14-C10	-2.41	115.49	120.50
37	b	616	IHT	C30-C27-C23	2.41	130.65	127.28
38	n	611	KC2	C1D-CHD-C4C	-2.41	120.59	126.25
28	f	602	CLA	CHB-C4A-NA	2.41	127.87	124.40
36	l	316	II0	C31-C33-C35	-2.41	119.77	126.36
28	B	828	CLA	CHB-C1B-NB	2.41	127.66	124.05
36	J	104	II0	C37-C35-C33	2.41	121.76	118.09
28	k	614	CLA	CHB-C4A-NA	2.40	127.87	124.40
36	e	612	II0	C17-C04-C10	-2.40	106.21	110.52
28	m	610	CLA	O2D-CGD-CBD	2.40	115.43	111.23
36	m	615	II0	C12-C14-C10	-2.40	115.50	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	k	609	CLA	CMB-C2B-C3B	2.40	132.20	126.55
28	A	813	CLA	CMB-C2B-C3B	2.40	132.20	126.55
36	h	311	II0	C19-C13-C09	-2.40	119.67	124.16
36	a	316	II0	C32-C34-C36	-2.40	119.78	126.36
30	A	849	LHG	O8-C23-C24	2.40	119.16	111.83
36	b	614	II0	C41-C39-C35	-2.40	123.91	127.28
36	i	314	II0	C31-C29-C25	-2.40	119.90	126.61
28	l	307	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	Q	303	CLA	CHB-C1B-C2B	-2.40	120.46	127.43
28	B	811	CLA	C7-C6-C5	-2.40	106.87	113.26
28	b	607	CLA	C1-C2-C3	-2.40	122.27	126.20
37	c	616	IHT	C19-C10-C09	2.40	118.71	113.60
28	h	301	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	g	310	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
28	B	805	CLA	CMB-C2B-C3B	2.40	132.19	126.55
28	A	834	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	b	601	CLA	CHB-C4A-NA	2.40	127.86	124.40
31	h	309	WVN	C19-C22-C26	2.40	122.78	119.01
28	c	604	CLA	CMB-C2B-C3B	2.40	132.19	126.55
28	f	603	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
28	a	313	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	d	303	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	B	809	CLA	CHB-C4A-NA	2.40	127.86	124.40
36	n	615	II0	C32-C34-C36	-2.40	119.80	126.36
28	B	807	CLA	C1-C2-C3	-2.40	122.27	126.20
28	B	838	CLA	C3B-C4B-NB	-2.39	108.39	110.53
28	c	606	CLA	C3B-C4B-NB	-2.39	108.39	110.53
28	B	809	CLA	CAB-C3B-C2B	2.39	129.90	123.53
31	F	204	WVN	C02-C11-C19	-2.39	120.85	124.58
28	A	802	CLA	CHB-C4A-NA	2.39	127.86	124.40
28	B	821	CLA	CBA-CAA-C2A	2.39	120.92	113.79
31	L	206	WVN	C06-C13-C15	-2.39	119.36	122.64
28	A	828	CLA	C1-O2A-CGA	-2.39	110.86	116.65
38	g	312	KC2	CAA-CBA-CGA	-2.39	114.88	127.05
28	A	834	CLA	CAA-CBA-CGA	-2.39	106.41	113.21
37	b	615	IHT	C31-C29-C26	-2.39	119.92	126.61
28	j	602	CLA	CHB-C4A-NA	2.39	127.85	124.40
36	b	613	II0	C30-C32-C34	-2.39	116.27	123.20
28	j	604	CLA	C7-C6-C5	-2.39	106.89	113.26
28	A	851	CLA	C4D-C3D-CAD	-2.39	105.51	108.11
28	h	301	CLA	CHB-C1B-NB	2.39	127.64	124.05
36	j	615	II0	C32-C34-C36	-2.39	119.81	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	811	CLA	C3B-C4B-NB	-2.39	108.40	110.53
28	e	610	CLA	CAA-CBA-CGA	-2.39	106.42	113.21
35	L	209	LMG	C1-C2-C3	2.39	115.04	110.01
28	b	607	CLA	CMC-C2C-C3C	2.39	132.61	126.15
36	i	314	II0	C37-C35-C33	2.39	121.74	118.09
28	B	803	CLA	CHB-C4A-NA	2.39	127.84	124.40
28	B	807	CLA	CHB-C4A-NA	2.39	127.84	124.40
28	j	607	CLA	C3B-C4B-NB	-2.39	108.40	110.53
28	a	308	CLA	CAA-C2A-C1A	-2.39	104.16	111.97
31	s	205	WVN	C40-C39-C36	-2.39	118.64	123.52
31	L	205	WVN	C38-C34-C33	2.39	121.73	118.09
30	i	318	LHG	C5-O7-C7	-2.39	112.09	117.80
28	B	825	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
31	R	202	WVN	C12-C14-C15	-2.38	109.80	114.06
38	n	611	KC2	CAB-C3B-C2B	2.38	136.18	128.43
28	d	308	CLA	CHB-C4A-NA	2.38	127.84	124.40
28	B	811	CLA	CMB-C2B-C3B	2.38	132.16	126.55
28	c	605	CLA	C3B-C4B-NB	-2.38	108.40	110.53
28	b	601	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
30	a	319	LHG	O8-C23-O10	-2.38	117.67	123.63
28	c	604	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
28	Q	303	CLA	C3B-C4B-NB	-2.38	108.40	110.53
28	A	832	CLA	C6-C7-C8	-2.38	108.05	115.97
28	a	303	CLA	CHB-C4A-NA	2.38	127.84	124.40
34	B	843	DGD	C2G-O2G-C1B	-2.38	112.09	117.80
38	g	313	KC2	O2D-CGD-O1D	-2.38	119.21	123.85
28	a	313	CLA	C3B-C4B-NB	-2.38	108.40	110.53
28	g	315	CLA	C3B-C4B-NB	-2.38	108.40	110.53
28	n	602	CLA	C3B-C4B-NB	-2.38	108.40	110.53
28	B	832	CLA	CHB-C1B-NB	2.38	127.62	124.05
28	A	841	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
30	A	844	LHG	C5-O7-C7	-2.38	112.10	117.80
28	A	817	CLA	CHB-C1B-NB	2.38	127.62	124.05
31	B	847	WVN	C39-C36-C32	-2.38	123.94	127.28
28	n	609	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
36	j	615	II0	C38-C36-C34	2.38	121.72	118.09
28	b	606	CLA	C4-C3-C5	2.38	119.36	115.23
28	i	309	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
28	b	604	CLA	O1D-CGD-CBD	2.38	129.21	124.52
28	m	606	CLA	CHB-C4A-NA	2.38	127.83	124.40
31	I	101	WVN	C27-C25-C23	2.38	121.72	118.09
28	A	818	CLA	O2D-CGD-CBD	2.38	115.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	304	CLA	CHB-C4A-NA	2.37	127.83	124.40
28	f	613	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
36	d	315	II0	C03-C05-C07	2.37	118.80	113.59
36	d	316	II0	C31-C33-C35	-2.37	119.85	126.36
31	J	101	WVN	C24-C22-C19	-2.37	114.46	118.09
28	A	824	CLA	CHA-C1A-NA	-2.37	121.02	126.39
28	A	832	CLA	C3B-C4B-NB	-2.37	108.41	110.53
38	k	613	KC2	C1D-CHD-C4C	-2.37	120.67	126.25
28	i	302	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
28	B	834	CLA	CHB-C4A-NA	2.37	127.82	124.40
28	A	814	CLA	CMB-C2B-C3B	2.37	132.12	126.55
31	B	844	WVN	C02-C05-C09	-2.37	118.55	121.47
30	A	849	LHG	C5-O7-C7	-2.37	112.12	117.80
35	O	205	LMG	C8-O7-C10	-2.37	112.12	117.80
36	O	203	II0	C20-C14-C12	2.37	118.78	114.42
37	k	618	IHT	C19-C10-C09	2.37	118.65	113.60
38	g	313	KC2	CBC-CAC-C3C	-2.37	115.69	127.53
36	d	316	II0	C32-C30-C26	-2.37	119.99	126.61
28	d	306	CLA	CMB-C2B-C3B	2.37	132.12	126.55
28	b	604	CLA	CHB-C4A-NA	2.37	127.82	124.40
31	e	615	WVN	C29-C26-C22	-2.37	123.96	127.28
28	g	310	CLA	O2D-CGD-CBD	2.37	115.36	111.23
30	l	317	LHG	O8-C23-C24	2.36	119.05	111.83
36	m	615	II0	C30-C32-C34	-2.36	116.35	123.20
28	i	304	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
36	l	316	II0	C37-C35-C33	2.36	121.70	118.09
36	g	317	II0	C38-C36-C34	2.36	121.70	118.09
28	m	601	CLA	CAA-C2A-C1A	-2.36	106.92	112.14
28	h	305	CLA	CMB-C2B-C3B	2.36	132.10	126.55
36	m	614	II0	C29-C31-C33	-2.36	116.36	123.20
36	d	316	II0	C12-C14-C10	-2.36	115.59	120.50
30	e	617	LHG	O4-P-O5	2.36	123.42	112.44
30	a	319	LHG	C25-C24-C23	-2.36	105.05	113.69
28	g	306	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
28	L	203	CLA	O2D-CGD-CBD	2.36	115.35	111.23
38	d	311	KC2	CAC-C3C-C4C	2.36	134.81	124.39
28	j	601	CLA	CHB-C4A-NA	2.36	127.80	124.40
36	l	312	II0	C42-C41-C39	-2.36	118.70	123.52
36	c	615	II0	C12-C14-C10	-2.36	115.59	120.50
31	B	845	WVN	C30-C33-C34	-2.36	119.90	126.36
28	h	307	CLA	CHB-C4A-NA	2.36	127.80	124.40
31	e	615	WVN	C29-C31-C32	-2.36	119.90	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	610	CLA	C4-C3-C5	2.36	119.32	115.23
36	c	613	II0	C20-C14-C10	-2.36	119.76	124.16
28	B	812	CLA	CHA-C1A-NA	-2.36	121.06	126.39
28	d	305	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
28	A	821	CLA	CHB-C4A-NA	2.35	127.80	124.40
30	A	849	LHG	C6-C5-C4	-2.35	106.30	111.78
28	b	605	CLA	CBA-CAA-C2A	-2.35	106.79	113.79
36	d	315	II0	C38-C36-C40	-2.35	119.00	122.82
28	m	609	CLA	C1-C2-C3	-2.35	122.34	126.20
38	m	611	KC2	O2D-CGD-O1D	-2.35	119.27	123.85
28	B	833	CLA	O2D-CGD-CBD	2.35	115.34	111.23
28	c	606	CLA	CHB-C1B-NB	2.35	127.58	124.05
29	B	842	PQN	C2M-C2-C3	-2.35	120.58	124.45
28	A	832	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
28	B	801	CLA	C3B-C4B-NB	-2.35	108.43	110.53
28	A	830	CLA	CHB-C1B-NB	2.35	127.58	124.05
36	e	614	II0	C05-C03-C09	2.35	114.12	109.49
31	B	846	WVN	C11-C19-C22	-2.35	121.27	126.32
28	K	101	CLA	CAA-CBA-CGA	-2.35	106.53	113.21
28	f	613	CLA	CHB-C4A-NA	2.35	127.79	124.40
28	L	204	CLA	C3B-C4B-NB	-2.35	108.43	110.53
28	f	612	CLA	CMB-C2B-C3B	2.35	132.07	126.55
31	K	104	WVN	C07-C01-C02	2.35	113.10	109.55
31	A	847	WVN	C03-C04-C09	-2.35	108.13	112.07
30	l	317	LHG	O4-P-O5	2.35	123.36	112.44
28	O	202	CLA	CBC-CAC-C3C	2.35	118.78	112.42
28	k	602	CLA	CBC-CAC-C3C	2.35	118.78	112.42
28	b	603	CLA	C3B-C4B-NB	-2.35	108.44	110.53
28	A	814	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
31	h	309	WVN	C39-C40-C37	-2.35	118.72	123.52
36	n	616	II0	C32-C34-C36	-2.35	119.93	126.36
36	m	615	II0	C31-C29-C25	-2.35	120.05	126.61
37	O	204	IHT	C31-C29-C26	-2.35	120.05	126.61
28	l	304	CLA	CMB-C2B-C1B	-2.35	121.85	125.42
31	J	102	WVN	C39-C40-C37	-2.34	118.72	123.52
28	m	613	CLA	O1D-CGD-CBD	2.34	129.14	124.52
30	g	321	LHG	C5-O7-C7	-2.34	112.18	117.80
28	O	201	CLA	CHB-C4A-NA	2.34	127.78	124.40
28	d	301	CLA	CMB-C2B-C3B	2.34	132.06	126.55
28	g	322	CLA	CBC-CAC-C3C	2.34	118.77	112.42
31	A	847	WVN	C35-C32-C31	2.34	121.67	118.09
36	i	314	II0	C29-C31-C33	-2.34	116.42	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	616	IHT	C40-C41-C38	-2.34	118.73	123.52
36	h	311	II0	C30-C32-C34	-2.34	116.42	123.20
28	i	307	CLA	O1D-CGD-CBD	2.34	129.13	124.52
36	h	310	II0	C19-C13-C09	-2.34	119.79	124.16
36	m	618	II0	C32-C30-C26	-2.34	120.07	126.61
28	g	303	CLA	CBA-CAA-C2A	2.34	120.75	113.79
32	A	850	LMT	O1B-C4'-C3'	2.34	113.17	107.23
31	i	316	WVN	C07-C01-C02	2.34	113.09	109.55
31	J	102	WVN	C23-C20-C13	-2.34	120.75	127.00
28	F	202	CLA	O2D-CGD-CBD	2.34	115.31	111.23
28	b	611	CLA	CHB-C4A-NA	2.34	127.77	124.40
31	A	846	WVN	C03-C04-C09	-2.34	108.15	112.07
29	A	842	PQN	C26-C25-C23	-2.34	108.20	115.97
36	l	313	II0	C34-C36-C40	2.34	122.68	119.01
38	i	319	KC2	CAB-C3B-C2B	2.33	136.02	128.43
28	B	840	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
28	A	829	CLA	CHB-C1B-NB	2.33	127.55	124.05
36	i	320	II0	C15-C03-C09	-2.33	106.34	110.52
31	l	301	WVN	C19-C22-C26	-2.33	115.34	119.01
36	f	614	II0	C19-C13-C09	-2.33	119.80	124.16
31	i	316	WVN	C38-C34-C37	-2.33	119.04	122.82
38	k	613	KC2	CMB-C2B-C1B	2.33	128.84	124.73
28	j	603	CLA	CHB-C4A-NA	2.33	127.77	124.40
28	n	602	CLA	CHB-C4A-NA	2.33	127.77	124.40
31	K	104	WVN	C20-C23-C25	-2.33	122.79	126.23
28	A	812	CLA	C6-C5-C3	-2.33	107.79	113.47
36	d	314	II0	C05-C03-C09	2.33	114.08	109.49
39	i	301	LMU	O1B-C1B-C2B	2.33	113.82	108.09
28	B	828	CLA	CHB-C1B-C2B	-2.33	120.66	127.43
28	b	603	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
36	c	613	II0	C32-C34-C36	-2.33	119.97	126.36
36	a	314	II0	C31-C33-C35	-2.33	119.98	126.36
31	L	206	WVN	C38-C34-C37	-2.33	119.04	122.82
36	f	618	II0	C38-C36-C34	2.33	121.64	118.09
28	Q	302	CLA	C7-C6-C5	-2.33	107.06	113.26
37	m	617	IHT	C20-C15-C12	2.33	118.70	114.42
31	B	848	WVN	C28-C30-C33	-2.33	116.46	123.20
31	B	844	WVN	C14-C15-C13	-2.33	119.56	122.70
28	n	602	CLA	O2D-CGD-CBD	2.33	115.30	111.23
28	R	203	CLA	C2A-C1A-CHA	2.33	127.90	123.87
28	m	613	CLA	C3B-C4B-NB	-2.33	108.45	110.53
28	B	827	CLA	C1-C2-C3	-2.32	123.00	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	g	313	KC2	C1D-CHD-C4C	-2.32	120.78	126.25
36	a	318	II0	C05-C03-C09	2.32	114.07	109.49
28	f	603	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
28	B	840	CLA	CHD-C1D-ND	-2.32	121.53	124.80
28	b	602	CLA	CMB-C2B-C3B	2.32	132.01	126.55
31	L	201	WVN	C28-C30-C33	-2.32	116.47	123.20
31	h	309	WVN	C35-C32-C36	-2.32	119.05	122.82
31	L	201	WVN	C02-C05-C09	-2.32	118.61	121.47
28	g	302	CLA	C2A-C1A-CHA	2.32	127.90	123.87
38	i	310	KC2	O2D-CGD-O1D	-2.32	119.33	123.85
28	s	203	CLA	CBA-CAA-C2A	-2.32	106.88	113.79
28	l	305	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
28	A	813	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
28	i	309	CLA	O2D-CGD-CBD	2.32	115.29	111.23
36	k	617	II0	C16-C03-C09	-2.32	106.36	110.52
28	L	203	CLA	CHB-C4A-NA	2.32	127.75	124.40
28	h	313	CLA	CHB-C4A-NA	2.32	127.75	124.40
28	A	812	CLA	C7-C6-C5	2.32	119.44	113.26
37	j	616	IHT	C31-C29-C26	-2.32	120.13	126.61
36	d	315	II0	C42-C41-C39	2.32	128.26	123.52
31	e	615	WVN	C30-C33-C34	-2.32	120.01	126.36
28	k	605	CLA	CMC-C2C-C1C	-2.32	121.42	125.03
28	f	601	CLA	C2A-C1A-CHA	2.31	127.88	123.87
36	m	616	II0	C32-C34-C36	-2.31	120.02	126.36
35	c	619	LMG	O1-C7-C8	2.31	116.44	110.82
31	K	102	WVN	C29-C26-C22	-2.31	124.03	127.28
28	B	832	CLA	CHB-C4A-NA	2.31	127.74	124.40
31	i	316	WVN	C14-C15-C13	-2.31	119.58	122.70
36	i	313	II0	C05-C03-C09	2.31	114.05	109.49
28	l	307	CLA	O1D-CGD-CBD	2.31	129.08	124.52
38	k	611	KC2	CAB-C3B-C4B	-2.31	119.30	124.82
36	k	619	II0	C37-C35-C33	2.31	121.62	118.09
28	l	305	CLA	C1-C2-C3	-2.31	122.41	126.20
36	c	614	II0	C29-C31-C33	-2.31	116.50	123.20
28	A	808	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
36	c	615	II0	C27-C25-C29	-2.31	119.70	124.18
28	B	827	CLA	CHD-C1D-ND	-2.31	121.55	124.80
28	B	824	CLA	CAA-C2A-C1A	2.31	119.54	111.97
31	s	207	WVN	C26-C29-C31	-2.31	116.51	123.20
31	A	845	WVN	C30-C33-C34	-2.31	120.03	126.36
30	n	619	LHG	O8-C23-C24	2.31	118.88	111.83
28	A	839	CLA	CMB-C2B-C1B	-2.31	121.91	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	802	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
31	J	101	WVN	C02-C05-C09	-2.31	118.63	121.47
28	A	841	CLA	C3A-C2A-C1A	2.31	104.79	101.34
28	c	603	CLA	CHD-C1D-ND	-2.31	121.56	124.80
28	c	612	CLA	C1-C2-C3	-2.30	122.42	126.20
36	i	314	II0	C42-C40-C36	-2.30	124.05	127.28
28	A	826	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
30	m	619	LHG	O8-C23-C24	2.30	118.86	111.83
36	n	618	II0	C38-C36-C34	2.30	121.61	118.09
28	m	612	CLA	C2A-C1A-CHA	2.30	127.86	123.87
28	A	840	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
36	e	613	II0	C31-C29-C25	-2.30	120.18	126.61
36	n	614	II0	C19-C13-C11	2.30	118.65	114.42
36	e	612	II0	C38-C36-C34	2.30	121.60	118.09
31	M	101	WVN	C04-C09-C05	-2.30	122.64	124.83
28	h	305	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
35	c	619	LMG	C4-C3-C2	2.30	114.86	110.83
38	i	319	KC2	O2D-CGD-O1D	-2.30	119.38	123.85
28	j	610	CLA	CHB-C4A-NA	2.30	127.72	124.40
28	B	833	CLA	C3B-C4B-NB	-2.30	108.48	110.53
28	m	610	CLA	CMC-C2C-C3C	2.30	132.36	126.15
36	c	617	II0	C27-C25-C29	-2.30	119.72	124.18
31	J	101	WVN	C40-C37-C34	-2.30	124.06	127.28
31	L	206	WVN	C02-C05-C09	-2.30	118.64	121.47
36	i	317	II0	C38-C36-C34	2.30	121.60	118.09
28	A	806	CLA	C11-C10-C8	-2.30	108.33	115.97
36	n	618	II0	C08-C12-C14	2.30	117.89	112.18
28	l	311	CLA	C4-C3-C5	2.30	119.21	115.23
28	A	855	CLA	C3A-C2A-C1A	2.30	105.53	101.64
38	i	310	KC2	CAA-CBA-CGA	-2.30	115.38	127.05
28	c	606	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
28	B	836	CLA	CAA-CBA-CGA	-2.29	106.69	113.21
36	m	616	II0	C17-C04-C10	-2.29	106.41	110.52
28	K	103	CLA	C2A-C1A-CHA	2.29	127.85	123.87
36	e	616	II0	C12-C14-C10	-2.29	115.72	120.50
31	A	847	WVN	C24-C22-C19	2.29	121.59	118.09
28	A	816	CLA	C6-C7-C8	-2.29	108.34	115.97
28	B	827	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
28	k	602	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
36	c	615	II0	C37-C35-C33	2.29	121.59	118.09
28	k	606	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
30	a	301	LHG	O4-P-O5	2.29	123.11	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	828	CLA	O2D-CGD-CBD	2.29	115.23	111.23
37	c	616	IHT	C20-C15-C12	2.29	118.63	114.42
28	b	607	CLA	CHD-C4C-NC	2.29	127.78	124.23
31	B	848	WVN	C10-C06-C13	2.29	113.77	110.44
28	B	817	CLA	CHB-C4A-NA	2.29	127.70	124.40
28	A	837	CLA	C6-C5-C3	-2.29	107.89	113.47
28	A	803	CLA	C3B-C4B-NB	-2.29	108.49	110.53
28	e	611	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
31	R	202	WVN	C04-C09-C05	-2.29	122.64	124.83
28	A	805	CLA	CMB-C2B-C3B	2.29	131.93	126.55
31	L	201	WVN	C29-C31-C32	-2.29	120.09	126.36
36	n	618	II0	C37-C35-C33	2.29	121.58	118.09
28	A	809	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
28	K	103	CLA	O1D-CGD-CBD	2.29	129.03	124.52
28	a	307	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
28	A	827	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
28	B	841	CLA	O2D-CGD-CBD	2.29	115.23	111.23
31	l	301	WVN	C35-C32-C31	2.29	121.58	118.09
28	e	604	CLA	O2D-CGD-CBD	2.29	115.22	111.23
28	k	607	CLA	O2D-CGD-CBD	2.29	115.22	111.23
28	e	608	CLA	C3B-C4B-NB	-2.29	108.49	110.53
28	A	852	CLA	CMA-C3A-C2A	-2.29	105.15	113.98
31	l	315	WVN	C40-C39-C36	-2.28	118.84	123.52
38	s	201	KC2	C1D-CHD-C4C	-2.28	120.88	126.25
28	l	306	CLA	CAA-C2A-C1A	2.28	119.46	111.97
28	s	202	CLA	CHB-C1B-NB	2.28	127.47	124.05
36	f	618	II0	C19-C13-C09	-2.28	119.89	124.16
37	n	617	IHT	C31-C29-C26	-2.28	120.23	126.61
31	h	309	WVN	C29-C31-C32	-2.28	120.10	126.36
28	d	303	CLA	C1-C2-C3	-2.28	122.46	126.20
28	e	606	CLA	C2A-C1A-CHA	2.28	127.83	123.87
28	A	817	CLA	CHB-C4A-NA	2.28	127.69	124.40
28	B	821	CLA	O1A-CGA-CBA	2.28	132.70	123.78
36	i	313	II0	C38-C36-C40	-2.28	119.12	122.82
31	B	847	WVN	C27-C25-C23	2.28	121.57	118.09
35	Q	301	LMG	O7-C10-O9	-2.28	118.38	123.70
31	L	205	WVN	C27-C25-C28	-2.28	119.12	122.82
28	B	811	CLA	C11-C12-C13	-2.28	108.39	115.97
36	g	316	II0	C12-C14-C10	-2.28	115.76	120.50
28	B	802	CLA	C3B-C4B-NB	-2.28	108.50	110.53
28	A	852	CLA	CHB-C1B-NB	2.28	127.47	124.05
31	s	207	WVN	C02-C05-C09	-2.28	118.67	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	s	202	CLA	CMB-C2B-C3B	2.28	131.91	126.55
28	A	812	CLA	CAC-C3C-C4C	2.28	127.75	124.79
28	c	608	CLA	O2D-CGD-CBD	2.28	115.21	111.23
28	j	612	CLA	CHB-C1B-C2B	-2.28	120.82	127.43
28	L	202	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
28	d	309	CLA	CHB-C4A-NA	2.28	127.69	124.40
36	j	615	II0	C12-C14-C10	-2.28	115.76	120.50
38	l	310	KC2	CMB-C2B-C1B	2.28	128.74	124.73
36	d	316	II0	C19-C13-C09	-2.28	119.91	124.16
37	m	617	IHT	C40-C41-C38	-2.28	118.86	123.52
36	h	311	II0	C32-C30-C26	-2.28	120.25	126.61
28	O	201	CLA	O2D-CGD-CBD	2.27	115.21	111.23
28	B	818	CLA	CAA-CBA-CGA	-2.27	106.75	113.21
38	m	611	KC2	C2B-C1B-NB	2.27	112.38	110.13
31	F	203	WVN	C27-C25-C23	2.27	121.56	118.09
28	A	836	CLA	O2D-CGD-CBD	2.27	115.20	111.23
28	B	841	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
28	A	802	CLA	CHB-C1B-C2B	-2.27	120.83	127.43
28	i	309	CLA	CMB-C2B-C3B	2.27	131.90	126.55
28	m	609	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
36	J	104	II0	C20-C14-C12	2.27	118.60	114.42
31	B	846	WVN	C23-C20-C13	-2.27	120.93	127.00
31	A	845	WVN	C24-C22-C19	2.27	121.56	118.09
35	J	105	LMG	O8-C28-C29	2.27	118.76	111.83
28	c	607	CLA	CHB-C4A-NA	2.27	127.68	124.40
37	m	617	IHT	C02-C07-C18	2.27	121.81	115.65
36	k	617	II0	C31-C33-C35	-2.27	120.14	126.36
28	B	807	CLA	CHB-C1B-NB	2.27	127.45	124.05
28	m	602	CLA	CMB-C2B-C3B	2.27	131.89	126.55
28	B	816	CLA	CAA-CBA-CGA	-2.27	106.77	113.21
36	l	313	II0	C33-C35-C39	2.27	122.58	119.01
28	i	304	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
38	m	611	KC2	CAA-CBA-CGA	-2.27	115.51	127.05
28	f	608	CLA	CHB-C4A-NA	2.27	127.67	124.40
36	l	316	II0	C32-C34-C36	-2.27	120.15	126.36
38	j	611	KC2	CAA-CBA-CGA	-2.27	115.53	127.05
28	n	610	CLA	O2D-CGD-CBD	2.26	115.19	111.23
28	j	612	CLA	CHB-C4A-NA	2.26	127.67	124.40
36	h	312	II0	C06-C04-C10	2.26	113.95	109.49
28	j	609	CLA	C1-C2-C3	-2.26	122.49	126.20
31	s	205	WVN	C21-C15-C14	2.26	118.42	113.60
28	A	837	CLA	CHC-C4B-NB	2.26	127.44	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	601	CLA	C3B-C4B-NB	-2.26	108.51	110.53
31	h	309	WVN	C12-C14-C15	-2.26	110.03	114.06
28	l	305	CLA	CMB-C2B-C3B	2.26	131.87	126.55
28	n	605	CLA	CMB-C2B-C3B	2.26	131.87	126.55
28	B	840	CLA	CHB-C4A-NA	2.26	127.66	124.40
28	O	202	CLA	C3B-C4B-NB	-2.26	108.51	110.53
31	s	205	WVN	C26-C29-C31	-2.26	116.66	123.20
36	i	314	II0	C32-C34-C36	-2.26	120.17	126.36
28	f	607	CLA	CHB-C1B-NB	2.26	127.43	124.05
28	m	612	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
28	A	808	CLA	CAA-CBA-CGA	-2.26	106.80	113.21
28	a	308	CLA	C3B-C4B-NB	-2.25	108.52	110.53
28	A	815	CLA	O1D-CGD-CBD	2.25	128.96	124.52
31	s	205	WVN	C19-C22-C26	-2.25	115.47	119.01
28	a	313	CLA	CHB-C1B-NB	2.25	127.43	124.05
38	s	201	KC2	CMD-C2D-C3D	2.25	132.77	125.67
37	n	617	IHT	C02-C07-C18	2.25	121.76	115.65
36	b	617	II0	C19-C13-C09	-2.25	119.95	124.16
28	h	313	CLA	C3B-C4B-NB	-2.25	108.52	110.53
28	A	808	CLA	CAA-C2A-C1A	2.25	119.35	111.97
36	d	316	II0	C06-C04-C10	2.25	113.92	109.49
38	c	610	KC2	CHD-C1D-C2D	2.25	133.95	127.43
36	i	314	II0	C34-C36-C40	-2.25	115.47	119.01
28	m	609	CLA	O2D-CGD-CBD	2.25	115.16	111.23
28	d	312	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
31	J	101	WVN	C02-C11-C19	2.25	128.08	124.58
31	F	203	WVN	C16-C05-C09	-2.25	114.81	122.37
28	O	206	CLA	CHA-C1A-NA	-2.25	121.30	126.39
36	a	316	II0	C31-C33-C35	-2.25	120.20	126.36
34	B	843	DGD	O6D-C5D-C6D	2.25	111.15	106.69
28	A	819	CLA	CMC-C2C-C1C	-2.25	121.52	125.03
37	k	618	IHT	C20-C15-C11	-2.25	119.96	124.16
37	j	616	IHT	C41-C40-C37	-2.25	118.92	123.52
28	s	202	CLA	C3B-C4B-NB	-2.25	108.53	110.53
28	A	828	CLA	CHB-C4A-NA	2.25	127.64	124.40
28	i	305	CLA	CHB-C4A-NA	2.25	127.64	124.40
28	h	308	CLA	CBA-CAA-C2A	2.25	120.47	113.79
31	B	846	WVN	C20-C13-C15	-2.25	116.38	121.56
36	d	315	II0	C32-C30-C26	-2.25	120.33	126.61
28	f	608	CLA	C3B-C4B-NB	-2.24	108.53	110.53
28	B	824	CLA	C2A-C1A-CHA	2.24	127.76	123.87
38	i	310	KC2	CMB-C2B-C1B	2.24	128.68	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	606	CLA	C4-C3-C5	2.24	118.77	116.13
28	A	816	CLA	CAA-C2A-C3A	-2.24	106.94	113.00
38	g	313	KC2	CAB-C3B-C4B	-2.24	119.47	124.82
31	s	205	WVN	C14-C15-C13	-2.24	119.68	122.70
36	d	313	II0	C19-C13-C09	-2.24	119.97	124.16
38	g	313	KC2	CAA-CBA-CGA	-2.24	115.65	127.05
28	a	311	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
36	b	617	II0	C29-C31-C33	-2.24	116.71	123.20
28	a	311	CLA	CAA-CBA-CGA	-2.24	106.85	113.21
28	A	813	CLA	O2A-CGA-O1A	-2.24	117.57	123.33
28	n	610	CLA	CHB-C4A-NA	2.24	127.63	124.40
36	e	613	II0	C31-C33-C35	-2.24	120.23	126.36
28	b	609	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
28	b	606	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
28	B	815	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
30	L	208	LHG	O8-C23-C24	2.24	118.66	111.83
28	B	839	CLA	C16-C15-C13	-2.24	108.53	115.97
38	m	611	KC2	CAB-C3B-C4B	-2.24	119.48	124.82
28	A	817	CLA	CMB-C2B-C3B	2.24	131.81	126.55
38	s	201	KC2	C2A-C1A-NA	2.24	112.93	109.34
28	A	825	CLA	C3B-C4B-NB	-2.24	108.53	110.53
28	e	605	CLA	CMD-C2D-C1D	-2.24	120.79	124.73
28	B	812	CLA	O2D-CGD-CBD	2.24	115.14	111.23
28	n	602	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
28	i	305	CLA	O1D-CGD-CBD	2.23	128.93	124.52
28	e	601	CLA	C2A-C1A-CHA	2.23	127.74	123.87
37	n	617	IHT	C20-C15-C11	-2.23	119.98	124.16
28	a	303	CLA	CMB-C2B-C3B	2.23	131.80	126.55
31	e	615	WVN	C20-C13-C15	-2.23	116.41	121.56
28	e	602	CLA	CMB-C2B-C3B	2.23	131.80	126.55
36	a	314	II0	C38-C36-C34	2.23	121.50	118.09
28	B	840	CLA	CBC-CAC-C3C	2.23	118.47	112.42
28	L	204	CLA	CMB-C2B-C3B	2.23	131.80	126.55
28	A	820	CLA	CHB-C1B-NB	2.23	127.40	124.05
28	B	802	CLA	C11-C10-C8	-2.23	108.55	115.97
35	b	621	LMG	C1-C2-C3	2.23	114.70	110.01
28	A	813	CLA	CHB-C4A-NA	2.23	127.62	124.40
28	c	604	CLA	CHB-C4A-NA	2.23	127.62	124.40
28	i	312	CLA	C2A-C1A-CHA	2.23	127.74	123.87
28	B	814	CLA	C3B-C4B-NB	-2.23	108.54	110.53
28	m	608	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
28	m	606	CLA	C1-C2-C3	-2.23	122.54	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	d	314	II0	C38-C36-C40	-2.23	119.20	122.82
28	g	309	CLA	C1-C2-C3	-2.23	122.55	126.20
38	e	609	KC2	CAA-CBA-CGA	-2.23	115.72	127.05
28	k	609	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
38	i	310	KC2	CHD-C1D-C2D	2.23	133.89	127.43
28	h	308	CLA	CHA-C1A-NA	-2.23	121.35	126.39
28	A	837	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
28	A	831	CLA	O1D-CGD-CBD	2.23	128.91	124.52
28	A	816	CLA	C16-C15-C13	-2.23	108.57	115.97
28	l	302	CLA	C3B-C4B-NB	-2.23	108.54	110.53
36	i	313	II0	C15-C03-C09	-2.23	106.53	110.52
36	d	315	II0	C32-C34-C36	-2.23	120.26	126.36
38	s	201	KC2	CAB-C3B-C2B	2.22	135.66	128.43
38	j	611	KC2	C2B-C1B-NB	2.22	112.33	110.13
28	A	834	CLA	C3A-C2A-C1A	2.22	104.67	101.34
28	A	808	CLA	C2A-C1A-CHA	2.22	127.72	123.87
28	l	311	CLA	CHB-C4A-NA	2.22	127.61	124.40
29	B	842	PQN	C17-C16-C15	-2.22	107.34	113.26
38	s	201	KC2	CAA-CBA-CGA	-2.22	115.75	127.05
28	h	304	CLA	O2D-CGD-CBD	2.22	115.11	111.23
28	B	811	CLA	CHB-C4A-NA	2.22	127.60	124.40
38	k	611	KC2	CAA-CBA-CGA	-2.22	115.76	127.05
28	A	805	CLA	C3A-C2A-C1A	2.22	104.66	101.34
35	c	619	LMG	O8-C28-C29	2.22	118.60	111.83
28	A	832	CLA	CMB-C2B-C3B	2.22	131.77	126.55
28	e	610	CLA	CMB-C2B-C3B	2.22	131.77	126.55
36	h	311	II0	C31-C29-C25	-2.22	120.41	126.61
28	l	302	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
28	e	605	CLA	C1-C2-C3	-2.22	122.56	126.20
28	m	602	CLA	C3B-C4B-NB	-2.22	108.55	110.53
38	d	311	KC2	CAA-CBA-CGA	-2.22	115.77	127.05
28	s	206	CLA	C2A-C1A-CHA	2.22	127.72	123.87
36	m	615	II0	C20-C14-C12	2.22	118.50	114.42
28	g	310	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
31	A	846	WVN	C12-C14-C15	-2.22	110.10	114.06
31	R	201	WVN	C23-C25-C28	2.22	122.50	119.01
36	n	614	II0	C20-C14-C12	2.22	118.50	114.42
37	k	618	IHT	C30-C32-C33	-2.22	120.28	126.36
28	O	202	CLA	C1-C2-C3	-2.22	122.57	126.20
28	n	605	CLA	C2A-C1A-CHA	2.22	127.71	123.87
36	h	311	II0	C11-C13-C09	-2.22	115.89	120.50
36	i	313	II0	C19-C13-C11	2.22	118.50	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	g	318	II0	C05-C03-C09	2.22	113.85	109.49
28	e	604	CLA	O1D-CGD-CBD	2.22	128.89	124.52
28	A	817	CLA	C6-C7-C8	-2.21	108.60	115.97
28	B	809	CLA	O2D-CGD-CBD	2.21	115.10	111.23
28	B	802	CLA	CHB-C4A-NA	2.21	127.60	124.40
28	B	804	CLA	O2D-CGD-CBD	2.21	115.10	111.23
28	j	602	CLA	C1-C2-C3	-2.21	123.18	126.76
28	L	204	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
28	B	829	CLA	CHB-C4A-NA	2.21	127.59	124.40
28	b	607	CLA	O2D-CGD-CBD	2.21	115.10	111.23
28	b	602	CLA	O2A-CGA-CBA	2.21	118.58	111.83
38	k	613	KC2	CHD-C1D-C2D	2.21	133.85	127.43
28	Q	302	CLA	C14-C13-C12	-2.21	103.39	111.27
28	g	309	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
28	b	607	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
36	h	311	II0	C17-C04-C10	-2.21	106.56	110.52
38	d	311	KC2	CHD-C1D-C2D	2.21	133.84	127.43
36	e	613	II0	C42-C41-C39	-2.21	119.00	123.52
28	c	604	CLA	C3A-C2A-C1A	2.21	104.65	101.34
35	b	621	LMG	O8-C28-C29	2.21	118.57	111.83
28	B	835	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
36	d	315	II0	C37-C35-C39	-2.21	119.24	122.82
28	m	613	CLA	CMB-C2B-C3B	2.21	131.75	126.55
28	h	306	CLA	C3B-C4B-NB	-2.21	108.56	110.53
28	B	811	CLA	C1-C2-C3	-2.21	122.58	126.20
38	d	310	KC2	CHD-C1D-C2D	2.21	133.84	127.43
36	l	314	II0	C32-C30-C26	-2.21	120.44	126.61
31	K	104	WVN	C19-C22-C26	-2.21	115.54	119.01
37	O	204	IHT	C04-C02-C07	2.21	113.64	110.44
28	b	606	CLA	O1D-CGD-CBD	2.21	128.87	124.52
31	A	847	WVN	C21-C15-C14	2.21	118.30	113.60
28	A	829	CLA	C4B-C3B-C2B	-2.21	104.56	107.30
36	l	314	II0	C27-C25-C29	-2.21	119.90	124.18
28	B	816	CLA	CHB-C4A-NA	2.21	127.58	124.40
28	A	826	CLA	CAA-C2A-C3A	-2.21	107.04	113.00
36	a	314	II0	C29-C31-C33	-2.21	116.81	123.20
28	f	609	CLA	CAC-C3C-C4C	2.21	127.66	124.79
30	A	844	LHG	C9-C8-C7	-2.21	105.61	113.69
35	L	209	LMG	C30-C29-C28	-2.21	105.61	113.69
36	O	203	II0	C30-C32-C34	-2.20	116.81	123.20
30	b	620	LHG	O8-C23-C24	2.20	118.56	111.83
28	A	812	CLA	C4-C3-C5	2.20	119.06	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	202	CLA	O2D-CGD-CBD	2.20	115.08	111.23
28	f	608	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
28	B	832	CLA	CHB-C1B-C2B	-2.20	121.03	127.43
28	n	610	CLA	C3B-C4B-NB	-2.20	108.56	110.53
28	g	302	CLA	CHA-C1A-NA	-2.20	121.40	126.39
36	i	317	II0	C30-C32-C34	-2.20	116.82	123.20
36	i	315	II0	C29-C31-C33	-2.20	116.82	123.20
31	l	301	WVN	C12-C14-C15	-2.20	110.13	114.06
28	l	303	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
28	b	608	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
36	e	616	II0	C11-C13-C09	-2.20	115.92	120.50
28	h	306	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
31	F	204	WVN	C31-C32-C36	-2.20	115.55	119.01
28	i	312	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
28	A	816	CLA	O2D-CGD-CBD	2.20	115.07	111.23
28	A	840	CLA	CHB-C4A-NA	2.20	127.57	124.40
28	c	608	CLA	CED-O2D-CGD	2.20	120.90	115.92
31	R	202	WVN	C23-C20-C13	-2.20	121.13	127.00
28	a	310	CLA	C3B-C4B-NB	-2.20	108.57	110.53
38	i	319	KC2	C2B-C1B-NB	2.20	112.30	110.13
31	s	205	WVN	C39-C40-C37	-2.20	119.02	123.52
28	A	838	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
31	F	203	WVN	C18-C06-C17	-2.20	102.34	108.63
28	s	202	CLA	C11-C12-C13	-2.20	108.66	115.97
28	n	601	CLA	O2A-CGA-O1A	-2.20	117.68	123.33
36	c	615	II0	C30-C32-C34	-2.20	116.84	123.20
36	a	316	II0	C31-C29-C25	-2.20	120.47	126.61
28	L	204	CLA	CHB-C4A-NA	2.20	127.57	124.40
28	B	808	CLA	CHB-C1B-NB	2.20	127.34	124.05
28	c	609	CLA	C3B-C4B-NB	-2.20	108.57	110.53
28	i	312	CLA	C1-C2-C3	-2.20	122.60	126.20
28	O	202	CLA	C2A-C1A-CHA	2.20	127.68	123.87
36	l	314	II0	C12-C14-C10	-2.20	115.93	120.50
28	g	311	CLA	C5-C3-C2	2.20	126.09	121.17
36	i	315	II0	C30-C32-C34	-2.19	116.84	123.20
28	f	602	CLA	CAC-C3C-C4C	2.19	127.64	124.79
28	b	605	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
36	l	316	II0	C27-C25-C29	-2.19	119.92	124.18
36	l	314	II0	C15-C03-C09	-2.19	106.59	110.52
36	c	617	II0	C28-C26-C30	-2.19	119.92	124.18
28	B	828	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
31	A	846	WVN	C35-C32-C31	-2.19	114.74	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	608	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
28	k	608	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
37	g	319	IHT	C31-C29-C26	-2.19	120.48	126.61
38	c	610	KC2	C1D-CHD-C4C	-2.19	121.09	126.25
28	A	823	CLA	CHB-C4A-NA	2.19	127.56	124.40
28	n	603	CLA	CAA-CBA-CGA	-2.19	106.99	113.21
36	m	614	II0	C11-C13-C09	-2.19	115.94	120.50
37	k	618	IHT	C20-C15-C12	2.19	118.45	114.42
28	k	601	CLA	C3B-C4B-NB	-2.19	108.58	110.53
38	j	611	KC2	CAB-C3B-C4B	-2.19	119.59	124.82
28	A	801	CLA	C2A-C1A-CHA	2.19	127.67	123.87
28	F	201	CLA	C1-C2-C3	-2.19	122.61	126.20
37	a	317	IHT	C20-C15-C11	-2.19	120.07	124.16
28	h	305	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
28	e	610	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
28	A	824	CLA	O2D-CGD-CBD	2.19	115.06	111.23
28	i	304	CLA	CMB-C2B-C3B	2.19	131.70	126.55
36	l	316	II0	C06-C04-C10	2.19	113.80	109.49
30	k	620	LHG	O8-C23-O10	-2.19	118.16	123.63
31	R	201	WVN	C24-C22-C19	2.19	121.43	118.09
35	c	619	LMG	C1-O6-C5	2.19	117.99	113.72
28	A	826	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
28	A	852	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
36	k	619	II0	C11-C13-C09	-2.19	115.95	120.50
28	f	608	CLA	CHB-C1B-NB	2.19	127.33	124.05
28	e	608	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
28	n	603	CLA	C3B-C4B-NB	-2.19	108.58	110.53
28	B	813	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
36	b	617	II0	C41-C42-C40	-2.19	119.05	123.52
38	s	204	KC2	CAB-C3B-C4B	-2.18	119.61	124.82
28	A	819	CLA	O2D-CGD-CBD	2.18	115.05	111.23
28	g	303	CLA	CMD-C2D-C3D	2.18	132.70	127.69
28	f	608	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
28	B	812	CLA	CHB-C4A-NA	2.18	127.55	124.40
28	b	608	CLA	CHD-C1D-ND	-2.18	121.73	124.80
36	k	621	II0	C37-C35-C33	2.18	121.42	118.09
37	O	204	IHT	C29-C31-C34	-2.18	116.88	123.20
28	n	609	CLA	CMC-C2C-C1C	2.18	128.44	125.03
37	a	317	IHT	C18-C22-C23	-2.18	123.01	126.23
28	s	206	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
36	c	617	II0	C42-C41-C39	-2.18	119.06	123.52
36	d	315	II0	C27-C25-C29	-2.18	119.95	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	816	CLA	C3B-C4B-NB	-2.18	108.58	110.53
36	n	616	II0	C31-C29-C25	-2.18	120.52	126.61
31	s	205	WVN	C12-C14-C15	-2.18	110.17	114.06
28	B	809	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
31	L	201	WVN	C11-C19-C22	-2.18	121.64	126.32
38	d	310	KC2	CAB-C3B-C4B	-2.18	119.62	124.82
38	i	319	KC2	CAA-CBA-CGA	-2.18	115.98	127.05
28	f	603	CLA	CMB-C2B-C3B	2.18	131.67	126.55
28	e	606	CLA	O1D-CGD-CBD	2.18	128.81	124.52
28	B	839	CLA	C3A-C2A-C1A	2.18	104.60	101.34
28	l	304	CLA	C3B-C4B-NB	-2.18	108.59	110.53
28	A	851	CLA	CAA-CBA-CGA	-2.17	107.03	113.21
38	i	310	KC2	C2B-C1B-NB	2.17	112.28	110.13
28	s	208	CLA	C1-C2-C3	-2.17	122.64	126.20
28	h	306	CLA	O1D-CGD-CBD	2.17	128.81	124.52
36	l	313	II0	C17-C04-C10	-2.17	106.62	110.52
36	n	614	II0	C32-C34-C36	-2.17	120.40	126.36
28	c	603	CLA	C3B-C4B-NB	-2.17	108.59	110.53
28	g	303	CLA	C3B-C4B-NB	-2.17	108.59	110.53
28	B	803	CLA	CHB-C1B-NB	2.17	127.31	124.05
28	g	311	CLA	O1D-CGD-CBD	2.17	128.80	124.52
31	A	847	WVN	C14-C15-C13	-2.17	119.77	122.70
28	A	833	CLA	CHC-C4B-NB	2.17	127.31	124.05
28	b	602	CLA	C3B-C4B-NB	-2.17	108.59	110.53
36	b	613	II0	C41-C42-C40	-2.17	119.08	123.52
36	k	617	II0	C30-C32-C34	-2.17	116.91	123.20
28	a	309	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
31	L	205	WVN	C19-C22-C26	2.17	122.42	119.01
30	g	321	LHG	C25-C24-C23	-2.17	105.75	113.69
28	m	606	CLA	C3B-C4B-NB	-2.17	108.59	110.53
37	O	204	IHT	C14-C02-C07	-2.17	106.84	110.24
28	b	612	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
28	n	601	CLA	CHB-C4A-NA	2.17	127.53	124.40
28	b	611	CLA	C3B-C4B-NB	-2.17	108.59	110.53
28	s	208	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
28	B	832	CLA	C1-C2-C3	-2.17	122.65	126.20
36	O	203	II0	C32-C30-C26	-2.17	120.55	126.61
28	A	810	CLA	C3B-C4B-NB	-2.17	108.60	110.53
28	A	827	CLA	C3B-C4B-NB	-2.17	108.60	110.53
36	g	318	II0	C20-C14-C12	2.16	118.40	114.42
28	B	802	CLA	CHC-C4B-NB	2.16	127.29	124.05
38	s	204	KC2	CAA-C2A-C1A	2.16	134.12	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	609	CLA	C4-C3-C5	2.16	118.98	115.23
31	i	316	WVN	C12-C14-C15	-2.16	110.20	114.06
28	k	604	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
38	l	310	KC2	CAB-C3B-C4B	-2.16	119.66	124.82
28	a	305	CLA	CAA-C2A-C1A	-2.16	104.89	111.97
31	L	205	WVN	C21-C15-C13	-2.16	122.13	124.48
38	k	612	KC2	CBC-CAC-C3C	-2.16	116.73	127.53
28	O	206	CLA	O2D-CGD-CBD	2.16	115.00	111.23
28	A	823	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
28	h	304	CLA	CHA-C1A-NA	-2.16	121.50	126.39
36	m	618	II0	C12-C14-C10	-2.16	116.01	120.50
28	A	804	CLA	C6-C7-C8	-2.16	108.79	115.97
28	e	602	CLA	CHB-C1B-NB	2.16	127.29	124.05
36	d	315	II0	C12-C14-C10	-2.16	116.01	120.50
28	e	604	CLA	CHC-C4B-NB	2.16	127.28	124.05
28	j	601	CLA	C3B-C4B-NB	-2.16	108.61	110.53
36	i	314	II0	C15-C03-C09	-2.15	106.66	110.52
28	g	308	CLA	C4-C3-C5	2.15	118.96	115.23
28	A	802	CLA	CHD-C1D-ND	-2.15	121.77	124.80
31	l	301	WVN	C14-C15-C13	-2.15	119.80	122.70
28	B	830	CLA	C3B-C4B-NB	-2.15	108.61	110.53
28	B	811	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
36	k	619	II0	C19-C13-C09	-2.15	120.14	124.16
28	h	307	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
36	m	616	II0	C38-C36-C34	2.15	121.37	118.09
28	l	305	CLA	CAA-CBA-CGA	-2.15	107.10	113.21
31	s	205	WVN	C07-C01-C02	2.15	112.80	109.55
28	L	204	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
36	h	312	II0	C29-C31-C33	-2.15	116.97	123.20
28	B	830	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
28	k	602	CLA	C3B-C4B-NB	-2.15	108.61	110.53
28	B	820	CLA	CHD-C1D-ND	-2.15	121.78	124.80
36	e	613	II0	C12-C14-C10	-2.15	116.03	120.50
28	a	308	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
28	l	311	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
28	l	311	CLA	C1-C2-C3	-2.15	122.68	126.20
28	B	825	CLA	CHB-C4A-NA	2.15	127.50	124.40
30	j	617	LHG	C5-O7-C7	-2.15	112.66	117.80
28	A	808	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
36	a	315	II0	C05-C03-C09	2.15	113.72	109.49
31	F	203	WVN	C30-C28-C25	-2.15	124.27	127.28
38	e	609	KC2	CHD-C1D-C2D	2.15	133.65	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	f	614	II0	C20-C14-C12	2.14	118.36	114.42
28	A	801	CLA	C1-C2-C3	-2.14	122.68	126.20
28	j	608	CLA	C3B-C4B-NB	-2.14	108.62	110.53
28	B	820	CLA	O1D-CGD-CBD	2.14	128.75	124.52
36	e	616	II0	C29-C31-C33	-2.14	116.99	123.20
28	A	831	CLA	C3B-C4B-NB	-2.14	108.62	110.53
28	B	814	CLA	O2D-CGD-CBD	2.14	114.98	111.23
28	A	837	CLA	CHB-C4A-NA	2.14	127.49	124.40
28	a	309	CLA	CHD-C4C-NC	2.14	127.55	124.23
28	d	305	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
28	B	834	CLA	O2D-CGD-CBD	2.14	114.97	111.23
28	B	813	CLA	C2A-C1A-CHA	2.14	127.58	123.87
36	n	614	II0	C41-C39-C35	-2.14	124.28	127.28
31	I	101	WVN	C12-C14-C15	-2.14	110.24	114.06
38	n	611	KC2	C2B-C1B-NB	2.14	112.24	110.13
28	A	811	CLA	O2D-CGD-CBD	2.14	114.97	111.23
31	K	104	WVN	C21-C15-C13	-2.14	122.15	124.48
28	A	801	CLA	CHB-C4A-NA	2.14	127.48	124.40
28	c	611	CLA	CMB-C2B-C3B	2.14	131.58	126.55
31	B	848	WVN	C16-C05-C09	-2.14	115.19	122.37
28	k	603	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
31	s	205	WVN	C30-C33-C34	-2.13	120.51	126.36
36	m	616	II0	C30-C32-C34	-2.13	117.01	123.20
31	l	315	WVN	C03-C04-C09	-2.13	108.49	112.07
28	B	840	CLA	CHB-C1B-NB	2.13	127.25	124.05
37	b	616	IHT	C19-C10-C07	-2.13	122.16	124.48
37	f	617	IHT	C29-C31-C34	-2.13	117.02	123.20
28	f	610	CLA	O2D-CGD-CBD	2.13	114.96	111.23
36	n	615	II0	C19-C13-C11	2.13	118.34	114.42
28	B	832	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
28	A	801	CLA	CHC-C4B-NB	2.13	127.25	124.05
28	i	302	CLA	C3B-C4B-NB	-2.13	108.63	110.53
36	a	314	II0	C34-C36-C40	-2.13	115.66	119.01
28	m	612	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
31	s	207	WVN	C40-C39-C36	-2.13	119.16	123.52
36	k	621	II0	C20-C14-C12	2.13	118.34	114.42
28	B	808	CLA	C11-C12-C13	-2.13	108.88	115.97
31	M	101	WVN	C40-C39-C36	-2.13	119.16	123.52
28	d	304	CLA	C1-C2-C3	-2.13	122.71	126.20
37	b	616	IHT	C19-C10-C09	2.13	118.14	113.60
36	k	615	II0	C16-C03-C09	-2.13	106.70	110.52
28	g	322	CLA	CHD-C1D-ND	-2.13	121.81	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	605	CLA	C2A-C1A-CHA	2.13	127.56	123.87
36	l	313	II0	C31-C29-C25	-2.13	120.66	126.61
36	m	614	II0	C20-C14-C12	2.13	118.33	114.42
28	O	206	CLA	C7-C6-C5	-2.13	107.59	113.26
28	L	202	CLA	CHB-C1B-NB	2.13	127.24	124.05
28	B	809	CLA	CMB-C2B-C3B	2.13	129.19	123.53
36	g	317	II0	C32-C34-C36	-2.13	120.53	126.36
38	k	611	KC2	C2B-C1B-NB	2.13	112.23	110.13
28	A	805	CLA	CHB-C4A-NA	2.13	127.47	124.40
31	J	102	WVN	C29-C31-C32	-2.13	120.53	126.36
28	m	607	CLA	O2D-CGD-CBD	2.13	114.95	111.23
28	f	602	CLA	O2D-CGD-CBD	2.13	114.95	111.23
28	m	605	CLA	C3B-C4B-NB	-2.13	108.63	110.53
38	l	310	KC2	C2B-C1B-NB	2.13	112.23	110.13
28	Q	302	CLA	C3B-C4B-NB	-2.13	108.63	110.53
31	F	204	WVN	C38-C34-C37	-2.12	119.37	122.82
31	R	201	WVN	C16-C05-C09	-2.12	115.23	122.37
28	B	836	CLA	C4-C3-C5	2.12	118.92	115.23
28	f	610	CLA	CHB-C4A-NA	2.12	127.47	124.40
31	J	102	WVN	C27-C25-C28	-2.12	119.38	122.82
28	a	307	CLA	C2A-C1A-CHA	2.12	127.55	123.87
28	f	609	CLA	O2D-CGD-CBD	2.12	114.94	111.23
30	i	318	LHG	O8-C23-O10	-2.12	118.32	123.63
36	e	614	II0	C29-C31-C33	-2.12	117.05	123.20
28	k	602	CLA	C1-O2A-CGA	-2.12	111.51	116.65
36	l	312	II0	C06-C04-C10	2.12	113.67	109.49
28	n	609	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
28	A	840	CLA	CHC-C4B-NB	2.12	127.23	124.05
28	Q	302	CLA	CMD-C2D-C1D	-2.12	120.99	124.73
36	k	617	II0	C29-C31-C33	-2.12	117.06	123.20
28	A	814	CLA	O2D-CGD-CBD	2.12	114.94	111.23
38	d	311	KC2	CMB-C2B-C1B	2.12	128.46	124.73
28	b	611	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
28	B	840	CLA	C3B-C4B-NB	-2.12	108.64	110.53
36	k	621	II0	C05-C03-C09	2.12	113.67	109.49
28	B	804	CLA	C11-C12-C13	-2.12	108.92	115.97
28	m	607	CLA	C1-C2-C3	-2.12	122.72	126.20
31	R	201	WVN	C26-C29-C31	-2.12	117.06	123.20
31	e	615	WVN	C01-C02-C11	-2.12	110.39	112.83
31	A	845	WVN	C10-C12-C14	2.12	115.93	111.28
28	l	308	CLA	CHD-C1D-ND	-2.12	121.82	124.80
28	B	811	CLA	C14-C13-C12	-2.12	103.72	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	601	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
28	s	208	CLA	C3B-C4B-NB	-2.12	108.64	110.53
28	B	808	CLA	CHC-C4B-NB	2.12	127.22	124.05
28	h	313	CLA	CHB-C1B-NB	2.12	127.22	124.05
37	g	319	IHT	C40-C41-C38	-2.12	119.19	123.52
28	a	312	CLA	C3A-C2A-C1A	2.12	104.51	101.34
28	f	610	CLA	CBC-CAC-C3C	-2.12	106.68	112.42
31	K	102	WVN	C23-C20-C13	-2.12	121.35	127.00
28	e	602	CLA	O1D-CGD-CBD	2.12	128.69	124.52
36	f	614	II0	C12-C14-C10	-2.12	116.10	120.50
36	c	615	II0	C38-C36-C40	-2.12	119.39	122.82
28	A	834	CLA	C3B-C4B-NB	-2.11	108.64	110.53
28	k	603	CLA	C3B-C4B-NB	-2.11	108.64	110.53
28	A	805	CLA	C1-C2-C3	-2.11	122.73	126.20
28	A	815	CLA	CHC-C4B-NB	2.11	127.22	124.05
38	n	612	KC2	CAB-C3B-C4B	-2.11	119.78	124.82
28	L	204	CLA	O2D-CGD-CBD	2.11	114.92	111.23
28	d	312	CLA	C2A-C1A-CHA	2.11	127.53	123.87
31	M	101	WVN	C16-C05-C09	-2.11	115.27	122.37
28	f	602	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
28	d	308	CLA	C3B-C4B-NB	-2.11	108.64	110.53
28	b	612	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
31	F	204	WVN	C28-C30-C33	2.11	129.32	123.20
28	B	836	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
39	i	301	LMU	O5'-C5'-C4'	2.11	114.09	109.72
28	f	601	CLA	CHA-C1A-NA	-2.11	121.61	126.39
28	l	308	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
28	d	312	CLA	CAC-C3C-C4C	2.11	127.54	124.79
28	c	606	CLA	C1-C2-C3	-2.11	122.74	126.20
28	b	602	CLA	C1-O2A-CGA	-2.11	111.54	116.65
36	i	313	II0	C18-C04-C10	-2.11	106.74	110.52
31	l	301	WVN	C30-C33-C34	-2.11	120.58	126.36
28	a	304	CLA	O2D-CGD-CBD	2.11	114.92	111.23
28	n	608	CLA	CHA-C4D-ND	2.11	136.90	132.55
36	d	314	II0	C20-C14-C12	2.11	118.30	114.42
28	A	808	CLA	CHA-C1A-NA	-2.11	121.62	126.39
28	e	607	CLA	O2D-CGD-CBD	2.11	114.92	111.23
28	A	831	CLA	C11-C10-C8	-2.11	108.96	115.97
36	b	614	II0	C32-C30-C26	-2.11	120.72	126.61
28	Q	302	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
38	g	314	KC2	CAA-CBA-CGA	-2.11	116.33	127.05
36	g	316	II0	C05-C03-C09	2.11	113.64	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	k	604	CLA	C1-C2-C3	-2.11	122.74	126.20
28	A	819	CLA	C2A-C1A-CHA	2.11	127.52	123.87
36	c	614	II0	C12-C14-C10	-2.11	116.11	120.50
35	L	209	LMG	O8-C28-O10	-2.11	118.36	123.63
28	e	611	CLA	C3B-C4B-NB	-2.11	108.65	110.53
38	e	609	KC2	C2B-C1B-NB	2.11	112.21	110.13
36	n	618	II0	C37-C35-C39	-2.11	119.41	122.82
28	A	815	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
28	j	603	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
36	h	311	II0	C32-C34-C36	-2.11	120.59	126.36
28	A	828	CLA	C3B-C4B-NB	-2.10	108.65	110.53
38	j	611	KC2	CHD-C1D-C2D	2.10	133.53	127.43
28	A	815	CLA	CHB-C4A-NA	2.10	127.44	124.40
28	f	609	CLA	C4-C3-C5	2.10	118.88	115.23
28	B	827	CLA	CHC-C4B-NB	2.10	127.20	124.05
36	k	619	II0	C38-C36-C34	2.10	121.30	118.09
28	n	603	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
28	g	307	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
38	n	612	KC2	CHD-C1D-C2D	2.10	133.53	127.43
28	h	301	CLA	CMA-C3A-C2A	-2.10	105.86	113.98
28	a	305	CLA	C3A-C2A-C1A	2.10	104.49	101.34
29	A	842	PQN	C14-C13-C15	2.10	118.88	115.23
38	c	610	KC2	C2B-C1B-NB	2.10	112.21	110.13
28	B	833	CLA	CBA-CAA-C2A	2.10	120.05	113.79
38	g	313	KC2	CHD-C1D-C2D	2.10	133.52	127.43
35	J	105	LMG	O1-C7-C8	-2.10	105.71	110.82
28	j	603	CLA	CHB-C1B-NB	2.10	127.20	124.05
31	l	315	WVN	C16-C05-C09	-2.10	115.31	122.37
36	i	313	II0	C11-C13-C09	-2.10	116.13	120.50
28	B	841	CLA	C16-C15-C13	-2.10	108.98	115.97
31	e	615	WVN	C23-C20-C13	-2.10	121.39	127.00
28	A	821	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
38	k	611	KC2	CHD-C1D-C2D	2.10	133.52	127.43
28	A	840	CLA	O1D-CGD-CBD	2.10	128.66	124.52
36	a	316	II0	C16-C03-C09	-2.10	106.76	110.52
28	B	801	CLA	C1-C2-C3	-2.10	122.76	126.20
36	n	616	II0	C30-C32-C34	-2.10	117.12	123.20
28	A	812	CLA	O2D-CGD-CBD	2.10	114.90	111.23
36	l	314	II0	C04-C06-C08	2.10	118.19	113.59
38	n	611	KC2	C4D-CHA-C1A	-2.10	116.06	122.45
31	L	201	WVN	C27-C25-C23	2.10	121.29	118.09
28	j	613	CLA	C1-C2-C3	-2.10	122.76	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	j	604	CLA	C11-C12-C13	-2.10	109.00	115.97
28	m	603	CLA	CAA-CBA-CGA	-2.10	107.26	113.21
38	c	610	KC2	CAB-C3B-C4B	-2.09	119.82	124.82
28	i	304	CLA	C3B-C4B-NB	-2.09	108.66	110.53
28	g	303	CLA	O2D-CGD-CBD	2.09	114.89	111.23
28	a	307	CLA	CHB-C1B-NB	2.09	127.19	124.05
28	m	602	CLA	O2D-CGD-CBD	2.09	114.89	111.23
30	e	617	LHG	O7-C7-O9	-2.09	118.81	123.70
28	B	818	CLA	O2D-CGD-CBD	2.09	114.89	111.23
38	d	310	KC2	C2B-C1B-NB	2.09	112.20	110.13
28	A	807	CLA	C11-C10-C8	-2.09	109.01	115.97
28	B	831	CLA	CHB-C4A-NA	2.09	127.42	124.40
28	n	606	CLA	C3B-C4B-NB	-2.09	108.66	110.53
28	A	831	CLA	C2A-C1A-CHA	2.09	127.50	123.87
28	g	308	CLA	CHC-C4B-NB	2.09	127.19	124.05
28	c	604	CLA	CHB-C1B-NB	2.09	127.19	124.05
28	A	806	CLA	CHB-C4A-NA	2.09	127.42	124.40
28	A	825	CLA	CHB-C4A-NA	2.09	127.42	124.40
28	B	822	CLA	CHB-C4A-NA	2.09	127.42	124.40
28	j	610	CLA	C1-C2-C3	-2.09	122.78	126.20
38	k	611	KC2	O1D-CGD-CBD	-2.09	120.40	124.52
28	f	609	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
28	f	605	CLA	O2A-CGA-O1A	-2.09	117.96	123.33
30	g	301	LHG	O9-C7-C8	-2.09	115.62	123.78
28	f	603	CLA	C3B-C4B-NB	-2.09	108.67	110.53
36	g	316	II0	C06-C04-C10	2.09	113.60	109.49
36	m	614	II0	C19-C13-C11	2.09	118.26	114.42
38	k	612	KC2	CAB-C3B-C4B	-2.09	119.84	124.82
30	g	321	LHG	C9-C8-C7	-2.09	106.05	113.69
31	R	202	WVN	C40-C37-C34	-2.09	124.35	127.28
28	i	303	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
28	O	206	CLA	C1-O2A-CGA	-2.08	111.60	116.65
28	B	821	CLA	C3B-C4B-NB	-2.08	108.67	110.53
38	j	611	KC2	CMB-C2B-C1B	2.08	128.40	124.73
28	A	836	CLA	CHC-C4B-NB	2.08	127.18	124.05
28	k	614	CLA	O2D-CGD-CBD	2.08	114.87	111.23
31	A	848	WVN	C12-C14-C15	-2.08	110.34	114.06
37	b	615	IHT	C29-C31-C34	-2.08	117.16	123.20
36	f	614	II0	C18-C04-C10	-2.08	106.79	110.52
36	g	320	II0	C38-C36-C34	2.08	121.27	118.09
28	b	606	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
36	h	311	II0	C05-C03-C09	2.08	113.59	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	k	621	II0	C15-C03-C09	-2.08	106.79	110.52
37	R	204	IHT	C20-C15-C12	2.08	118.25	114.42
36	d	315	II0	C31-C33-C35	-2.08	120.65	126.36
28	j	612	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
28	A	832	CLA	CHB-C1B-NB	2.08	127.17	124.05
38	g	314	KC2	CAB-C3B-C4B	-2.08	119.85	124.82
28	A	840	CLA	C3B-C4B-NB	-2.08	108.67	110.53
36	f	616	II0	C19-C13-C11	2.08	118.25	114.42
28	A	838	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
28	A	806	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
28	A	818	CLA	CBC-CAC-C3C	2.08	118.06	112.42
28	K	103	CLA	CAC-C3C-C4C	2.08	127.50	124.79
28	m	613	CLA	CAC-C3C-C4C	-2.08	122.08	124.79
28	a	312	CLA	C3B-C4B-NB	-2.08	108.67	110.53
28	a	310	CLA	CHC-C4B-NB	2.08	127.17	124.05
28	k	605	CLA	CMC-C2C-C3C	2.08	131.77	126.15
28	B	820	CLA	C1-C2-C3	-2.08	122.79	126.20
28	B	808	CLA	C4-C3-C5	2.08	118.83	115.23
28	f	610	CLA	CMD-C2D-C3D	2.08	132.45	127.69
35	c	619	LMG	O6-C5-C6	2.08	111.59	106.44
36	i	320	II0	C32-C30-C26	-2.08	120.80	126.61
28	h	303	CLA	O2D-CGD-CBD	2.08	114.86	111.23
38	c	610	KC2	CAA-CBA-CGA	-2.08	116.49	127.05
28	B	834	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
28	d	308	CLA	O2D-CGD-CBD	2.08	114.86	111.23
28	b	608	CLA	C7-C6-C5	-2.08	107.73	113.26
36	k	617	II0	C32-C34-C36	-2.07	120.67	126.36
28	B	840	CLA	CHC-C4B-NB	2.07	127.16	124.05
28	B	821	CLA	CHA-C1A-NA	-2.07	121.70	126.39
29	B	842	PQN	C6-C5-C10	2.07	121.59	119.26
37	k	618	IHT	C36-C33-C32	2.07	121.25	118.09
28	f	607	CLA	C3B-C4B-NB	-2.07	108.68	110.53
28	b	612	CLA	C1-C2-C3	-2.07	122.80	126.20
38	s	204	KC2	CAC-C3C-C4C	2.07	133.54	124.39
36	a	314	II0	C42-C41-C39	-2.07	119.28	123.52
28	b	612	CLA	CMB-C2B-C3B	2.07	131.42	126.55
28	j	603	CLA	C3B-C4B-NB	-2.07	108.68	110.53
36	k	617	II0	C20-C14-C12	2.07	118.22	114.42
28	j	612	CLA	O2D-CGD-CBD	2.07	114.85	111.23
36	m	616	II0	C29-C31-C33	-2.07	117.21	123.20
28	O	206	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
28	m	608	CLA	O2A-CGA-O1A	-2.07	118.45	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	816	CLA	O2D-CGD-CBD	2.07	114.84	111.23
37	g	319	IHT	C28-C26-C29	-2.07	120.17	124.18
28	d	308	CLA	CMA-C3A-C2A	-2.07	111.49	116.23
36	g	320	II0	C37-C35-C33	2.07	121.25	118.09
28	g	306	CLA	CHB-C4A-NA	2.07	127.38	124.40
36	n	615	II0	C05-C03-C09	2.07	113.56	109.49
36	c	617	II0	C17-C04-C10	-2.07	106.82	110.52
28	B	823	CLA	C7-C6-C5	-2.07	107.75	113.26
28	K	101	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
38	l	310	KC2	CAA-CBA-CGA	-2.07	116.54	127.05
28	l	308	CLA	O2D-CGD-CBD	2.07	114.84	111.23
28	b	603	CLA	C4-C3-C5	2.07	118.81	115.23
28	A	852	CLA	C11-C12-C13	-2.07	109.10	115.97
28	m	610	CLA	CMC-C2C-C1C	-2.07	121.81	125.03
36	k	616	II0	C19-C13-C09	-2.06	120.30	124.16
28	h	308	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
30	i	318	LHG	O4-P-O5	2.06	122.05	112.44
28	B	812	CLA	C1-C2-C3	-2.06	122.82	126.20
28	g	306	CLA	C3B-C4B-NB	-2.06	108.69	110.53
28	B	818	CLA	CHB-C4A-NA	2.06	127.38	124.40
30	A	844	LHG	O8-C23-O10	-2.06	118.47	123.63
28	A	821	CLA	CHD-C1D-ND	-2.06	121.90	124.80
28	l	307	CLA	C6-C7-C8	-2.06	109.11	115.97
28	h	301	CLA	C7-C6-C5	-2.06	107.77	113.26
28	l	307	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
28	n	607	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
28	B	818	CLA	C3B-C4B-NB	-2.06	108.69	110.53
28	A	811	CLA	CHB-C1B-NB	2.06	127.14	124.05
28	m	602	CLA	CHB-C4A-NA	2.06	127.37	124.40
38	s	201	KC2	CAC-C3C-C4C	2.06	133.50	124.39
28	B	827	CLA	O2D-CGD-CBD	2.06	114.83	111.23
28	f	608	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
28	n	609	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
38	g	314	KC2	CHD-C1D-C2D	2.06	133.41	127.43
28	j	601	CLA	O2D-CGD-CBD	2.06	114.83	111.23
28	g	304	CLA	C3B-C4B-NB	-2.06	108.69	110.53
30	j	617	LHG	O7-C7-O9	-2.06	118.89	123.70
36	i	313	II0	C31-C29-C25	-2.06	120.86	126.61
36	g	320	II0	C11-C13-C09	-2.06	116.22	120.50
31	A	847	WVN	C39-C36-C32	-2.06	124.39	127.28
36	n	615	II0	C42-C41-C39	-2.06	119.31	123.52
36	d	313	II0	C11-C13-C09	-2.06	116.22	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	101	WVN	C35-C32-C31	2.06	121.23	118.09
38	i	319	KC2	CAC-C3C-C4C	2.06	133.48	124.39
28	g	307	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
39	i	301	LMU	C1'-C2'-C3'	2.06	114.33	110.01
28	a	310	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
31	J	102	WVN	C16-C05-C09	-2.05	115.46	122.37
28	B	823	CLA	C16-C15-C13	-2.05	109.14	115.97
36	l	316	II0	C28-C26-C30	-2.05	120.19	124.18
36	d	316	II0	C27-C25-C29	-2.05	120.19	124.18
36	c	614	II0	C17-C04-C10	2.05	114.20	110.52
28	B	805	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
28	n	602	CLA	CHA-C1A-NA	-2.05	121.74	126.39
36	c	615	II0	C38-C36-C34	2.05	121.22	118.09
28	n	609	CLA	C6-C7-C8	-2.05	109.14	115.97
36	k	619	II0	C20-C14-C12	2.05	118.20	114.42
36	j	614	II0	C19-C13-C11	2.05	118.20	114.42
28	m	604	CLA	O2D-CGD-CBD	2.05	114.82	111.23
38	i	319	KC2	CHD-C1D-C2D	2.05	133.38	127.43
36	j	615	II0	C20-C14-C12	2.05	118.19	114.42
36	m	616	II0	C06-C04-C10	2.05	113.53	109.49
28	B	818	CLA	CHD-C1D-ND	-2.05	121.92	124.80
28	A	801	CLA	C3B-C4B-NB	-2.05	108.70	110.53
32	A	850	LMT	O5'-C1'-O1'	-2.05	105.20	110.04
28	e	602	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
28	g	307	CLA	O2D-CGD-CBD	2.05	114.81	111.23
28	B	810	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
28	B	803	CLA	CHC-C1C-NC	2.05	127.40	124.31
28	A	851	CLA	CHA-C1A-NA	-2.05	121.75	126.39
38	g	312	KC2	CAB-C3B-C2B	2.05	135.09	128.43
28	l	309	CLA	C2A-C1A-CHA	2.05	127.42	123.87
31	B	847	WVN	C29-C26-C22	-2.05	124.41	127.28
38	n	612	KC2	CAC-C3C-C4C	2.05	133.44	124.39
28	b	608	CLA	CMB-C2B-C3B	2.05	131.36	126.55
30	j	617	LHG	O8-C23-O10	-2.05	118.51	123.63
28	A	815	CLA	C3B-C4B-NB	-2.05	108.70	110.53
28	c	607	CLA	C4A-NA-C1A	2.05	107.61	106.68
28	a	304	CLA	CMA-C3A-C2A	-2.04	106.08	113.98
28	m	603	CLA	O1D-CGD-CBD	2.04	128.55	124.52
31	i	316	WVN	C06-C13-C20	2.04	121.20	115.65
28	m	610	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
28	d	312	CLA	CHD-C1D-ND	-2.04	121.93	124.80
28	B	839	CLA	C11-C10-C8	-2.04	109.17	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	j	613	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
28	j	608	CLA	O1D-CGD-CBD	2.04	128.55	124.52
36	n	616	II0	C06-C04-C10	2.04	113.52	109.49
28	A	807	CLA	C3B-C4B-NB	-2.04	108.71	110.53
36	l	314	II0	C05-C03-C09	2.04	113.52	109.49
30	A	843	LHG	O8-C23-O10	-2.04	118.52	123.63
36	b	613	II0	C33-C35-C39	-2.04	115.80	119.01
28	A	816	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
28	k	601	CLA	CAC-C3C-C4C	2.04	127.45	124.79
28	b	609	CLA	CHD-C1D-ND	-2.04	121.93	124.80
28	B	815	CLA	O2D-CGD-CBD	2.04	114.80	111.23
38	i	319	KC2	C4D-CHA-C1A	-2.04	116.23	122.45
38	s	204	KC2	CAA-CBA-CGA	-2.04	116.67	127.05
36	n	616	II0	C12-C14-C10	-2.04	116.25	120.50
28	g	309	CLA	C11-C10-C8	-2.04	109.18	115.97
28	n	609	CLA	CMB-C2B-C3B	2.04	131.35	126.55
31	J	101	WVN	C03-C04-C09	-2.04	108.64	112.07
36	n	616	II0	C27-C25-C29	-2.04	120.22	124.18
28	K	103	CLA	CHA-C1A-NA	-2.04	121.77	126.39
28	n	602	CLA	CHD-C1D-ND	-2.04	121.93	124.80
36	e	614	II0	C18-C04-C10	-2.04	106.87	110.52
28	B	806	CLA	C1-C2-C3	-2.04	122.86	126.20
28	B	837	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
28	A	827	CLA	O1D-CGD-CBD	2.04	128.54	124.52
28	A	806	CLA	CHB-C1B-NB	2.04	127.11	124.05
28	A	831	CLA	CHC-C4B-NB	2.04	127.11	124.05
28	a	311	CLA	C1-C2-C3	-2.04	122.86	126.20
28	j	602	CLA	C3B-C4B-NB	-2.04	108.71	110.53
28	d	302	CLA	CHB-C1B-NB	2.04	127.10	124.05
28	B	823	CLA	O2D-CGD-CBD	2.04	114.79	111.23
28	d	301	CLA	O2A-CGA-CBA	2.04	118.04	111.83
28	d	301	CLA	C1-O2A-CGA	-2.04	111.72	116.65
38	g	312	KC2	C2B-C1B-NB	2.04	112.14	110.13
28	a	305	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
36	m	614	II0	C38-C36-C34	2.04	121.20	118.09
36	c	613	II0	C08-C12-C14	2.04	117.25	112.18
28	A	836	CLA	C4-C3-C5	2.04	118.76	115.23
28	m	609	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
30	g	321	LHG	O8-C23-O10	-2.03	118.54	123.63
36	k	615	II0	C38-C36-C40	-2.03	119.52	122.82
30	c	620	LHG	O7-C7-O9	-2.03	118.95	123.70
28	f	612	CLA	CAC-C3C-C2C	-2.03	123.82	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	810	CLA	CHD-C1D-ND	-2.03	121.94	124.80
28	O	201	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
28	A	801	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
35	c	619	LMG	O1-C1-C2	2.03	111.36	108.27
28	B	829	CLA	CHA-C1A-NA	-2.03	121.79	126.39
36	h	311	II0	C29-C31-C33	-2.03	117.31	123.20
28	B	830	CLA	CHC-C4B-NB	2.03	127.10	124.05
28	a	303	CLA	O2D-CGD-CBD	2.03	114.78	111.23
28	k	601	CLA	O2D-CGD-CBD	2.03	114.78	111.23
38	n	611	KC2	CAA-CBA-CGA	-2.03	116.72	127.05
36	d	314	II0	C32-C30-C26	-2.03	120.94	126.61
36	e	613	II0	C16-C03-C09	-2.03	106.88	110.52
31	R	201	WVN	C03-C04-C09	-2.03	108.66	112.07
28	A	828	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
28	c	607	CLA	C3B-C4B-NB	-2.03	108.72	110.53
36	i	317	II0	C16-C03-C15	-2.03	102.83	108.63
28	A	818	CLA	CHB-C4A-NA	2.03	127.33	124.40
31	i	316	WVN	C02-C05-C09	2.03	123.96	121.47
28	h	306	CLA	CMA-C3A-C2A	-2.03	106.14	113.98
36	m	615	II0	C31-C33-C35	-2.03	120.81	126.36
28	i	302	CLA	CBC-CAC-C3C	-2.03	106.93	112.42
38	m	611	KC2	CAA-C2A-C1A	2.03	133.52	124.64
28	f	602	CLA	O2A-CGA-CBA	2.03	118.01	111.83
36	c	615	II0	C16-C03-C09	-2.03	106.89	110.52
28	B	821	CLA	C5-C3-C2	2.03	125.71	121.17
28	k	607	CLA	CED-O2D-CGD	2.03	120.51	115.92
28	l	304	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
36	a	314	II0	C37-C35-C33	2.02	121.18	118.09
28	B	841	CLA	C11-C12-C13	-2.02	109.24	115.97
28	k	604	CLA	C4-C3-C5	2.02	118.74	115.23
38	e	609	KC2	CAB-C3B-C4B	-2.02	119.99	124.82
31	h	309	WVN	C35-C32-C31	2.02	121.18	118.09
28	n	606	CLA	C1-C2-C3	-2.02	122.88	126.20
28	B	802	CLA	O2D-CGD-CBD	2.02	114.77	111.23
30	J	106	LHG	O7-C7-O9	-2.02	118.98	123.70
28	O	202	CLA	CHA-C1A-NA	-2.02	121.81	126.39
28	f	610	CLA	C4-C3-C5	2.02	118.74	115.23
28	g	307	CLA	CMB-C2B-C3B	2.02	131.31	126.55
30	i	318	LHG	O7-C7-O9	-2.02	118.98	123.70
36	h	310	II0	C05-C03-C09	2.02	113.47	109.49
28	e	602	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
28	j	606	CLA	C1-C2-C3	-2.02	122.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	k	614	CLA	C2A-C1A-CHA	2.02	127.37	123.87
28	F	201	CLA	CHA-C1A-NA	-2.02	121.81	126.39
28	B	832	CLA	C1-O2A-CGA	2.02	121.54	116.65
31	J	101	WVN	C28-C30-C33	-2.02	117.34	123.20
28	j	605	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
28	A	840	CLA	CMB-C2B-C3B	2.02	131.30	126.55
37	R	204	IHT	C36-C33-C37	-2.02	119.54	122.82
28	L	203	CLA	CMB-C2B-C3B	2.02	131.30	126.55
37	b	616	IHT	C41-C38-C35	-2.02	124.45	127.28
38	i	319	KC2	CMB-C2B-C1B	2.02	128.28	124.73
28	g	310	CLA	CHD-C1D-ND	-2.02	121.96	124.80
28	l	308	CLA	CHD-C1D-C2D	2.02	129.69	125.49
28	B	841	CLA	C1-C2-C3	-2.02	122.89	126.20
28	c	602	CLA	CHB-C1B-NB	2.02	127.08	124.05
28	b	605	CLA	CAA-C2A-C1A	2.02	118.59	111.97
31	R	202	WVN	C16-C05-C09	-2.02	115.59	122.37
30	j	617	LHG	O4-P-O5	2.02	121.83	112.44
38	s	204	KC2	C2B-C1B-NB	2.02	112.12	110.13
31	B	848	WVN	C21-C15-C14	2.02	117.89	113.60
31	L	206	WVN	C16-C05-C09	-2.02	115.59	122.37
28	k	607	CLA	C3B-C4B-NB	-2.02	108.73	110.53
31	l	315	WVN	C30-C33-C34	-2.01	120.84	126.36
28	b	605	CLA	CHA-C1A-NA	-2.01	121.83	126.39
31	L	201	WVN	C38-C34-C33	2.01	121.17	118.09
28	c	606	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
38	m	611	KC2	CHD-C1D-C2D	2.01	133.27	127.43
30	n	619	LHG	C5-O7-C7	-2.01	112.98	117.80
28	c	601	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
28	f	612	CLA	CAA-C2A-C1A	2.01	118.57	111.97
28	g	305	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
28	n	605	CLA	CAC-C3C-C4C	2.01	127.41	124.79
28	K	103	CLA	CHA-C4D-ND	2.01	136.70	132.55
28	e	608	CLA	O2D-CGD-CBD	2.01	114.75	111.23
31	A	846	WVN	C40-C37-C34	-2.01	124.45	127.28
38	i	310	KC2	CAB-C3B-C2B	2.01	134.97	128.43
28	b	609	CLA	CAC-C3C-C4C	2.01	127.41	124.79
31	J	101	WVN	C23-C20-C13	-2.01	121.62	127.00
28	d	302	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
28	F	201	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
28	A	840	CLA	C11-C12-C13	-2.01	109.28	115.97
28	m	607	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
36	k	617	II0	C27-C25-C29	-2.01	120.28	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	604	CLA	CHC-C4B-NB	2.01	127.06	124.05
38	f	611	KC2	CAC-C3C-C4C	2.01	133.27	124.39
28	B	816	CLA	CHC-C4B-NB	2.01	127.06	124.05
28	A	819	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
28	k	605	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
28	a	311	CLA	C3A-C2A-C1A	2.01	104.35	101.34
28	B	801	CLA	CHB-C4A-NA	2.01	127.30	124.40
28	n	605	CLA	CHA-C1A-NA	-2.01	121.85	126.39
28	Q	303	CLA	CHB-C4A-NA	2.01	127.30	124.40
28	a	306	CLA	O1D-CGD-CBD	2.01	128.48	124.52
31	R	202	WVN	C20-C13-C15	-2.01	116.93	121.56
28	B	817	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
36	f	618	II0	C37-C35-C39	-2.01	119.57	122.82
31	J	101	WVN	C12-C10-C06	-2.01	107.33	114.43
35	J	105	LMG	O8-C28-O10	-2.01	118.61	123.63
28	c	609	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
36	h	311	II0	C31-C33-C35	-2.00	120.87	126.36
28	A	815	CLA	C2D-C1D-ND	-2.00	108.14	110.13
31	J	102	WVN	C02-C05-C09	-2.00	119.00	121.47
28	c	611	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
28	l	304	CLA	CMB-C2B-C3B	2.00	131.26	126.55
30	n	619	LHG	O7-C7-O9	-2.00	119.02	123.70
31	M	101	WVN	C29-C31-C32	-2.00	120.87	126.36
28	A	852	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
36	c	613	II0	C05-C03-C09	2.00	113.44	109.49
35	J	105	LMG	C6-C5-C4	-2.00	108.10	113.02
28	m	601	CLA	O2D-CGD-CBD	2.00	114.73	111.23
28	h	313	CLA	C1-C2-C3	-2.00	122.92	126.20
38	s	204	KC2	C2D-C1D-ND	-2.00	108.25	110.33
35	O	205	LMG	O7-C10-O9	-2.00	119.03	123.70
28	B	832	CLA	C3A-C2A-C1A	2.00	104.34	101.34
31	B	845	WVN	C19-C22-C26	-2.00	115.86	119.01
28	f	606	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (217) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	A	801	CLA	ND
28	A	802	CLA	ND
28	A	803	CLA	ND
28	A	804	CLA	ND
28	A	805	CLA	ND

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Mol	Chain	Res	Type	Atom
28	A	806	CLA	ND
28	A	807	CLA	ND
28	A	808	CLA	ND
28	A	809	CLA	ND
28	A	810	CLA	ND
28	A	812	CLA	ND
28	A	813	CLA	ND
28	A	815	CLA	ND
28	A	816	CLA	ND
28	A	817	CLA	ND
28	A	818	CLA	ND
28	A	819	CLA	ND
28	A	820	CLA	ND
28	A	822	CLA	ND
28	A	824	CLA	ND
28	A	826	CLA	ND
28	A	827	CLA	ND
28	A	829	CLA	ND
28	A	831	CLA	ND
28	A	832	CLA	ND
28	A	833	CLA	ND
28	A	834	CLA	ND
28	A	835	CLA	ND
28	A	837	CLA	ND
28	A	838	CLA	ND
28	A	839	CLA	ND
28	A	840	CLA	ND
28	A	841	CLA	ND
28	A	851	CLA	ND
28	A	852	CLA	ND
28	A	854	CLA	ND
28	A	855	CLA	ND
28	B	801	CLA	ND
28	B	802	CLA	ND
28	B	803	CLA	ND
28	B	804	CLA	ND
28	B	805	CLA	ND
28	B	806	CLA	ND
28	B	807	CLA	ND
28	B	808	CLA	ND
28	B	809	CLA	ND
28	B	810	CLA	ND

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Mol	Chain	Res	Type	Atom
28	B	811	CLA	ND
28	B	812	CLA	ND
28	B	813	CLA	ND
28	B	815	CLA	ND
28	B	817	CLA	ND
28	B	820	CLA	ND
28	B	821	CLA	ND
28	B	823	CLA	ND
28	B	824	CLA	ND
28	B	825	CLA	ND
28	B	826	CLA	ND
28	B	828	CLA	ND
28	B	830	CLA	ND
28	B	831	CLA	ND
28	B	832	CLA	ND
28	B	833	CLA	ND
28	B	834	CLA	ND
28	B	835	CLA	ND
28	B	836	CLA	ND
28	B	837	CLA	ND
28	B	838	CLA	ND
28	B	839	CLA	ND
28	B	840	CLA	ND
28	F	201	CLA	ND
28	F	202	CLA	ND
28	J	103	CLA	ND
28	L	202	CLA	ND
28	L	207	CLA	ND
28	O	201	CLA	ND
28	O	202	CLA	ND
28	O	206	CLA	ND
28	K	101	CLA	ND
28	K	103	CLA	ND
28	s	202	CLA	ND
28	s	206	CLA	ND
28	s	208	CLA	ND
28	c	601	CLA	ND
28	c	602	CLA	ND
28	c	603	CLA	ND
28	c	605	CLA	ND
28	c	607	CLA	ND
28	c	608	CLA	ND

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Mol	Chain	Res	Type	Atom
28	c	609	CLA	ND
28	c	612	CLA	ND
28	a	303	CLA	ND
28	a	304	CLA	ND
28	a	305	CLA	ND
28	a	306	CLA	ND
28	a	307	CLA	ND
28	a	308	CLA	ND
28	a	309	CLA	ND
28	a	310	CLA	ND
28	a	311	CLA	ND
28	a	312	CLA	ND
28	b	601	CLA	ND
28	b	602	CLA	ND
28	b	603	CLA	ND
28	b	605	CLA	ND
28	b	606	CLA	ND
28	b	607	CLA	ND
28	b	608	CLA	ND
28	b	609	CLA	ND
28	b	610	CLA	ND
28	b	611	CLA	ND
28	b	612	CLA	ND
28	h	302	CLA	ND
28	h	303	CLA	ND
28	h	304	CLA	ND
28	h	305	CLA	ND
28	h	306	CLA	ND
28	h	307	CLA	ND
28	h	308	CLA	ND
28	h	313	CLA	ND
28	m	601	CLA	ND
28	m	602	CLA	ND
28	m	603	CLA	ND
28	m	606	CLA	ND
28	m	607	CLA	ND
28	m	608	CLA	ND
28	m	609	CLA	ND
28	m	610	CLA	ND
28	m	612	CLA	ND
28	m	613	CLA	ND
28	e	601	CLA	ND

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Mol	Chain	Res	Type	Atom
28	e	603	CLA	ND
28	e	606	CLA	ND
28	e	607	CLA	ND
28	e	608	CLA	ND
28	e	610	CLA	ND
28	e	611	CLA	ND
28	l	302	CLA	ND
28	l	303	CLA	ND
28	l	304	CLA	ND
28	l	305	CLA	ND
28	l	306	CLA	ND
28	l	307	CLA	ND
28	l	308	CLA	ND
28	l	309	CLA	ND
28	l	311	CLA	ND
28	k	602	CLA	ND
28	k	603	CLA	ND
28	k	604	CLA	ND
28	k	605	CLA	ND
28	k	607	CLA	ND
28	k	608	CLA	ND
28	k	609	CLA	ND
28	k	610	CLA	ND
28	k	614	CLA	ND
28	f	601	CLA	ND
28	f	602	CLA	ND
28	f	603	CLA	ND
28	f	604	CLA	ND
28	f	608	CLA	ND
28	f	609	CLA	ND
28	f	610	CLA	ND
28	f	612	CLA	ND
28	f	613	CLA	ND
28	i	302	CLA	ND
28	i	303	CLA	ND
28	i	304	CLA	ND
28	i	306	CLA	ND
28	i	307	CLA	ND
28	i	308	CLA	ND
28	i	309	CLA	ND
28	i	311	CLA	ND
28	i	312	CLA	ND

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Mol	Chain	Res	Type	Atom
28	j	601	CLA	ND
28	j	602	CLA	ND
28	j	603	CLA	ND
28	j	605	CLA	ND
28	j	606	CLA	ND
28	j	607	CLA	ND
28	j	608	CLA	ND
28	j	609	CLA	ND
28	j	610	CLA	ND
28	j	612	CLA	ND
28	j	613	CLA	ND
28	d	301	CLA	ND
28	d	302	CLA	ND
28	d	303	CLA	ND
28	d	304	CLA	ND
28	d	305	CLA	ND
28	d	306	CLA	ND
28	d	307	CLA	ND
28	d	308	CLA	ND
28	d	309	CLA	ND
28	g	302	CLA	ND
28	g	303	CLA	ND
28	g	304	CLA	ND
28	g	306	CLA	ND
28	g	307	CLA	ND
28	g	308	CLA	ND
28	g	309	CLA	ND
28	g	310	CLA	ND
28	g	311	CLA	ND
28	g	315	CLA	ND
28	g	322	CLA	ND
28	R	203	CLA	ND
28	n	601	CLA	ND
28	n	603	CLA	ND
28	n	604	CLA	ND
28	n	605	CLA	ND
28	n	606	CLA	ND
28	n	607	CLA	ND
28	n	608	CLA	ND
28	n	609	CLA	ND
28	n	610	CLA	ND
28	n	613	CLA	ND

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Mol	Chain	Res	Type	Atom
28	Q	302	CLA	ND
28	Q	303	CLA	ND

All (3727) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	801	CLA	CBD-CGD-O2D-CED
28	A	802	CLA	C1A-C2A-CAA-CBA
28	A	802	CLA	CBA-CGA-O2A-C1
28	A	802	CLA	O1A-CGA-O2A-C1
28	A	803	CLA	C1A-C2A-CAA-CBA
28	A	803	CLA	C3A-C2A-CAA-CBA
28	A	804	CLA	C3A-C2A-CAA-CBA
28	A	804	CLA	CAD-CBD-CGD-O2D
28	A	805	CLA	C1A-C2A-CAA-CBA
28	A	807	CLA	CHA-CBD-CGD-O1D
28	A	807	CLA	CHA-CBD-CGD-O2D
28	A	809	CLA	C1A-C2A-CAA-CBA
28	A	810	CLA	C1A-C2A-CAA-CBA
28	A	810	CLA	C3A-C2A-CAA-CBA
28	A	811	CLA	CBA-CGA-O2A-C1
28	A	813	CLA	C1A-C2A-CAA-CBA
28	A	813	CLA	CBD-CGD-O2D-CED
28	A	815	CLA	CBD-CGD-O2D-CED
28	A	815	CLA	O1D-CGD-O2D-CED
28	A	816	CLA	C1A-C2A-CAA-CBA
28	A	816	CLA	CHA-CBD-CGD-O1D
28	A	816	CLA	CHA-CBD-CGD-O2D
28	A	817	CLA	C1A-C2A-CAA-CBA
28	A	817	CLA	C3A-C2A-CAA-CBA
28	A	818	CLA	C3A-C2A-CAA-CBA
28	A	822	CLA	C4B-C3B-CAB-CBB
28	A	827	CLA	C11-C12-C13-C14
28	A	829	CLA	CHA-CBD-CGD-O1D
28	A	829	CLA	CHA-CBD-CGD-O2D
28	A	831	CLA	C1A-C2A-CAA-CBA
28	A	831	CLA	C2B-C3B-CAB-CBB
28	A	831	CLA	C4B-C3B-CAB-CBB
28	A	832	CLA	CHA-CBD-CGD-O1D
28	A	832	CLA	CHA-CBD-CGD-O2D
28	A	837	CLA	C3A-C2A-CAA-CBA
28	A	841	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	A	852	CLA	C14-C13-C15-C16
28	A	854	CLA	CBA-CGA-O2A-C1
28	A	854	CLA	O1A-CGA-O2A-C1
28	A	855	CLA	C2B-C3B-CAB-CBB
28	A	855	CLA	C4B-C3B-CAB-CBB
28	B	802	CLA	CBD-CGD-O2D-CED
28	B	804	CLA	C3A-C2A-CAA-CBA
28	B	805	CLA	CBD-CGD-O2D-CED
28	B	807	CLA	CHA-CBD-CGD-O1D
28	B	807	CLA	CHA-CBD-CGD-O2D
28	B	807	CLA	C14-C13-C15-C16
28	B	813	CLA	CAD-CBD-CGD-O1D
28	B	814	CLA	C1A-C2A-CAA-CBA
28	B	816	CLA	C3A-C2A-CAA-CBA
28	B	818	CLA	C1A-C2A-CAA-CBA
28	B	818	CLA	C3A-C2A-CAA-CBA
28	B	820	CLA	C2B-C3B-CAB-CBB
28	B	820	CLA	C4B-C3B-CAB-CBB
28	B	821	CLA	CHA-CBD-CGD-O1D
28	B	821	CLA	CHA-CBD-CGD-O2D
28	B	825	CLA	C1A-C2A-CAA-CBA
28	B	825	CLA	C3A-C2A-CAA-CBA
28	B	827	CLA	C1A-C2A-CAA-CBA
28	B	827	CLA	C3A-C2A-CAA-CBA
28	B	827	CLA	C4B-C3B-CAB-CBB
28	B	829	CLA	C4B-C3B-CAB-CBB
28	B	831	CLA	C1A-C2A-CAA-CBA
28	B	831	CLA	C2B-C3B-CAB-CBB
28	B	831	CLA	C4B-C3B-CAB-CBB
28	B	832	CLA	C1A-C2A-CAA-CBA
28	B	840	CLA	C1A-C2A-CAA-CBA
28	F	201	CLA	C6-C7-C8-C10
28	F	202	CLA	C1A-C2A-CAA-CBA
28	F	202	CLA	C3A-C2A-CAA-CBA
28	J	103	CLA	C1A-C2A-CAA-CBA
28	L	202	CLA	C1A-C2A-CAA-CBA
28	L	202	CLA	C3A-C2A-CAA-CBA
28	L	202	CLA	CBD-CGD-O2D-CED
28	L	203	CLA	C11-C12-C13-C14
28	L	204	CLA	C1A-C2A-CAA-CBA
28	L	204	CLA	C3A-C2A-CAA-CBA
28	L	207	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	L	207	CLA	C4-C3-C5-C6
28	O	201	CLA	C1A-C2A-CAA-CBA
28	O	201	CLA	C3A-C2A-CAA-CBA
28	O	201	CLA	C4-C3-C5-C6
28	O	202	CLA	C1A-C2A-CAA-CBA
28	O	202	CLA	CAD-CBD-CGD-O1D
28	O	202	CLA	CAD-CBD-CGD-O2D
28	O	202	CLA	CBD-CGD-O2D-CED
28	O	206	CLA	C1A-C2A-CAA-CBA
28	O	206	CLA	C3A-C2A-CAA-CBA
28	K	103	CLA	C3A-C2A-CAA-CBA
28	K	103	CLA	CBD-CGD-O2D-CED
28	s	202	CLA	C4B-C3B-CAB-CBB
28	s	203	CLA	C1A-C2A-CAA-CBA
28	s	206	CLA	C1A-C2A-CAA-CBA
28	s	208	CLA	C2B-C3B-CAB-CBB
28	s	208	CLA	C4B-C3B-CAB-CBB
28	c	601	CLA	C1A-C2A-CAA-CBA
28	c	602	CLA	C3A-C2A-CAA-CBA
28	c	602	CLA	CHA-CBD-CGD-O1D
28	c	602	CLA	CHA-CBD-CGD-O2D
28	c	605	CLA	C2B-C3B-CAB-CBB
28	c	605	CLA	C4B-C3B-CAB-CBB
28	c	605	CLA	C2-C3-C5-C6
28	c	605	CLA	C4-C3-C5-C6
28	c	606	CLA	C1A-C2A-CAA-CBA
28	c	608	CLA	C3A-C2A-CAA-CBA
28	c	608	CLA	CBD-CGD-O2D-CED
28	c	608	CLA	C14-C13-C15-C16
28	a	303	CLA	C3A-C2A-CAA-CBA
28	a	304	CLA	C1A-C2A-CAA-CBA
28	a	304	CLA	C3A-C2A-CAA-CBA
28	a	305	CLA	C2-C3-C5-C6
28	a	305	CLA	C4-C3-C5-C6
28	a	306	CLA	CAD-CBD-CGD-O2D
28	a	307	CLA	C2B-C3B-CAB-CBB
28	a	307	CLA	C4B-C3B-CAB-CBB
28	a	308	CLA	C1A-C2A-CAA-CBA
28	a	308	CLA	CHA-CBD-CGD-O2D
28	a	309	CLA	CHA-CBD-CGD-O1D
28	a	309	CLA	CHA-CBD-CGD-O2D
28	a	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	a	310	CLA	C4B-C3B-CAB-CBB
28	a	311	CLA	CHA-CBD-CGD-O2D
28	a	312	CLA	C1A-C2A-CAA-CBA
28	a	312	CLA	C2B-C3B-CAB-CBB
28	a	312	CLA	C4B-C3B-CAB-CBB
28	a	312	CLA	C11-C12-C13-C14
28	a	312	CLA	C14-C13-C15-C16
28	a	313	CLA	C2B-C3B-CAB-CBB
28	a	313	CLA	C4B-C3B-CAB-CBB
28	b	601	CLA	CHA-CBD-CGD-O1D
28	b	601	CLA	CHA-CBD-CGD-O2D
28	b	602	CLA	C3A-C2A-CAA-CBA
28	b	602	CLA	CHA-CBD-CGD-O1D
28	b	602	CLA	CHA-CBD-CGD-O2D
28	b	605	CLA	C2B-C3B-CAB-CBB
28	b	605	CLA	C4B-C3B-CAB-CBB
28	b	605	CLA	C14-C13-C15-C16
28	b	606	CLA	C2B-C3B-CAB-CBB
28	b	606	CLA	C4B-C3B-CAB-CBB
28	b	606	CLA	CBD-CGD-O2D-CED
28	b	607	CLA	C2B-C3B-CAB-CBB
28	b	607	CLA	C4B-C3B-CAB-CBB
28	b	608	CLA	C4-C3-C5-C6
28	b	609	CLA	CBD-CGD-O2D-CED
28	b	610	CLA	C1A-C2A-CAA-CBA
28	b	610	CLA	C2B-C3B-CAB-CBB
28	b	610	CLA	C4B-C3B-CAB-CBB
28	b	611	CLA	CBD-CGD-O2D-CED
28	b	612	CLA	CBA-CGA-O2A-C1
28	b	612	CLA	O1A-CGA-O2A-C1
28	b	612	CLA	C2B-C3B-CAB-CBB
28	b	612	CLA	C4B-C3B-CAB-CBB
28	b	612	CLA	C2-C3-C5-C6
28	h	303	CLA	C2B-C3B-CAB-CBB
28	h	303	CLA	C4B-C3B-CAB-CBB
28	h	304	CLA	C1A-C2A-CAA-CBA
28	h	304	CLA	C3A-C2A-CAA-CBA
28	h	304	CLA	CHA-CBD-CGD-O1D
28	h	304	CLA	CHA-CBD-CGD-O2D
28	h	305	CLA	C1A-C2A-CAA-CBA
28	h	305	CLA	C2-C3-C5-C6
28	h	305	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	h	306	CLA	CBD-CGD-O2D-CED
28	h	308	CLA	C2B-C3B-CAB-CBB
28	h	308	CLA	C4B-C3B-CAB-CBB
28	m	602	CLA	C1A-C2A-CAA-CBA
28	m	602	CLA	C3A-C2A-CAA-CBA
28	m	602	CLA	CHA-CBD-CGD-O1D
28	m	602	CLA	CHA-CBD-CGD-O2D
28	m	603	CLA	CBD-CGD-O2D-CED
28	m	605	CLA	C1A-C2A-CAA-CBA
28	m	605	CLA	C3A-C2A-CAA-CBA
28	m	607	CLA	C1A-C2A-CAA-CBA
28	m	607	CLA	C3A-C2A-CAA-CBA
28	m	607	CLA	CHA-CBD-CGD-O2D
28	m	608	CLA	C1A-C2A-CAA-CBA
28	m	608	CLA	C3A-C2A-CAA-CBA
28	m	609	CLA	C3A-C2A-CAA-CBA
28	m	610	CLA	C1A-C2A-CAA-CBA
28	m	610	CLA	C3A-C2A-CAA-CBA
28	m	610	CLA	C2B-C3B-CAB-CBB
28	m	610	CLA	C4B-C3B-CAB-CBB
28	m	612	CLA	C1A-C2A-CAA-CBA
28	m	612	CLA	C2-C3-C5-C6
28	m	613	CLA	CBD-CGD-O2D-CED
28	e	601	CLA	C1A-C2A-CAA-CBA
28	e	601	CLA	C3A-C2A-CAA-CBA
28	e	602	CLA	C3A-C2A-CAA-CBA
28	e	604	CLA	CBD-CGD-O2D-CED
28	e	605	CLA	C2B-C3B-CAB-CBB
28	e	605	CLA	C4B-C3B-CAB-CBB
28	e	607	CLA	C1A-C2A-CAA-CBA
28	e	608	CLA	C1A-C2A-CAA-CBA
28	e	608	CLA	C2B-C3B-CAB-CBB
28	e	608	CLA	C4B-C3B-CAB-CBB
28	e	611	CLA	C2B-C3B-CAB-CBB
28	e	611	CLA	C4B-C3B-CAB-CBB
28	e	611	CLA	C12-C13-C15-C16
28	l	302	CLA	C2B-C3B-CAB-CBB
28	l	302	CLA	C4B-C3B-CAB-CBB
28	l	303	CLA	C1A-C2A-CAA-CBA
28	l	303	CLA	C3A-C2A-CAA-CBA
28	l	303	CLA	C4B-C3B-CAB-CBB
28	l	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	l	303	CLA	CHA-CBD-CGD-O2D
28	l	305	CLA	CBD-CGD-O2D-CED
28	l	306	CLA	CBA-CGA-O2A-C1
28	l	306	CLA	O1A-CGA-O2A-C1
28	l	306	CLA	C2B-C3B-CAB-CBB
28	l	306	CLA	C4B-C3B-CAB-CBB
28	l	307	CLA	C1A-C2A-CAA-CBA
28	l	307	CLA	C3A-C2A-CAA-CBA
28	l	308	CLA	C3A-C2A-CAA-CBA
28	k	601	CLA	CBA-CGA-O2A-C1
28	k	601	CLA	O1A-CGA-O2A-C1
28	k	601	CLA	C2B-C3B-CAB-CBB
28	k	601	CLA	C4B-C3B-CAB-CBB
28	k	601	CLA	CBD-CGD-O2D-CED
28	k	601	CLA	C2-C3-C5-C6
28	k	602	CLA	C3A-C2A-CAA-CBA
28	k	602	CLA	CBD-CGD-O2D-CED
28	k	606	CLA	C1A-C2A-CAA-CBA
28	k	606	CLA	C2B-C3B-CAB-CBB
28	k	606	CLA	C4B-C3B-CAB-CBB
28	k	606	CLA	CBD-CGD-O2D-CED
28	k	607	CLA	C1A-C2A-CAA-CBA
28	k	607	CLA	CBA-CGA-O2A-C1
28	k	607	CLA	O1A-CGA-O2A-C1
28	k	607	CLA	CBD-CGD-O2D-CED
28	k	607	CLA	C2-C3-C5-C6
28	k	608	CLA	C1A-C2A-CAA-CBA
28	k	608	CLA	C3A-C2A-CAA-CBA
28	k	608	CLA	C2B-C3B-CAB-CBB
28	k	608	CLA	C4B-C3B-CAB-CBB
28	k	609	CLA	CBD-CGD-O2D-CED
28	k	610	CLA	C1A-C2A-CAA-CBA
28	k	610	CLA	C3A-C2A-CAA-CBA
28	k	610	CLA	C2B-C3B-CAB-CBB
28	k	610	CLA	C4B-C3B-CAB-CBB
28	k	610	CLA	CBD-CGD-O2D-CED
28	k	614	CLA	C2B-C3B-CAB-CBB
28	k	614	CLA	C4B-C3B-CAB-CBB
28	k	614	CLA	CBD-CGD-O2D-CED
28	f	602	CLA	C1A-C2A-CAA-CBA
28	f	602	CLA	C3A-C2A-CAA-CBA
28	f	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	f	602	CLA	C4B-C3B-CAB-CBB
28	f	606	CLA	C2-C3-C5-C6
28	f	607	CLA	C1A-C2A-CAA-CBA
28	f	607	CLA	C3A-C2A-CAA-CBA
28	f	607	CLA	C11-C12-C13-C14
28	f	609	CLA	CBD-CGD-O2D-CED
28	f	610	CLA	C1A-C2A-CAA-CBA
28	f	610	CLA	C3A-C2A-CAA-CBA
28	f	610	CLA	C2B-C3B-CAB-CBB
28	f	610	CLA	C4B-C3B-CAB-CBB
28	f	612	CLA	CBD-CGD-O2D-CED
28	f	612	CLA	C2-C3-C5-C6
28	f	613	CLA	CBD-CGD-O2D-CED
28	i	302	CLA	C3A-C2A-CAA-CBA
28	i	303	CLA	C3A-C2A-CAA-CBA
28	i	303	CLA	CHA-CBD-CGD-O1D
28	i	303	CLA	CHA-CBD-CGD-O2D
28	i	304	CLA	CBD-CGD-O2D-CED
28	i	305	CLA	CBD-CGD-O2D-CED
28	i	306	CLA	C1A-C2A-CAA-CBA
28	i	306	CLA	C3A-C2A-CAA-CBA
28	i	306	CLA	C2B-C3B-CAB-CBB
28	i	306	CLA	C4B-C3B-CAB-CBB
28	i	309	CLA	C1A-C2A-CAA-CBA
28	i	309	CLA	CBD-CGD-O2D-CED
28	i	311	CLA	C3A-C2A-CAA-CBA
28	i	312	CLA	C1A-C2A-CAA-CBA
28	j	604	CLA	CAD-CBD-CGD-O1D
28	j	604	CLA	CAD-CBD-CGD-O2D
28	j	606	CLA	CHA-CBD-CGD-O1D
28	j	606	CLA	CHA-CBD-CGD-O2D
28	j	607	CLA	CHA-CBD-CGD-O1D
28	j	607	CLA	CHA-CBD-CGD-O2D
28	j	610	CLA	C1A-C2A-CAA-CBA
28	j	610	CLA	C3A-C2A-CAA-CBA
28	j	612	CLA	CAD-CBD-CGD-O1D
28	j	612	CLA	CAD-CBD-CGD-O2D
28	j	613	CLA	CBD-CGD-O2D-CED
28	j	613	CLA	C14-C13-C15-C16
28	d	301	CLA	C1A-C2A-CAA-CBA
28	d	301	CLA	C3A-C2A-CAA-CBA
28	d	302	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	d	302	CLA	CHA-CBD-CGD-O2D
28	d	302	CLA	CBD-CGD-O2D-CED
28	d	303	CLA	C1A-C2A-CAA-CBA
28	d	303	CLA	C3A-C2A-CAA-CBA
28	d	303	CLA	C4-C3-C5-C6
28	d	305	CLA	C2B-C3B-CAB-CBB
28	d	305	CLA	C4B-C3B-CAB-CBB
28	d	305	CLA	CHA-CBD-CGD-O1D
28	d	305	CLA	CHA-CBD-CGD-O2D
28	d	306	CLA	C1A-C2A-CAA-CBA
28	d	306	CLA	C3A-C2A-CAA-CBA
28	d	306	CLA	CAD-CBD-CGD-O1D
28	d	306	CLA	CAD-CBD-CGD-O2D
28	d	309	CLA	CBD-CGD-O2D-CED
28	d	312	CLA	CHA-CBD-CGD-O1D
28	d	312	CLA	CHA-CBD-CGD-O2D
28	d	312	CLA	CBD-CGD-O2D-CED
28	g	303	CLA	C3A-C2A-CAA-CBA
28	g	306	CLA	C1A-C2A-CAA-CBA
28	g	310	CLA	C1A-C2A-CAA-CBA
28	g	310	CLA	CBA-CGA-O2A-C1
28	g	310	CLA	O1A-CGA-O2A-C1
28	g	310	CLA	CHA-CBD-CGD-O1D
28	g	310	CLA	CHA-CBD-CGD-O2D
28	g	315	CLA	C1A-C2A-CAA-CBA
28	g	315	CLA	C3A-C2A-CAA-CBA
28	g	315	CLA	C2B-C3B-CAB-CBB
28	g	315	CLA	C4B-C3B-CAB-CBB
28	g	322	CLA	CHA-CBD-CGD-O1D
28	g	322	CLA	CHA-CBD-CGD-O2D
28	n	601	CLA	C1A-C2A-CAA-CBA
28	n	601	CLA	C4B-C3B-CAB-CBB
28	n	603	CLA	C1A-C2A-CAA-CBA
28	n	604	CLA	C1A-C2A-CAA-CBA
28	n	605	CLA	C1A-C2A-CAA-CBA
28	n	605	CLA	C3A-C2A-CAA-CBA
28	n	606	CLA	C1A-C2A-CAA-CBA
28	n	606	CLA	C3A-C2A-CAA-CBA
28	n	606	CLA	CBA-CGA-O2A-C1
28	n	606	CLA	O1A-CGA-O2A-C1
28	n	607	CLA	CHA-CBD-CGD-O1D
28	n	607	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	n	608	CLA	C3A-C2A-CAA-CBA
28	n	608	CLA	C4B-C3B-CAB-CBB
28	n	610	CLA	C1A-C2A-CAA-CBA
28	n	610	CLA	C3A-C2A-CAA-CBA
28	n	610	CLA	C14-C13-C15-C16
28	n	613	CLA	C1A-C2A-CAA-CBA
28	Q	302	CLA	C2B-C3B-CAB-CBB
28	Q	302	CLA	C4B-C3B-CAB-CBB
28	Q	302	CLA	CBD-CGD-O2D-CED
28	Q	303	CLA	C1A-C2A-CAA-CBA
28	Q	303	CLA	C3A-C2A-CAA-CBA
30	A	843	LHG	C4-O6-P-O3
30	A	844	LHG	O1-C1-C2-C3
30	A	844	LHG	C3-O3-P-O5
30	A	849	LHG	C3-O3-P-O5
30	A	849	LHG	C3-O3-P-O6
30	A	849	LHG	C4-O6-P-O3
30	A	849	LHG	C4-O6-P-O4
30	A	849	LHG	C4-O6-P-O5
30	A	849	LHG	C8-C7-O7-C5
30	J	106	LHG	C1-C2-C3-O3
30	J	106	LHG	C3-O3-P-O4
30	J	106	LHG	C3-O3-P-O6
30	L	208	LHG	C3-O3-P-O5
30	L	208	LHG	C3-O3-P-O6
30	L	208	LHG	C4-O6-P-O3
30	c	618	LHG	C4-O6-P-O3
30	c	618	LHG	C4-O6-P-O4
30	c	618	LHG	O9-C7-O7-C5
30	c	618	LHG	C8-C7-O7-C5
30	c	620	LHG	O1-C1-C2-C3
30	c	620	LHG	C3-O3-P-O4
30	c	620	LHG	C4-O6-P-O3
30	c	620	LHG	C4-O6-P-O4
30	a	301	LHG	C3-O3-P-O6
30	a	301	LHG	O9-C7-O7-C5
30	b	619	LHG	C3-O3-P-O4
30	b	619	LHG	C3-O3-P-O6
30	b	619	LHG	O9-C7-O7-C5
30	m	619	LHG	C4-O6-P-O3
30	m	619	LHG	C4-O6-P-O4
30	e	617	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
30	e	617	LHG	O9-C7-O7-C5
30	l	317	LHG	C3-O3-P-O6
30	k	620	LHG	O1-C1-C2-O2
30	k	620	LHG	O1-C1-C2-C3
30	k	620	LHG	C3-O3-P-O4
30	k	620	LHG	C3-O3-P-O5
30	k	620	LHG	C3-O3-P-O6
30	k	620	LHG	C8-C7-O7-C5
30	f	619	LHG	C3-O3-P-O5
30	f	619	LHG	C3-O3-P-O6
30	f	619	LHG	C4-O6-P-O5
30	f	619	LHG	O9-C7-O7-C5
30	i	318	LHG	C3-O3-P-O6
30	i	318	LHG	C8-C7-O7-C5
30	i	318	LHG	O10-C23-O8-C6
30	i	318	LHG	C24-C23-O8-C6
30	j	617	LHG	C4-O6-P-O3
30	j	617	LHG	C4-O6-P-O4
30	d	317	LHG	C1-C2-C3-O3
30	d	317	LHG	C3-O3-P-O4
30	d	317	LHG	C3-O3-P-O6
30	d	317	LHG	C4-O6-P-O3
30	d	317	LHG	C4-O6-P-O5
30	d	317	LHG	C8-C7-O7-C5
30	g	301	LHG	C3-O3-P-O4
30	g	301	LHG	C3-O3-P-O5
30	g	301	LHG	C3-O3-P-O6
30	g	301	LHG	C4-O6-P-O5
30	g	321	LHG	C3-O3-P-O4
30	g	321	LHG	C3-O3-P-O6
30	g	321	LHG	C4-O6-P-O3
30	g	321	LHG	C4-O6-P-O4
30	g	321	LHG	O9-C7-O7-C5
30	g	321	LHG	C8-C7-O7-C5
30	n	619	LHG	C3-O3-P-O6
30	n	619	LHG	C4-O6-P-O3
30	n	619	LHG	C4-O6-P-O4
30	n	619	LHG	C4-O6-P-O5
31	A	845	WVN	C01-C02-C11-C19
31	A	845	WVN	C05-C02-C11-C19
31	A	846	WVN	C20-C23-C25-C27
31	A	846	WVN	C20-C23-C25-C28

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Mol	Chain	Res	Type	Atoms
31	A	846	WVN	C30-C33-C34-C37
31	A	846	WVN	C30-C33-C34-C38
31	A	848	WVN	C20-C23-C25-C27
31	A	848	WVN	C20-C23-C25-C28
31	A	848	WVN	C30-C33-C34-C37
31	B	844	WVN	C20-C23-C25-C27
31	B	844	WVN	C30-C33-C34-C37
31	B	846	WVN	C05-C02-C11-C19
31	B	848	WVN	C05-C02-C11-C19
31	B	848	WVN	C11-C19-C22-C26
31	B	848	WVN	C29-C31-C32-C35
31	B	848	WVN	C29-C31-C32-C36
31	F	203	WVN	C11-C19-C22-C24
31	F	203	WVN	C11-C19-C22-C26
31	F	203	WVN	C22-C26-C29-C31
31	F	204	WVN	C05-C02-C11-C19
31	F	204	WVN	C15-C13-C20-C23
31	I	101	WVN	C05-C02-C11-C19
31	I	101	WVN	C11-C19-C22-C24
31	I	101	WVN	C11-C19-C22-C26
31	I	101	WVN	C29-C31-C32-C36
31	J	101	WVN	C01-C02-C11-C19
31	J	101	WVN	C05-C02-C11-C19
31	J	101	WVN	C06-C13-C20-C23
31	J	101	WVN	C20-C23-C25-C27
31	J	101	WVN	C20-C23-C25-C28
31	J	102	WVN	C01-C02-C11-C19
31	J	102	WVN	C05-C02-C11-C19
31	J	102	WVN	C11-C19-C22-C24
31	J	102	WVN	C11-C19-C22-C26
31	J	102	WVN	C20-C23-C25-C27
31	J	102	WVN	C20-C23-C25-C28
31	J	102	WVN	C30-C33-C34-C37
31	J	102	WVN	C30-C33-C34-C38
31	L	201	WVN	C05-C02-C11-C19
31	L	201	WVN	C15-C13-C20-C23
31	L	201	WVN	C11-C19-C22-C26
31	L	205	WVN	C06-C13-C20-C23
31	L	205	WVN	C11-C19-C22-C24
31	L	205	WVN	C11-C19-C22-C26
31	M	101	WVN	C05-C02-C11-C19
31	M	101	WVN	C15-C13-C20-C23

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Mol	Chain	Res	Type	Atoms
31	M	101	WVN	C20-C23-C25-C27
31	M	101	WVN	C20-C23-C25-C28
31	M	101	WVN	C30-C33-C34-C37
31	M	101	WVN	C30-C33-C34-C38
31	K	102	WVN	C22-C26-C29-C31
31	s	207	WVN	C01-C02-C11-C19
31	h	309	WVN	C20-C23-C25-C27
31	h	309	WVN	C20-C23-C25-C28
31	h	309	WVN	C30-C33-C34-C37
31	h	309	WVN	C30-C33-C34-C38
31	e	615	WVN	C01-C02-C11-C19
31	e	615	WVN	C05-C02-C11-C19
31	e	615	WVN	C15-C13-C20-C23
31	e	615	WVN	C30-C33-C34-C37
31	l	315	WVN	C15-C13-C20-C23
31	l	315	WVN	C29-C31-C32-C35
31	l	315	WVN	C29-C31-C32-C36
31	i	316	WVN	C29-C31-C32-C36
31	R	202	WVN	C01-C02-C11-C19
31	R	202	WVN	C05-C02-C11-C19
31	R	202	WVN	C06-C13-C20-C23
31	R	202	WVN	C20-C23-C25-C28
32	A	850	LMT	C2'-C1'-O1'-C1
32	A	850	LMT	O5'-C1'-O1'-C1
32	a	302	LMT	O5'-C1'-O1'-C1
32	b	618	LMT	O5'-C1'-O1'-C1
35	L	209	LMG	C2-C1-O1-C7
35	L	209	LMG	O6-C1-O1-C7
35	b	621	LMG	O9-C10-O7-C8
35	b	621	LMG	C11-C10-O7-C8
35	n	620	LMG	C2-C1-O1-C7
35	n	620	LMG	O7-C8-C9-O8
35	Q	301	LMG	C11-C10-O7-C8
36	J	104	II0	C25-C29-C31-C33
36	J	104	II0	C26-C30-C32-C34
36	J	104	II0	C32-C34-C36-C38
36	J	104	II0	C32-C34-C36-C40
36	c	613	II0	C26-C30-C32-C34
36	c	617	II0	C32-C34-C36-C40
36	a	318	II0	C31-C33-C35-C37
36	a	318	II0	C31-C33-C35-C39
36	a	318	II0	C36-C40-C42-C41

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Mol	Chain	Res	Type	Atoms
36	b	614	II0	C31-C33-C35-C39
36	h	311	II0	C26-C30-C32-C34
36	h	311	II0	C32-C34-C36-C40
36	h	312	II0	C25-C29-C31-C33
36	m	614	II0	C32-C34-C36-C38
36	m	614	II0	C32-C34-C36-C40
36	m	615	II0	C26-C30-C32-C34
36	m	615	II0	C31-C33-C35-C39
36	m	618	II0	C31-C33-C35-C39
36	e	612	II0	C26-C30-C32-C34
36	e	612	II0	C32-C34-C36-C38
36	e	612	II0	C32-C34-C36-C40
36	e	614	II0	C26-C30-C32-C34
36	e	614	II0	C32-C34-C36-C38
36	e	614	II0	C32-C34-C36-C40
36	l	312	II0	C32-C34-C36-C38
36	l	312	II0	C32-C34-C36-C40
36	l	313	II0	C31-C33-C35-C39
36	l	314	II0	C32-C34-C36-C38
36	l	314	II0	C32-C34-C36-C40
36	l	316	II0	C31-C33-C35-C39
36	l	316	II0	C32-C34-C36-C40
36	k	616	II0	C25-C29-C31-C33
36	k	616	II0	C31-C33-C35-C39
36	k	616	II0	C32-C34-C36-C38
36	k	616	II0	C32-C34-C36-C40
36	k	617	II0	C25-C29-C31-C33
36	k	619	II0	C31-C33-C35-C39
36	k	619	II0	C32-C34-C36-C40
36	k	621	II0	C31-C33-C35-C37
36	k	621	II0	C31-C33-C35-C39
36	k	621	II0	C32-C34-C36-C38
36	k	621	II0	C32-C34-C36-C40
36	f	614	II0	C26-C30-C32-C34
36	f	615	II0	C32-C34-C36-C40
36	f	616	II0	C31-C33-C35-C37
36	f	616	II0	C31-C33-C35-C39
36	f	618	II0	C25-C29-C31-C33
36	f	618	II0	C32-C34-C36-C40
36	i	314	II0	C32-C34-C36-C38
36	i	314	II0	C32-C34-C36-C40
36	i	315	II0	C32-C34-C36-C40

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Mol	Chain	Res	Type	Atoms
36	i	317	II0	C31-C33-C35-C37
36	i	317	II0	C31-C33-C35-C39
36	i	320	II0	C31-C33-C35-C37
36	i	320	II0	C31-C33-C35-C39
36	j	614	II0	C31-C33-C35-C37
36	j	614	II0	C31-C33-C35-C39
36	d	316	II0	C25-C29-C31-C33
36	d	316	II0	C32-C34-C36-C38
36	d	316	II0	C32-C34-C36-C40
36	g	317	II0	C32-C34-C36-C38
36	g	317	II0	C32-C34-C36-C40
36	g	320	II0	C26-C30-C32-C34
36	g	320	II0	C32-C34-C36-C38
36	g	320	II0	C32-C34-C36-C40
36	n	615	II0	C31-C33-C35-C39
36	n	616	II0	C36-C40-C42-C41
36	n	618	II0	C31-C33-C35-C37
36	n	618	II0	C31-C33-C35-C39
37	c	616	IHT	C30-C32-C33-C36
37	c	616	IHT	C30-C32-C33-C37
37	b	616	IHT	C10-C07-C18-C22
37	m	617	IHT	C31-C34-C35-C38
37	k	618	IHT	C33-C37-C40-C41
37	f	617	IHT	C30-C32-C33-C36
37	f	617	IHT	C30-C32-C33-C37
37	j	616	IHT	C30-C32-C33-C37
37	g	319	IHT	C10-C07-C18-C22
37	R	204	IHT	C10-C07-C18-C22
37	n	617	IHT	C02-C07-C18-C22
37	n	617	IHT	C18-C22-C23-C25
37	n	617	IHT	C18-C22-C23-C27
38	s	201	KC2	C3A-C2A-CAA-CBA
38	s	201	KC2	C2C-C3C-CAC-CBC
38	s	201	KC2	C4C-C3C-CAC-CBC
38	s	201	KC2	CHA-CBD-CGD-O1D
38	s	204	KC2	C1A-C2A-CAA-CBA
38	s	204	KC2	C3A-C2A-CAA-CBA
38	s	204	KC2	C2C-C3C-CAC-CBC
38	s	204	KC2	C4C-C3C-CAC-CBC
38	c	610	KC2	C3A-C2A-CAA-CBA
38	c	610	KC2	C2C-C3C-CAC-CBC
38	c	610	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
38	c	610	KC2	C2A-CAA-CBA-CGA
38	c	610	KC2	CHA-CBD-CGD-O2D
38	m	611	KC2	C3A-C2A-CAA-CBA
38	m	611	KC2	C2A-CAA-CBA-CGA
38	e	609	KC2	C1A-C2A-CAA-CBA
38	e	609	KC2	C2C-C3C-CAC-CBC
38	e	609	KC2	C4C-C3C-CAC-CBC
38	e	609	KC2	CBD-CGD-O2D-CED
38	l	310	KC2	C2C-C3C-CAC-CBC
38	k	611	KC2	C2C-C3C-CAC-CBC
38	k	611	KC2	C4C-C3C-CAC-CBC
38	k	611	KC2	CHA-CBD-CGD-O2D
38	k	611	KC2	CBD-CGD-O2D-CED
38	k	613	KC2	C1A-C2A-CAA-CBA
38	k	613	KC2	C3A-C2A-CAA-CBA
38	k	613	KC2	C2C-C3C-CAC-CBC
38	k	613	KC2	C4C-C3C-CAC-CBC
38	f	611	KC2	C2C-C3C-CAC-CBC
38	f	611	KC2	C4C-C3C-CAC-CBC
38	f	611	KC2	C2A-CAA-CBA-CGA
38	f	611	KC2	CHA-CBD-CGD-O1D
38	f	611	KC2	CHA-CBD-CGD-O2D
38	i	310	KC2	C3A-C2A-CAA-CBA
38	i	310	KC2	C2B-C3B-CAB-CBB
38	i	310	KC2	C4B-C3B-CAB-CBB
38	i	310	KC2	C2C-C3C-CAC-CBC
38	i	310	KC2	C4C-C3C-CAC-CBC
38	i	319	KC2	C2C-C3C-CAC-CBC
38	i	319	KC2	C4C-C3C-CAC-CBC
38	j	611	KC2	C3A-C2A-CAA-CBA
38	j	611	KC2	C2C-C3C-CAC-CBC
38	j	611	KC2	C2A-CAA-CBA-CGA
38	d	310	KC2	C2C-C3C-CAC-CBC
38	d	310	KC2	C2A-CAA-CBA-CGA
38	d	310	KC2	CHA-CBD-CGD-O1D
38	d	310	KC2	CHA-CBD-CGD-O2D
38	d	311	KC2	C3A-C2A-CAA-CBA
38	d	311	KC2	C2A-CAA-CBA-CGA
38	g	312	KC2	C2B-C3B-CAB-CBB
38	g	312	KC2	CBD-CGD-O2D-CED
38	g	314	KC2	C3A-C2A-CAA-CBA
38	n	611	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
38	n	611	KC2	C2C-C3C-CAC-CBC
38	n	611	KC2	C2A-CAA-CBA-CGA
38	n	612	KC2	C3A-C2A-CAA-CBA
38	n	612	KC2	C2C-C3C-CAC-CBC
38	n	612	KC2	C4C-C3C-CAC-CBC
38	n	612	KC2	C2A-CAA-CBA-CGA
38	n	612	KC2	CHA-CBD-CGD-O1D
38	n	612	KC2	CHA-CBD-CGD-O2D
28	A	855	CLA	O1D-CGD-O2D-CED
28	c	608	CLA	O1D-CGD-O2D-CED
28	k	601	CLA	O1D-CGD-O2D-CED
28	k	614	CLA	O1D-CGD-O2D-CED
28	d	306	CLA	O1D-CGD-O2D-CED
38	e	609	KC2	O1D-CGD-O2D-CED
38	g	312	KC2	O1D-CGD-O2D-CED
32	A	850	LMT	O5B-C1B-O1B-C4'
39	i	301	LMU	O5B-C1B-O1B-C4'
28	A	801	CLA	O1D-CGD-O2D-CED
28	c	603	CLA	O1D-CGD-O2D-CED
28	c	611	CLA	O1D-CGD-O2D-CED
28	l	307	CLA	O1D-CGD-O2D-CED
28	k	607	CLA	O1D-CGD-O2D-CED
28	k	609	CLA	O1D-CGD-O2D-CED
28	f	613	CLA	O1D-CGD-O2D-CED
28	i	306	CLA	O1D-CGD-O2D-CED
28	i	309	CLA	O1D-CGD-O2D-CED
28	d	309	CLA	O1D-CGD-O2D-CED
38	k	611	KC2	O1D-CGD-O2D-CED
28	A	808	CLA	CBD-CGD-O2D-CED
28	A	816	CLA	CBD-CGD-O2D-CED
28	A	817	CLA	CBD-CGD-O2D-CED
28	A	831	CLA	CBD-CGD-O2D-CED
28	A	840	CLA	CBD-CGD-O2D-CED
28	A	855	CLA	CBD-CGD-O2D-CED
28	B	803	CLA	CBD-CGD-O2D-CED
28	B	812	CLA	CBD-CGD-O2D-CED
28	B	813	CLA	CBD-CGD-O2D-CED
28	B	821	CLA	CBD-CGD-O2D-CED
28	s	203	CLA	CBD-CGD-O2D-CED
28	c	603	CLA	CBD-CGD-O2D-CED
28	c	611	CLA	CBD-CGD-O2D-CED
28	c	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	b	608	CLA	CBD-CGD-O2D-CED
28	b	610	CLA	CBD-CGD-O2D-CED
28	h	302	CLA	CBD-CGD-O2D-CED
28	m	612	CLA	CBD-CGD-O2D-CED
28	e	606	CLA	CBD-CGD-O2D-CED
28	e	607	CLA	CBD-CGD-O2D-CED
28	e	611	CLA	CBD-CGD-O2D-CED
28	l	307	CLA	CBD-CGD-O2D-CED
28	k	604	CLA	CBD-CGD-O2D-CED
28	f	606	CLA	CBD-CGD-O2D-CED
28	i	306	CLA	CBD-CGD-O2D-CED
28	i	311	CLA	CBD-CGD-O2D-CED
28	i	312	CLA	CBD-CGD-O2D-CED
28	j	603	CLA	CBD-CGD-O2D-CED
28	j	608	CLA	CBD-CGD-O2D-CED
28	d	306	CLA	CBD-CGD-O2D-CED
28	d	308	CLA	CBD-CGD-O2D-CED
28	g	315	CLA	CBD-CGD-O2D-CED
28	n	601	CLA	CBD-CGD-O2D-CED
28	n	603	CLA	CBD-CGD-O2D-CED
28	n	613	CLA	CBD-CGD-O2D-CED
28	Q	303	CLA	CBD-CGD-O2D-CED
28	A	811	CLA	O1A-CGA-O2A-C1
28	A	841	CLA	O1A-CGA-O2A-C1
28	B	830	CLA	O1A-CGA-O2A-C1
28	F	201	CLA	O1A-CGA-O2A-C1
28	a	311	CLA	O1A-CGA-O2A-C1
28	a	312	CLA	O1A-CGA-O2A-C1
28	h	303	CLA	O1A-CGA-O2A-C1
28	e	606	CLA	O1A-CGA-O2A-C1
28	e	611	CLA	O1A-CGA-O2A-C1
30	A	849	LHG	O10-C23-O8-C6
30	e	617	LHG	O10-C23-O8-C6
28	d	307	CLA	O1A-CGA-O2A-C1
28	B	803	CLA	C2C-C3C-CAC-CBC
28	K	103	CLA	O1D-CGD-O2D-CED
28	f	610	CLA	C5-C6-C7-C8
28	d	307	CLA	CBA-CGA-O2A-C1
28	m	613	CLA	C4C-C3C-CAC-CBC
28	b	608	CLA	O1D-CGD-O2D-CED
28	e	606	CLA	O1D-CGD-O2D-CED
28	i	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	n	613	CLA	O1D-CGD-O2D-CED
28	A	821	CLA	CBA-CGA-O2A-C1
28	A	841	CLA	CBA-CGA-O2A-C1
28	a	311	CLA	CBA-CGA-O2A-C1
28	a	312	CLA	CBA-CGA-O2A-C1
28	h	303	CLA	CBA-CGA-O2A-C1
28	e	606	CLA	CBA-CGA-O2A-C1
28	e	611	CLA	CBA-CGA-O2A-C1
30	A	849	LHG	C24-C23-O8-C6
30	e	617	LHG	C24-C23-O8-C6
28	g	302	CLA	CBD-CGD-O2D-CED
28	g	306	CLA	CBD-CGD-O2D-CED
28	A	803	CLA	O1A-CGA-O2A-C1
28	A	814	CLA	O1A-CGA-O2A-C1
28	A	821	CLA	O1A-CGA-O2A-C1
28	A	835	CLA	O1A-CGA-O2A-C1
28	B	812	CLA	O1A-CGA-O2A-C1
28	B	813	CLA	O1A-CGA-O2A-C1
28	b	606	CLA	O1A-CGA-O2A-C1
28	h	302	CLA	O1A-CGA-O2A-C1
28	h	305	CLA	O1A-CGA-O2A-C1
28	l	307	CLA	O1A-CGA-O2A-C1
28	i	304	CLA	O1A-CGA-O2A-C1
28	j	607	CLA	O1A-CGA-O2A-C1
30	c	618	LHG	O10-C23-O8-C6
30	k	620	LHG	O10-C23-O8-C6
35	b	621	LMG	O10-C28-O8-C9
35	Q	301	LMG	O10-C28-O8-C9
28	e	604	CLA	C10-C11-C12-C13
28	B	803	CLA	O1D-CGD-O2D-CED
28	s	203	CLA	O1D-CGD-O2D-CED
28	b	610	CLA	O1D-CGD-O2D-CED
28	k	602	CLA	O1D-CGD-O2D-CED
28	i	304	CLA	O1D-CGD-O2D-CED
28	i	312	CLA	O1D-CGD-O2D-CED
28	j	613	CLA	O1D-CGD-O2D-CED
38	k	612	KC2	CAA-CBA-CGA-O1A
28	A	813	CLA	O1D-CGD-O2D-CED
28	B	805	CLA	O1D-CGD-O2D-CED
28	O	202	CLA	O1D-CGD-O2D-CED
28	b	606	CLA	O1D-CGD-O2D-CED
28	b	609	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	m	603	CLA	O1D-CGD-O2D-CED
28	m	613	CLA	O1D-CGD-O2D-CED
28	l	305	CLA	O1D-CGD-O2D-CED
28	k	606	CLA	O1D-CGD-O2D-CED
28	i	305	CLA	O1D-CGD-O2D-CED
28	d	302	CLA	O1D-CGD-O2D-CED
28	d	312	CLA	O1D-CGD-O2D-CED
28	i	302	CLA	CBD-CGD-O2D-CED
28	B	810	CLA	O1A-CGA-O2A-C1
28	m	613	CLA	C2C-C3C-CAC-CBC
30	A	849	LHG	O9-C7-O7-C5
30	k	620	LHG	O9-C7-O7-C5
30	i	318	LHG	O9-C7-O7-C5
30	d	317	LHG	O9-C7-O7-C5
35	Q	301	LMG	O9-C10-O7-C8
28	c	607	CLA	O1A-CGA-O2A-C1
28	A	802	CLA	C3-C5-C6-C7
28	A	820	CLA	C3-C5-C6-C7
28	A	839	CLA	C3-C5-C6-C7
28	B	802	CLA	C3-C5-C6-C7
28	B	807	CLA	C3-C5-C6-C7
28	B	830	CLA	C3-C5-C6-C7
28	B	836	CLA	C3-C5-C6-C7
28	O	202	CLA	C3-C5-C6-C7
28	a	309	CLA	C3-C5-C6-C7
28	b	607	CLA	C3-C5-C6-C7
28	e	605	CLA	C3-C5-C6-C7
28	l	303	CLA	C3-C5-C6-C7
28	l	309	CLA	C3-C5-C6-C7
28	k	608	CLA	C3-C5-C6-C7
28	f	610	CLA	C3-C5-C6-C7
28	i	305	CLA	C3-C5-C6-C7
28	Q	302	CLA	C3-C5-C6-C7
28	h	306	CLA	O1D-CGD-O2D-CED
28	A	803	CLA	CBA-CGA-O2A-C1
28	A	830	CLA	CBA-CGA-O2A-C1
28	B	812	CLA	CBA-CGA-O2A-C1
28	F	201	CLA	CBA-CGA-O2A-C1
28	c	608	CLA	CBA-CGA-O2A-C1
28	h	302	CLA	CBA-CGA-O2A-C1
28	l	307	CLA	CBA-CGA-O2A-C1
28	i	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	j	607	CLA	CBA-CGA-O2A-C1
28	g	308	CLA	CBA-CGA-O2A-C1
30	k	620	LHG	C24-C23-O8-C6
35	b	621	LMG	C29-C28-O8-C9
35	Q	301	LMG	C29-C28-O8-C9
39	i	301	LMU	O5'-C5'-C6'-O6'
28	A	814	CLA	CBD-CGD-O2D-CED
28	A	822	CLA	CBD-CGD-O2D-CED
28	A	827	CLA	CBD-CGD-O2D-CED
28	A	837	CLA	CBD-CGD-O2D-CED
28	B	804	CLA	CBD-CGD-O2D-CED
28	B	809	CLA	CBD-CGD-O2D-CED
28	B	819	CLA	CBD-CGD-O2D-CED
28	B	830	CLA	CBD-CGD-O2D-CED
28	B	835	CLA	CBD-CGD-O2D-CED
28	B	837	CLA	CBD-CGD-O2D-CED
28	B	839	CLA	CBD-CGD-O2D-CED
28	a	305	CLA	CBD-CGD-O2D-CED
28	b	601	CLA	CBD-CGD-O2D-CED
28	b	607	CLA	CBD-CGD-O2D-CED
28	h	304	CLA	CBD-CGD-O2D-CED
28	h	313	CLA	CBD-CGD-O2D-CED
28	e	602	CLA	CBD-CGD-O2D-CED
28	e	610	CLA	CBD-CGD-O2D-CED
28	l	302	CLA	CBD-CGD-O2D-CED
28	l	303	CLA	CBD-CGD-O2D-CED
28	l	311	CLA	CBD-CGD-O2D-CED
28	k	608	CLA	CBD-CGD-O2D-CED
28	f	602	CLA	CBD-CGD-O2D-CED
28	i	303	CLA	CBD-CGD-O2D-CED
28	j	612	CLA	CBD-CGD-O2D-CED
28	d	304	CLA	CBD-CGD-O2D-CED
28	g	307	CLA	CBD-CGD-O2D-CED
38	g	314	KC2	CBD-CGD-O2D-CED
30	a	301	LHG	C8-C7-O7-C5
30	b	619	LHG	C8-C7-O7-C5
30	e	617	LHG	C8-C7-O7-C5
30	f	619	LHG	C8-C7-O7-C5
28	L	202	CLA	O1D-CGD-O2D-CED
28	b	611	CLA	O1D-CGD-O2D-CED
28	k	610	CLA	O1D-CGD-O2D-CED
28	f	609	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	f	612	CLA	O1D-CGD-O2D-CED
28	n	603	CLA	O1D-CGD-O2D-CED
28	Q	302	CLA	O1D-CGD-O2D-CED
28	f	602	CLA	O1A-CGA-O2A-C1
28	B	836	CLA	C2C-C3C-CAC-CBC
28	B	802	CLA	O1D-CGD-O2D-CED
28	j	603	CLA	O1D-CGD-O2D-CED
38	e	609	KC2	CAA-CBA-CGA-O2A
38	l	310	KC2	CAA-CBA-CGA-O2A
38	i	319	KC2	CAA-CBA-CGA-O2A
28	A	811	CLA	C4-C3-C5-C6
28	A	816	CLA	C4-C3-C5-C6
28	A	829	CLA	C4-C3-C5-C6
28	A	839	CLA	C4-C3-C5-C6
28	B	801	CLA	C4-C3-C5-C6
28	b	603	CLA	C4-C3-C5-C6
28	m	608	CLA	C4-C3-C5-C6
28	k	604	CLA	C4-C3-C5-C6
28	f	602	CLA	C4-C3-C5-C6
28	n	609	CLA	C4-C3-C5-C6
28	A	829	CLA	C2-C3-C5-C6
28	A	839	CLA	C2-C3-C5-C6
28	B	801	CLA	C2-C3-C5-C6
28	O	201	CLA	C2-C3-C5-C6
28	b	603	CLA	C2-C3-C5-C6
28	b	608	CLA	C2-C3-C5-C6
28	m	608	CLA	C2-C3-C5-C6
28	k	604	CLA	C2-C3-C5-C6
28	d	303	CLA	C2-C3-C5-C6
28	n	609	CLA	C2-C3-C5-C6
28	F	202	CLA	CBD-CGD-O2D-CED
28	a	308	CLA	CBD-CGD-O2D-CED
28	c	612	CLA	O1D-CGD-O2D-CED
28	e	604	CLA	O1D-CGD-O2D-CED
28	A	841	CLA	C2A-CAA-CBA-CGA
28	B	808	CLA	C2A-CAA-CBA-CGA
28	A	823	CLA	O1A-CGA-O2A-C1
28	B	822	CLA	C3-C5-C6-C7
28	g	322	CLA	C3-C5-C6-C7
28	A	814	CLA	CBA-CGA-O2A-C1
28	A	835	CLA	CBA-CGA-O2A-C1
28	A	839	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	810	CLA	CBA-CGA-O2A-C1
28	B	813	CLA	CBA-CGA-O2A-C1
28	B	828	CLA	CBA-CGA-O2A-C1
28	B	830	CLA	CBA-CGA-O2A-C1
28	B	837	CLA	CBA-CGA-O2A-C1
28	O	206	CLA	CBA-CGA-O2A-C1
28	c	606	CLA	CBA-CGA-O2A-C1
28	a	310	CLA	CBA-CGA-O2A-C1
28	b	606	CLA	CBA-CGA-O2A-C1
28	h	305	CLA	CBA-CGA-O2A-C1
28	f	607	CLA	CBA-CGA-O2A-C1
28	f	610	CLA	CBA-CGA-O2A-C1
28	i	307	CLA	CBA-CGA-O2A-C1
28	j	606	CLA	CBA-CGA-O2A-C1
28	j	612	CLA	CBA-CGA-O2A-C1
28	n	605	CLA	CBA-CGA-O2A-C1
30	c	618	LHG	C24-C23-O8-C6
36	O	203	II0	C25-C29-C31-C33
36	a	318	II0	C25-C29-C31-C33
36	h	311	II0	C36-C40-C42-C41
36	m	616	II0	C26-C30-C32-C34
36	m	618	II0	C25-C29-C31-C33
36	k	621	II0	C25-C29-C31-C33
36	d	313	II0	C25-C29-C31-C33
37	c	616	IHT	C23-C27-C30-C32
37	c	616	IHT	C35-C38-C41-C40
37	b	615	IHT	C23-C27-C30-C32
37	b	615	IHT	C26-C29-C31-C34
37	k	618	IHT	C23-C27-C30-C32
37	g	319	IHT	C23-C27-C30-C32
37	n	617	IHT	C23-C27-C30-C32
28	B	837	CLA	O1A-CGA-O2A-C1
28	c	601	CLA	O1A-CGA-O2A-C1
28	c	605	CLA	O1A-CGA-O2A-C1
28	c	608	CLA	O1A-CGA-O2A-C1
28	b	601	CLA	O1A-CGA-O2A-C1
28	g	308	CLA	O1A-CGA-O2A-C1
28	c	607	CLA	CBA-CGA-O2A-C1
28	A	831	CLA	O1D-CGD-O2D-CED
28	e	611	CLA	O1D-CGD-O2D-CED
28	j	608	CLA	O1D-CGD-O2D-CED
38	f	611	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	A	829	CLA	C3-C5-C6-C7
28	b	604	CLA	C3-C5-C6-C7
28	e	611	CLA	C3-C5-C6-C7
28	A	832	CLA	CBD-CGD-O2D-CED
28	A	852	CLA	CBD-CGD-O2D-CED
28	B	801	CLA	CBD-CGD-O2D-CED
28	B	816	CLA	CBD-CGD-O2D-CED
28	B	826	CLA	CBD-CGD-O2D-CED
28	k	605	CLA	CBD-CGD-O2D-CED
28	f	608	CLA	CBD-CGD-O2D-CED
28	d	301	CLA	CBD-CGD-O2D-CED
30	e	617	LHG	C26-C27-C28-C29
30	J	106	LHG	O2-C2-C3-O3
30	a	319	LHG	O2-C2-C3-O3
30	d	317	LHG	O2-C2-C3-O3
28	Q	303	CLA	O1D-CGD-O2D-CED
28	A	818	CLA	CBA-CGA-O2A-C1
28	B	802	CLA	CBA-CGA-O2A-C1
28	c	605	CLA	CBA-CGA-O2A-C1
28	b	601	CLA	CBA-CGA-O2A-C1
28	b	611	CLA	CBA-CGA-O2A-C1
28	m	602	CLA	CBA-CGA-O2A-C1
28	f	602	CLA	CBA-CGA-O2A-C1
28	f	613	CLA	CBA-CGA-O2A-C1
28	d	312	CLA	CBA-CGA-O2A-C1
28	g	322	CLA	CBA-CGA-O2A-C1
28	n	609	CLA	CBA-CGA-O2A-C1
30	g	301	LHG	C24-C23-O8-C6
28	A	839	CLA	O1A-CGA-O2A-C1
28	B	828	CLA	O1A-CGA-O2A-C1
28	f	610	CLA	O1A-CGA-O2A-C1
28	j	606	CLA	O1A-CGA-O2A-C1
28	n	605	CLA	O1A-CGA-O2A-C1
28	A	840	CLA	O1D-CGD-O2D-CED
28	B	821	CLA	O1D-CGD-O2D-CED
39	i	301	LMU	C4'-C5'-C6'-O6'
28	J	103	CLA	CBD-CGD-O2D-CED
28	h	307	CLA	CBD-CGD-O2D-CED
28	j	605	CLA	CBD-CGD-O2D-CED
28	j	609	CLA	CBD-CGD-O2D-CED
28	b	607	CLA	C2C-C3C-CAC-CBC
28	m	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	a	310	CLA	O1A-CGA-O2A-C1
28	A	816	CLA	O1D-CGD-O2D-CED
28	B	812	CLA	O1D-CGD-O2D-CED
28	f	606	CLA	O1D-CGD-O2D-CED
28	n	601	CLA	O1D-CGD-O2D-CED
28	B	811	CLA	C3-C5-C6-C7
28	O	206	CLA	C3-C5-C6-C7
28	a	308	CLA	C3-C5-C6-C7
28	s	208	CLA	CBD-CGD-O2D-CED
28	a	313	CLA	CBD-CGD-O2D-CED
28	l	304	CLA	CBD-CGD-O2D-CED
28	l	308	CLA	CBD-CGD-O2D-CED
38	k	612	KC2	CBD-CGD-O2D-CED
32	b	618	LMT	O5'-C5'-C6'-O6'
35	b	621	LMG	O6-C5-C6-O5
28	h	302	CLA	O1D-CGD-O2D-CED
28	d	308	CLA	O1D-CGD-O2D-CED
28	g	315	CLA	O1D-CGD-O2D-CED
28	A	823	CLA	CBA-CGA-O2A-C1
28	c	601	CLA	CBA-CGA-O2A-C1
28	A	812	CLA	C4-C3-C5-C6
28	B	836	CLA	C4-C3-C5-C6
28	c	606	CLA	C4-C3-C5-C6
28	b	610	CLA	C4-C3-C5-C6
28	f	607	CLA	C4-C3-C5-C6
28	f	610	CLA	C4-C3-C5-C6
28	A	811	CLA	C2-C3-C5-C6
28	A	816	CLA	C2-C3-C5-C6
28	A	854	CLA	C2-C3-C5-C6
28	B	836	CLA	C2-C3-C5-C6
28	b	610	CLA	C2-C3-C5-C6
28	f	607	CLA	C2-C3-C5-C6
28	f	610	CLA	C2-C3-C5-C6
28	A	830	CLA	O1A-CGA-O2A-C1
28	c	606	CLA	O1A-CGA-O2A-C1
28	b	611	CLA	O1A-CGA-O2A-C1
28	m	602	CLA	O1A-CGA-O2A-C1
28	f	613	CLA	O1A-CGA-O2A-C1
30	g	301	LHG	O10-C23-O8-C6
28	A	812	CLA	CBD-CGD-O2D-CED
28	A	818	CLA	CBD-CGD-O2D-CED
28	B	811	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	f	605	CLA	CBD-CGD-O2D-CED
28	i	308	CLA	CBD-CGD-O2D-CED
28	e	607	CLA	O1D-CGD-O2D-CED
28	A	819	CLA	C2A-CAA-CBA-CGA
28	A	821	CLA	C2A-CAA-CBA-CGA
28	i	306	CLA	C2A-CAA-CBA-CGA
35	Q	301	LMG	C13-C14-C15-C16
28	k	604	CLA	O1D-CGD-O2D-CED
28	A	818	CLA	O1A-CGA-O2A-C1
28	B	804	CLA	O1A-CGA-O2A-C1
28	B	808	CLA	O1A-CGA-O2A-C1
28	f	607	CLA	O1A-CGA-O2A-C1
28	i	307	CLA	O1A-CGA-O2A-C1
28	j	612	CLA	O1A-CGA-O2A-C1
28	d	312	CLA	O1A-CGA-O2A-C1
28	g	322	CLA	O1A-CGA-O2A-C1
35	c	619	LMG	O6-C1-O1-C7
35	n	620	LMG	O6-C1-O1-C7
28	A	808	CLA	O1D-CGD-O2D-CED
28	A	817	CLA	O1D-CGD-O2D-CED
28	B	816	CLA	CBA-CGA-O2A-C1
28	B	822	CLA	CBA-CGA-O2A-C1
28	B	827	CLA	CBA-CGA-O2A-C1
28	c	602	CLA	CBA-CGA-O2A-C1
28	m	607	CLA	CBA-CGA-O2A-C1
28	f	603	CLA	CBA-CGA-O2A-C1
28	n	607	CLA	CBA-CGA-O2A-C1
30	f	619	LHG	C28-C29-C30-C31
28	A	802	CLA	CBD-CGD-O2D-CED
28	A	823	CLA	CBD-CGD-O2D-CED
28	A	839	CLA	CBD-CGD-O2D-CED
28	c	601	CLA	CBD-CGD-O2D-CED
28	b	602	CLA	CBD-CGD-O2D-CED
28	l	309	CLA	CBD-CGD-O2D-CED
28	d	303	CLA	CBD-CGD-O2D-CED
38	k	613	KC2	CBD-CGD-O2D-CED
38	n	611	KC2	CBD-CGD-O2D-CED
35	J	105	LMG	C28-C29-C30-C31
38	k	612	KC2	CAA-CBA-CGA-O2A
28	n	609	CLA	O1A-CGA-O2A-C1
28	g	306	CLA	O1D-CGD-O2D-CED
30	l	317	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	B	829	CLA	CBD-CGD-O2D-CED
28	B	836	CLA	CBD-CGD-O2D-CED
28	c	606	CLA	CBD-CGD-O2D-CED
28	b	603	CLA	CBD-CGD-O2D-CED
28	j	602	CLA	CBD-CGD-O2D-CED
28	n	605	CLA	CBD-CGD-O2D-CED
28	A	818	CLA	C4C-C3C-CAC-CBC
31	h	309	WVN	C34-C37-C40-C39
31	e	615	WVN	C25-C28-C30-C33
31	l	315	WVN	C22-C26-C29-C31
36	c	617	II0	C26-C30-C32-C34
36	a	316	II0	C25-C29-C31-C33
36	a	318	II0	C35-C39-C41-C42
36	h	311	II0	C35-C39-C41-C42
36	e	616	II0	C36-C40-C42-C41
36	l	312	II0	C26-C30-C32-C34
36	k	619	II0	C25-C29-C31-C33
36	f	616	II0	C25-C29-C31-C33
36	i	317	II0	C26-C30-C32-C34
36	d	315	II0	C36-C40-C42-C41
36	n	615	II0	C25-C29-C31-C33
37	c	616	IHT	C33-C37-C40-C41
37	k	618	IHT	C26-C29-C31-C34
28	B	802	CLA	O1A-CGA-O2A-C1
28	B	816	CLA	O1A-CGA-O2A-C1
28	B	827	CLA	O1A-CGA-O2A-C1
30	b	620	LHG	C1-C2-C3-O3
28	A	801	CLA	CBA-CGA-O2A-C1
28	A	822	CLA	CBA-CGA-O2A-C1
28	A	837	CLA	CBA-CGA-O2A-C1
28	A	840	CLA	CBA-CGA-O2A-C1
28	B	804	CLA	CBA-CGA-O2A-C1
28	B	808	CLA	CBA-CGA-O2A-C1
28	B	814	CLA	CBA-CGA-O2A-C1
28	B	826	CLA	CBA-CGA-O2A-C1
28	B	838	CLA	CBA-CGA-O2A-C1
28	F	202	CLA	CBA-CGA-O2A-C1
28	k	606	CLA	CBA-CGA-O2A-C1
28	k	610	CLA	CBA-CGA-O2A-C1
28	f	601	CLA	CBA-CGA-O2A-C1
28	f	609	CLA	CBA-CGA-O2A-C1
28	f	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	n	608	CLA	CBA-CGA-O2A-C1
30	g	321	LHG	C24-C23-O8-C6
35	c	619	LMG	C29-C28-O8-C9
32	b	618	LMT	C4'-C5'-C6'-O6'
30	f	619	LHG	C33-C34-C35-C36
32	a	320	LMT	C3-C4-C5-C6
32	a	320	LMT	C11-C10-C9-C8
28	k	608	CLA	O1D-CGD-O2D-CED
28	i	302	CLA	O1D-CGD-O2D-CED
28	g	302	CLA	O1D-CGD-O2D-CED
30	b	619	LHG	C26-C27-C28-C29
28	k	605	CLA	C2C-C3C-CAC-CBC
28	c	602	CLA	O1A-CGA-O2A-C1
28	B	813	CLA	O1D-CGD-O2D-CED
38	s	201	KC2	CAA-CBA-CGA-O1A
38	s	201	KC2	CAA-CBA-CGA-O2A
28	A	835	CLA	C4-C3-C5-C6
28	A	854	CLA	C4-C3-C5-C6
28	b	606	CLA	C4-C3-C5-C6
28	l	311	CLA	C4-C3-C5-C6
28	A	835	CLA	C2-C3-C5-C6
28	c	606	CLA	C2-C3-C5-C6
28	b	606	CLA	C2-C3-C5-C6
28	l	311	CLA	C2-C3-C5-C6
28	f	602	CLA	C2-C3-C5-C6
28	A	802	CLA	C11-C10-C8-C9
28	A	809	CLA	C6-C7-C8-C9
28	A	812	CLA	C11-C12-C13-C14
28	A	817	CLA	C11-C10-C8-C9
28	A	824	CLA	C11-C12-C13-C14
28	A	825	CLA	C6-C7-C8-C9
28	A	827	CLA	C14-C13-C15-C16
28	A	838	CLA	C11-C10-C8-C9
28	A	838	CLA	C14-C13-C15-C16
28	A	839	CLA	C14-C13-C15-C16
28	B	802	CLA	C11-C12-C13-C14
28	B	804	CLA	C14-C13-C15-C16
28	B	806	CLA	C6-C7-C8-C9
28	B	811	CLA	C14-C13-C15-C16
28	B	821	CLA	C14-C13-C15-C16
28	B	836	CLA	C6-C7-C8-C9
28	B	837	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	B	839	CLA	C6-C7-C8-C9
28	B	839	CLA	C11-C12-C13-C14
28	F	201	CLA	C11-C10-C8-C9
28	F	201	CLA	C11-C12-C13-C14
28	L	203	CLA	C6-C7-C8-C9
28	O	202	CLA	C11-C10-C8-C9
28	s	206	CLA	C14-C13-C15-C16
28	c	608	CLA	C11-C10-C8-C9
28	a	308	CLA	C11-C10-C8-C9
28	a	308	CLA	C14-C13-C15-C16
28	b	605	CLA	C6-C7-C8-C9
28	b	607	CLA	C14-C13-C15-C16
28	b	611	CLA	C11-C12-C13-C14
28	h	306	CLA	C11-C10-C8-C9
28	e	605	CLA	C11-C10-C8-C9
28	e	605	CLA	C11-C12-C13-C14
28	e	606	CLA	C6-C7-C8-C9
28	e	606	CLA	C11-C10-C8-C9
28	e	607	CLA	C11-C10-C8-C9
28	e	610	CLA	C11-C12-C13-C14
28	e	611	CLA	C11-C12-C13-C14
28	k	608	CLA	C6-C7-C8-C9
28	k	608	CLA	C11-C10-C8-C9
28	f	602	CLA	C14-C13-C15-C16
28	f	607	CLA	C6-C7-C8-C9
28	f	607	CLA	C14-C13-C15-C16
28	f	608	CLA	C11-C10-C8-C9
28	f	609	CLA	C11-C10-C8-C9
28	f	613	CLA	C11-C12-C13-C14
28	j	604	CLA	C11-C10-C8-C9
28	j	610	CLA	C6-C7-C8-C9
28	d	303	CLA	C14-C13-C15-C16
28	g	308	CLA	C6-C7-C8-C9
28	g	308	CLA	C11-C12-C13-C14
28	n	604	CLA	C6-C7-C8-C9
28	n	607	CLA	C14-C13-C15-C16
28	n	609	CLA	C14-C13-C15-C16
28	A	814	CLA	O1D-CGD-O2D-CED
28	l	303	CLA	O1D-CGD-O2D-CED
28	l	311	CLA	O1D-CGD-O2D-CED
28	j	612	CLA	O1D-CGD-O2D-CED
28	d	304	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	b	618	LMT	C2'-C1'-O1'-C1
35	c	619	LMG	C2-C1-O1-C7
30	J	106	LHG	C23-C24-C25-C26
30	b	620	LHG	O2-C2-C3-O3
28	f	602	CLA	O1D-CGD-O2D-CED
28	i	303	CLA	O1D-CGD-O2D-CED
35	Q	301	LMG	C29-C30-C31-C32
28	m	607	CLA	O1A-CGA-O2A-C1
28	n	607	CLA	O1A-CGA-O2A-C1
28	B	815	CLA	CBD-CGD-O2D-CED
28	f	604	CLA	CBD-CGD-O2D-CED
28	g	304	CLA	CBD-CGD-O2D-CED
28	B	837	CLA	O1D-CGD-O2D-CED
31	A	846	WVN	C29-C31-C32-C35
31	A	848	WVN	C11-C19-C22-C24
31	A	848	WVN	C30-C33-C34-C38
31	B	844	WVN	C30-C33-C34-C38
31	B	848	WVN	C11-C19-C22-C24
31	F	203	WVN	C29-C31-C32-C35
31	F	204	WVN	C11-C19-C22-C24
31	F	204	WVN	C29-C31-C32-C35
31	I	101	WVN	C29-C31-C32-C35
31	L	201	WVN	C11-C19-C22-C24
31	L	205	WVN	C20-C23-C25-C27
31	K	102	WVN	C11-C19-C22-C24
31	K	102	WVN	C29-C31-C32-C35
31	e	615	WVN	C20-C23-C25-C27
31	e	615	WVN	C30-C33-C34-C38
31	l	315	WVN	C11-C19-C22-C24
31	i	316	WVN	C29-C31-C32-C35
31	R	201	WVN	C11-C19-C22-C24
31	R	202	WVN	C20-C23-C25-C27
36	J	104	II0	C31-C33-C35-C37
36	c	613	II0	C32-C34-C36-C38
36	c	617	II0	C32-C34-C36-C38
36	a	314	II0	C32-C34-C36-C38
36	a	318	II0	C32-C34-C36-C38
36	b	614	II0	C31-C33-C35-C37
36	h	311	II0	C32-C34-C36-C38
36	m	615	II0	C31-C33-C35-C37
36	m	615	II0	C32-C34-C36-C38
36	e	613	II0	C31-C33-C35-C37

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Mol	Chain	Res	Type	Atoms
36	l	313	II0	C31-C33-C35-C37
36	l	316	II0	C31-C33-C35-C37
36	l	316	II0	C32-C34-C36-C38
36	k	616	II0	C31-C33-C35-C37
36	k	619	II0	C31-C33-C35-C37
36	k	619	II0	C32-C34-C36-C38
36	f	614	II0	C32-C34-C36-C38
36	f	615	II0	C32-C34-C36-C38
36	f	618	II0	C32-C34-C36-C38
36	i	313	II0	C32-C34-C36-C38
36	i	315	II0	C32-C34-C36-C38
36	i	317	II0	C32-C34-C36-C38
36	i	320	II0	C32-C34-C36-C38
36	d	313	II0	C32-C34-C36-C38
36	d	316	II0	C31-C33-C35-C37
36	g	316	II0	C32-C34-C36-C38
36	n	615	II0	C31-C33-C35-C37
37	O	204	IHT	C18-C22-C23-C25
37	O	204	IHT	C31-C34-C35-C39
37	c	616	IHT	C18-C22-C23-C25
37	c	616	IHT	C31-C34-C35-C39
37	a	317	IHT	C18-C22-C23-C25
37	a	317	IHT	C30-C32-C33-C36
37	b	615	IHT	C18-C22-C23-C25
37	m	617	IHT	C18-C22-C23-C25
37	m	617	IHT	C31-C34-C35-C39
37	k	618	IHT	C30-C32-C33-C36
37	k	618	IHT	C31-C34-C35-C39
37	j	616	IHT	C30-C32-C33-C36
31	A	846	WVN	C29-C31-C32-C36
31	A	847	WVN	C20-C23-C25-C28
31	B	844	WVN	C20-C23-C25-C28
31	L	205	WVN	C20-C23-C25-C28
31	K	102	WVN	C29-C31-C32-C36
31	h	309	WVN	C11-C19-C22-C26
31	e	615	WVN	C20-C23-C25-C28
31	l	315	WVN	C11-C19-C22-C26
31	R	201	WVN	C11-C19-C22-C26
36	J	104	II0	C31-C33-C35-C39
36	O	203	II0	C31-C33-C35-C39
36	c	613	II0	C32-C34-C36-C40
36	a	318	II0	C32-C34-C36-C40

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Mol	Chain	Res	Type	Atoms
36	m	615	II0	C32-C34-C36-C40
36	m	616	II0	C32-C34-C36-C40
36	f	614	II0	C32-C34-C36-C40
36	i	320	II0	C32-C34-C36-C40
36	d	313	II0	C32-C34-C36-C40
36	d	316	II0	C31-C33-C35-C39
36	g	316	II0	C32-C34-C36-C40
37	O	204	IHT	C18-C22-C23-C27
37	O	204	IHT	C31-C34-C35-C38
37	c	616	IHT	C18-C22-C23-C27
37	c	616	IHT	C31-C34-C35-C38
37	a	317	IHT	C18-C22-C23-C27
37	a	317	IHT	C30-C32-C33-C37
37	b	615	IHT	C18-C22-C23-C27
37	m	617	IHT	C18-C22-C23-C27
37	k	618	IHT	C18-C22-C23-C27
37	k	618	IHT	C30-C32-C33-C37
37	k	618	IHT	C31-C34-C35-C38
35	Q	301	LMG	C16-C17-C18-C19
28	a	303	CLA	C3-C5-C6-C7
28	k	605	CLA	C2A-CAA-CBA-CGA
28	B	804	CLA	O1D-CGD-O2D-CED
28	b	601	CLA	O1D-CGD-O2D-CED
28	B	814	CLA	O1A-CGA-O2A-C1
28	O	206	CLA	O1A-CGA-O2A-C1
28	k	606	CLA	O1A-CGA-O2A-C1
28	k	610	CLA	O1A-CGA-O2A-C1
28	n	608	CLA	O1A-CGA-O2A-C1
35	c	619	LMG	O10-C28-O8-C9
28	A	832	CLA	C15-C16-C17-C18
30	a	319	LHG	O7-C5-C6-O8
32	a	320	LMT	C4B-C5B-C6B-O6B
28	A	805	CLA	CBA-CGA-O2A-C1
28	A	832	CLA	CBA-CGA-O2A-C1
28	j	610	CLA	CBA-CGA-O2A-C1
35	O	205	LMG	C29-C28-O8-C9
28	h	306	CLA	C8-C10-C11-C12
28	B	830	CLA	C2-C1-O2A-CGA
28	h	301	CLA	C2-C1-O2A-CGA
28	A	837	CLA	O1D-CGD-O2D-CED
28	B	819	CLA	O1D-CGD-O2D-CED
28	B	830	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	a	305	CLA	O1D-CGD-O2D-CED
28	l	302	CLA	O1D-CGD-O2D-CED
30	f	619	LHG	C12-C13-C14-C15
28	O	206	CLA	C15-C16-C17-C18
28	b	602	CLA	C5-C6-C7-C8
28	b	605	CLA	C8-C10-C11-C12
28	f	602	CLA	C8-C10-C11-C12
28	h	304	CLA	O1D-CGD-O2D-CED
28	l	306	CLA	CBD-CGD-O2D-CED
28	A	818	CLA	C2C-C3C-CAC-CBC
28	A	810	CLA	C11-C10-C8-C7
28	A	812	CLA	C6-C7-C8-C10
28	A	818	CLA	C12-C13-C15-C16
28	A	825	CLA	C11-C12-C13-C15
28	A	836	CLA	C6-C7-C8-C10
28	A	838	CLA	C11-C12-C13-C15
28	A	839	CLA	C11-C12-C13-C15
28	B	805	CLA	C11-C12-C13-C15
28	B	811	CLA	C11-C10-C8-C7
28	L	203	CLA	C12-C13-C15-C16
28	a	308	CLA	C11-C12-C13-C15
28	a	312	CLA	C6-C7-C8-C10
28	b	603	CLA	C12-C13-C15-C16
28	b	608	CLA	C11-C10-C8-C7
28	b	610	CLA	C11-C10-C8-C7
28	b	611	CLA	C6-C7-C8-C10
28	h	301	CLA	C11-C12-C13-C15
28	h	306	CLA	C6-C7-C8-C10
28	e	605	CLA	C12-C13-C15-C16
28	e	606	CLA	C11-C12-C13-C15
28	l	303	CLA	C6-C7-C8-C10
28	k	604	CLA	C11-C12-C13-C15
28	n	607	CLA	C6-C7-C8-C10
28	n	607	CLA	C11-C12-C13-C15
28	Q	302	CLA	C12-C13-C15-C16
28	A	826	CLA	CBA-CGA-O2A-C1
28	A	828	CLA	CBA-CGA-O2A-C1
28	e	607	CLA	CBA-CGA-O2A-C1
38	e	609	KC2	CAA-CBA-CGA-O1A
28	b	603	CLA	C15-C16-C17-C18
28	B	809	CLA	O1D-CGD-O2D-CED
30	i	318	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	K	104	WVN	C32-C36-C39-C40
31	s	207	WVN	C25-C28-C30-C33
31	h	309	WVN	C25-C28-C30-C33
36	c	615	II0	C25-C29-C31-C33
36	e	613	II0	C25-C29-C31-C33
36	l	314	II0	C26-C30-C32-C34
36	i	313	II0	C26-C30-C32-C34
36	i	314	II0	C26-C30-C32-C34
36	i	317	II0	C25-C29-C31-C33
36	i	320	II0	C25-C29-C31-C33
36	d	315	II0	C26-C30-C32-C34
36	g	317	II0	C25-C29-C31-C33
36	g	318	II0	C25-C29-C31-C33
37	O	204	IHT	C26-C29-C31-C34
37	k	618	IHT	C35-C38-C41-C40
37	j	616	IHT	C23-C27-C30-C32
28	B	839	CLA	O1D-CGD-O2D-CED
35	L	209	LMG	C38-C39-C40-C41
28	l	306	CLA	C3-C5-C6-C7
28	m	606	CLA	C5-C6-C7-C8
28	f	609	CLA	C15-C16-C17-C18
28	f	613	CLA	C10-C11-C12-C13
30	l	317	LHG	C23-C24-C25-C26
28	B	838	CLA	O1A-CGA-O2A-C1
28	F	202	CLA	O1A-CGA-O2A-C1
30	g	321	LHG	O10-C23-O8-C6
28	a	304	CLA	CBD-CGD-O2D-CED
28	f	601	CLA	CBD-CGD-O2D-CED
30	n	619	LHG	C8-C7-O7-C5
28	A	802	CLA	C5-C6-C7-C8
28	A	841	CLA	C15-C16-C17-C18
28	B	836	CLA	C13-C15-C16-C17
28	B	838	CLA	C5-C6-C7-C8
28	b	611	CLA	C5-C6-C7-C8
28	e	607	CLA	C5-C6-C7-C8
28	l	303	CLA	C10-C11-C12-C13
28	l	303	CLA	C15-C16-C17-C18
28	l	306	CLA	C13-C15-C16-C17
28	k	604	CLA	C13-C15-C16-C17
28	B	803	CLA	C4C-C3C-CAC-CBC
28	A	811	CLA	C2A-CAA-CBA-CGA
28	A	822	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	B	812	CLA	C2A-CAA-CBA-CGA
28	B	835	CLA	C2A-CAA-CBA-CGA
28	L	204	CLA	C2A-CAA-CBA-CGA
28	s	202	CLA	C2A-CAA-CBA-CGA
28	s	206	CLA	C2A-CAA-CBA-CGA
28	c	602	CLA	C2A-CAA-CBA-CGA
28	c	608	CLA	C2A-CAA-CBA-CGA
28	c	611	CLA	C2A-CAA-CBA-CGA
28	a	312	CLA	C2A-CAA-CBA-CGA
28	b	611	CLA	C2A-CAA-CBA-CGA
28	h	302	CLA	C2A-CAA-CBA-CGA
28	h	307	CLA	C2A-CAA-CBA-CGA
28	l	307	CLA	C2A-CAA-CBA-CGA
28	f	612	CLA	C2A-CAA-CBA-CGA
28	i	303	CLA	C2A-CAA-CBA-CGA
28	i	311	CLA	C2A-CAA-CBA-CGA
28	g	315	CLA	C2A-CAA-CBA-CGA
28	g	322	CLA	C2A-CAA-CBA-CGA
28	F	201	CLA	C5-C6-C7-C8
28	b	603	CLA	C8-C10-C11-C12
28	b	606	CLA	C10-C11-C12-C13
28	b	607	CLA	C13-C15-C16-C17
28	e	604	CLA	C5-C6-C7-C8
28	e	606	CLA	C15-C16-C17-C18
28	e	611	CLA	C5-C6-C7-C8
28	f	607	CLA	C15-C16-C17-C18
28	f	609	CLA	C5-C6-C7-C8
29	A	842	PQN	C25-C26-C27-C28
30	a	301	LHG	C7-C8-C9-C10
35	F	205	LMG	C10-C11-C12-C13
28	e	602	CLA	O1D-CGD-O2D-CED
28	A	801	CLA	O1A-CGA-O2A-C1
28	A	822	CLA	O1A-CGA-O2A-C1
28	A	837	CLA	O1A-CGA-O2A-C1
28	f	612	CLA	O1A-CGA-O2A-C1
28	A	838	CLA	C3-C5-C6-C7
28	B	831	CLA	CBD-CGD-O2D-CED
28	A	822	CLA	O1D-CGD-O2D-CED
28	A	852	CLA	O1D-CGD-O2D-CED
28	h	313	CLA	O1D-CGD-O2D-CED
28	A	826	CLA	C5-C6-C7-C8
28	B	836	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	b	603	CLA	C5-C6-C7-C8
28	b	604	CLA	C5-C6-C7-C8
28	b	604	CLA	C13-C15-C16-C17
28	b	611	CLA	C8-C10-C11-C12
28	h	306	CLA	C15-C16-C17-C18
28	m	603	CLA	C15-C16-C17-C18
28	l	305	CLA	C10-C11-C12-C13
28	f	602	CLA	C13-C15-C16-C17
29	A	842	PQN	C18-C20-C21-C22
30	m	619	LHG	O2-C2-C3-O3
30	e	617	LHG	O2-C2-C3-O3
30	f	619	LHG	O2-C2-C3-O3
28	h	306	CLA	CBA-CGA-O2A-C1
28	k	614	CLA	CBA-CGA-O2A-C1
28	g	306	CLA	CBA-CGA-O2A-C1
35	c	619	LMG	C37-C38-C39-C40
28	A	840	CLA	O1A-CGA-O2A-C1
28	B	822	CLA	O1A-CGA-O2A-C1
28	B	826	CLA	O1A-CGA-O2A-C1
28	f	601	CLA	O1A-CGA-O2A-C1
28	f	603	CLA	O1A-CGA-O2A-C1
28	B	819	CLA	C5-C6-C7-C8
28	B	841	CLA	C13-C15-C16-C17
28	c	604	CLA	C13-C15-C16-C17
28	a	308	CLA	C15-C16-C17-C18
28	b	610	CLA	C5-C6-C7-C8
28	e	610	CLA	C10-C11-C12-C13
28	f	613	CLA	C15-C16-C17-C18
28	i	305	CLA	C5-C6-C7-C8
30	n	619	LHG	O9-C7-O7-C5
28	A	832	CLA	O1D-CGD-O2D-CED
32	a	320	LMT	O1'-C1-C2-C3
28	e	604	CLA	C3-C5-C6-C7
28	A	827	CLA	O1D-CGD-O2D-CED
28	B	835	CLA	O1D-CGD-O2D-CED
28	a	308	CLA	O1D-CGD-O2D-CED
28	e	610	CLA	O1D-CGD-O2D-CED
28	g	307	CLA	O1D-CGD-O2D-CED
28	A	802	CLA	C8-C10-C11-C12
28	e	610	CLA	C5-C6-C7-C8
28	l	305	CLA	C8-C10-C11-C12
28	e	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	e	617	LHG	C7-C8-C9-C10
30	f	619	LHG	C23-C24-C25-C26
34	B	843	DGD	C1B-C2B-C3B-C4B
28	B	816	CLA	O1D-CGD-O2D-CED
28	B	826	CLA	O1D-CGD-O2D-CED
28	F	202	CLA	O1D-CGD-O2D-CED
28	b	607	CLA	O1D-CGD-O2D-CED
28	k	605	CLA	O1D-CGD-O2D-CED
28	d	301	CLA	O1D-CGD-O2D-CED
28	k	605	CLA	C4C-C3C-CAC-CBC
28	A	807	CLA	C8-C10-C11-C12
28	B	833	CLA	C13-C15-C16-C17
28	O	202	CLA	C5-C6-C7-C8
28	e	604	CLA	C13-C15-C16-C17
28	g	322	CLA	C5-C6-C7-C8
28	A	838	CLA	CBA-CGA-O2A-C1
28	L	203	CLA	CBA-CGA-O2A-C1
28	i	302	CLA	CBA-CGA-O2A-C1
28	B	834	CLA	CBD-CGD-O2D-CED
28	c	602	CLA	CBD-CGD-O2D-CED
28	f	607	CLA	CBD-CGD-O2D-CED
35	c	619	LMG	C11-C10-O7-C8
38	k	611	KC2	C2A-CAA-CBA-CGA
38	k	612	KC2	C2A-CAA-CBA-CGA
38	k	613	KC2	C2A-CAA-CBA-CGA
32	b	618	LMT	C7-C8-C9-C10
28	A	826	CLA	O1A-CGA-O2A-C1
28	e	607	CLA	O1A-CGA-O2A-C1
28	f	609	CLA	O1A-CGA-O2A-C1
28	f	608	CLA	O1D-CGD-O2D-CED
28	j	605	CLA	O1D-CGD-O2D-CED
30	e	617	LHG	C23-C24-C25-C26
35	b	621	LMG	C4-C5-C6-O5
28	s	203	CLA	C3-C5-C6-C7
28	f	613	CLA	C3-C5-C6-C7
28	j	609	CLA	O1D-CGD-O2D-CED
28	B	816	CLA	C8-C10-C11-C12
30	g	321	LHG	C25-C26-C27-C28
31	F	203	WVN	C32-C36-C39-C40
31	F	204	WVN	C22-C26-C29-C31
36	l	313	II0	C25-C29-C31-C33
36	k	621	II0	C36-C40-C42-C41

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Mol	Chain	Res	Type	Atoms
36	g	316	II0	C26-C30-C32-C34
36	n	618	II0	C25-C29-C31-C33
37	c	616	IHT	C26-C29-C31-C34
37	a	317	IHT	C23-C27-C30-C32
28	O	206	CLA	C10-C11-C12-C13
28	b	607	CLA	C15-C16-C17-C18
28	m	604	CLA	C15-C16-C17-C18
28	m	608	CLA	C13-C15-C16-C17
32	a	320	LMT	O5B-C5B-C6B-O6B
30	m	619	LHG	C1-C2-C3-O3
30	e	617	LHG	C1-C2-C3-O3
30	f	619	LHG	C1-C2-C3-O3
28	B	827	CLA	C2A-CAA-CBA-CGA
28	F	202	CLA	C2A-CAA-CBA-CGA
28	h	303	CLA	C2A-CAA-CBA-CGA
28	j	606	CLA	C2A-CAA-CBA-CGA
28	A	809	CLA	CBA-CGA-O2A-C1
28	l	305	CLA	CBA-CGA-O2A-C1
28	b	607	CLA	C4C-C3C-CAC-CBC
28	A	835	CLA	C15-C16-C17-C18
28	B	824	CLA	C13-C15-C16-C17
28	F	201	CLA	C15-C16-C17-C18
28	b	608	CLA	C13-C15-C16-C17
28	b	610	CLA	C10-C11-C12-C13
28	h	306	CLA	C10-C11-C12-C13
28	f	610	CLA	C15-C16-C17-C18
28	g	305	CLA	C13-C15-C16-C17
28	n	607	CLA	C15-C16-C17-C18
28	B	808	CLA	CBD-CGD-O2D-CED
28	B	824	CLA	CBD-CGD-O2D-CED
28	s	202	CLA	CBD-CGD-O2D-CED
28	a	303	CLA	CBD-CGD-O2D-CED
28	J	103	CLA	O1D-CGD-O2D-CED
28	a	313	CLA	O1D-CGD-O2D-CED
28	A	829	CLA	C8-C10-C11-C12
28	c	612	CLA	C8-C10-C11-C12
28	m	608	CLA	C15-C16-C17-C18
28	f	602	CLA	C10-C11-C12-C13
30	d	317	LHG	C24-C25-C26-C27
28	A	841	CLA	C8-C10-C11-C12
28	b	604	CLA	C10-C11-C12-C13
28	e	606	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	k	608	CLA	C8-C10-C11-C12
28	f	604	CLA	C8-C10-C11-C12
28	f	608	CLA	C15-C16-C17-C18
28	j	610	CLA	C10-C11-C12-C13
28	j	610	CLA	O1A-CGA-O2A-C1
28	h	307	CLA	O1D-CGD-O2D-CED
28	k	604	CLA	C5-C6-C7-C8
28	f	613	CLA	C8-C10-C11-C12
28	n	604	CLA	CBD-CGD-O2D-CED
28	g	308	CLA	C14-C13-C15-C16
28	n	604	CLA	C11-C10-C8-C9
35	L	209	LMG	O9-C10-O7-C8
35	c	619	LMG	O9-C10-O7-C8
32	a	302	LMT	C2'-C1'-O1'-C1
35	Q	301	LMG	C2-C1-O1-C7
39	i	301	LMU	C2'-C1'-O1'-C1
28	i	308	CLA	O1D-CGD-O2D-CED
30	n	619	LHG	C24-C23-O8-C6
28	n	604	CLA	C11-C12-C13-C14
28	g	322	CLA	C2C-C3C-CAC-CBC
28	A	829	CLA	C15-C16-C17-C18
35	O	205	LMG	O10-C28-O8-C9
28	b	611	CLA	C3-C5-C6-C7
28	k	609	CLA	C3-C5-C6-C7
28	B	806	CLA	C5-C6-C7-C8
31	A	845	WVN	C20-C23-C25-C27
31	A	847	WVN	C20-C23-C25-C27
31	A	847	WVN	C29-C31-C32-C35
31	B	847	WVN	C30-C33-C34-C38
31	L	201	WVN	C20-C23-C25-C27
31	s	205	WVN	C20-C23-C25-C27
31	h	309	WVN	C11-C19-C22-C24
31	e	615	WVN	C11-C19-C22-C24
31	i	316	WVN	C20-C23-C25-C27
36	O	203	II0	C31-C33-C35-C37
36	h	310	II0	C32-C34-C36-C38
36	h	312	II0	C31-C33-C35-C37
36	m	616	II0	C32-C34-C36-C38
36	j	614	II0	C32-C34-C36-C38
36	d	315	II0	C31-C33-C35-C37
37	b	615	IHT	C30-C32-C33-C36
37	k	618	IHT	C18-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
37	j	616	IHT	C18-C22-C23-C25
37	n	617	IHT	C30-C32-C33-C36
31	A	845	WVN	C20-C23-C25-C28
31	A	848	WVN	C11-C19-C22-C26
31	F	204	WVN	C11-C19-C22-C26
31	F	204	WVN	C29-C31-C32-C36
31	L	201	WVN	C20-C23-C25-C28
31	K	102	WVN	C11-C19-C22-C26
31	i	316	WVN	C20-C23-C25-C28
36	h	310	II0	C32-C34-C36-C40
36	h	312	II0	C31-C33-C35-C39
36	i	313	II0	C32-C34-C36-C40
36	d	315	II0	C31-C33-C35-C39
37	b	615	IHT	C30-C32-C33-C37
37	j	616	IHT	C18-C22-C23-C27
37	n	617	IHT	C30-C32-C33-C37
28	A	805	CLA	O1A-CGA-O2A-C1
28	A	828	CLA	O1A-CGA-O2A-C1
28	A	808	CLA	C2A-CAA-CBA-CGA
28	A	828	CLA	C2A-CAA-CBA-CGA
28	B	814	CLA	C2A-CAA-CBA-CGA
28	B	815	CLA	C2A-CAA-CBA-CGA
28	B	840	CLA	C2A-CAA-CBA-CGA
28	a	303	CLA	C2A-CAA-CBA-CGA
28	b	602	CLA	C2A-CAA-CBA-CGA
28	m	604	CLA	C2A-CAA-CBA-CGA
28	m	610	CLA	C2A-CAA-CBA-CGA
28	m	612	CLA	C2A-CAA-CBA-CGA
28	f	607	CLA	C2A-CAA-CBA-CGA
28	f	613	CLA	C2A-CAA-CBA-CGA
28	O	206	CLA	C13-C15-C16-C17
30	J	106	LHG	O1-C1-C2-C3
30	b	619	LHG	O1-C1-C2-C3
30	m	619	LHG	O1-C1-C2-C3
30	e	617	LHG	O1-C1-C2-C3
30	l	317	LHG	O1-C1-C2-C3
30	f	619	LHG	O1-C1-C2-C3
30	g	301	LHG	O1-C1-C2-C3
28	s	208	CLA	O1D-CGD-O2D-CED
28	l	304	CLA	O1D-CGD-O2D-CED
28	s	203	CLA	C16-C17-C18-C19
30	l	317	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
28	A	832	CLA	O1A-CGA-O2A-C1
28	A	805	CLA	C3-C5-C6-C7
28	a	312	CLA	C8-C10-C11-C12
35	Q	301	LMG	O6-C1-O1-C7
39	i	301	LMU	O5'-C1'-O1'-C1
30	b	620	LHG	C8-C7-O7-C5
30	m	619	LHG	C8-C7-O7-C5
35	L	209	LMG	C11-C10-O7-C8
28	b	608	CLA	C15-C16-C17-C18
28	B	801	CLA	O1D-CGD-O2D-CED
28	f	605	CLA	O1D-CGD-O2D-CED
28	A	809	CLA	O1A-CGA-O2A-C1
28	B	811	CLA	O1D-CGD-O2D-CED
28	l	308	CLA	O1D-CGD-O2D-CED
28	B	805	CLA	CBA-CGA-O2A-C1
28	A	809	CLA	C5-C6-C7-C8
30	b	619	LHG	C23-C24-C25-C26
28	A	812	CLA	O1D-CGD-O2D-CED
28	A	818	CLA	O1D-CGD-O2D-CED
28	e	607	CLA	C2-C1-O2A-CGA
28	B	801	CLA	C16-C17-C18-C20
28	B	833	CLA	C16-C17-C18-C19
28	b	611	CLA	C16-C17-C18-C19
28	d	303	CLA	C16-C17-C18-C19
28	L	203	CLA	O1A-CGA-O2A-C1
28	k	614	CLA	O1A-CGA-O2A-C1
28	i	302	CLA	O1A-CGA-O2A-C1
28	B	836	CLA	C5-C6-C7-C8
28	m	606	CLA	C13-C15-C16-C17
28	e	606	CLA	C5-C6-C7-C8
29	B	842	PQN	C25-C26-C27-C28
30	e	617	LHG	C28-C29-C30-C31
30	m	619	LHG	C29-C30-C31-C32
28	A	802	CLA	O1D-CGD-O2D-CED
28	b	602	CLA	O1D-CGD-O2D-CED
28	A	839	CLA	C10-C11-C12-C13
38	n	611	KC2	CAA-CBA-CGA-O2A
30	A	843	LHG	C11-C12-C13-C14
28	h	306	CLA	O1A-CGA-O2A-C1
28	i	303	CLA	CBA-CGA-O2A-C1
30	A	849	LHG	C11-C10-C9-C8
30	a	301	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	f	619	LHG	C26-C27-C28-C29
30	A	844	LHG	O1-C1-C2-O2
30	c	620	LHG	O1-C1-C2-O2
30	l	317	LHG	O1-C1-C2-O2
32	A	850	LMT	C2-C1-O1'-C1'
36	l	316	II0	C09-C21-C23-C25
39	i	301	LMU	C2-C1-O1'-C1'
35	L	209	LMG	C18-C19-C20-C21
28	m	603	CLA	C5-C6-C7-C8
28	e	611	CLA	C13-C15-C16-C17
28	g	322	CLA	C8-C10-C11-C12
28	A	810	CLA	C4B-C3B-CAB-CBB
28	A	823	CLA	C4B-C3B-CAB-CBB
28	A	852	CLA	C4B-C3B-CAB-CBB
28	B	838	CLA	C4B-C3B-CAB-CBB
28	K	103	CLA	C4B-C3B-CAB-CBB
28	a	305	CLA	C4B-C3B-CAB-CBB
28	b	601	CLA	C4B-C3B-CAB-CBB
28	m	601	CLA	C4B-C3B-CAB-CBB
28	m	613	CLA	C4B-C3B-CAB-CBB
28	e	607	CLA	C4B-C3B-CAB-CBB
28	l	309	CLA	C4B-C3B-CAB-CBB
28	l	311	CLA	C4B-C3B-CAB-CBB
28	j	610	CLA	C4B-C3B-CAB-CBB
28	g	302	CLA	C4B-C3B-CAB-CBB
28	g	306	CLA	C4B-C3B-CAB-CBB
28	g	307	CLA	C4B-C3B-CAB-CBB
30	b	619	LHG	C11-C10-C9-C8
30	k	620	LHG	C28-C29-C30-C31
35	b	621	LMG	C21-C22-C23-C24
28	A	835	CLA	C16-C17-C18-C19
28	B	812	CLA	C11-C12-C13-C15
28	B	823	CLA	C16-C17-C18-C19
28	B	833	CLA	C16-C17-C18-C20
28	a	306	CLA	C16-C17-C18-C19
28	n	604	CLA	C11-C12-C13-C15
28	n	610	CLA	C16-C17-C18-C19
28	n	610	CLA	C16-C17-C18-C20
28	g	306	CLA	O1A-CGA-O2A-C1
28	A	817	CLA	C2A-CAA-CBA-CGA
28	k	610	CLA	C2A-CAA-CBA-CGA
28	k	614	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	e	617	LHG	C9-C10-C11-C12
35	J	105	LMG	C13-C14-C15-C16
28	e	605	CLA	C5-C6-C7-C8
30	c	620	LHG	C8-C7-O7-C5
30	e	617	LHG	C30-C31-C32-C33
28	A	831	CLA	C11-C12-C13-C15
28	A	840	CLA	C6-C7-C8-C10
28	A	854	CLA	C11-C10-C8-C7
28	B	817	CLA	C6-C7-C8-C10
28	B	830	CLA	C6-C7-C8-C10
28	B	839	CLA	C11-C10-C8-C7
28	h	307	CLA	C6-C7-C8-C10
28	e	611	CLA	C11-C10-C8-C7
28	k	608	CLA	C12-C13-C15-C16
28	k	609	CLA	C11-C12-C13-C15
28	f	608	CLA	C12-C13-C15-C16
28	f	613	CLA	C12-C13-C15-C16
28	g	322	CLA	C6-C7-C8-C10
28	B	806	CLA	C15-C16-C17-C18
28	a	306	CLA	C15-C16-C17-C18
30	f	619	LHG	C10-C11-C12-C13
32	A	850	LMT	C7-C8-C9-C10
28	A	838	CLA	O1A-CGA-O2A-C1
28	A	813	CLA	C3A-C2A-CAA-CBA
28	A	814	CLA	C3A-C2A-CAA-CBA
28	A	816	CLA	C3A-C2A-CAA-CBA
28	A	831	CLA	C3A-C2A-CAA-CBA
28	A	834	CLA	C3A-C2A-CAA-CBA
28	A	841	CLA	C3A-C2A-CAA-CBA
28	B	811	CLA	C3A-C2A-CAA-CBA
28	B	812	CLA	C3A-C2A-CAA-CBA
28	B	831	CLA	C3A-C2A-CAA-CBA
28	B	832	CLA	C3A-C2A-CAA-CBA
28	B	839	CLA	C3A-C2A-CAA-CBA
28	O	202	CLA	C3A-C2A-CAA-CBA
28	s	202	CLA	C3A-C2A-CAA-CBA
28	s	203	CLA	C3A-C2A-CAA-CBA
28	c	601	CLA	C3A-C2A-CAA-CBA
28	a	307	CLA	C3A-C2A-CAA-CBA
28	a	308	CLA	C3A-C2A-CAA-CBA
28	b	605	CLA	C4-C3-C5-C6
28	b	612	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	h	305	CLA	C3A-C2A-CAA-CBA
28	h	307	CLA	C3A-C2A-CAA-CBA
28	m	613	CLA	C3A-C2A-CAA-CBA
28	e	607	CLA	C3A-C2A-CAA-CBA
28	k	606	CLA	C3A-C2A-CAA-CBA
28	k	607	CLA	C3A-C2A-CAA-CBA
28	f	605	CLA	C3A-C2A-CAA-CBA
28	i	309	CLA	C3A-C2A-CAA-CBA
28	j	606	CLA	C3A-C2A-CAA-CBA
28	j	608	CLA	C3A-C2A-CAA-CBA
28	g	306	CLA	C3A-C2A-CAA-CBA
28	n	601	CLA	C3A-C2A-CAA-CBA
28	n	603	CLA	C3A-C2A-CAA-CBA
28	n	604	CLA	C3A-C2A-CAA-CBA
35	b	621	LMG	C12-C13-C14-C15
28	A	812	CLA	C2-C3-C5-C6
32	A	850	LMT	C1-C2-C3-C4
28	A	823	CLA	O1D-CGD-O2D-CED
28	f	604	CLA	O1D-CGD-O2D-CED
35	Q	301	LMG	C14-C15-C16-C17
31	B	848	WVN	C22-C26-C29-C31
36	m	614	II0	C26-C30-C32-C34
36	e	616	II0	C35-C39-C41-C42
36	f	618	II0	C35-C39-C41-C42
36	n	614	II0	C36-C40-C42-C41
37	O	204	IHT	C35-C38-C41-C40
37	f	617	IHT	C23-C27-C30-C32
37	g	319	IHT	C35-C38-C41-C40
28	b	611	CLA	C16-C17-C18-C20
32	a	320	LMT	C6-C7-C8-C9
28	A	839	CLA	C5-C6-C7-C8
28	a	310	CLA	O2A-C1-C2-C3
30	e	617	LHG	C11-C12-C13-C14
28	A	817	CLA	CBA-CGA-O2A-C1
28	m	612	CLA	CBA-CGA-O2A-C1
35	F	205	LMG	C7-C8-C9-O8
32	b	618	LMT	C4-C5-C6-C7
28	L	203	CLA	C3-C5-C6-C7
30	c	620	LHG	C7-C8-C9-C10
28	g	322	CLA	C10-C11-C12-C13
30	f	619	LHG	C11-C10-C9-C8
28	B	840	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	A	839	CLA	O1D-CGD-O2D-CED
28	c	601	CLA	O1D-CGD-O2D-CED
28	l	309	CLA	O1D-CGD-O2D-CED
28	j	602	CLA	O1D-CGD-O2D-CED
39	i	301	LMU	C1-C2-C3-C4
28	d	303	CLA	O1D-CGD-O2D-CED
28	s	203	CLA	C16-C17-C18-C20
28	h	306	CLA	C16-C17-C18-C20
28	g	309	CLA	C16-C17-C18-C19
35	b	621	LMG	C28-C29-C30-C31
28	B	805	CLA	O1A-CGA-O2A-C1
28	A	822	CLA	C2B-C3B-CAB-CBB
28	A	823	CLA	C2B-C3B-CAB-CBB
28	B	838	CLA	C2B-C3B-CAB-CBB
28	s	202	CLA	C2B-C3B-CAB-CBB
28	b	601	CLA	C2B-C3B-CAB-CBB
28	m	601	CLA	C2B-C3B-CAB-CBB
28	m	613	CLA	C2B-C3B-CAB-CBB
28	l	303	CLA	C2B-C3B-CAB-CBB
28	l	309	CLA	C2B-C3B-CAB-CBB
28	j	610	CLA	C2B-C3B-CAB-CBB
28	g	302	CLA	C2B-C3B-CAB-CBB
28	n	601	CLA	C2B-C3B-CAB-CBB
28	n	608	CLA	C2B-C3B-CAB-CBB
31	A	845	WVN	C15-C13-C20-C23
31	A	846	WVN	C06-C13-C20-C23
31	A	846	WVN	C15-C13-C20-C23
31	A	847	WVN	C15-C13-C20-C23
31	A	848	WVN	C15-C13-C20-C23
31	J	102	WVN	C15-C13-C20-C23
31	L	205	WVN	C15-C13-C20-C23
31	M	101	WVN	C06-C13-C20-C23
31	K	104	WVN	C06-C13-C20-C23
31	s	205	WVN	C15-C13-C20-C23
31	s	207	WVN	C06-C13-C20-C23
31	s	207	WVN	C15-C13-C20-C23
31	e	615	WVN	C06-C13-C20-C23
37	O	204	IHT	C10-C07-C18-C22
37	a	317	IHT	C02-C07-C18-C22
37	k	618	IHT	C02-C07-C18-C22
37	n	617	IHT	C10-C07-C18-C22
28	g	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	O	202	CLA	CBA-CGA-O2A-C1
28	A	829	CLA	C5-C6-C7-C8
30	L	208	LHG	C14-C15-C16-C17
35	L	209	LMG	C19-C20-C21-C22
28	l	306	CLA	C2C-C3C-CAC-CBC
28	n	605	CLA	O1D-CGD-O2D-CED
28	B	825	CLA	C2A-CAA-CBA-CGA
28	L	202	CLA	C2A-CAA-CBA-CGA
28	d	306	CLA	C2A-CAA-CBA-CGA
28	i	303	CLA	O1A-CGA-O2A-C1
30	n	619	LHG	O10-C23-O8-C6
30	c	620	LHG	C28-C29-C30-C31
30	m	619	LHG	O9-C7-O7-C5
38	m	611	KC2	CAA-CBA-CGA-O2A
28	b	611	CLA	C4-C3-C5-C6
35	b	621	LMG	C33-C34-C35-C36
28	B	817	CLA	C13-C15-C16-C17
28	b	607	CLA	C5-C6-C7-C8
28	b	605	CLA	C2-C3-C5-C6
30	l	317	LHG	C10-C11-C12-C13
30	f	619	LHG	C19-C20-C21-C22
28	A	839	CLA	C16-C17-C18-C20
30	f	619	LHG	C17-C18-C19-C20
30	l	317	LHG	C7-C8-C9-C10
28	a	313	CLA	CBA-CGA-O2A-C1
28	A	808	CLA	C6-C7-C8-C9
28	A	841	CLA	C14-C13-C15-C16
28	B	801	CLA	C11-C10-C8-C9
28	B	801	CLA	C11-C12-C13-C14
28	B	838	CLA	C11-C10-C8-C9
28	b	611	CLA	C14-C13-C15-C16
35	L	209	LMG	C32-C33-C34-C35
35	b	621	LMG	C22-C23-C24-C25
28	g	309	CLA	C5-C6-C7-C8
28	O	206	CLA	C2C-C3C-CAC-CBC
30	J	106	LHG	C12-C13-C14-C15
28	k	609	CLA	C8-C10-C11-C12
39	i	301	LMU	C4-C5-C6-C7
35	F	205	LMG	C11-C12-C13-C14
35	Q	301	LMG	C11-C12-C13-C14
28	l	306	CLA	C5-C6-C7-C8
31	l	301	WVN	C22-C26-C29-C31

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Mol	Chain	Res	Type	Atoms
36	h	312	II0	C26-C30-C32-C34
36	e	612	II0	C25-C29-C31-C33
36	k	615	II0	C26-C30-C32-C34
36	i	313	II0	C25-C29-C31-C33
36	i	315	II0	C25-C29-C31-C33
36	d	313	II0	C36-C40-C42-C41
29	A	842	PQN	C26-C27-C28-C29
28	A	836	CLA	CBD-CGD-O2D-CED
28	d	305	CLA	CBD-CGD-O2D-CED
30	L	208	LHG	C8-C7-O7-C5
28	O	202	CLA	O1A-CGA-O2A-C1
30	a	319	LHG	C23-C24-C25-C26
28	A	818	CLA	C13-C15-C16-C17
28	a	308	CLA	C5-C6-C7-C8
28	b	605	CLA	C10-C11-C12-C13
30	c	620	LHG	O9-C7-O7-C5
30	b	620	LHG	O9-C7-O7-C5
35	n	620	LMG	C17-C18-C19-C20
30	c	620	LHG	C31-C32-C33-C34
30	f	619	LHG	C35-C36-C37-C38
31	s	207	WVN	C20-C23-C25-C27
31	i	316	WVN	C11-C19-C22-C24
36	m	618	II0	C31-C33-C35-C37
36	f	618	II0	C31-C33-C35-C37
37	b	616	IHT	C30-C32-C33-C36
28	A	832	CLA	C4C-C3C-CAC-CBC
35	F	205	LMG	O6-C5-C6-O5
31	s	207	WVN	C20-C23-C25-C28
31	e	615	WVN	C11-C19-C22-C26
31	i	316	WVN	C11-C19-C22-C26
36	j	614	II0	C32-C34-C36-C40
37	b	616	IHT	C30-C32-C33-C37
28	n	603	CLA	CBA-CGA-O2A-C1
28	e	607	CLA	C2A-CAA-CBA-CGA
28	b	606	CLA	C14-C13-C15-C16
28	m	608	CLA	C4C-C3C-CAC-CBC
28	B	806	CLA	C16-C17-C18-C19
28	B	837	CLA	C16-C17-C18-C19
28	B	837	CLA	C16-C17-C18-C20
28	e	606	CLA	C16-C17-C18-C19
38	m	611	KC2	C2C-C3C-CAC-CBC
38	d	311	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
38	g	313	KC2	C2C-C3C-CAC-CBC
32	b	618	LMT	C3-C4-C5-C6
28	c	606	CLA	O1D-CGD-O2D-CED
28	B	836	CLA	C8-C10-C11-C12
28	b	605	CLA	C15-C16-C17-C18
28	A	817	CLA	O1A-CGA-O2A-C1
28	m	612	CLA	O1A-CGA-O2A-C1
28	l	305	CLA	O1A-CGA-O2A-C1
28	B	808	CLA	C3-C5-C6-C7
28	j	604	CLA	C3-C5-C6-C7
35	O	205	LMG	O6-C5-C6-O5
28	A	840	CLA	C10-C11-C12-C13
28	c	608	CLA	C13-C15-C16-C17
28	a	308	CLA	C8-C10-C11-C12
28	f	610	CLA	C8-C10-C11-C12
28	Q	302	CLA	C15-C16-C17-C18
30	A	849	LHG	C9-C10-C11-C12
35	L	209	LMG	C34-C35-C36-C37
28	L	207	CLA	CBA-CGA-O2A-C1
30	g	301	LHG	C7-C8-C9-C10
30	c	618	LHG	C5-C6-O8-C23
28	B	804	CLA	C10-C11-C12-C13
38	s	201	KC2	C2A-CAA-CBA-CGA
38	s	204	KC2	C2A-CAA-CBA-CGA
38	l	310	KC2	C4C-C3C-CAC-CBC
38	j	611	KC2	C4C-C3C-CAC-CBC
38	d	310	KC2	C4C-C3C-CAC-CBC
38	g	312	KC2	C4B-C3B-CAB-CBB
38	n	611	KC2	C4C-C3C-CAC-CBC
28	B	806	CLA	C16-C17-C18-C20
30	e	617	LHG	C27-C28-C29-C30
28	B	836	CLA	O1D-CGD-O2D-CED
32	a	320	LMT	O5'-C5'-C6'-O6'
30	c	620	LHG	C23-C24-C25-C26
28	b	603	CLA	C10-C11-C12-C13
30	c	620	LHG	O7-C5-C6-O8
35	F	205	LMG	O7-C8-C9-O8
28	j	610	CLA	C4C-C3C-CAC-CBC
30	f	619	LHG	C31-C32-C33-C34
32	A	850	LMT	C3-C4-C5-C6
28	f	607	CLA	C10-C11-C12-C13
30	b	619	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
35	c	619	LMG	C35-C36-C37-C38
28	d	304	CLA	C2-C1-O2A-CGA
28	B	830	CLA	C16-C17-C18-C19
28	a	306	CLA	C16-C17-C18-C20
28	m	610	CLA	C5-C6-C7-C8
38	f	611	KC2	CAA-CBA-CGA-O2A
28	B	813	CLA	C4-C3-C5-C6
28	e	607	CLA	C4-C3-C5-C6
28	B	813	CLA	C3-C5-C6-C7
28	b	611	CLA	C2-C3-C5-C6
28	e	606	CLA	C2-C3-C5-C6
30	L	208	LHG	O9-C7-O7-C5
28	B	813	CLA	C8-C10-C11-C12
30	i	318	LHG	C27-C28-C29-C30
30	g	301	LHG	C24-C25-C26-C27
35	J	105	LMG	C20-C21-C22-C23
28	A	815	CLA	C2A-CAA-CBA-CGA
28	B	801	CLA	C2A-CAA-CBA-CGA
28	B	837	CLA	C2A-CAA-CBA-CGA
28	O	201	CLA	C2A-CAA-CBA-CGA
28	k	602	CLA	C2A-CAA-CBA-CGA
28	f	610	CLA	C2A-CAA-CBA-CGA
28	A	809	CLA	CBD-CGD-O2D-CED
28	h	301	CLA	CBD-CGD-O2D-CED
28	b	602	CLA	CBA-CGA-O2A-C1
32	A	850	LMT	O5'-C5'-C6'-O6'
30	c	620	LHG	C26-C27-C28-C29
28	b	603	CLA	O1D-CGD-O2D-CED
28	g	304	CLA	O1D-CGD-O2D-CED
28	Q	302	CLA	C5-C6-C7-C8
28	s	203	CLA	C5-C6-C7-C8
30	J	106	LHG	O1-C1-C2-O2
28	m	609	CLA	O1A-CGA-O2A-C1
28	f	609	CLA	C3-C5-C6-C7
38	j	611	KC2	CAA-CBA-CGA-O2A
28	A	804	CLA	C1A-C2A-CAA-CBA
28	A	808	CLA	C1A-C2A-CAA-CBA
28	A	814	CLA	C1A-C2A-CAA-CBA
28	A	818	CLA	C1A-C2A-CAA-CBA
28	A	822	CLA	C1A-C2A-CAA-CBA
28	A	830	CLA	C1A-C2A-CAA-CBA
28	A	833	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	A	834	CLA	C1A-C2A-CAA-CBA
28	A	837	CLA	C1A-C2A-CAA-CBA
28	A	840	CLA	C1A-C2A-CAA-CBA
28	A	841	CLA	C1A-C2A-CAA-CBA
28	A	854	CLA	C1A-C2A-CAA-CBA
28	B	804	CLA	C1A-C2A-CAA-CBA
28	B	811	CLA	C1A-C2A-CAA-CBA
28	B	812	CLA	C1A-C2A-CAA-CBA
28	B	816	CLA	C1A-C2A-CAA-CBA
28	B	819	CLA	C1A-C2A-CAA-CBA
28	B	824	CLA	C1A-C2A-CAA-CBA
28	B	828	CLA	C1A-C2A-CAA-CBA
28	B	830	CLA	C1A-C2A-CAA-CBA
28	B	836	CLA	C1A-C2A-CAA-CBA
28	B	839	CLA	C1A-C2A-CAA-CBA
28	L	207	CLA	C1A-C2A-CAA-CBA
28	s	202	CLA	C1A-C2A-CAA-CBA
28	c	602	CLA	C1A-C2A-CAA-CBA
28	c	608	CLA	C1A-C2A-CAA-CBA
28	a	303	CLA	C1A-C2A-CAA-CBA
28	a	307	CLA	C1A-C2A-CAA-CBA
28	a	310	CLA	C1A-C2A-CAA-CBA
28	b	602	CLA	C1A-C2A-CAA-CBA
28	b	612	CLA	C1A-C2A-CAA-CBA
28	h	302	CLA	C1A-C2A-CAA-CBA
28	h	307	CLA	C1A-C2A-CAA-CBA
28	h	308	CLA	C1A-C2A-CAA-CBA
28	m	609	CLA	C1A-C2A-CAA-CBA
28	m	613	CLA	C1A-C2A-CAA-CBA
28	e	602	CLA	C1A-C2A-CAA-CBA
28	l	308	CLA	C1A-C2A-CAA-CBA
28	l	311	CLA	C1A-C2A-CAA-CBA
28	k	601	CLA	C1A-C2A-CAA-CBA
28	k	602	CLA	C1A-C2A-CAA-CBA
28	k	614	CLA	C1A-C2A-CAA-CBA
28	f	605	CLA	C1A-C2A-CAA-CBA
28	i	302	CLA	C1A-C2A-CAA-CBA
28	i	303	CLA	C1A-C2A-CAA-CBA
28	i	311	CLA	C1A-C2A-CAA-CBA
28	j	601	CLA	C1A-C2A-CAA-CBA
28	j	606	CLA	C1A-C2A-CAA-CBA
28	d	307	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	g	303	CLA	C1A-C2A-CAA-CBA
28	n	608	CLA	C1A-C2A-CAA-CBA
28	A	839	CLA	C8-C10-C11-C12
28	j	604	CLA	C5-C6-C7-C8
28	j	610	CLA	C5-C6-C7-C8
28	A	806	CLA	C8-C10-C11-C12
28	B	836	CLA	C15-C16-C17-C18
30	g	301	LHG	O6-C4-C5-C6
28	c	612	CLA	C3-C5-C6-C7
28	A	806	CLA	C6-C7-C8-C10
28	A	807	CLA	C12-C13-C15-C16
28	A	810	CLA	C11-C12-C13-C15
28	A	817	CLA	C11-C10-C8-C7
28	A	826	CLA	C12-C13-C15-C16
28	A	829	CLA	C11-C10-C8-C7
28	A	831	CLA	C12-C13-C15-C16
28	A	835	CLA	C6-C7-C8-C10
28	A	852	CLA	C11-C10-C8-C7
28	B	802	CLA	C11-C12-C13-C15
28	B	816	CLA	C11-C10-C8-C7
28	B	821	CLA	C6-C7-C8-C10
28	B	833	CLA	C12-C13-C15-C16
28	F	201	CLA	C11-C12-C13-C15
28	O	206	CLA	C6-C7-C8-C10
28	s	202	CLA	C11-C10-C8-C7
28	c	608	CLA	C11-C10-C8-C7
28	c	612	CLA	C11-C12-C13-C15
28	a	306	CLA	C6-C7-C8-C10
28	b	604	CLA	C11-C12-C13-C15
28	b	605	CLA	C12-C13-C15-C16
28	b	607	CLA	C12-C13-C15-C16
28	b	610	CLA	C11-C12-C13-C15
28	e	606	CLA	C6-C7-C8-C10
28	e	606	CLA	C11-C10-C8-C7
28	e	607	CLA	C11-C10-C8-C7
28	e	611	CLA	C6-C7-C8-C10
28	l	305	CLA	C12-C13-C15-C16
28	l	309	CLA	C11-C12-C13-C15
28	f	610	CLA	C6-C7-C8-C10
28	f	613	CLA	C6-C7-C8-C10
28	i	305	CLA	C11-C10-C8-C7
28	j	604	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	n	607	CLA	C12-C13-C15-C16
28	n	610	CLA	C12-C13-C15-C16
28	Q	302	CLA	C6-C7-C8-C10
29	A	842	PQN	C21-C22-C23-C25
30	J	106	LHG	C29-C30-C31-C32
28	B	801	CLA	C16-C17-C18-C19
28	B	836	CLA	C16-C17-C18-C20
28	f	604	CLA	C16-C17-C18-C19
28	n	609	CLA	C13-C15-C16-C17
28	n	603	CLA	O1A-CGA-O2A-C1
28	J	103	CLA	C3A-C2A-CAA-CBA
28	b	609	CLA	CBA-CGA-O2A-C1
30	A	849	LHG	C16-C17-C18-C19
28	j	601	CLA	CBD-CGD-O2D-CED
30	k	620	LHG	C23-C24-C25-C26
35	c	619	LMG	C38-C39-C40-C41
28	e	606	CLA	C4-C3-C5-C6
28	A	840	CLA	C2-C3-C5-C6
28	a	304	CLA	O1D-CGD-O2D-CED
28	B	822	CLA	C5-C6-C7-C8
28	A	851	CLA	C2A-CAA-CBA-CGA
28	e	602	CLA	C2A-CAA-CBA-CGA
28	l	308	CLA	C2A-CAA-CBA-CGA
28	i	302	CLA	C2A-CAA-CBA-CGA
28	R	203	CLA	C2A-CAA-CBA-CGA
28	A	806	CLA	C6-C7-C8-C9
28	A	810	CLA	C11-C12-C13-C14
28	A	824	CLA	C11-C10-C8-C9
28	A	825	CLA	C11-C10-C8-C9
28	A	829	CLA	C11-C10-C8-C9
28	A	831	CLA	C14-C13-C15-C16
28	A	838	CLA	C11-C12-C13-C14
28	A	839	CLA	C11-C12-C13-C14
28	A	852	CLA	C11-C10-C8-C9
28	A	854	CLA	C6-C7-C8-C9
28	B	806	CLA	C11-C10-C8-C9
28	B	812	CLA	C6-C7-C8-C9
28	B	816	CLA	C11-C10-C8-C9
28	B	817	CLA	C11-C12-C13-C14
28	B	821	CLA	C6-C7-C8-C9
28	B	822	CLA	C11-C12-C13-C14
28	s	202	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	s	202	CLA	C11-C12-C13-C14
28	c	612	CLA	C11-C12-C13-C14
28	a	309	CLA	C14-C13-C15-C16
28	e	607	CLA	C11-C12-C13-C14
28	e	610	CLA	C6-C7-C8-C9
28	e	611	CLA	C14-C13-C15-C16
28	f	610	CLA	C6-C7-C8-C9
28	f	613	CLA	C6-C7-C8-C9
28	i	307	CLA	C6-C7-C8-C9
28	j	613	CLA	C6-C7-C8-C9
28	d	303	CLA	C11-C12-C13-C14
28	g	305	CLA	C11-C10-C8-C9
28	Q	302	CLA	C14-C13-C15-C16
28	B	820	CLA	CBA-CGA-O2A-C1
28	B	829	CLA	CBA-CGA-O2A-C1
28	s	208	CLA	CBA-CGA-O2A-C1
28	m	609	CLA	CBA-CGA-O2A-C1
30	c	620	LHG	C24-C23-O8-C6
28	A	818	CLA	C8-C10-C11-C12
28	l	311	CLA	C8-C10-C11-C12
28	e	603	CLA	O1D-CGD-O2D-CED
28	a	312	CLA	C15-C16-C17-C18
30	f	619	LHG	C7-C8-C9-C10
30	L	208	LHG	C4-C5-C6-O8
30	m	619	LHG	C4-C5-C6-O8
30	k	620	LHG	C4-C5-C6-O8
35	O	205	LMG	C7-C8-C9-O8
35	n	620	LMG	C7-C8-C9-O8
35	L	209	LMG	C36-C37-C38-C39
28	b	611	CLA	C10-C11-C12-C13
28	m	604	CLA	C2C-C3C-CAC-CBC
28	k	609	CLA	CBA-CGA-O2A-C1
28	d	304	CLA	CBA-CGA-O2A-C1
30	J	106	LHG	C24-C23-O8-C6
28	A	839	CLA	C16-C17-C18-C19
28	B	814	CLA	C6-C7-C8-C10
28	f	604	CLA	C16-C17-C18-C20
28	i	307	CLA	C5-C6-C7-C8
28	a	313	CLA	O1A-CGA-O2A-C1
30	J	106	LHG	C9-C10-C11-C12
28	f	601	CLA	O1D-CGD-O2D-CED
28	B	822	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	m	604	CLA	C10-C11-C12-C13
28	j	610	CLA	C8-C10-C11-C12
38	d	310	KC2	CAA-CBA-CGA-O2A
28	L	207	CLA	O1A-CGA-O2A-C1
28	A	840	CLA	C4-C3-C5-C6
28	l	303	CLA	C4-C3-C5-C6
28	A	841	CLA	CBD-CGD-O2D-CED
28	B	835	CLA	C10-C11-C12-C13
28	Q	302	CLA	C10-C11-C12-C13
31	L	206	WVN	C20-C23-C25-C27
31	l	301	WVN	C20-C23-C25-C27
36	k	615	II0	C32-C34-C36-C38
37	f	617	IHT	C18-C22-C23-C25
30	J	106	LHG	C15-C16-C17-C18
28	m	608	CLA	C16-C17-C18-C20
31	K	104	WVN	C20-C23-C25-C28
31	s	205	WVN	C20-C23-C25-C28
31	R	201	WVN	C20-C23-C25-C28
36	e	613	II0	C31-C33-C35-C39
36	f	618	II0	C31-C33-C35-C39
37	f	617	IHT	C18-C22-C23-C27
28	c	605	CLA	C2A-CAA-CBA-CGA
28	e	610	CLA	C2A-CAA-CBA-CGA
30	m	619	LHG	C26-C27-C28-C29
30	b	619	LHG	C13-C14-C15-C16
35	F	205	LMG	C19-C20-C21-C22
30	L	208	LHG	O1-C1-C2-C3
28	B	815	CLA	O1D-CGD-O2D-CED
28	c	602	CLA	O1D-CGD-O2D-CED
28	A	829	CLA	CBA-CGA-O2A-C1
28	h	301	CLA	CBA-CGA-O2A-C1
28	g	311	CLA	CBA-CGA-O2A-C1
28	g	322	CLA	O2A-C1-C2-C3
32	b	618	LMT	C2-C3-C4-C5
36	c	615	II0	C36-C40-C42-C41
36	a	315	II0	C26-C30-C32-C34
36	e	613	II0	C26-C30-C32-C34
36	j	614	II0	C25-C29-C31-C33
36	d	314	II0	C36-C40-C42-C41
28	B	814	CLA	CBD-CGD-O2D-CED
30	g	301	LHG	C30-C31-C32-C33
28	n	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	J	106	LHG	C33-C34-C35-C36
28	A	828	CLA	C2-C3-C5-C6
35	b	621	LMG	C14-C15-C16-C17
28	A	812	CLA	C16-C17-C18-C20
28	m	604	CLA	C16-C17-C18-C20
28	m	606	CLA	C16-C17-C18-C20
35	J	105	LMG	C18-C19-C20-C21
30	m	619	LHG	O7-C5-C6-O8
35	Q	301	LMG	O7-C8-C9-O8
30	l	317	LHG	C9-C10-C11-C12
28	B	825	CLA	CBA-CGA-O2A-C1
28	B	836	CLA	CBA-CGA-O2A-C1
30	e	617	LHG	C31-C32-C33-C34
30	a	319	LHG	C31-C32-C33-C34
35	F	205	LMG	C15-C16-C17-C18
28	n	613	CLA	CAA-CBA-CGA-O2A
30	A	849	LHG	C10-C11-C12-C13
30	f	619	LHG	C27-C28-C29-C30
32	A	850	LMT	C4'-C5'-C6'-O6'
28	k	614	CLA	C2-C1-O2A-CGA
28	m	608	CLA	C16-C17-C18-C19
28	B	829	CLA	O1A-CGA-O2A-C1
35	Q	301	LMG	C17-C18-C19-C20
28	A	806	CLA	CBA-CGA-O2A-C1
28	A	812	CLA	CBA-CGA-O2A-C1
28	e	602	CLA	CBA-CGA-O2A-C1
30	f	619	LHG	C24-C23-O8-C6
30	a	319	LHG	C19-C20-C21-C22
28	n	602	CLA	CBD-CGD-O2D-CED
30	g	301	LHG	C8-C7-O7-C5
35	L	209	LMG	C22-C23-C24-C25
28	c	612	CLA	C10-C11-C12-C13
28	a	311	CLA	C15-C16-C17-C18
30	c	620	LHG	C9-C10-C11-C12
28	l	306	CLA	O1D-CGD-O2D-CED
28	A	835	CLA	C13-C15-C16-C17
28	B	802	CLA	C5-C6-C7-C8
28	f	609	CLA	C10-C11-C12-C13
28	B	829	CLA	O1D-CGD-O2D-CED
28	f	607	CLA	O1D-CGD-O2D-CED
31	J	101	WVN	C22-C26-C29-C31
36	m	618	II0	C35-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
28	k	602	CLA	C4C-C3C-CAC-CBC
28	b	608	CLA	C16-C17-C18-C19
30	c	620	LHG	O10-C23-O8-C6
28	B	819	CLA	C2-C3-C5-C6
28	l	305	CLA	C2-C3-C5-C6
28	h	307	CLA	CBA-CGA-O2A-C1
28	k	603	CLA	CBA-CGA-O2A-C1
28	g	307	CLA	CBA-CGA-O2A-C1
28	n	604	CLA	CBA-CGA-O2A-C1
28	B	835	CLA	C8-C10-C11-C12
28	b	606	CLA	C5-C6-C7-C8
30	J	106	LHG	C25-C26-C27-C28
32	a	320	LMT	C2-C1-O1'-C1'
36	a	315	II0	C10-C22-C24-C26
36	l	312	II0	C09-C21-C23-C25
36	f	618	II0	C09-C21-C23-C25
36	d	315	II0	C09-C21-C23-C25
36	g	317	II0	C09-C21-C23-C25
36	n	618	II0	C10-C22-C24-C26
28	A	804	CLA	C14-C13-C15-C16
28	A	805	CLA	C11-C10-C8-C9
28	A	818	CLA	C14-C13-C15-C16
28	A	825	CLA	C14-C13-C15-C16
28	A	835	CLA	C6-C7-C8-C9
28	B	802	CLA	C6-C7-C8-C9
28	B	803	CLA	C6-C7-C8-C9
28	B	805	CLA	C14-C13-C15-C16
28	B	812	CLA	C11-C10-C8-C9
28	B	835	CLA	C11-C10-C8-C9
28	B	836	CLA	C11-C12-C13-C14
28	B	836	CLA	C14-C13-C15-C16
28	B	839	CLA	C11-C10-C8-C9
28	O	206	CLA	C6-C7-C8-C9
28	s	203	CLA	C6-C7-C8-C9
28	a	308	CLA	C11-C12-C13-C14
28	b	604	CLA	C11-C12-C13-C14
28	b	610	CLA	C11-C12-C13-C14
28	h	306	CLA	C11-C12-C13-C14
28	h	307	CLA	C11-C10-C8-C9
28	m	603	CLA	C11-C10-C8-C9
28	m	606	CLA	C11-C12-C13-C14
28	m	608	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	e	604	CLA	C6-C7-C8-C9
28	e	606	CLA	C11-C12-C13-C14
28	l	305	CLA	C14-C13-C15-C16
28	l	309	CLA	C11-C12-C13-C14
28	k	609	CLA	C11-C12-C13-C14
28	f	613	CLA	C14-C13-C15-C16
28	i	305	CLA	C11-C10-C8-C9
28	j	604	CLA	C14-C13-C15-C16
28	d	303	CLA	C11-C10-C8-C9
28	n	610	CLA	C11-C12-C13-C14
28	Q	302	CLA	C6-C7-C8-C9
29	A	842	PQN	C21-C22-C23-C24
28	A	801	CLA	C4B-C3B-CAB-CBB
28	A	832	CLA	C4B-C3B-CAB-CBB
28	B	802	CLA	C4B-C3B-CAB-CBB
28	B	819	CLA	C4B-C3B-CAB-CBB
28	b	604	CLA	C4B-C3B-CAB-CBB
28	h	301	CLA	C4B-C3B-CAB-CBB
28	m	605	CLA	C4B-C3B-CAB-CBB
28	m	606	CLA	C4B-C3B-CAB-CBB
28	f	605	CLA	C4B-C3B-CAB-CBB
28	j	607	CLA	C4B-C3B-CAB-CBB
28	j	613	CLA	C4B-C3B-CAB-CBB
30	g	301	LHG	C25-C26-C27-C28
35	J	105	LMG	C41-C42-C43-C44
28	s	202	CLA	O1D-CGD-O2D-CED
28	B	838	CLA	CAA-CBA-CGA-O2A
28	A	841	CLA	C10-C11-C12-C13
28	l	309	CLA	C10-C11-C12-C13
28	b	603	CLA	CBA-CGA-O2A-C1
35	b	621	LMG	C36-C37-C38-C39
28	c	612	CLA	C2A-CAA-CBA-CGA
28	l	305	CLA	C2A-CAA-CBA-CGA
28	f	602	CLA	C2A-CAA-CBA-CGA
28	n	610	CLA	C2A-CAA-CBA-CGA
32	a	320	LMT	C4-C5-C6-C7
35	n	620	LMG	C18-C19-C20-C21
30	J	106	LHG	O6-C4-C5-C6
30	e	617	LHG	O6-C4-C5-C6
30	n	619	LHG	O6-C4-C5-C6
28	B	834	CLA	O1D-CGD-O2D-CED
28	B	804	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	A	824	CLA	C11-C10-C8-C7
28	A	825	CLA	C11-C10-C8-C7
28	A	838	CLA	C11-C10-C8-C7
28	A	840	CLA	C12-C13-C15-C16
28	A	854	CLA	C6-C7-C8-C10
28	B	802	CLA	C6-C7-C8-C10
28	B	803	CLA	C6-C7-C8-C10
28	B	805	CLA	C12-C13-C15-C16
28	B	806	CLA	C11-C10-C8-C7
28	B	811	CLA	C12-C13-C15-C16
28	B	812	CLA	C6-C7-C8-C10
28	B	817	CLA	C11-C12-C13-C15
28	B	821	CLA	C12-C13-C15-C16
28	B	835	CLA	C11-C10-C8-C7
28	B	836	CLA	C11-C12-C13-C15
28	B	836	CLA	C12-C13-C15-C16
28	L	203	CLA	C6-C7-C8-C10
28	O	202	CLA	C11-C10-C8-C7
28	s	202	CLA	C6-C7-C8-C10
28	s	202	CLA	C11-C12-C13-C15
28	s	203	CLA	C6-C7-C8-C10
28	c	608	CLA	C12-C13-C15-C16
28	a	309	CLA	C11-C12-C13-C15
28	a	312	CLA	C12-C13-C15-C16
28	b	605	CLA	C6-C7-C8-C10
28	b	607	CLA	C11-C12-C13-C15
28	h	306	CLA	C11-C12-C13-C15
28	m	603	CLA	C11-C10-C8-C7
28	m	606	CLA	C11-C12-C13-C15
28	m	608	CLA	C12-C13-C15-C16
28	e	604	CLA	C6-C7-C8-C10
28	e	605	CLA	C11-C10-C8-C7
28	e	607	CLA	C11-C12-C13-C15
28	e	610	CLA	C6-C7-C8-C10
28	k	604	CLA	C12-C13-C15-C16
28	f	607	CLA	C11-C12-C13-C15
28	f	607	CLA	C12-C13-C15-C16
28	f	608	CLA	C11-C12-C13-C15
28	f	613	CLA	C11-C12-C13-C15
28	i	307	CLA	C6-C7-C8-C10
28	j	613	CLA	C6-C7-C8-C10
28	d	303	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
28	d	303	CLA	C11-C12-C13-C15
28	g	305	CLA	C11-C10-C8-C7
28	g	309	CLA	C12-C13-C15-C16
28	n	604	CLA	C6-C7-C8-C10
28	n	607	CLA	C11-C10-C8-C7
28	n	610	CLA	C11-C12-C13-C15
28	a	308	CLA	C10-C11-C12-C13
30	L	208	LHG	C35-C36-C37-C38
28	a	312	CLA	C16-C17-C18-C20
30	c	620	LHG	C10-C11-C12-C13
35	c	619	LMG	C29-C30-C31-C32
30	J	106	LHG	O10-C23-O8-C6
28	A	802	CLA	C3A-C2A-CAA-CBA
28	A	805	CLA	C3A-C2A-CAA-CBA
28	A	809	CLA	C3A-C2A-CAA-CBA
28	A	828	CLA	C4-C3-C5-C6
28	A	830	CLA	C3A-C2A-CAA-CBA
28	B	808	CLA	C3A-C2A-CAA-CBA
28	B	819	CLA	C4-C3-C5-C6
28	B	836	CLA	C3A-C2A-CAA-CBA
28	c	611	CLA	C3A-C2A-CAA-CBA
28	g	310	CLA	C3A-C2A-CAA-CBA
28	A	841	CLA	C13-C15-C16-C17
28	k	608	CLA	C13-C15-C16-C17
30	n	619	LHG	C12-C13-C14-C15
28	g	306	CLA	CAA-CBA-CGA-O2A
28	A	829	CLA	O1A-CGA-O2A-C1
28	b	609	CLA	O1A-CGA-O2A-C1
28	d	304	CLA	O1A-CGA-O2A-C1
28	m	606	CLA	CBA-CGA-O2A-C1
28	n	613	CLA	CBA-CGA-O2A-C1
31	A	848	WVN	C25-C28-C30-C33
31	J	101	WVN	C34-C37-C40-C39
36	a	314	II0	C26-C30-C32-C34
36	b	613	II0	C26-C30-C32-C34
36	b	614	II0	C25-C29-C31-C33
36	b	614	II0	C26-C30-C32-C34
36	h	310	II0	C36-C40-C42-C41
36	m	615	II0	C25-C29-C31-C33
36	k	616	II0	C26-C30-C32-C34
36	k	616	II0	C36-C40-C42-C41
36	k	621	II0	C35-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
36	f	615	II0	C25-C29-C31-C33
36	i	320	II0	C26-C30-C32-C34
36	j	614	II0	C36-C40-C42-C41
36	j	615	II0	C35-C39-C41-C42
36	d	316	II0	C36-C40-C42-C41
36	n	616	II0	C26-C30-C32-C34
37	g	319	IHT	C33-C37-C40-C41
28	b	608	CLA	C16-C17-C18-C20
31	F	204	WVN	C30-C33-C34-C38
36	h	311	II0	C31-C33-C35-C37
37	g	319	IHT	C31-C34-C35-C39
28	a	308	CLA	CAA-CBA-CGA-O2A
28	m	612	CLA	C4-C3-C5-C6
28	k	601	CLA	C4-C3-C5-C6
28	f	606	CLA	C4-C3-C5-C6
28	f	612	CLA	C4-C3-C5-C6
28	A	812	CLA	O1A-CGA-O2A-C1
28	b	602	CLA	O1A-CGA-O2A-C1
28	h	301	CLA	O1A-CGA-O2A-C1
28	k	609	CLA	O1A-CGA-O2A-C1
28	n	602	CLA	O1A-CGA-O2A-C1
28	n	604	CLA	O1A-CGA-O2A-C1
28	A	852	CLA	C8-C10-C11-C12
36	i	317	II0	C32-C34-C36-C40
35	Q	301	LMG	C15-C16-C17-C18
30	c	618	LHG	C4-C5-C6-O8
30	a	319	LHG	C4-C5-C6-O8
30	b	620	LHG	C4-C5-C6-O8
30	e	617	LHG	C4-C5-C6-O8
30	f	619	LHG	C4-C5-C6-O8
30	g	321	LHG	C4-C5-C6-O8
28	A	812	CLA	C16-C17-C18-C19
28	h	306	CLA	C16-C17-C18-C19
28	A	806	CLA	C15-C16-C17-C18
28	A	829	CLA	C10-C11-C12-C13
28	g	311	CLA	O1A-CGA-O2A-C1
30	a	301	LHG	C27-C28-C29-C30
35	c	619	LMG	C31-C32-C33-C34
38	i	319	KC2	CAA-CBA-CGA-O1A
30	b	619	LHG	C24-C25-C26-C27
28	l	305	CLA	C4-C3-C5-C6
28	i	307	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	L	204	CLA	CBA-CGA-O2A-C1
28	B	833	CLA	CBD-CGD-O2D-CED
35	c	619	LMG	C39-C40-C41-C42
28	a	303	CLA	O1D-CGD-O2D-CED
28	B	810	CLA	C6-C7-C8-C10
28	B	830	CLA	C16-C17-C18-C20
28	a	312	CLA	C16-C17-C18-C19
28	b	604	CLA	C16-C17-C18-C20
28	e	610	CLA	C16-C17-C18-C19
30	J	106	LHG	O6-C4-C5-O7
30	e	617	LHG	O6-C4-C5-O7
28	B	838	CLA	C8-C10-C11-C12
28	A	810	CLA	C2B-C3B-CAB-CBB
28	m	606	CLA	C2B-C3B-CAB-CBB
31	F	204	WVN	C06-C13-C20-C23
31	l	301	WVN	C15-C13-C20-C23
31	l	315	WVN	C06-C13-C20-C23
31	i	316	WVN	C06-C13-C20-C23
28	e	604	CLA	C8-C10-C11-C12
28	l	309	CLA	C14-C13-C15-C16
28	b	610	CLA	C15-C16-C17-C18
29	A	842	PQN	C15-C16-C17-C18
28	B	808	CLA	O1D-CGD-O2D-CED
35	Q	301	LMG	C30-C31-C32-C33
30	f	619	LHG	C14-C15-C16-C17
28	A	806	CLA	C16-C17-C18-C20
28	B	812	CLA	C11-C12-C13-C14
28	B	814	CLA	C6-C7-C8-C9
28	b	604	CLA	C16-C17-C18-C19
28	m	606	CLA	C16-C17-C18-C19
28	e	610	CLA	C16-C17-C18-C20
28	g	309	CLA	C16-C17-C18-C20
29	A	842	PQN	C26-C27-C28-C30
28	B	803	CLA	C2A-CAA-CBA-CGA
28	B	810	CLA	C2A-CAA-CBA-CGA
28	B	831	CLA	O1D-CGD-O2D-CED
30	L	208	LHG	O7-C5-C6-O8
30	k	620	LHG	O7-C5-C6-O8
30	g	321	LHG	O7-C5-C6-O8
30	b	619	LHG	C28-C29-C30-C31
30	k	620	LHG	C30-C31-C32-C33
30	f	619	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	m	619	LHG	C27-C28-C29-C30
30	g	301	LHG	O9-C7-O7-C5
28	e	607	CLA	C2-C3-C5-C6
28	O	206	CLA	C16-C17-C18-C19
28	m	610	CLA	C6-C7-C8-C9
30	L	208	LHG	C32-C33-C34-C35
35	J	105	LMG	C42-C43-C44-C45
28	A	832	CLA	C2C-C3C-CAC-CBC
28	A	837	CLA	C14-C13-C15-C16
28	A	840	CLA	C14-C13-C15-C16
28	B	824	CLA	C6-C7-C8-C9
28	B	832	CLA	C11-C10-C8-C9
28	B	833	CLA	C14-C13-C15-C16
28	c	612	CLA	C11-C10-C8-C9
28	e	604	CLA	C11-C12-C13-C14
28	k	604	CLA	C14-C13-C15-C16
28	n	607	CLA	C6-C7-C8-C9
28	n	607	CLA	C11-C10-C8-C9
28	R	203	CLA	CAA-CBA-CGA-O2A
28	B	824	CLA	O1D-CGD-O2D-CED
28	B	823	CLA	C16-C17-C18-C20
28	B	839	CLA	C16-C17-C18-C20
28	e	606	CLA	C16-C17-C18-C20
28	f	607	CLA	C16-C17-C18-C20
28	f	608	CLA	C16-C17-C18-C20
28	A	809	CLA	O1D-CGD-O2D-CED
28	d	305	CLA	O1D-CGD-O2D-CED
28	L	202	CLA	O2A-C1-C2-C3
28	B	820	CLA	O1A-CGA-O2A-C1
28	i	302	CLA	CAA-CBA-CGA-O2A
30	J	106	LHG	C16-C17-C18-C19
30	J	106	LHG	C11-C10-C9-C8
28	B	811	CLA	C4-C3-C5-C6
28	B	824	CLA	C4-C3-C5-C6
36	c	614	II0	C25-C29-C31-C33
37	m	617	IHT	C23-C27-C30-C32
28	m	604	CLA	C16-C17-C18-C19
28	d	303	CLA	C16-C17-C18-C20
28	e	610	CLA	C8-C10-C11-C12
28	A	836	CLA	O1D-CGD-O2D-CED
28	j	601	CLA	O1D-CGD-O2D-CED
30	n	619	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	a	319	LHG	C15-C16-C17-C18
28	Q	302	CLA	C13-C15-C16-C17
30	a	319	LHG	C1-C2-C3-O3
30	k	620	LHG	C1-C2-C3-O3
30	d	317	LHG	C27-C28-C29-C30
35	b	621	LMG	C13-C14-C15-C16
28	s	208	CLA	O1A-CGA-O2A-C1
28	g	307	CLA	O1A-CGA-O2A-C1
28	A	826	CLA	C3-C5-C6-C7
28	A	801	CLA	CAA-CBA-CGA-O2A
30	L	208	LHG	O6-C4-C5-C6
28	n	604	CLA	O1D-CGD-O2D-CED
28	A	835	CLA	C16-C17-C18-C20
28	B	810	CLA	C6-C7-C8-C9
28	B	811	CLA	C16-C17-C18-C19
31	K	104	WVN	C20-C23-C25-C27
31	R	201	WVN	C20-C23-C25-C27
37	R	204	IHT	C18-C22-C23-C25
35	Q	301	LMG	C31-C32-C33-C34
28	A	812	CLA	C12-C13-C15-C16
28	A	816	CLA	C11-C10-C8-C7
28	A	827	CLA	C11-C12-C13-C15
28	A	837	CLA	C12-C13-C15-C16
28	A	838	CLA	C12-C13-C15-C16
28	A	852	CLA	C11-C12-C13-C15
28	A	852	CLA	C12-C13-C15-C16
28	B	804	CLA	C11-C12-C13-C15
28	B	807	CLA	C12-C13-C15-C16
28	B	812	CLA	C11-C10-C8-C7
28	B	824	CLA	C6-C7-C8-C10
28	B	832	CLA	C11-C10-C8-C7
28	B	836	CLA	C6-C7-C8-C10
28	F	201	CLA	C12-C13-C15-C16
28	O	206	CLA	C12-C13-C15-C16
28	c	612	CLA	C11-C10-C8-C7
28	a	308	CLA	C11-C10-C8-C7
28	a	308	CLA	C12-C13-C15-C16
28	b	603	CLA	C11-C12-C13-C15
28	b	604	CLA	C6-C7-C8-C10
28	b	608	CLA	C12-C13-C15-C16
28	b	610	CLA	C6-C7-C8-C10
28	m	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	e	604	CLA	C11-C12-C13-C15
28	l	305	CLA	C11-C10-C8-C7
28	l	307	CLA	C6-C7-C8-C10
28	l	309	CLA	C6-C7-C8-C10
28	f	608	CLA	C11-C10-C8-C7
28	j	604	CLA	C11-C10-C8-C7
28	j	610	CLA	C6-C7-C8-C10
28	j	610	CLA	C11-C10-C8-C7
28	g	308	CLA	C11-C10-C8-C7
28	n	609	CLA	C12-C13-C15-C16
30	L	208	LHG	C23-C24-C25-C26
28	B	805	CLA	C15-C16-C17-C18
31	A	847	WVN	C29-C31-C32-C36
31	F	203	WVN	C29-C31-C32-C36
31	L	206	WVN	C20-C23-C25-C28
31	l	301	WVN	C20-C23-C25-C28
36	a	314	II0	C32-C34-C36-C40
37	R	204	IHT	C18-C22-C23-C27
30	a	301	LHG	C24-C23-O8-C6
30	J	106	LHG	C34-C35-C36-C37
30	a	319	LHG	C14-C15-C16-C17
28	B	825	CLA	O1A-CGA-O2A-C1
28	b	603	CLA	O1A-CGA-O2A-C1
28	A	807	CLA	C2A-CAA-CBA-CGA
28	l	306	CLA	C2A-CAA-CBA-CGA
28	n	609	CLA	C2A-CAA-CBA-CGA
28	B	836	CLA	C4C-C3C-CAC-CBC
28	B	811	CLA	C16-C17-C18-C20
28	B	839	CLA	C16-C17-C18-C19
28	A	807	CLA	CBD-CGD-O2D-CED
30	l	317	LHG	C8-C7-O7-C5
28	B	807	CLA	C4-C3-C5-C6
28	b	607	CLA	C4-C3-C5-C6
28	d	303	CLA	CAA-CBA-CGA-O2A
28	g	307	CLA	CAA-CBA-CGA-O2A
28	h	307	CLA	O1A-CGA-O2A-C1
28	B	813	CLA	C2-C3-C5-C6
38	g	312	KC2	C2C-C3C-CAC-CBC
38	g	314	KC2	C2C-C3C-CAC-CBC
28	g	305	CLA	C2C-C3C-CAC-CBC
35	Q	301	LMG	C4-C5-C6-O5
28	h	301	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	e	617	LHG	C6-C5-O7-C7
28	m	606	CLA	O1A-CGA-O2A-C1
30	a	301	LHG	C14-C15-C16-C17
31	I	101	WVN	C34-C37-C40-C39
31	J	101	WVN	C32-C36-C39-C40
36	k	616	II0	C35-C39-C41-C42
28	B	836	CLA	O1A-CGA-O2A-C1
28	e	602	CLA	O1A-CGA-O2A-C1
28	k	603	CLA	O1A-CGA-O2A-C1
28	n	613	CLA	O1A-CGA-O2A-C1
30	f	619	LHG	O10-C23-O8-C6
28	k	602	CLA	CBA-CGA-O2A-C1
28	g	309	CLA	O1D-CGD-O2D-CED
30	L	208	LHG	O6-C4-C5-O7
30	b	620	LHG	O6-C4-C5-O7
30	n	619	LHG	O6-C4-C5-O7
35	Q	301	LMG	C7-C8-C9-O8
38	d	311	KC2	C4C-C3C-CAC-CBC
38	g	312	KC2	C4C-C3C-CAC-CBC
38	g	313	KC2	C4C-C3C-CAC-CBC
28	B	802	CLA	C16-C17-C18-C20
28	B	801	CLA	C3-C5-C6-C7
28	A	841	CLA	O1D-CGD-O2D-CED
28	B	807	CLA	C2-C3-C5-C6
28	B	824	CLA	C2-C3-C5-C6
28	b	603	CLA	C3-C5-C6-C7
28	n	610	CLA	C3-C5-C6-C7
30	c	618	LHG	O7-C5-C6-O8
30	f	619	LHG	O7-C5-C6-O8
30	g	301	LHG	O7-C5-C6-O8
28	B	813	CLA	C5-C6-C7-C8
28	s	203	CLA	C15-C16-C17-C18
28	A	808	CLA	C11-C12-C13-C14
28	A	820	CLA	C11-C10-C8-C9
28	B	804	CLA	C11-C12-C13-C14
28	B	815	CLA	C11-C10-C8-C9
28	L	203	CLA	C14-C13-C15-C16
28	b	603	CLA	C11-C12-C13-C14
28	b	603	CLA	C14-C13-C15-C16
28	b	606	CLA	C6-C7-C8-C9
28	b	607	CLA	C11-C12-C13-C14
28	b	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	e	611	CLA	C6-C7-C8-C9
28	l	306	CLA	C14-C13-C15-C16
28	k	604	CLA	C11-C12-C13-C14
28	j	613	CLA	C11-C12-C13-C14
28	g	309	CLA	C11-C10-C8-C9
29	B	842	PQN	C16-C17-C18-C19
28	B	836	CLA	C16-C17-C18-C19
28	m	610	CLA	C6-C7-C8-C10
28	A	806	CLA	O1A-CGA-O2A-C1
35	F	205	LMG	C32-C33-C34-C35
28	B	802	CLA	C15-C16-C17-C18
28	c	604	CLA	C5-C6-C7-C8
28	a	312	CLA	C5-C6-C7-C8
28	k	609	CLA	C15-C16-C17-C18
31	B	844	WVN	C02-C11-C19-C22
31	K	102	WVN	C02-C11-C19-C22
30	L	208	LHG	C7-C8-C9-C10
28	F	202	CLA	C2-C1-O2A-CGA
28	O	206	CLA	C16-C17-C18-C20
28	l	303	CLA	C16-C17-C18-C20
28	f	608	CLA	C16-C17-C18-C19
28	h	313	CLA	C5-C6-C7-C8
28	g	322	CLA	C15-C16-C17-C18
28	B	811	CLA	C2-C3-C5-C6
28	b	607	CLA	C2-C3-C5-C6
30	l	317	LHG	O9-C7-O7-C5
28	l	311	CLA	CBA-CGA-O2A-C1
28	A	807	CLA	C16-C17-C18-C20
28	B	808	CLA	C16-C17-C18-C19
28	f	609	CLA	C16-C17-C18-C20
28	L	204	CLA	O1A-CGA-O2A-C1
28	A	854	CLA	C3-C5-C6-C7
28	j	610	CLA	C2C-C3C-CAC-CBC
38	i	310	KC2	CAA-CBA-CGA-O2A
35	F	205	LMG	C23-C24-C25-C26
35	L	209	LMG	C17-C18-C19-C20
28	g	322	CLA	C16-C17-C18-C20
36	i	313	II0	C09-C21-C23-C25
28	m	604	CLA	C4C-C3C-CAC-CBC
28	A	817	CLA	C4B-C3B-CAB-CBB
28	B	826	CLA	C1A-C2A-CAA-CBA
28	B	834	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	B	835	CLA	C4B-C3B-CAB-CBB
28	F	202	CLA	C4B-C3B-CAB-CBB
28	L	203	CLA	C1A-C2A-CAA-CBA
28	c	601	CLA	C4B-C3B-CAB-CBB
28	b	606	CLA	C1A-C2A-CAA-CBA
28	b	611	CLA	C4B-C3B-CAB-CBB
28	h	307	CLA	C4B-C3B-CAB-CBB
28	k	607	CLA	C4B-C3B-CAB-CBB
28	k	609	CLA	C1A-C2A-CAA-CBA
28	f	613	CLA	C1A-C2A-CAA-CBA
28	j	602	CLA	C1A-C2A-CAA-CBA
28	j	608	CLA	C1A-C2A-CAA-CBA
28	d	307	CLA	C4B-C3B-CAB-CBB
28	g	308	CLA	C1A-C2A-CAA-CBA
28	g	311	CLA	C4B-C3B-CAB-CBB
28	n	606	CLA	C4B-C3B-CAB-CBB
28	m	608	CLA	CBA-CGA-O2A-C1
28	l	303	CLA	CBA-CGA-O2A-C1
28	s	206	CLA	C4-C3-C5-C6
31	R	201	WVN	C30-C33-C34-C37
37	g	319	IHT	C31-C34-C35-C38
31	F	203	WVN	C34-C37-C40-C39
30	b	620	LHG	C9-C10-C11-C12
30	d	317	LHG	C28-C29-C30-C31
30	f	619	LHG	O6-C4-C5-C6
28	a	311	CLA	CBD-CGD-O2D-CED
28	A	807	CLA	O1D-CGD-O2D-CED
28	B	814	CLA	O1D-CGD-O2D-CED
28	l	311	CLA	O1A-CGA-O2A-C1
28	b	601	CLA	C2-C3-C5-C6
28	h	308	CLA	C2-C3-C5-C6
28	m	609	CLA	C2-C3-C5-C6
28	j	612	CLA	C2-C3-C5-C6
28	d	305	CLA	C2-C3-C5-C6
28	R	203	CLA	C2-C3-C5-C6
28	n	603	CLA	C2-C3-C5-C6
30	b	619	LHG	C9-C10-C11-C12
28	A	809	CLA	C6-C7-C8-C10
28	A	812	CLA	C11-C12-C13-C15
28	A	816	CLA	C12-C13-C15-C16
28	A	817	CLA	C11-C12-C13-C15
28	A	828	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	A	838	CLA	C6-C7-C8-C10
28	B	813	CLA	C11-C10-C8-C7
28	B	815	CLA	C11-C10-C8-C7
28	B	830	CLA	C11-C10-C8-C7
28	B	835	CLA	C6-C7-C8-C10
28	B	837	CLA	C11-C10-C8-C7
28	B	839	CLA	C6-C7-C8-C10
28	B	839	CLA	C11-C12-C13-C15
28	O	206	CLA	C11-C12-C13-C15
28	s	206	CLA	C11-C12-C13-C15
28	a	306	CLA	C11-C10-C8-C7
28	a	309	CLA	C12-C13-C15-C16
28	a	311	CLA	C6-C7-C8-C10
28	e	605	CLA	C11-C12-C13-C15
28	e	611	CLA	C11-C12-C13-C15
28	l	303	CLA	C11-C12-C13-C15
28	k	604	CLA	C6-C7-C8-C10
28	k	608	CLA	C11-C10-C8-C7
28	f	607	CLA	C6-C7-C8-C10
28	g	308	CLA	C11-C12-C13-C15
28	n	610	CLA	C6-C7-C8-C10
28	Q	302	CLA	C11-C12-C13-C15
28	A	806	CLA	C16-C17-C18-C19
28	A	807	CLA	C16-C17-C18-C19
28	h	301	CLA	C16-C17-C18-C20
28	f	613	CLA	C16-C17-C18-C20
28	a	311	CLA	O1D-CGD-O2D-CED
28	h	307	CLA	CAA-CBA-CGA-O2A
28	s	202	CLA	CBA-CGA-O2A-C1
28	h	301	CLA	O1D-CGD-O2D-CED
28	s	202	CLA	O1A-CGA-O2A-C1
30	L	208	LHG	C2-C3-O3-P
30	n	619	LHG	C5-C4-O6-P
28	f	613	CLA	C3A-C2A-CAA-CBA
28	g	305	CLA	C15-C16-C17-C18
30	b	619	LHG	C30-C31-C32-C33
30	f	619	LHG	O6-C4-C5-O7
30	g	301	LHG	O6-C4-C5-O7
28	A	816	CLA	C11-C10-C8-C9
28	B	805	CLA	C11-C10-C8-C9
28	B	811	CLA	C11-C10-C8-C9
28	c	612	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	a	306	CLA	C6-C7-C8-C9
28	a	309	CLA	C11-C12-C13-C14
28	h	306	CLA	C6-C7-C8-C9
28	m	602	CLA	C6-C7-C8-C9
28	l	305	CLA	C11-C10-C8-C9
28	f	608	CLA	C11-C12-C13-C14
30	J	106	LHG	C14-C15-C16-C17
36	h	312	II0	C35-C39-C41-C42
36	h	312	II0	C36-C40-C42-C41
36	m	618	II0	C26-C30-C32-C34
36	i	313	II0	C35-C39-C41-C42
28	A	821	CLA	C1-C2-C3-C4
28	B	828	CLA	C1-C2-C3-C4
38	j	611	KC2	C1A-C2A-CAA-CBA
38	g	314	KC2	C1A-C2A-CAA-CBA
30	l	317	LHG	C26-C27-C28-C29
30	b	620	LHG	O7-C5-C6-O8
30	e	617	LHG	O7-C5-C6-O8
28	A	821	CLA	O2A-C1-C2-C3
28	d	306	CLA	CBA-CGA-O2A-C1
30	c	620	LHG	C4-C5-C6-O8
35	Q	301	LMG	O1-C7-C8-C9
28	m	604	CLA	C8-C10-C11-C12
28	h	301	CLA	CAA-CBA-CGA-O2A
28	A	814	CLA	CAD-CBD-CGD-O2D
28	A	854	CLA	CAD-CBD-CGD-O2D
28	B	813	CLA	CAD-CBD-CGD-O2D
28	b	604	CLA	CAD-CBD-CGD-O2D
28	h	308	CLA	CAD-CBD-CGD-O2D
28	j	605	CLA	CAD-CBD-CGD-O2D
28	g	305	CLA	CAD-CBD-CGD-O2D
30	c	620	LHG	O2-C2-C3-O3
28	d	306	CLA	O1A-CGA-O2A-C1
30	b	619	LHG	C29-C30-C31-C32
28	Q	302	CLA	CBA-CGA-O2A-C1
35	L	209	LMG	C41-C42-C43-C44
28	A	803	CLA	C6-C7-C8-C10
28	A	840	CLA	C16-C17-C18-C20
28	k	601	CLA	C2A-CAA-CBA-CGA
28	k	606	CLA	C2A-CAA-CBA-CGA
28	j	601	CLA	C2A-CAA-CBA-CGA
28	l	309	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	n	620	LMG	C22-C23-C24-C25
30	e	617	LHG	C10-C11-C12-C13
30	c	620	LHG	C30-C31-C32-C33
28	A	804	CLA	CAD-CBD-CGD-O1D
28	A	813	CLA	CAD-CBD-CGD-O1D
28	A	814	CLA	CAD-CBD-CGD-O1D
28	A	821	CLA	CHA-CBD-CGD-O1D
28	A	821	CLA	CHA-CBD-CGD-O2D
28	A	841	CLA	CHA-CBD-CGD-O1D
28	A	854	CLA	CAD-CBD-CGD-O1D
28	B	841	CLA	CAD-CBD-CGD-O1D
28	s	208	CLA	CHA-CBD-CGD-O1D
28	s	208	CLA	CHA-CBD-CGD-O2D
28	a	303	CLA	CHA-CBD-CGD-O1D
28	a	303	CLA	CHA-CBD-CGD-O2D
28	a	306	CLA	CAD-CBD-CGD-O1D
28	a	308	CLA	CHA-CBD-CGD-O1D
28	a	311	CLA	CHA-CBD-CGD-O1D
28	b	604	CLA	CAD-CBD-CGD-O1D
28	h	308	CLA	CAD-CBD-CGD-O1D
28	m	607	CLA	CHA-CBD-CGD-O1D
28	f	607	CLA	CHA-CBD-CGD-O1D
28	f	607	CLA	CHA-CBD-CGD-O2D
28	i	306	CLA	CAD-CBD-CGD-O1D
28	j	601	CLA	CHA-CBD-CGD-O1D
28	j	601	CLA	CHA-CBD-CGD-O2D
28	j	602	CLA	CHA-CBD-CGD-O1D
28	j	602	CLA	CHA-CBD-CGD-O2D
28	j	605	CLA	CAD-CBD-CGD-O1D
28	g	305	CLA	CAD-CBD-CGD-O1D
28	g	308	CLA	CHA-CBD-CGD-O1D
28	g	308	CLA	CHA-CBD-CGD-O2D
28	g	309	CLA	CAD-CBD-CGD-O1D
30	A	843	LHG	C4-O6-P-O5
30	A	849	LHG	C3-O3-P-O4
30	L	208	LHG	C4-O6-P-O5
30	c	618	LHG	C4-O6-P-O5
30	c	620	LHG	C3-O3-P-O5
30	c	620	LHG	C3-O3-P-O6
30	c	620	LHG	C4-O6-P-O5
30	a	301	LHG	C3-O3-P-O5
30	a	319	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
30	b	619	LHG	C4-O6-P-O5
30	b	620	LHG	C3-O3-P-O5
30	b	620	LHG	C4-O6-P-O3
30	m	619	LHG	C3-O3-P-O6
30	e	617	LHG	C4-O6-P-O5
30	l	317	LHG	C3-O3-P-O5
30	i	318	LHG	C3-O3-P-O5
30	i	318	LHG	C4-O6-P-O3
30	i	318	LHG	C4-O6-P-O5
30	j	617	LHG	C4-O6-P-O5
30	d	317	LHG	C3-O3-P-O5
30	d	317	LHG	C4-O6-P-O4
30	g	321	LHG	C3-O3-P-O5
30	n	619	LHG	C3-O3-P-O5
31	A	847	WVN	C22-C26-C29-C31
31	F	204	WVN	C25-C28-C30-C33
31	I	101	WVN	C32-C36-C39-C40
31	s	207	WVN	C05-C02-C11-C19
31	i	316	WVN	C32-C36-C39-C40
31	i	316	WVN	C34-C37-C40-C39
36	b	614	II0	C35-C39-C41-C42
36	m	615	II0	C35-C39-C41-C42
36	l	314	II0	C25-C29-C31-C33
36	l	316	II0	C35-C39-C41-C42
36	k	615	II0	C35-C39-C41-C42
36	g	316	II0	C36-C40-C42-C41
36	n	616	II0	C35-C39-C41-C42
37	m	617	IHT	C33-C37-C40-C41
38	s	201	KC2	CHA-CBD-CGD-O2D
38	s	204	KC2	CHA-CBD-CGD-O2D
38	c	610	KC2	CHA-CBD-CGD-O1D
38	l	310	KC2	CHA-CBD-CGD-O2D
38	l	310	KC2	CAA-CBA-CGA-O1A
28	F	201	CLA	C4-C3-C5-C6
28	A	817	CLA	C2B-C3B-CAB-CBB
28	A	852	CLA	C2B-C3B-CAB-CBB
28	B	827	CLA	C2B-C3B-CAB-CBB
28	B	829	CLA	C2B-C3B-CAB-CBB
28	K	103	CLA	C2B-C3B-CAB-CBB
28	b	611	CLA	C2B-C3B-CAB-CBB
28	h	301	CLA	C2B-C3B-CAB-CBB
28	h	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	e	607	CLA	C2B-C3B-CAB-CBB
28	l	311	CLA	C2B-C3B-CAB-CBB
28	j	607	CLA	C2B-C3B-CAB-CBB
28	j	613	CLA	C2B-C3B-CAB-CBB
28	g	306	CLA	C2B-C3B-CAB-CBB
28	g	307	CLA	C2B-C3B-CAB-CBB
28	g	311	CLA	C2B-C3B-CAB-CBB
28	n	606	CLA	C2B-C3B-CAB-CBB
35	c	619	LMG	C34-C35-C36-C37
30	A	849	LHG	C5-C4-O6-P
31	R	201	WVN	C30-C33-C34-C38
37	b	616	IHT	C18-C22-C23-C25
37	m	617	IHT	C30-C32-C33-C36
30	a	319	LHG	C10-C11-C12-C13
36	e	616	II0	C32-C34-C36-C40
37	b	616	IHT	C18-C22-C23-C27
28	m	608	CLA	O1A-CGA-O2A-C1
30	a	301	LHG	O10-C23-O8-C6
30	b	619	LHG	O1-C1-C2-O2
28	B	833	CLA	O1D-CGD-O2D-CED
28	b	610	CLA	C16-C17-C18-C19
28	f	607	CLA	C16-C17-C18-C19
30	n	619	LHG	O1-C1-C2-C3
28	m	610	CLA	C4C-C3C-CAC-CBC
35	J	105	LMG	C37-C38-C39-C40
28	A	838	CLA	C5-C6-C7-C8
29	A	842	PQN	C20-C21-C22-C23
30	f	619	LHG	C34-C35-C36-C37
30	g	301	LHG	C6-C5-O7-C7
31	L	206	WVN	C28-C30-C33-C34
28	B	815	CLA	CAA-CBA-CGA-O2A
28	B	841	CLA	CAA-CBA-CGA-O2A
28	j	610	CLA	CAA-CBA-CGA-O2A
28	s	203	CLA	C10-C11-C12-C13
28	l	303	CLA	C2-C3-C5-C6
31	I	101	WVN	C22-C26-C29-C31
31	L	201	WVN	C22-C26-C29-C31
37	a	317	IHT	C26-C29-C31-C34
28	e	605	CLA	C16-C17-C18-C19
28	f	609	CLA	C16-C17-C18-C19
28	m	608	CLA	C5-C6-C7-C8
28	l	311	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	f	608	CLA	C13-C15-C16-C17
29	B	842	PQN	C20-C21-C22-C23
30	b	620	LHG	O6-C4-C5-C6
30	A	843	LHG	C10-C11-C12-C13
28	A	802	CLA	C11-C12-C13-C14
28	A	806	CLA	C11-C12-C13-C14
28	A	812	CLA	C14-C13-C15-C16
28	A	836	CLA	C6-C7-C8-C9
28	B	808	CLA	C11-C12-C13-C14
28	B	822	CLA	C11-C10-C8-C9
28	F	201	CLA	C14-C13-C15-C16
28	O	206	CLA	C11-C12-C13-C14
28	s	203	CLA	C14-C13-C15-C16
28	b	610	CLA	C6-C7-C8-C9
28	b	610	CLA	C14-C13-C15-C16
28	e	607	CLA	C6-C7-C8-C9
28	l	306	CLA	C11-C12-C13-C14
28	l	309	CLA	C6-C7-C8-C9
28	j	610	CLA	C11-C10-C8-C9
28	g	308	CLA	C11-C10-C8-C9
28	g	309	CLA	C14-C13-C15-C16
35	J	105	LMG	C31-C32-C33-C34
28	A	808	CLA	C12-C13-C15-C16
28	A	827	CLA	C12-C13-C15-C16
28	A	832	CLA	C11-C12-C13-C15
28	A	839	CLA	C12-C13-C15-C16
28	B	803	CLA	C11-C10-C8-C7
28	B	837	CLA	C11-C12-C13-C15
28	F	201	CLA	C11-C10-C8-C7
28	a	312	CLA	C11-C12-C13-C15
28	b	610	CLA	C12-C13-C15-C16
28	e	604	CLA	C11-C10-C8-C7
30	c	618	LHG	C25-C26-C27-C28
28	A	803	CLA	C6-C7-C8-C9
28	L	203	CLA	C16-C17-C18-C19
28	A	841	CLA	C4-C3-C5-C6
28	B	825	CLA	C4-C3-C5-C6
30	e	617	LHG	C2-C3-O3-P
35	O	205	LMG	O7-C8-C9-O8
28	f	613	CLA	CAA-CBA-CGA-O2A
28	a	306	CLA	C13-C15-C16-C17
28	e	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	k	615	II0	C36-C40-C42-C41
36	i	313	II0	C36-C40-C42-C41
28	c	602	CLA	C2C-C3C-CAC-CBC
28	b	610	CLA	C16-C17-C18-C20
28	A	804	CLA	CAA-CBA-CGA-O2A
28	A	817	CLA	CAA-CBA-CGA-O2A
28	d	305	CLA	CAA-CBA-CGA-O2A
28	f	601	CLA	C2A-CAA-CBA-CGA
28	e	606	CLA	C8-C10-C11-C12
28	B	840	CLA	C3-C5-C6-C7
28	h	303	CLA	C2-C1-O2A-CGA
28	l	306	CLA	C4C-C3C-CAC-CBC
30	J	106	LHG	C30-C31-C32-C33
28	e	605	CLA	CBA-CGA-O2A-C1
34	B	843	DGD	C2A-C1A-O1G-C1G
28	j	613	CLA	C5-C6-C7-C8
28	A	817	CLA	C16-C17-C18-C19
28	A	840	CLA	C16-C17-C18-C19
28	A	824	CLA	C8-C10-C11-C12
28	f	604	CLA	C2C-C3C-CAC-CBC
34	B	843	DGD	C5D-C6D-O5D-C1E
28	s	206	CLA	C5-C6-C7-C8
28	e	601	CLA	C2A-CAA-CBA-CGA
28	e	604	CLA	C2A-CAA-CBA-CGA
28	g	305	CLA	C2A-CAA-CBA-CGA
31	F	204	WVN	C34-C37-C40-C39
37	n	617	IHT	C33-C37-C40-C41
28	B	808	CLA	C16-C17-C18-C20
28	e	611	CLA	C4-C3-C5-C6
38	i	319	KC2	C2B-C3B-CAB-CBB
34	B	843	DGD	C8B-C9B-CAB-CBB
28	K	101	CLA	CBA-CGA-O2A-C1
28	Q	302	CLA	O1A-CGA-O2A-C1
30	g	301	LHG	C31-C32-C33-C34
36	f	615	II0	C10-C22-C24-C26
28	A	801	CLA	C16-C17-C18-C20
28	A	820	CLA	C2C-C3C-CAC-CBC
28	A	812	CLA	C6-C7-C8-C9
28	A	852	CLA	C11-C12-C13-C14
28	B	805	CLA	C11-C12-C13-C14
28	B	835	CLA	C6-C7-C8-C9
28	B	837	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	a	306	CLA	C11-C10-C8-C9
28	a	311	CLA	C6-C7-C8-C9
28	b	604	CLA	C6-C7-C8-C9
28	l	303	CLA	C11-C12-C13-C14
28	l	307	CLA	C6-C7-C8-C9
28	k	604	CLA	C6-C7-C8-C9
28	j	613	CLA	C11-C10-C8-C9
28	n	610	CLA	C6-C7-C8-C9
28	B	835	CLA	CBA-CGA-O2A-C1
28	m	608	CLA	C2C-C3C-CAC-CBC
28	B	815	CLA	C4B-C3B-CAB-CBB
28	c	609	CLA	C4B-C3B-CAB-CBB
28	g	322	CLA	C4B-C3B-CAB-CBB
30	L	208	LHG	C33-C34-C35-C36
30	m	619	LHG	C10-C11-C12-C13
28	n	609	CLA	C3-C5-C6-C7
28	n	602	CLA	O1D-CGD-O2D-CED
28	f	603	CLA	CBD-CGD-O2D-CED
28	s	202	CLA	C16-C17-C18-C20
28	B	840	CLA	O1A-CGA-O2A-C1
28	k	602	CLA	O1A-CGA-O2A-C1
28	A	854	CLA	C2A-CAA-CBA-CGA
28	A	841	CLA	C2-C3-C5-C6
28	e	611	CLA	C2-C3-C5-C6
28	a	308	CLA	C13-C15-C16-C17
28	B	806	CLA	C3-C5-C6-C7
30	J	106	LHG	C27-C28-C29-C30
31	B	846	WVN	C25-C28-C30-C33
36	g	317	II0	C26-C30-C32-C34
28	a	310	CLA	O1D-CGD-O2D-CED
28	B	809	CLA	CBA-CGA-O2A-C1
38	m	611	KC2	C4C-C3C-CAC-CBC
38	i	319	KC2	C4B-C3B-CAB-CBB
38	g	314	KC2	C4C-C3C-CAC-CBC
28	A	818	CLA	C11-C12-C13-C15
28	A	829	CLA	C6-C7-C8-C10
28	A	851	CLA	C11-C10-C8-C7
28	B	807	CLA	C11-C10-C8-C7
28	B	808	CLA	C11-C12-C13-C15
28	h	313	CLA	C12-C13-C15-C16
30	L	208	LHG	O2-C2-C3-O3
28	A	801	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	f	619	LHG	C11-C12-C13-C14
28	A	812	CLA	C3A-C2A-CAA-CBA
28	A	840	CLA	C3A-C2A-CAA-CBA
28	B	840	CLA	C3A-C2A-CAA-CBA
28	s	206	CLA	C3A-C2A-CAA-CBA
28	c	606	CLA	C3A-C2A-CAA-CBA
28	a	311	CLA	C3A-C2A-CAA-CBA
28	e	608	CLA	C3A-C2A-CAA-CBA
28	g	308	CLA	C3A-C2A-CAA-CBA
28	n	613	CLA	C3A-C2A-CAA-CBA
28	m	606	CLA	CAA-CBA-CGA-O2A
30	k	620	LHG	C11-C12-C13-C14
28	A	816	CLA	C8-C10-C11-C12
28	s	202	CLA	C8-C10-C11-C12
31	A	846	WVN	C24-C22-C26-C29
31	B	846	WVN	C24-C22-C26-C29
31	J	101	WVN	C24-C22-C26-C29
36	l	313	II0	C38-C36-C40-C42
37	b	616	IHT	C25-C23-C27-C30
37	g	319	IHT	C25-C23-C27-C30
30	A	849	LHG	C24-C25-C26-C27
30	J	106	LHG	C32-C33-C34-C35
31	K	104	WVN	C22-C26-C29-C31
28	A	854	CLA	C16-C17-C18-C20
28	B	801	CLA	C13-C15-C16-C17
31	F	203	WVN	C30-C33-C34-C38
28	Q	303	CLA	CAA-CBA-CGA-O2A
28	k	606	CLA	C4-C3-C5-C6
28	j	612	CLA	C4-C3-C5-C6
28	d	305	CLA	C4-C3-C5-C6
28	n	603	CLA	C4-C3-C5-C6
32	b	618	LMT	O1'-C1-C2-C3
28	e	604	CLA	C4-C3-C5-C6
28	i	305	CLA	C2A-CAA-CBA-CGA
30	a	319	LHG	C29-C30-C31-C32
28	f	608	CLA	C3-C5-C6-C7
28	B	805	CLA	C10-C11-C12-C13
28	A	818	CLA	C11-C12-C13-C14
28	A	826	CLA	C11-C12-C13-C14
28	A	841	CLA	C6-C7-C8-C9
28	B	807	CLA	C11-C10-C8-C9
28	B	807	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	B	835	CLA	C11-C12-C13-C14
28	a	306	CLA	C14-C13-C15-C16
28	a	309	CLA	C6-C7-C8-C9
28	a	312	CLA	C6-C7-C8-C9
28	b	603	CLA	C6-C7-C8-C9
28	b	604	CLA	C11-C10-C8-C9
28	b	611	CLA	C6-C7-C8-C9
28	h	301	CLA	C11-C12-C13-C14
28	h	313	CLA	C6-C7-C8-C9
28	e	605	CLA	C6-C7-C8-C9
28	i	305	CLA	C6-C7-C8-C9
28	i	307	CLA	C11-C10-C8-C9
28	n	607	CLA	C11-C12-C13-C14
28	A	854	CLA	C16-C17-C18-C19
28	B	819	CLA	C6-C7-C8-C9
28	m	603	CLA	C13-C15-C16-C17
28	R	203	CLA	CBA-CGA-O2A-C1
30	b	619	LHG	C27-C28-C29-C30
35	F	205	LMG	C14-C15-C16-C17
35	Q	301	LMG	C9-C8-O7-C10
32	A	850	LMT	C2-C3-C4-C5
28	a	306	CLA	CBD-CGD-O2D-CED
28	i	312	CLA	CAA-CBA-CGA-O2A
30	m	619	LHG	O1-C1-C2-O2
30	g	301	LHG	O1-C1-C2-O2
35	L	209	LMG	C37-C38-C39-C40
28	b	604	CLA	C2A-CAA-CBA-CGA
28	k	607	CLA	C2A-CAA-CBA-CGA
28	i	312	CLA	C2A-CAA-CBA-CGA
28	d	303	CLA	C2A-CAA-CBA-CGA
34	B	843	DGD	O1A-C1A-O1G-C1G
28	A	812	CLA	C1A-C2A-CAA-CBA
28	B	808	CLA	C1A-C2A-CAA-CBA
28	a	311	CLA	C1A-C2A-CAA-CBA
28	h	301	CLA	C1A-C2A-CAA-CBA
31	A	846	WVN	C19-C22-C26-C29
31	B	846	WVN	C19-C22-C26-C29
31	J	101	WVN	C19-C22-C26-C29
36	l	313	II0	C34-C36-C40-C42
37	b	616	IHT	C22-C23-C27-C30
37	g	319	IHT	C22-C23-C27-C30
35	L	209	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
32	A	850	LMT	C6-C7-C8-C9
35	c	619	LMG	C14-C15-C16-C17
28	g	306	CLA	CAA-CBA-CGA-O1A
28	K	101	CLA	O1A-CGA-O2A-C1
28	A	832	CLA	C2B-C3B-CAB-CBB
28	A	833	CLA	C2B-C3B-CAB-CBB
28	B	815	CLA	C2B-C3B-CAB-CBB
28	B	834	CLA	C2B-C3B-CAB-CBB
28	B	835	CLA	C2B-C3B-CAB-CBB
28	F	202	CLA	C2B-C3B-CAB-CBB
28	L	203	CLA	C2B-C3B-CAB-CBB
28	s	203	CLA	C2B-C3B-CAB-CBB
28	c	609	CLA	C2B-C3B-CAB-CBB
28	a	305	CLA	C2B-C3B-CAB-CBB
28	b	604	CLA	C2B-C3B-CAB-CBB
28	m	612	CLA	C2B-C3B-CAB-CBB
28	e	602	CLA	C2B-C3B-CAB-CBB
28	f	605	CLA	C2B-C3B-CAB-CBB
28	d	307	CLA	C2B-C3B-CAB-CBB
28	n	603	CLA	C2B-C3B-CAB-CBB
28	Q	303	CLA	C2B-C3B-CAB-CBB
31	A	845	WVN	C06-C13-C20-C23
31	B	844	WVN	C15-C13-C20-C23
31	R	202	WVN	C15-C13-C20-C23
37	b	616	IHT	C02-C07-C18-C22
28	a	306	CLA	O1D-CGD-O2D-CED
28	A	825	CLA	CBA-CGA-O2A-C1
28	j	613	CLA	CBA-CGA-O2A-C1
30	J	106	LHG	C17-C18-C19-C20
30	a	301	LHG	C5-C4-O6-P
28	B	820	CLA	CBD-CGD-O2D-CED
28	a	303	CLA	C4-C3-C5-C6
28	a	309	CLA	C4-C3-C5-C6
31	l	315	WVN	C34-C37-C40-C39
28	A	802	CLA	C11-C12-C13-C15
28	A	825	CLA	C6-C7-C8-C10
28	A	826	CLA	C6-C7-C8-C10
28	A	840	CLA	C11-C12-C13-C15
28	B	802	CLA	C11-C10-C8-C7
28	s	203	CLA	C12-C13-C15-C16
28	b	611	CLA	C11-C12-C13-C15
28	h	306	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	m	603	CLA	C12-C13-C15-C16
28	g	305	CLA	C11-C12-C13-C15
28	A	837	CLA	C16-C17-C18-C20
28	b	603	CLA	C16-C17-C18-C20
28	h	306	CLA	C2A-CAA-CBA-CGA
28	k	609	CLA	C2A-CAA-CBA-CGA
30	d	317	LHG	C7-C8-C9-C10
35	J	105	LMG	O1-C7-C8-O7
32	a	302	LMT	C1-C2-C3-C4
32	a	320	LMT	C5-C6-C7-C8
28	s	202	CLA	C3-C5-C6-C7
28	B	802	CLA	CAA-CBA-CGA-O2A
28	B	807	CLA	C16-C17-C18-C20
28	b	606	CLA	C12-C13-C15-C16
28	l	309	CLA	C12-C13-C15-C16
31	B	846	WVN	C29-C31-C32-C35
31	L	201	WVN	C29-C31-C32-C35
36	b	614	II0	C32-C34-C36-C38
36	e	616	II0	C32-C34-C36-C38
36	n	618	II0	C32-C34-C36-C38
28	j	605	CLA	CAA-CBA-CGA-O2A
28	A	827	CLA	C4-C3-C5-C6
28	O	202	CLA	C4-C3-C5-C6
28	i	306	CLA	CAA-CBA-CGA-O2A
28	B	825	CLA	C2-C3-C5-C6
28	i	307	CLA	C2-C3-C5-C6
30	L	208	LHG	C12-C13-C14-C15
28	A	832	CLA	C2-C1-O2A-CGA
28	e	605	CLA	C15-C16-C17-C18
37	m	617	IHT	C30-C32-C33-C37
28	k	614	CLA	C2C-C3C-CAC-CBC
28	A	824	CLA	C13-C15-C16-C17
28	B	837	CLA	C15-C16-C17-C18
35	O	205	LMG	C28-C29-C30-C31
28	c	604	CLA	C2A-CAA-CBA-CGA
28	k	604	CLA	C2A-CAA-CBA-CGA
28	Q	303	CLA	CAA-CBA-CGA-O1A
28	m	608	CLA	C11-C10-C8-C9
32	a	302	LMT	C4-C5-C6-C7
28	g	322	CLA	C4C-C3C-CAC-CBC
35	n	620	LMG	C15-C16-C17-C18
28	A	840	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	L	203	CLA	C16-C17-C18-C20
30	l	317	LHG	C25-C26-C27-C28
28	n	613	CLA	CAA-CBA-CGA-O1A
28	g	305	CLA	C4C-C3C-CAC-CBC
28	f	604	CLA	C4C-C3C-CAC-CBC
28	A	802	CLA	C4-C3-C5-C6
30	f	619	LHG	C2-C3-O3-P
28	B	822	CLA	C10-C11-C12-C13
28	e	610	CLA	C15-C16-C17-C18
28	f	607	CLA	C5-C6-C7-C8
28	f	608	CLA	C10-C11-C12-C13
28	B	807	CLA	C16-C17-C18-C19
30	a	319	LHG	C33-C34-C35-C36
35	b	621	LMG	C16-C17-C18-C19
28	j	606	CLA	CAA-CBA-CGA-O2A
30	g	301	LHG	C11-C10-C9-C8
28	j	605	CLA	CAA-CBA-CGA-O1A
30	b	619	LHG	C18-C19-C20-C21
28	B	809	CLA	O1A-CGA-O2A-C1
28	R	203	CLA	O1A-CGA-O2A-C1
35	L	209	LMG	O10-C28-O8-C9
28	A	835	CLA	C2A-CAA-CBA-CGA
28	l	303	CLA	C2A-CAA-CBA-CGA
35	J	105	LMG	C19-C20-C21-C22
30	e	617	LHG	O1-C1-C2-O2
30	f	619	LHG	O1-C1-C2-O2
36	m	618	II0	C10-C22-C24-C26
36	e	612	II0	C10-C22-C24-C26
36	i	317	II0	C10-C22-C24-C26
36	j	615	II0	C10-C22-C24-C26
36	d	313	II0	C09-C21-C23-C25
36	d	316	II0	C10-C22-C24-C26
36	g	316	II0	C10-C22-C24-C26
36	g	318	II0	C09-C21-C23-C25
36	n	615	II0	C10-C22-C24-C26
36	n	616	II0	C09-C21-C23-C25
30	c	620	LHG	O6-C4-C5-O7
28	B	802	CLA	C16-C17-C18-C19
28	B	817	CLA	C16-C17-C18-C20
28	c	608	CLA	C15-C16-C17-C18
28	A	833	CLA	C4B-C3B-CAB-CBB
28	s	203	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	m	602	CLA	C4B-C3B-CAB-CBB
28	m	612	CLA	C4B-C3B-CAB-CBB
28	e	602	CLA	C4B-C3B-CAB-CBB
28	e	604	CLA	C4B-C3B-CAB-CBB
28	Q	303	CLA	C4B-C3B-CAB-CBB
28	l	303	CLA	O1A-CGA-O2A-C1
28	g	308	CLA	C8-C10-C11-C12
28	s	202	CLA	C16-C17-C18-C19
28	B	833	CLA	C5-C6-C7-C8
28	j	613	CLA	O1A-CGA-O2A-C1
28	B	824	CLA	C15-C16-C17-C18
35	L	209	LMG	C11-C12-C13-C14
28	f	603	CLA	O1D-CGD-O2D-CED
30	b	620	LHG	C25-C26-C27-C28
28	l	306	CLA	C16-C17-C18-C19
28	j	613	CLA	C16-C17-C18-C19
28	A	818	CLA	C4-C3-C5-C6
28	a	309	CLA	C8-C10-C11-C12
28	A	819	CLA	CAA-CBA-CGA-O2A
28	A	827	CLA	C2-C3-C5-C6
28	f	613	CLA	C11-C10-C8-C7
30	a	319	LHG	C24-C25-C26-C27
28	l	307	CLA	C5-C6-C7-C8
31	A	845	WVN	C32-C36-C39-C40
31	l	315	WVN	C32-C36-C39-C40
37	O	204	IHT	C23-C27-C30-C32
30	b	619	LHG	O2-C2-C3-O3
30	k	620	LHG	O2-C2-C3-O3
28	B	838	CLA	CAA-CBA-CGA-O1A
28	A	810	CLA	C11-C10-C8-C9
28	A	817	CLA	C11-C12-C13-C14
28	A	831	CLA	C11-C12-C13-C14
28	A	836	CLA	C11-C12-C13-C14
28	B	802	CLA	C11-C10-C8-C9
28	B	817	CLA	C14-C13-C15-C16
28	m	608	CLA	C6-C7-C8-C9
28	l	306	CLA	C11-C10-C8-C9
28	k	608	CLA	C14-C13-C15-C16
28	f	613	CLA	C13-C15-C16-C17
35	c	619	LMG	C32-C33-C34-C35
35	J	105	LMG	C8-C7-O1-C1
28	c	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	a	304	CLA	C2A-CAA-CBA-CGA
28	a	313	CLA	C2A-CAA-CBA-CGA
28	b	607	CLA	C2A-CAA-CBA-CGA
28	A	833	CLA	C2-C1-O2A-CGA
28	B	804	CLA	C2-C1-O2A-CGA
28	k	606	CLA	C2-C1-O2A-CGA
28	j	603	CLA	C2-C1-O2A-CGA
28	f	608	CLA	O1A-CGA-O2A-C1
28	A	841	CLA	C16-C17-C18-C20
28	e	605	CLA	C16-C17-C18-C20
28	A	851	CLA	C3A-C2A-CAA-CBA
28	B	814	CLA	C3A-C2A-CAA-CBA
28	a	313	CLA	C3A-C2A-CAA-CBA
28	b	610	CLA	C3A-C2A-CAA-CBA
28	e	605	CLA	C4-C3-C5-C6
28	f	601	CLA	C3A-C2A-CAA-CBA
28	e	604	CLA	O1A-CGA-O2A-C1
35	L	209	LMG	C39-C40-C41-C42
30	a	301	LHG	O1-C1-C2-C3
28	l	309	CLA	C5-C6-C7-C8
28	R	203	CLA	CAA-CBA-CGA-O1A
35	c	619	LMG	C17-C18-C19-C20
28	a	310	CLA	CBD-CGD-O2D-CED
35	c	619	LMG	C4-C5-C6-O5
28	k	606	CLA	CAA-CBA-CGA-O2A
28	A	818	CLA	C2-C3-C5-C6
28	h	306	CLA	C13-C15-C16-C17
28	i	302	CLA	CAA-CBA-CGA-O1A
30	f	619	LHG	C25-C26-C27-C28
35	c	619	LMG	C24-C25-C26-C27
28	B	817	CLA	CBA-CGA-O2A-C1
28	B	840	CLA	CBA-CGA-O2A-C1
28	e	604	CLA	CBA-CGA-O2A-C1
28	B	835	CLA	O1A-CGA-O2A-C1
28	A	819	CLA	CAA-CBA-CGA-O1A
28	a	304	CLA	CBA-CGA-O2A-C1
28	m	610	CLA	C2C-C3C-CAC-CBC
28	A	812	CLA	C8-C10-C11-C12
28	d	304	CLA	C2A-CAA-CBA-CGA
28	F	201	CLA	C2-C3-C5-C6
36	k	615	II0	C25-C29-C31-C33
28	A	812	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	m	606	CLA	C15-C16-C17-C18
28	l	302	CLA	C2-C1-O2A-CGA
28	f	612	CLA	C4C-C3C-CAC-CBC
28	A	816	CLA	C14-C13-C15-C16
28	A	828	CLA	C14-C13-C15-C16
28	A	832	CLA	C11-C12-C13-C14
28	B	813	CLA	C11-C10-C8-C9
28	F	201	CLA	C6-C7-C8-C9
28	e	611	CLA	C11-C10-C8-C9
28	l	306	CLA	C6-C7-C8-C9
28	A	841	CLA	C16-C17-C18-C19
28	B	817	CLA	C16-C17-C18-C19
28	l	303	CLA	C16-C17-C18-C19
28	j	604	CLA	C2C-C3C-CAC-CBC
28	B	805	CLA	CAA-CBA-CGA-O2A
31	B	847	WVN	C30-C33-C34-C37
36	k	615	II0	C32-C34-C36-C40
36	n	618	II0	C32-C34-C36-C40
35	F	205	LMG	C24-C25-C26-C27
28	d	303	CLA	CAA-CBA-CGA-O1A
28	c	608	CLA	CAA-CBA-CGA-O2A
28	l	307	CLA	CAA-CBA-CGA-O2A
28	c	609	CLA	CAA-CBA-CGA-O2A
28	A	801	CLA	C12-C13-C15-C16
28	A	824	CLA	C11-C12-C13-C15
28	B	804	CLA	C12-C13-C15-C16
28	B	806	CLA	C6-C7-C8-C10
28	B	807	CLA	C6-C7-C8-C10
28	B	817	CLA	C12-C13-C15-C16
28	B	822	CLA	C11-C12-C13-C15
28	B	838	CLA	C11-C10-C8-C7
28	s	206	CLA	C12-C13-C15-C16
28	m	608	CLA	C11-C10-C8-C7
28	e	610	CLA	C11-C12-C13-C15
28	l	311	CLA	C6-C7-C8-C10
28	f	602	CLA	C12-C13-C15-C16
28	i	307	CLA	C11-C12-C13-C15
28	j	613	CLA	C11-C12-C13-C15
28	d	303	CLA	C12-C13-C15-C16
28	A	825	CLA	O1A-CGA-O2A-C1
28	j	613	CLA	C3-C5-C6-C7
28	A	801	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	a	308	CLA	CAA-CBA-CGA-O1A
35	L	209	LMG	C23-C24-C25-C26
28	A	801	CLA	C2B-C3B-CAB-CBB
28	A	841	CLA	C2B-C3B-CAB-CBB
28	B	802	CLA	C2B-C3B-CAB-CBB
28	B	819	CLA	C2B-C3B-CAB-CBB
28	s	206	CLA	C2B-C3B-CAB-CBB
28	c	607	CLA	C2B-C3B-CAB-CBB
28	m	602	CLA	C2B-C3B-CAB-CBB
28	m	605	CLA	C2B-C3B-CAB-CBB
28	e	604	CLA	C2B-C3B-CAB-CBB
28	e	610	CLA	C2B-C3B-CAB-CBB
28	g	322	CLA	C2B-C3B-CAB-CBB
31	J	101	WVN	C15-C13-C20-C23
31	J	102	WVN	C06-C13-C20-C23
37	a	317	IHT	C10-C07-C18-C22
28	A	812	CLA	CAA-CBA-CGA-O2A
35	n	620	LMG	C32-C33-C34-C35
28	A	802	CLA	C2-C1-O2A-CGA
28	A	805	CLA	C2-C1-O2A-CGA
28	B	836	CLA	C2-C1-O2A-CGA
28	b	612	CLA	C2-C1-O2A-CGA
28	k	610	CLA	C2-C1-O2A-CGA
28	n	610	CLA	CAA-CBA-CGA-O2A
30	f	619	LHG	O7-C7-C8-C9
28	m	603	CLA	C4-C3-C5-C6
28	s	203	CLA	CAA-CBA-CGA-O2A
28	g	308	CLA	CAA-CBA-CGA-O2A
28	e	604	CLA	C2-C3-C5-C6
30	i	318	LHG	C26-C27-C28-C29
28	c	609	CLA	CAA-CBA-CGA-O1A
28	B	806	CLA	C2A-CAA-CBA-CGA
35	J	105	LMG	C34-C35-C36-C37
28	A	828	CLA	CAA-CBA-CGA-O2A
28	h	303	CLA	CAA-CBA-CGA-O2A
28	l	304	CLA	CAA-CBA-CGA-O2A
30	A	844	LHG	O7-C7-C8-C9
30	J	106	LHG	O7-C7-C8-C9
30	m	619	LHG	C31-C32-C33-C34
28	A	841	CLA	C5-C6-C7-C8
30	n	619	LHG	C32-C33-C34-C35
28	f	608	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	827	CLA	CAA-CBA-CGA-O2A
28	B	840	CLA	CAA-CBA-CGA-O2A
30	k	620	LHG	C7-C8-C9-C10
30	b	620	LHG	C11-C12-C13-C14
28	A	809	CLA	C11-C10-C8-C7
28	c	606	CLA	CAA-CBA-CGA-O2A
28	m	608	CLA	CAA-CBA-CGA-O2A
28	j	603	CLA	CAA-CBA-CGA-O2A
28	g	315	CLA	CAA-CBA-CGA-O2A
28	A	836	CLA	C8-C10-C11-C12
28	B	811	CLA	C2C-C3C-CAC-CBC
28	s	206	CLA	C2-C3-C5-C6
28	a	303	CLA	C2-C3-C5-C6
28	j	613	CLA	C2A-CAA-CBA-CGA
28	g	310	CLA	C2A-CAA-CBA-CGA
28	L	202	CLA	CAA-CBA-CGA-O2A
36	a	314	II0	C10-C22-C24-C26
36	b	613	II0	C10-C22-C24-C26
36	h	312	II0	C10-C22-C24-C26
36	k	621	II0	C10-C22-C24-C26
36	i	315	II0	C09-C21-C23-C25
36	i	320	II0	C10-C22-C24-C26
36	g	320	II0	C10-C22-C24-C26
28	e	601	CLA	CAA-CBA-CGA-O2A
28	B	803	CLA	C11-C12-C13-C14
28	B	804	CLA	C6-C7-C8-C9
28	B	817	CLA	C6-C7-C8-C9
28	h	301	CLA	C11-C10-C8-C9
28	e	607	CLA	C14-C13-C15-C16
28	l	311	CLA	C15-C16-C17-C18
30	i	318	LHG	C5-C4-O6-P
28	A	836	CLA	CAA-CBA-CGA-O2A
28	e	603	CLA	CAA-CBA-CGA-O2A
30	b	620	LHG	O7-C7-C8-C9
30	m	619	LHG	C25-C26-C27-C28
35	b	621	LMG	C7-C8-C9-O8
28	A	819	CLA	C4B-C3B-CAB-CBB
28	A	830	CLA	C4B-C3B-CAB-CBB
28	A	835	CLA	C4B-C3B-CAB-CBB
28	A	851	CLA	C1A-C2A-CAA-CBA
28	B	817	CLA	C4B-C3B-CAB-CBB
28	L	203	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	c	611	CLA	C1A-C2A-CAA-CBA
28	a	313	CLA	C1A-C2A-CAA-CBA
28	e	610	CLA	C4B-C3B-CAB-CBB
28	l	302	CLA	C1A-C2A-CAA-CBA
28	l	306	CLA	C1A-C2A-CAA-CBA
28	f	601	CLA	C1A-C2A-CAA-CBA
28	n	603	CLA	C4B-C3B-CAB-CBB
28	n	609	CLA	C1A-C2A-CAA-CBA
29	B	842	PQN	C13-C15-C16-C17
28	h	313	CLA	C4-C3-C5-C6
30	b	619	LHG	C10-C11-C12-C13
35	O	205	LMG	O6-C1-O1-C7
28	c	612	CLA	CAA-CBA-CGA-O2A
28	h	308	CLA	CAA-CBA-CGA-O2A
28	e	607	CLA	CAA-CBA-CGA-O2A
28	f	603	CLA	CAA-CBA-CGA-O2A
28	i	311	CLA	CAA-CBA-CGA-O2A
28	j	607	CLA	CAA-CBA-CGA-O2A
28	j	608	CLA	CAA-CBA-CGA-O2A
30	c	618	LHG	C27-C28-C29-C30
31	F	204	WVN	C30-C33-C34-C37
36	b	614	II0	C32-C34-C36-C40
36	h	311	II0	C31-C33-C35-C39
36	i	314	II0	C36-C40-C42-C41
37	f	617	IHT	C33-C37-C40-C41
30	m	619	LHG	C30-C31-C32-C33
30	L	208	LHG	C11-C10-C9-C8
28	i	305	CLA	C8-C10-C11-C12
28	B	836	CLA	CAA-CBA-CGA-O2A
28	m	604	CLA	CAA-CBA-CGA-O2A
30	i	318	LHG	O8-C23-C24-C25
30	j	617	LHG	O8-C23-C24-C25
28	m	609	CLA	C2A-CAA-CBA-CGA
28	f	604	CLA	C2A-CAA-CBA-CGA
35	c	619	LMG	C12-C13-C14-C15
28	g	308	CLA	C16-C17-C18-C20
28	c	605	CLA	CAA-CBA-CGA-O2A
28	B	804	CLA	CAA-CBA-CGA-O1A
35	n	620	LMG	C29-C30-C31-C32
35	Q	301	LMG	O6-C5-C6-O5
28	c	601	CLA	C2-C3-C5-C6
28	f	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	n	608	CLA	C2-C3-C5-C6
28	n	613	CLA	C2-C3-C5-C6
28	m	608	CLA	C8-C10-C11-C12
28	A	816	CLA	C2-C1-O2A-CGA
28	a	303	CLA	C2-C1-O2A-CGA
28	i	306	CLA	C2-C1-O2A-CGA
28	Q	302	CLA	C2-C1-O2A-CGA
28	A	802	CLA	C11-C10-C8-C7
28	A	824	CLA	C12-C13-C15-C16
28	L	203	CLA	C11-C12-C13-C15
28	h	306	CLA	C11-C10-C8-C7
28	k	609	CLA	C12-C13-C15-C16
28	g	308	CLA	C6-C7-C8-C10
28	g	309	CLA	C11-C12-C13-C15
28	A	854	CLA	C10-C11-C12-C13
28	f	601	CLA	C2-C1-O2A-CGA
28	A	840	CLA	C8-C10-C11-C12
28	e	606	CLA	C10-C11-C12-C13
31	B	844	WVN	C34-C37-C40-C39
28	j	602	CLA	C2A-CAA-CBA-CGA
28	B	828	CLA	O2A-C1-C2-C3
28	h	306	CLA	C5-C6-C7-C8
28	A	825	CLA	C8-C10-C11-C12
28	a	312	CLA	C3A-C2A-CAA-CBA
28	h	301	CLA	C3A-C2A-CAA-CBA
28	h	308	CLA	C3A-C2A-CAA-CBA
28	k	601	CLA	C3A-C2A-CAA-CBA
28	g	307	CLA	CAA-CBA-CGA-O1A
28	d	302	CLA	CAA-CBA-CGA-O2A
35	J	105	LMG	O8-C28-C29-C30
35	Q	301	LMG	C28-C29-C30-C31
28	f	601	CLA	C4C-C3C-CAC-CBC
28	n	610	CLA	C4C-C3C-CAC-CBC
32	A	850	LMT	C5'-C4'-O1B-C1B
28	B	840	CLA	CAA-CBA-CGA-O1A
28	c	608	CLA	CAA-CBA-CGA-O1A
28	l	304	CLA	CAA-CBA-CGA-O1A
28	g	308	CLA	CAA-CBA-CGA-O1A
30	J	106	LHG	O9-C7-C8-C9
28	j	604	CLA	C2A-CAA-CBA-CGA
35	c	619	LMG	C13-C14-C15-C16
28	m	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	A	825	CLA	C11-C12-C13-C14
28	A	838	CLA	C6-C7-C8-C9
28	A	840	CLA	C6-C7-C8-C9
28	A	840	CLA	C11-C12-C13-C14
28	B	802	CLA	C14-C13-C15-C16
28	B	830	CLA	C6-C7-C8-C9
28	B	830	CLA	C11-C10-C8-C9
28	s	206	CLA	C11-C12-C13-C14
28	m	603	CLA	C14-C13-C15-C16
28	k	608	CLA	C11-C12-C13-C14
28	f	613	CLA	C11-C10-C8-C9
28	i	307	CLA	C11-C12-C13-C14
28	g	322	CLA	C6-C7-C8-C9
28	Q	302	CLA	C11-C12-C13-C14
29	B	842	PQN	C21-C22-C23-C24
30	j	617	LHG	O10-C23-C24-C25
36	e	616	II0	C25-C29-C31-C33
35	n	620	LMG	C14-C15-C16-C17
28	j	606	CLA	O1D-CGD-O2D-CED
28	b	604	CLA	C8-C10-C11-C12
28	k	608	CLA	C4-C3-C5-C6
29	A	842	PQN	C14-C13-C15-C16
28	A	812	CLA	CAA-CBA-CGA-O1A
28	h	303	CLA	CAA-CBA-CGA-O1A
28	l	307	CLA	CAA-CBA-CGA-O1A
28	b	601	CLA	C4-C3-C5-C6
28	b	612	CLA	C4-C3-C5-C6
28	m	609	CLA	C4-C3-C5-C6
28	k	607	CLA	C4-C3-C5-C6
31	A	848	WVN	C01-C02-C11-C19
38	s	201	KC2	C1A-C2A-CAA-CBA
38	c	610	KC2	C1A-C2A-CAA-CBA
38	m	611	KC2	C1A-C2A-CAA-CBA
38	e	609	KC2	C3A-C2A-CAA-CBA
38	l	310	KC2	C3A-C2A-CAA-CBA
38	k	612	KC2	C3A-C2A-CAA-CBA
38	i	310	KC2	C1A-C2A-CAA-CBA
38	d	311	KC2	C1A-C2A-CAA-CBA
38	g	312	KC2	C3A-C2A-CAA-CBA
38	n	611	KC2	C1A-C2A-CAA-CBA
38	n	612	KC2	C1A-C2A-CAA-CBA
28	c	605	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	b	620	LHG	O9-C7-C8-C9
28	b	611	CLA	C15-C16-C17-C18
28	j	604	CLA	C4C-C3C-CAC-CBC
30	c	620	LHG	C11-C10-C9-C8
35	c	619	LMG	C40-C41-C42-C43
30	c	618	LHG	O7-C7-C8-C9
28	j	608	CLA	CAA-CBA-CGA-O1A
28	A	810	CLA	C10-C11-C12-C13
31	s	205	WVN	C30-C33-C34-C37
36	a	316	II0	C31-C33-C35-C39
28	A	828	CLA	CAA-CBA-CGA-O1A
28	B	805	CLA	CAA-CBA-CGA-O1A
28	L	202	CLA	CAA-CBA-CGA-O1A
28	s	203	CLA	CAA-CBA-CGA-O1A
28	g	315	CLA	CAA-CBA-CGA-O1A
28	n	610	CLA	CAA-CBA-CGA-O1A
30	A	844	LHG	O9-C7-C8-C9
30	a	301	LHG	O7-C5-C6-O8
35	n	620	LMG	O1-C7-C8-O7
35	n	620	LMG	C37-C38-C39-C40
28	j	603	CLA	CAA-CBA-CGA-O1A
30	f	619	LHG	O9-C7-C8-C9
28	A	824	CLA	CAA-CBA-CGA-O2A
28	b	609	CLA	CAA-CBA-CGA-O2A
28	g	308	CLA	C16-C17-C18-C19
28	A	836	CLA	CAA-CBA-CGA-O1A
28	e	607	CLA	CAA-CBA-CGA-O1A
28	b	603	CLA	C13-C15-C16-C17
28	f	601	CLA	C2C-C3C-CAC-CBC
28	k	610	CLA	CAA-CBA-CGA-O2A
35	b	621	LMG	O8-C28-C29-C30
28	A	802	CLA	C2-C3-C5-C6
28	m	603	CLA	C2-C3-C5-C6
28	c	606	CLA	CAA-CBA-CGA-O1A
28	h	308	CLA	CAA-CBA-CGA-O1A
28	m	608	CLA	CAA-CBA-CGA-O1A
28	d	302	CLA	CAA-CBA-CGA-O1A
28	A	810	CLA	CAD-CBD-CGD-O2D
28	A	833	CLA	CAD-CBD-CGD-O2D
28	A	834	CLA	CAD-CBD-CGD-O2D
28	B	840	CLA	CAD-CBD-CGD-O2D
28	B	841	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	L	207	CLA	CAD-CBD-CGD-O2D
28	K	101	CLA	CAD-CBD-CGD-O2D
28	a	304	CLA	CAD-CBD-CGD-O2D
28	i	304	CLA	CAD-CBD-CGD-O2D
28	i	306	CLA	CAD-CBD-CGD-O2D
28	g	309	CLA	CAD-CBD-CGD-O2D
28	g	315	CLA	CAD-CBD-CGD-O2D
28	a	303	CLA	C2C-C3C-CAC-CBC
28	s	206	CLA	CAA-CBA-CGA-O2A
28	B	810	CLA	C2C-C3C-CAC-CBC
28	m	604	CLA	CAA-CBA-CGA-O1A
28	e	603	CLA	CAA-CBA-CGA-O1A
28	i	311	CLA	CAA-CBA-CGA-O1A
28	e	605	CLA	C10-C11-C12-C13
28	e	606	CLA	C2-C1-O2A-CGA
28	l	306	CLA	C2-C1-O2A-CGA
28	B	827	CLA	CAA-CBA-CGA-O1A
28	B	820	CLA	O1D-CGD-O2D-CED
28	m	610	CLA	CAA-CBA-CGA-O2A
38	c	610	KC2	CAA-CBA-CGA-O2A
28	B	835	CLA	C15-C16-C17-C18
28	A	818	CLA	C2A-CAA-CBA-CGA
28	f	609	CLA	C2A-CAA-CBA-CGA
30	a	319	LHG	C25-C26-C27-C28
28	k	610	CLA	CAA-CBA-CGA-O1A
28	l	308	CLA	CAA-CBA-CGA-O2A
28	j	601	CLA	CAA-CBA-CGA-O2A
30	a	301	LHG	C26-C27-C28-C29
28	O	206	CLA	C5-C6-C7-C8
28	c	612	CLA	CAA-CBA-CGA-O1A
28	f	603	CLA	CAA-CBA-CGA-O1A
28	A	808	CLA	CAA-CBA-CGA-O2A
28	a	311	CLA	CAA-CBA-CGA-O2A
28	e	604	CLA	CAA-CBA-CGA-O2A
28	k	601	CLA	CAA-CBA-CGA-O2A
28	B	836	CLA	CAA-CBA-CGA-O1A
30	c	618	LHG	C10-C11-C12-C13

There are no ring outliers.

247 monomers are involved in 487 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	851	CLA	2	0
28	c	603	CLA	1	0
28	l	303	CLA	1	0
30	i	318	LHG	2	0
28	b	605	CLA	1	0
28	A	835	CLA	4	0
28	A	837	CLA	3	0
28	B	824	CLA	2	0
28	A	830	CLA	1	0
36	n	618	II0	1	0
30	L	208	LHG	2	0
28	b	606	CLA	5	0
28	B	808	CLA	1	0
31	L	206	WVN	1	0
36	m	615	II0	1	0
28	B	840	CLA	2	0
30	m	619	LHG	2	0
28	m	609	CLA	1	0
28	h	303	CLA	1	0
28	g	322	CLA	5	0
31	I	101	WVN	2	0
35	b	621	LMG	3	0
28	h	308	CLA	2	0
28	A	822	CLA	2	0
28	b	608	CLA	3	0
28	d	304	CLA	2	0
28	B	817	CLA	4	0
28	B	821	CLA	5	0
28	i	303	CLA	2	0
28	g	303	CLA	2	0
28	m	602	CLA	3	0
28	A	817	CLA	4	0
28	B	823	CLA	2	0
28	f	602	CLA	3	0
31	J	101	WVN	1	0
28	h	306	CLA	4	0
28	A	814	CLA	1	0
28	B	804	CLA	1	0
28	c	601	CLA	2	0
34	B	843	DGD	2	0
28	m	607	CLA	1	0
28	n	610	CLA	2	0
28	j	605	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	i	320	II0	1	0
28	j	607	CLA	3	0
28	i	305	CLA	1	0
28	i	308	CLA	1	0
28	A	806	CLA	2	0
30	j	617	LHG	2	0
28	O	202	CLA	4	0
28	B	811	CLA	2	0
28	B	828	CLA	1	0
28	m	612	CLA	2	0
28	d	307	CLA	1	0
28	g	310	CLA	2	0
28	O	206	CLA	8	0
28	b	601	CLA	2	0
28	a	304	CLA	2	0
28	n	602	CLA	2	0
28	h	302	CLA	1	0
28	B	825	CLA	2	0
28	e	607	CLA	3	0
28	B	806	CLA	1	0
28	L	207	CLA	2	0
28	B	820	CLA	1	0
28	A	803	CLA	2	0
28	k	606	CLA	1	0
28	B	810	CLA	1	0
28	A	855	CLA	1	0
38	f	611	KC2	1	0
28	b	611	CLA	2	0
28	k	608	CLA	3	0
30	a	319	LHG	2	0
28	c	602	CLA	2	0
30	c	620	LHG	1	0
29	A	842	PQN	1	0
32	b	618	LMT	2	0
28	i	302	CLA	3	0
36	k	621	II0	1	0
35	c	619	LMG	3	0
28	A	818	CLA	4	0
28	L	202	CLA	3	0
28	b	612	CLA	2	0
28	B	809	CLA	1	0
28	g	308	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	202	CLA	1	0
31	B	846	WVN	2	0
28	B	839	CLA	4	0
28	J	103	CLA	2	0
37	j	616	IHT	1	0
28	L	204	CLA	3	0
30	a	301	LHG	1	0
30	n	619	LHG	1	0
28	f	608	CLA	6	0
28	B	831	CLA	1	0
28	a	303	CLA	2	0
28	n	613	CLA	1	0
28	l	307	CLA	1	0
28	B	836	CLA	3	0
28	d	308	CLA	1	0
28	g	305	CLA	1	0
28	d	303	CLA	10	0
35	Q	301	LMG	4	0
36	d	316	II0	1	0
28	f	613	CLA	2	0
28	h	301	CLA	4	0
28	b	604	CLA	3	0
28	c	608	CLA	2	0
28	n	607	CLA	1	0
28	A	826	CLA	3	0
28	l	306	CLA	3	0
35	L	209	LMG	7	0
28	c	605	CLA	1	0
28	d	302	CLA	3	0
28	a	305	CLA	1	0
28	e	601	CLA	2	0
28	e	604	CLA	3	0
28	B	813	CLA	8	0
28	d	306	CLA	1	0
28	A	804	CLA	2	0
28	B	832	CLA	3	0
30	b	620	LHG	1	0
36	l	312	II0	1	0
28	B	807	CLA	2	0
28	B	833	CLA	4	0
28	A	810	CLA	1	0
28	n	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	b	619	LHG	1	0
28	B	801	CLA	5	0
28	f	601	CLA	1	0
28	A	819	CLA	1	0
35	n	620	LMG	3	0
36	d	315	II0	1	0
30	J	106	LHG	6	0
28	A	811	CLA	2	0
28	A	828	CLA	4	0
28	A	831	CLA	2	0
30	f	619	LHG	2	0
31	A	848	WVN	1	0
28	m	608	CLA	2	0
32	A	850	LMT	1	0
28	Q	302	CLA	7	0
28	A	809	CLA	2	0
28	L	203	CLA	4	0
35	F	205	LMG	4	0
28	n	604	CLA	2	0
31	A	847	WVN	3	0
28	F	201	CLA	5	0
28	A	852	CLA	3	0
35	J	105	LMG	4	0
28	h	304	CLA	2	0
28	B	827	CLA	2	0
28	A	838	CLA	3	0
30	A	849	LHG	3	0
28	A	813	CLA	1	0
28	A	815	CLA	1	0
28	i	306	CLA	2	0
28	n	609	CLA	3	0
31	A	846	WVN	1	0
31	R	202	WVN	7	0
28	b	610	CLA	3	0
28	c	606	CLA	2	0
28	e	611	CLA	3	0
37	n	617	IHT	2	0
28	a	312	CLA	1	0
28	B	830	CLA	3	0
28	A	827	CLA	1	0
28	A	840	CLA	2	0
28	h	307	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	i	319	KC2	10	0
28	s	208	CLA	1	0
28	e	610	CLA	2	0
28	a	307	CLA	1	0
28	b	603	CLA	2	0
28	R	203	CLA	1	0
28	k	607	CLA	2	0
28	i	307	CLA	3	0
28	B	815	CLA	6	0
38	g	312	KC2	3	0
38	s	201	KC2	1	0
28	O	201	CLA	1	0
28	m	610	CLA	2	0
29	B	842	PQN	1	0
28	f	607	CLA	4	0
28	A	836	CLA	5	0
28	m	604	CLA	1	0
28	A	821	CLA	3	0
28	f	610	CLA	4	0
28	a	309	CLA	1	0
28	j	604	CLA	1	0
28	B	837	CLA	3	0
28	B	802	CLA	1	0
28	A	820	CLA	3	0
28	A	841	CLA	4	0
28	A	802	CLA	7	0
28	A	823	CLA	2	0
28	B	841	CLA	1	0
28	k	601	CLA	1	0
28	e	605	CLA	2	0
28	l	305	CLA	2	0
28	A	816	CLA	3	0
28	e	606	CLA	6	0
28	B	835	CLA	5	0
28	l	308	CLA	1	0
28	n	603	CLA	4	0
28	A	807	CLA	2	0
28	a	308	CLA	2	0
28	f	606	CLA	1	0
28	B	822	CLA	4	0
30	l	317	LHG	1	0
28	k	609	CLA	2	0

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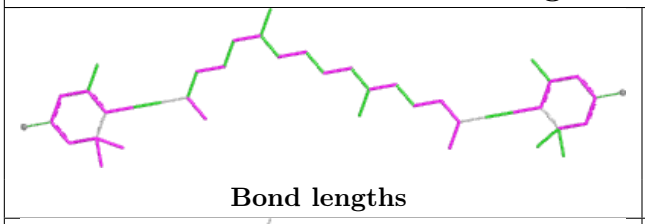
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	i	312	CLA	1	0
28	j	601	CLA	3	0
28	B	834	CLA	2	0
28	A	801	CLA	3	0
36	f	615	II0	1	0
28	a	311	CLA	2	0
37	f	617	IHT	1	0
28	m	603	CLA	5	0
37	b	615	IHT	1	0
28	c	604	CLA	2	0
28	A	854	CLA	5	0
28	B	819	CLA	1	0
28	m	606	CLA	1	0
28	A	834	CLA	2	0
28	s	202	CLA	5	0
28	i	311	CLA	1	0
28	l	311	CLA	2	0
28	A	824	CLA	3	0
28	k	610	CLA	2	0
30	g	301	LHG	2	0
28	j	610	CLA	3	0
28	b	602	CLA	1	0
28	g	315	CLA	1	0
28	A	829	CLA	2	0
28	B	803	CLA	4	0
28	c	612	CLA	2	0
28	A	839	CLA	5	0
28	B	814	CLA	1	0
28	g	309	CLA	6	0
28	b	607	CLA	4	0
31	K	102	WVN	1	0
28	n	605	CLA	1	0
28	B	805	CLA	3	0
28	k	602	CLA	3	0
28	d	301	CLA	2	0
39	i	301	LMU	2	0

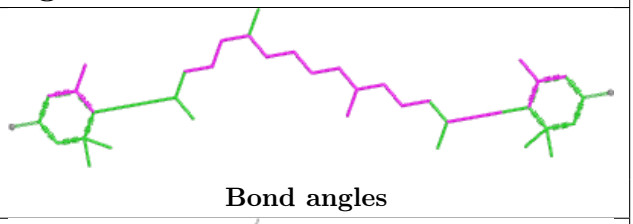
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

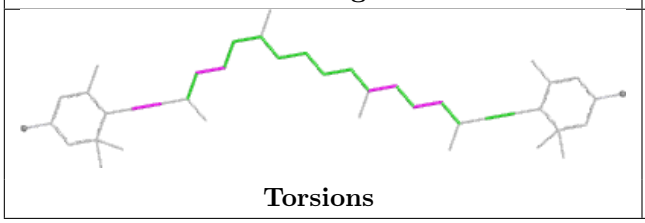
Ligand II0 g 317



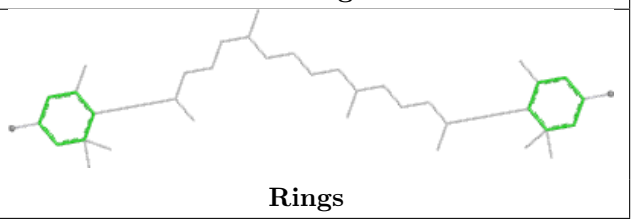
Bond lengths



Bond angles

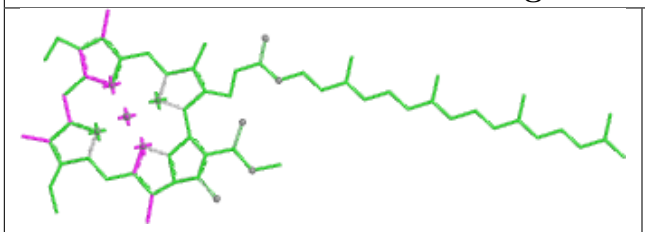


Torsions

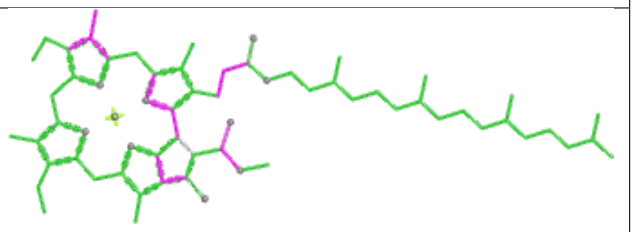


Rings

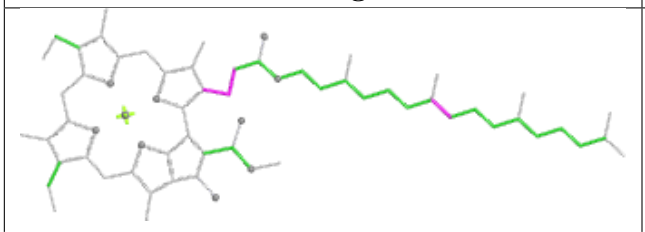
Ligand CLA A 851



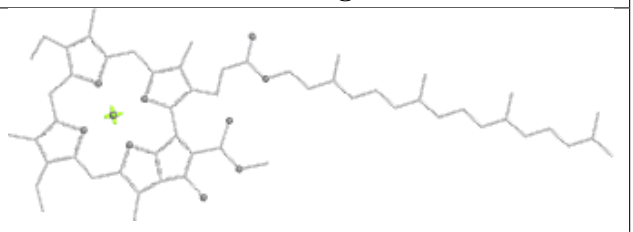
Bond lengths



Bond angles

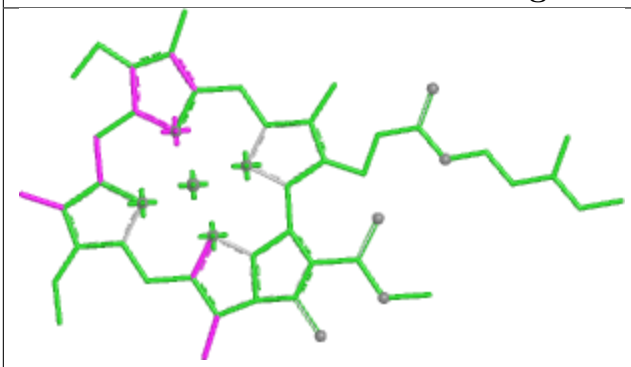


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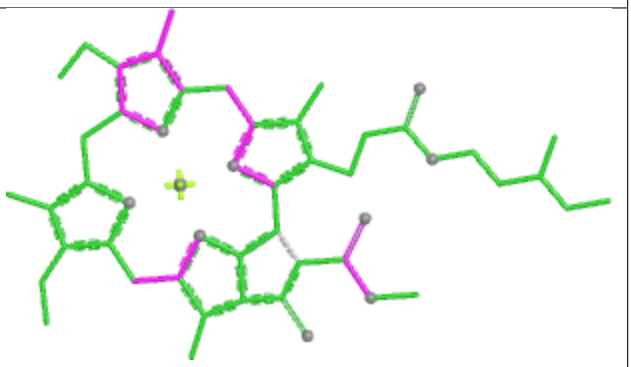


Rings

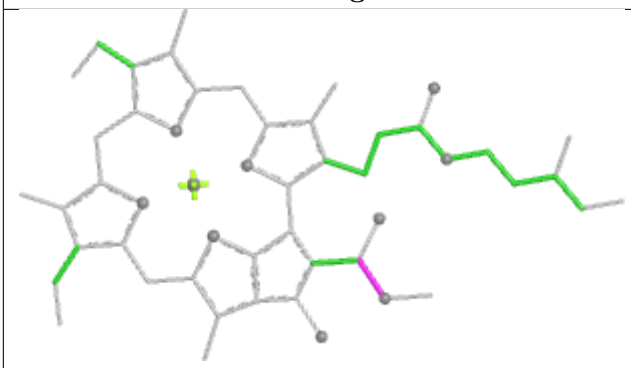
Ligand CLA c 603



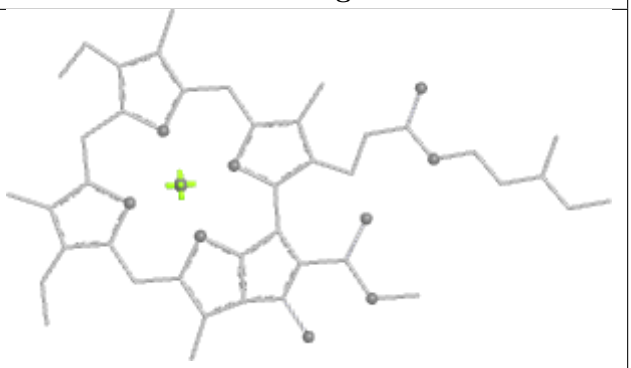
Bond lengths



Bond angles

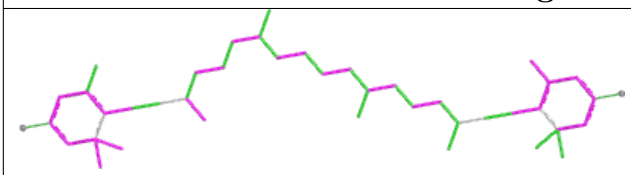


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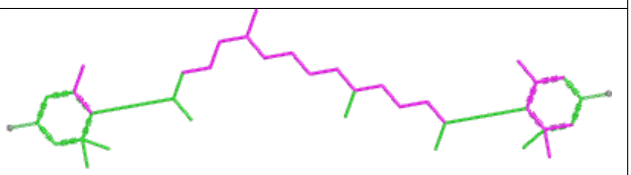


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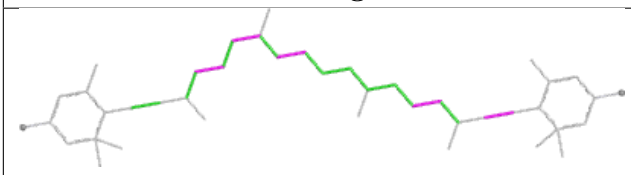
Ligand II0 m 618



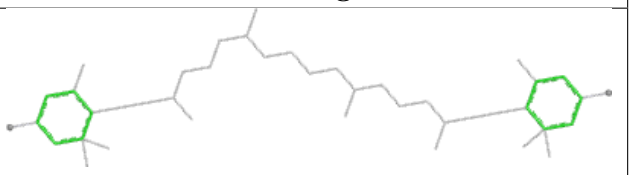
Bond lengths



Bond angles

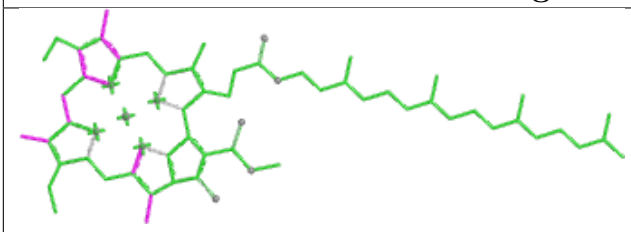


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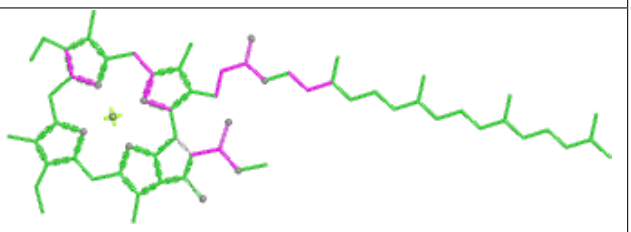


Rings

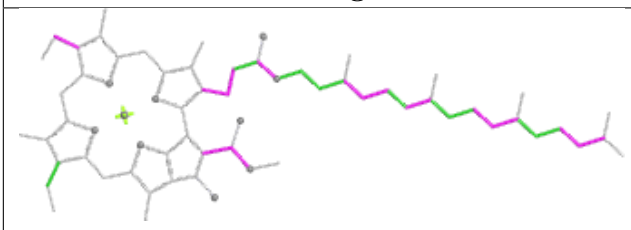
Ligand CLA l 303



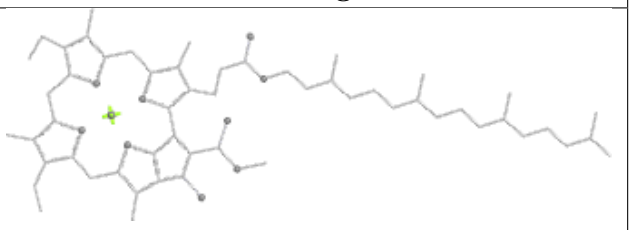
Bond lengths



Bond angles

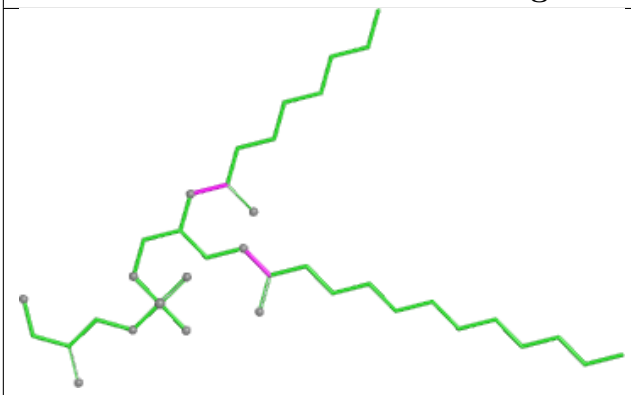


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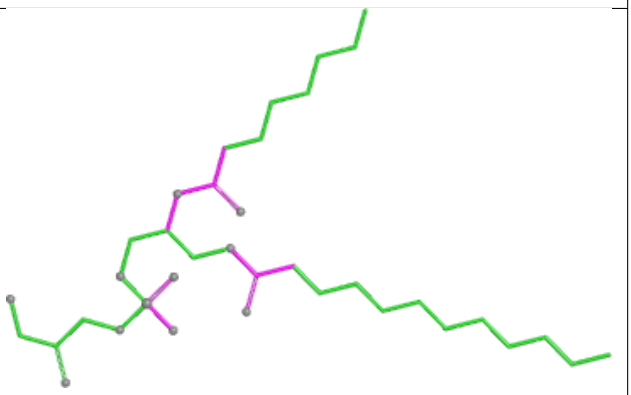


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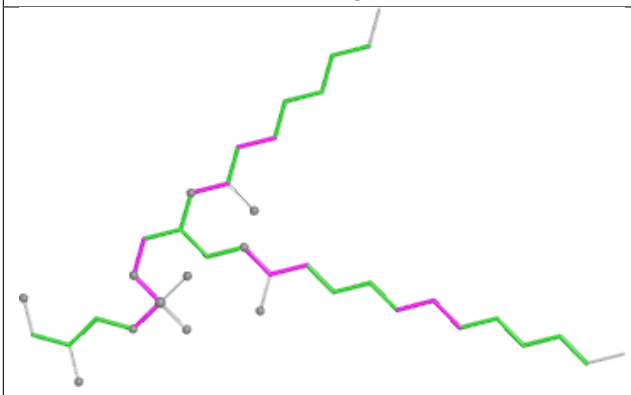
Ligand LHG i 318



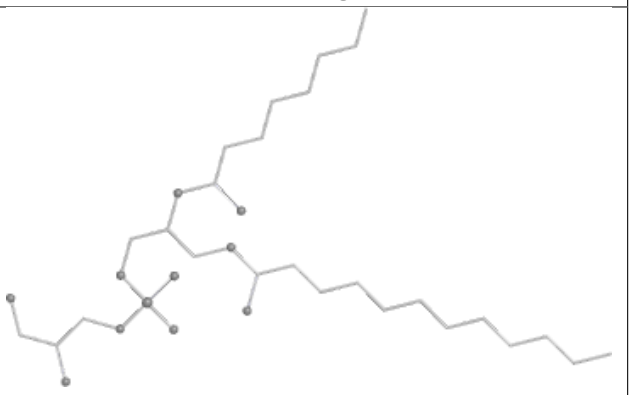
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Bond angles

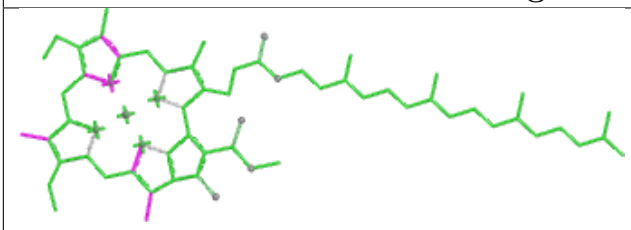


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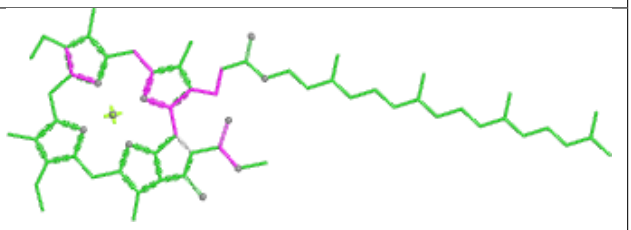


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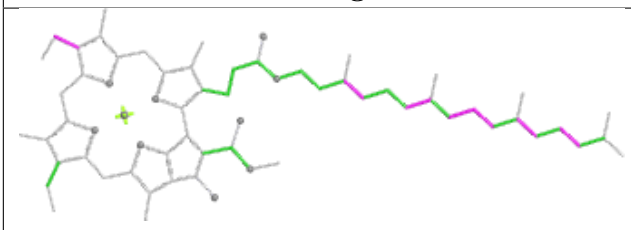
Ligand CLA b 605



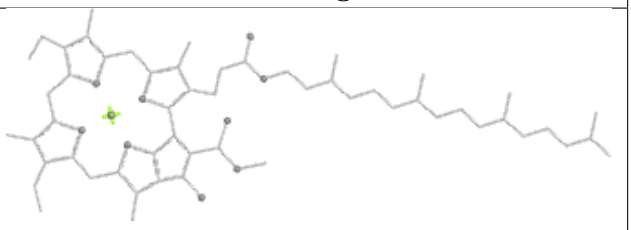
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Bond angles

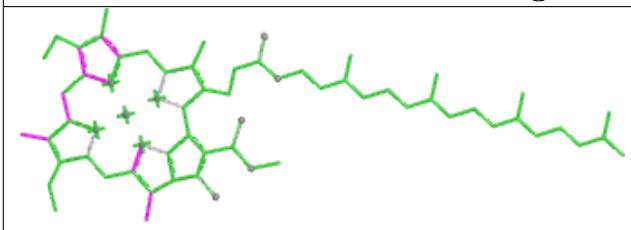


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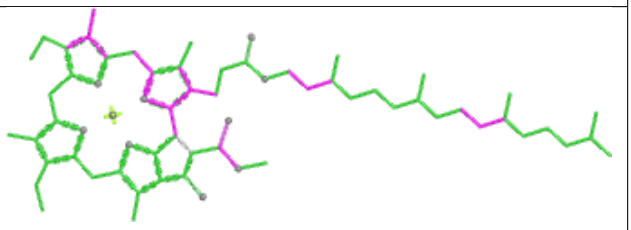


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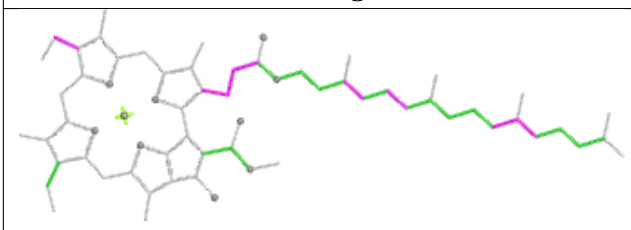
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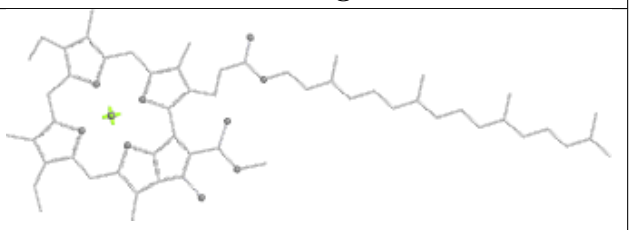
Bond lengths



Bond angles

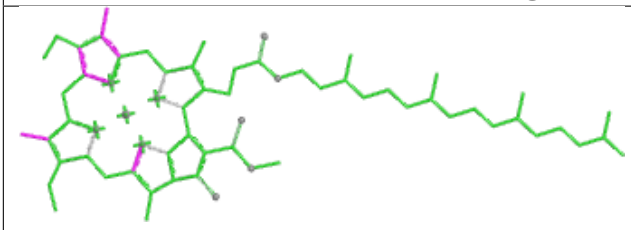


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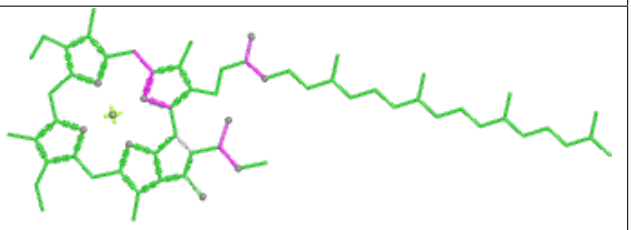


Rings

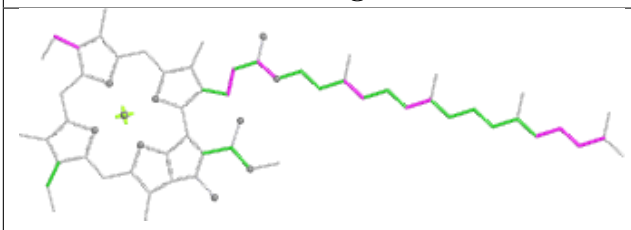
Ligand CLA A 835



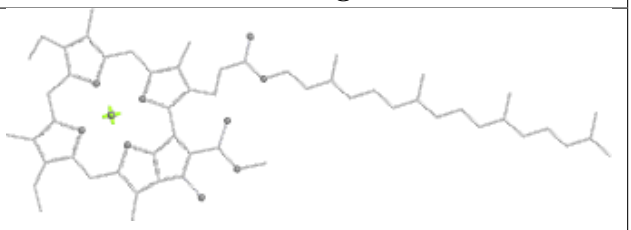
Bond lengths



Bond angles

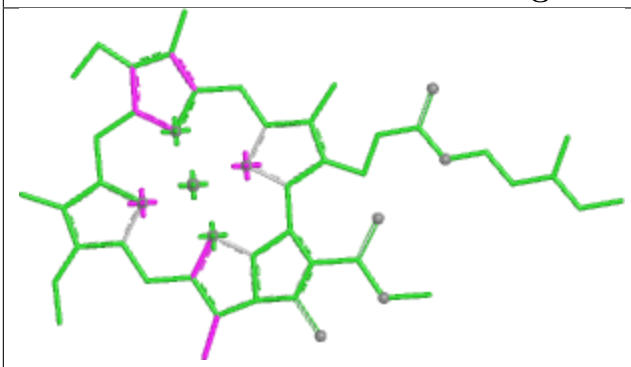


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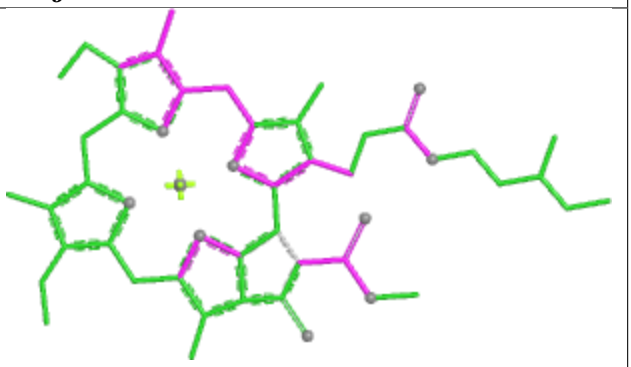


Rings

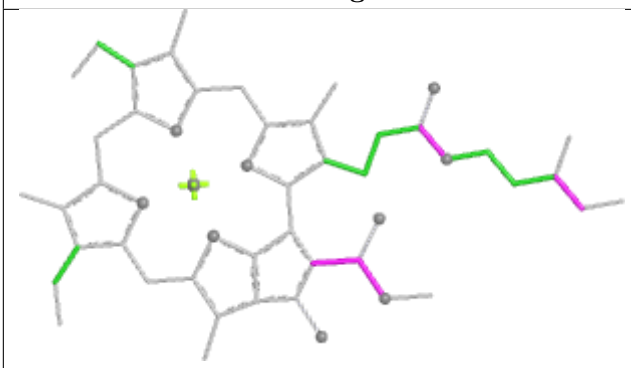
Ligand CLA j 612



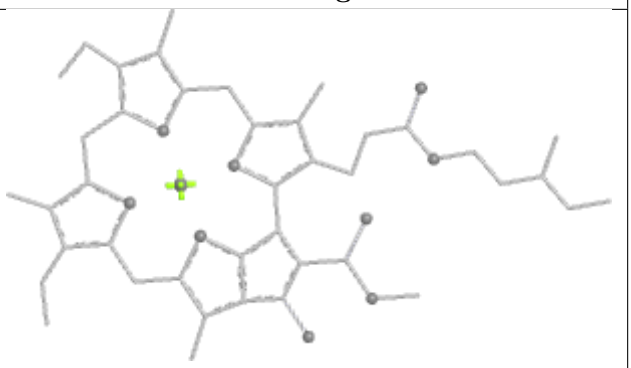
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Bond angles

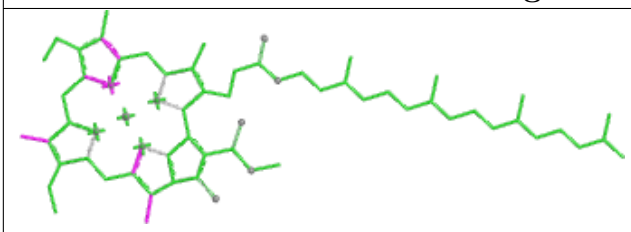


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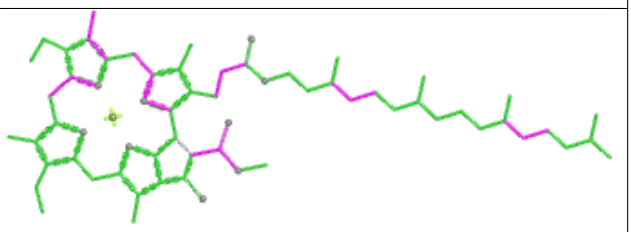


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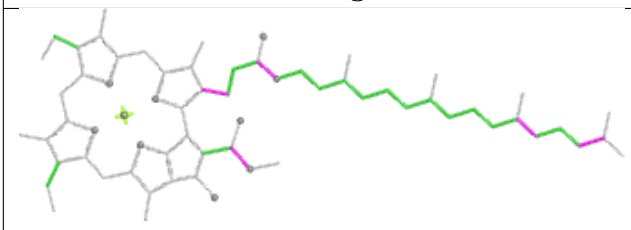
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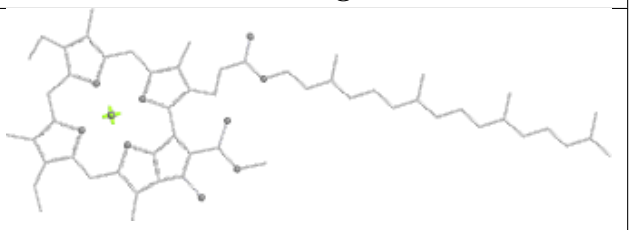
Bond lengths



Bond angles

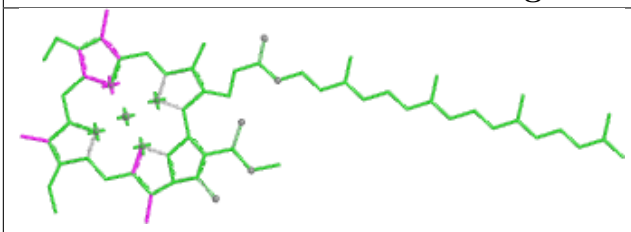


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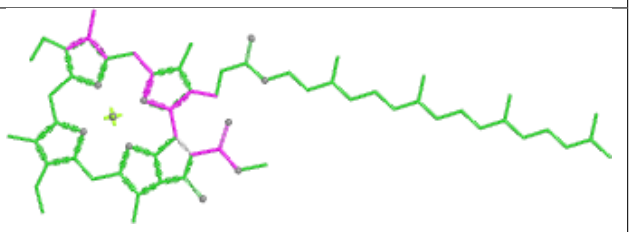


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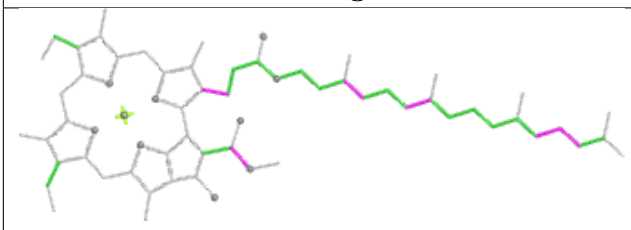
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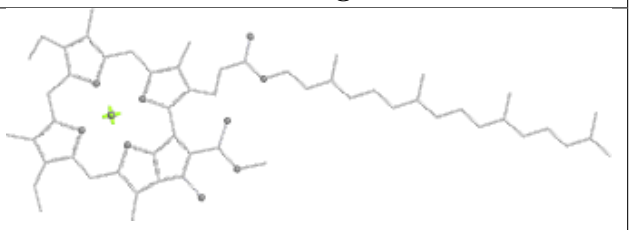
Bond lengths



Bond angles

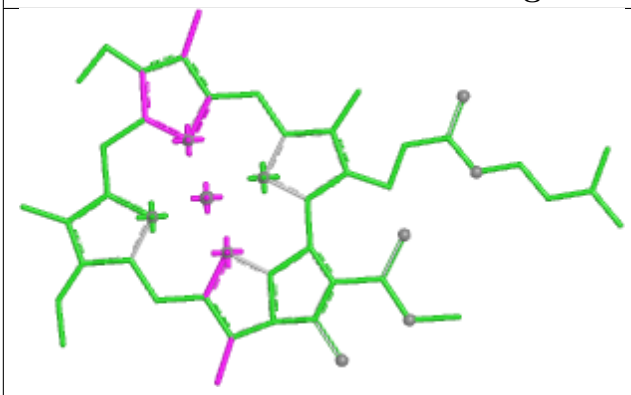


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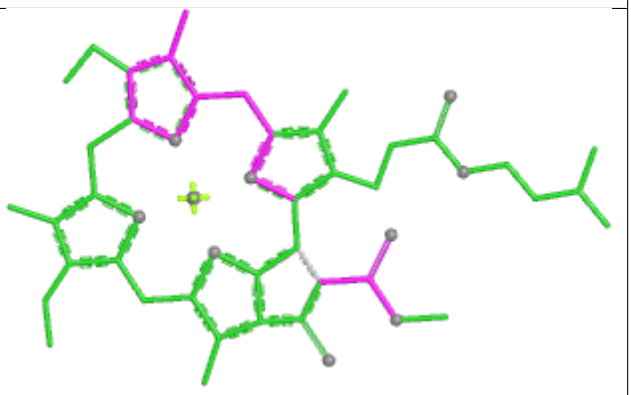


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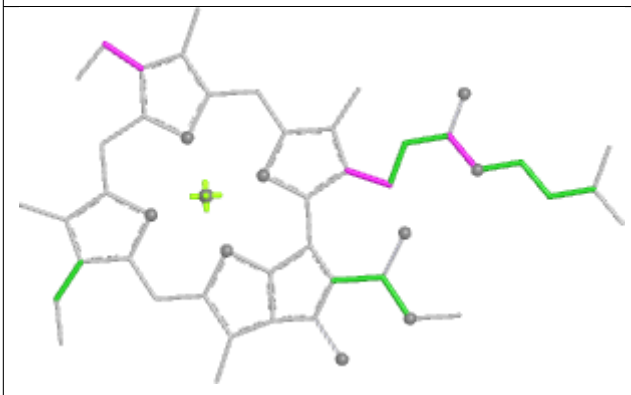
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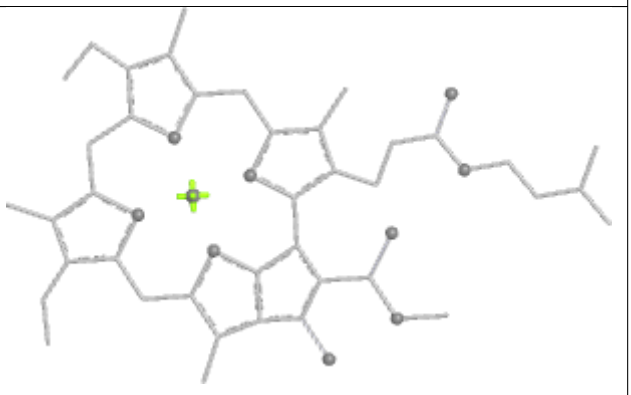
Bond lengths



Bond angles

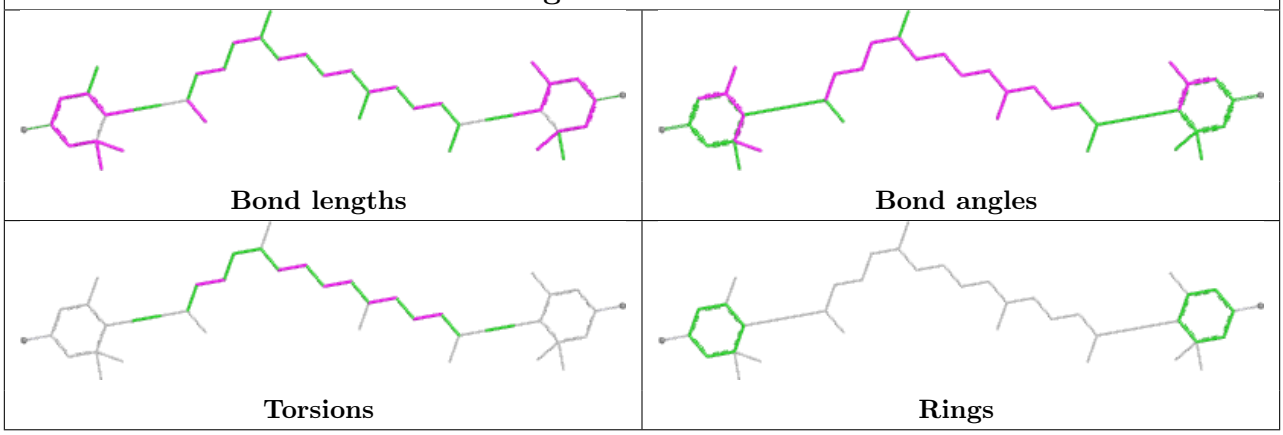


Torsions



Rings

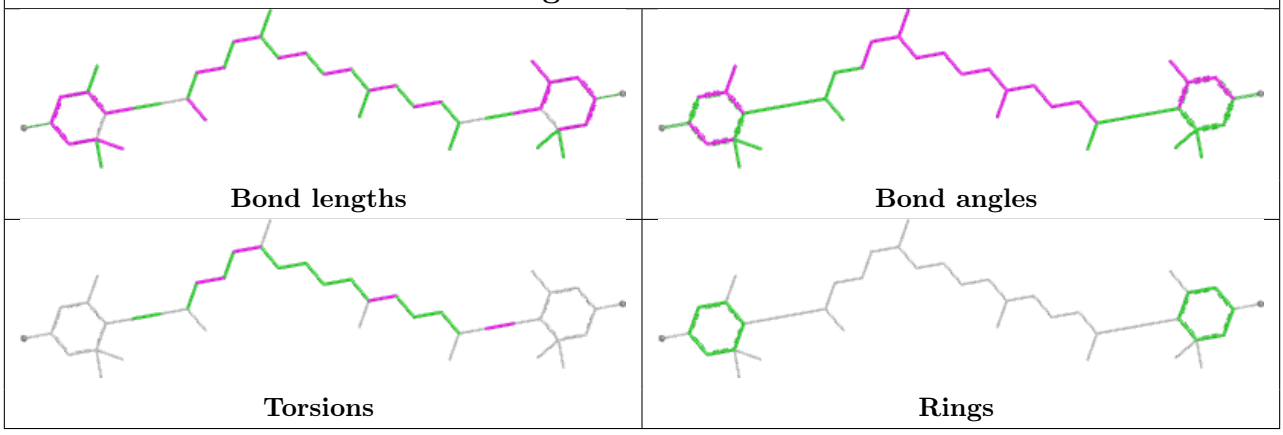
Ligand II0 k 615



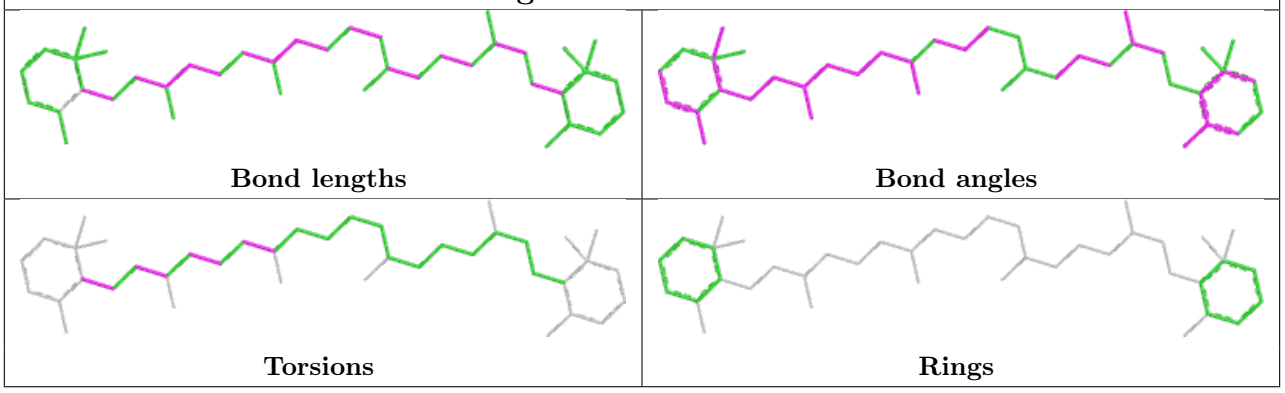
Ligand WVN R 201



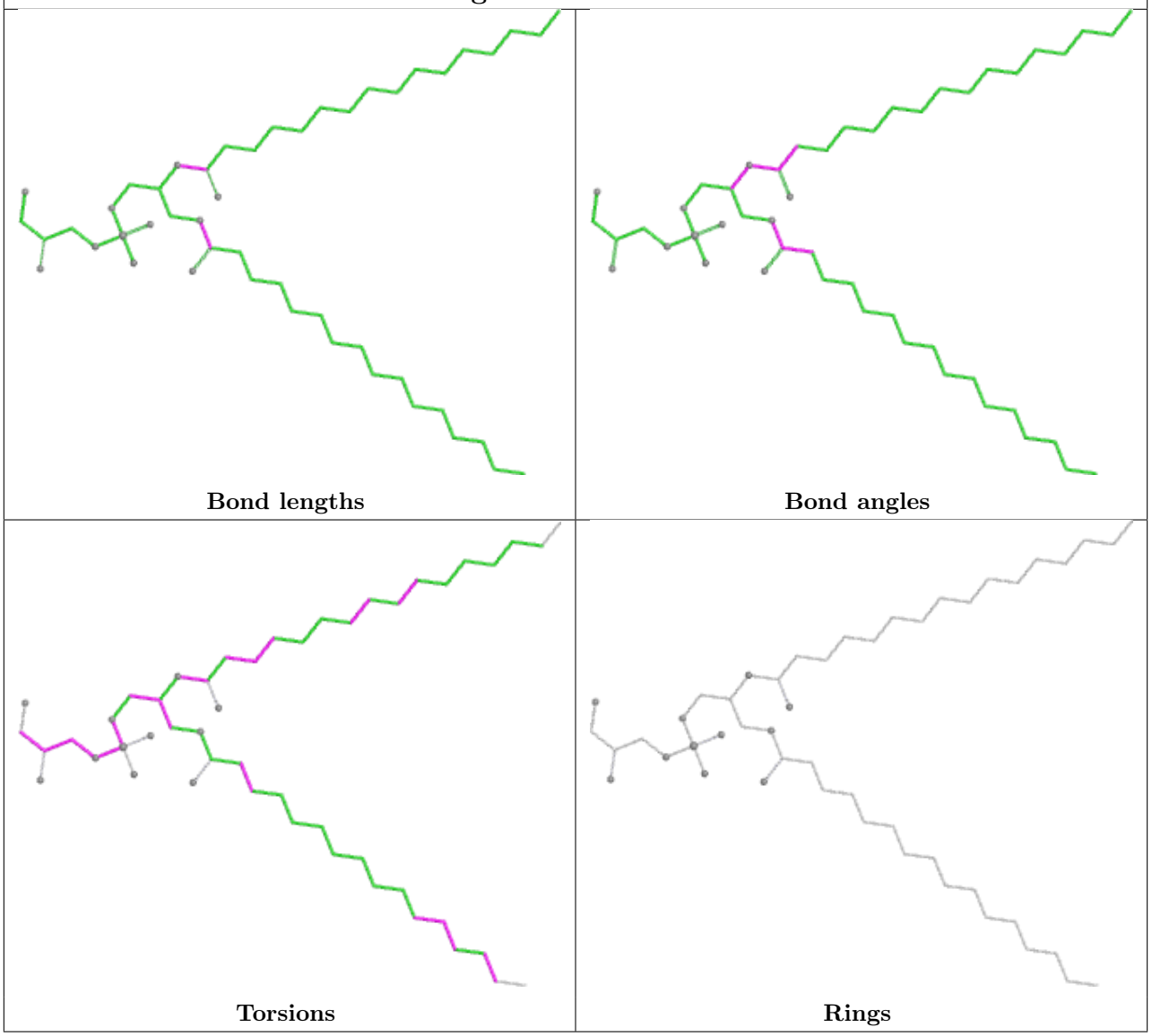
Ligand II0 n 618



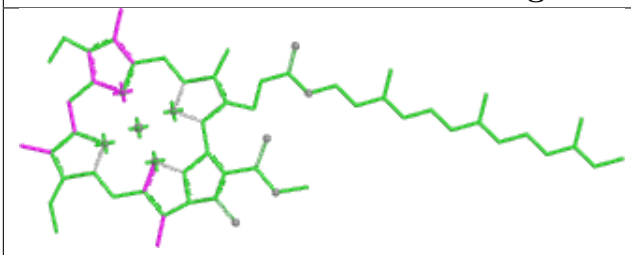
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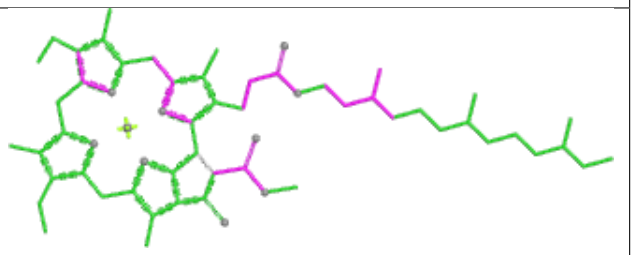
Ligand LHG L 208



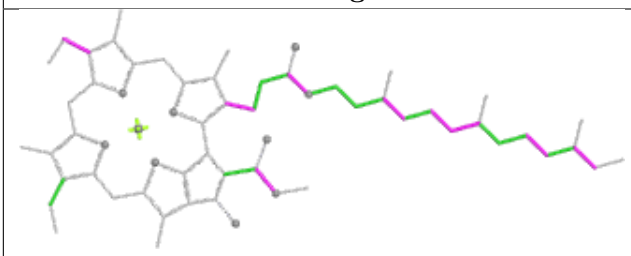
Ligand CLA b 606



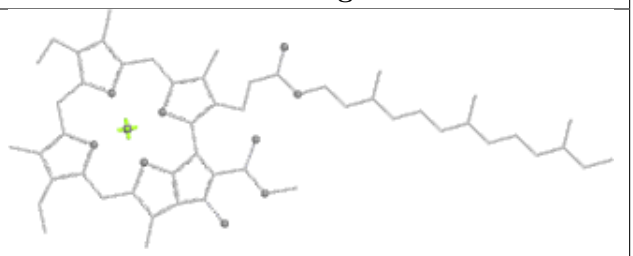
Bond lengths



Bond angles

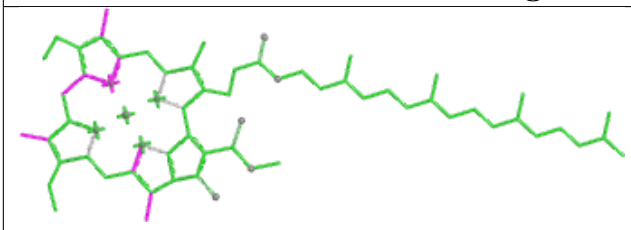


Torsions

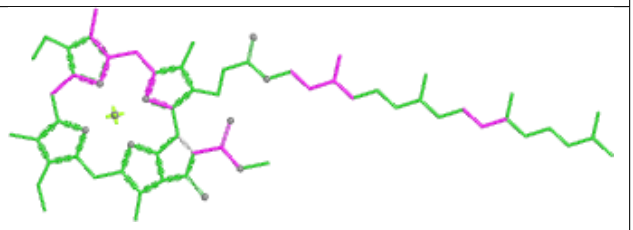


Rings

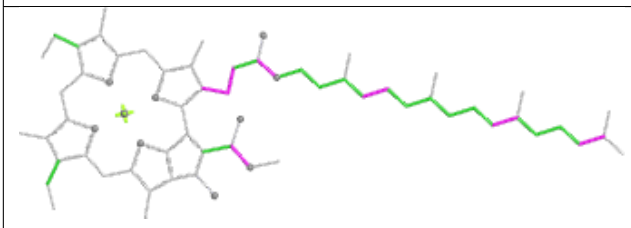
Ligand CLA B 808



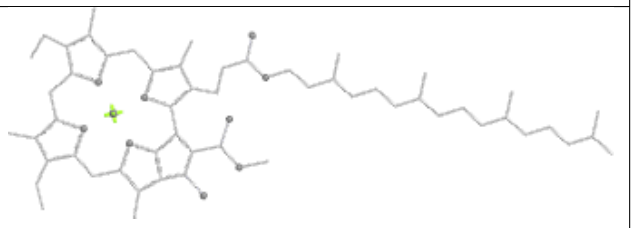
Bond lengths



Bond angles

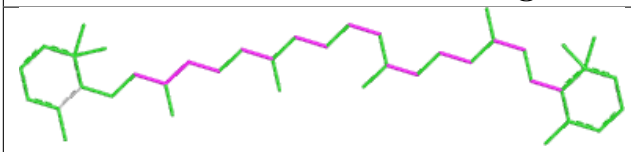


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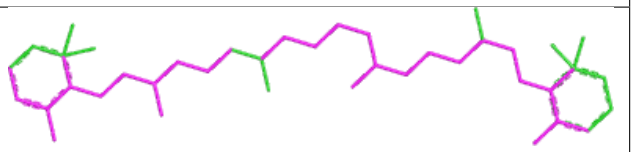


Rings

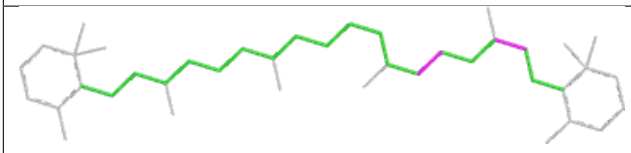
Ligand WVN L 206



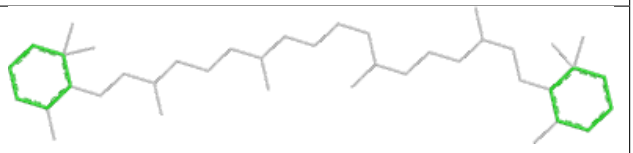
Bond lengths



Bond angles

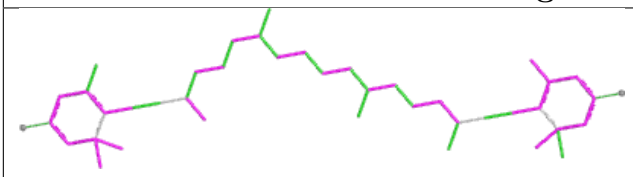


Torsions

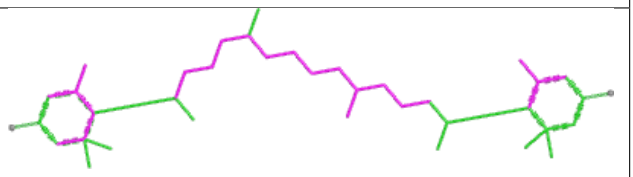


Rings

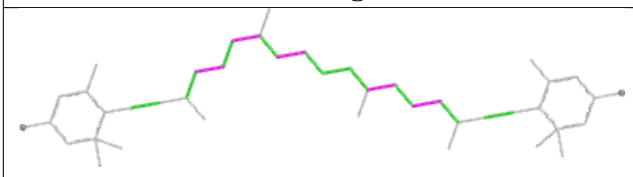
Ligand II0 m 615



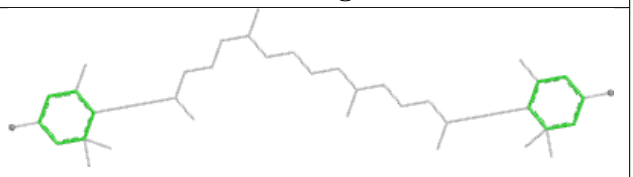
Bond lengths



Bond angles

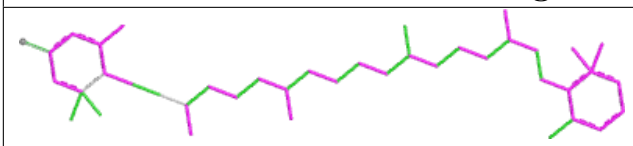


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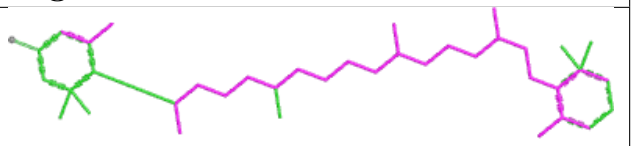


Rings

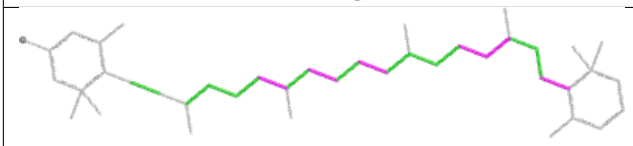
Ligand IHT g 319



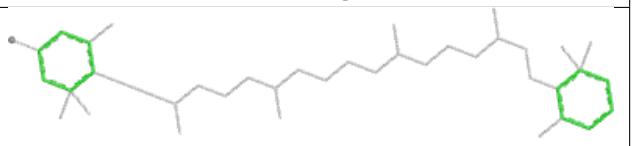
Bond lengths



Bond angles

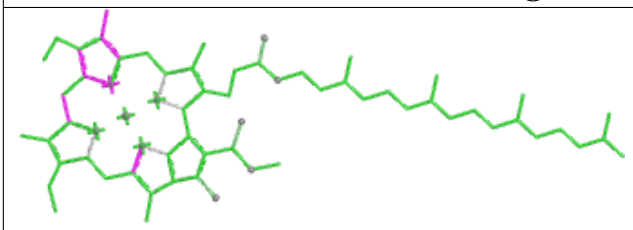


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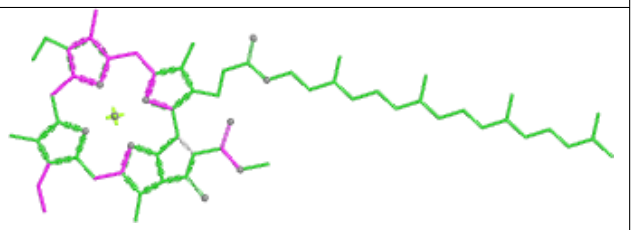


Rings

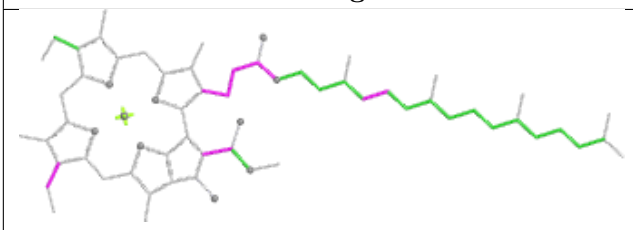
Ligand CLA B 840



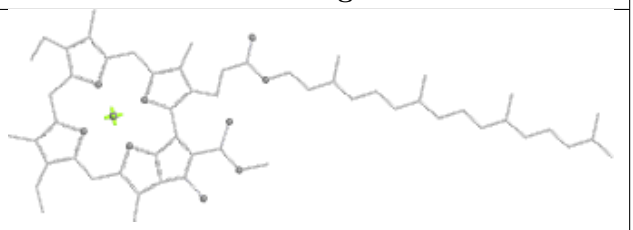
Bond lengths



Bond angles

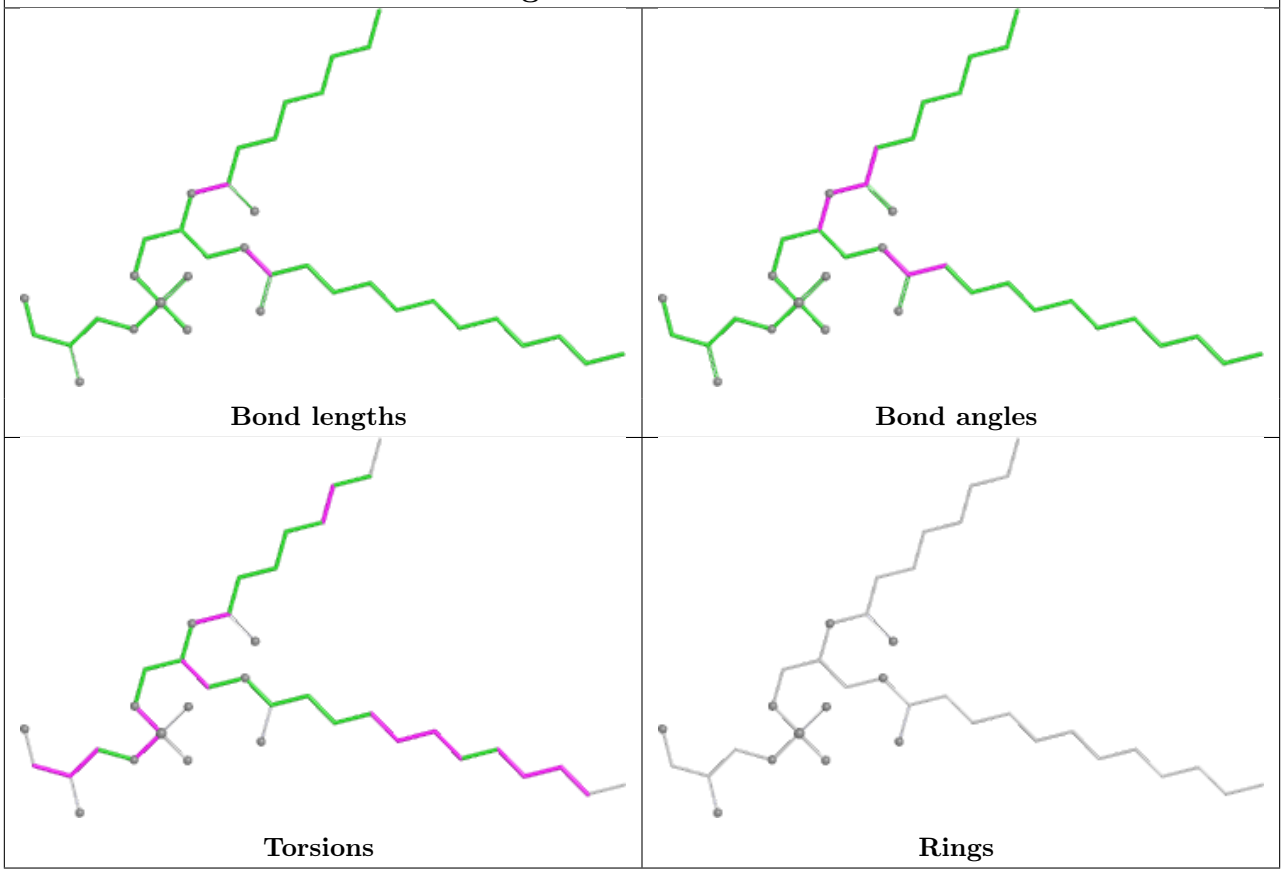


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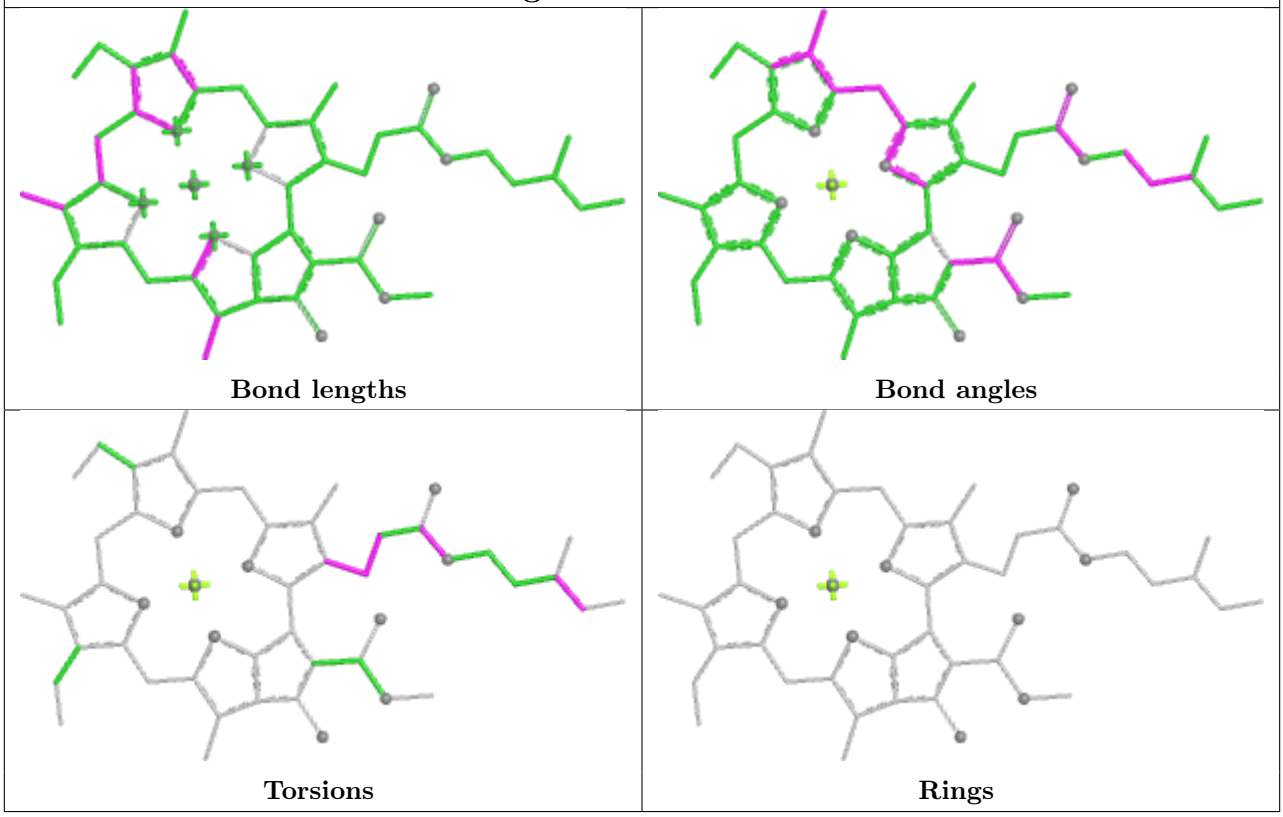


Rings

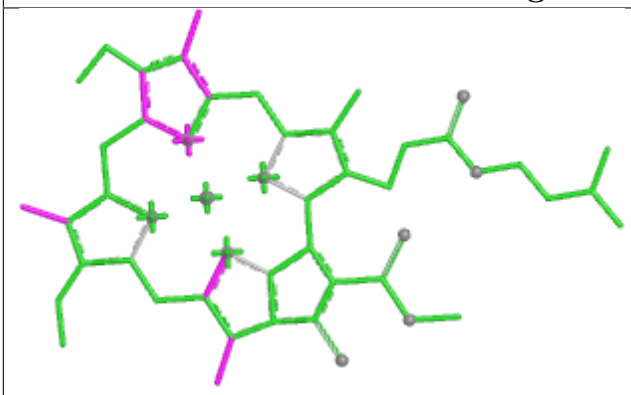
Ligand LHG m 619



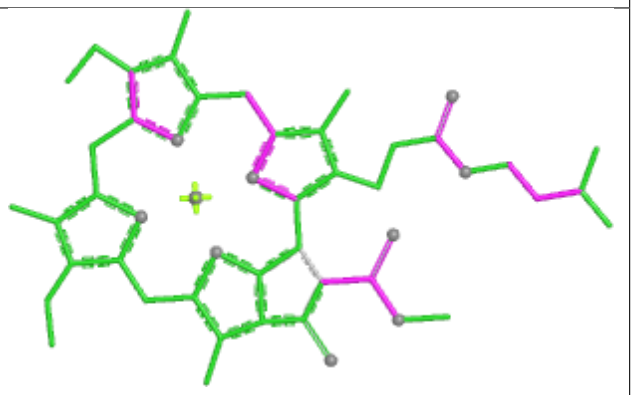
Ligand CLA m 609



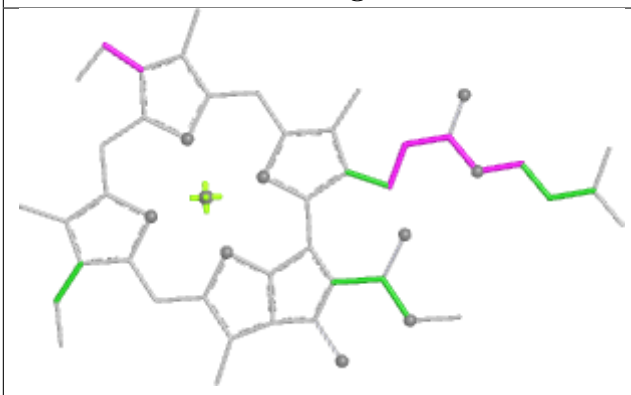
Ligand CLA h 303



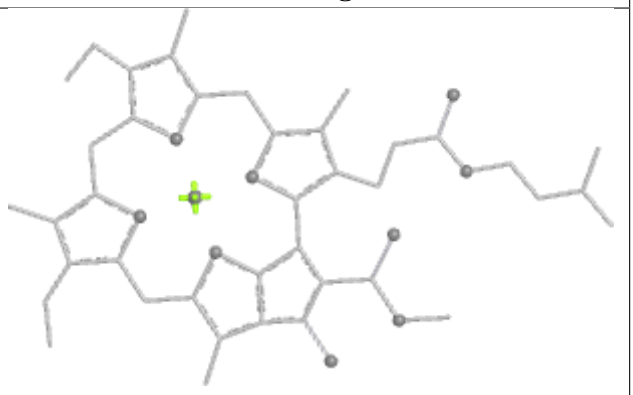
Bond lengths



Bond angles

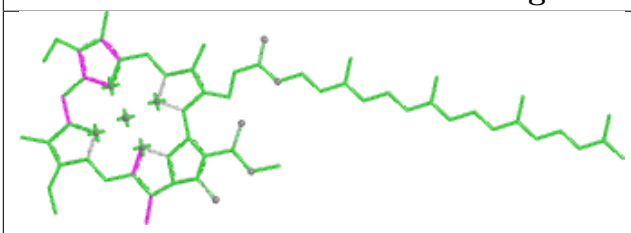


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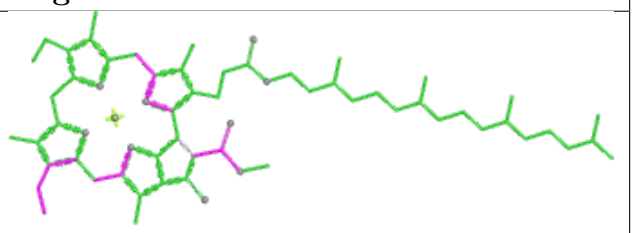


Rings

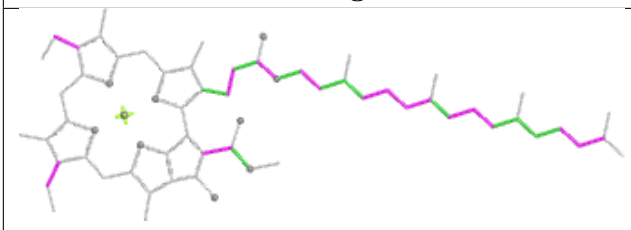
Ligand CLA g 322



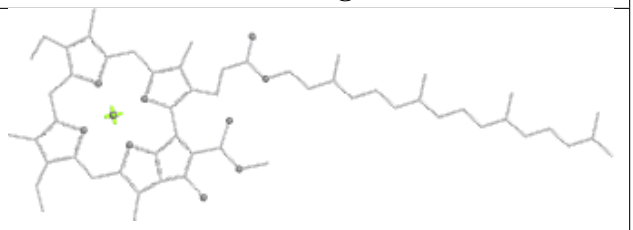
Bond lengths



Bond angles

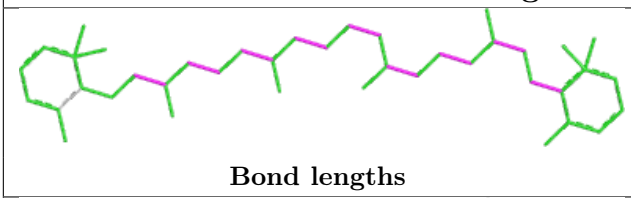


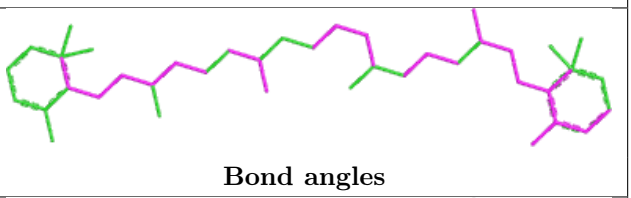
Torsions

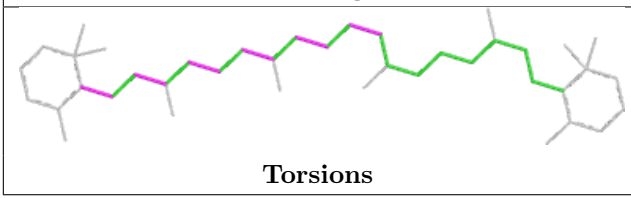


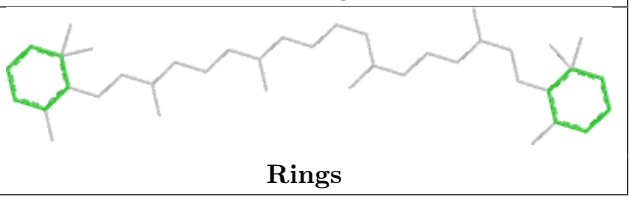
Rings

Ligand WVN I 101

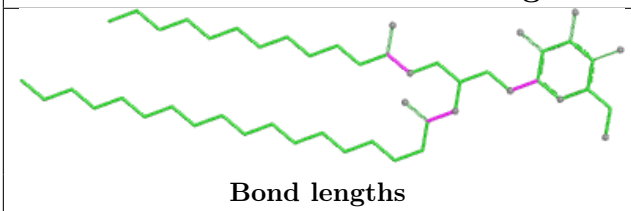

Bond lengths

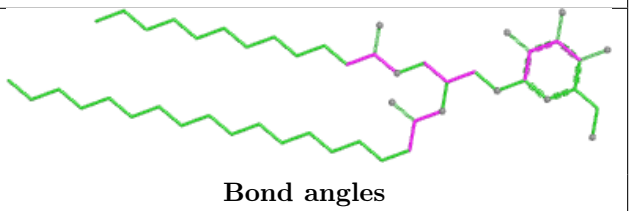

Bond angles

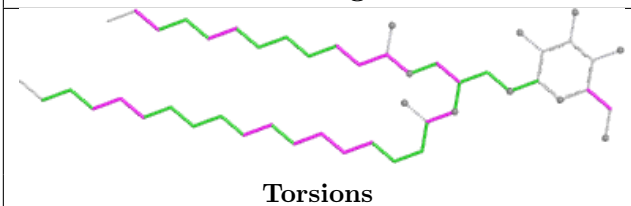

Torsions

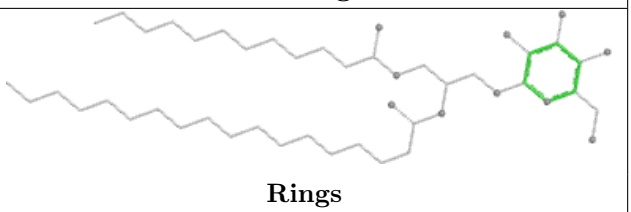

Rings

Ligand LMG b 621

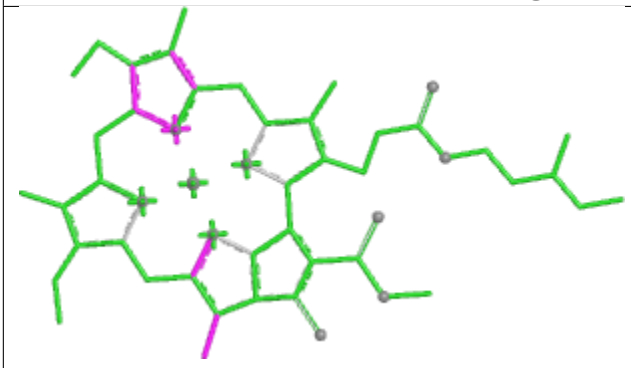

Bond lengths

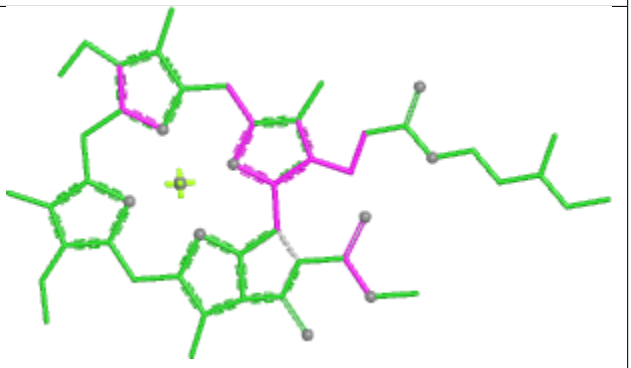

Bond angles

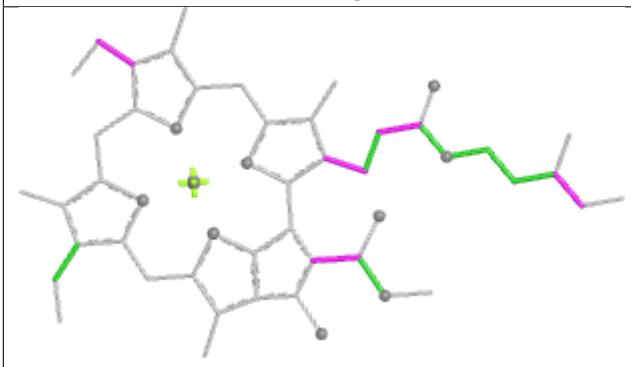

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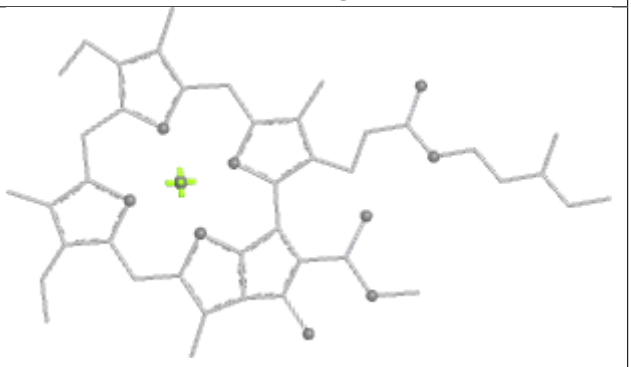

Rings

Ligand CLA h 308

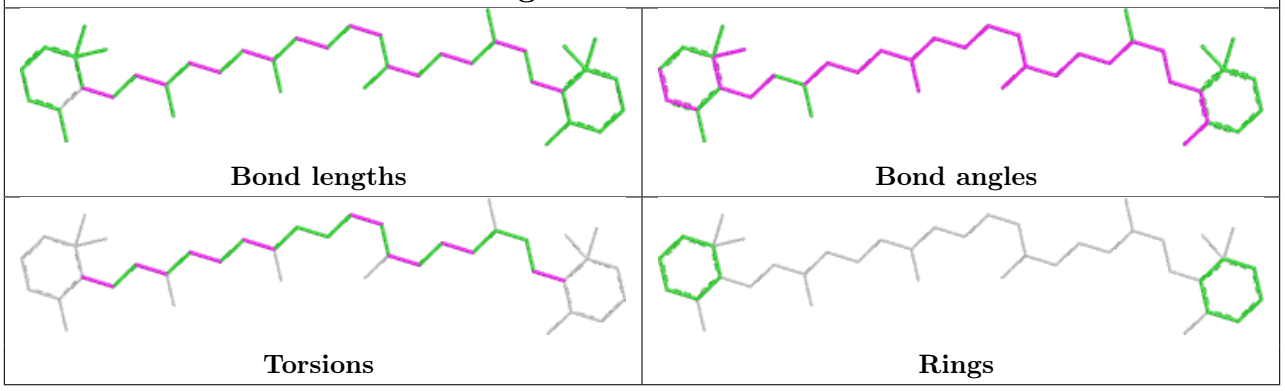

Bond lengths


Bond angles

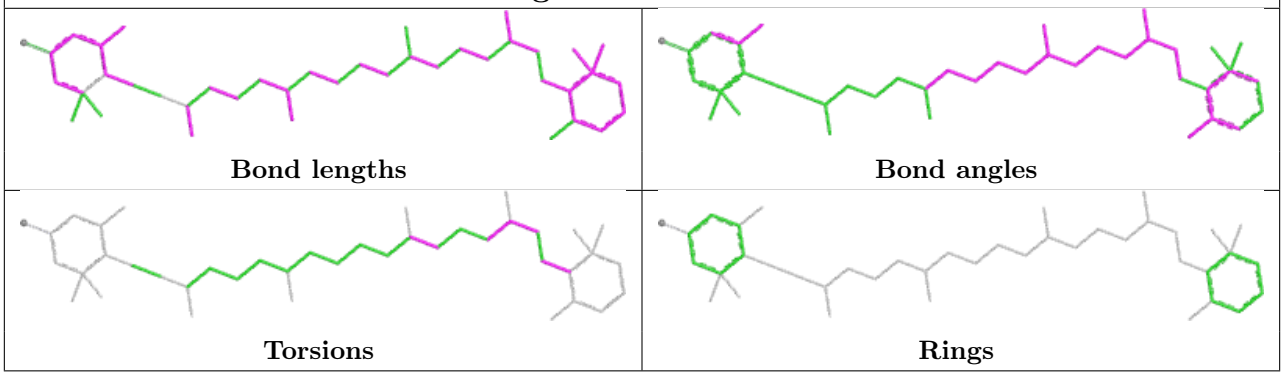

Torsions


Rings

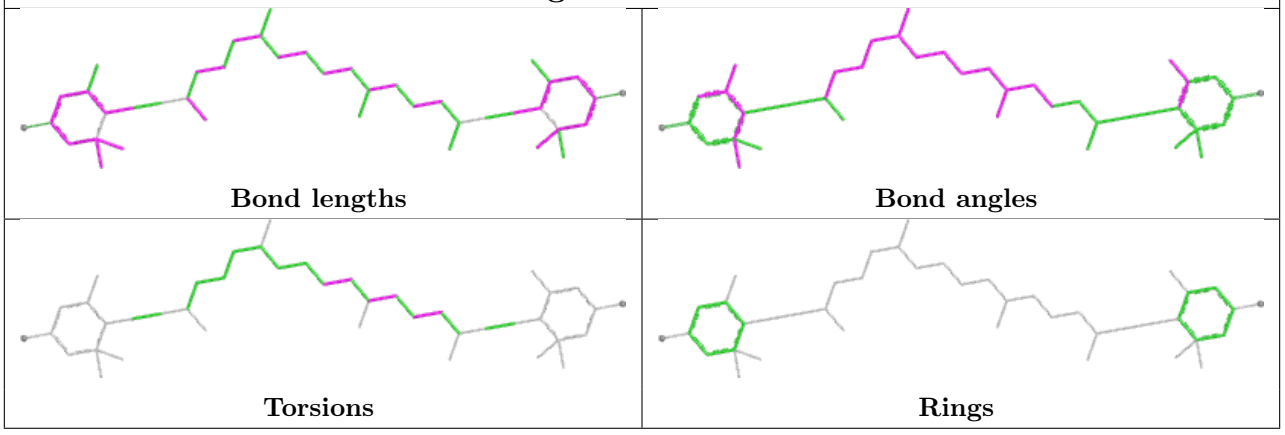
Ligand WVN F 204



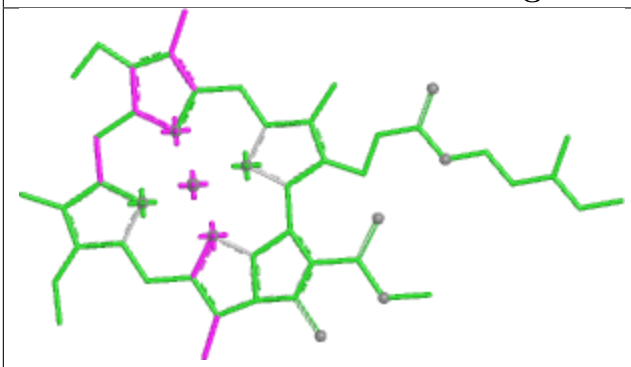
Ligand IHT b 616



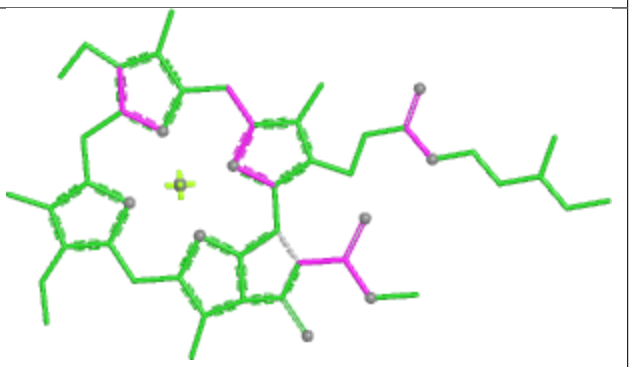
Ligand II0 i 314



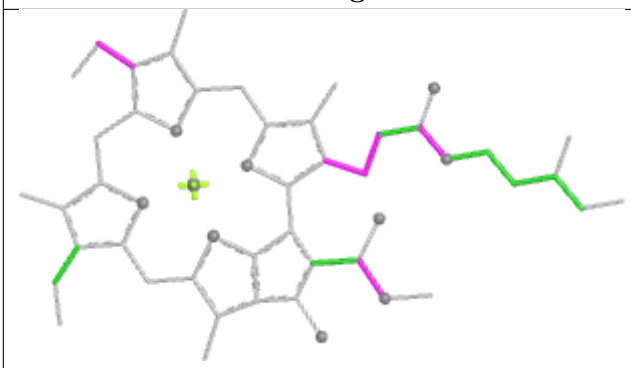
Ligand CLA A 822



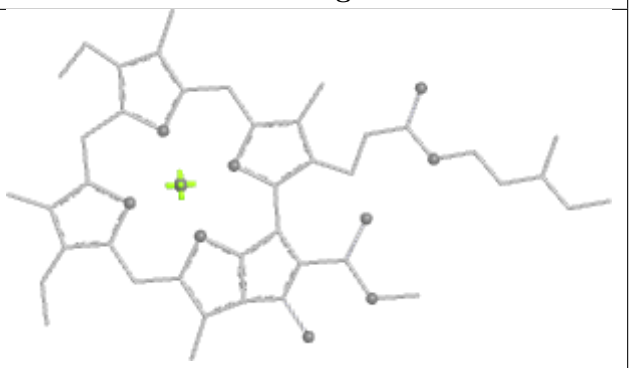
Bond lengths



Bond angles

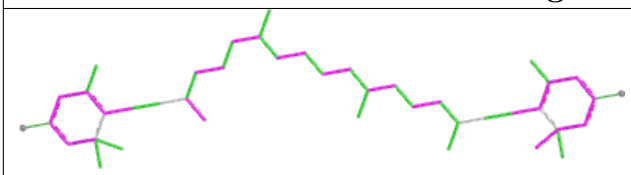


Torsions

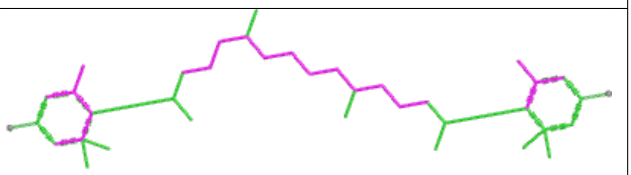


Rings

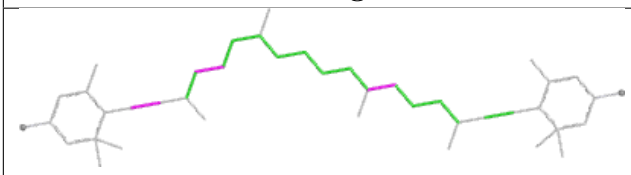
Ligand II0 i 315



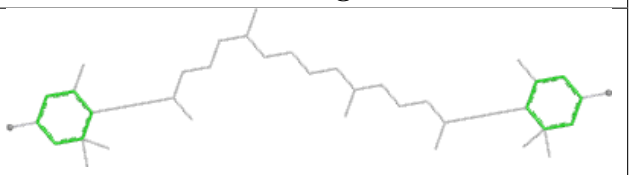
Bond lengths



Bond angles

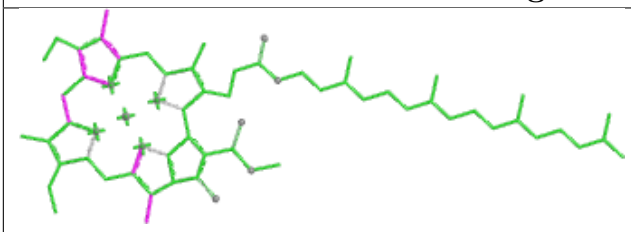


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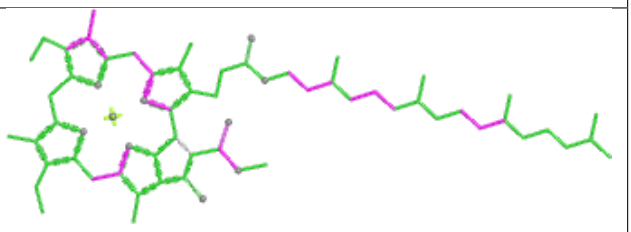


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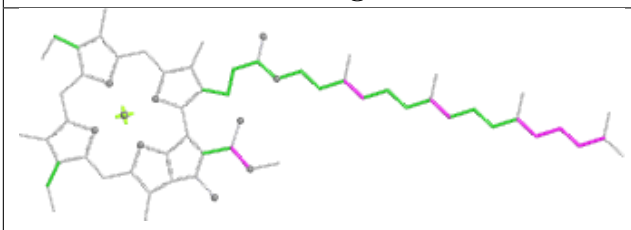
Ligand CLA b 608



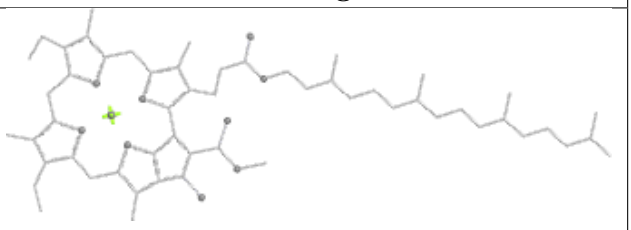
Bond lengths



Bond angles

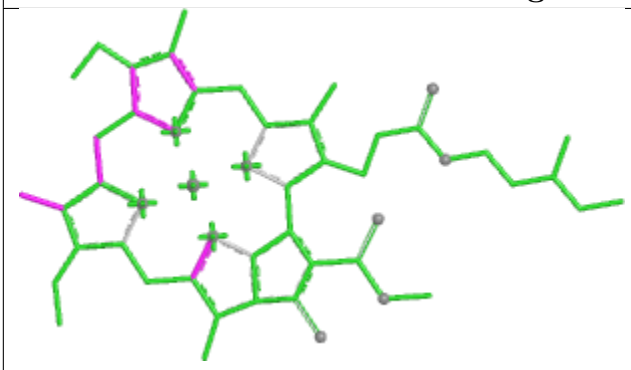


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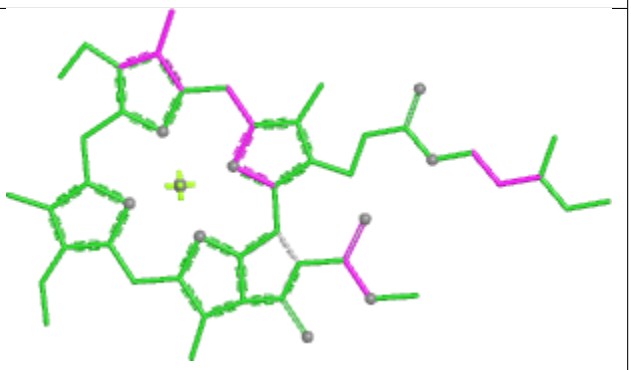


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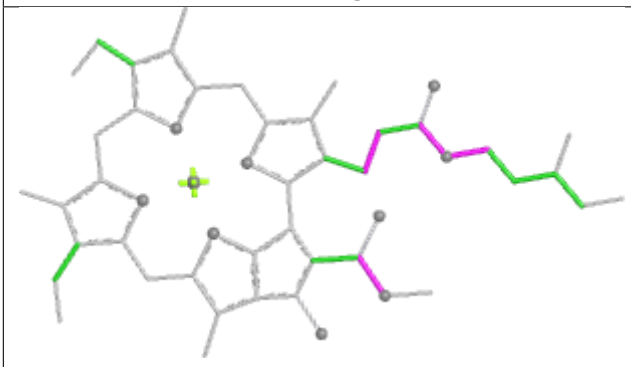
Ligand CLA d 304



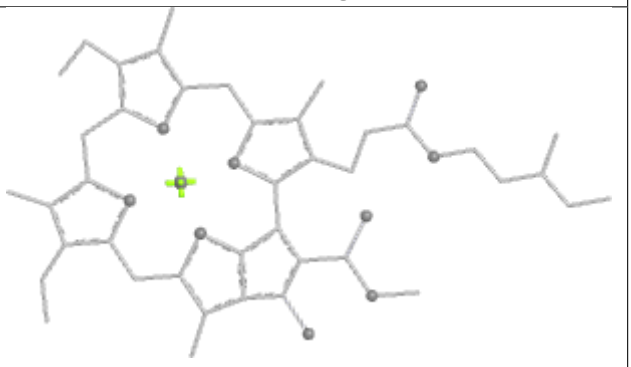
Bond lengths



Bond angles

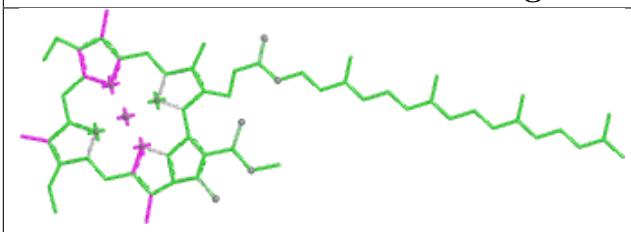


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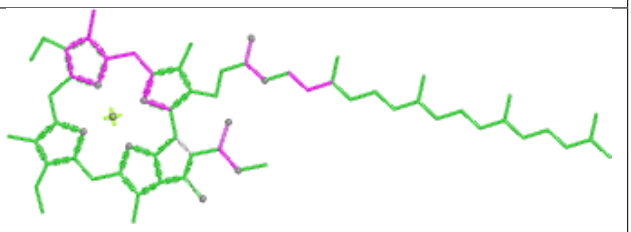


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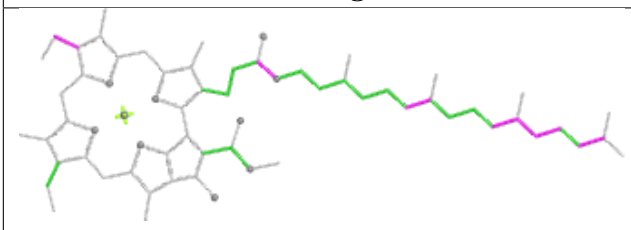
Ligand CLA B 817



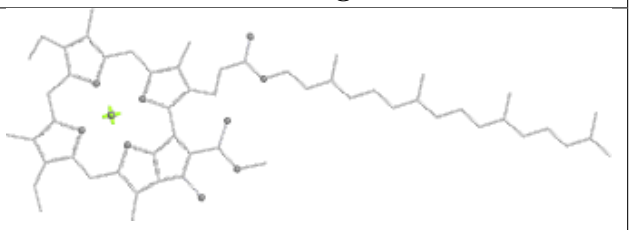
Bond lengths



Bond angles

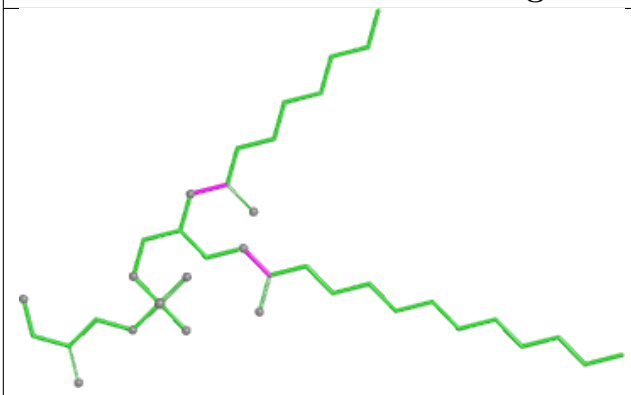


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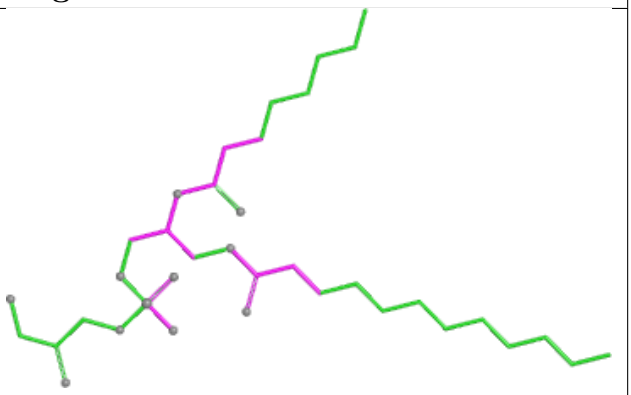


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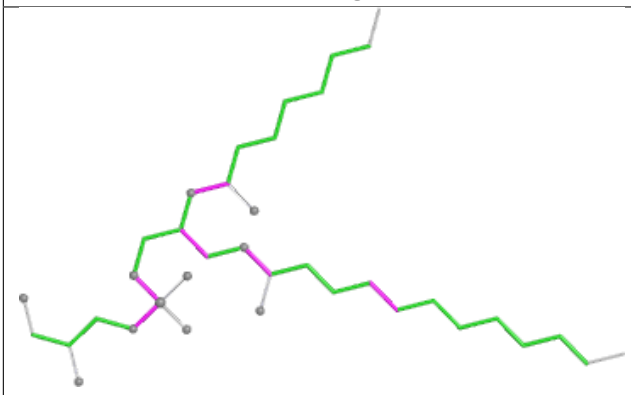
Ligand LHG g 321



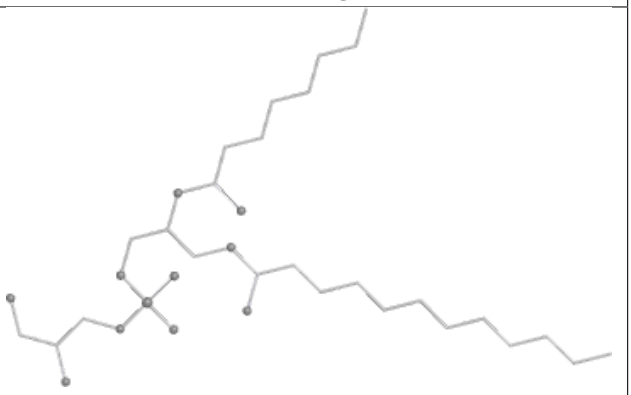
Bond lengths



Bond angles

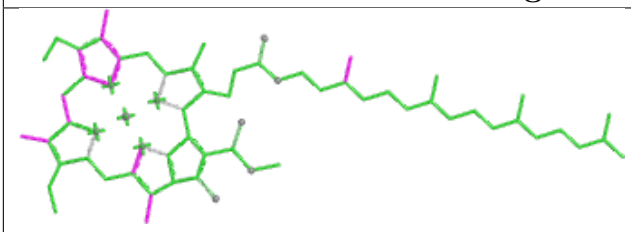


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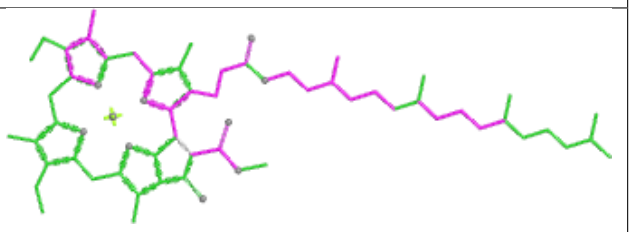


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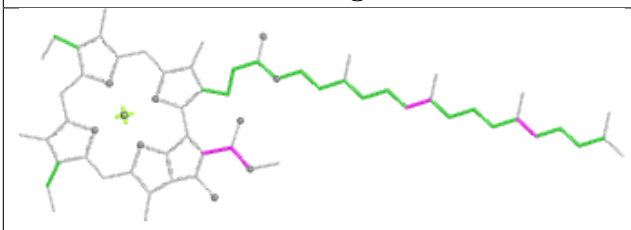
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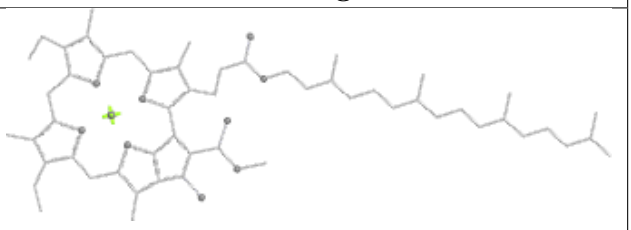
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Bond angles

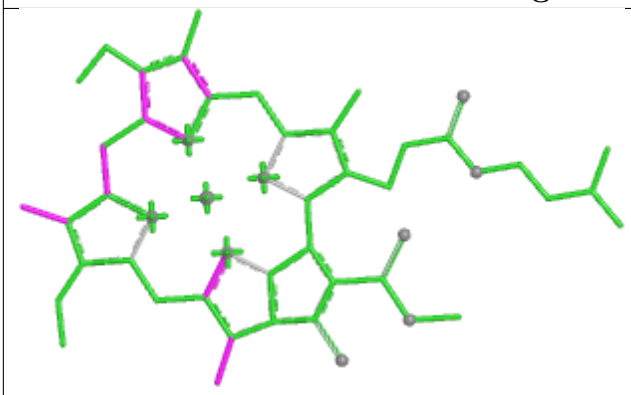


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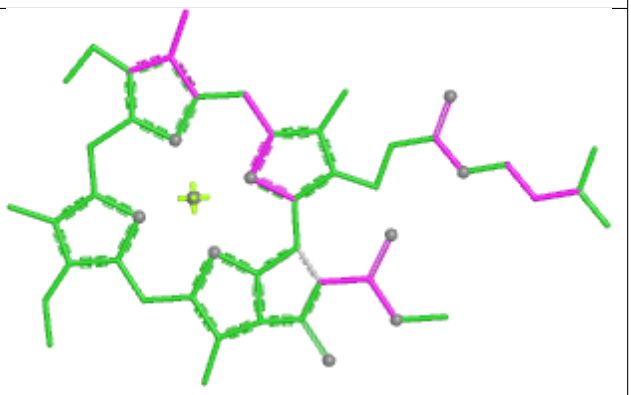


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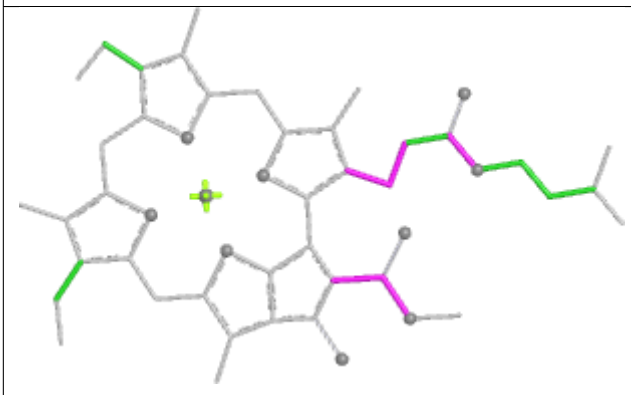
Ligand CLA i 303



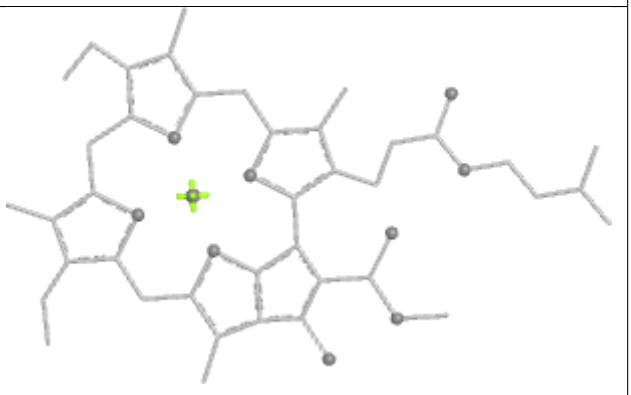
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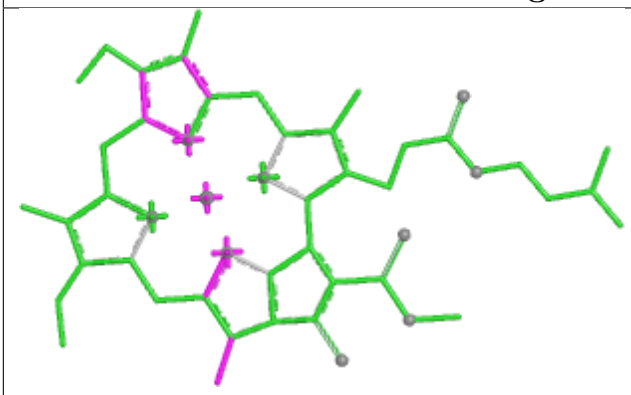


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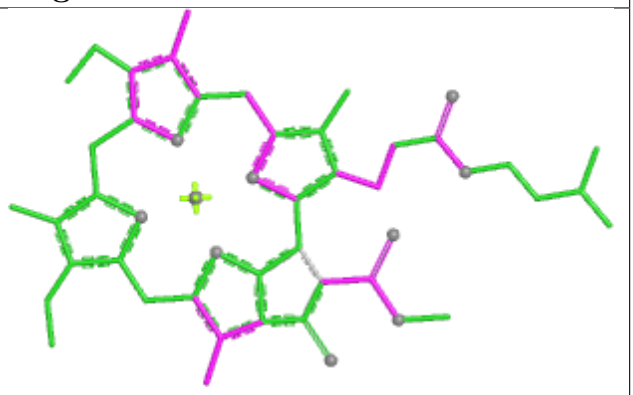


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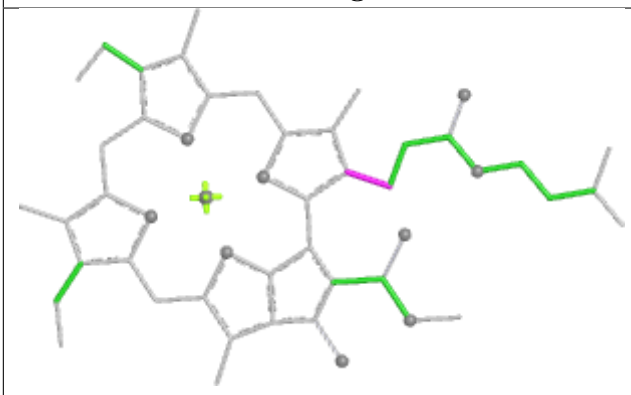
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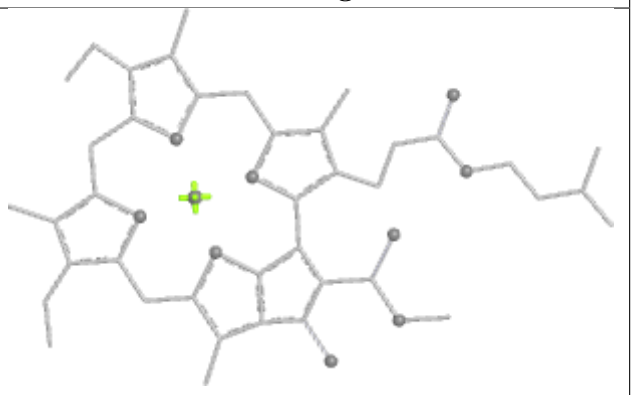
Bond lengths



Bond angles

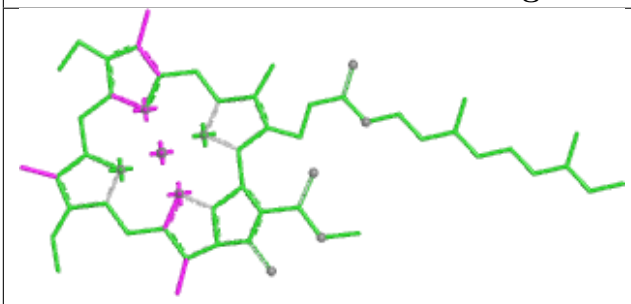


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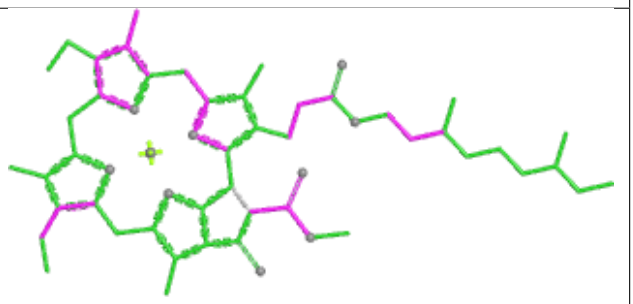


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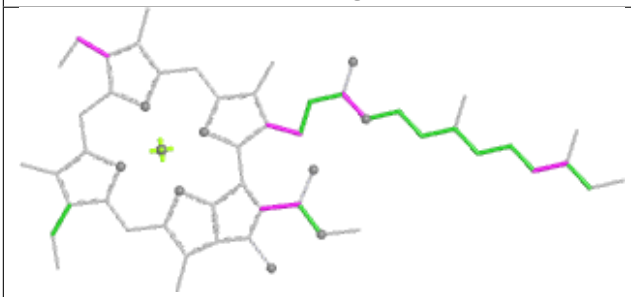
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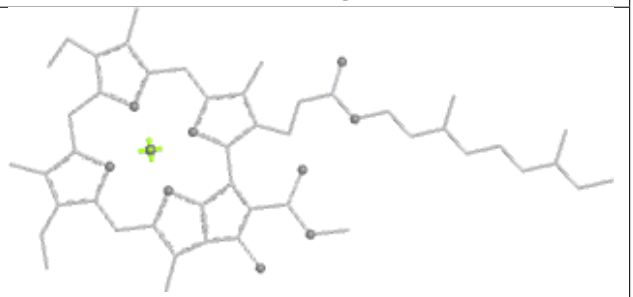
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Bond angles

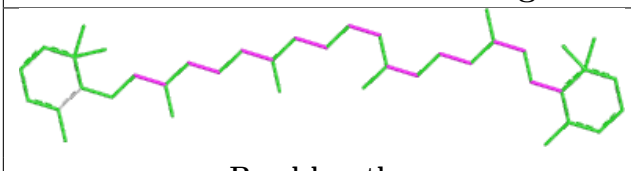


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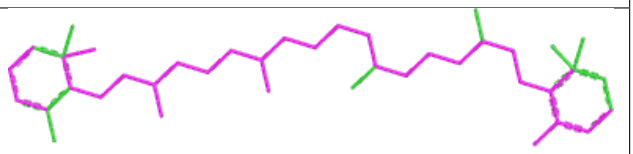


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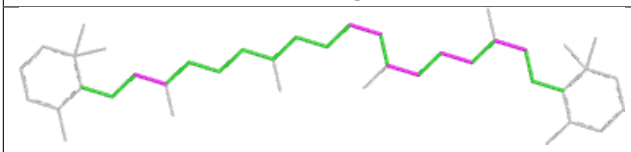
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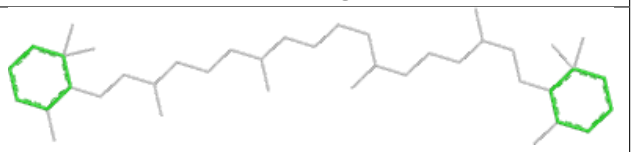
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Bond angles

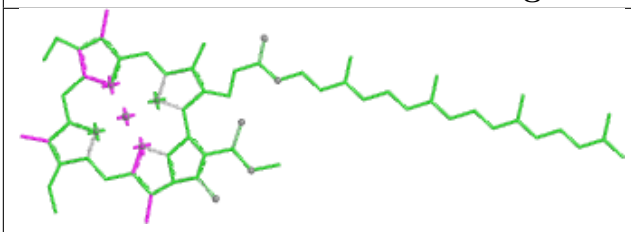


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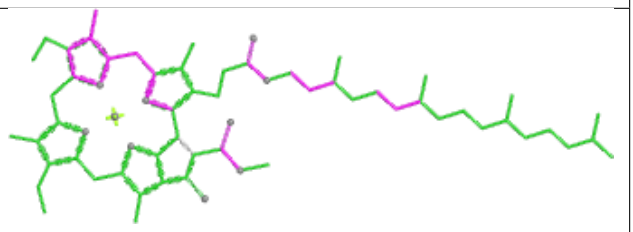


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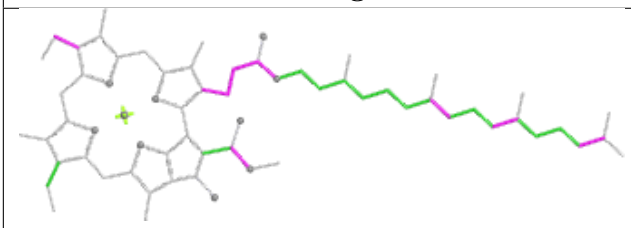
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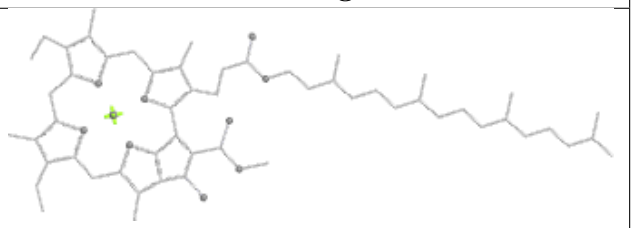
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Bond angles

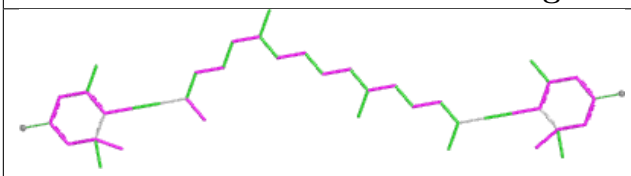


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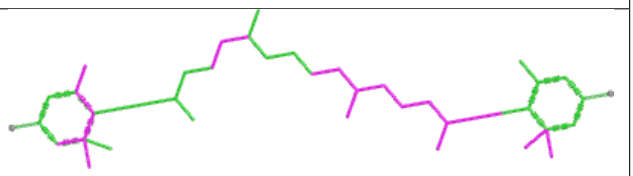


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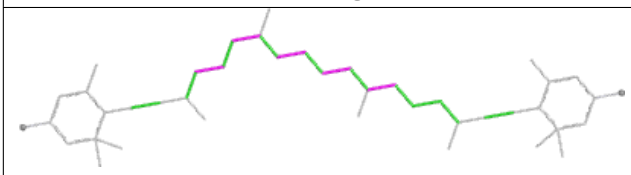
Ligand II0 a 318



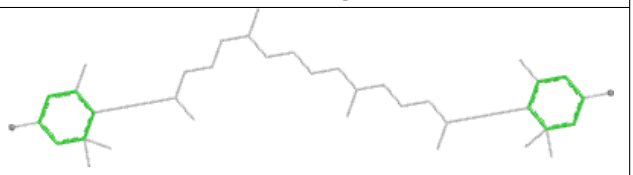
Bond lengths



Bond angles

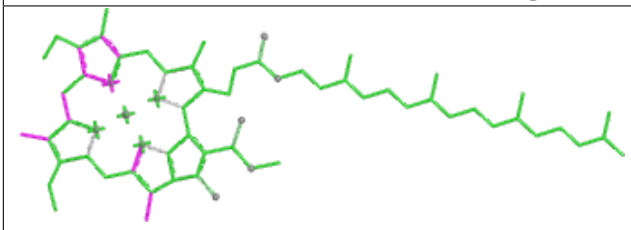


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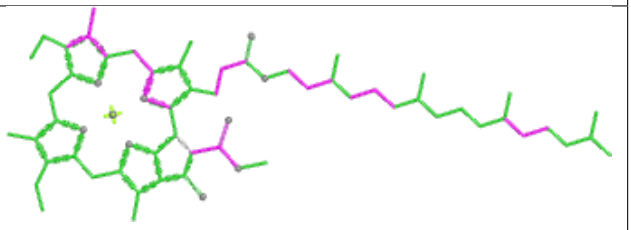


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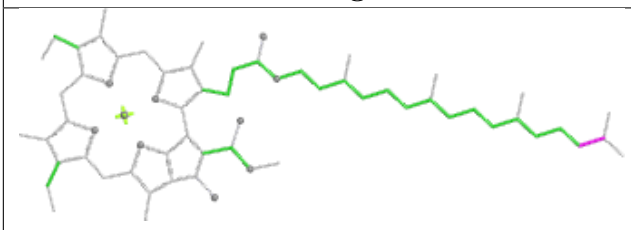
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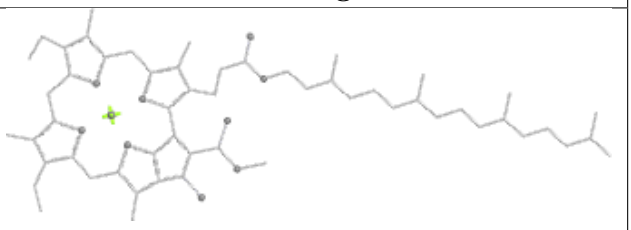
Bond lengths



Bond angles

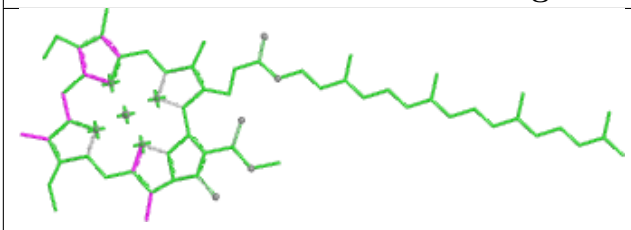


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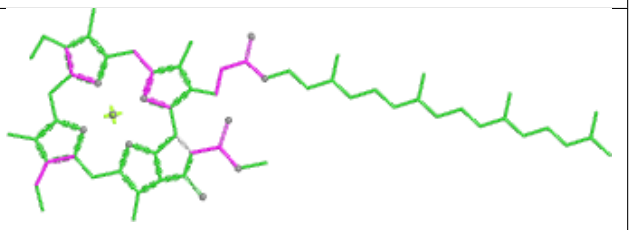


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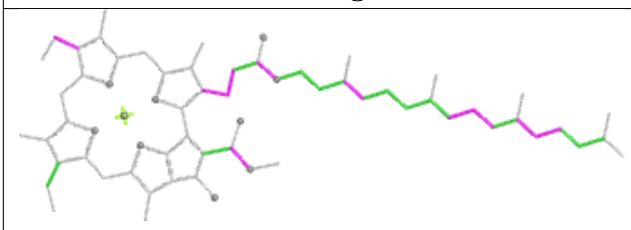
Ligand CLA f 602



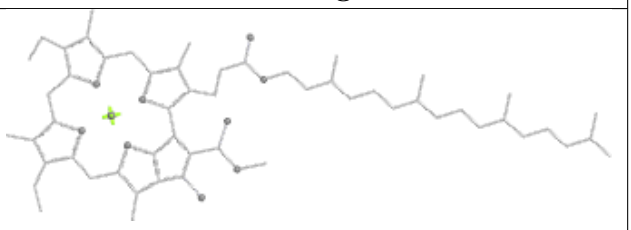
Bond lengths



Bond angles

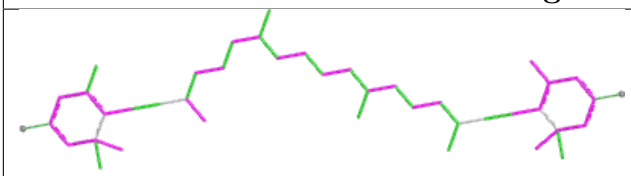


Torsions

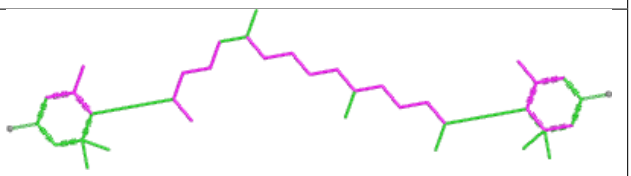


Rings

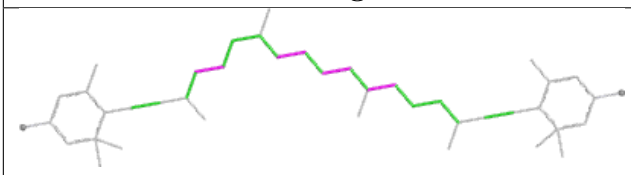
Ligand II0 e 616



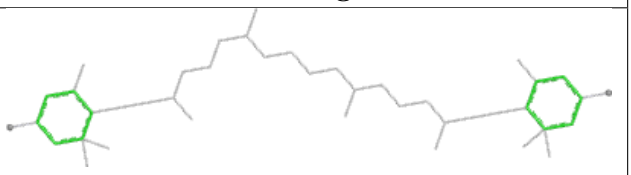
Bond lengths



Bond angles

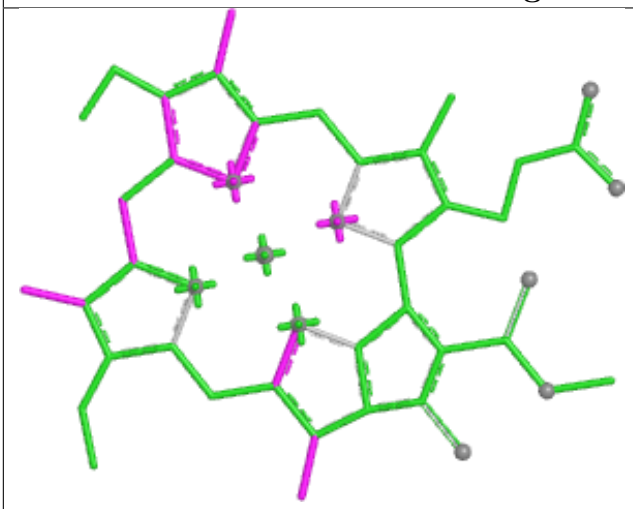


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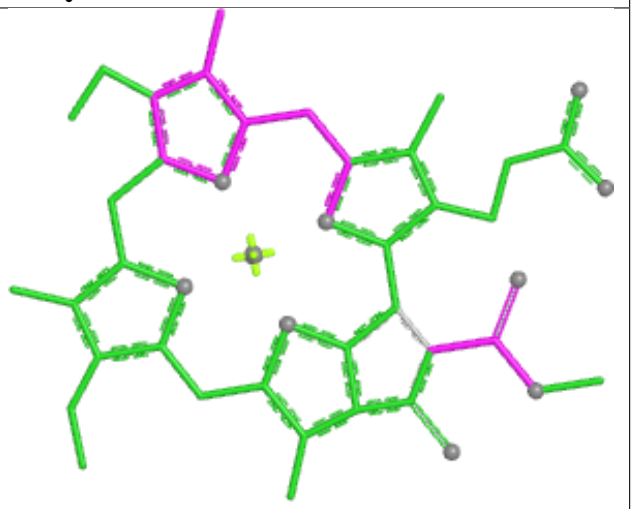


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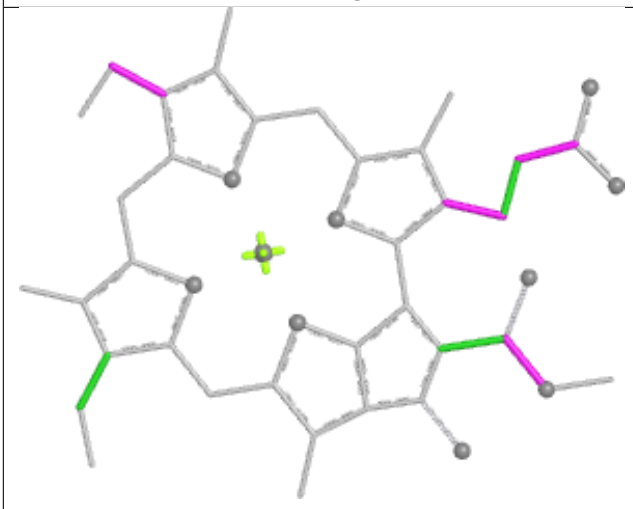
Ligand CLA Q 303



Bond lengths



Bond angles

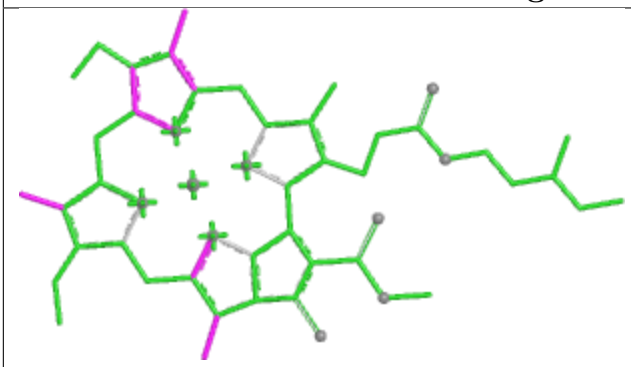


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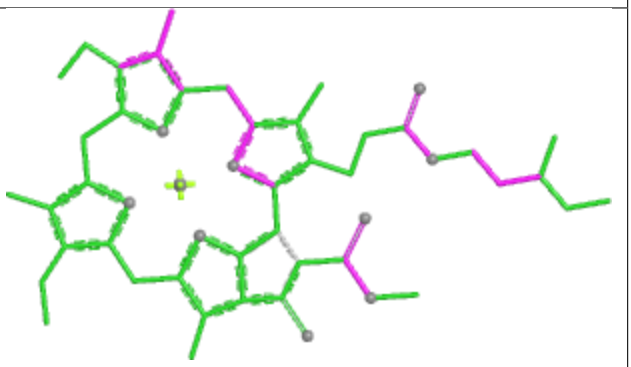


Rings

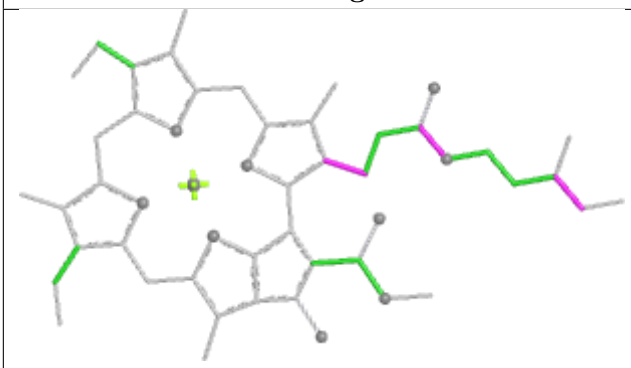
Ligand CLA h 305



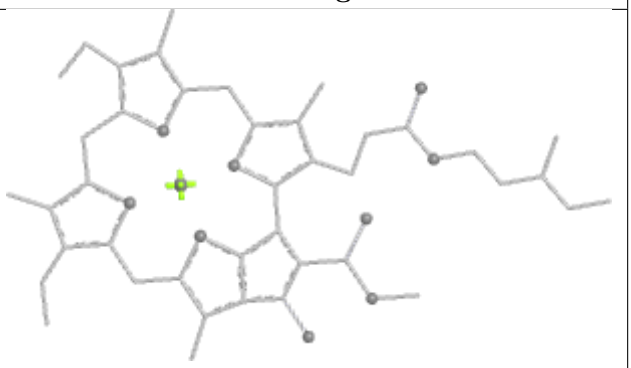
Bond lengths



Bond angles

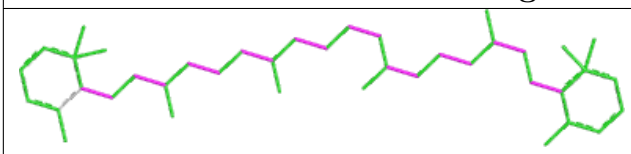


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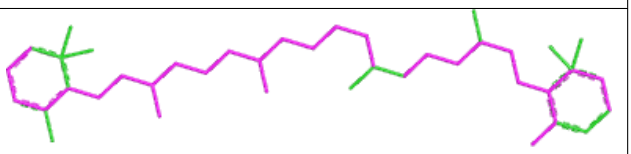


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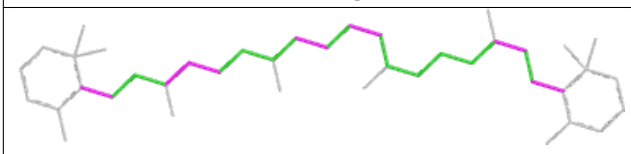
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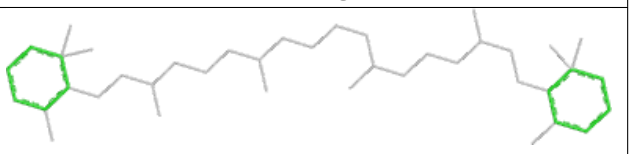
Bond lengths



Bond angles

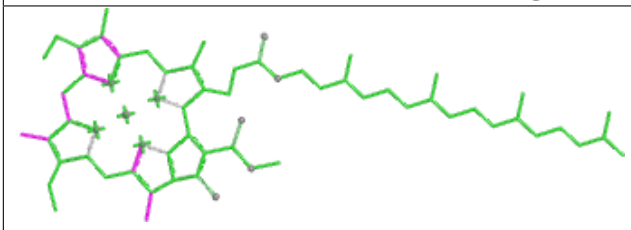


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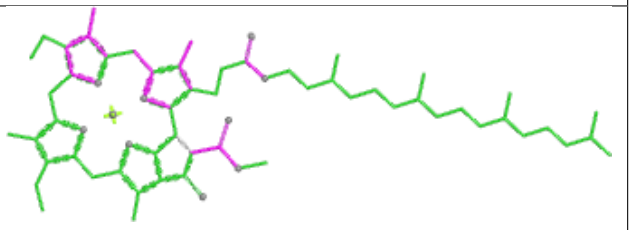


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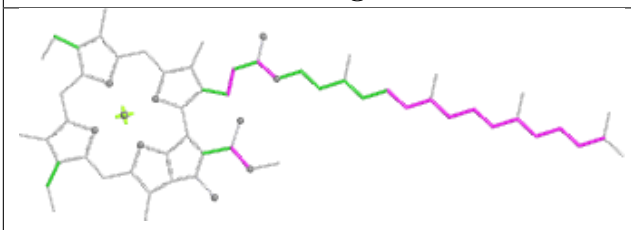
Ligand CLA h 306



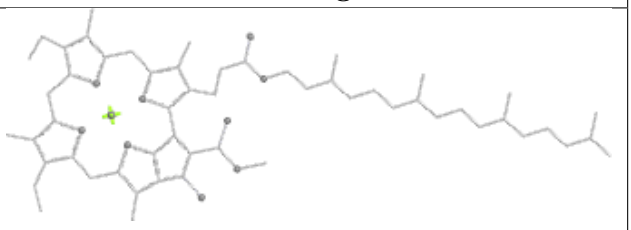
Bond lengths



Bond angles

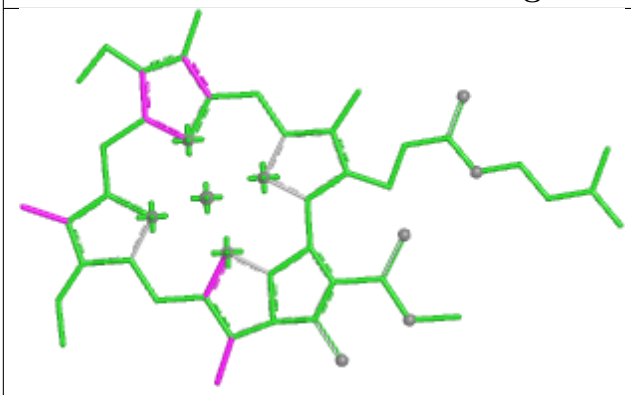


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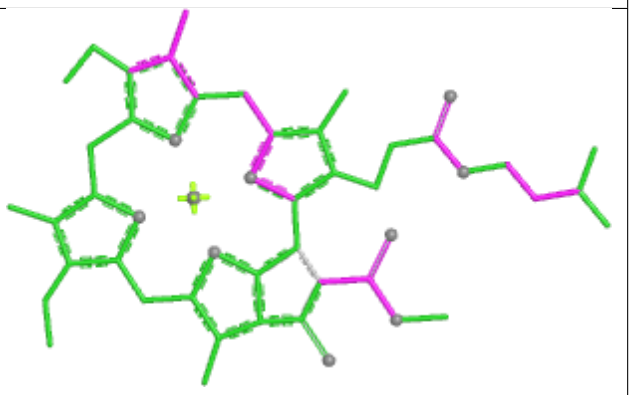


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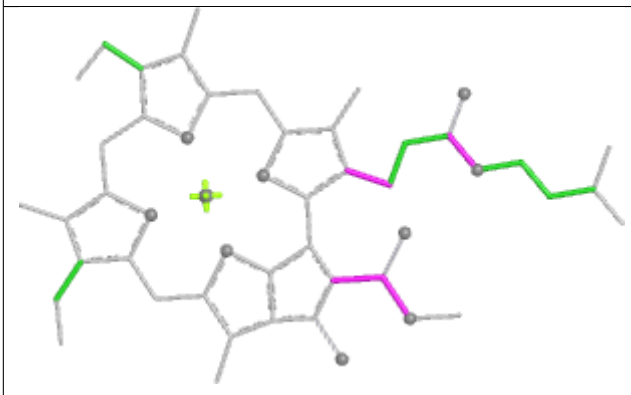
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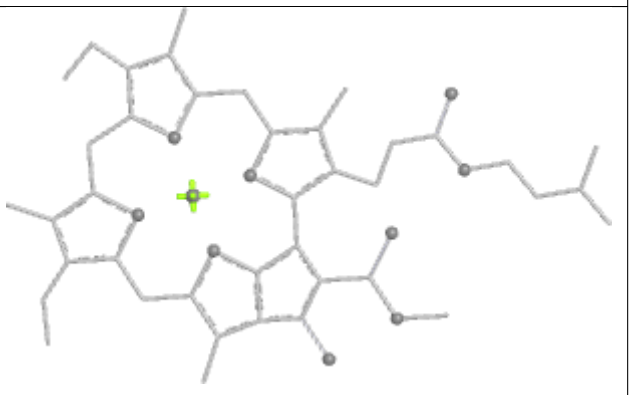
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Bond angles

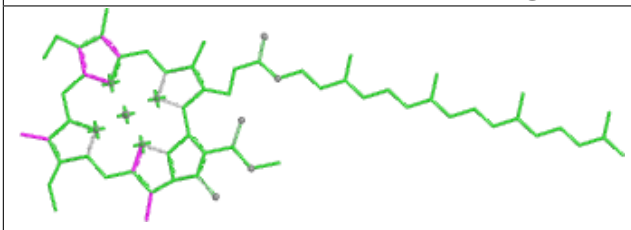


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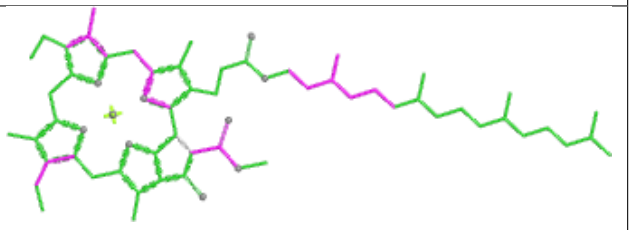


Rings

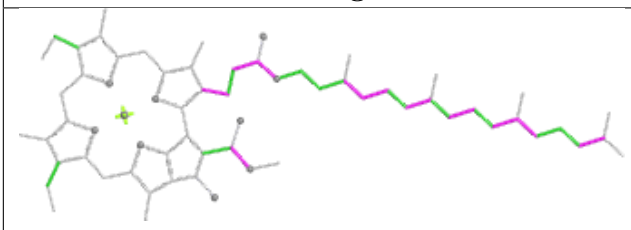
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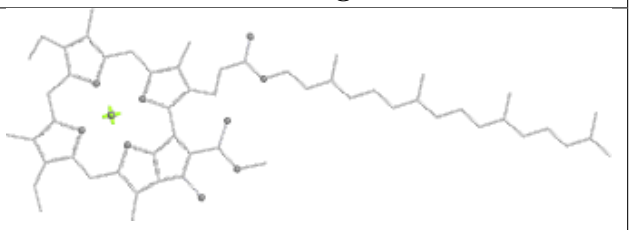
Bond lengths



Bond angles

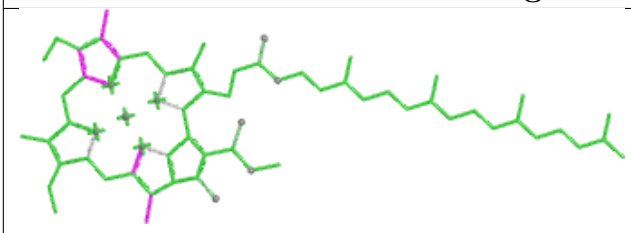


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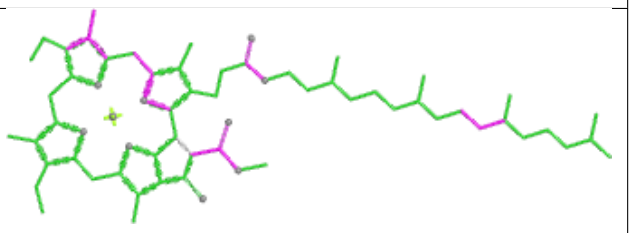


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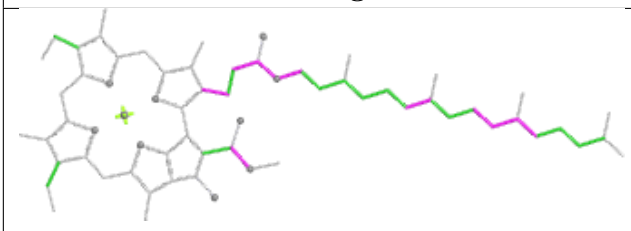
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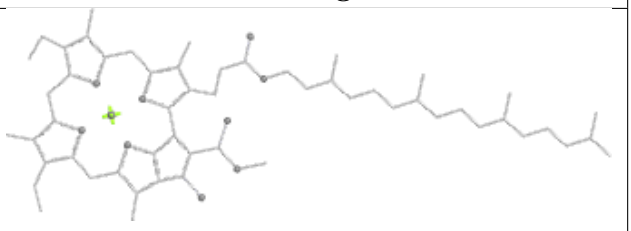
Bond lengths



Bond angles

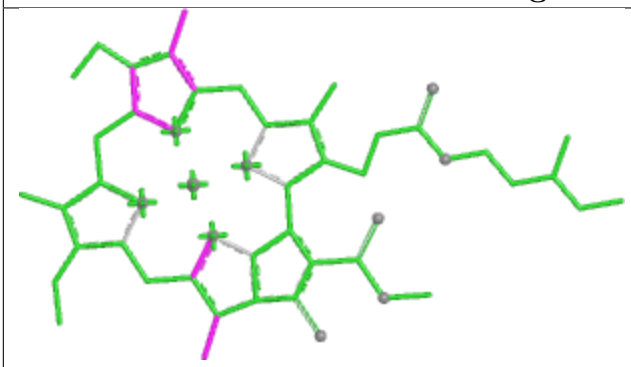


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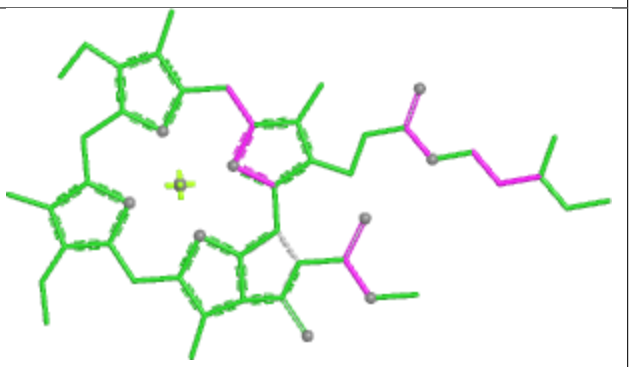


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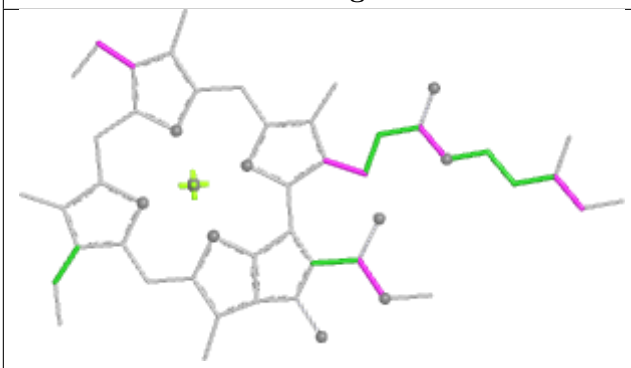
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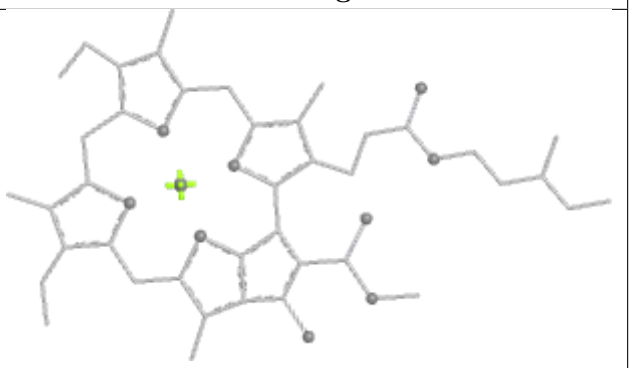
Bond lengths



Bond angles

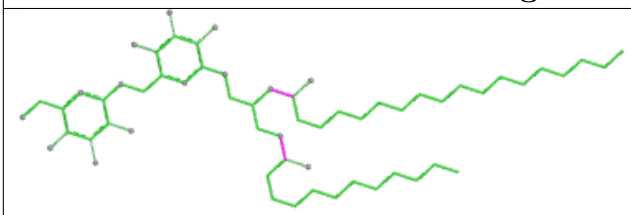


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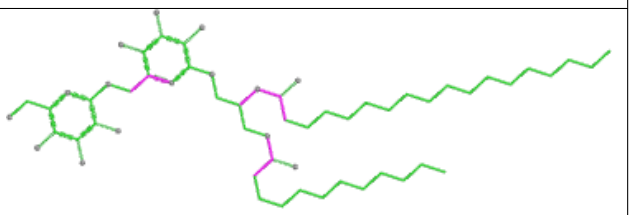


Rings

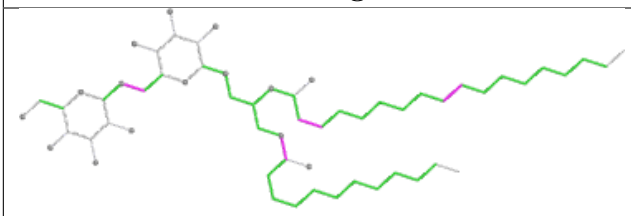
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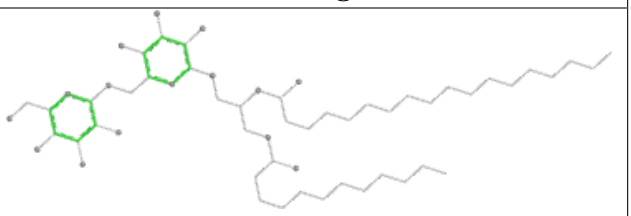
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Bond angles

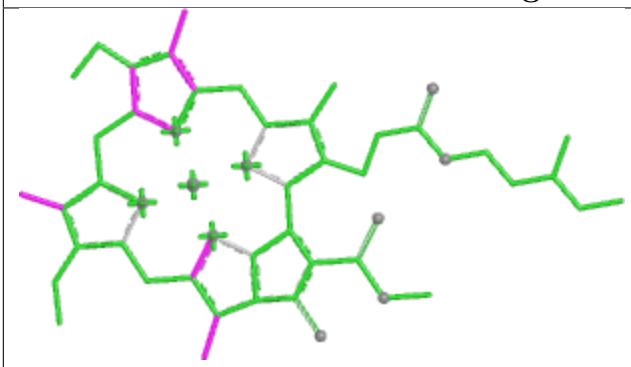


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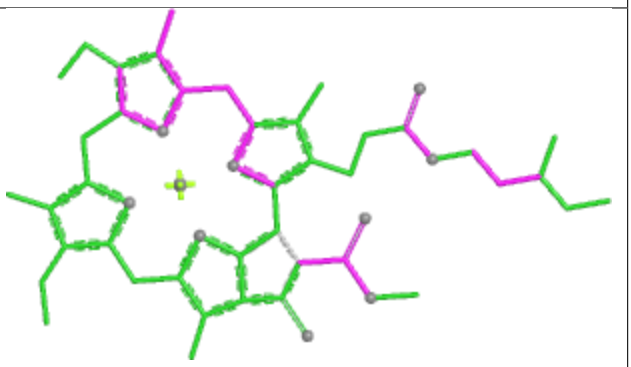


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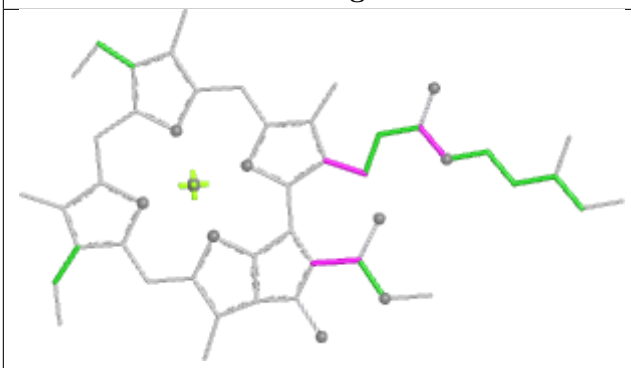
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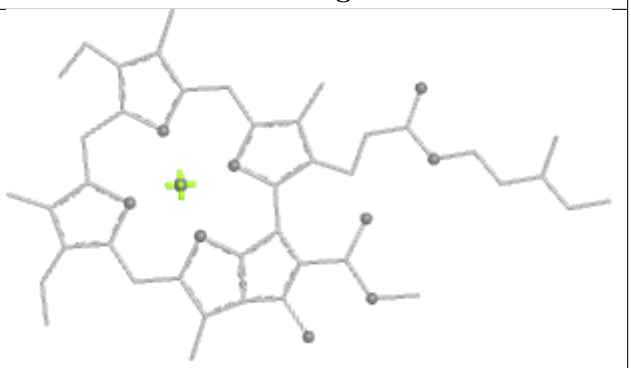
Bond lengths



Bond angles

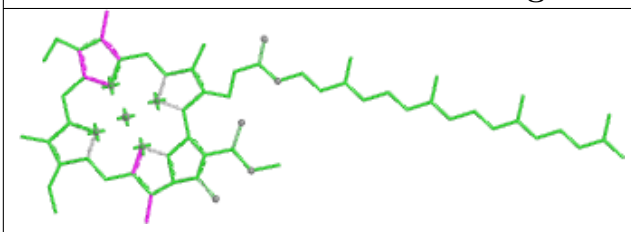


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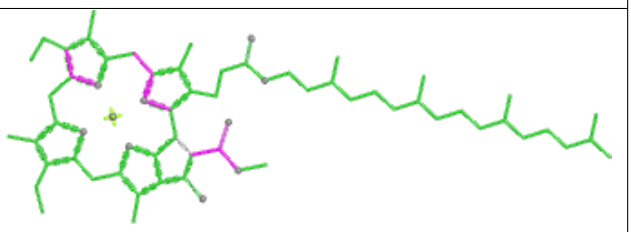


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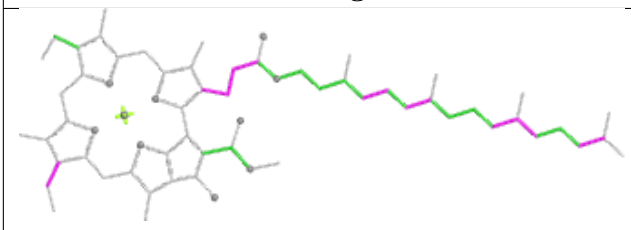
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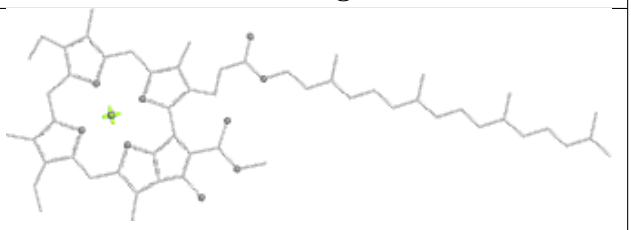
Bond lengths



Bond angles

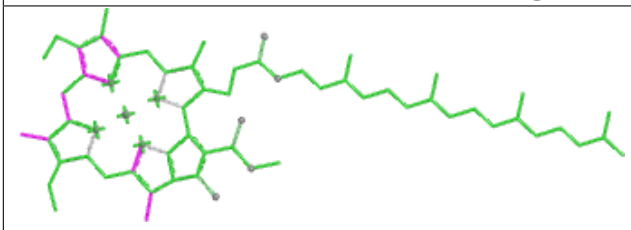


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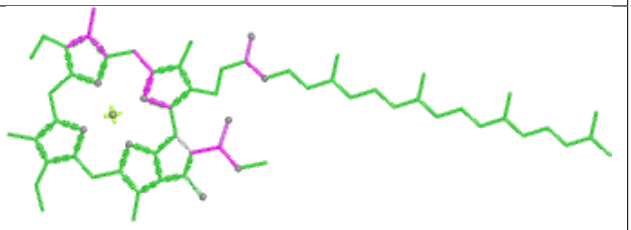


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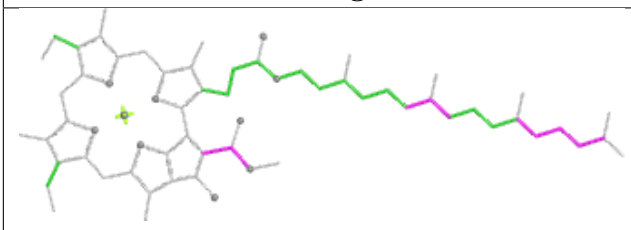
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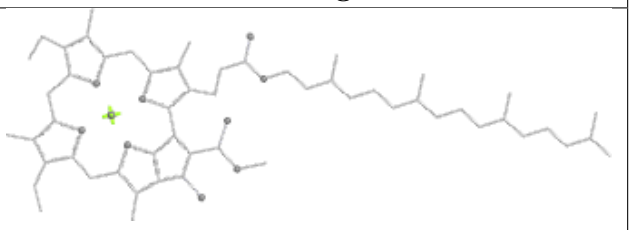
Bond lengths



Bond angles

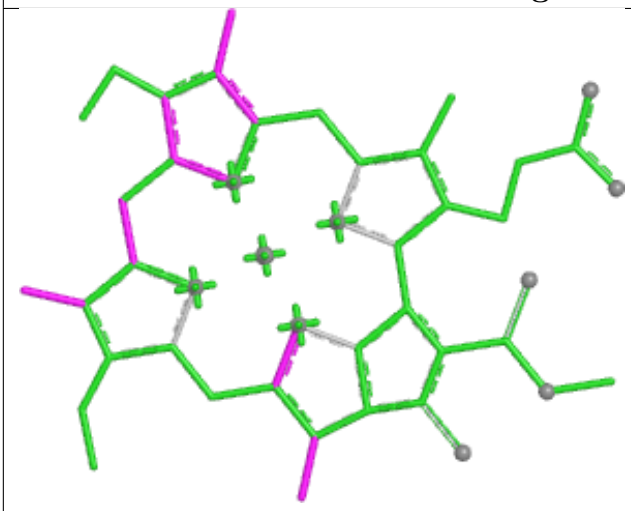


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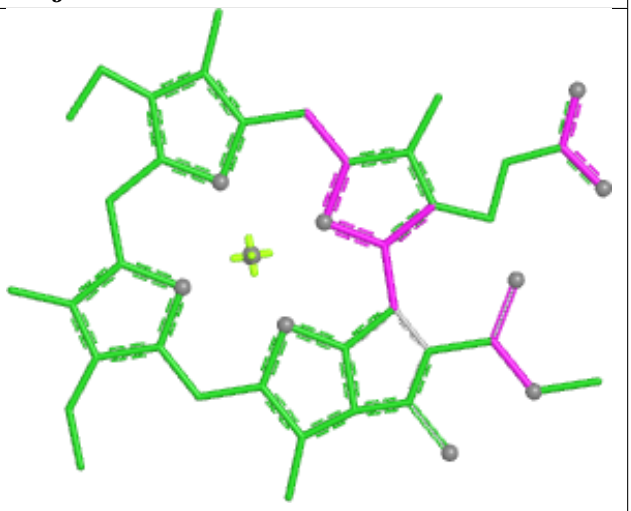


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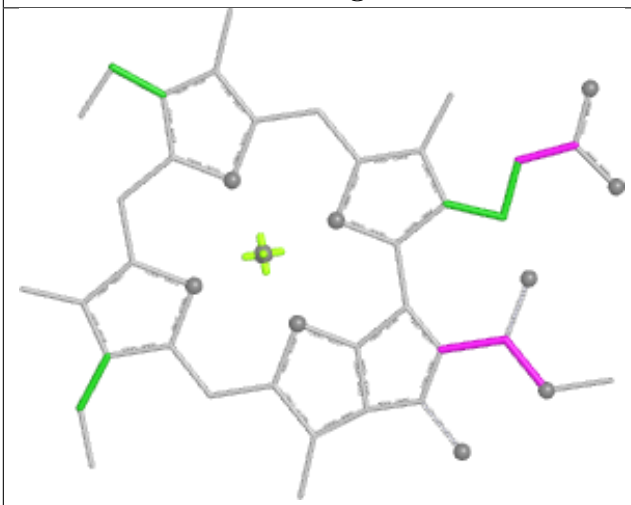
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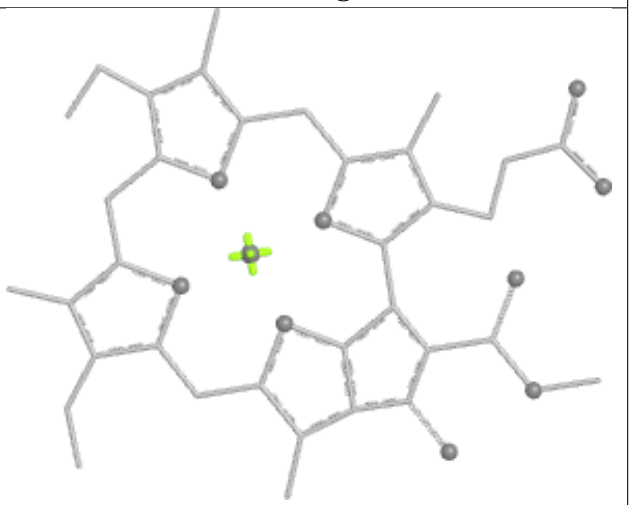
Bond lengths



Bond angles

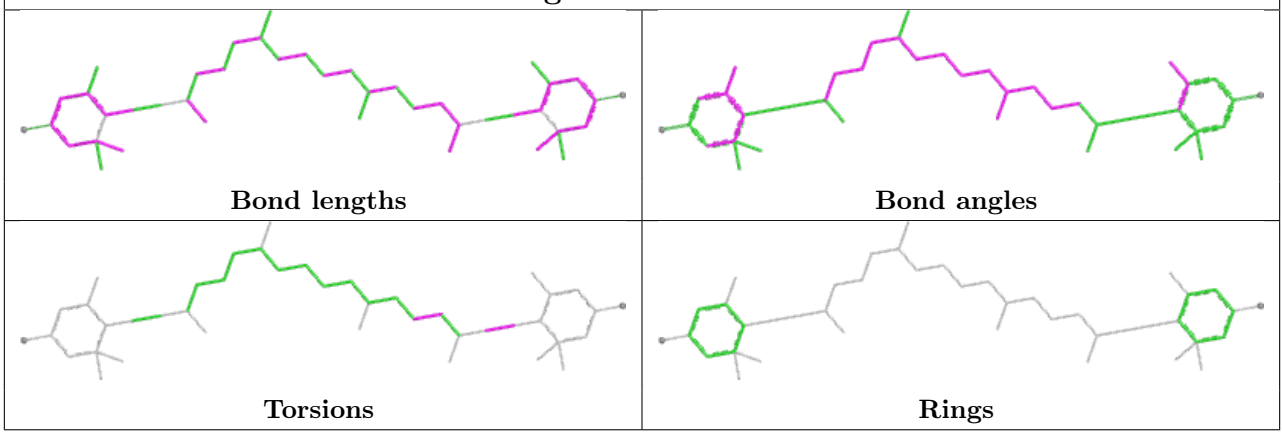


Torsions

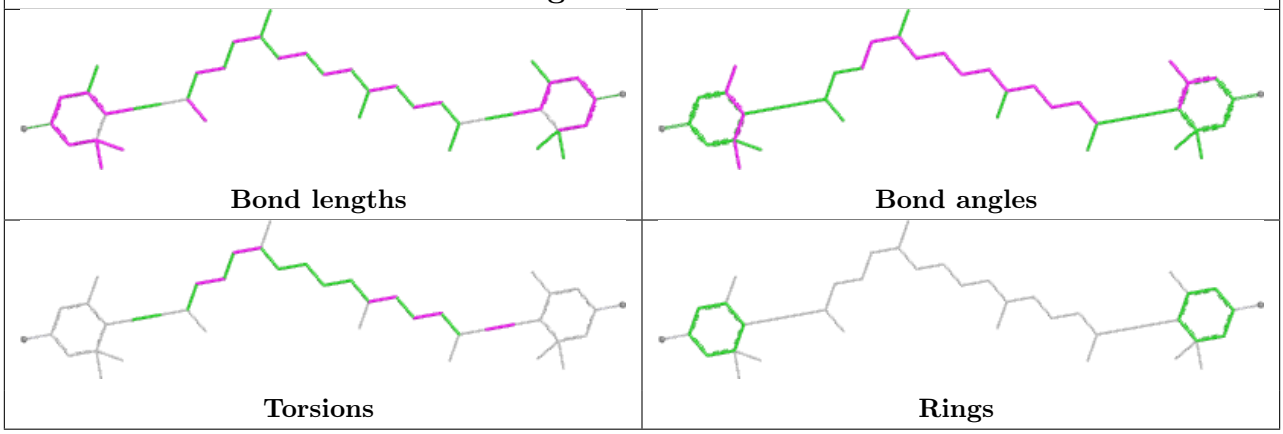


Rings

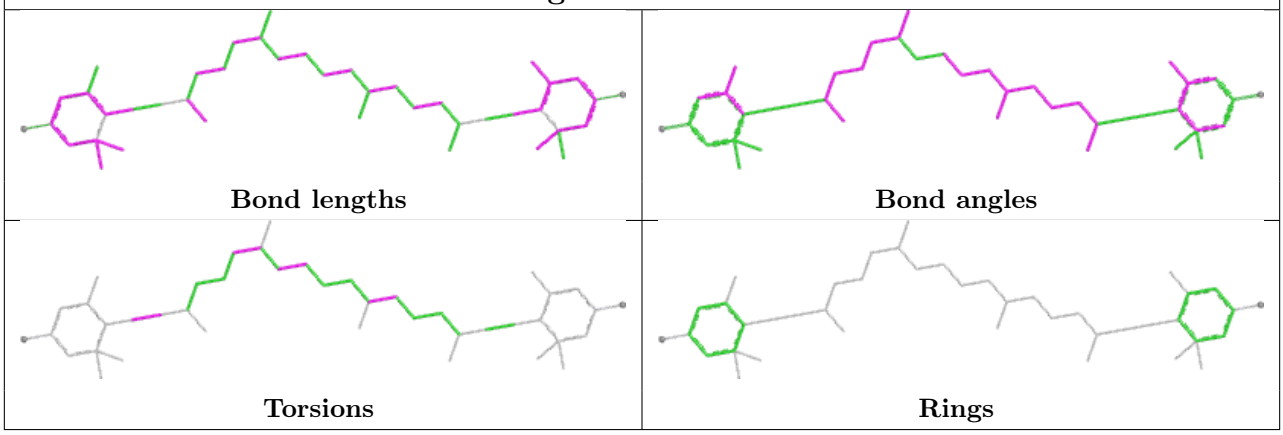
Ligand II0 a 315



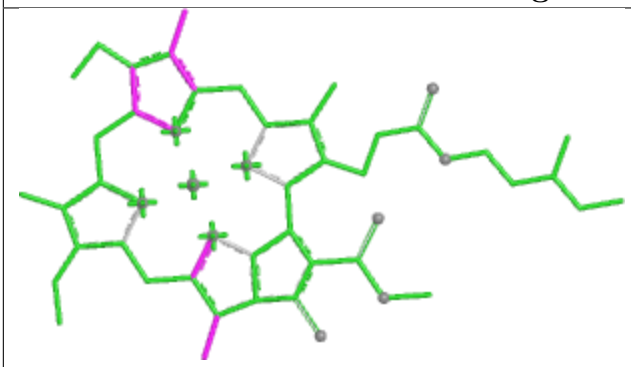
Ligand II0 i 320



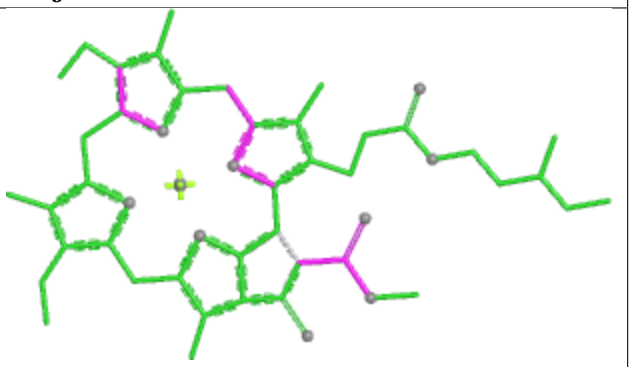
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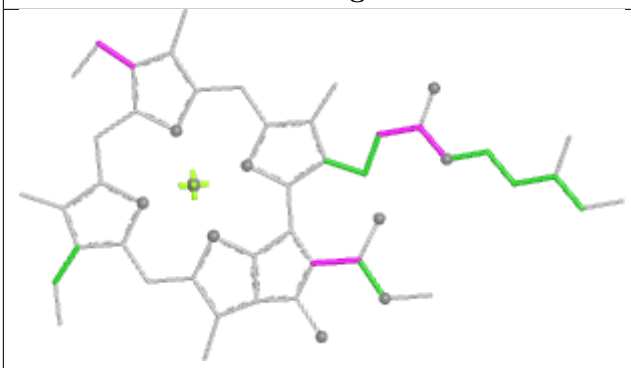
Ligand CLA j 607



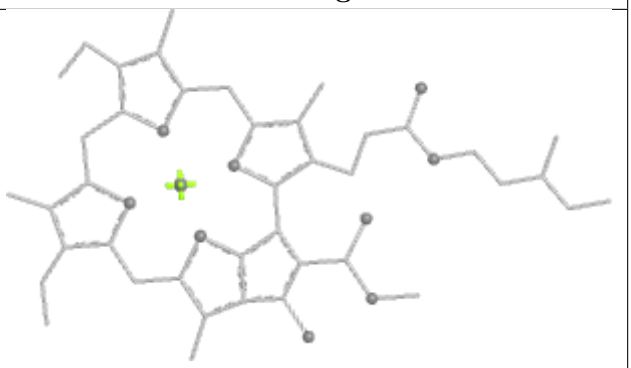
Bond lengths



Bond angles

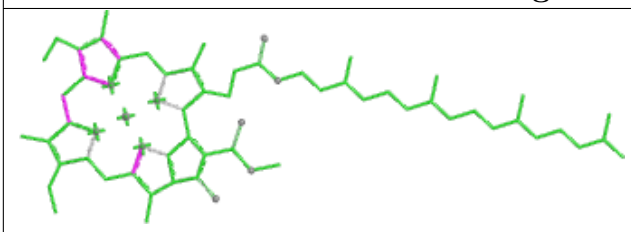


Torsions

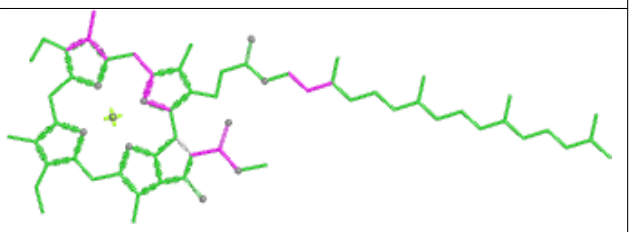


Rings

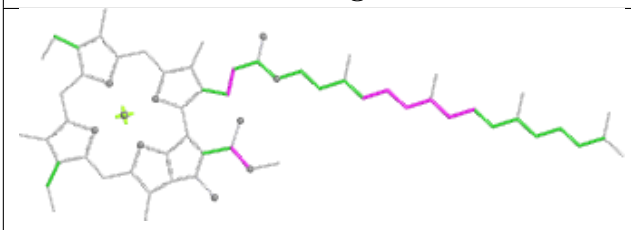
Ligand CLA i 305



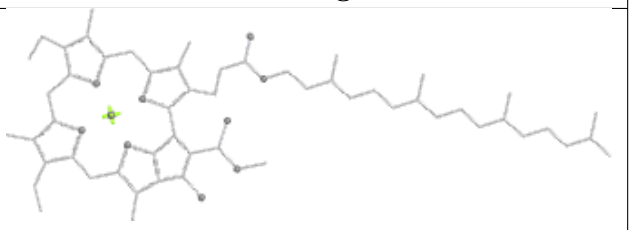
Bond lengths



Bond angles

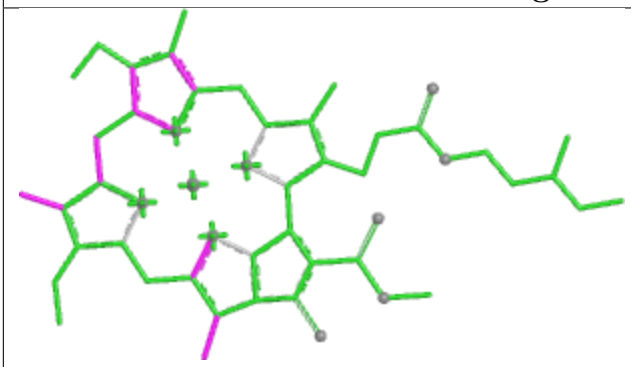


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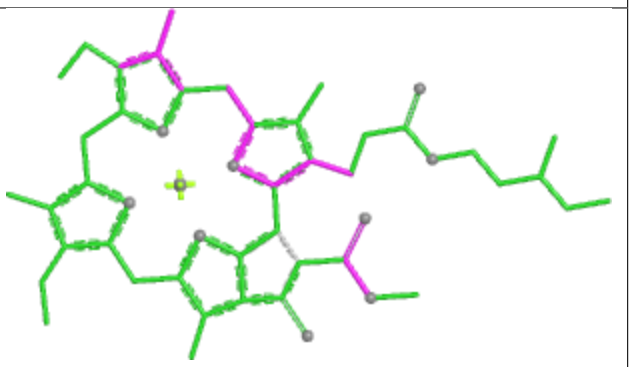


Rings

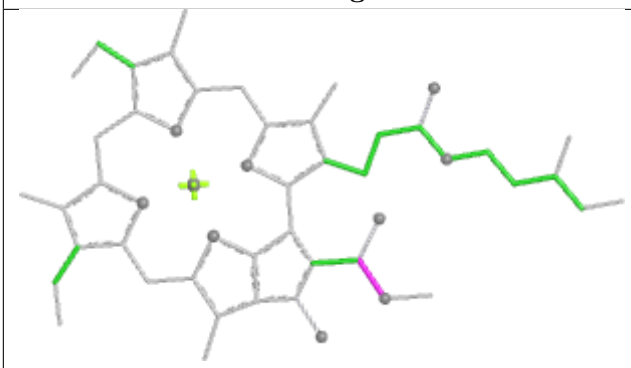
Ligand CLA i 308



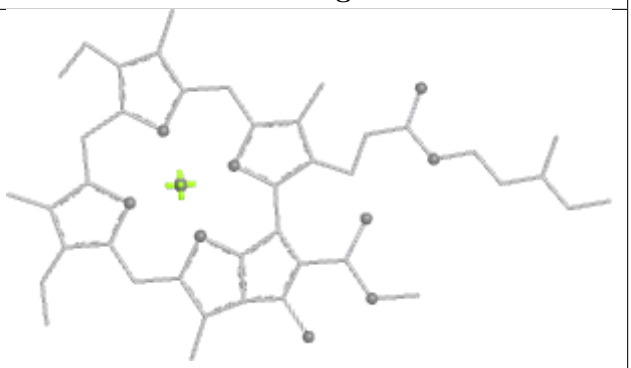
Bond lengths



Bond angles

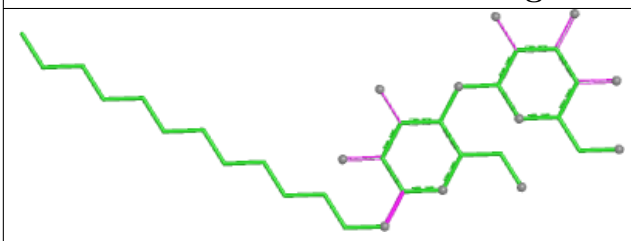


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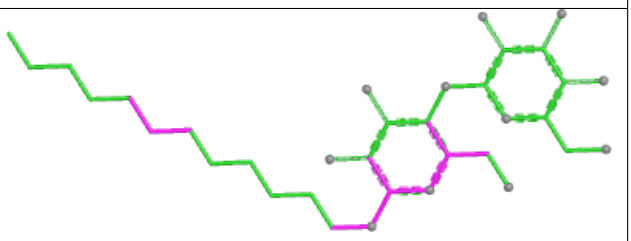


Rings

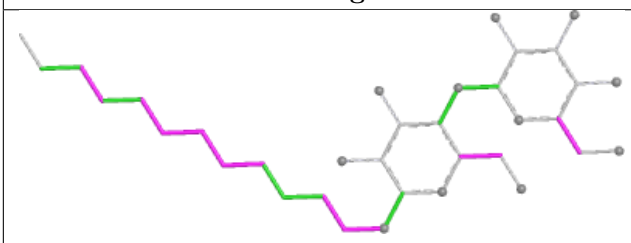
Ligand LMT a 320



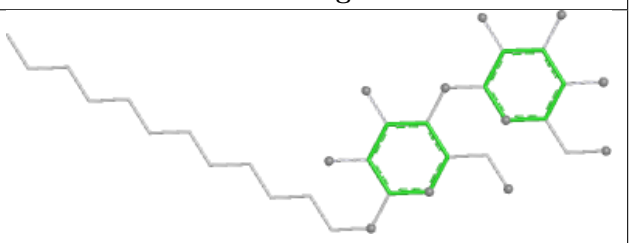
Bond lengths



Bond angles

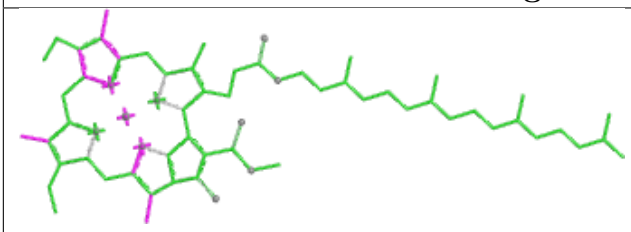


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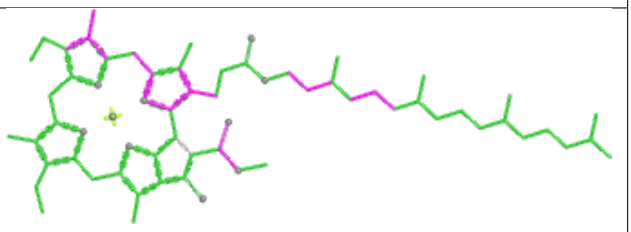


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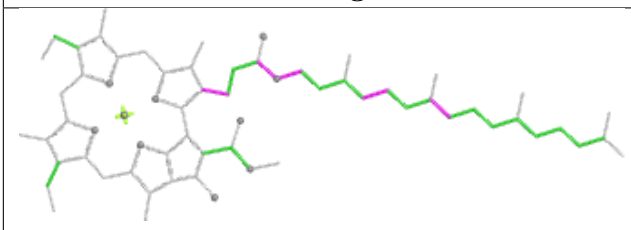
Ligand CLA A 805



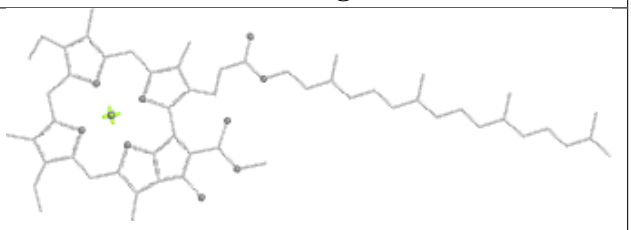
Bond lengths



Bond angles

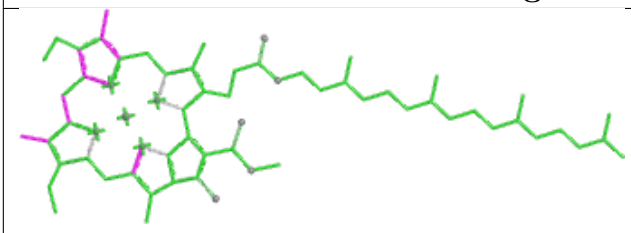


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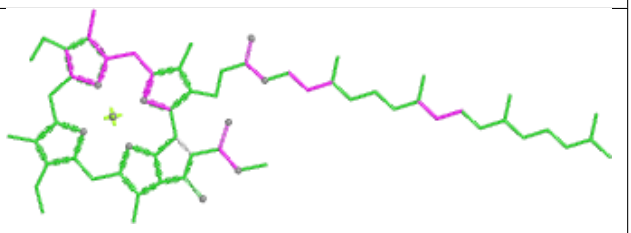


Rings

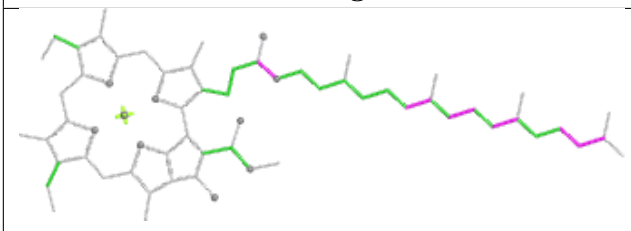
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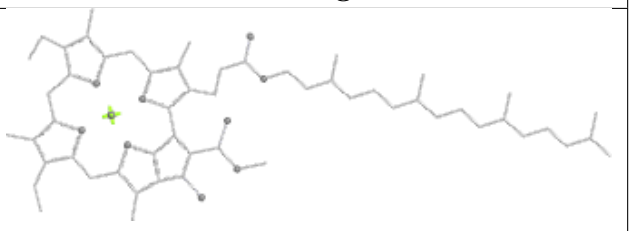
Bond lengths



Bond angles

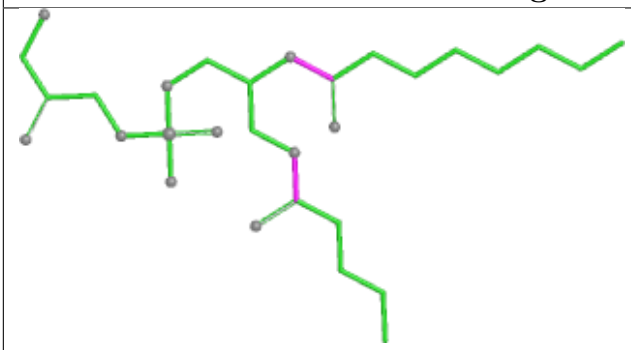


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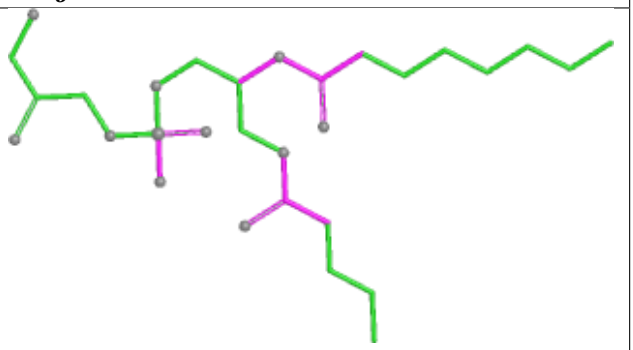


Rings

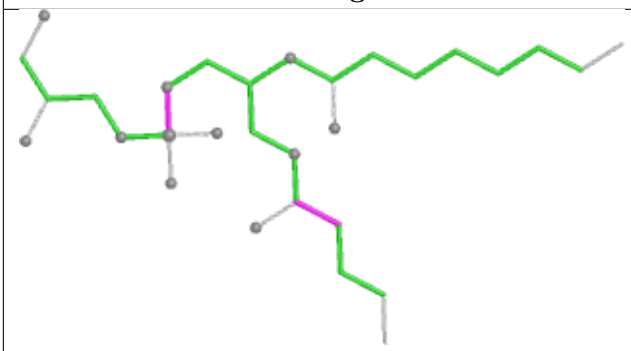
Ligand LHG j 617



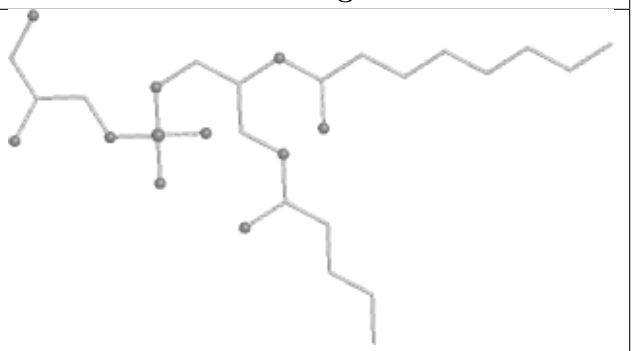
Bond lengths



Bond angles

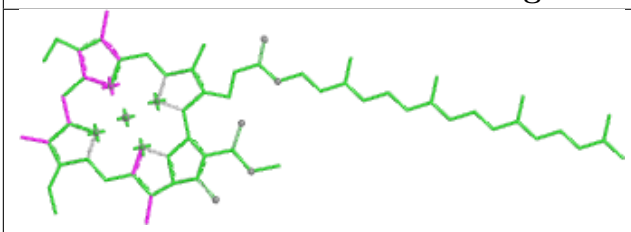


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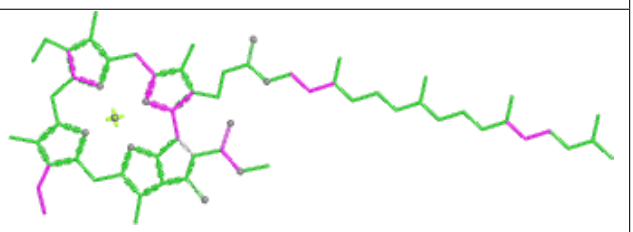


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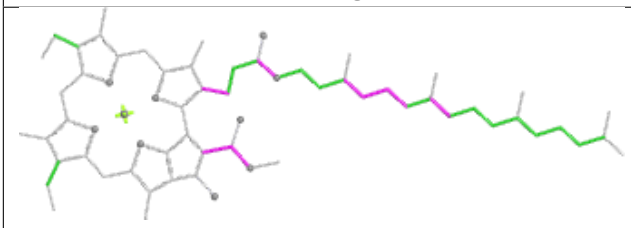
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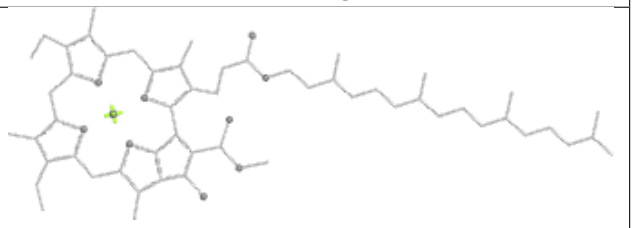
Bond lengths



Bond angles

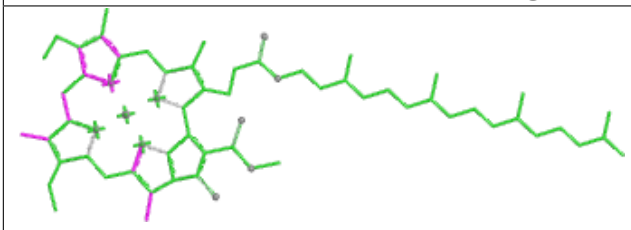


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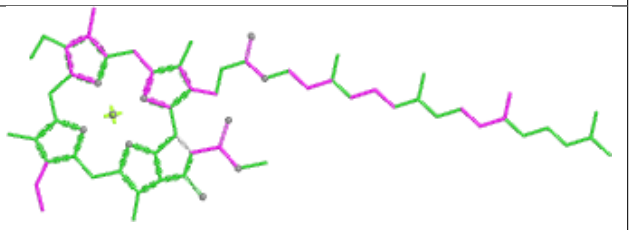


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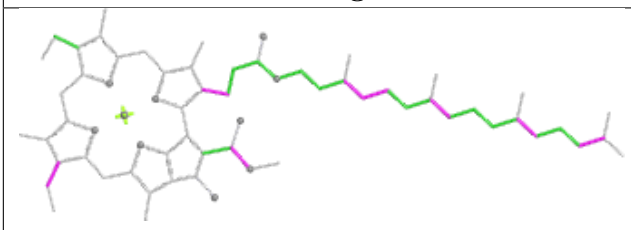
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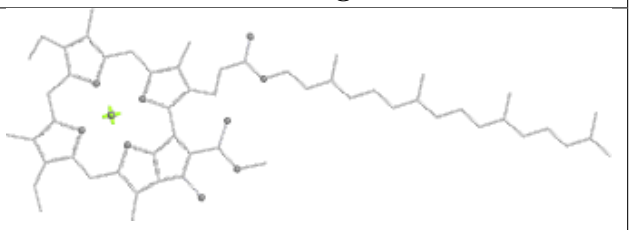
Bond lengths



Bond angles

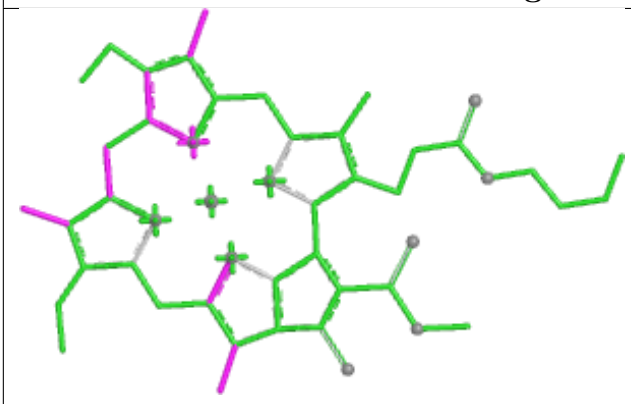


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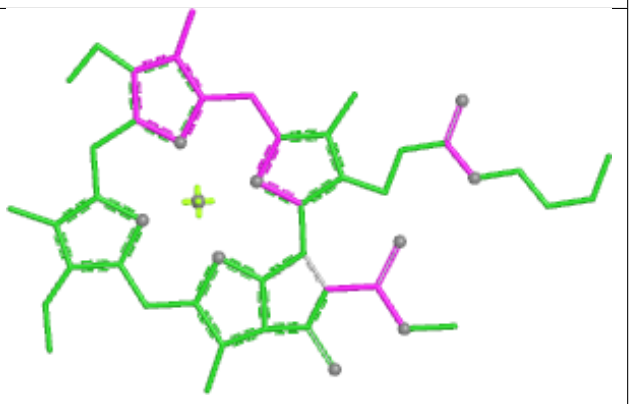


Rings

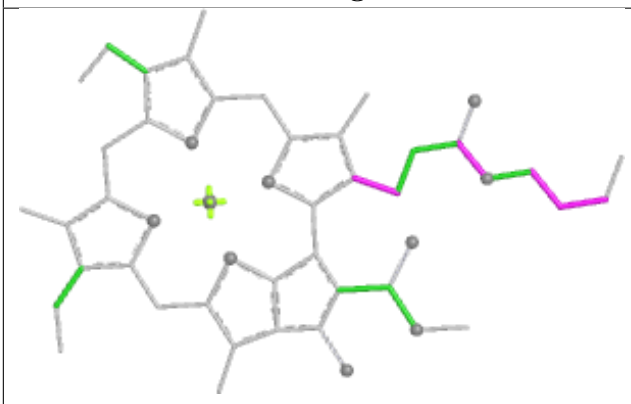
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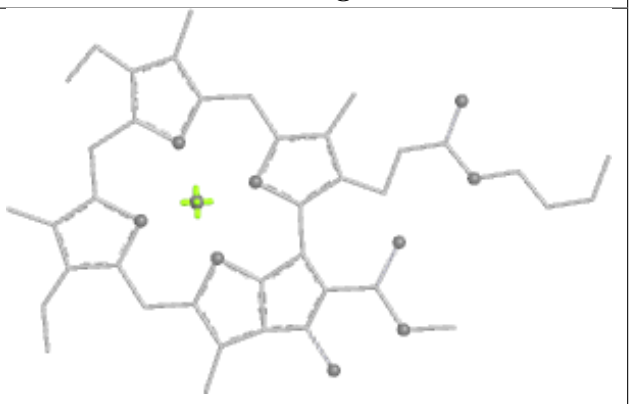
Bond lengths



Bond angles

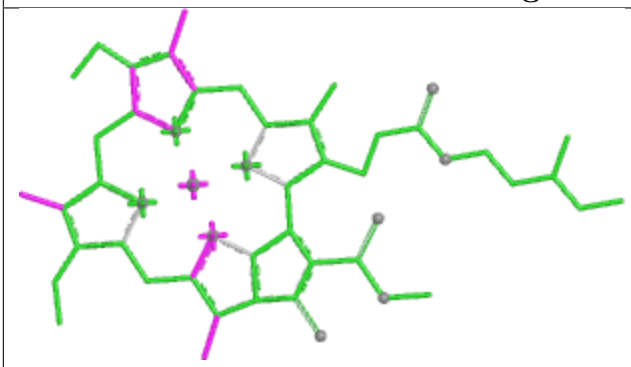


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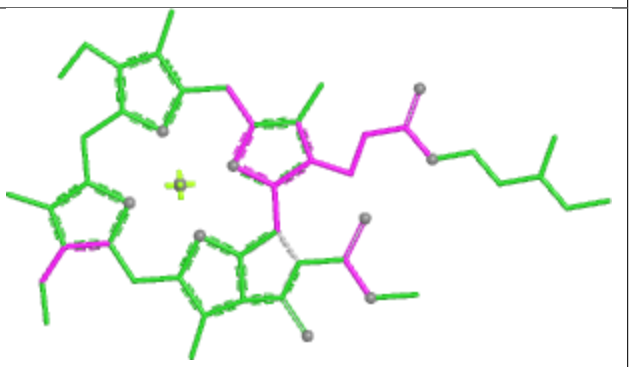


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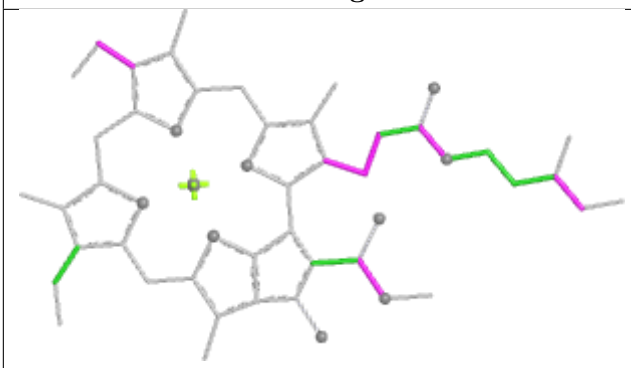
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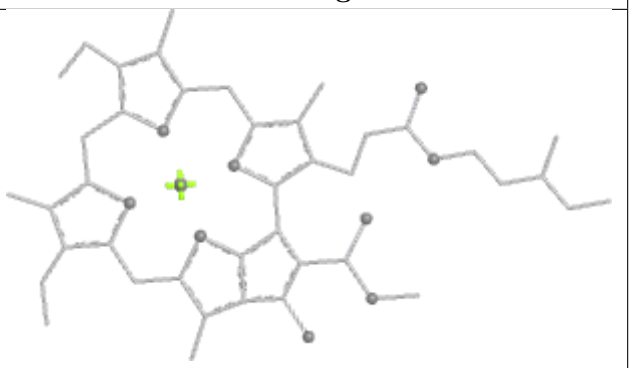
Bond lengths



Bond angles

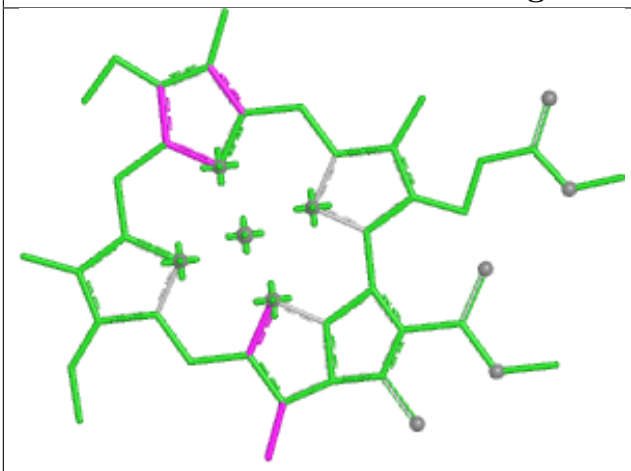


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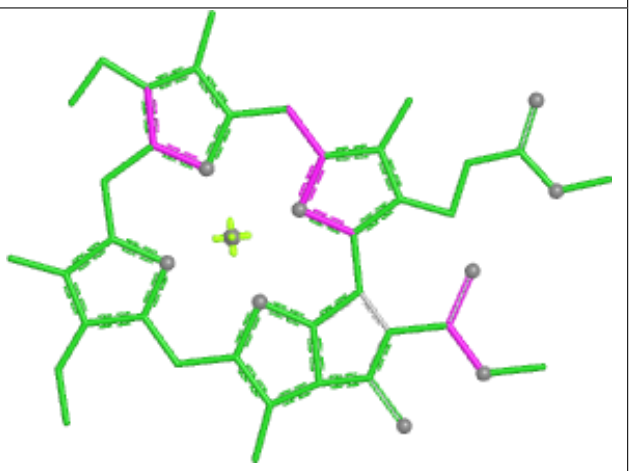


Rings

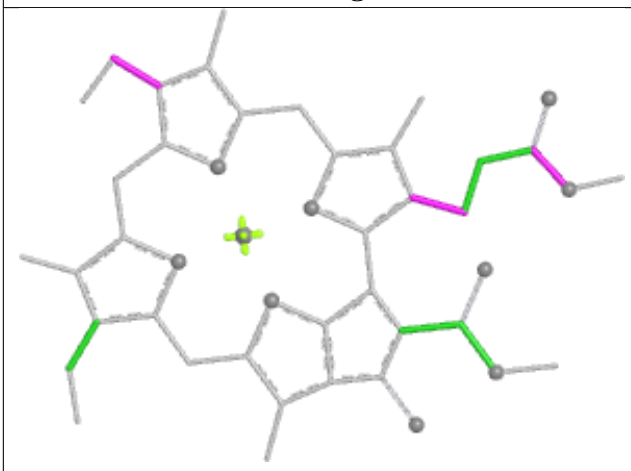
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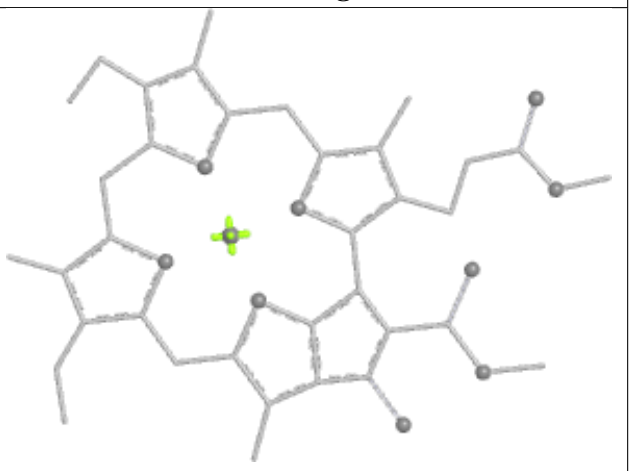
Bond lengths



Bond angles

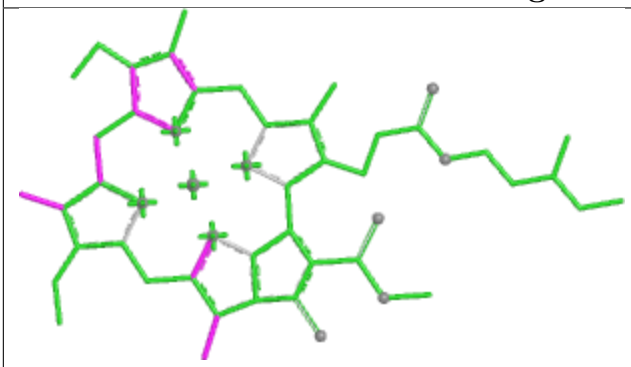


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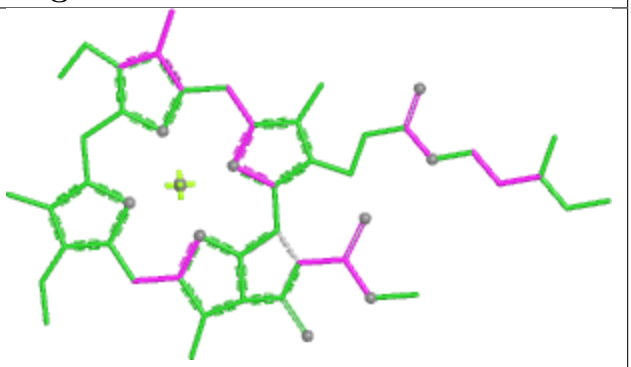


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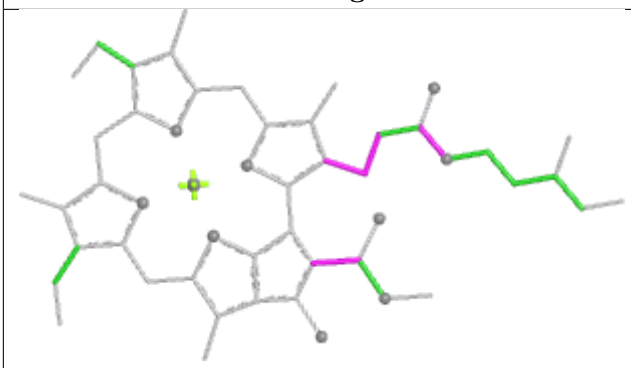
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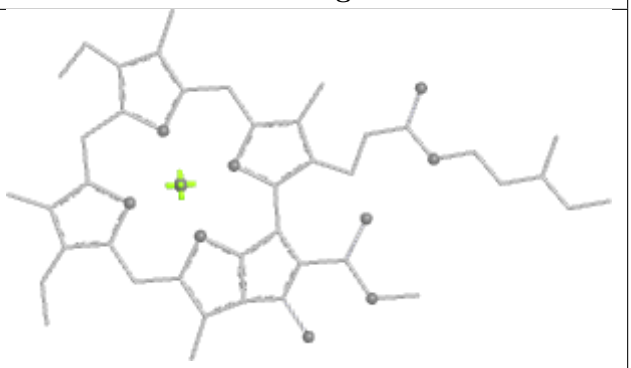
Bond lengths



Bond angles

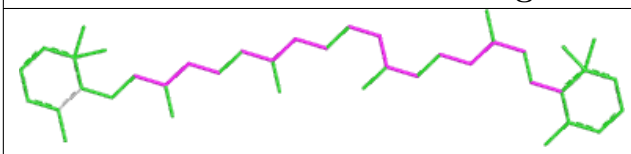


Torsions

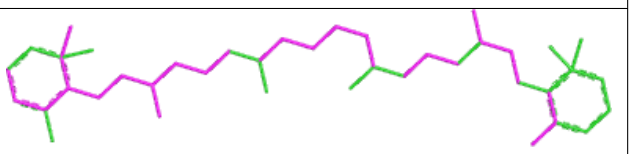


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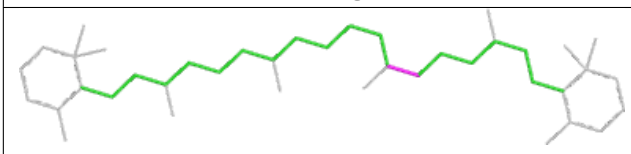
Ligand WVN B 847



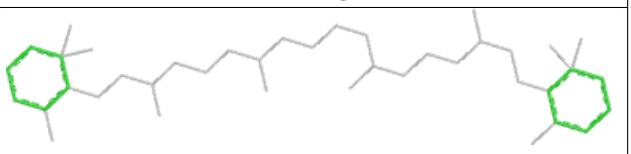
Bond lengths



Bond angles

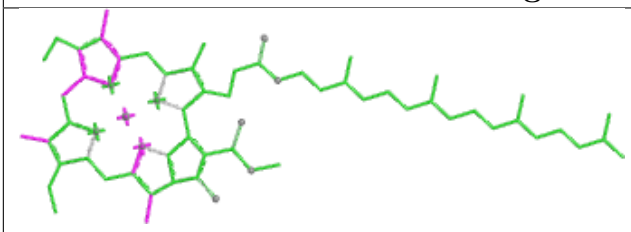


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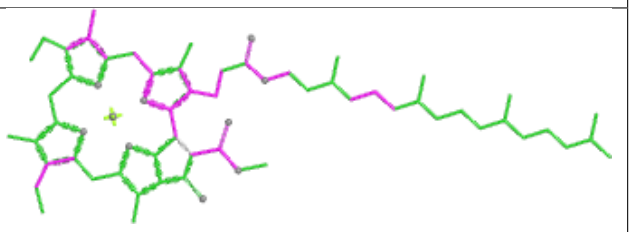


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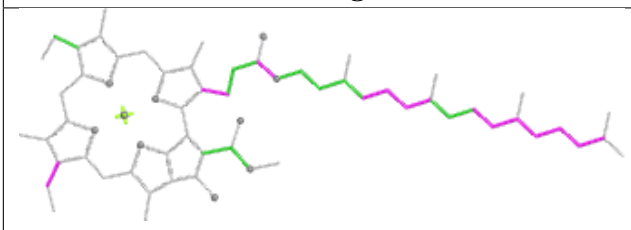
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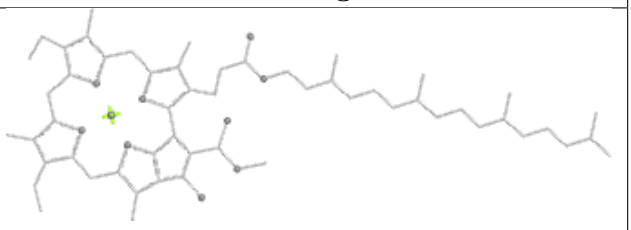
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Bond angles

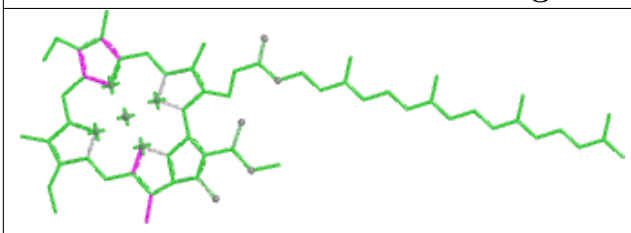


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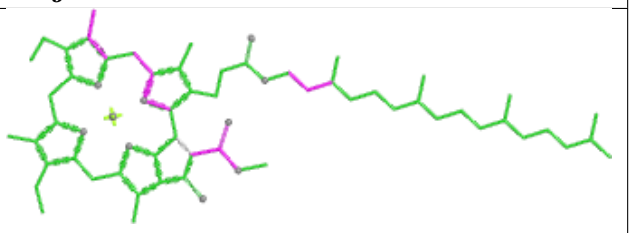


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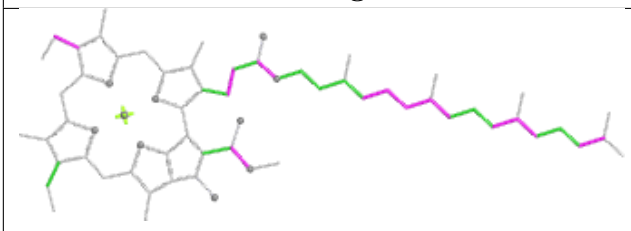
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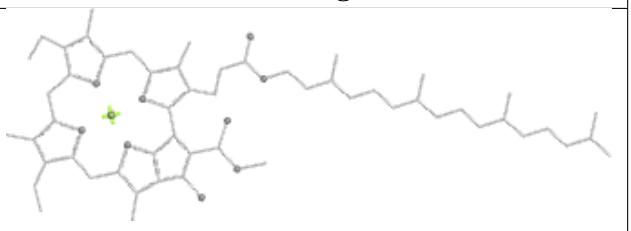
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Bond angles

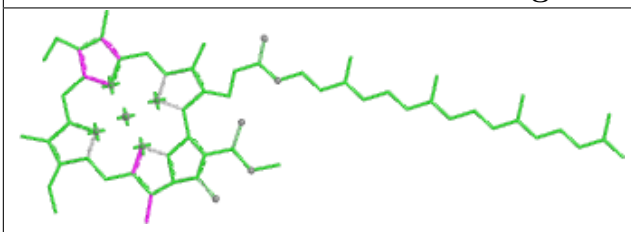


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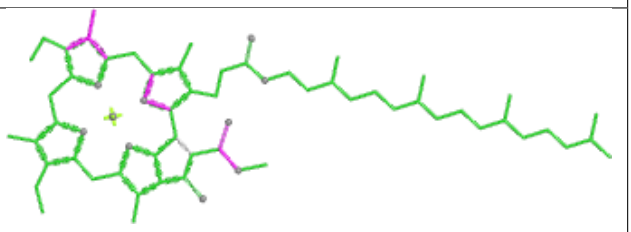


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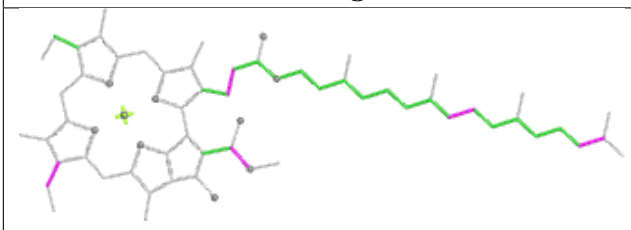
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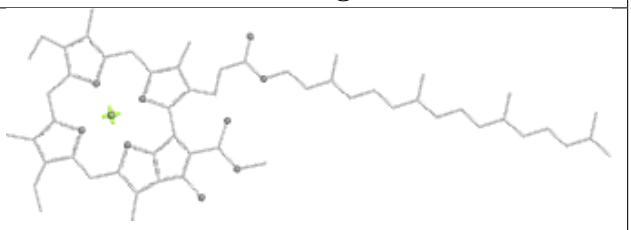
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Bond angles

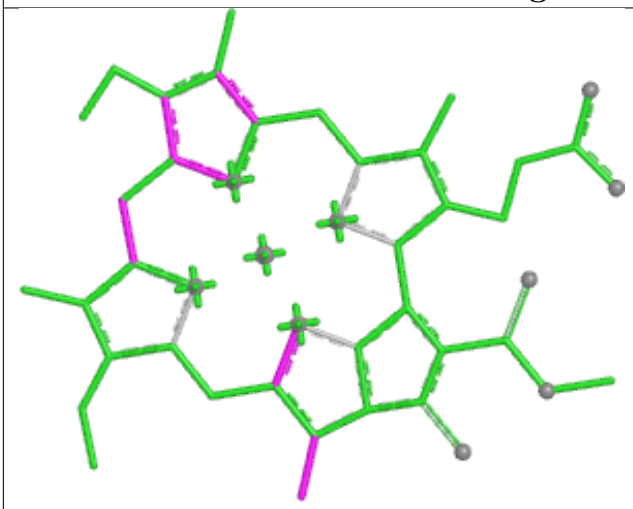


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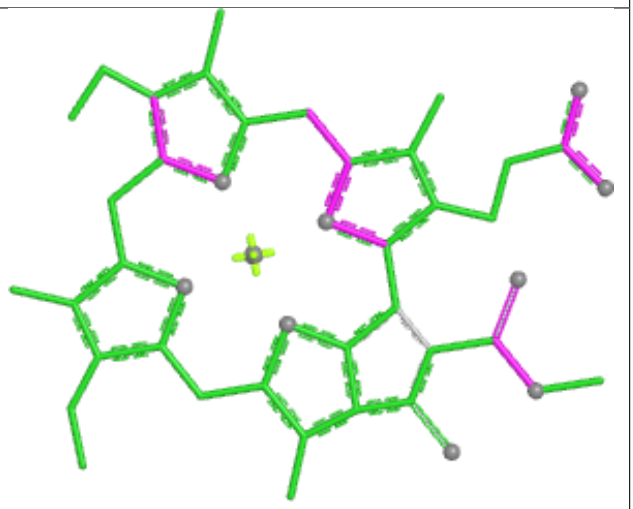


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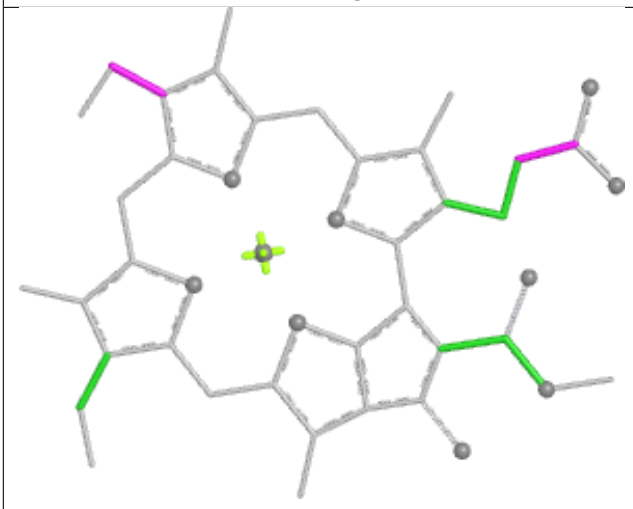
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Bond lengths



Bond angles

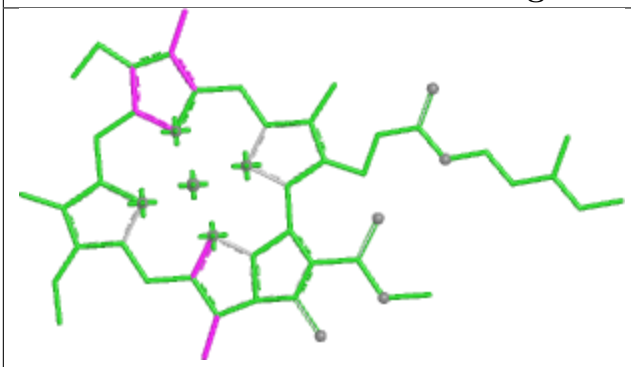


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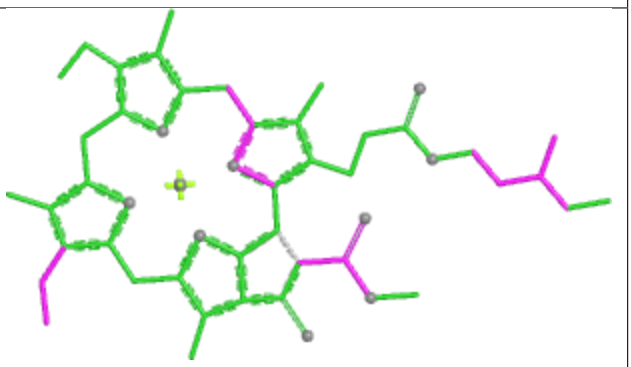


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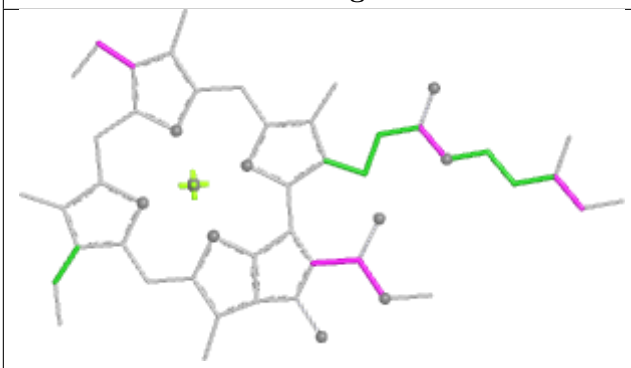
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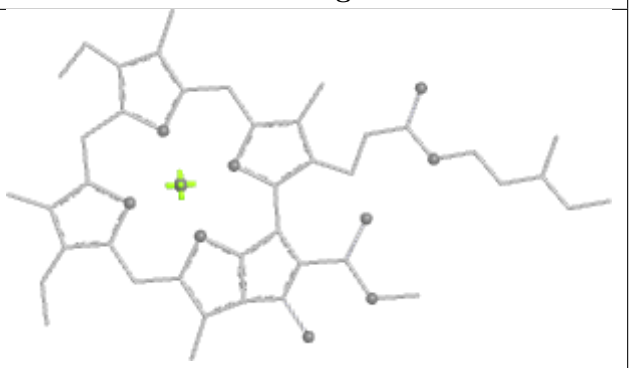
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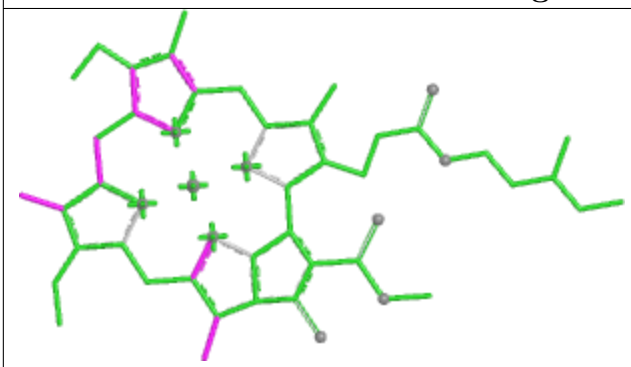


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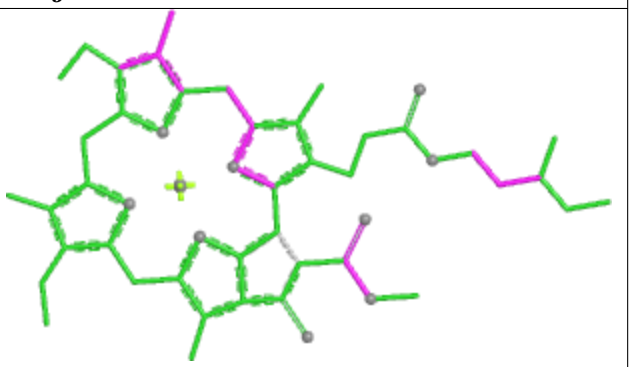


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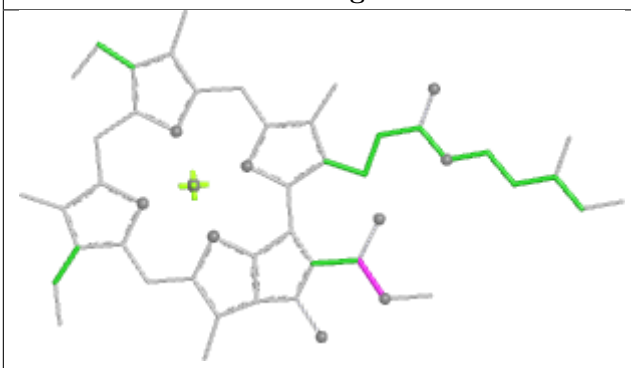
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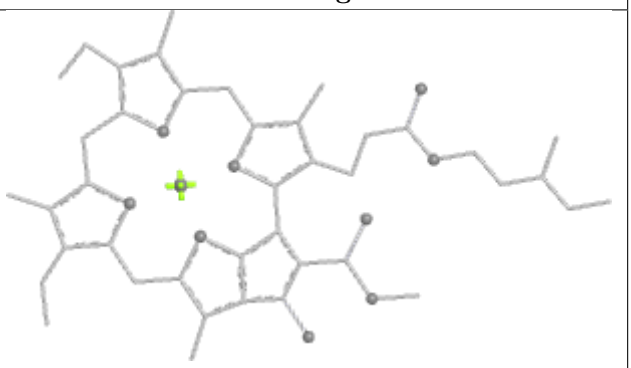
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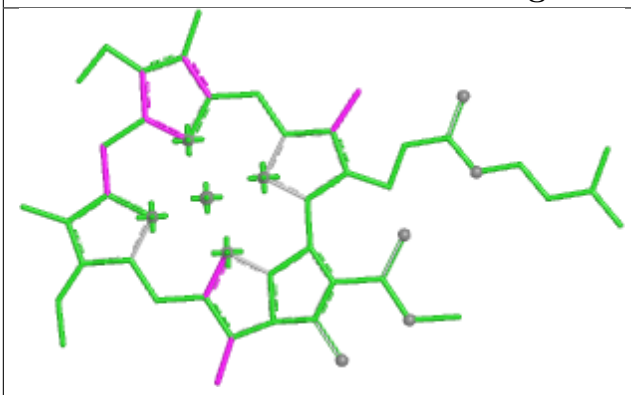


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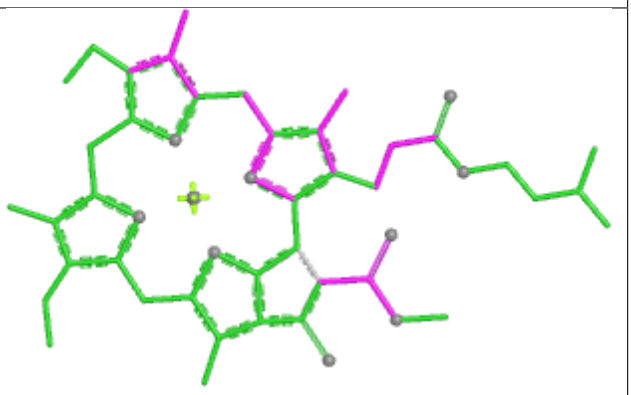


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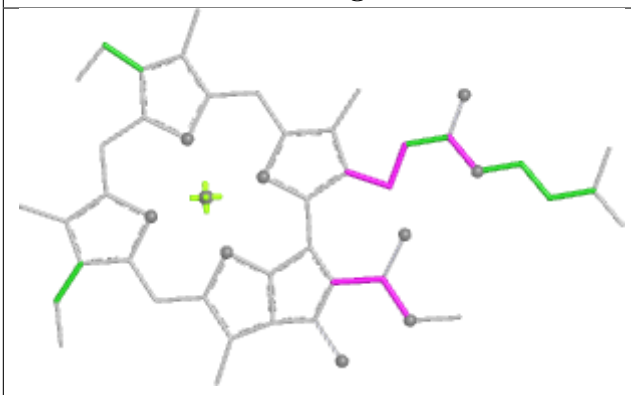
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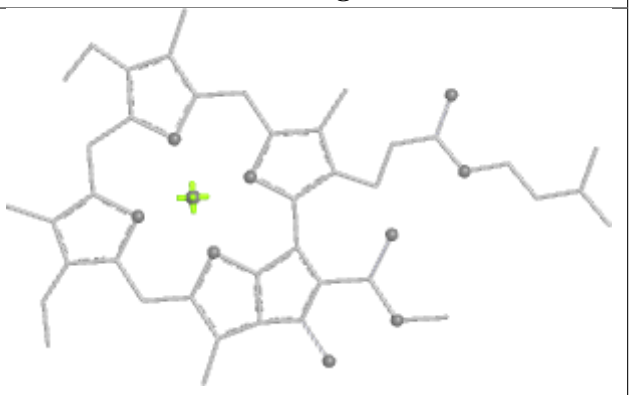
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Bond angles

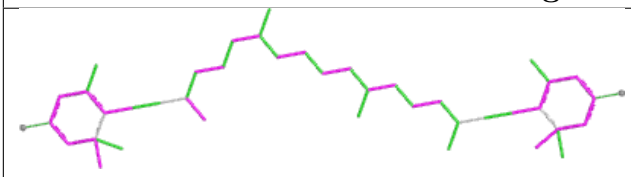


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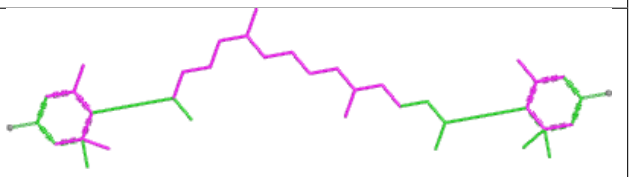


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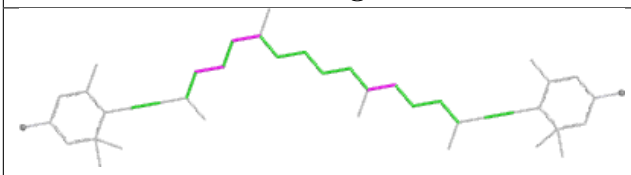
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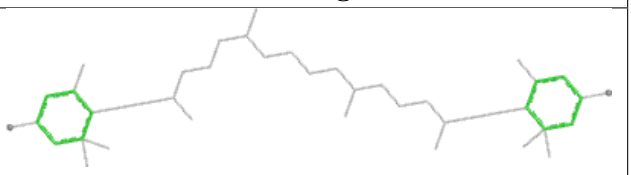
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Bond angles

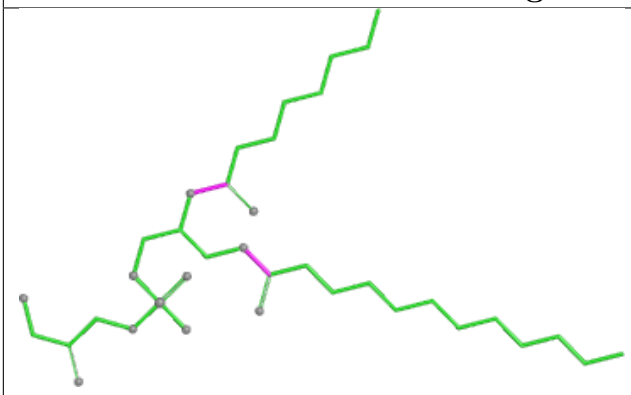


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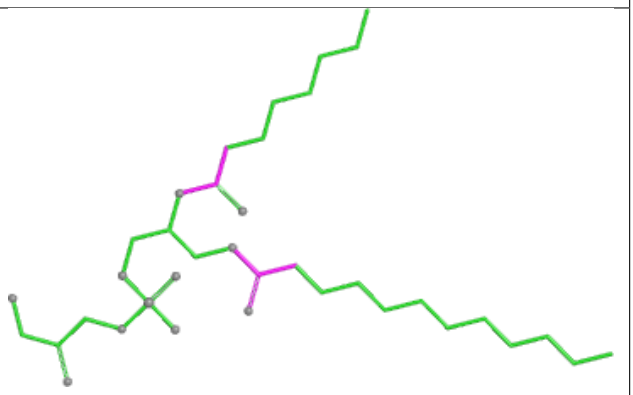


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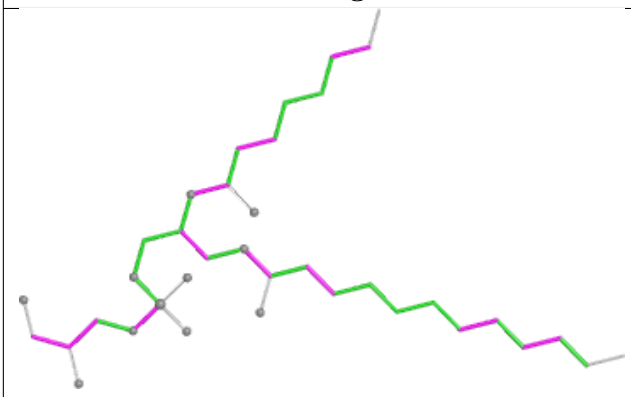
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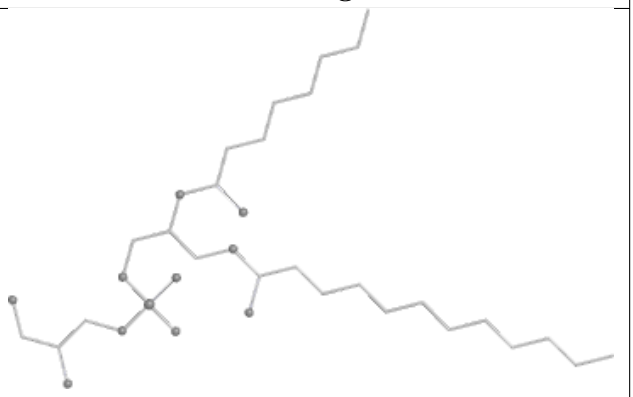
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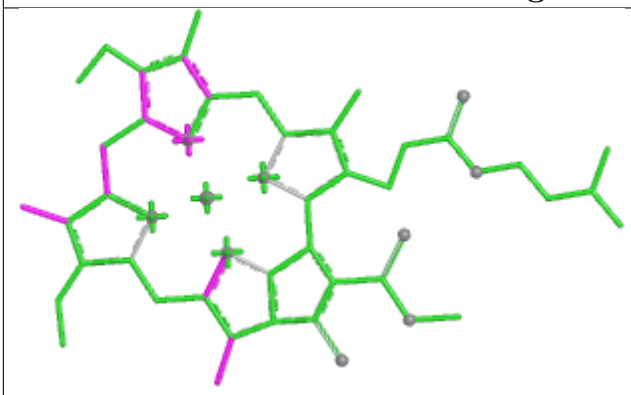


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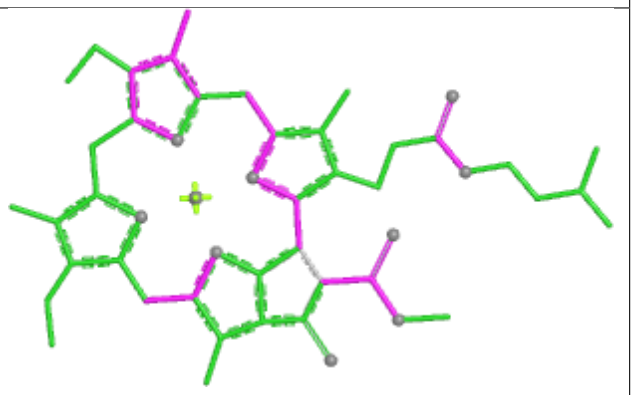


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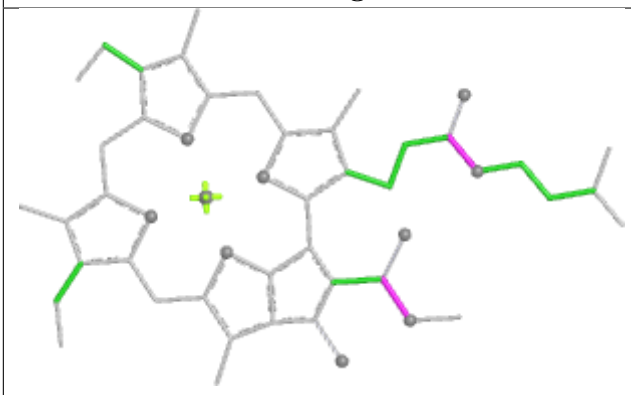
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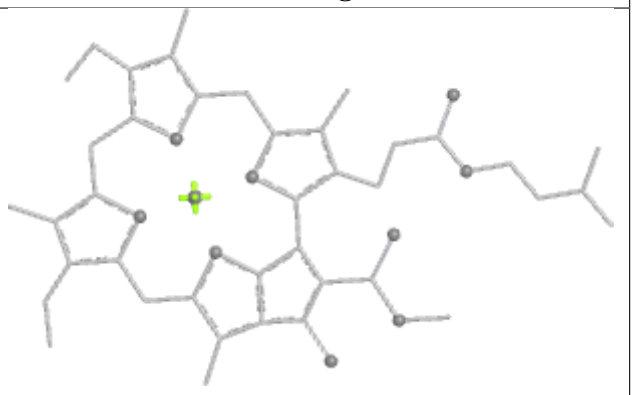
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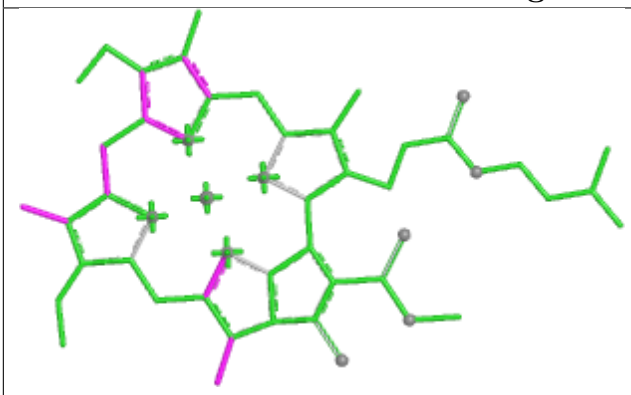


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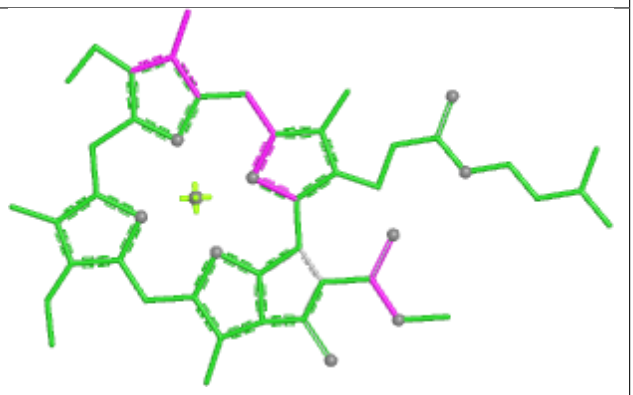


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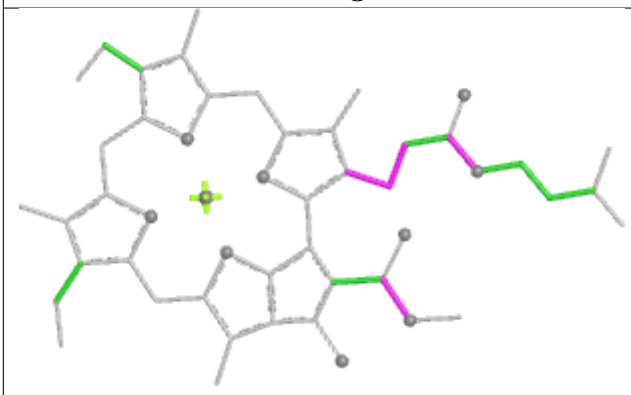
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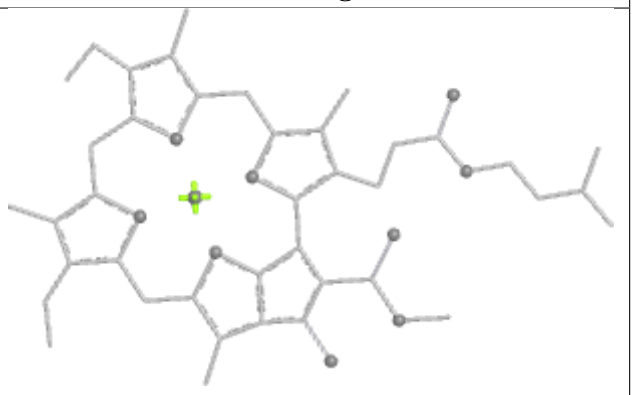
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Bond angles

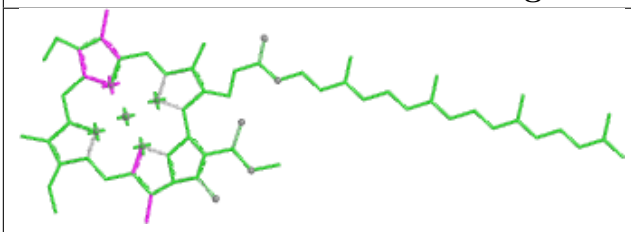


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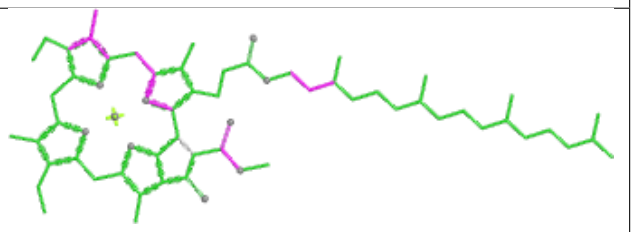


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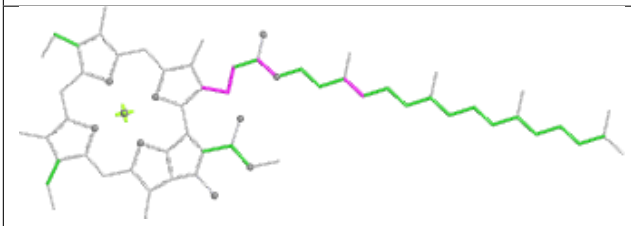
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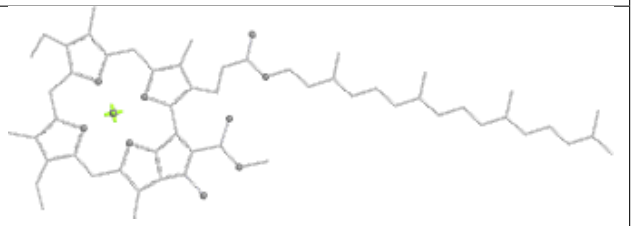
Bond lengths



Bond angles

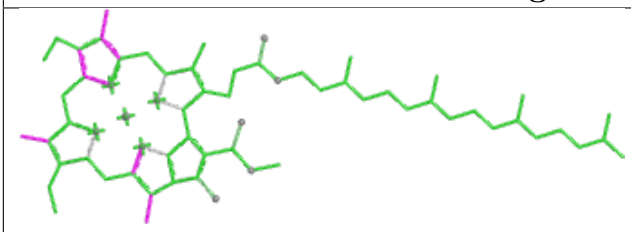


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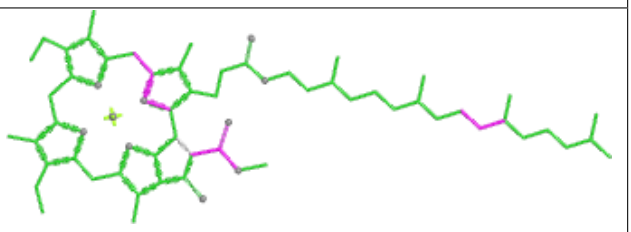


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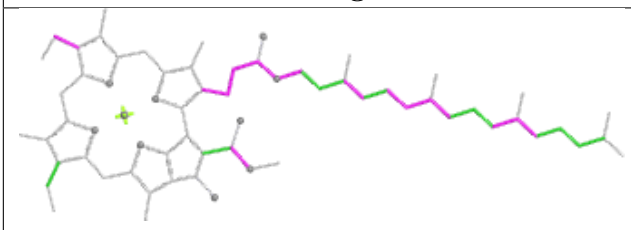
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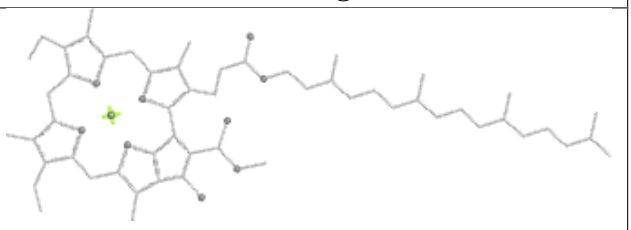
Bond lengths



Bond angles

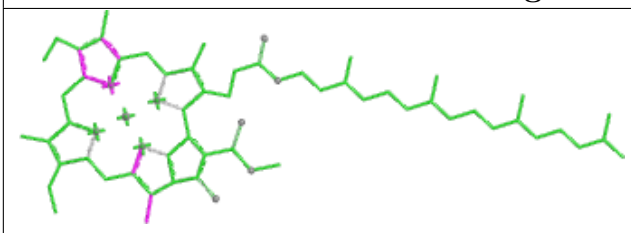


Torsions

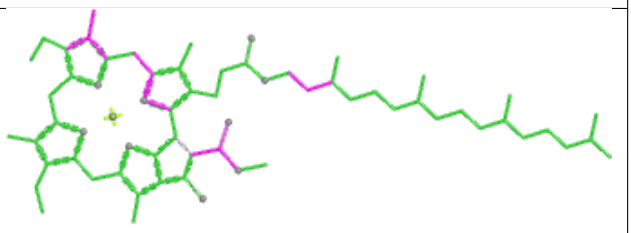


Rings

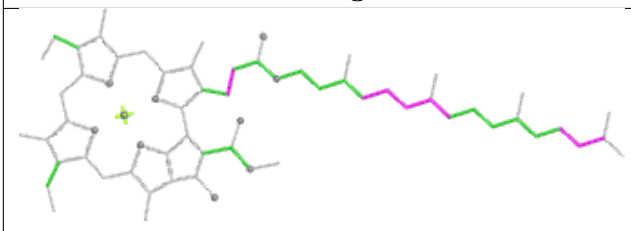
Ligand CLA B 806



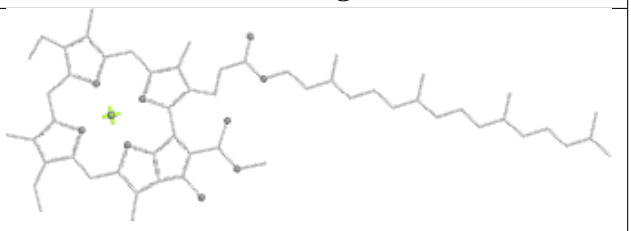
Bond lengths



Bond angles

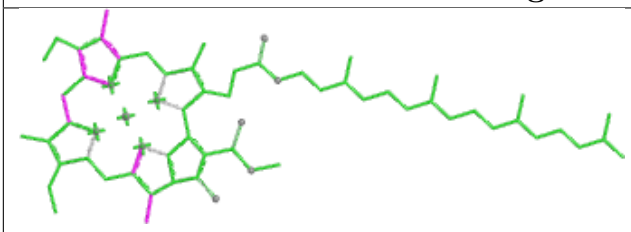


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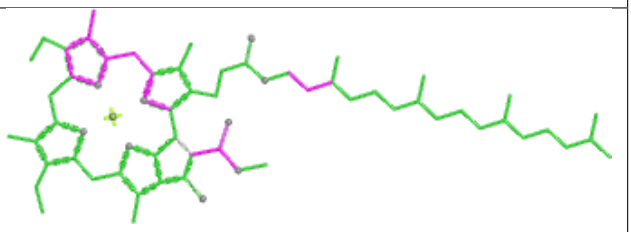


Rings

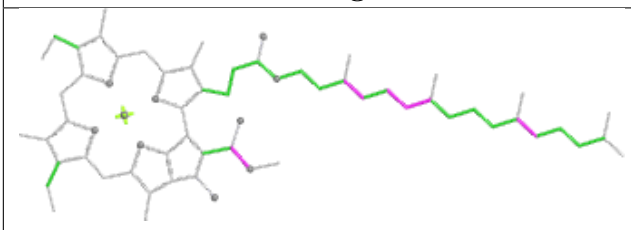
Ligand CLA h 313



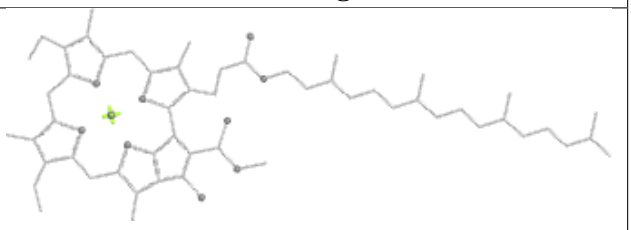
Bond lengths



Bond angles

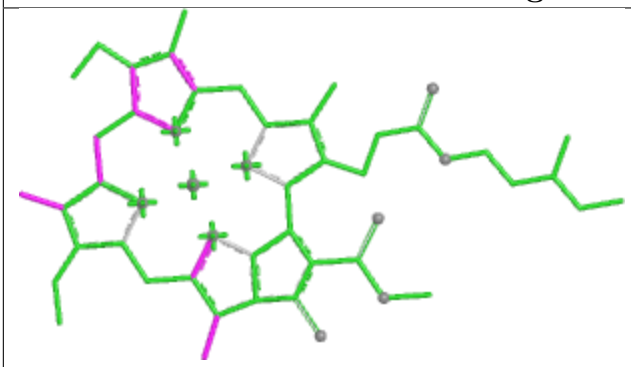


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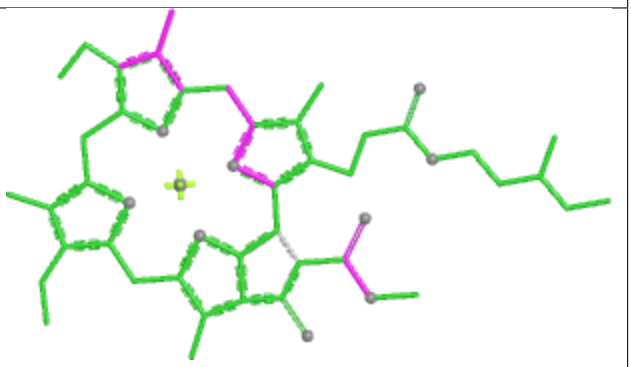


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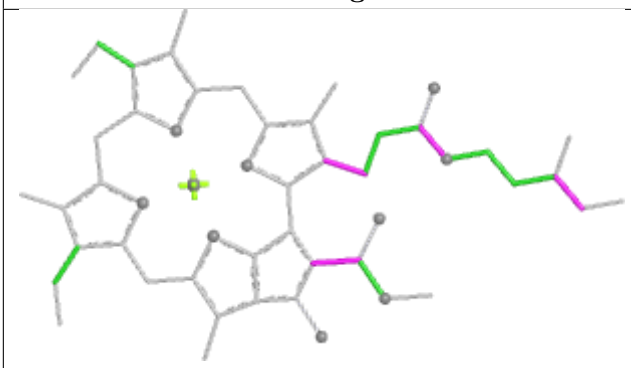
Ligand CLA L 207



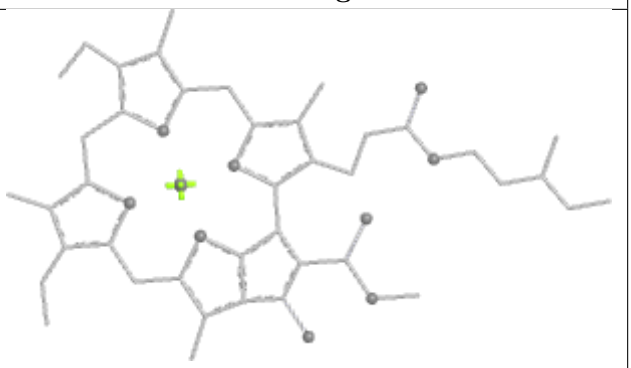
Bond lengths



Bond angles

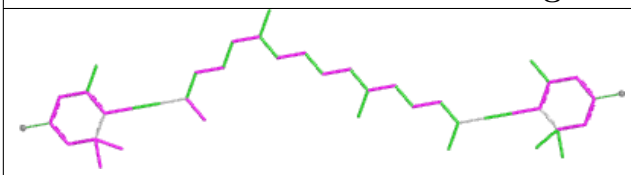


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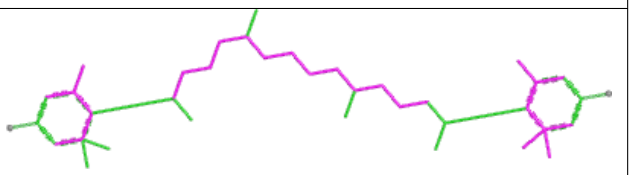


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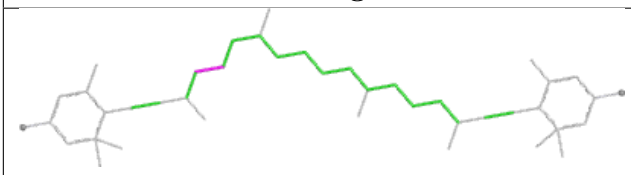
Ligand II0 c 614



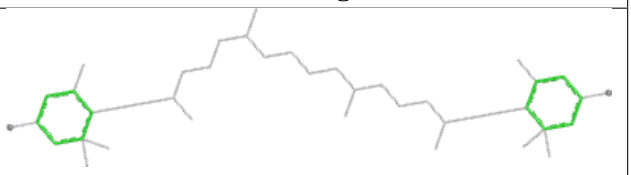
Bond lengths



Bond angles

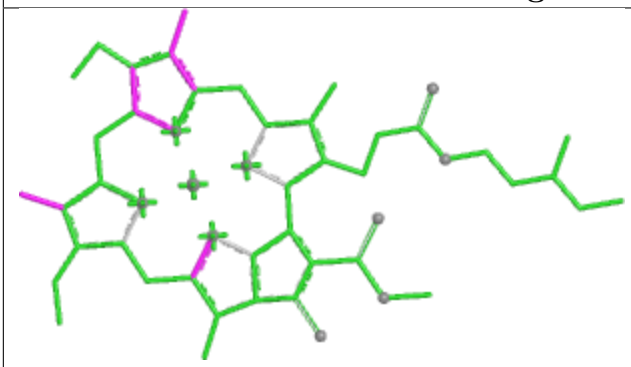


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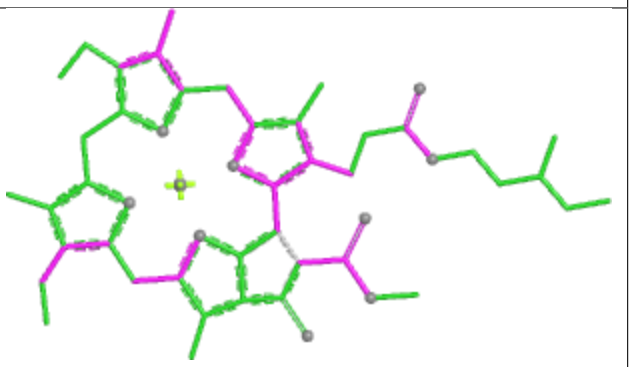


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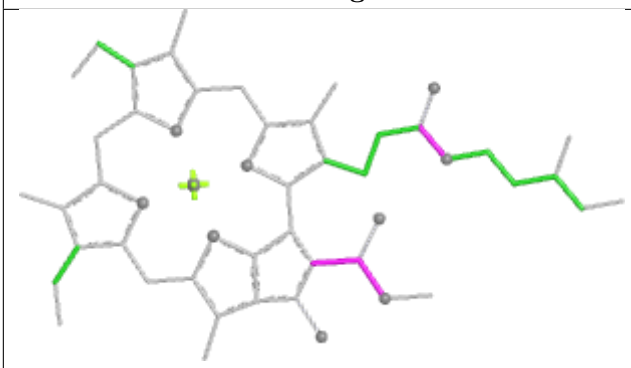
Ligand CLA d 312



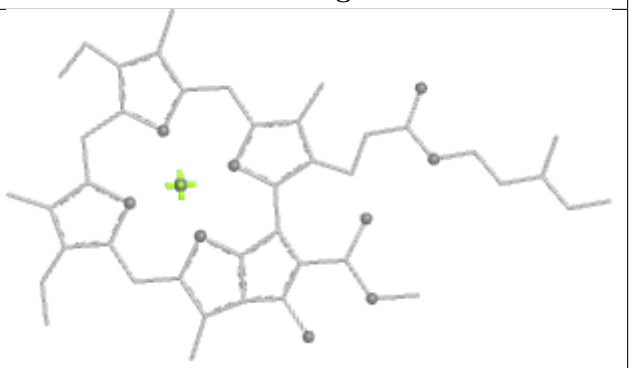
Bond lengths



Bond angles

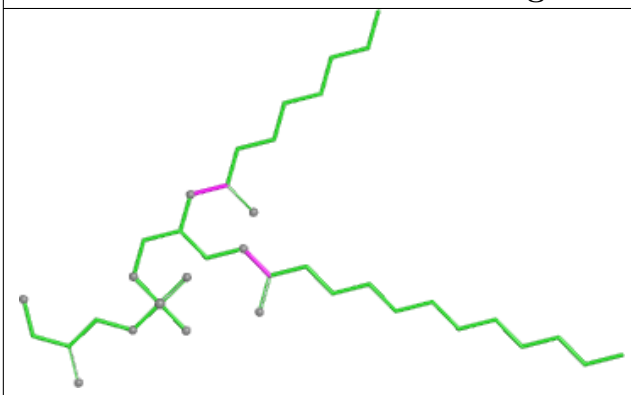


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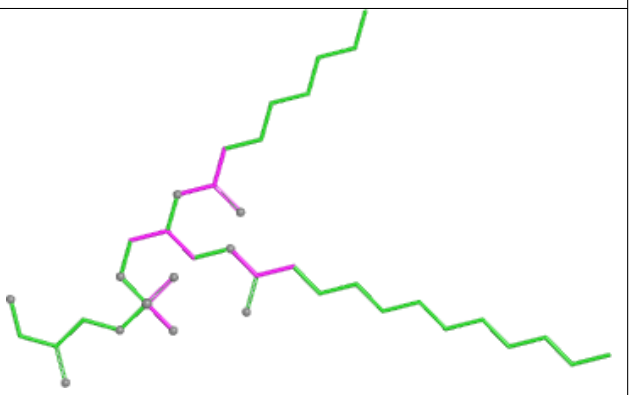


Rings

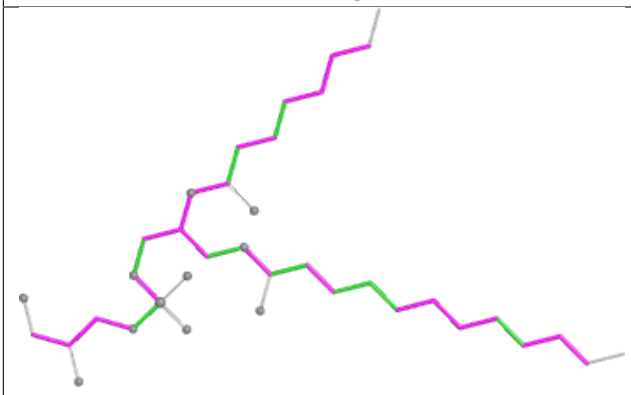
Ligand LHG e 617



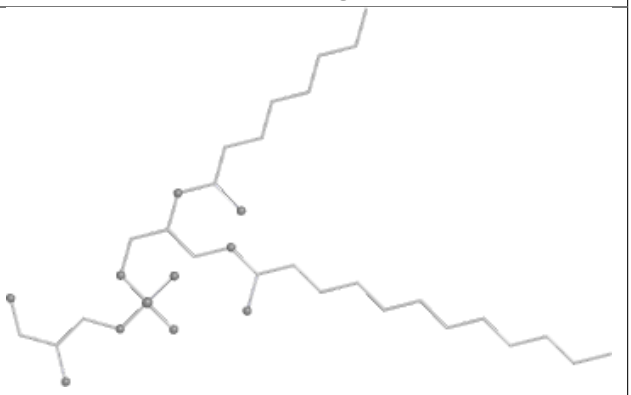
Bond lengths



Bond angles

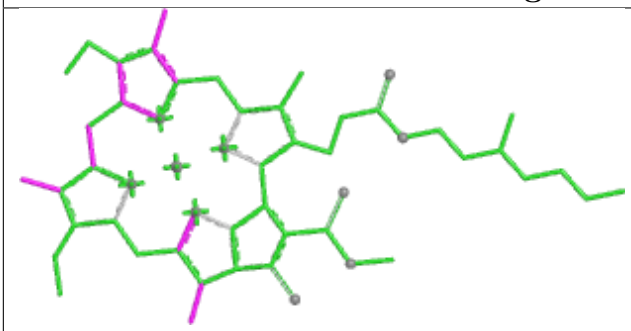


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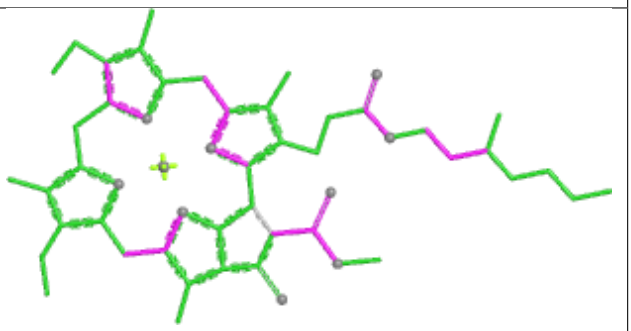


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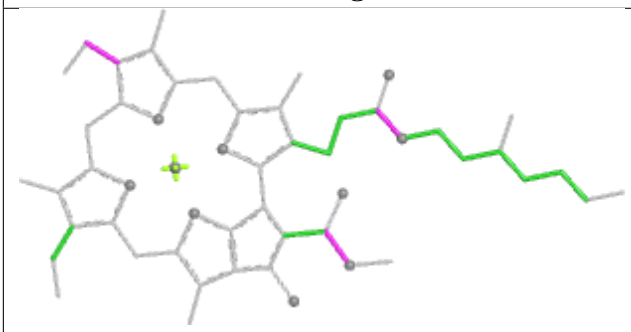
Ligand CLA B 820



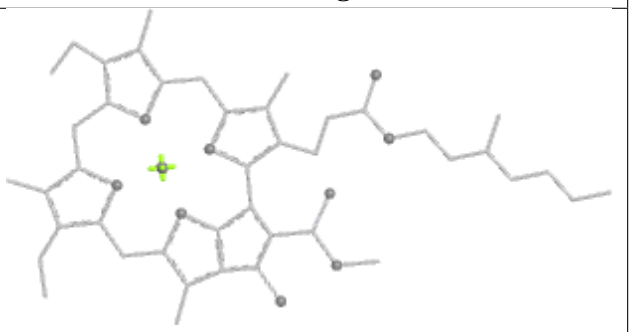
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Bond angles

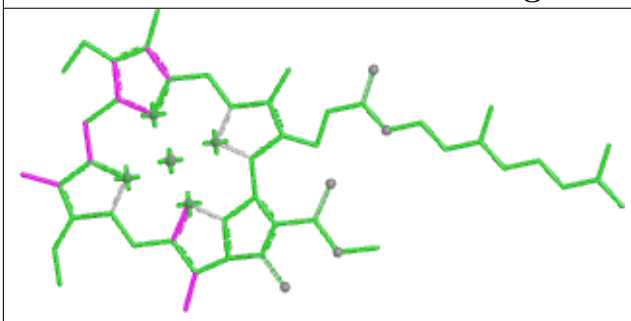


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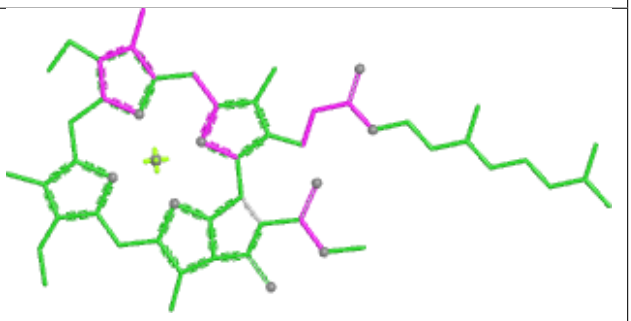


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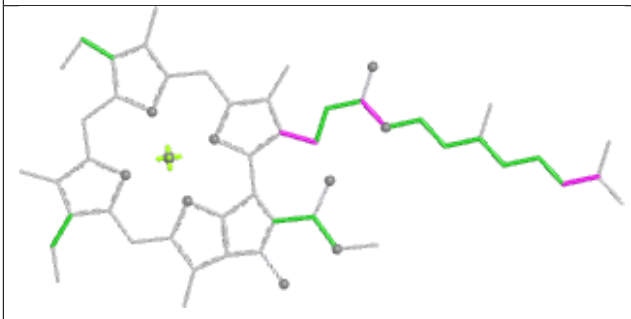
Ligand CLA A 803



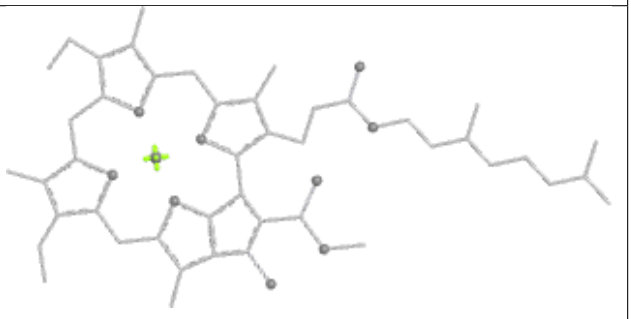
Bond lengths



Bond angles

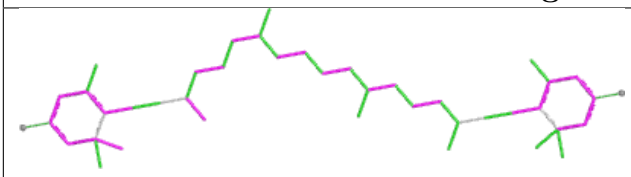


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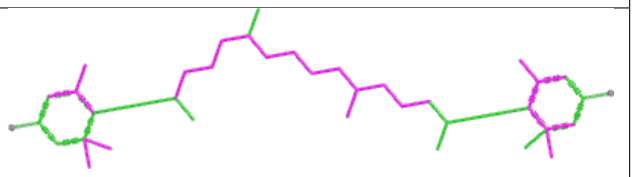


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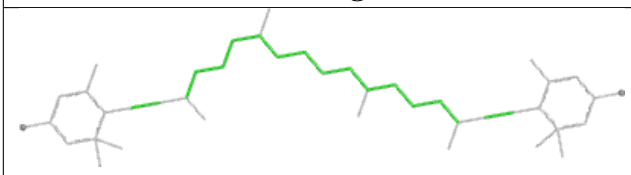
Ligand II0 b 617



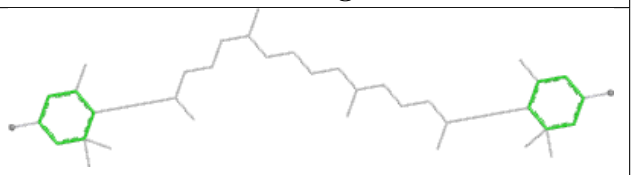
Bond lengths



Bond angles

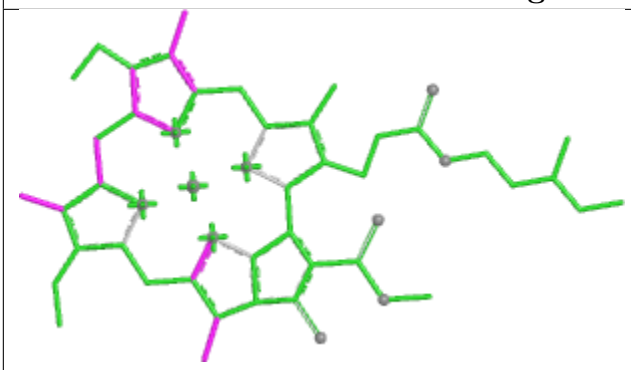


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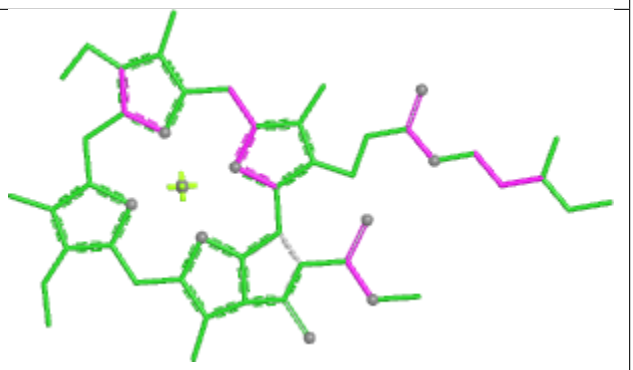


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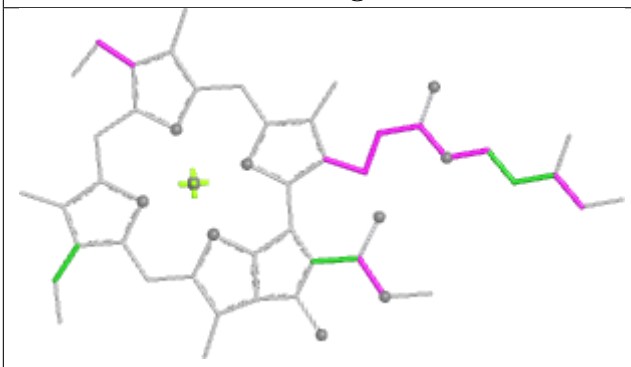
Ligand CLA k 606



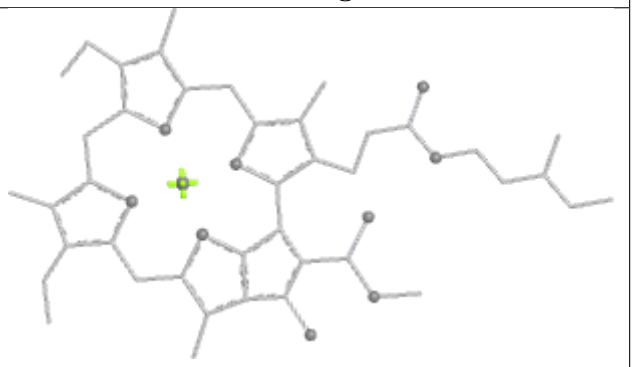
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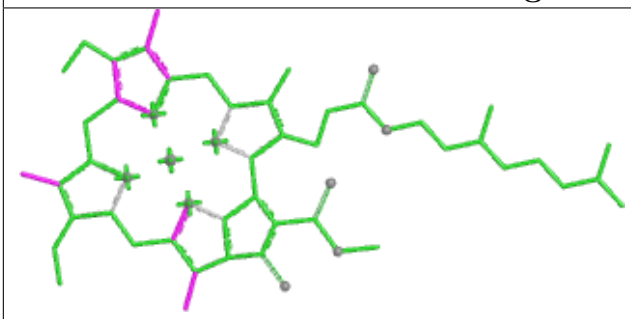
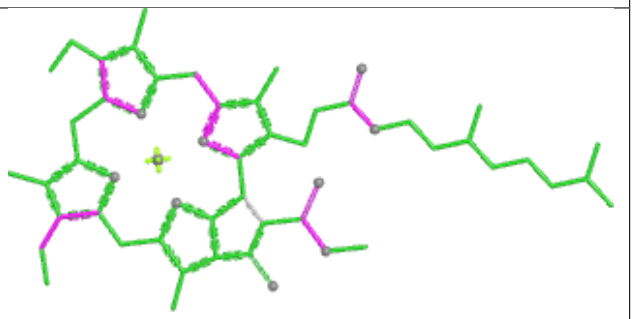
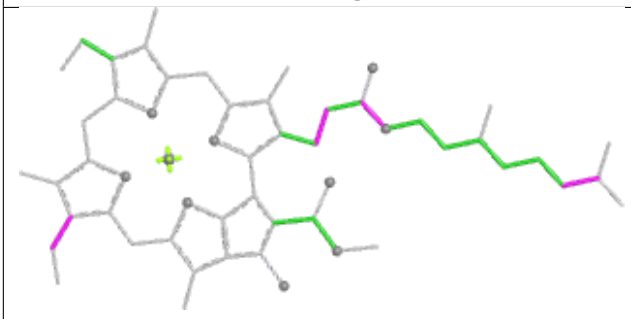
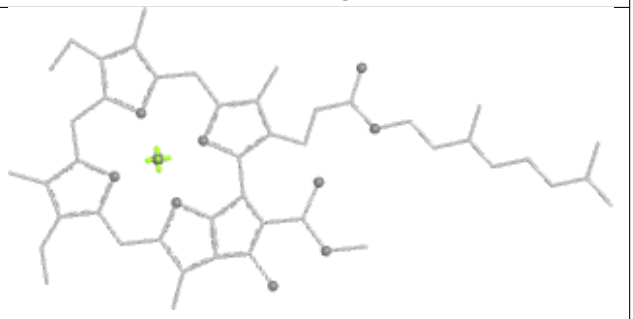
Bond angles



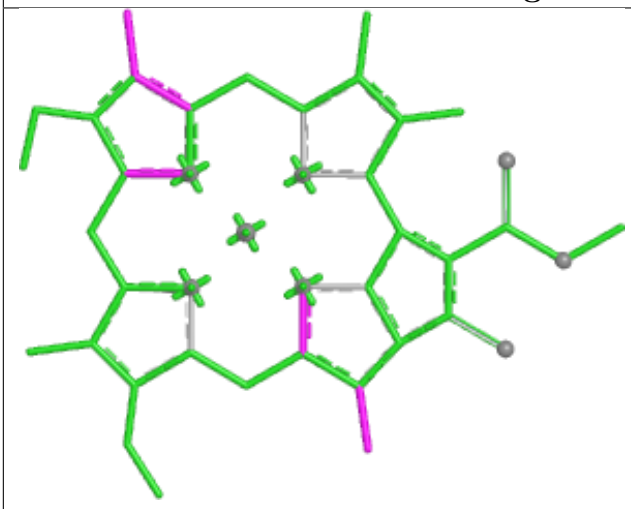
Torsions



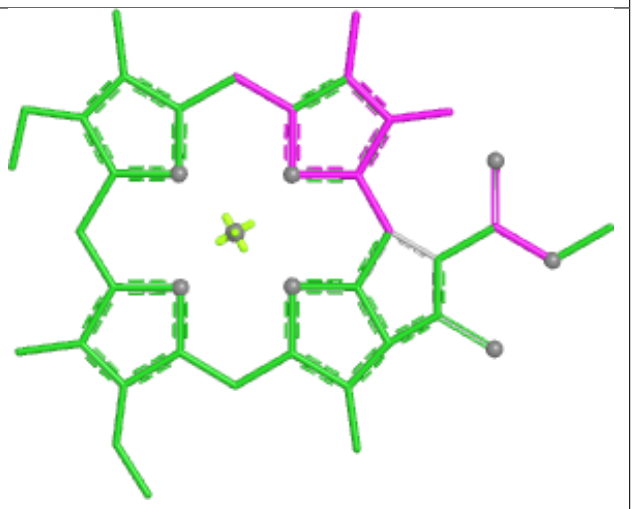
Rings

Ligand CLA B 810	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

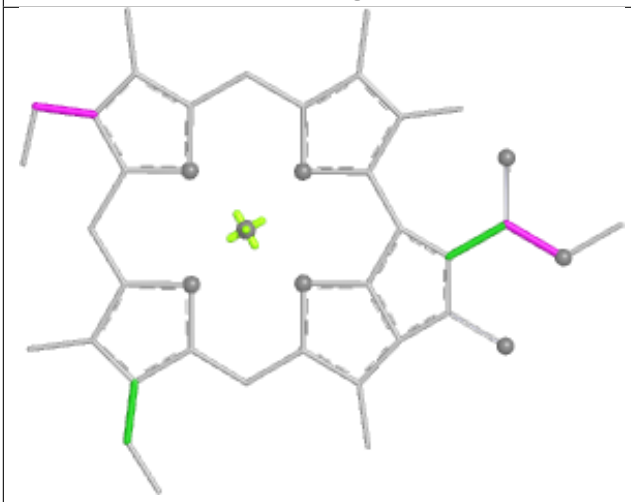
Ligand CLA A 855



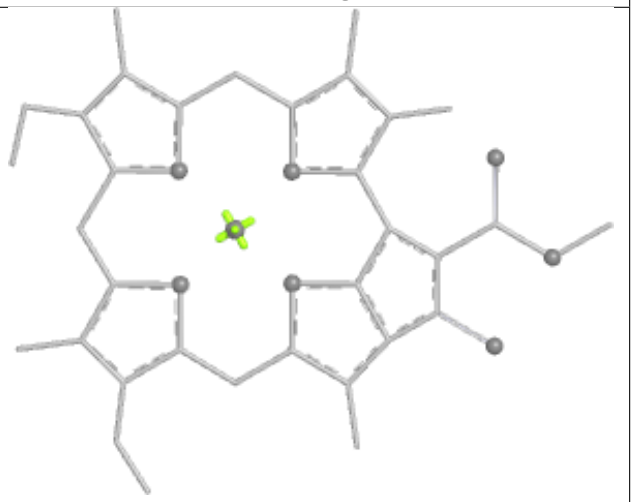
Bond lengths



Bond angles

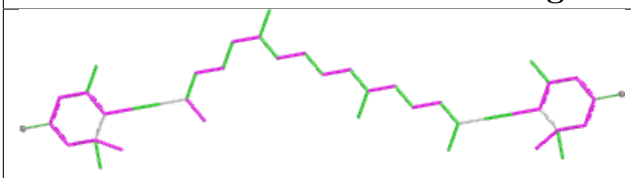


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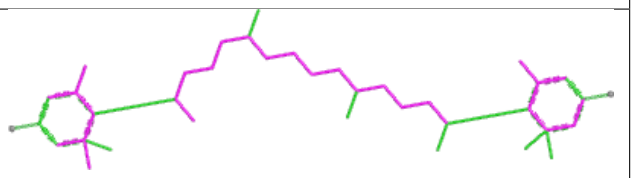


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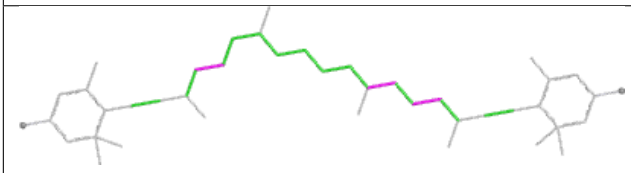
Ligand II0 l 314



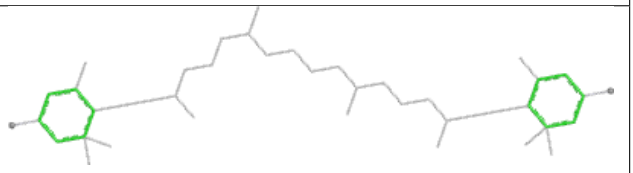
Bond lengths



Bond angles

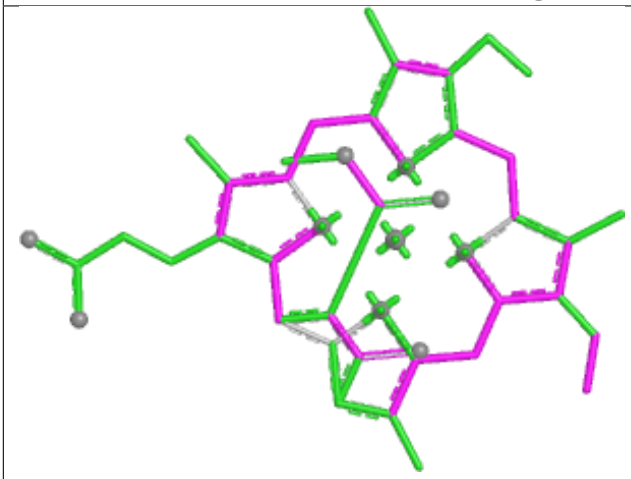


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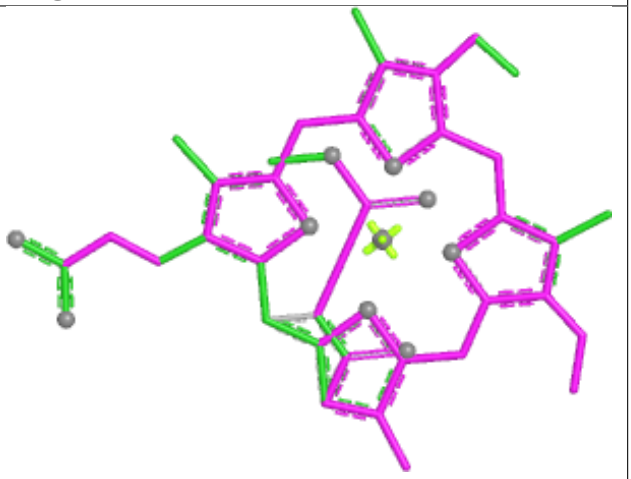


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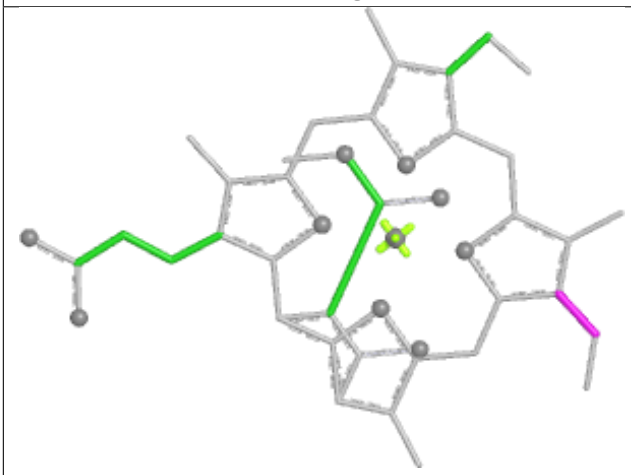
Ligand KC2 g 313



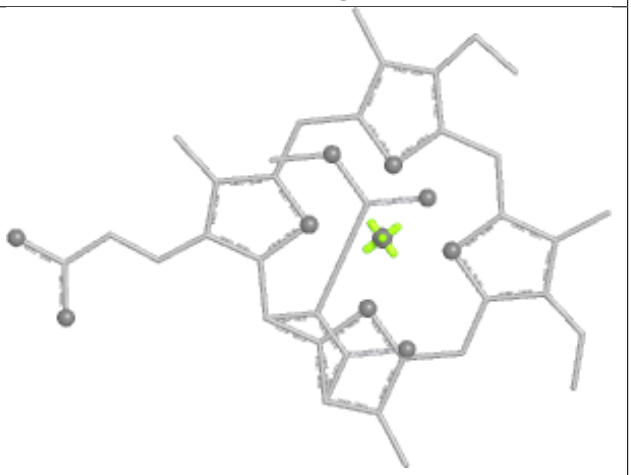
Bond lengths



Bond angles

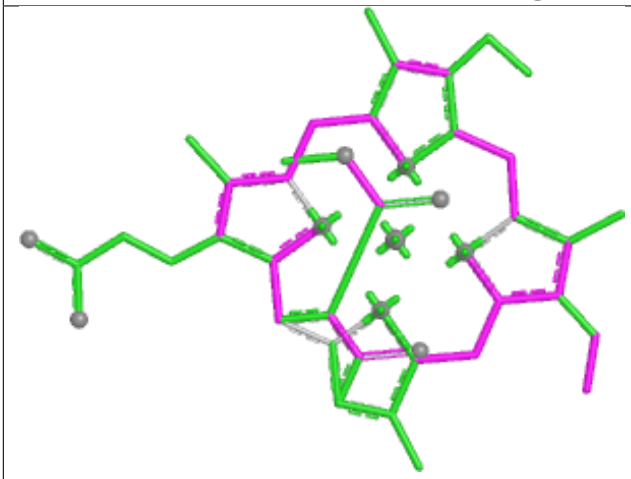


Torsions

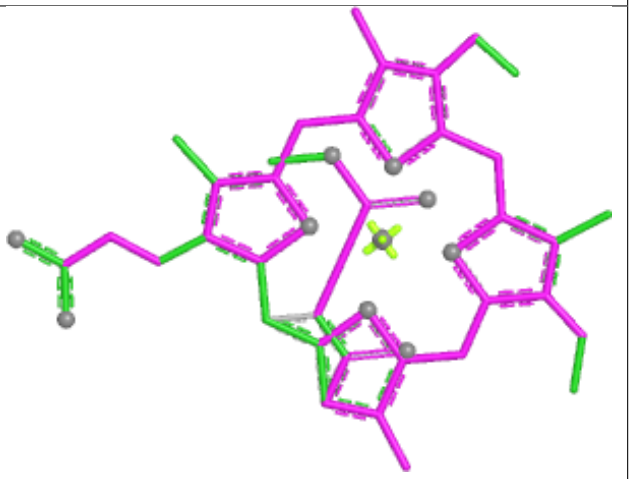


Rings

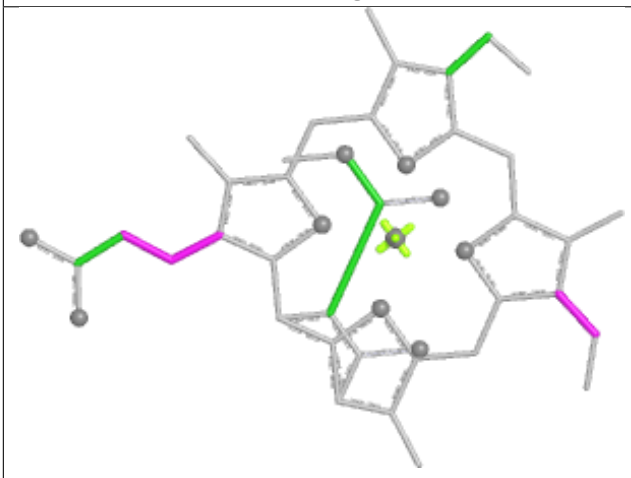
Ligand KC2 d 311



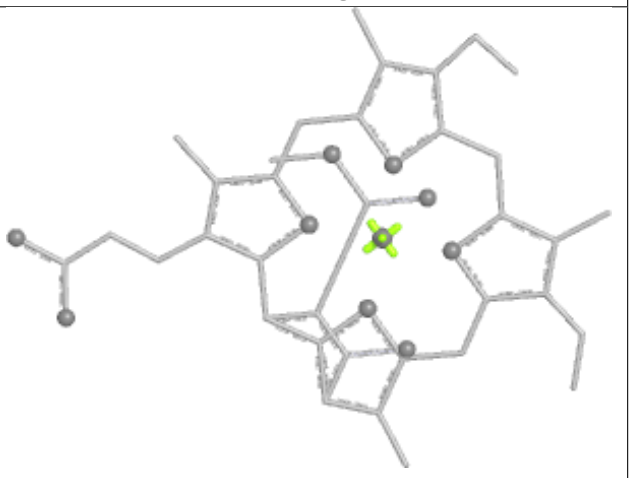
Bond lengths



Bond angles

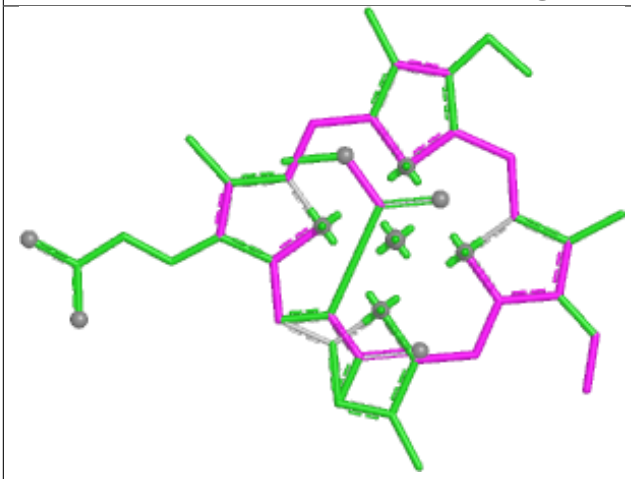


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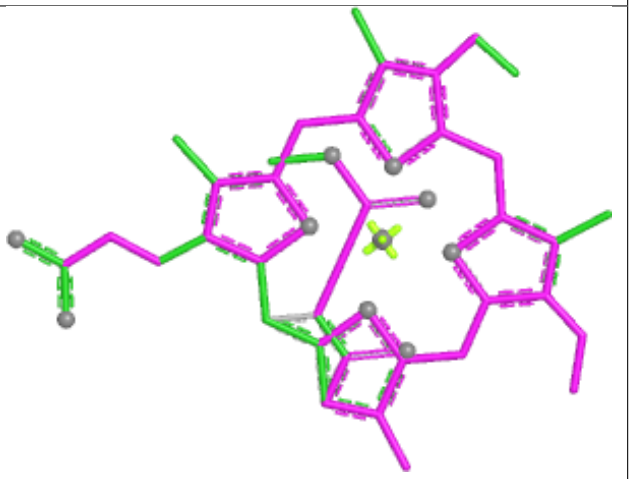


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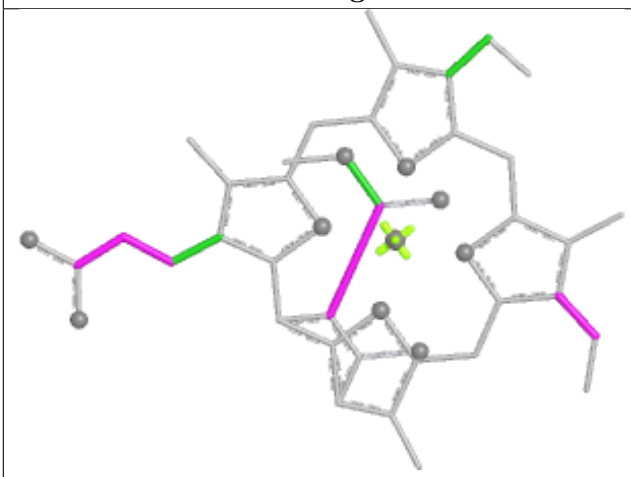
Ligand KC2 f 611



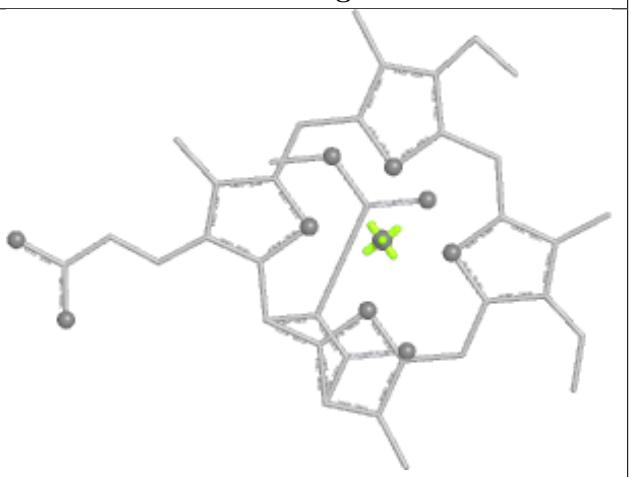
Bond lengths



Bond angles

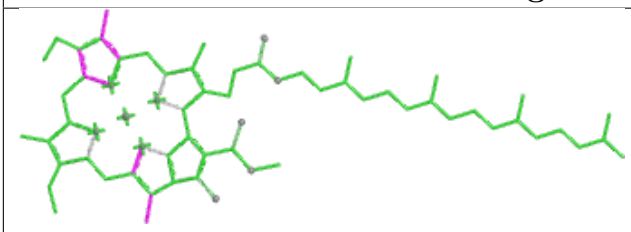


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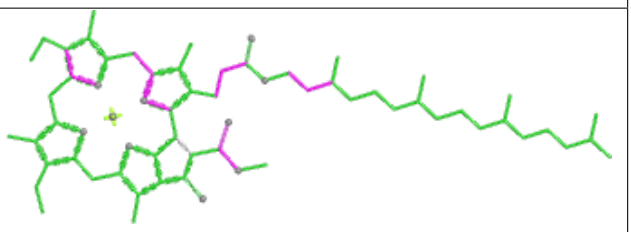


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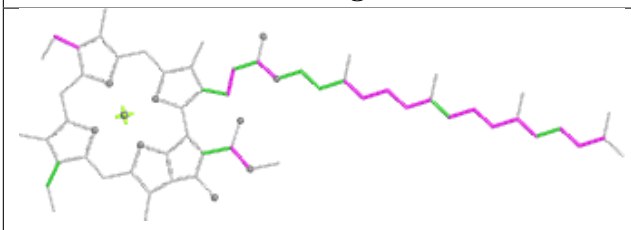
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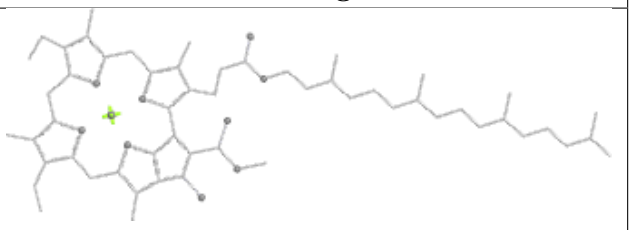
Bond lengths



Bond angles

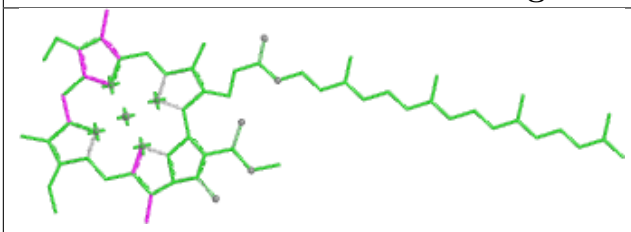


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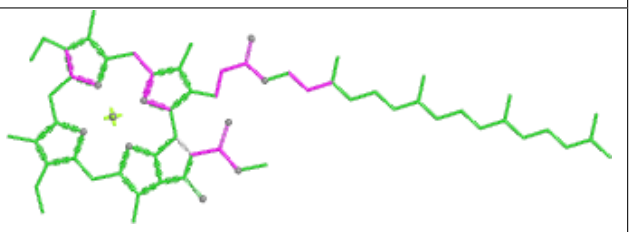


Rings

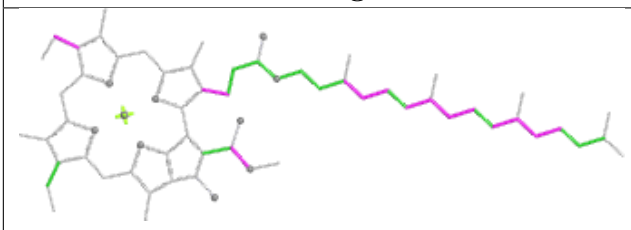
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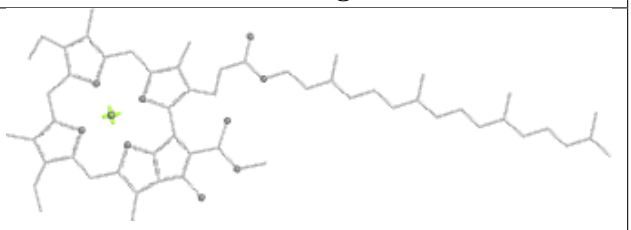
Bond lengths



Bond angles

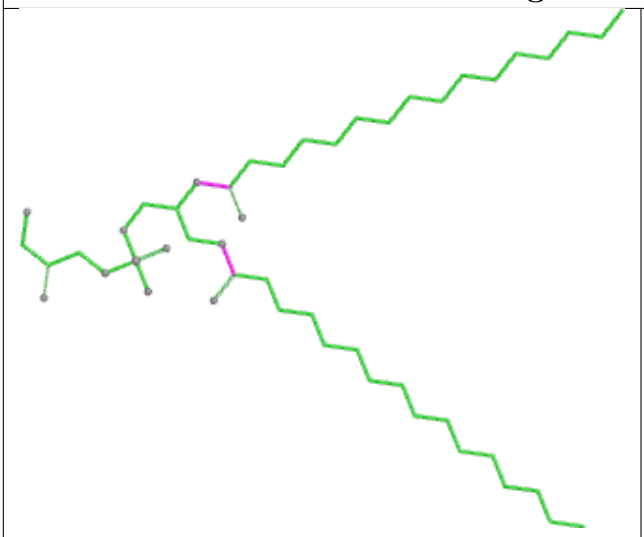


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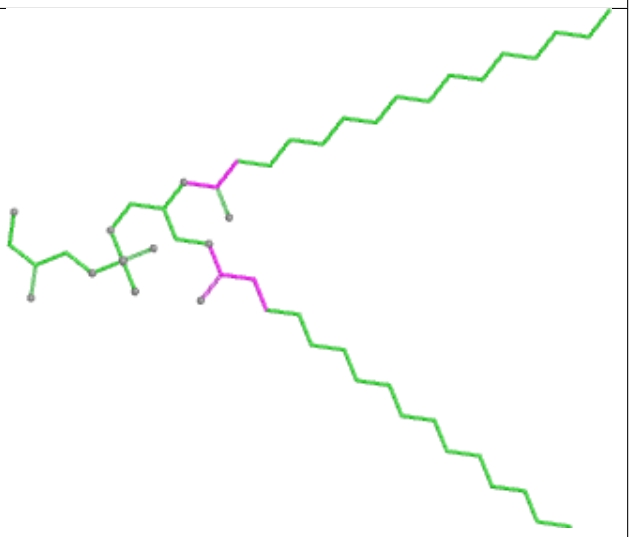


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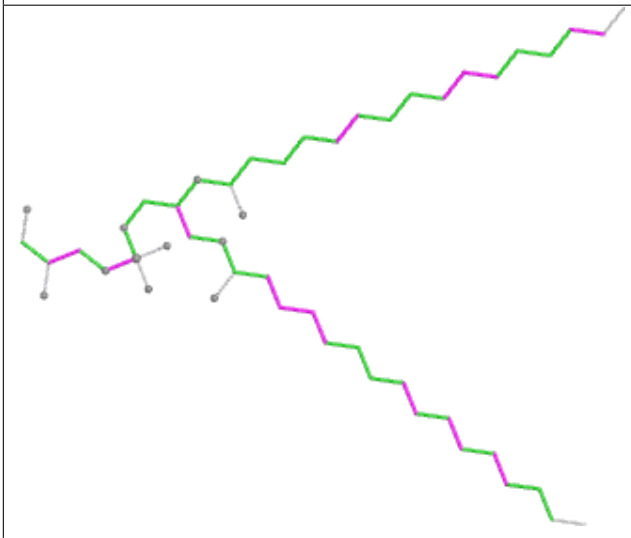
Ligand LHG a 319



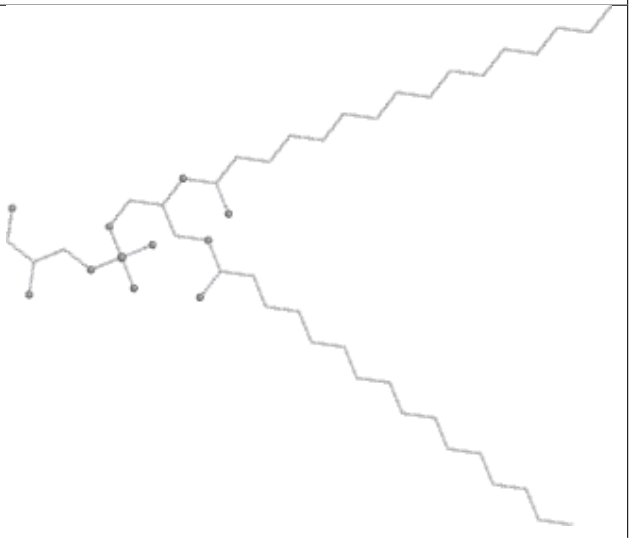
Bond lengths



Bond angles

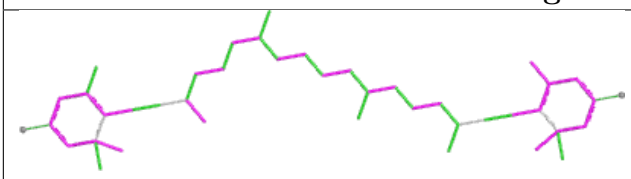


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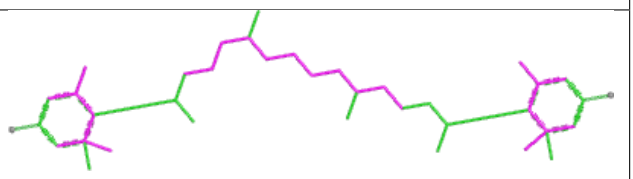


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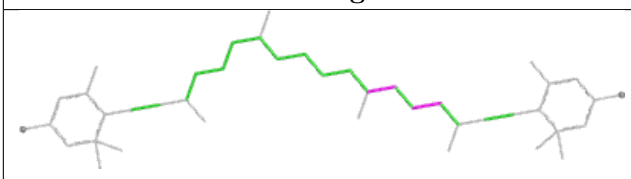
Ligand II0 e 614



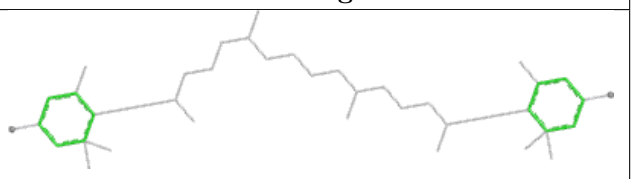
Bond lengths



Bond angles

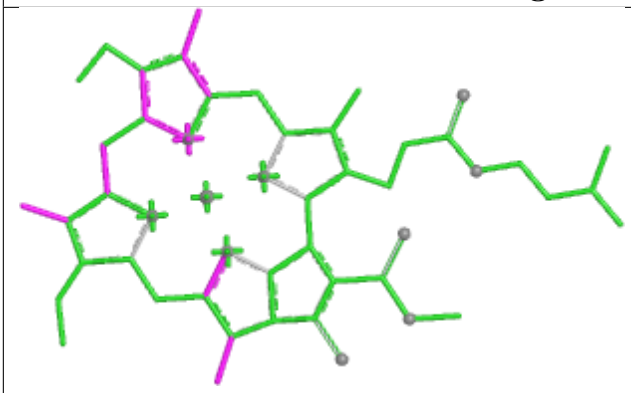


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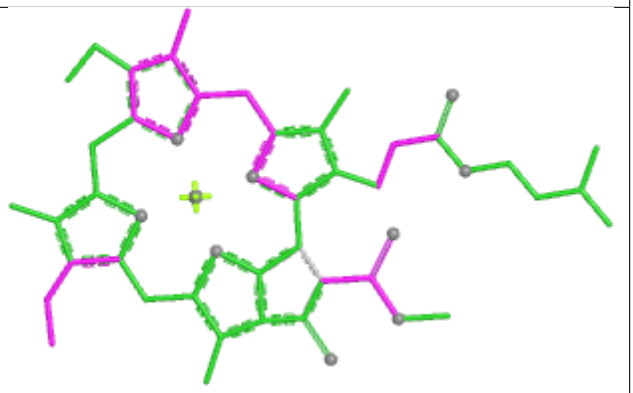


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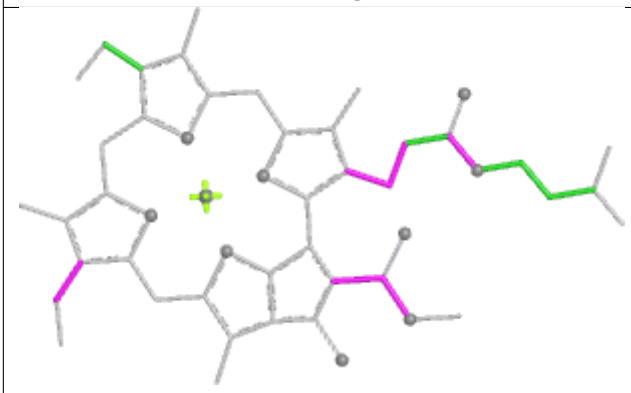
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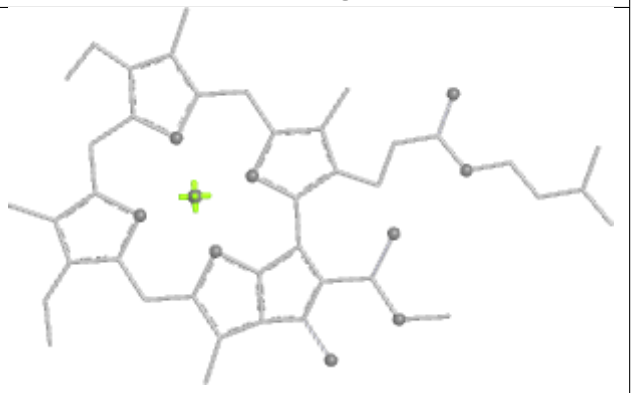
Bond lengths



Bond angles

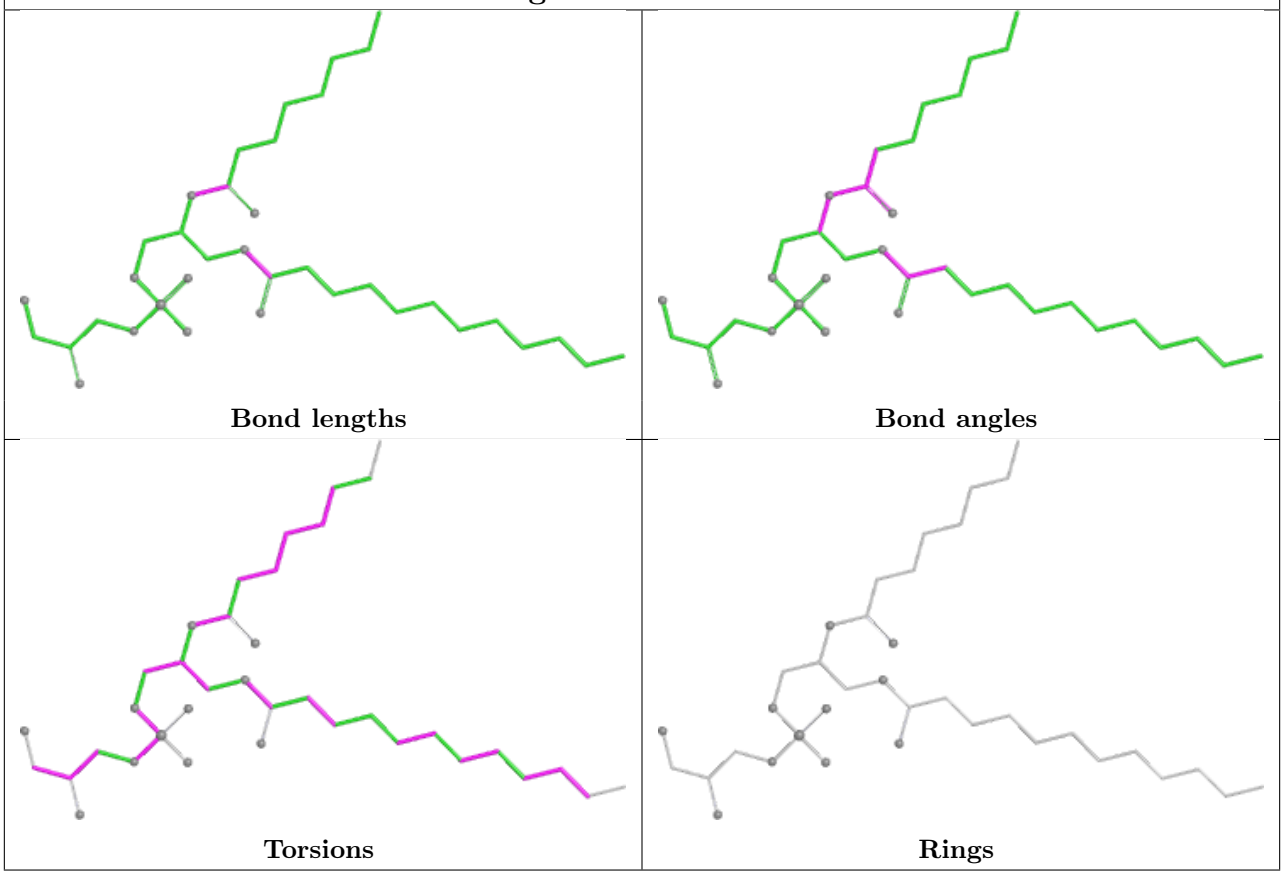


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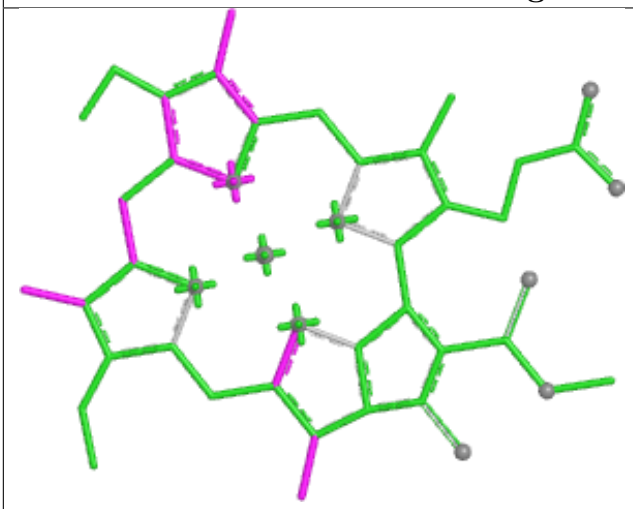


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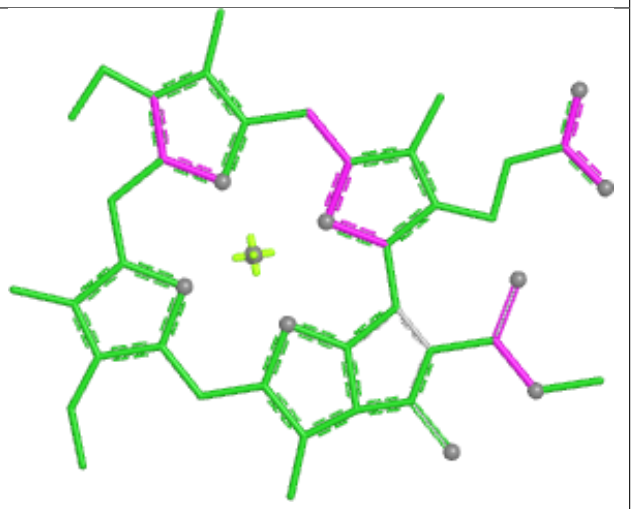
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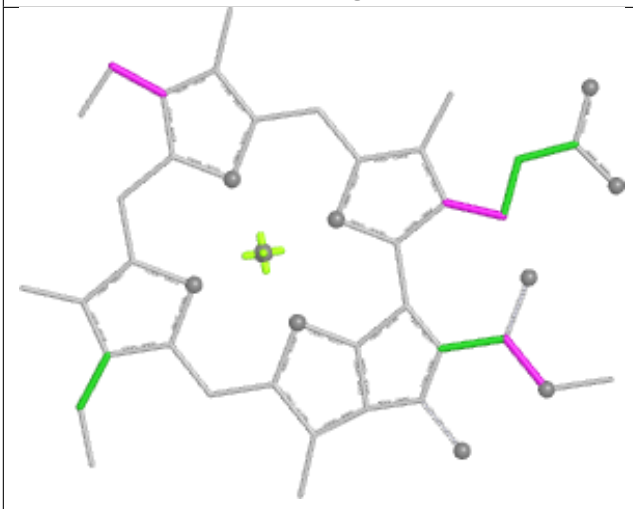
Ligand CLA n 601



Bond lengths



Bond angles

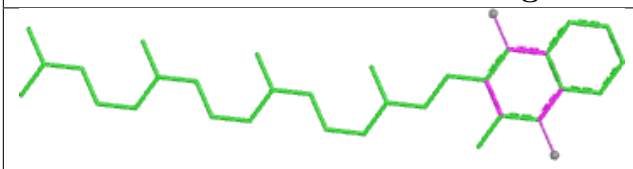


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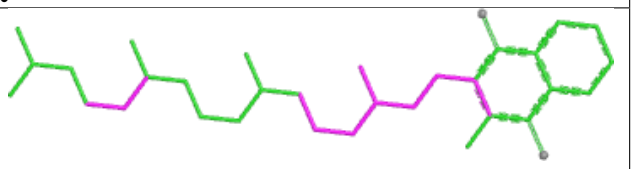


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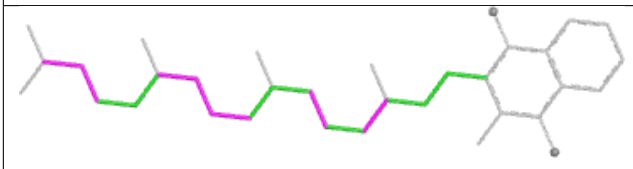
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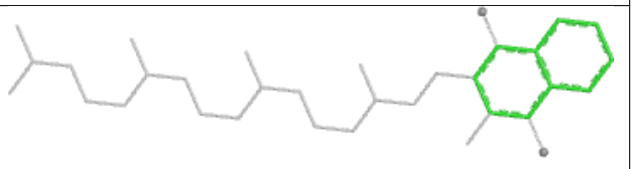
Bond lengths



Bond angles

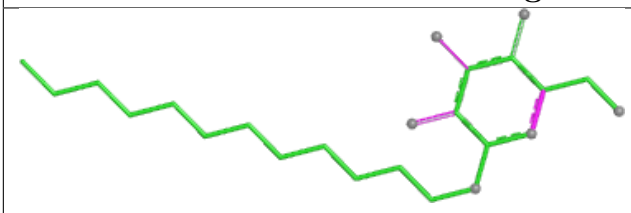


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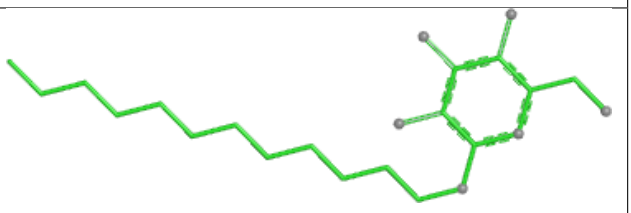


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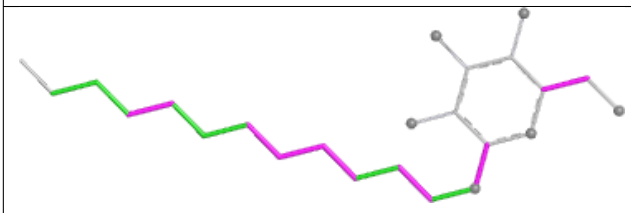
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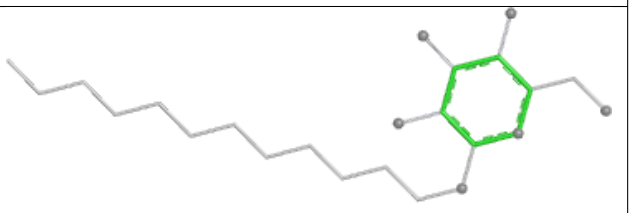
Bond lengths



Bond angles

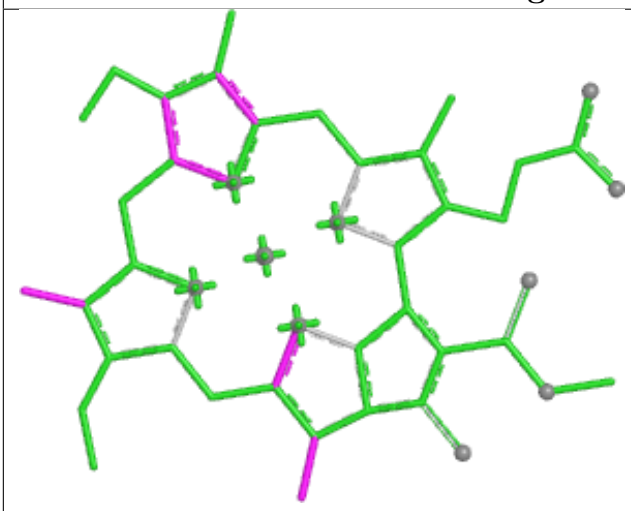


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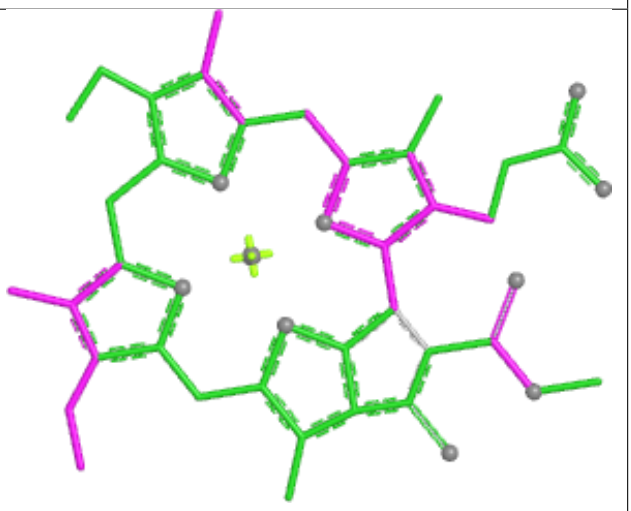


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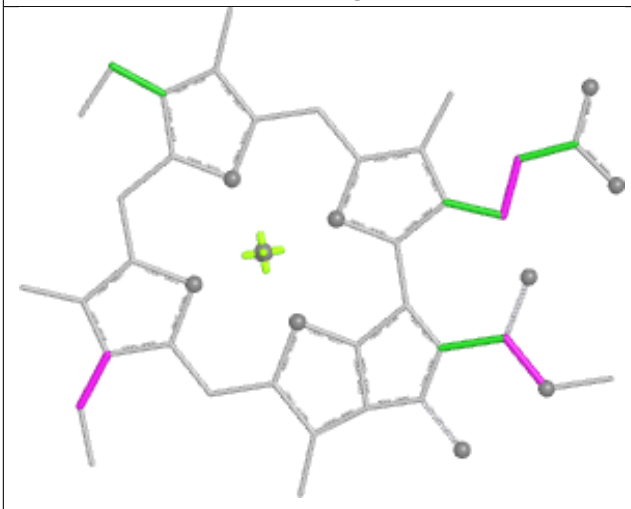
Ligand CLA k 605



Bond lengths



Bond angles

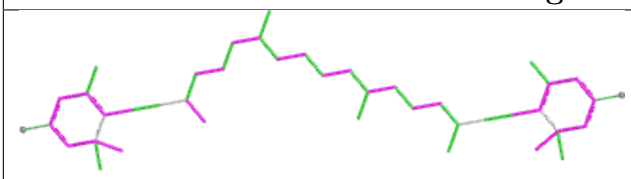


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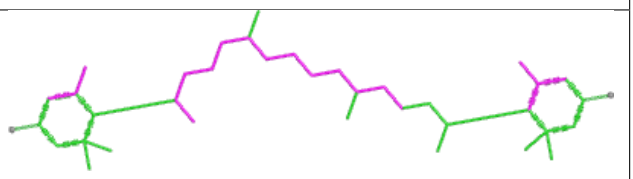


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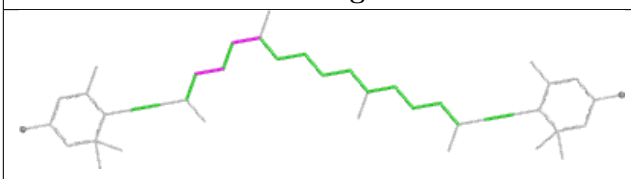
Ligand II0 f 616



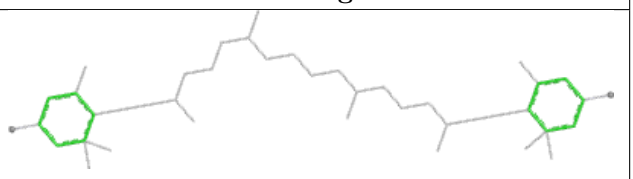
Bond lengths



Bond angles

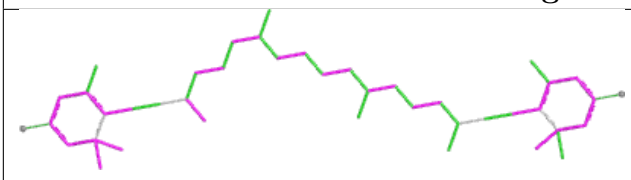


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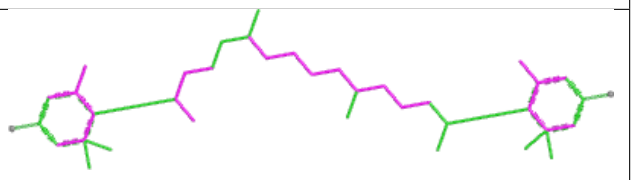


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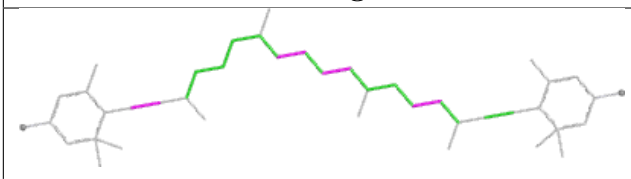
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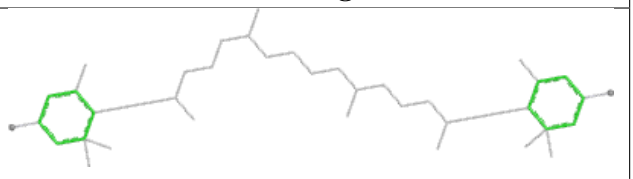
Bond lengths



Bond angles

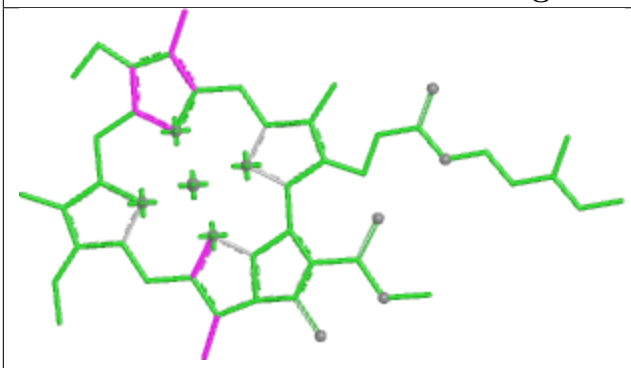


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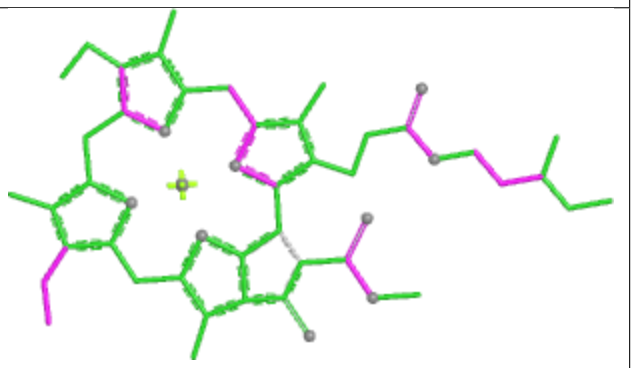


Rings

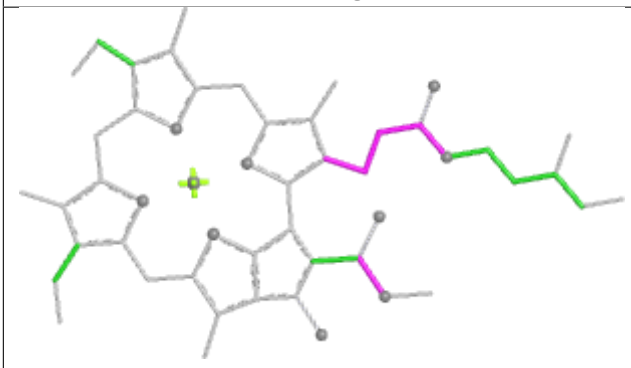
Ligand CLA i 302



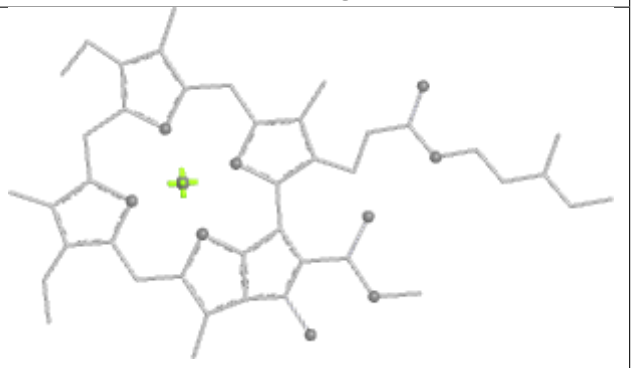
Bond lengths



Bond angles

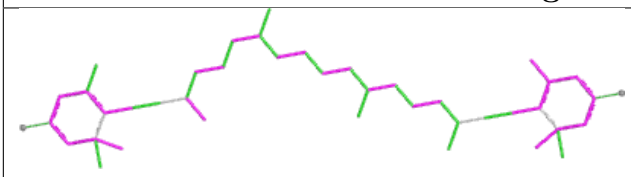


Torsions

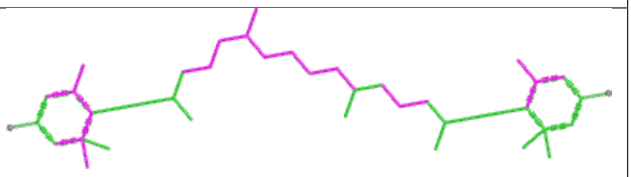


Rings

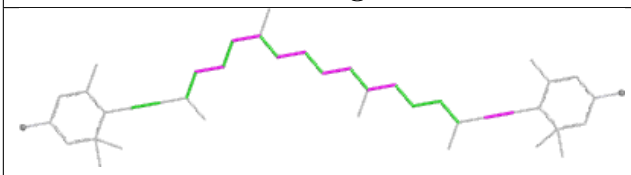
Ligand II0 k 621



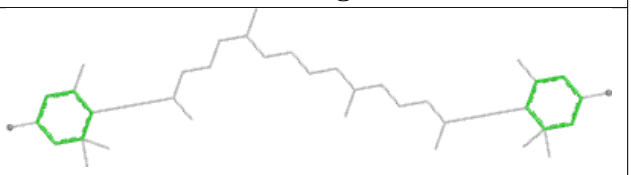
Bond lengths



Bond angles

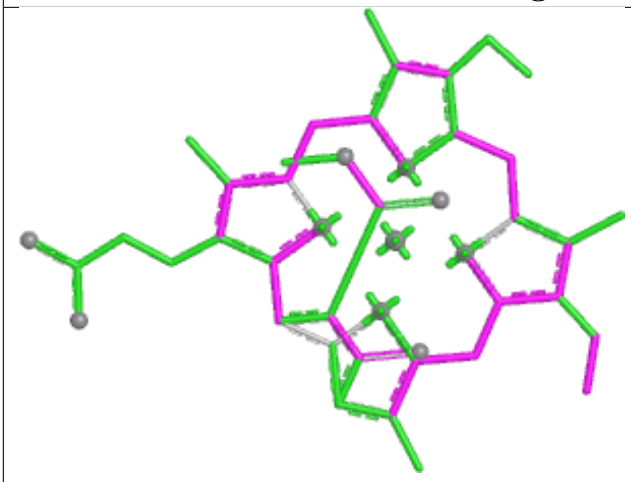


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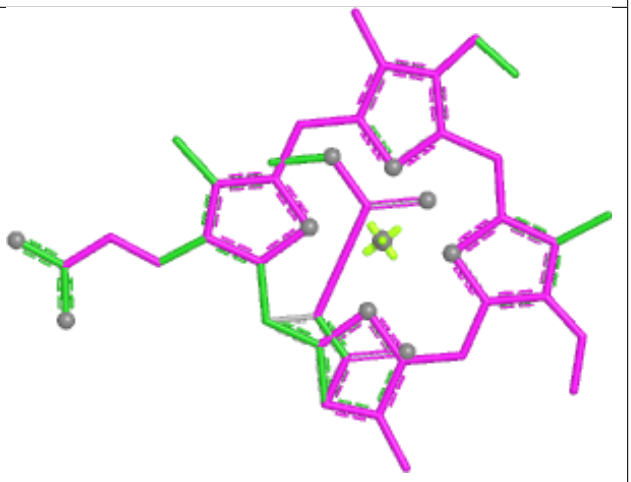


Rings

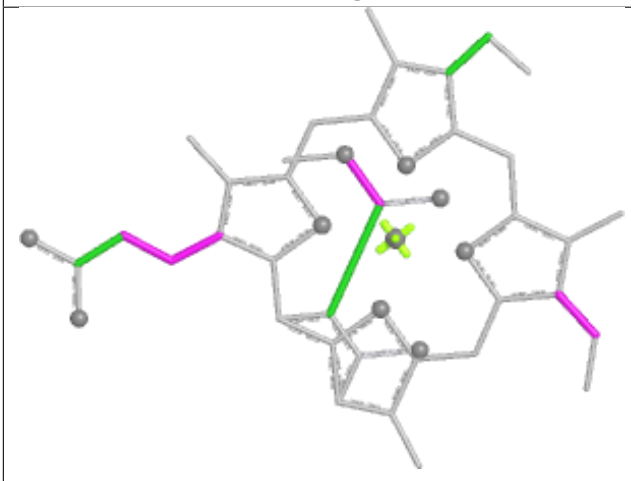
Ligand KC2 k 613



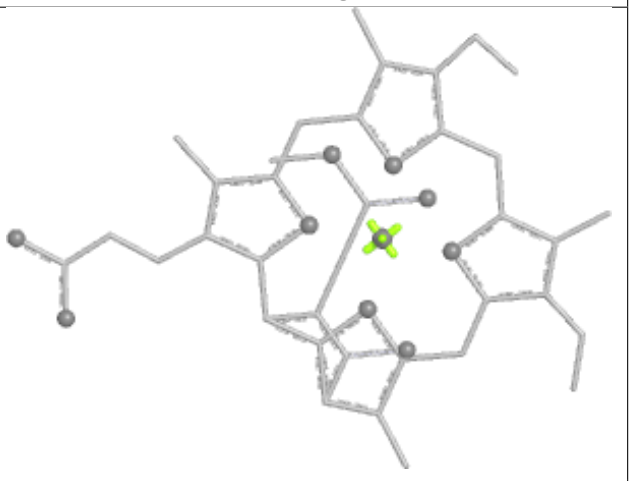
Bond lengths



Bond angles

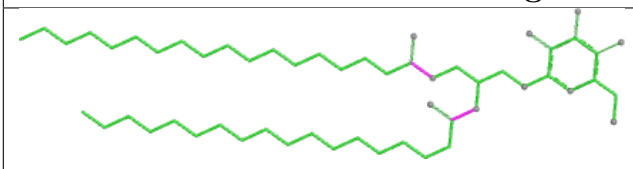


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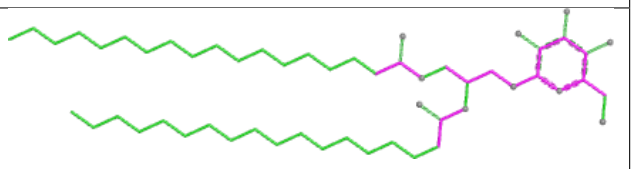


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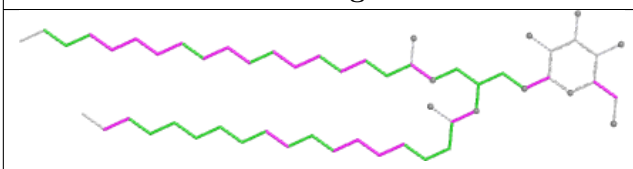
Ligand LMG c 619



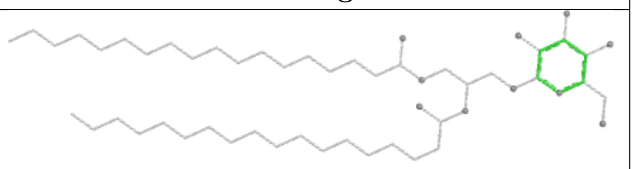
Bond lengths



Bond angles

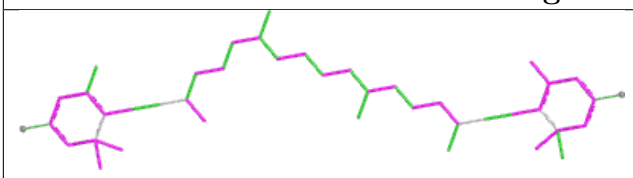


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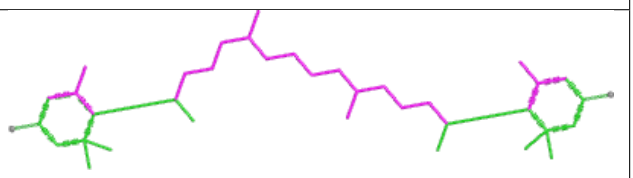


Rings

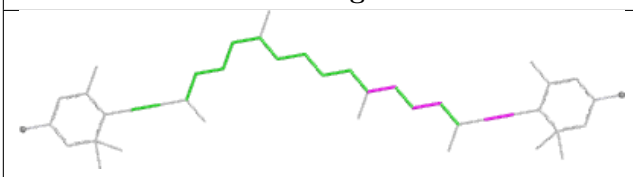
Ligand II0 a 314



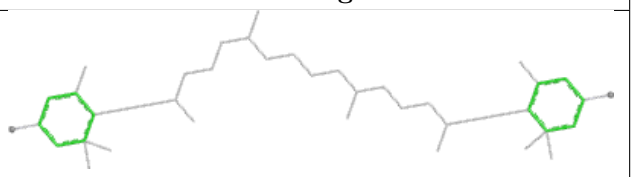
Bond lengths



Bond angles

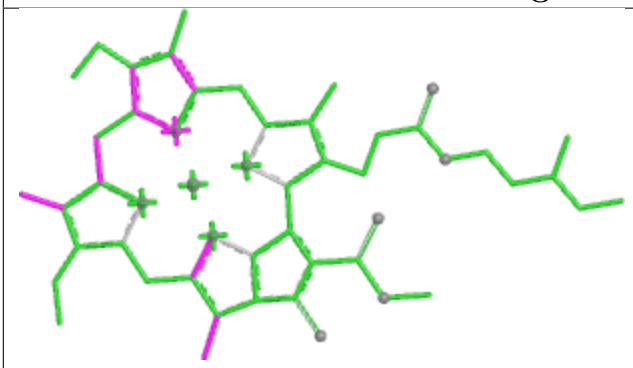


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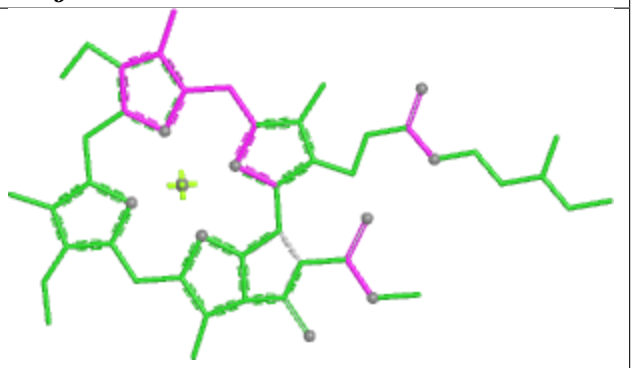


Rings

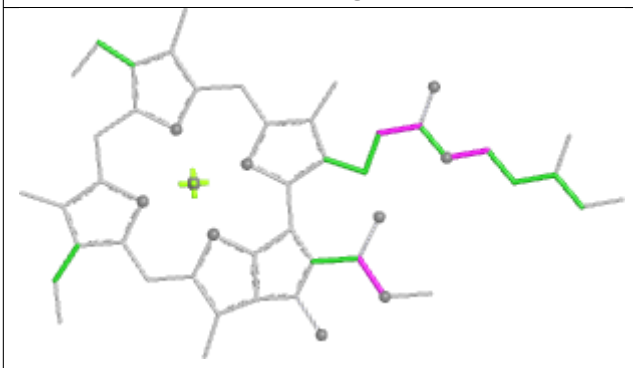
Ligand CLA j 603



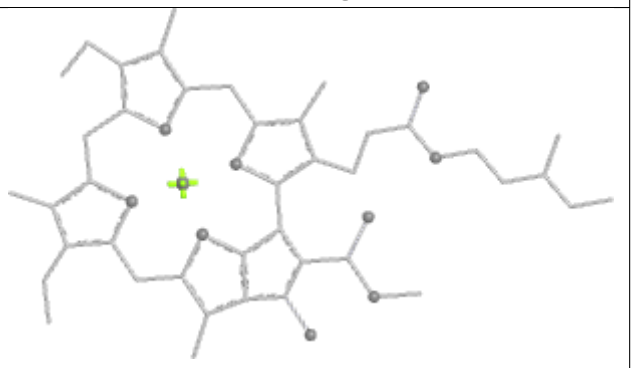
Bond lengths



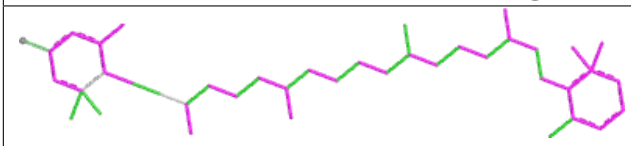
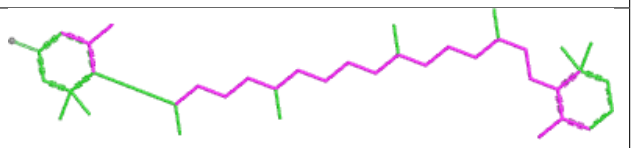
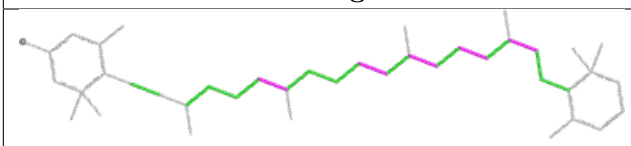
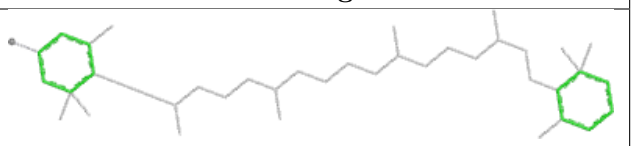
Bond angles

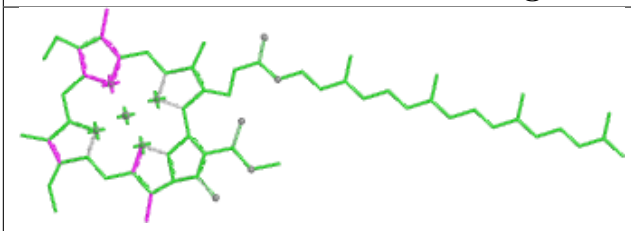
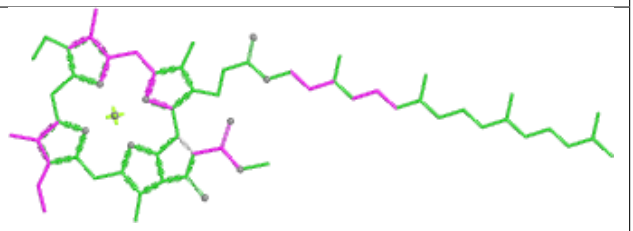
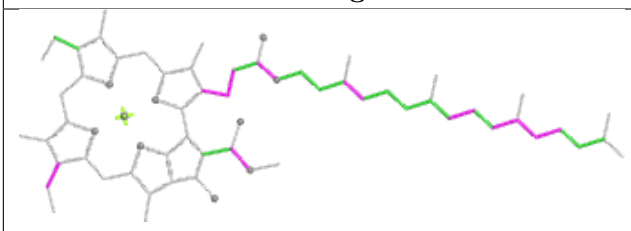
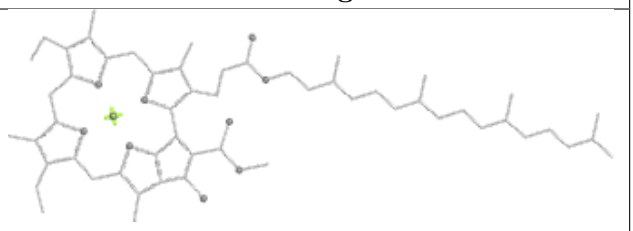


Torsions

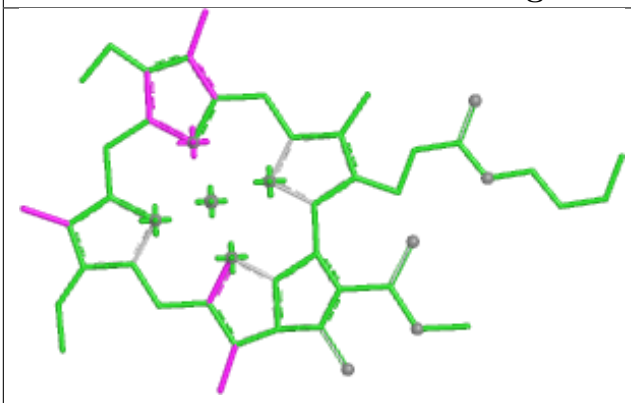


Rings

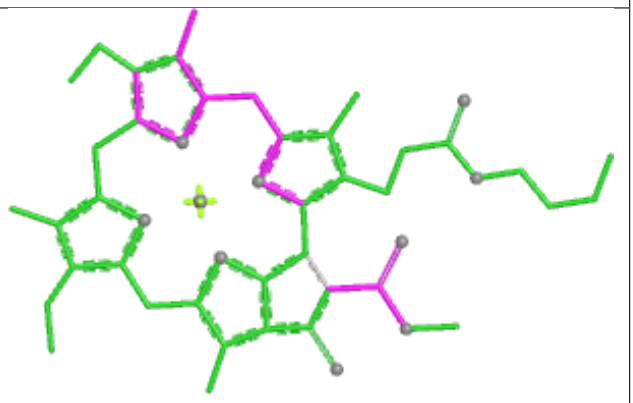
Ligand IHT m 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

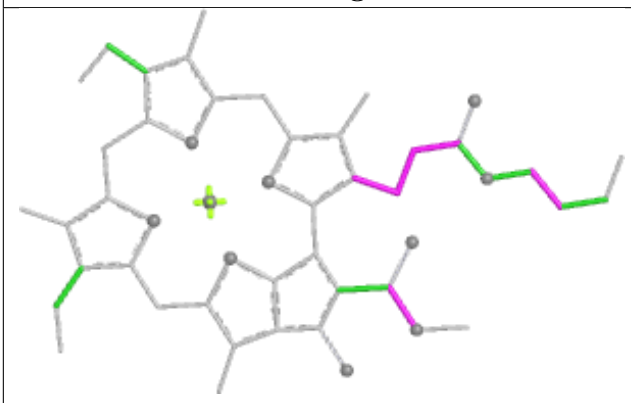
Ligand CLA L 202



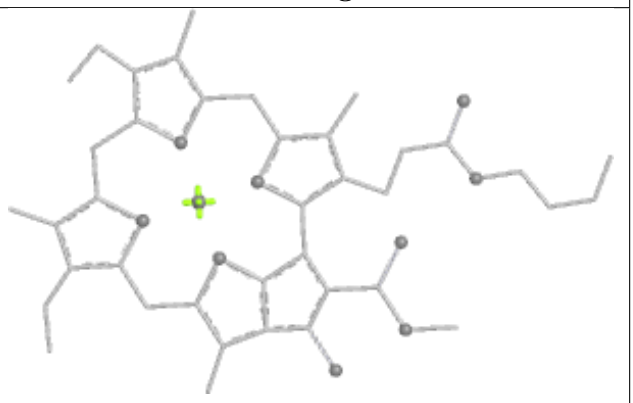
Bond lengths



Bond angles

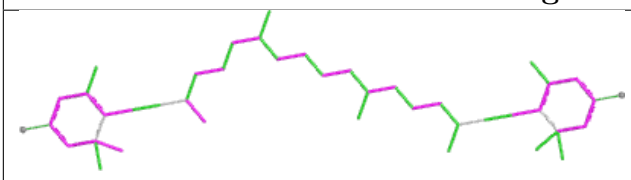


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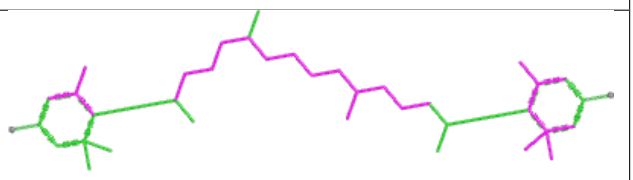


Rings

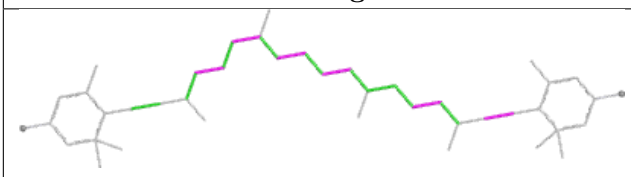
Ligand II0 h 312



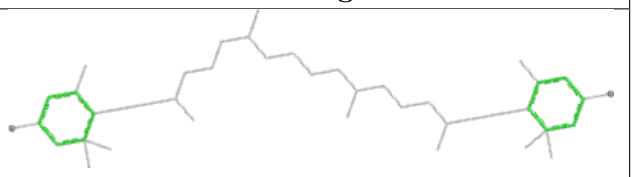
Bond lengths



Bond angles

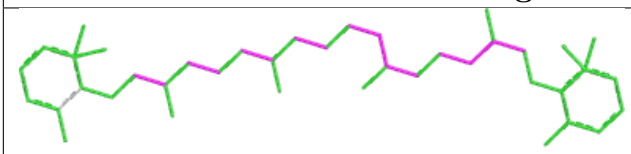


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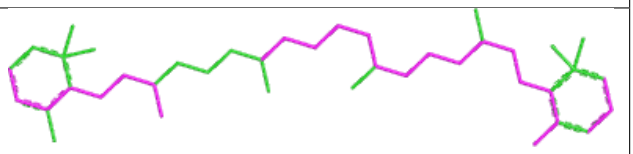


Rings

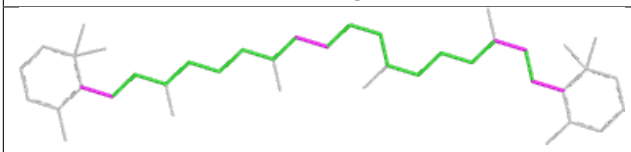
Ligand WVN A 845



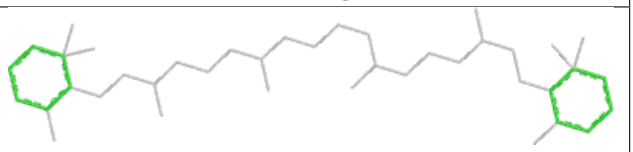
Bond lengths



Bond angles

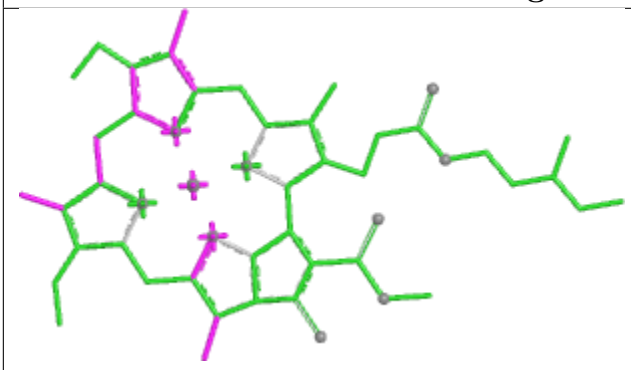


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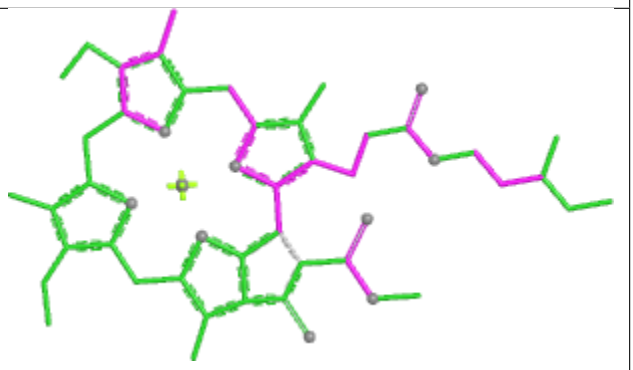


Rings

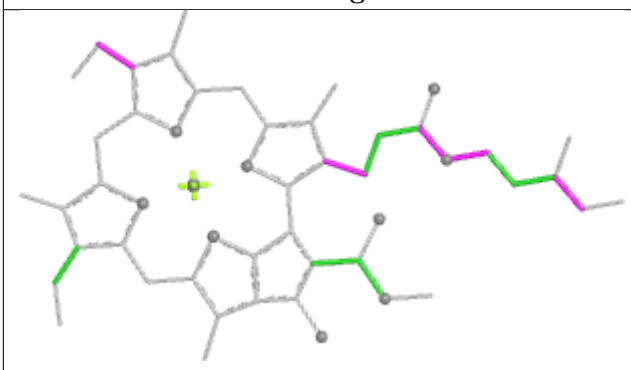
Ligand CLA b 612



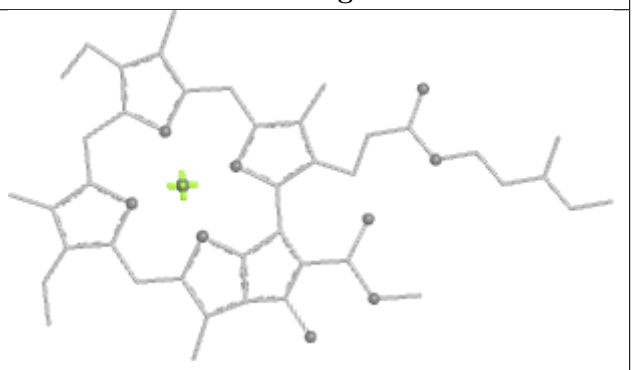
Bond lengths



Bond angles

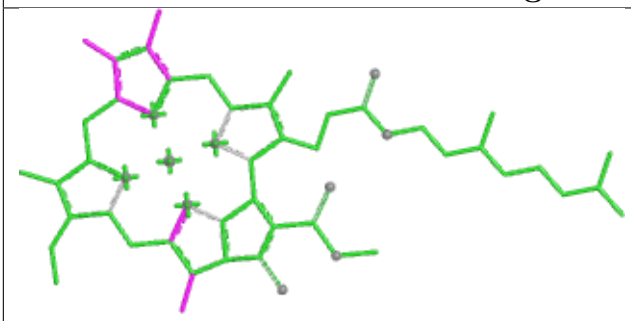


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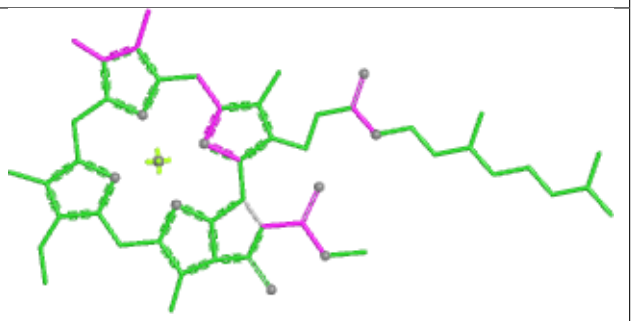


Rings

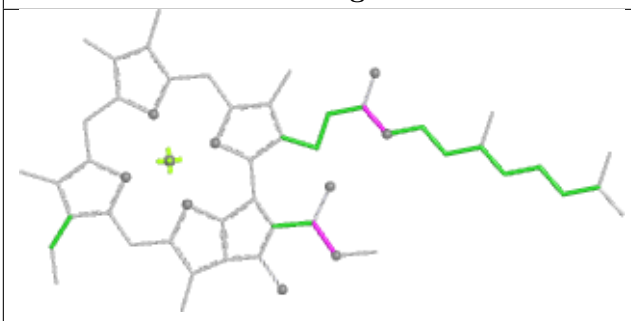
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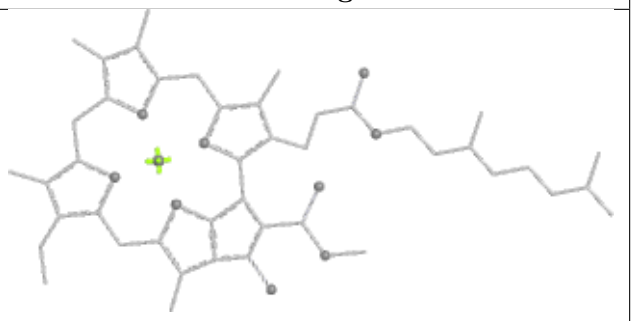
Bond lengths



Bond angles

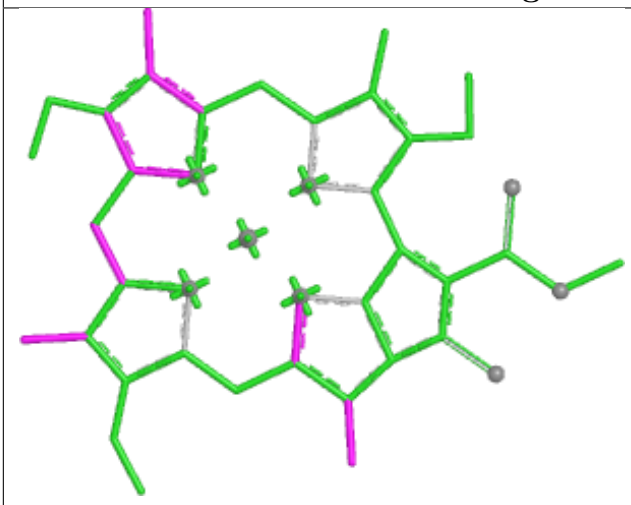


Torsions

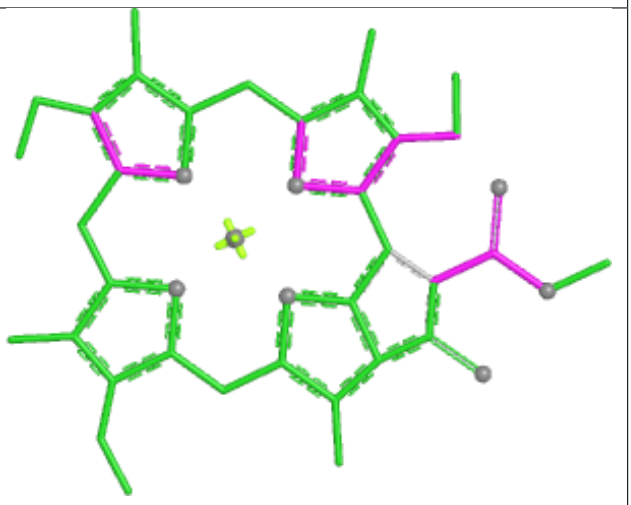


Rings

Ligand CLA m 601



Bond lengths



Bond angles

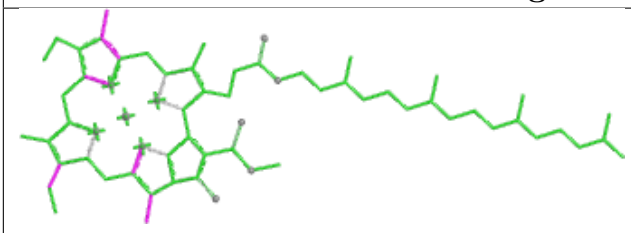


Torsions

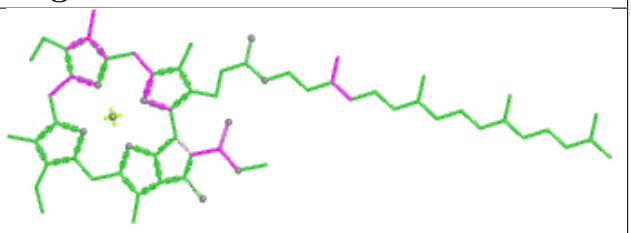


Rings

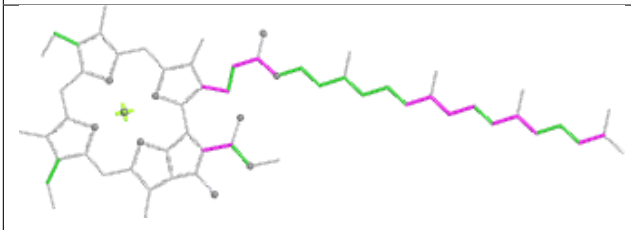
Ligand CLA g 308



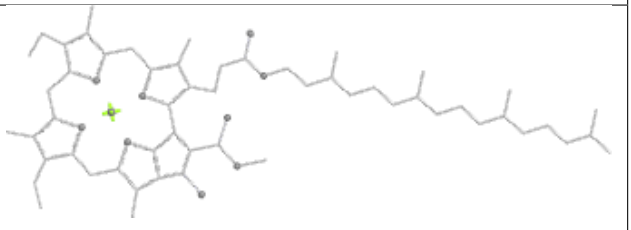
Bond lengths



Bond angles

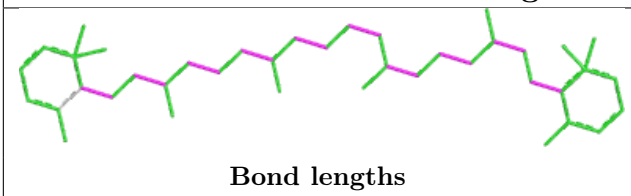


Torsions

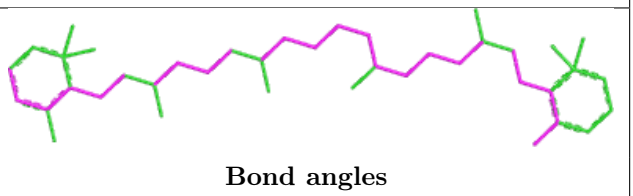


Rings

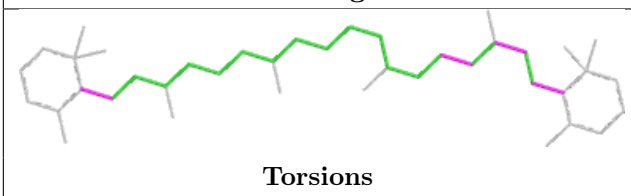
Ligand WVN s 207



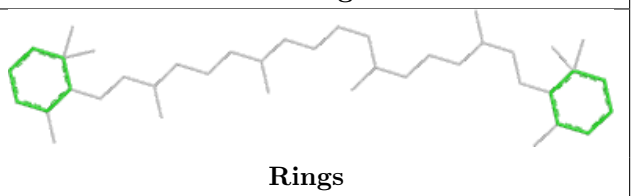
Bond lengths



Bond angles

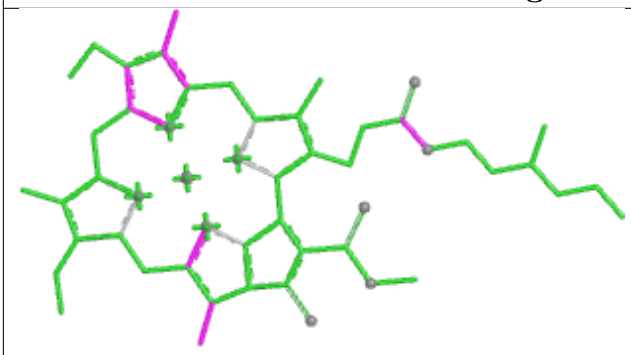


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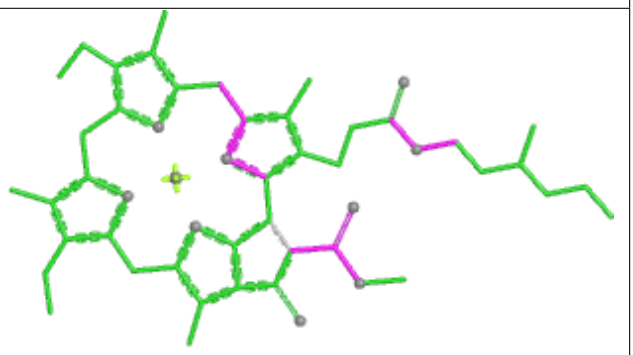


Rings

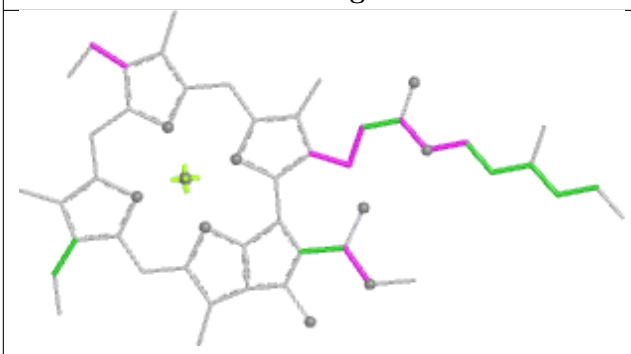
Ligand CLA F 202



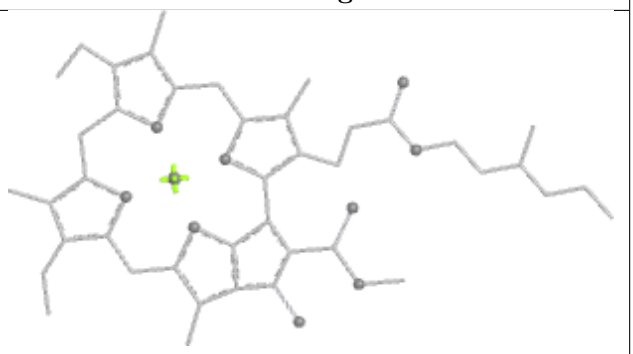
Bond lengths



Bond angles

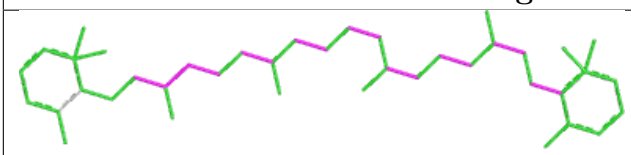


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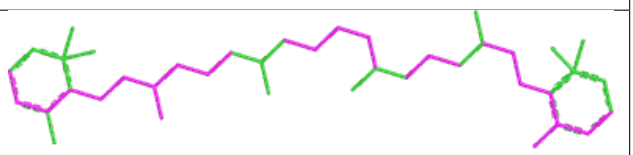


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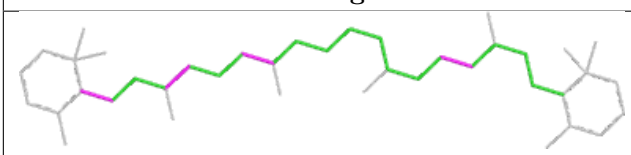
Ligand WVN B 846



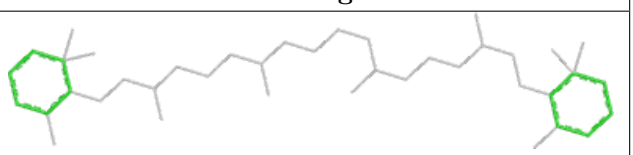
Bond lengths



Bond angles

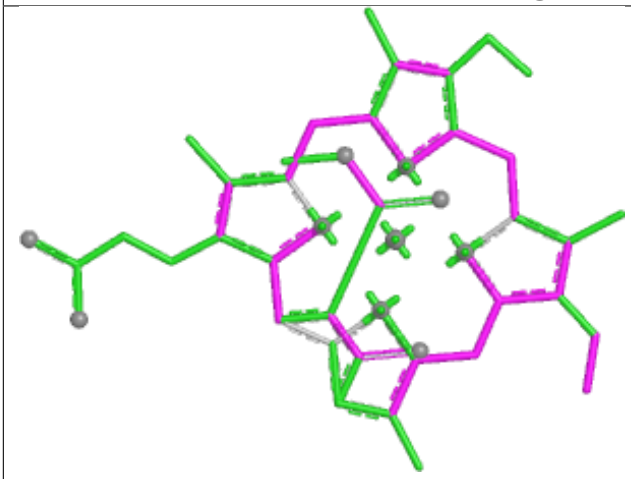


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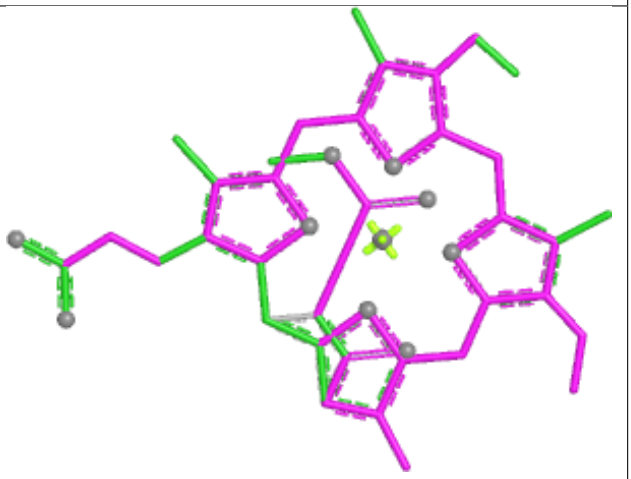


Rings

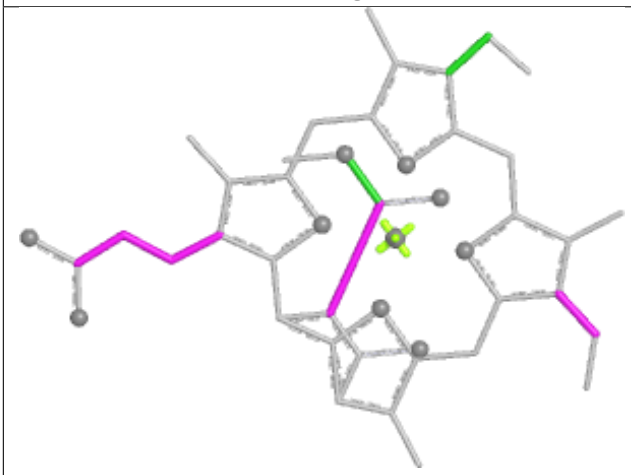
Ligand KC2 c 610



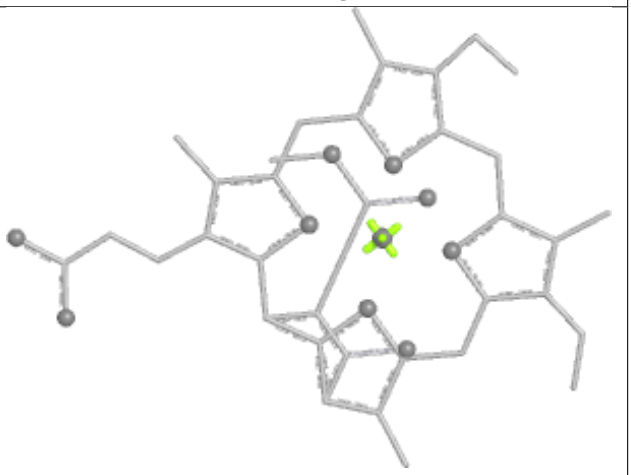
Bond lengths



Bond angles

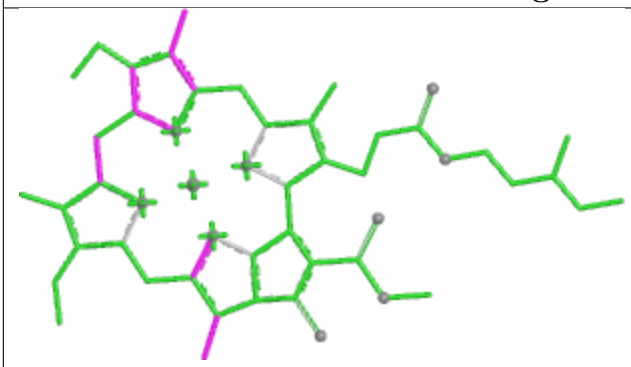


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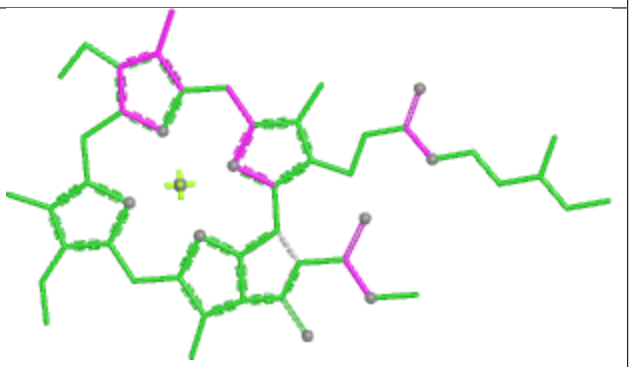


Rings

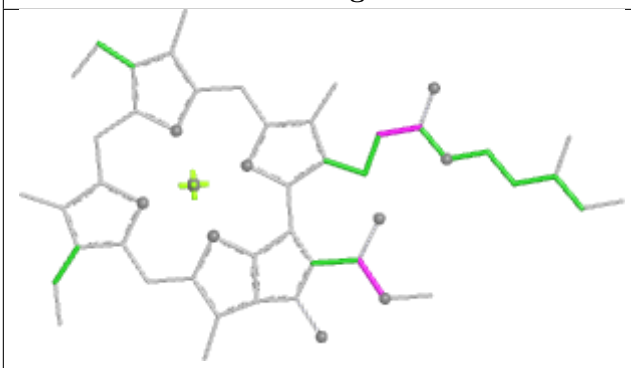
Ligand CLA l 304



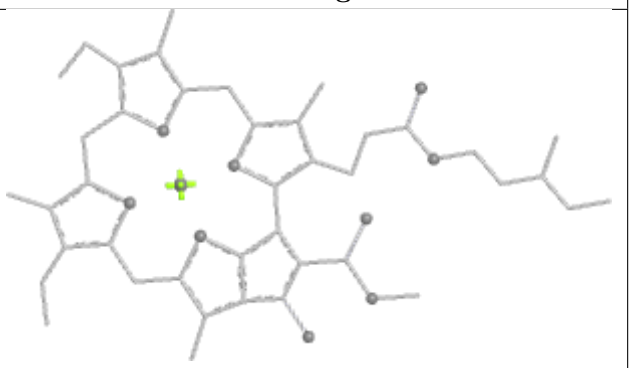
Bond lengths



Bond angles

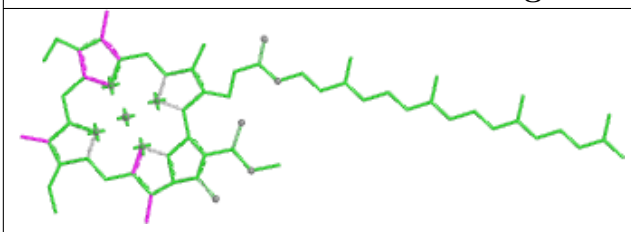


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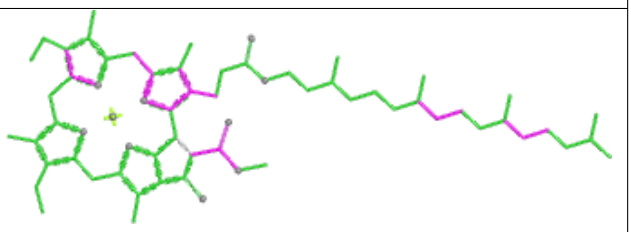


Rings

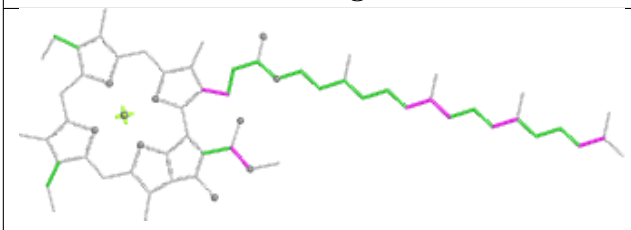
Ligand CLA B 839



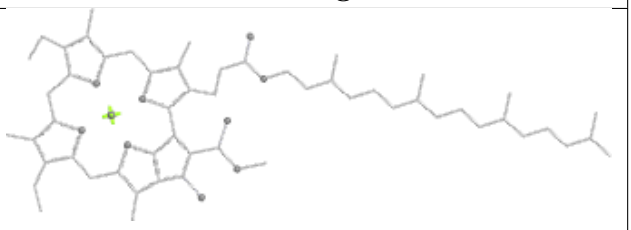
Bond lengths



Bond angles

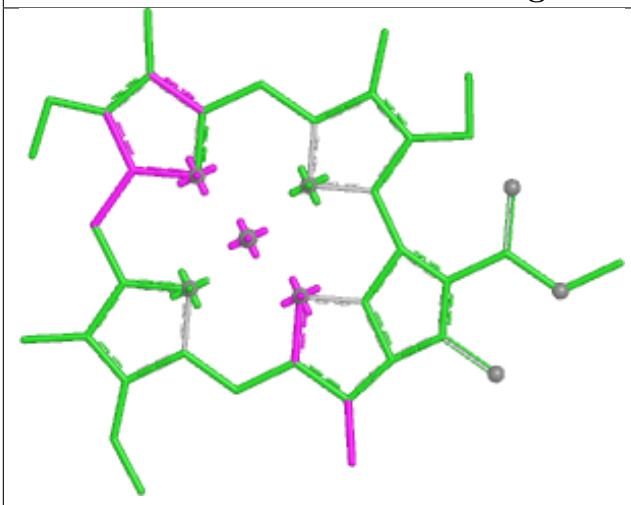


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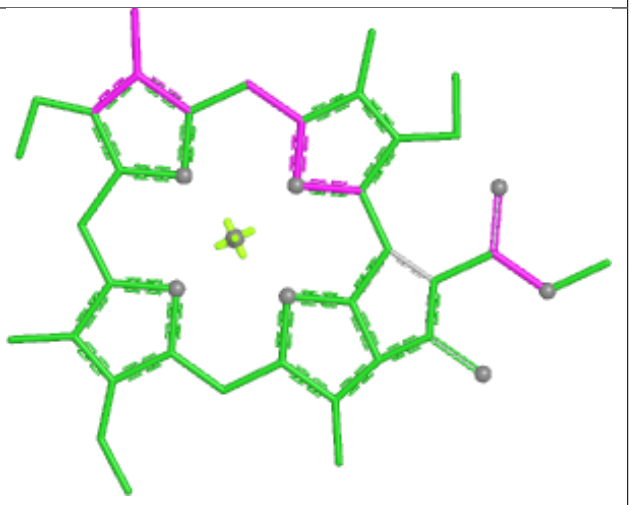


Rings

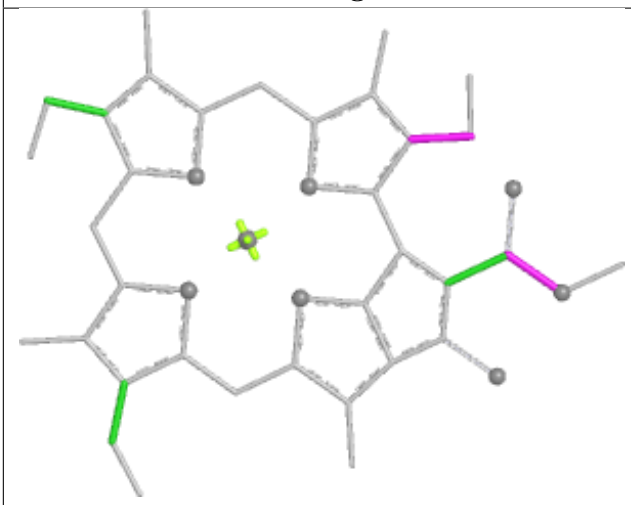
Ligand CLA J 103



Bond lengths



Bond angles

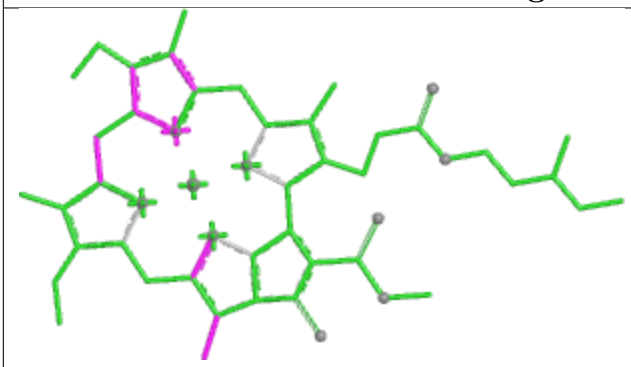


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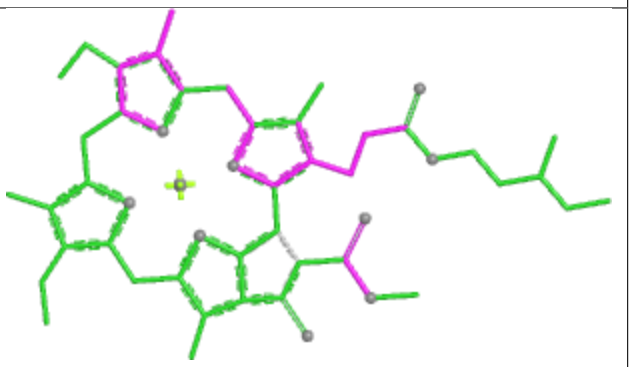


Rings

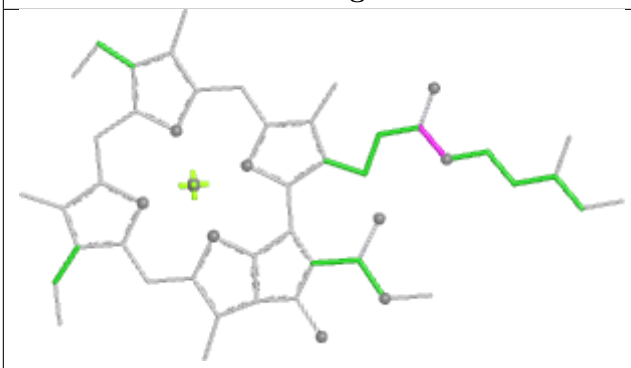
Ligand CLA k 603



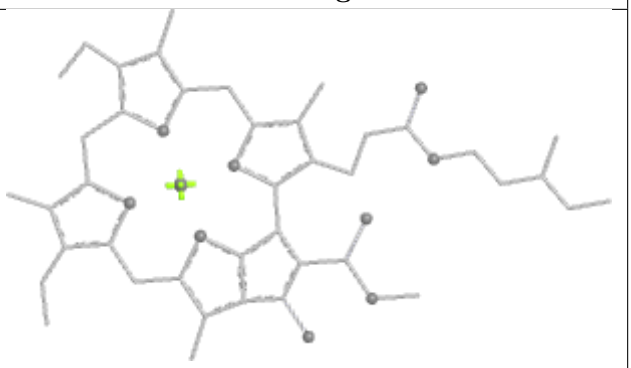
Bond lengths



Bond angles

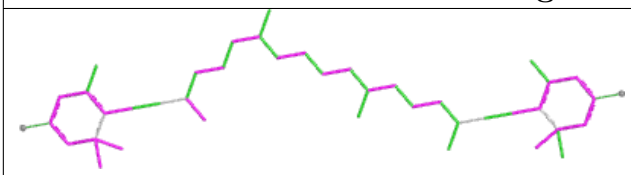


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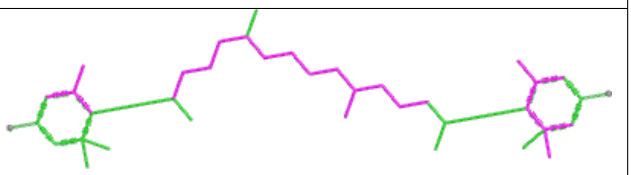


Rings

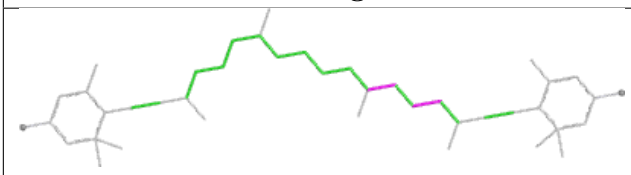
Ligand II0 m 616



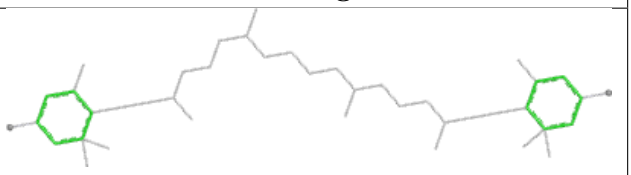
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Bond angles

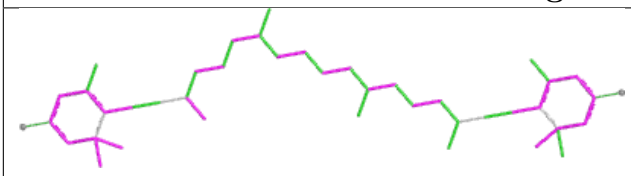


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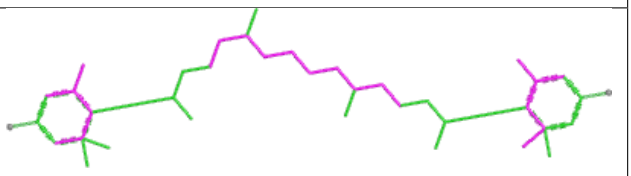


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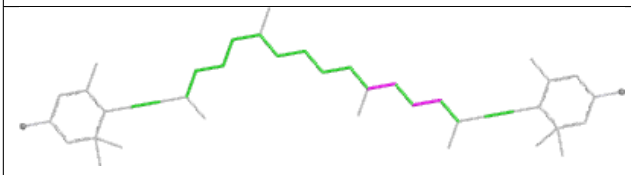
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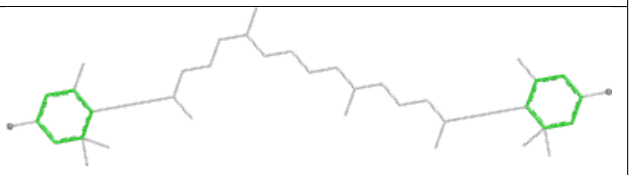
Bond lengths



Bond angles

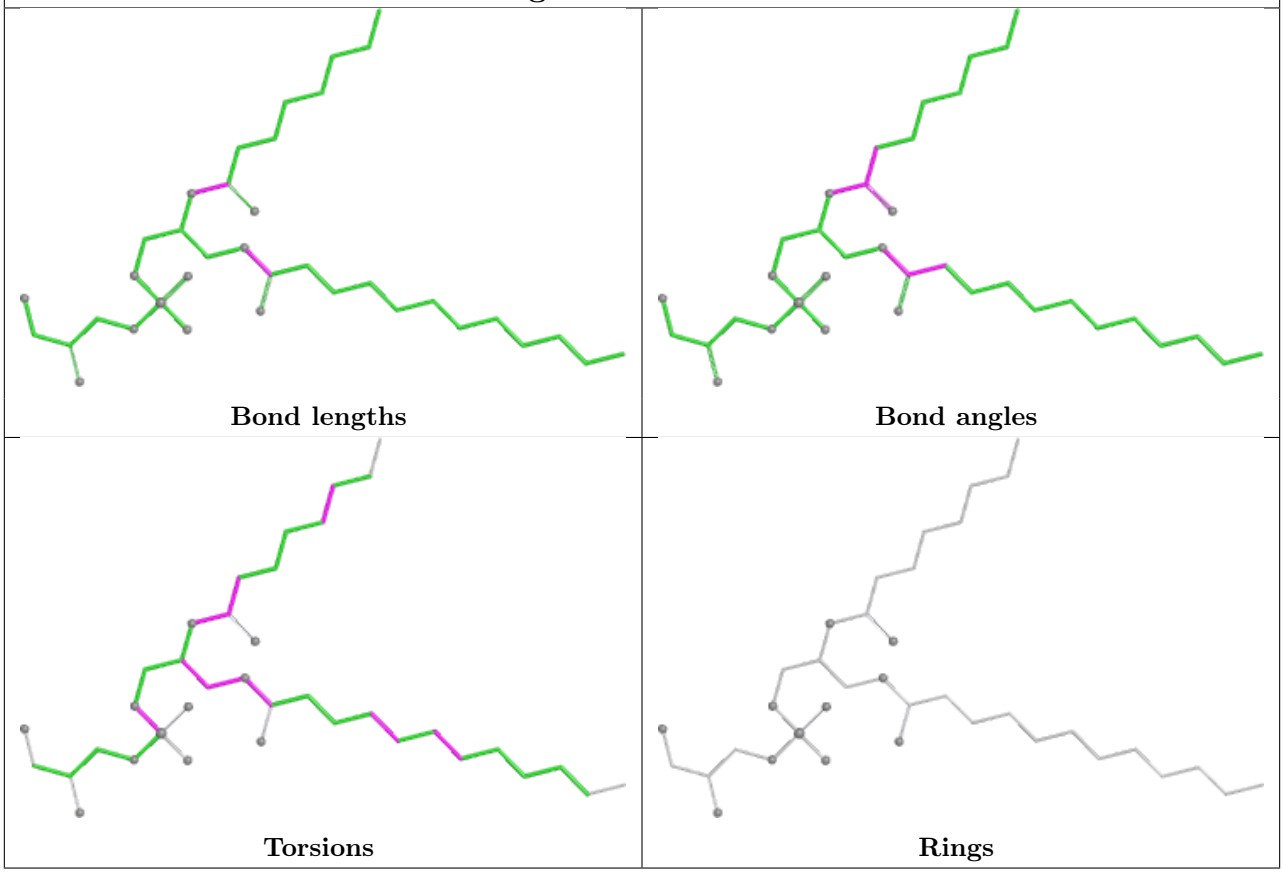


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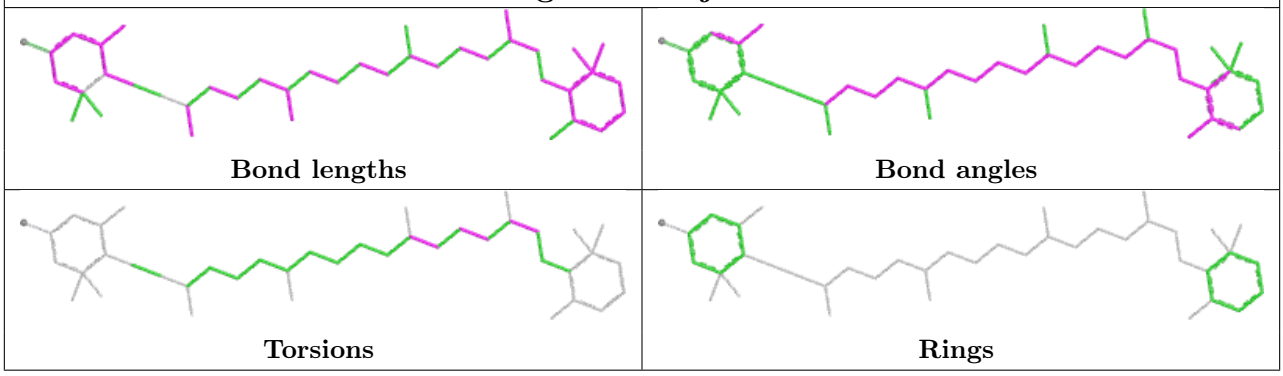


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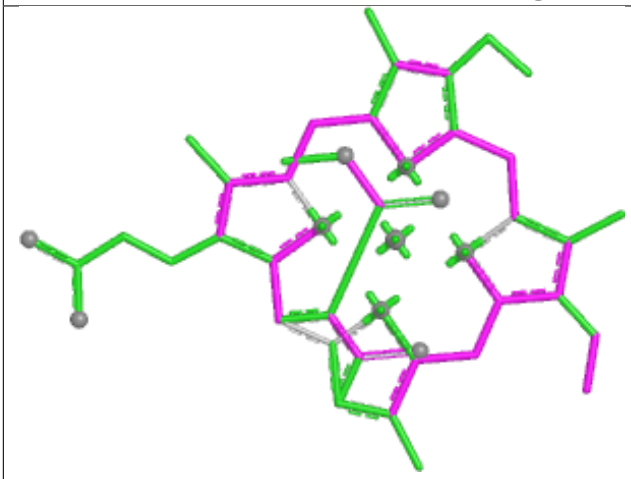
Ligand LHG c 618



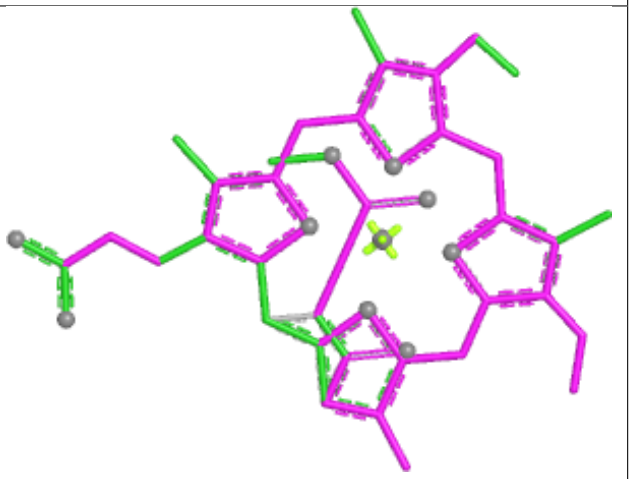
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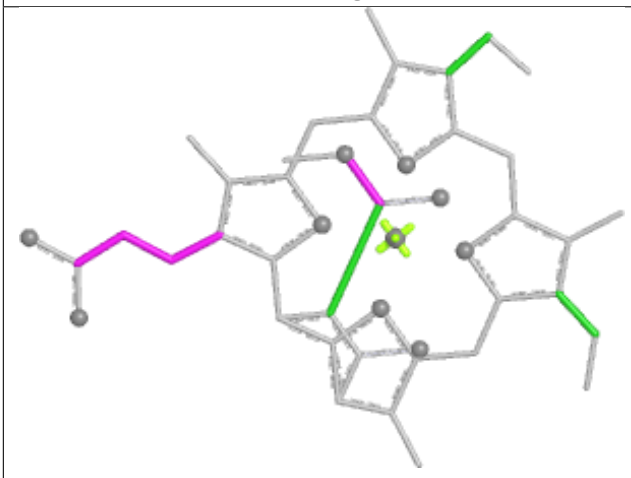
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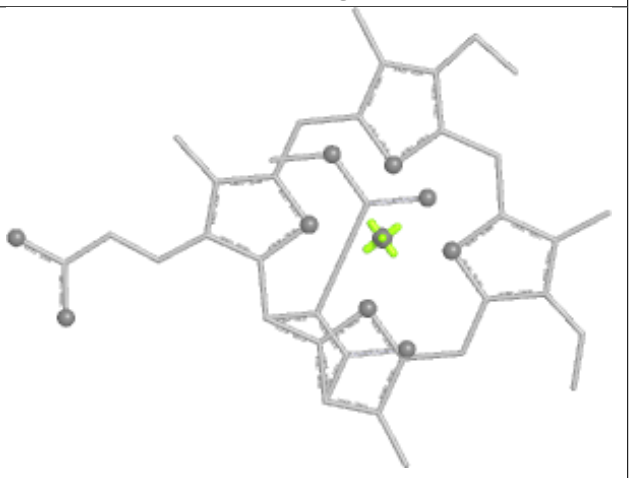
Bond lengths



Bond angles

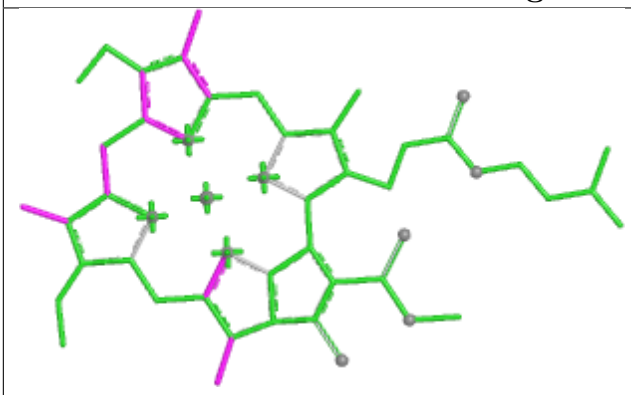


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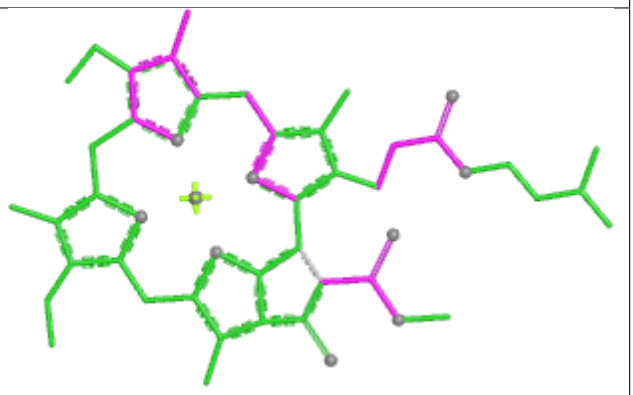


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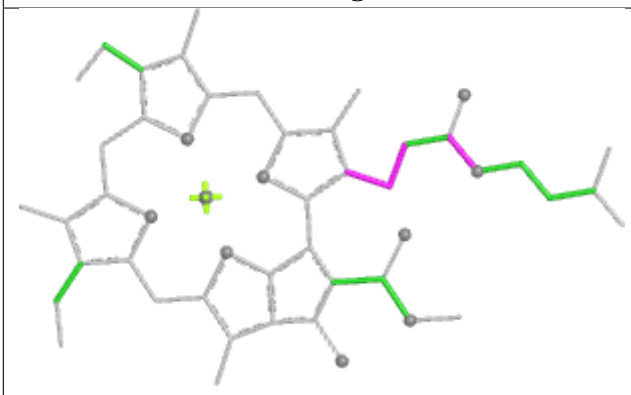
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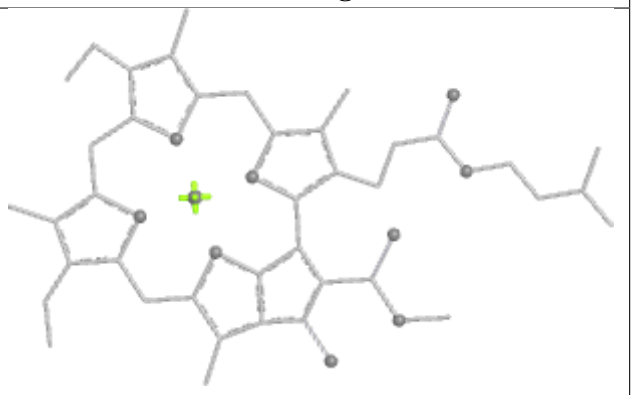
Bond lengths



Bond angles

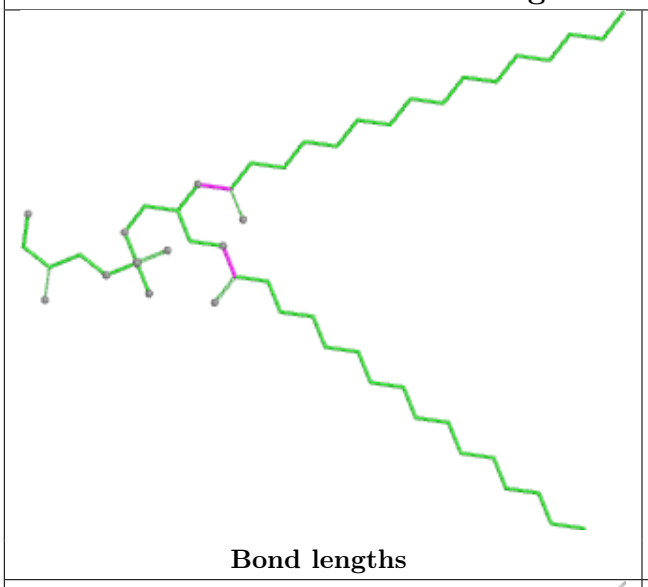


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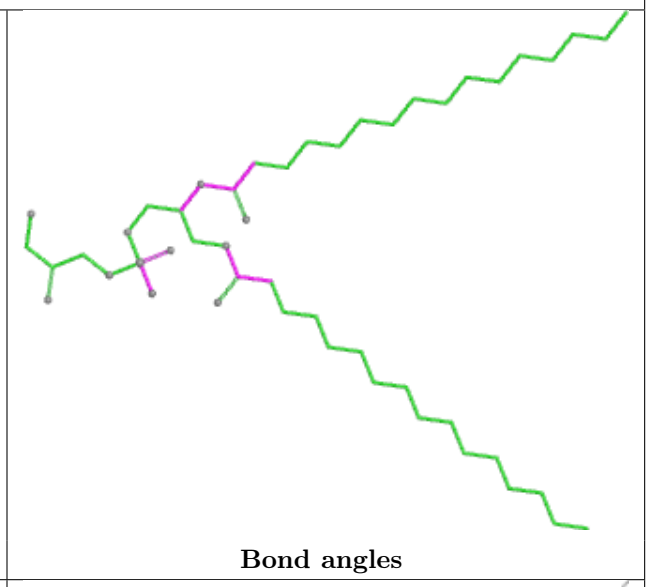


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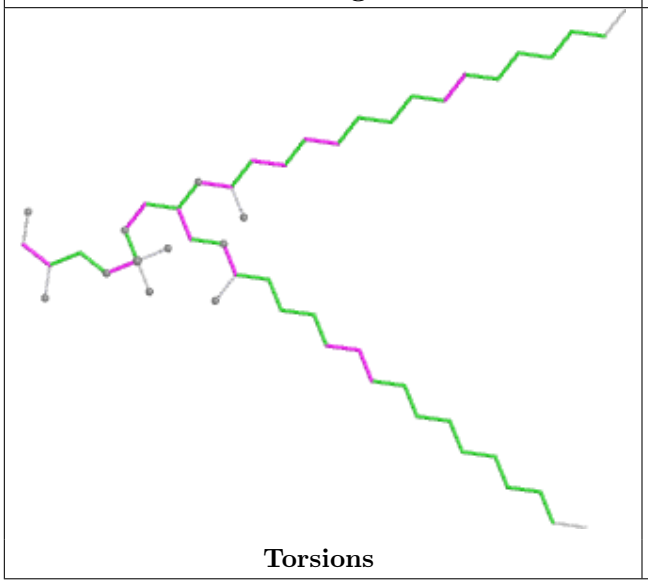
Ligand LHG a 301



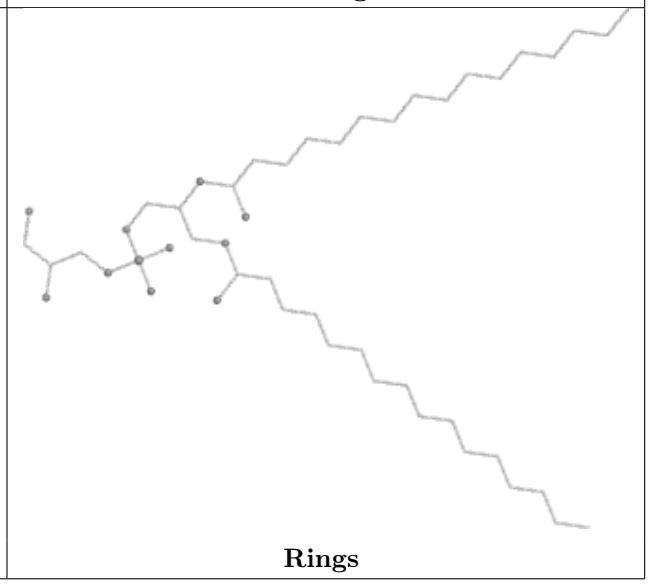
Bond lengths



Bond angles

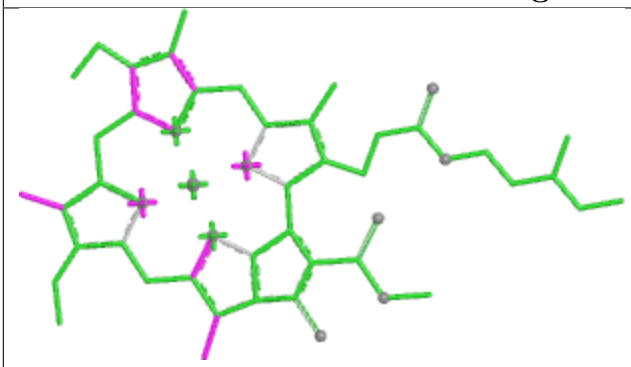


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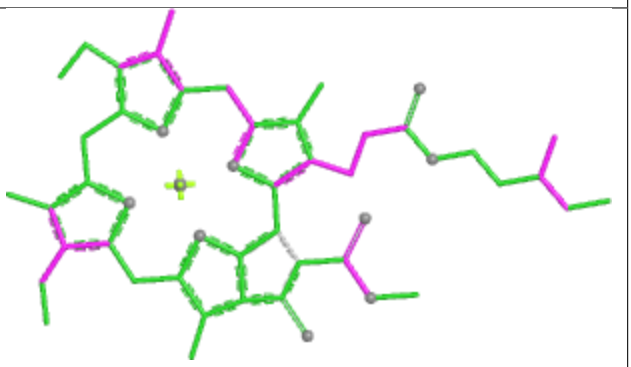


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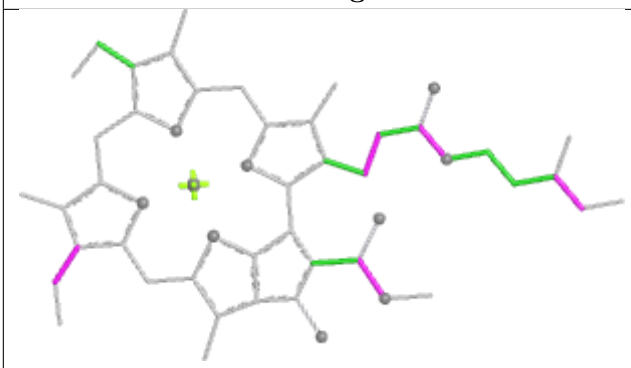
Ligand CLA f 612



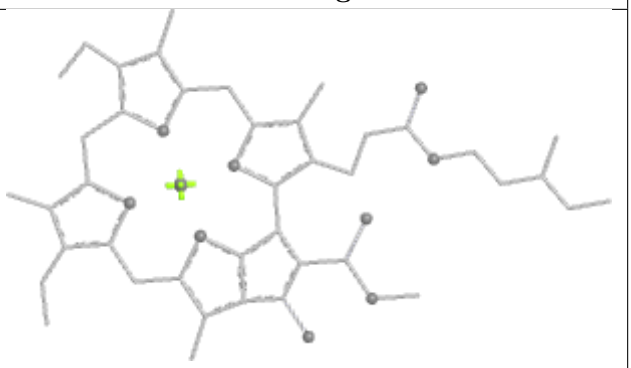
Bond lengths



Bond angles

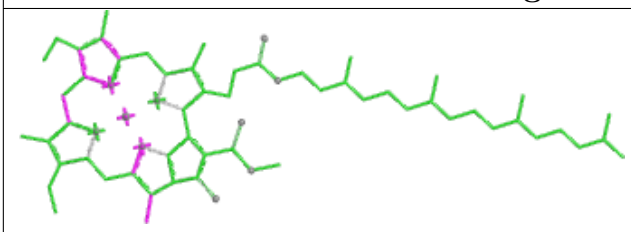


Torsions

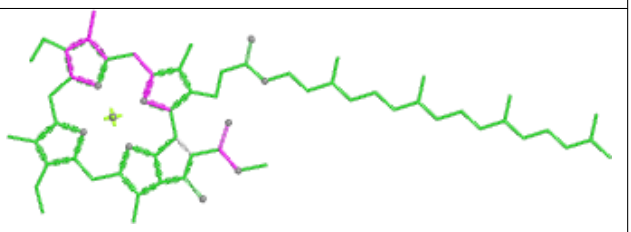


Rings

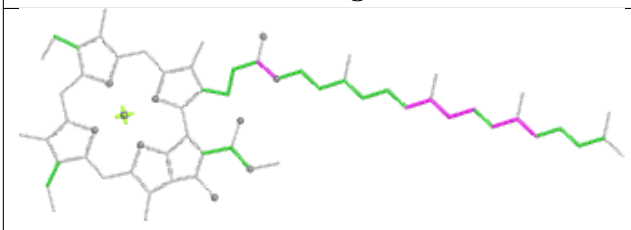
Ligand CLA A 825



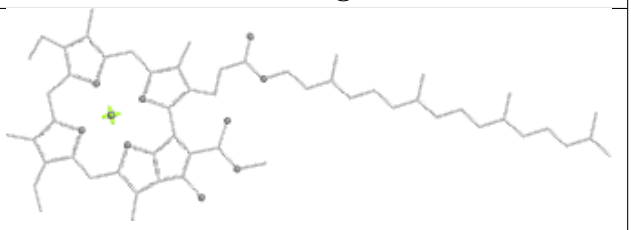
Bond lengths



Bond angles

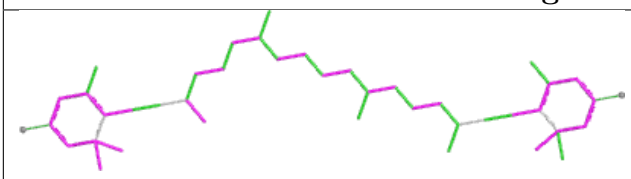


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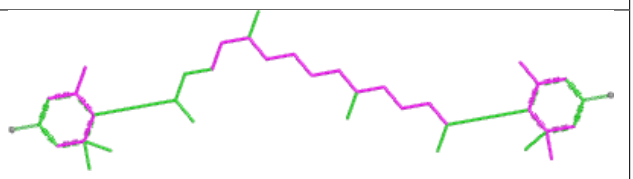


Rings

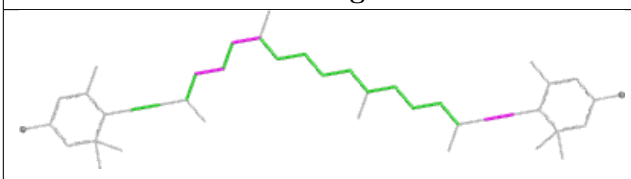
Ligand II0 n 615



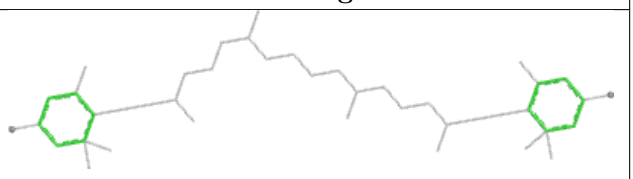
Bond lengths



Bond angles

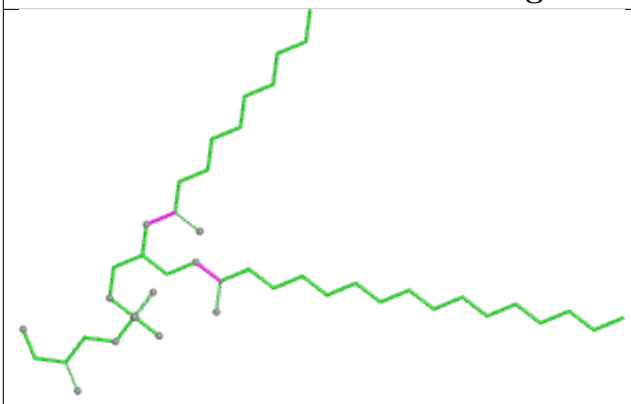


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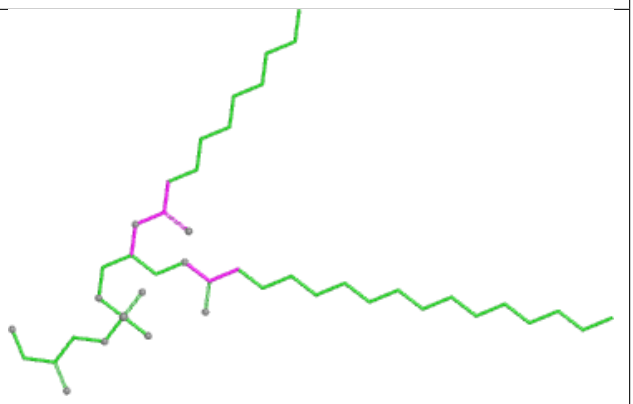


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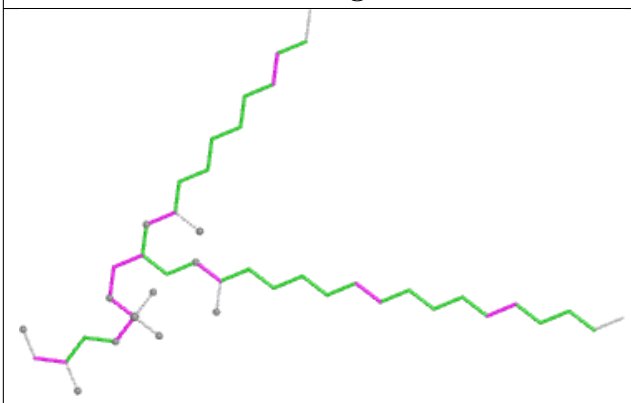
Ligand LHG n 619



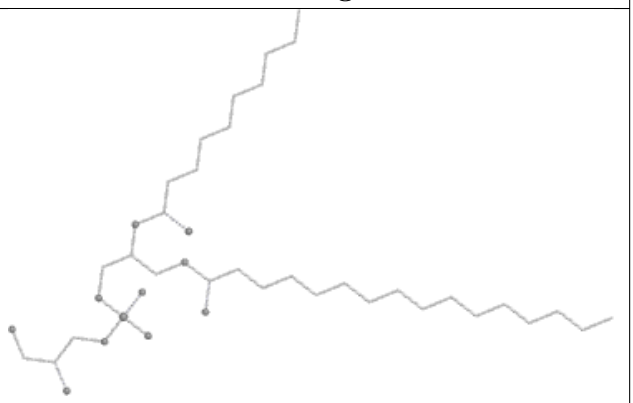
Bond lengths



Bond angles

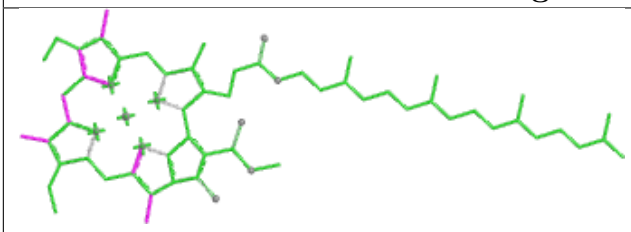


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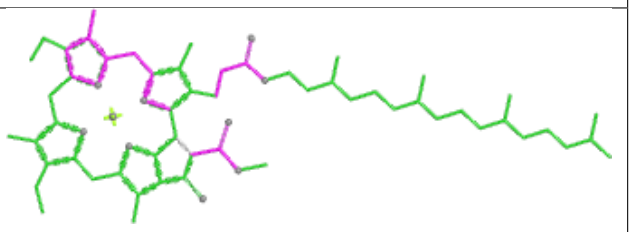


Rings

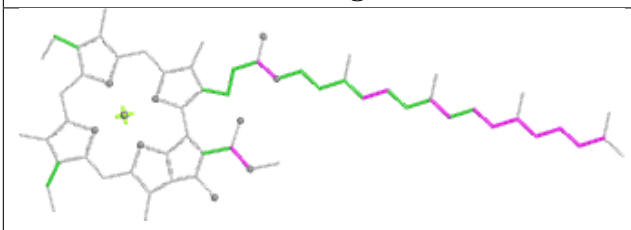
Ligand CLA f 608



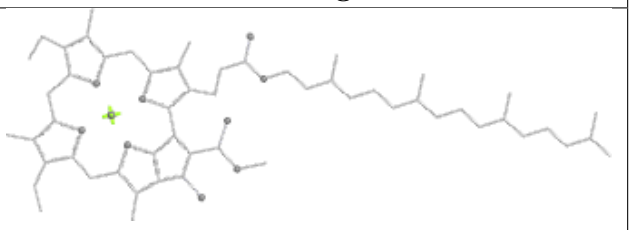
Bond lengths



Bond angles

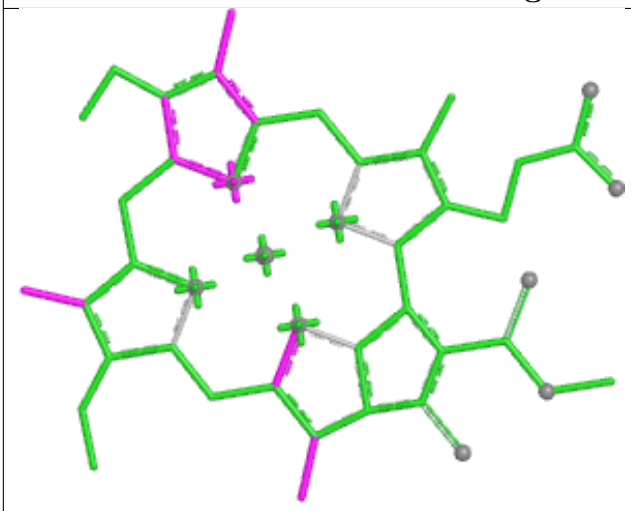


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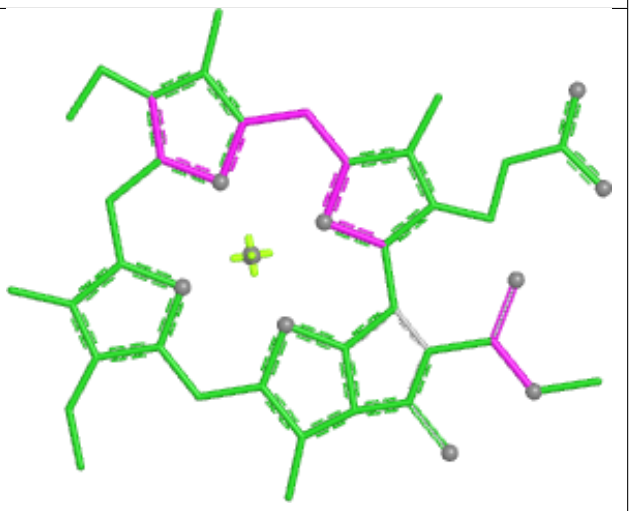


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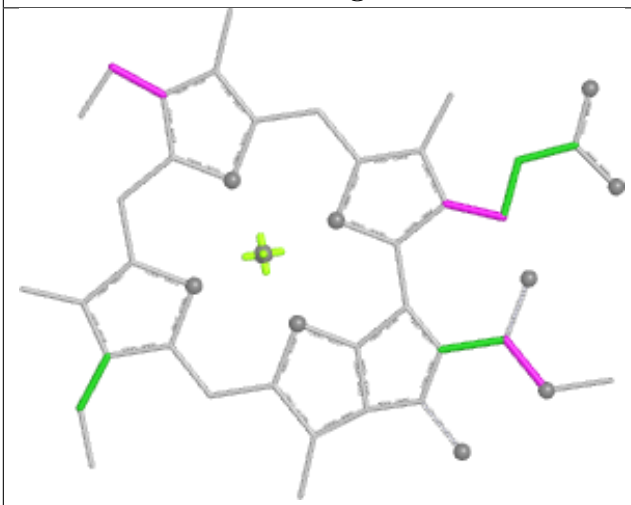
Ligand CLA B 831



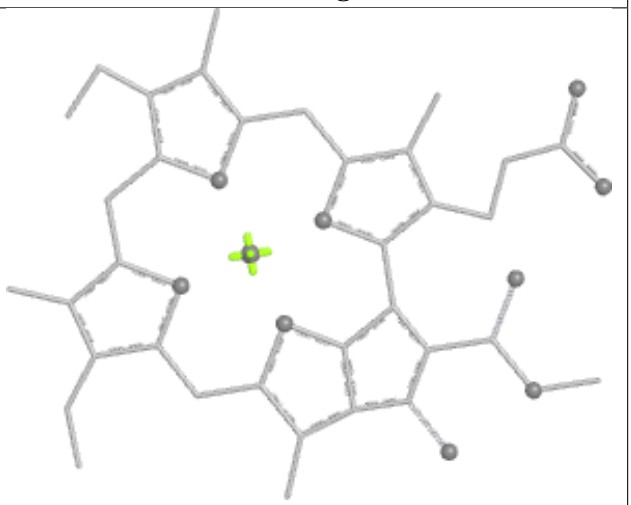
Bond lengths



Bond angles

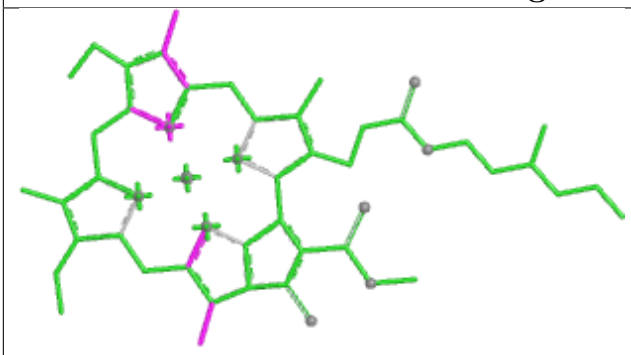


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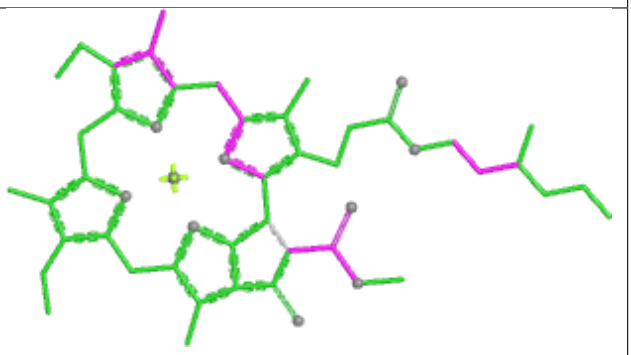


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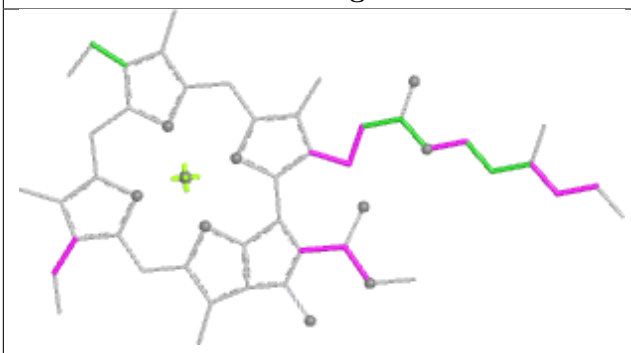
Ligand CLA a 303



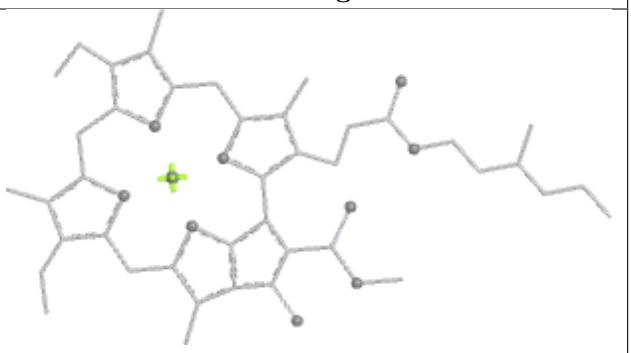
Bond lengths



Bond angles

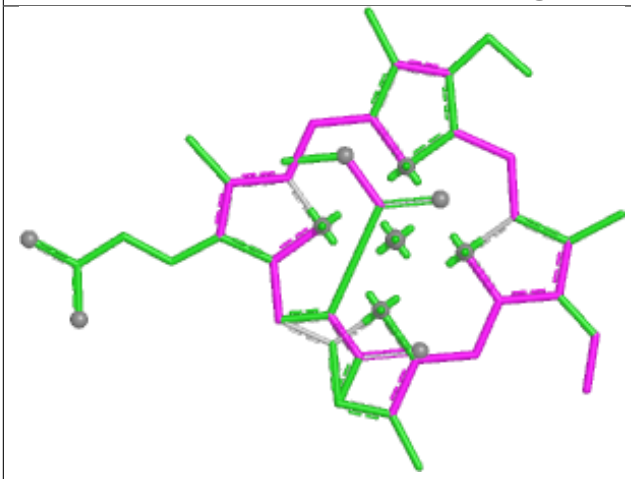


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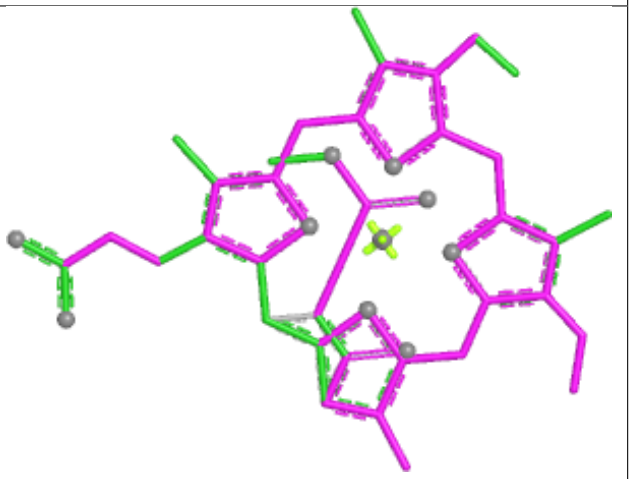


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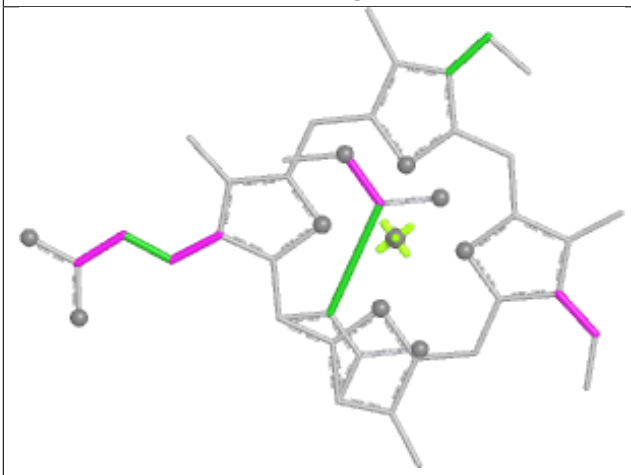
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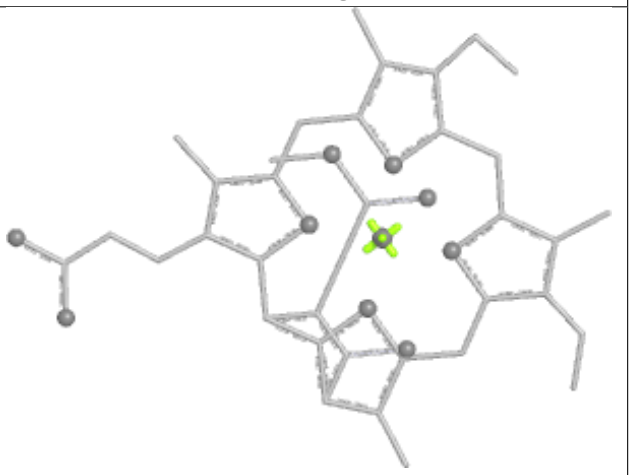
Bond lengths



Bond angles

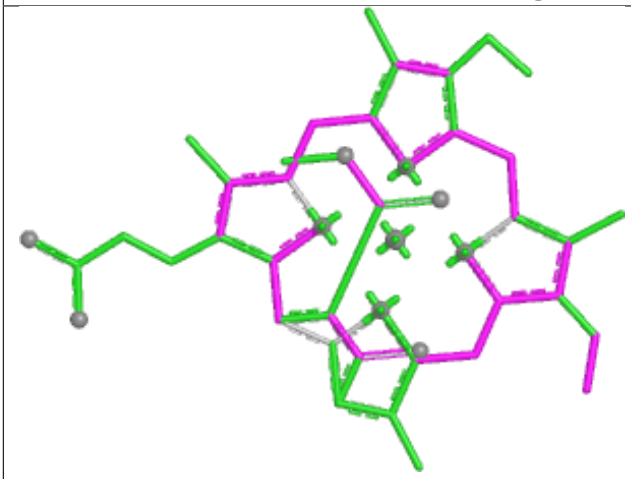


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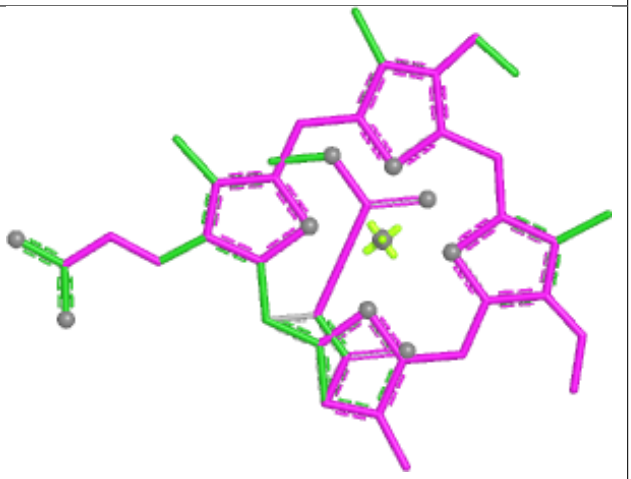


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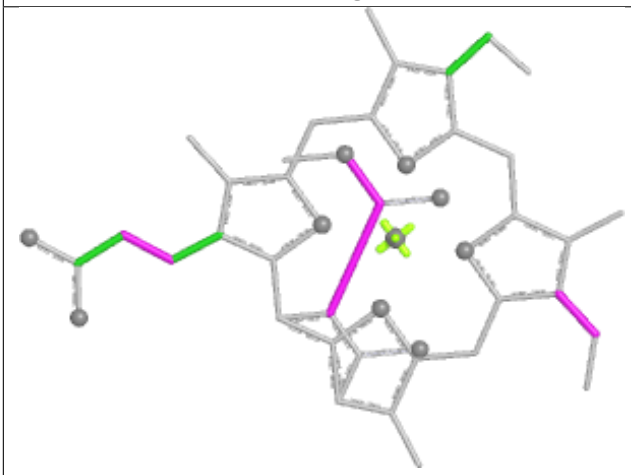
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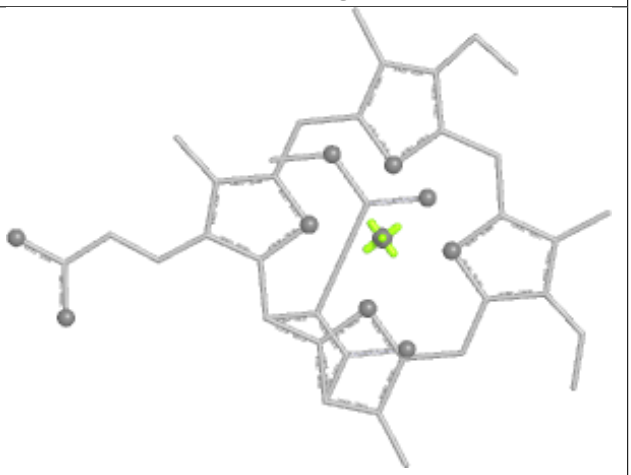
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Bond angles

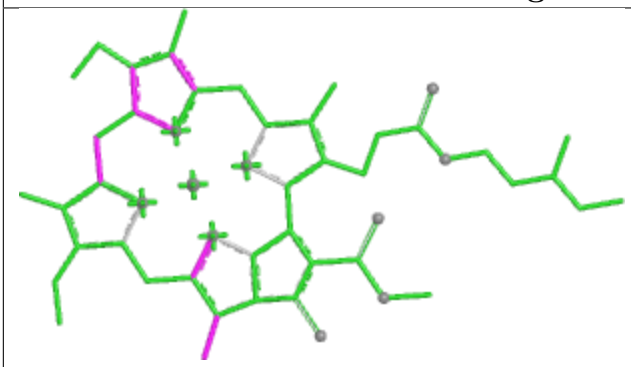


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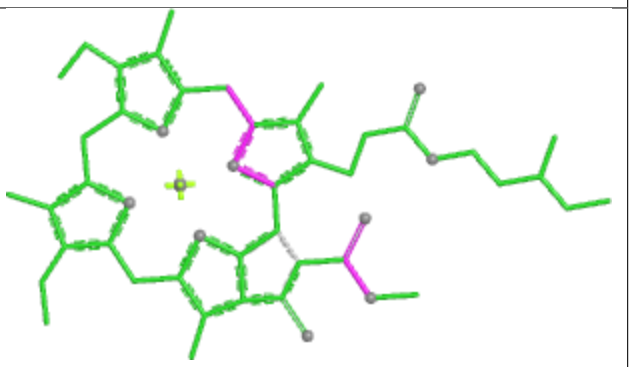


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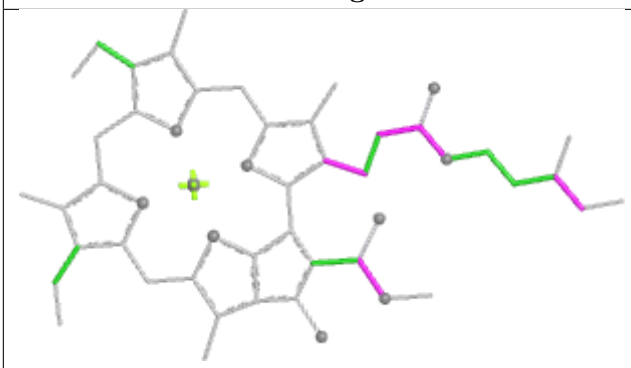
Ligand CLA n 613



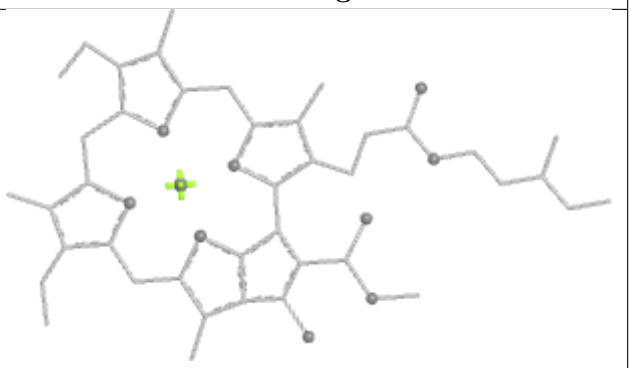
Bond lengths



Bond angles

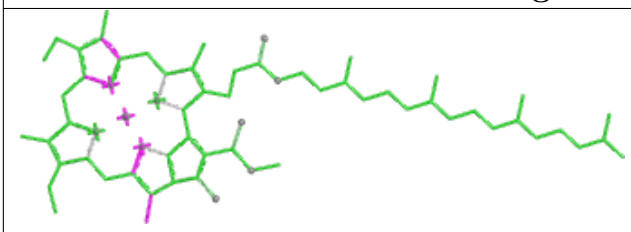


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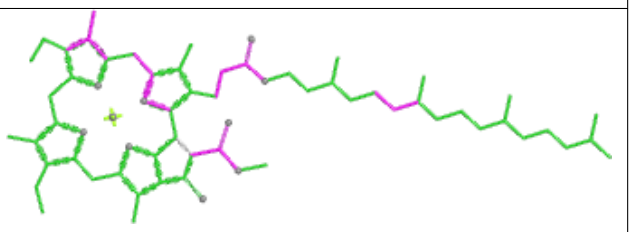


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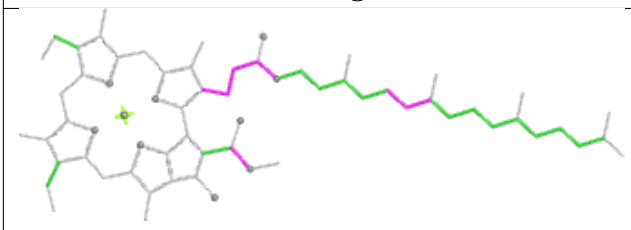
Ligand CLA l 307



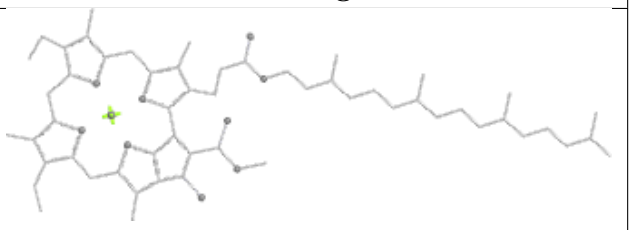
Bond lengths



Bond angles

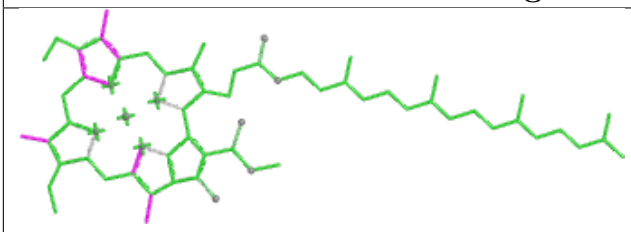


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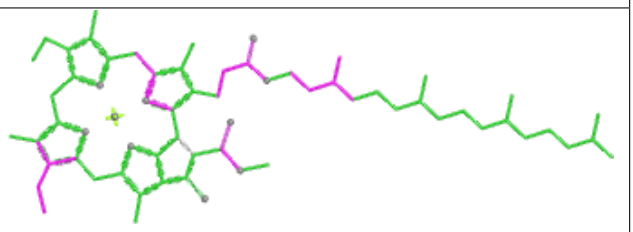


Rings

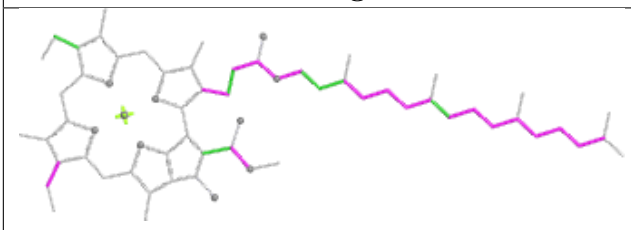
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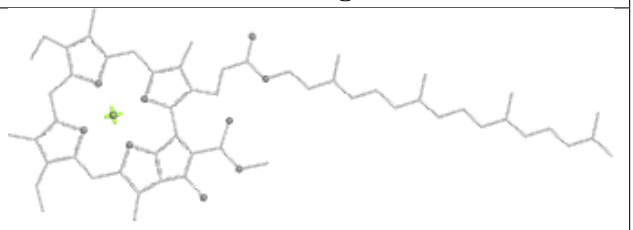
Bond lengths



Bond angles

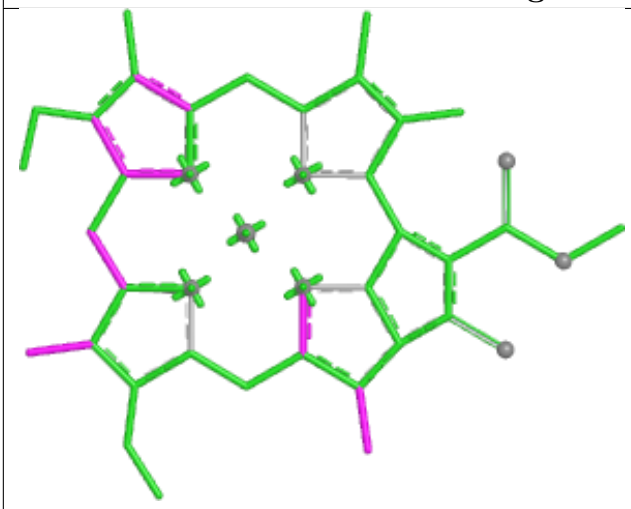


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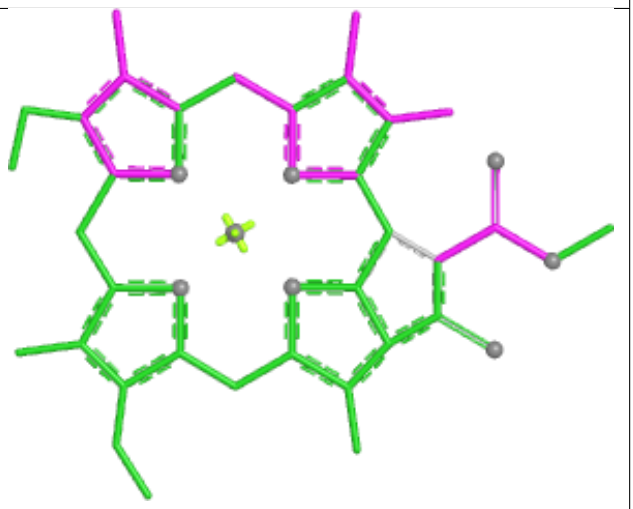


Rings

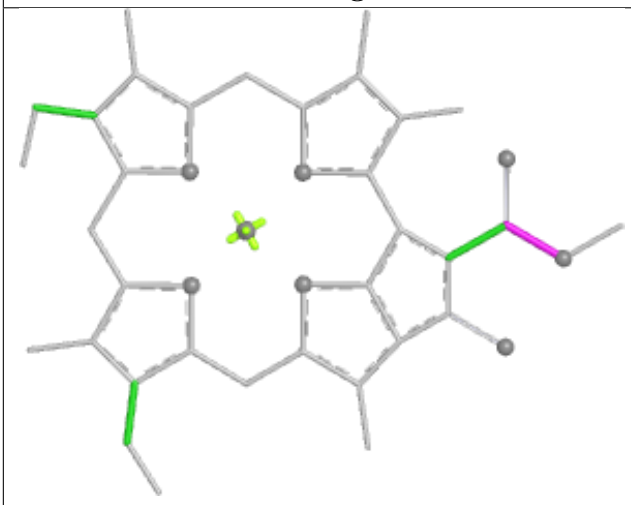
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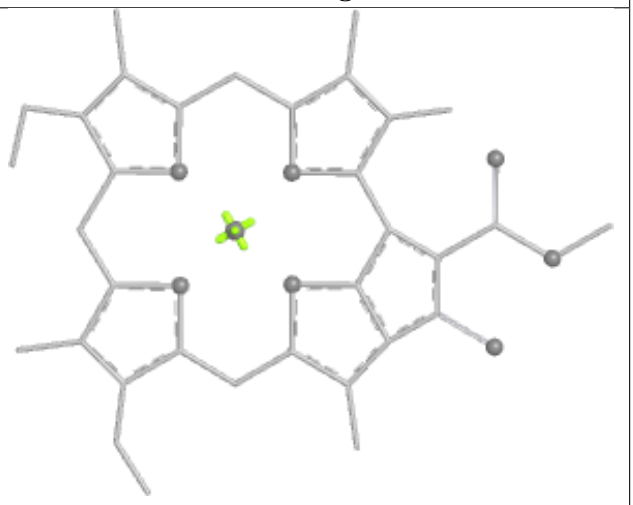
Bond lengths



Bond angles

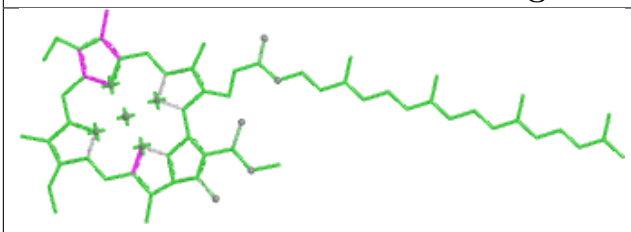


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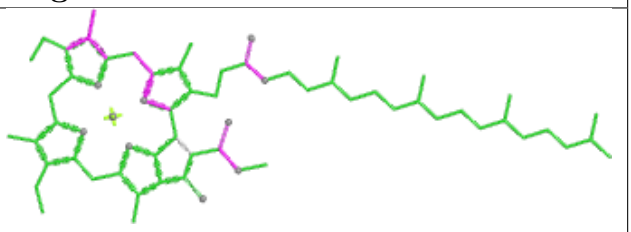


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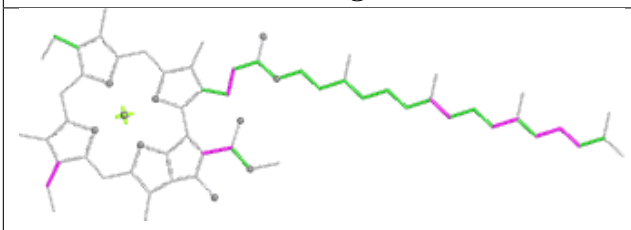
Ligand CLA g 305



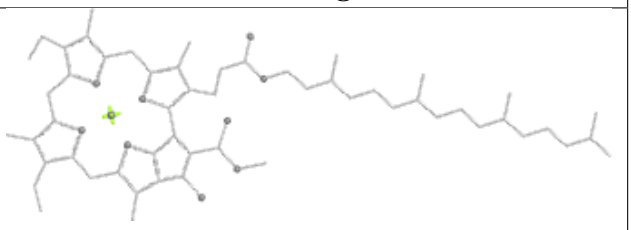
Bond lengths



Bond angles

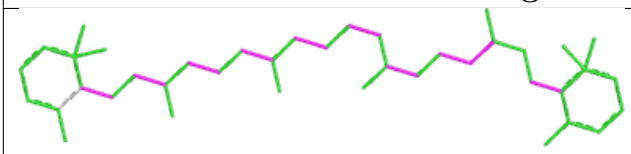


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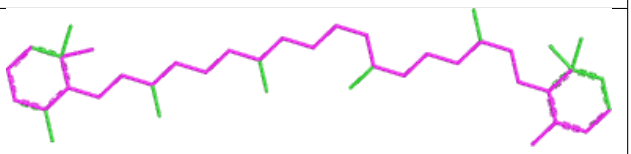


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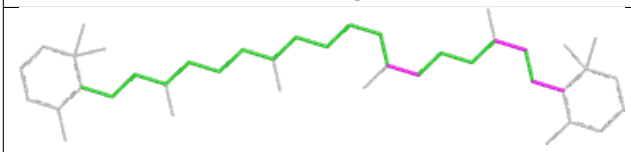
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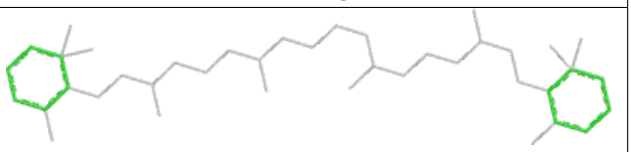
Bond lengths



Bond angles

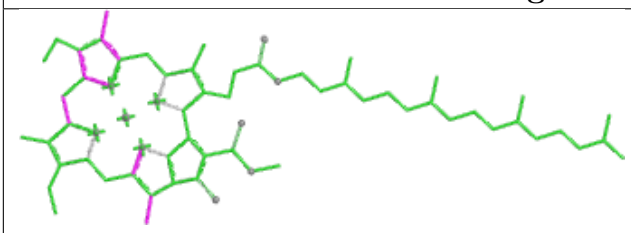


Torsions

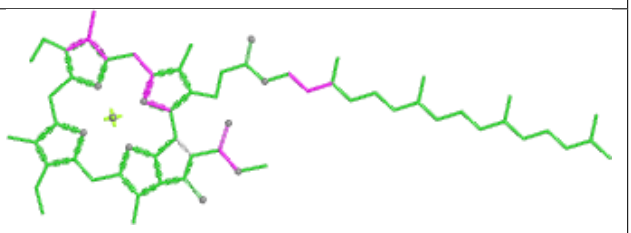


Rings

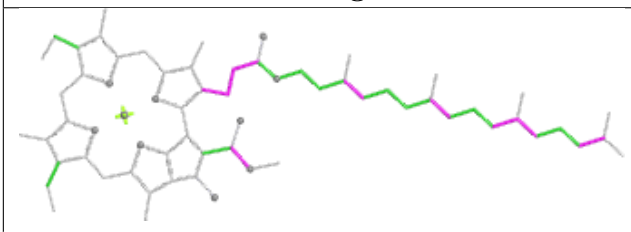
Ligand CLA d 303



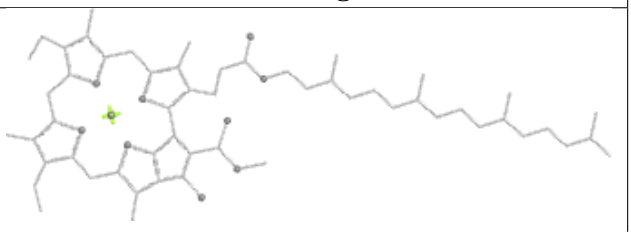
Bond lengths



Bond angles

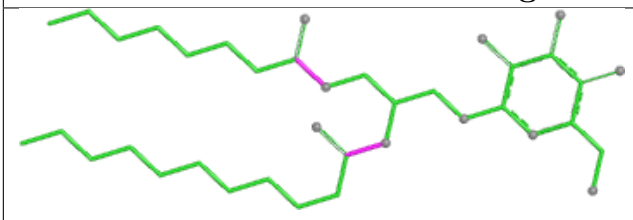


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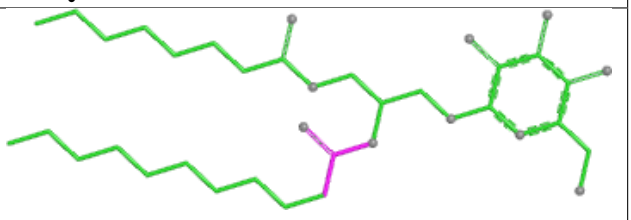


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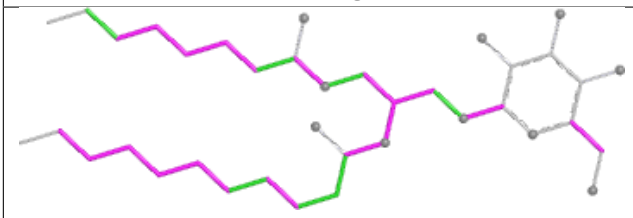
Ligand LMG Q 301



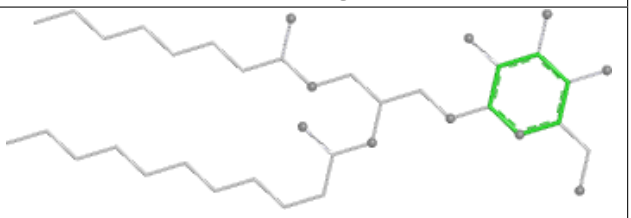
Bond lengths



Bond angles

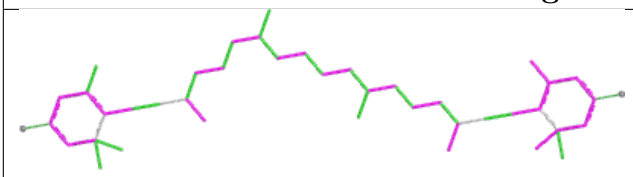


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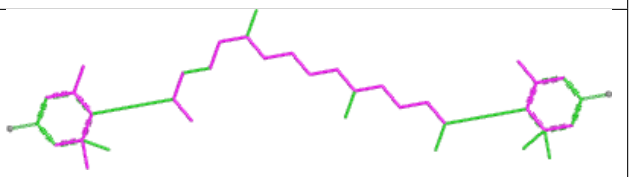


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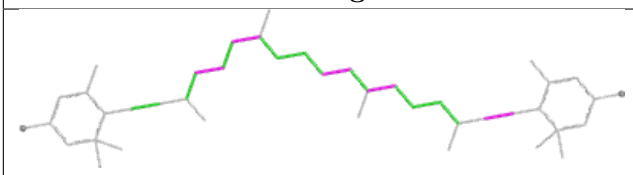
Ligand II0 d 316



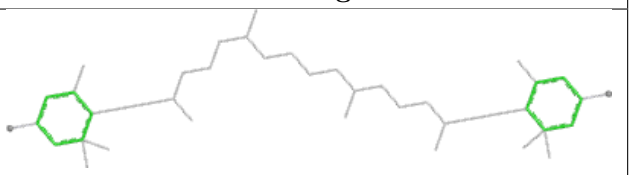
Bond lengths



Bond angles

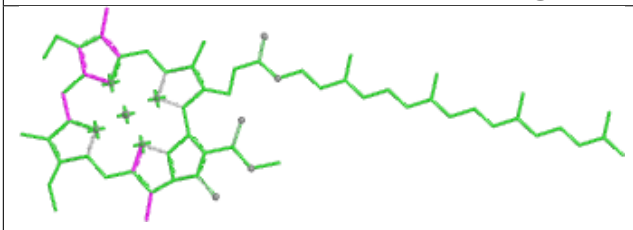


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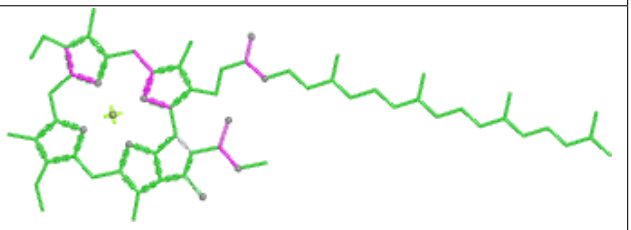


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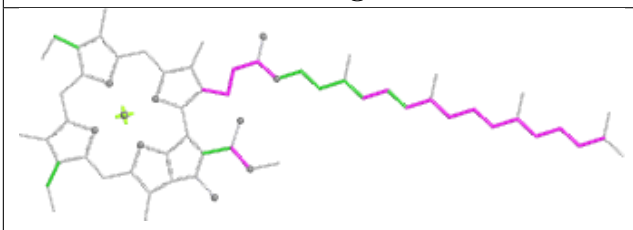
Ligand CLA f 613



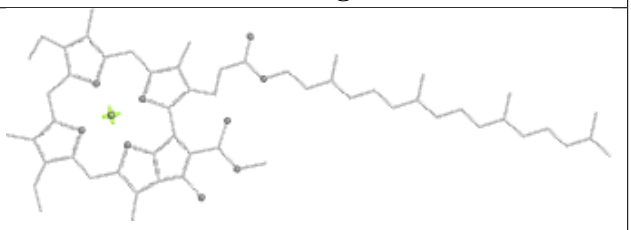
Bond lengths



Bond angles

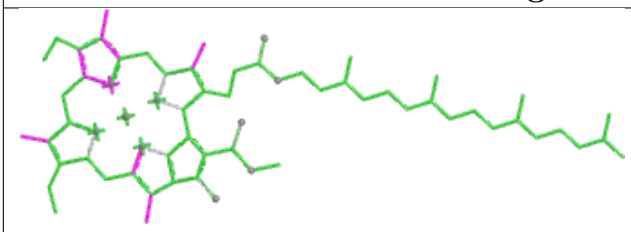


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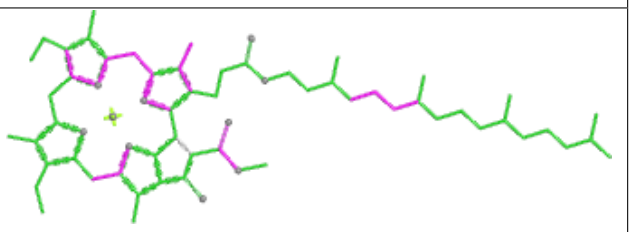


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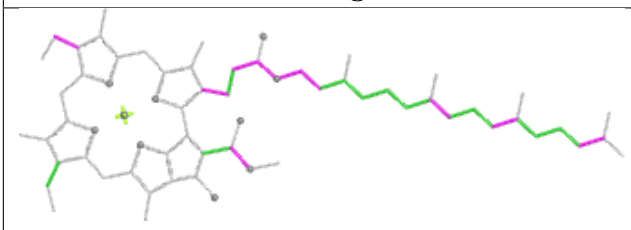
Ligand CLA h 301



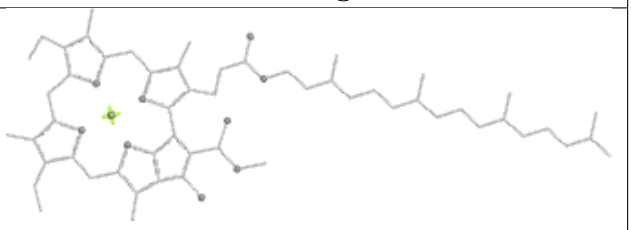
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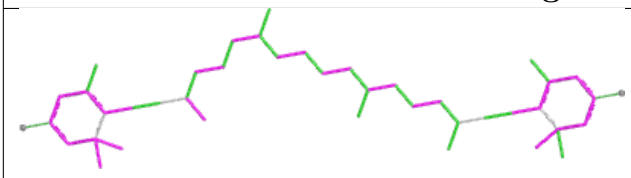


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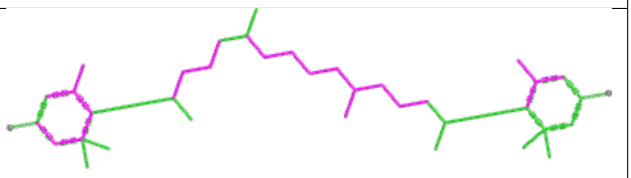


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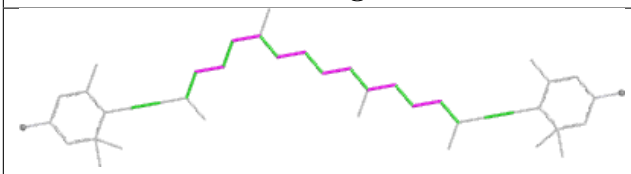
Ligand II0 k 616



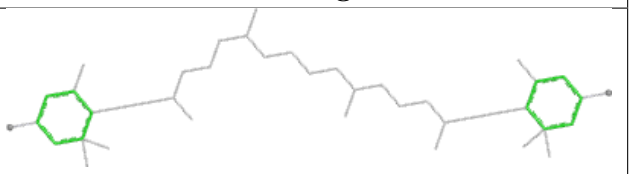
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Bond angles

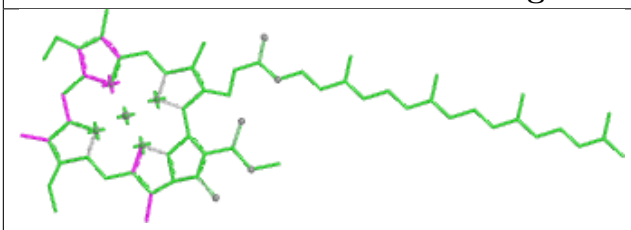


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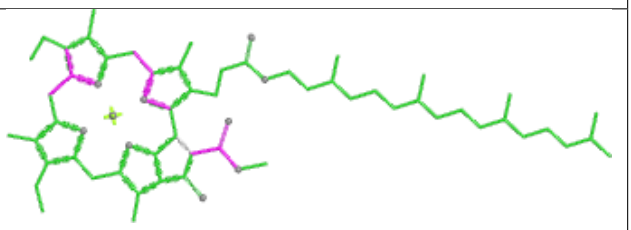


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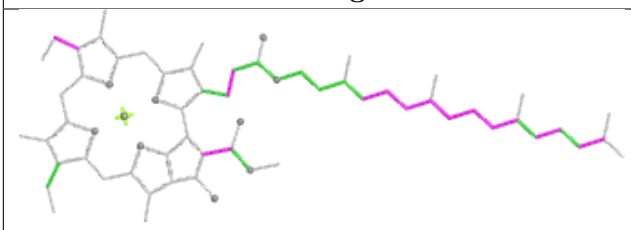
Ligand CLA b 604



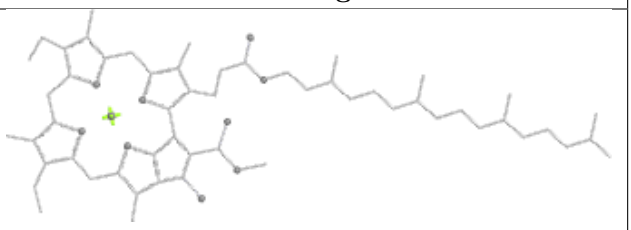
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Bond angles

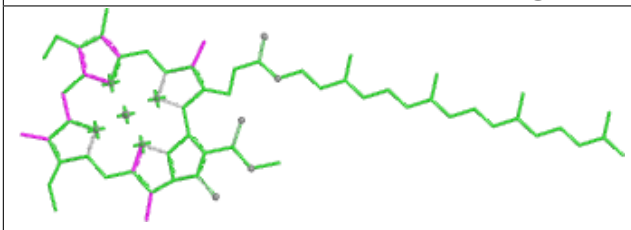


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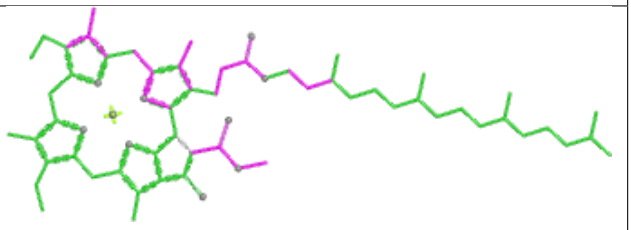


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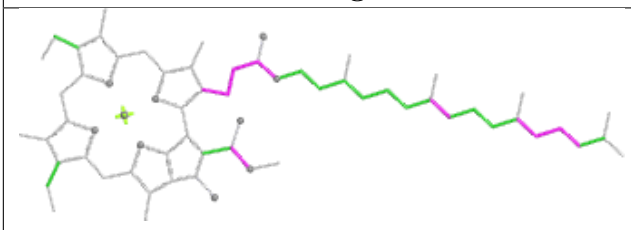
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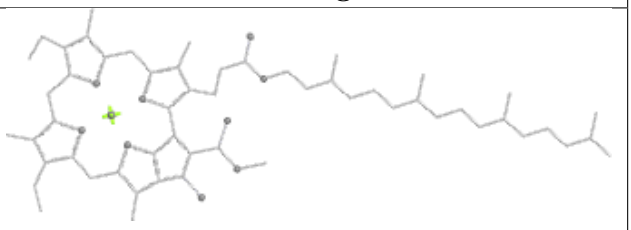
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Bond angles

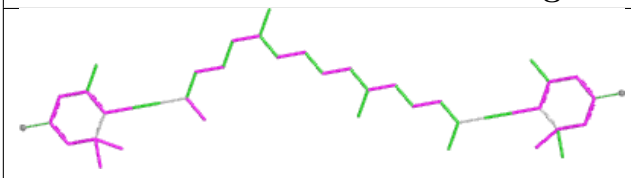


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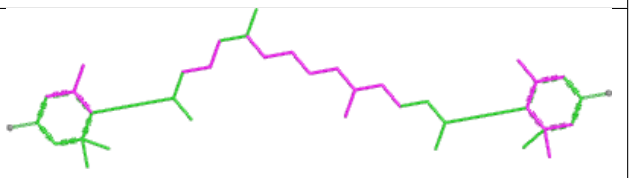


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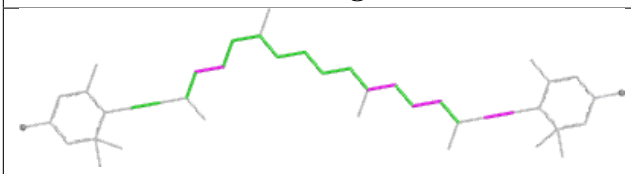
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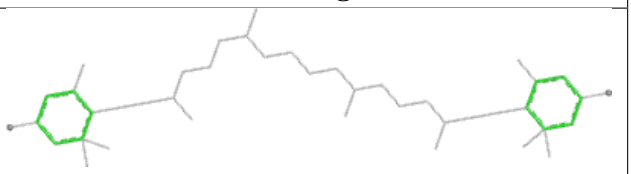
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Bond angles

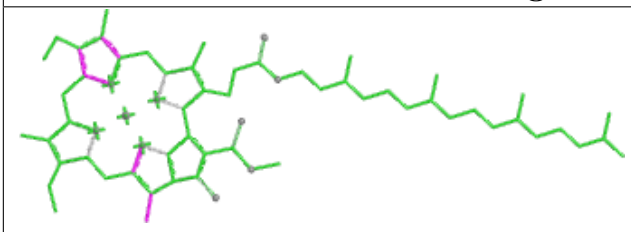


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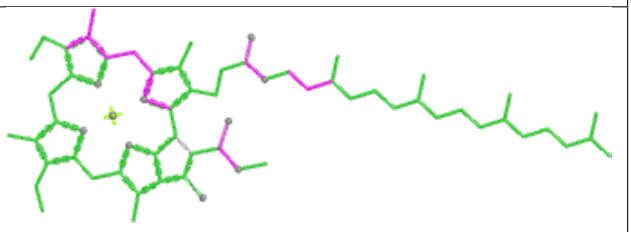


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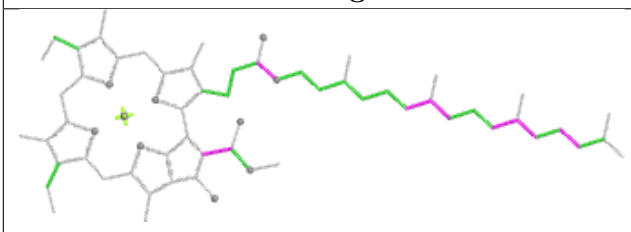
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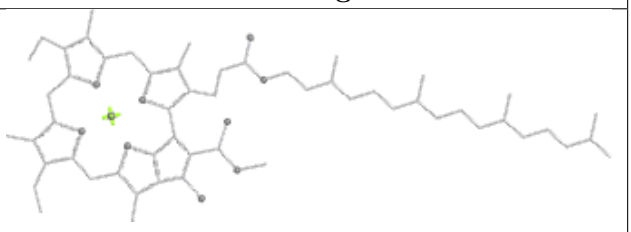
Bond lengths



Bond angles

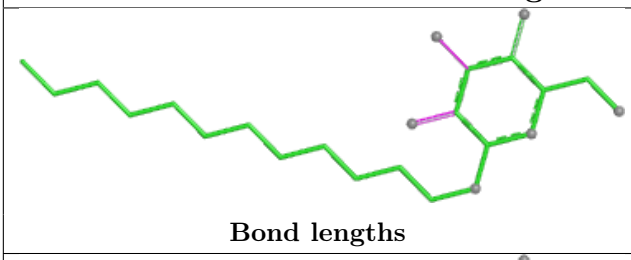


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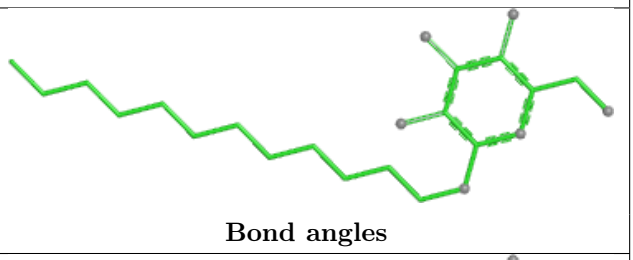


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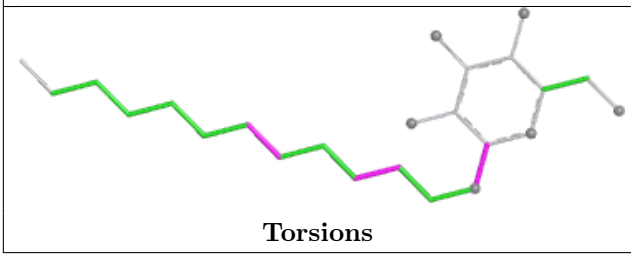
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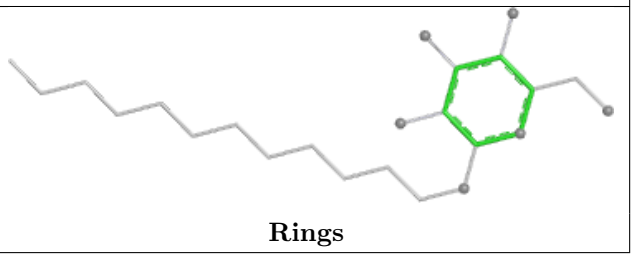
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Bond angles

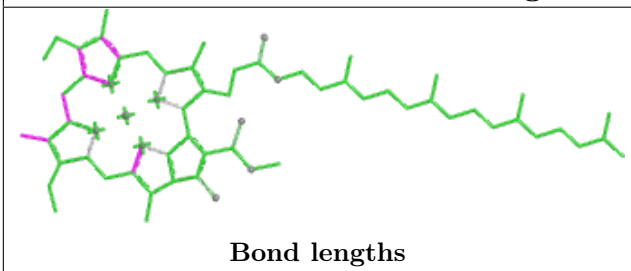


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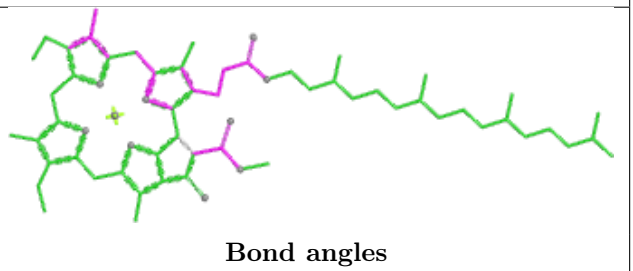


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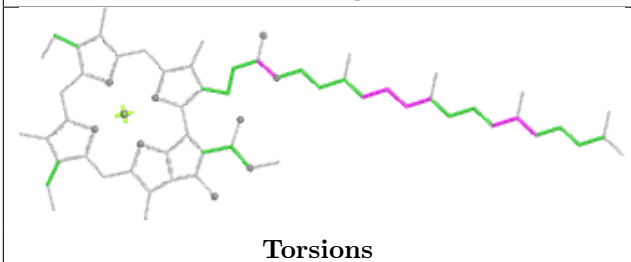
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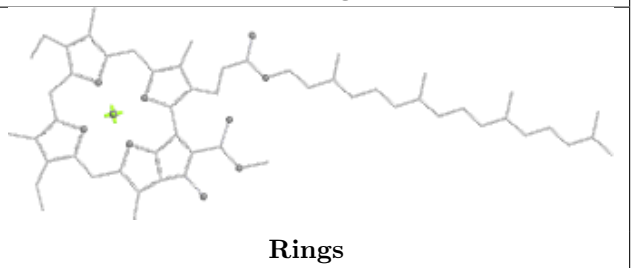
Bond lengths



Bond angles

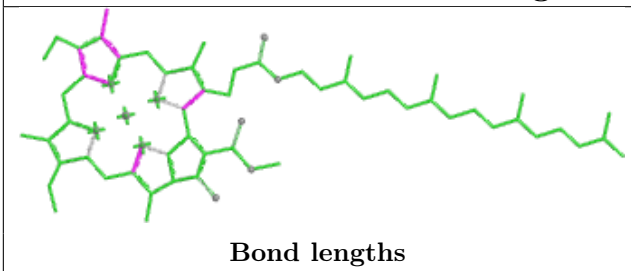


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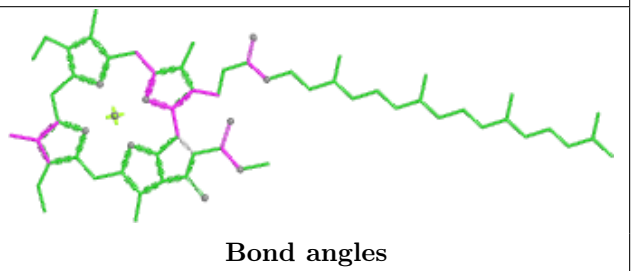


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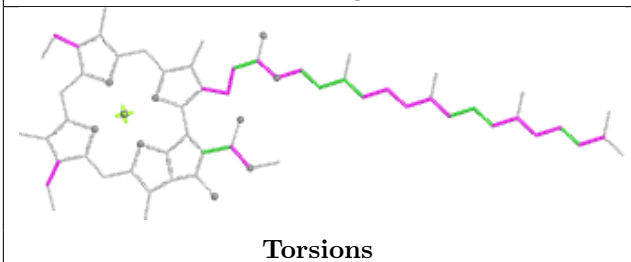
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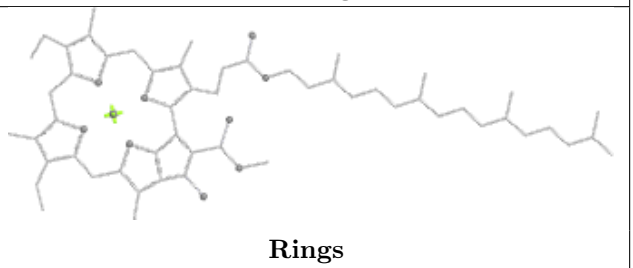
Bond lengths



Bond angles

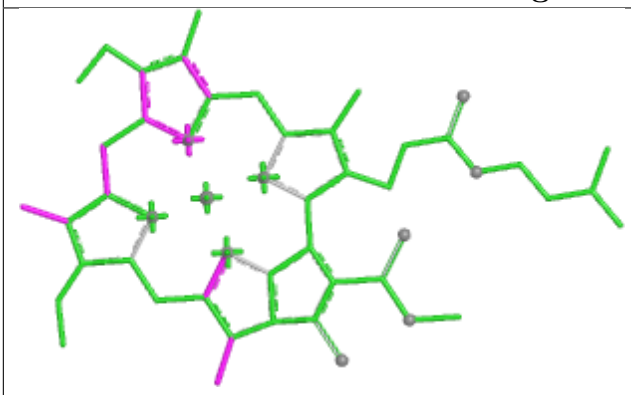


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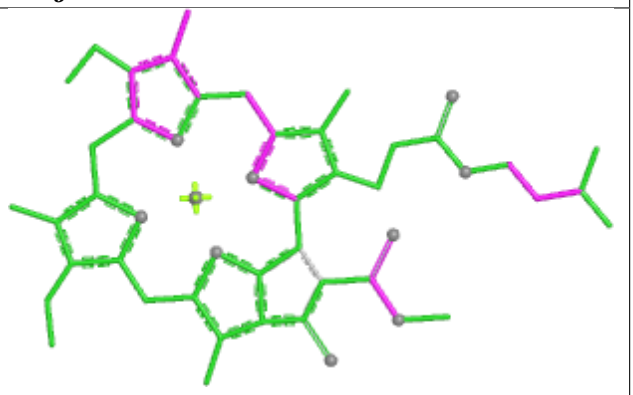


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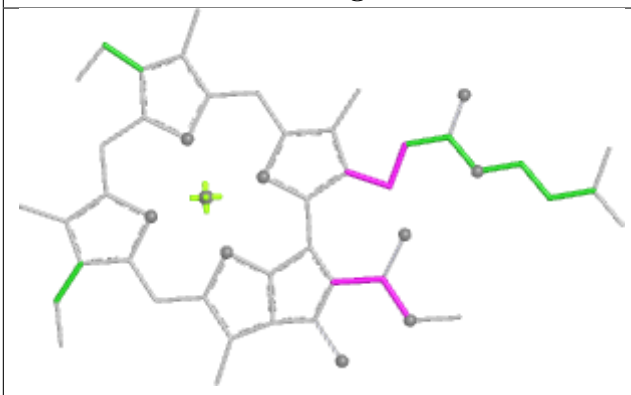
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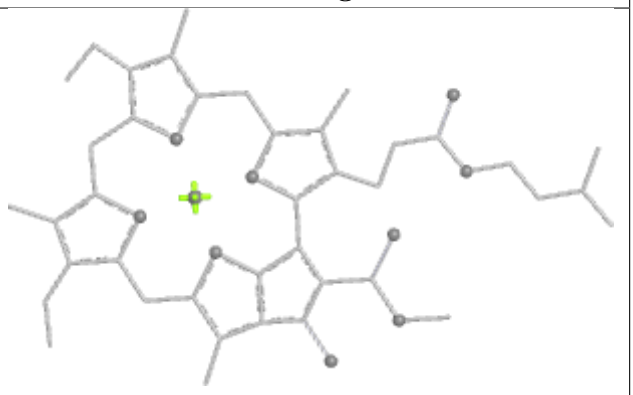
Bond lengths



Bond angles

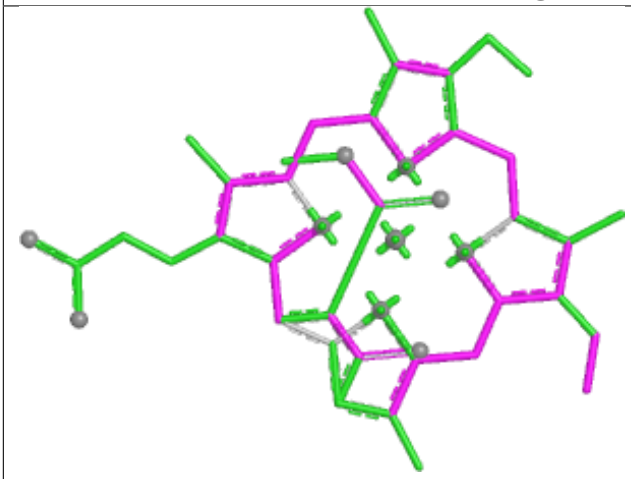


Torsions

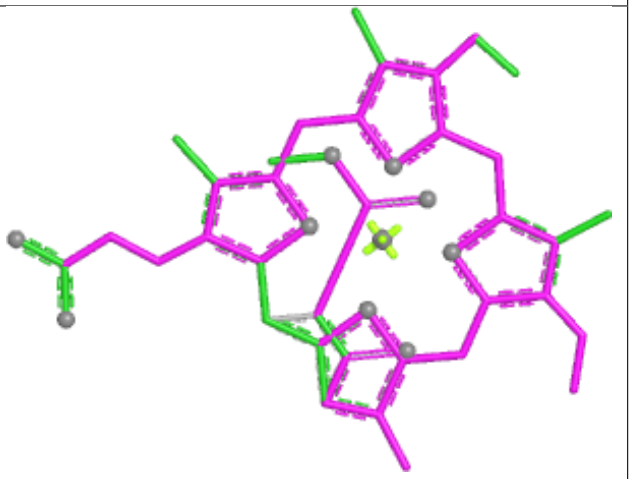


Rings

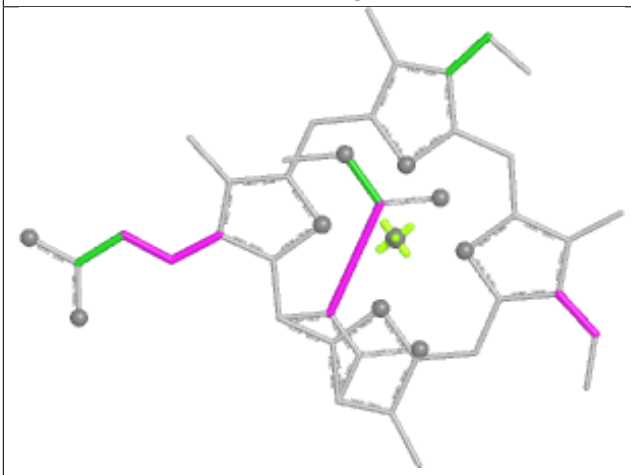
Ligand KC2 s 204



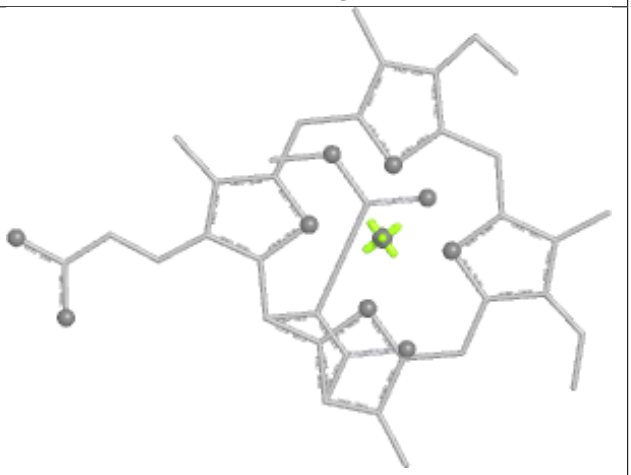
Bond lengths



Bond angles

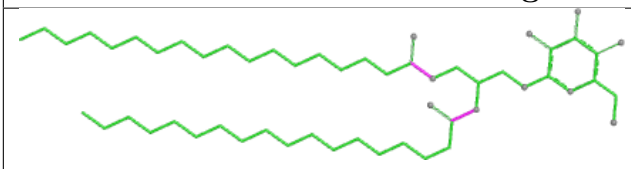


Torsions

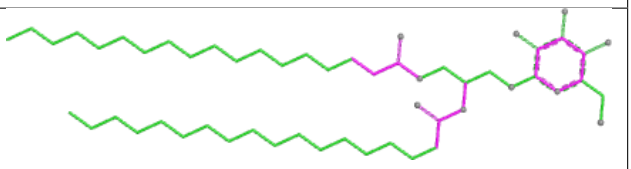


Rings

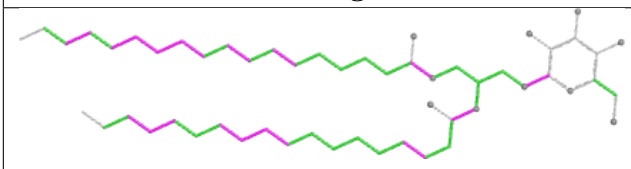
Ligand LMG L 209



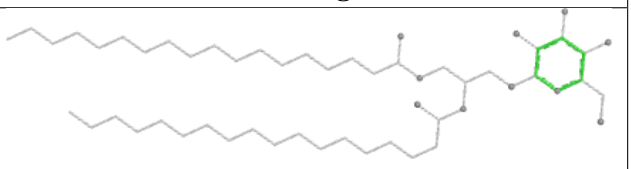
Bond lengths



Bond angles

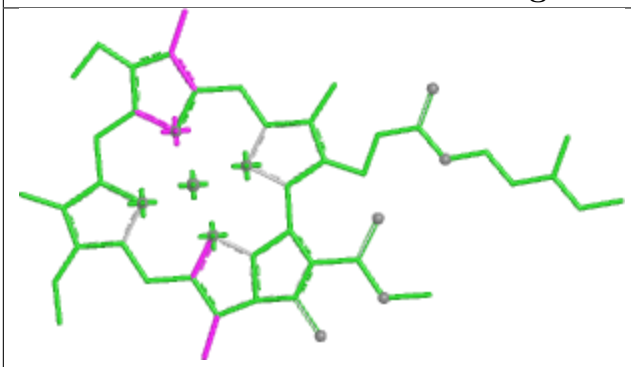


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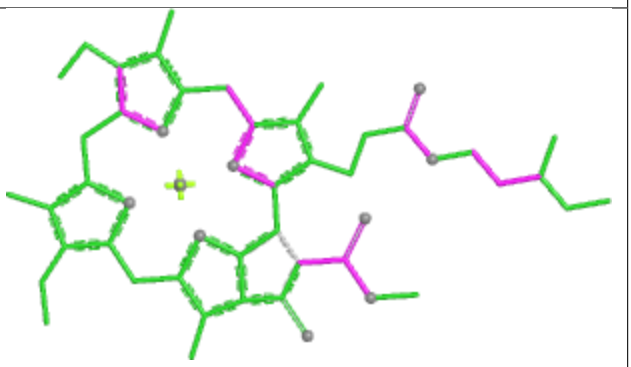


Rings

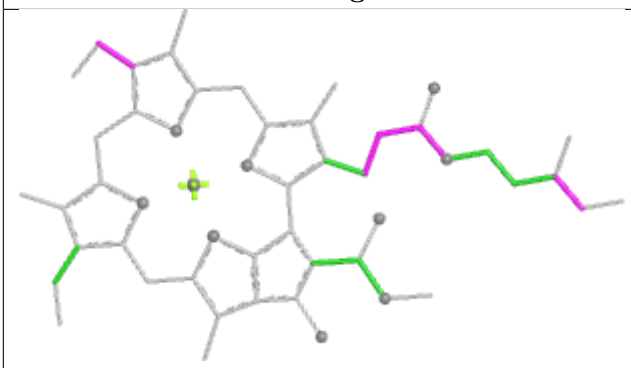
Ligand CLA c 605



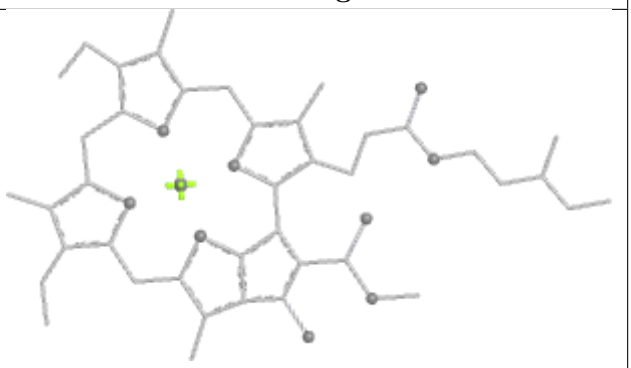
Bond lengths



Bond angles

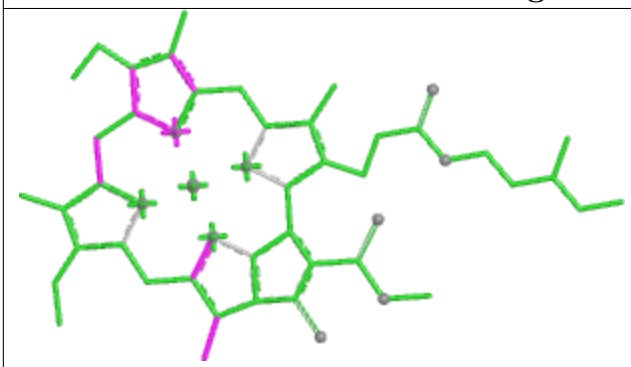


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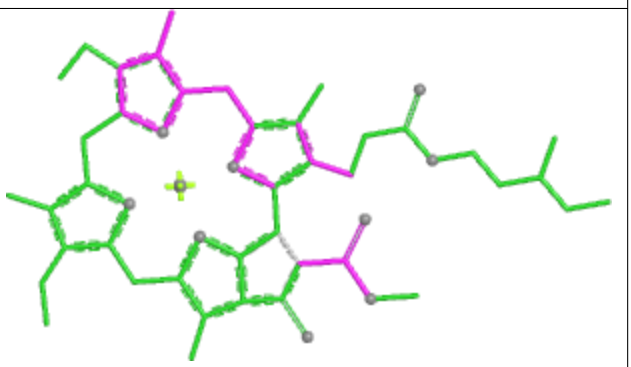


Rings

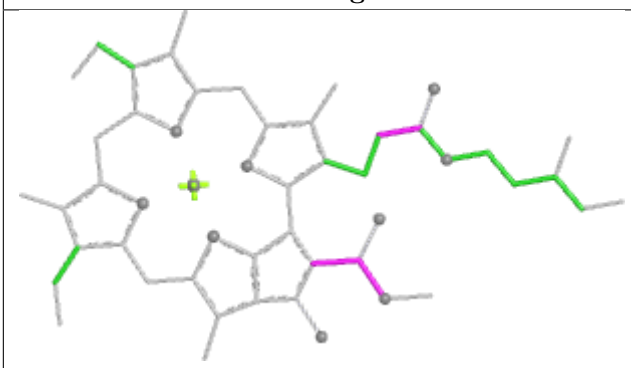
Ligand CLA d 302



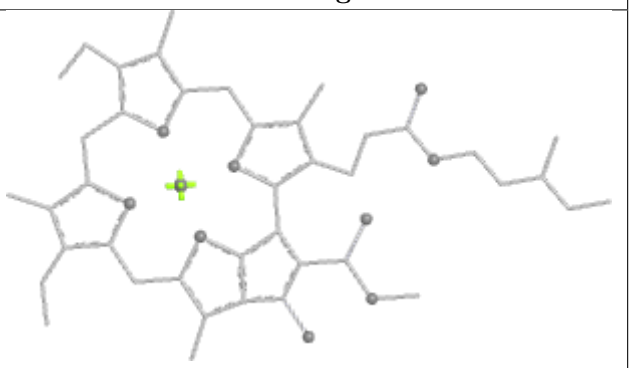
Bond lengths



Bond angles

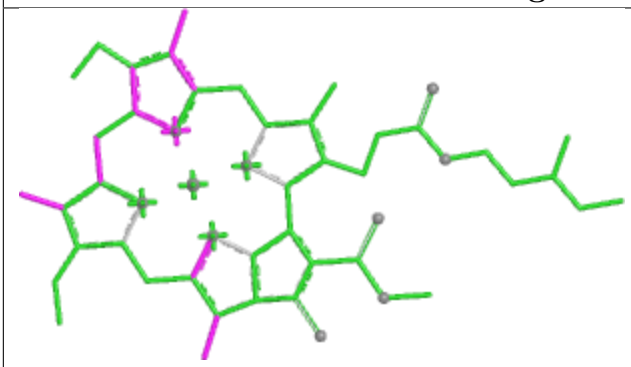


Torsions

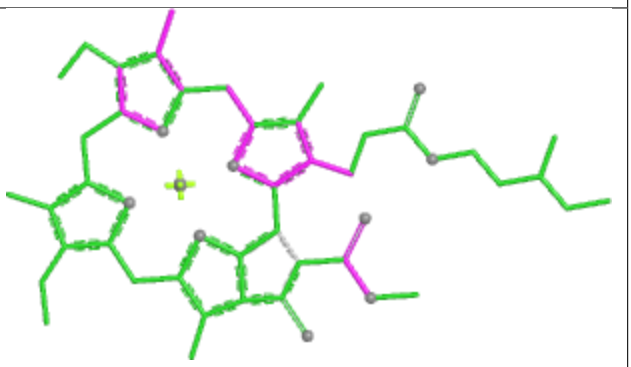


Rings

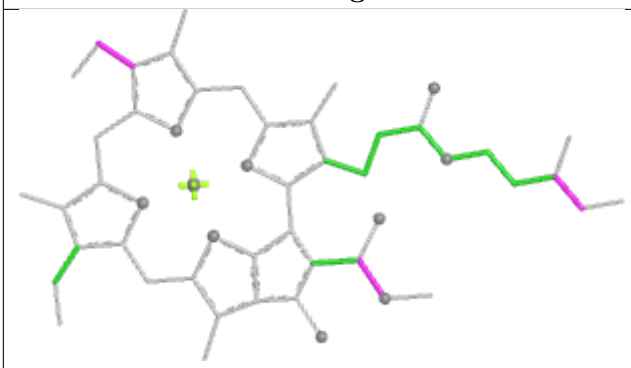
Ligand CLA a 305



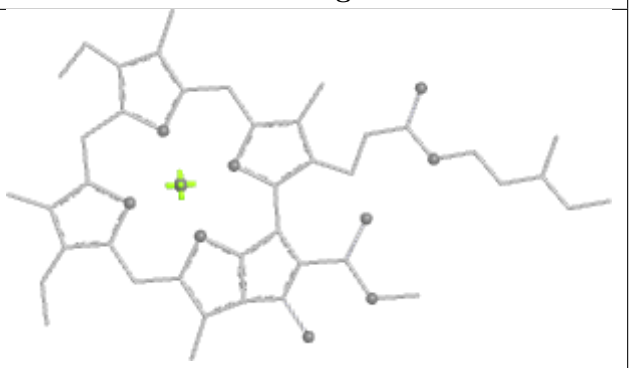
Bond lengths



Bond angles

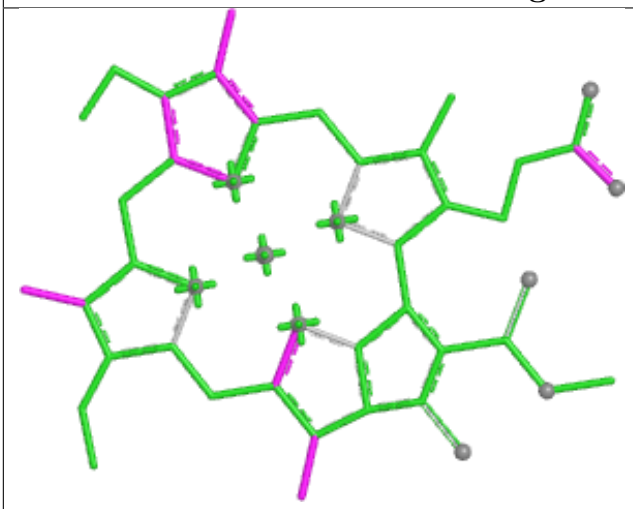


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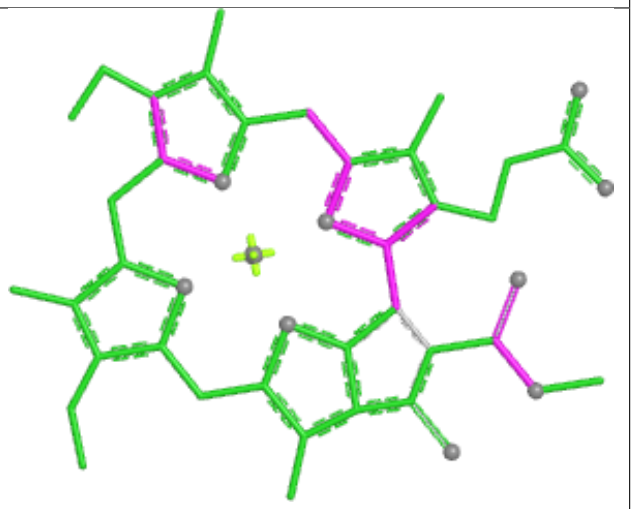


Rings

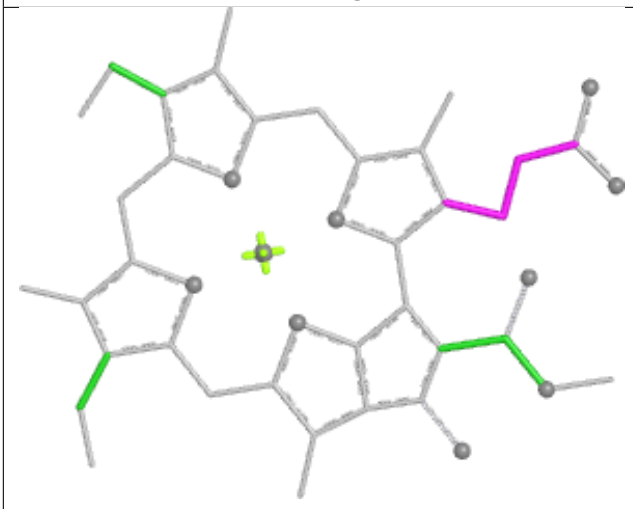
Ligand CLA e 601



Bond lengths



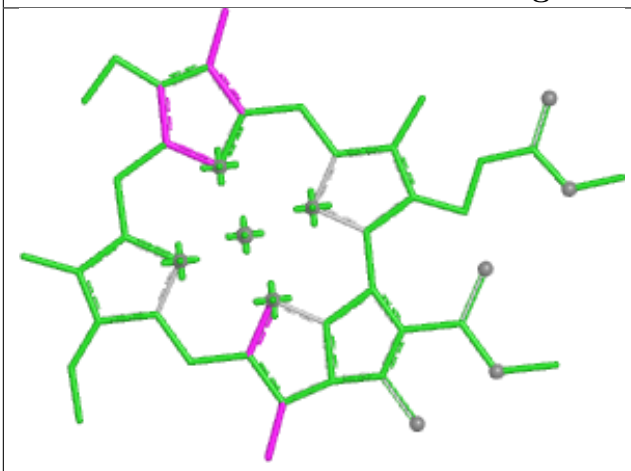
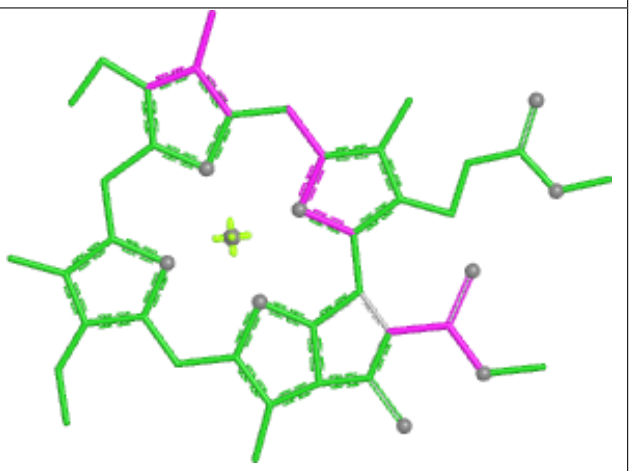
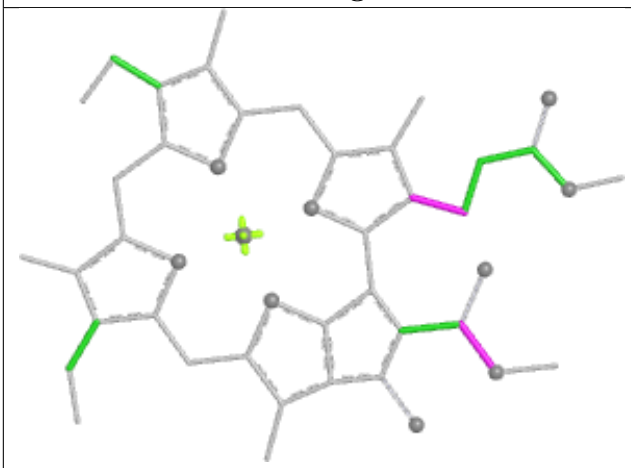
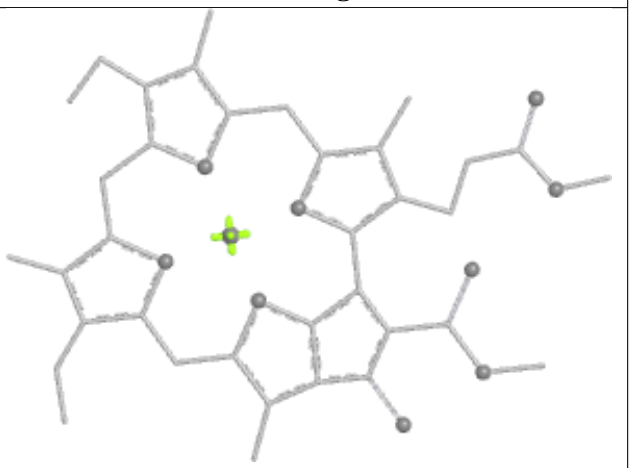
Bond angles

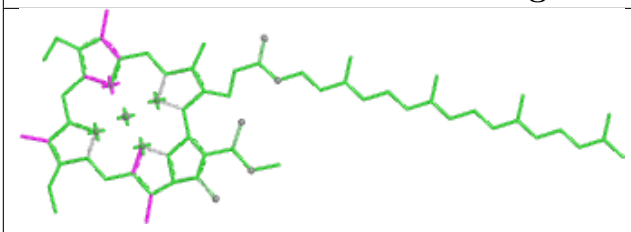
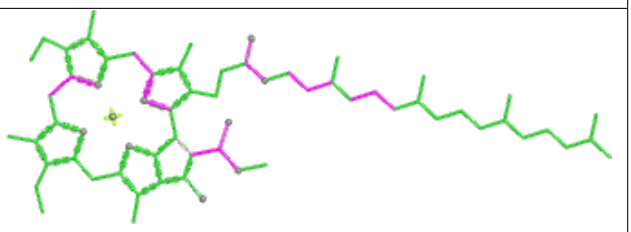
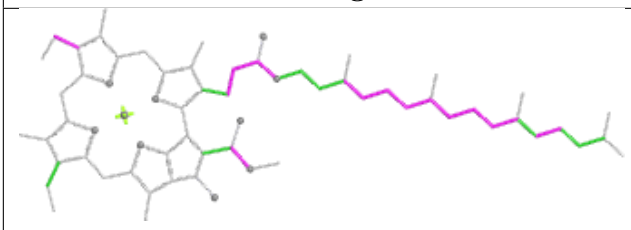
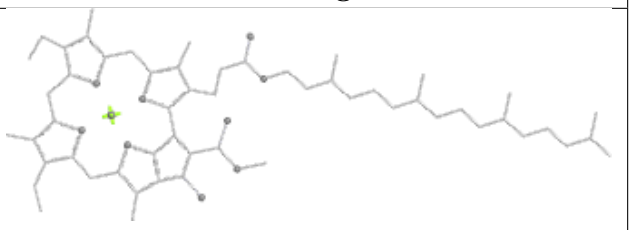


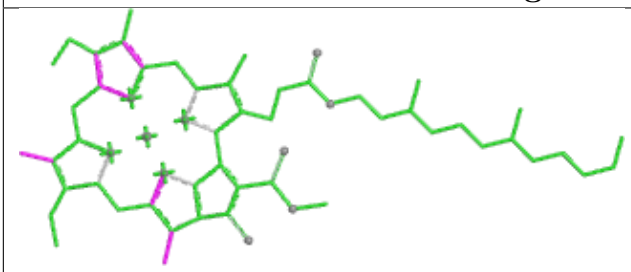
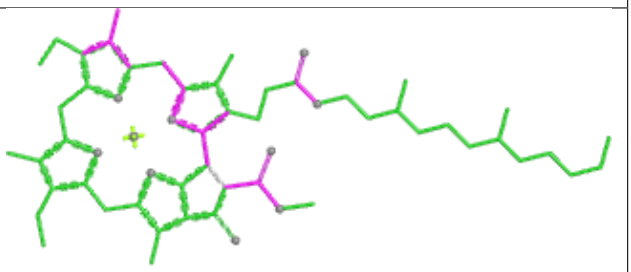
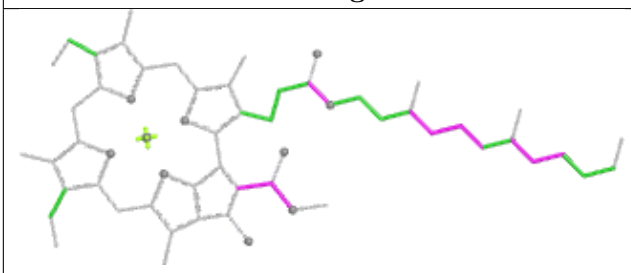
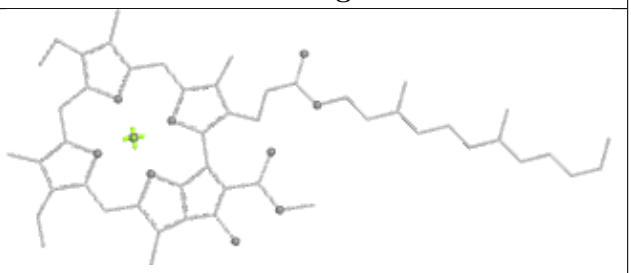
Torsions

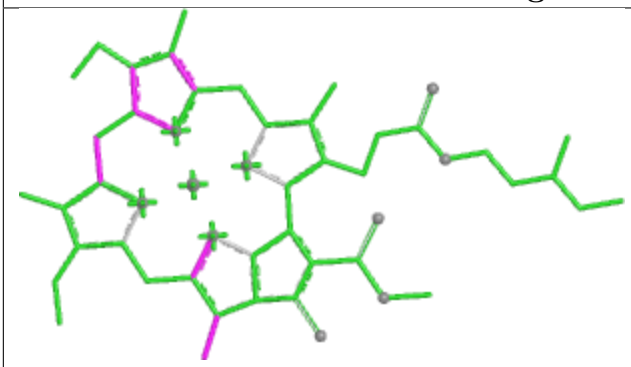
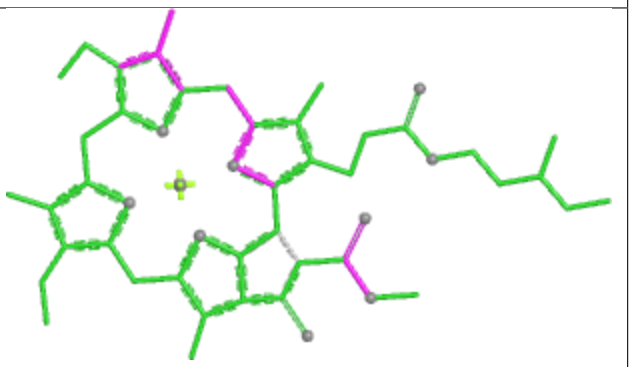
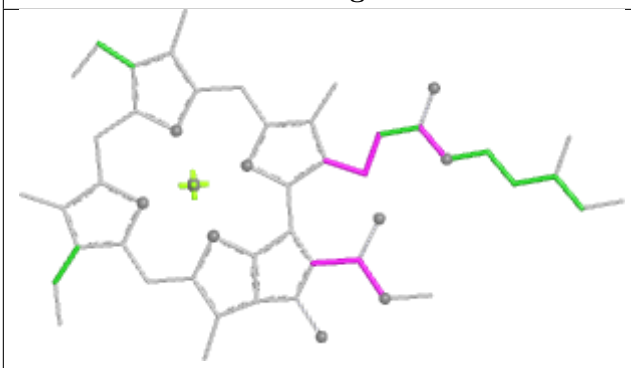
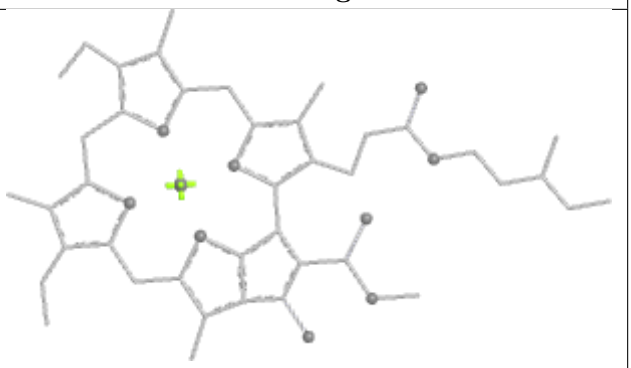


Rings

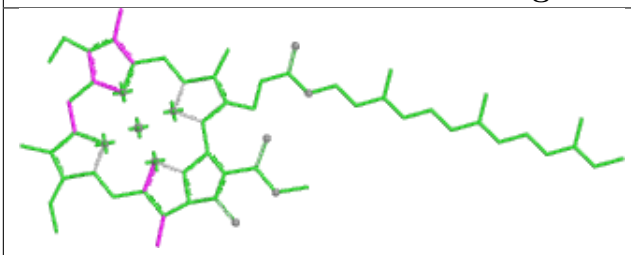
Ligand CLA i 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

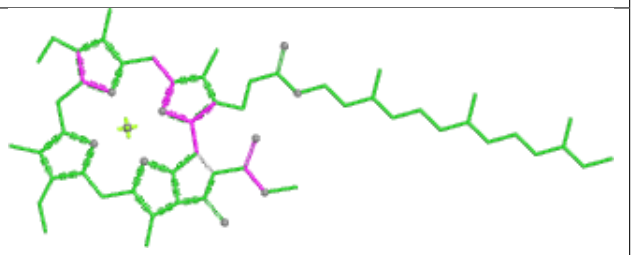
Ligand CLA B 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

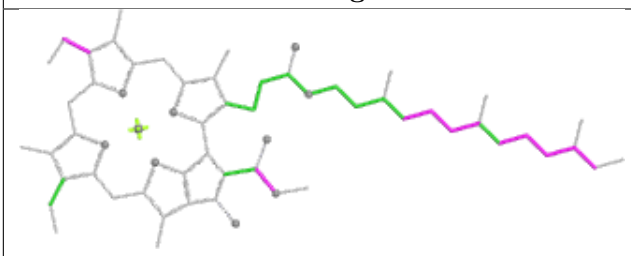
Ligand CLA l 309



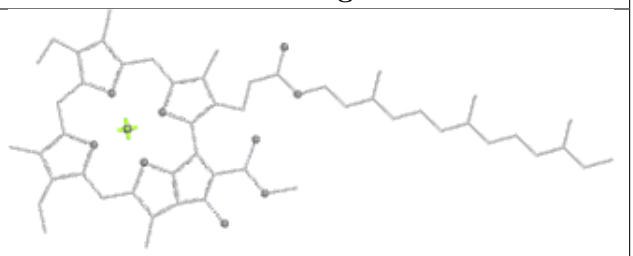
Bond lengths



Bond angles

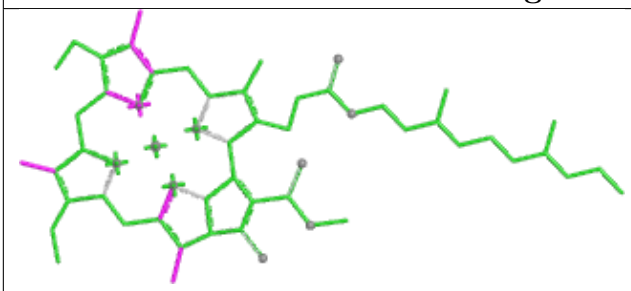


Torsions

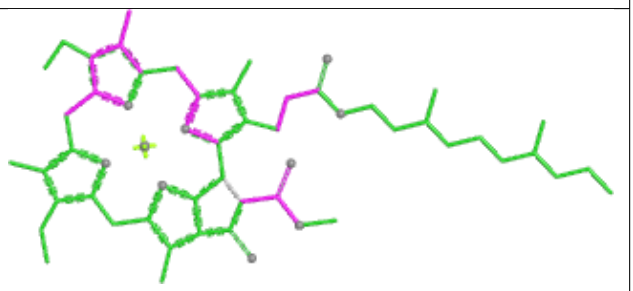


Rings

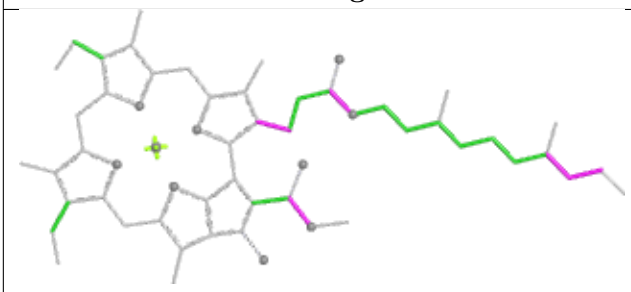
Ligand CLA B 816



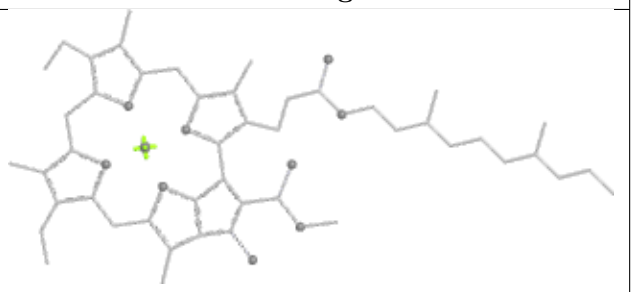
Bond lengths



Bond angles

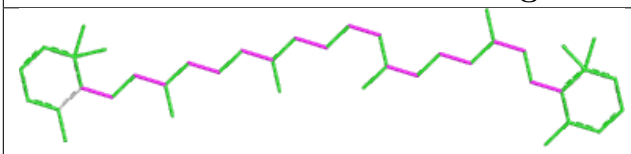


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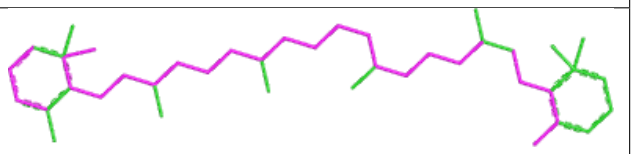


Rings

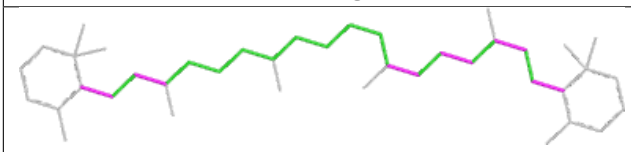
Ligand WVN e 615



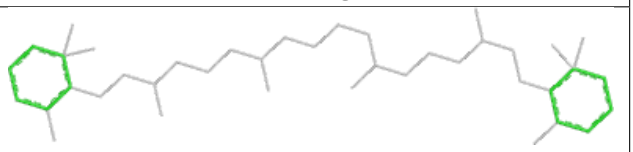
Bond lengths



Bond angles

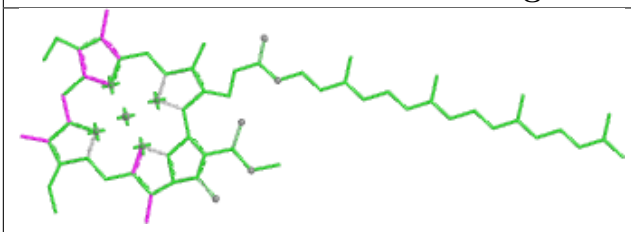


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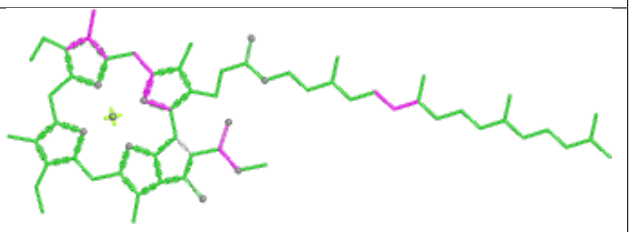


Rings

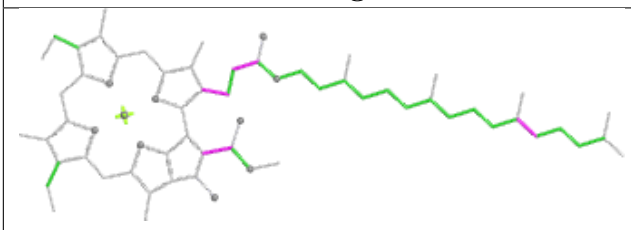
Ligand CLA A 804



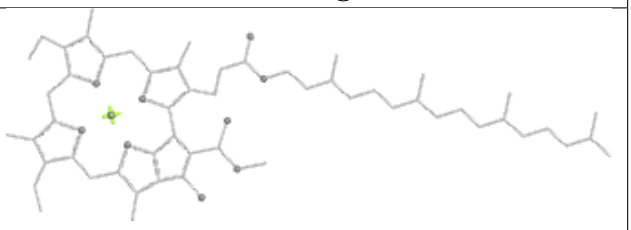
Bond lengths



Bond angles

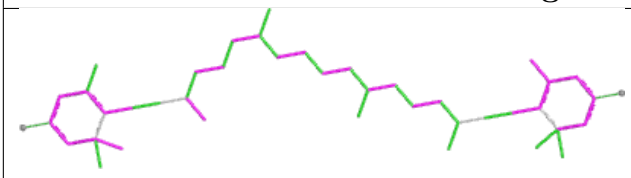


Torsions

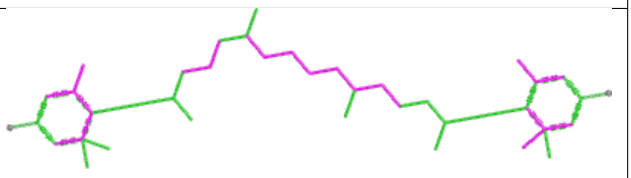


Rings

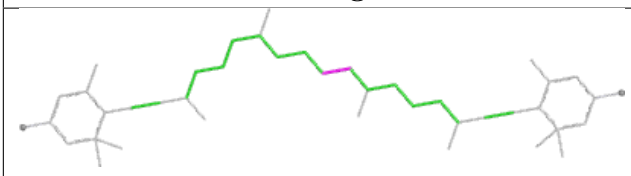
Ligand II0 n 614



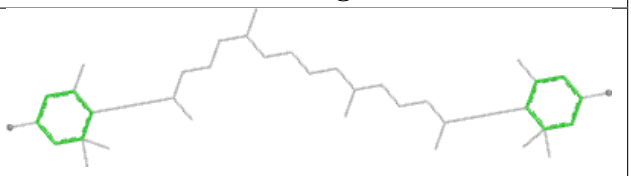
Bond lengths



Bond angles

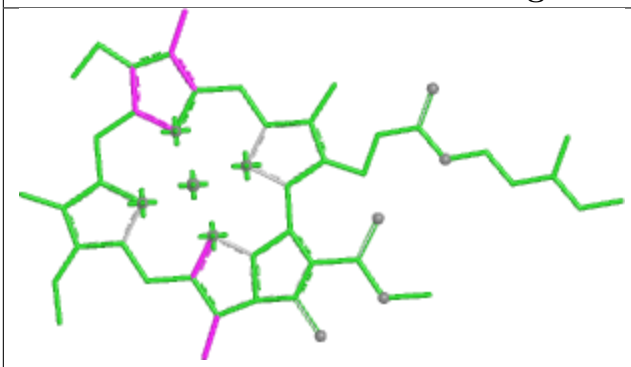


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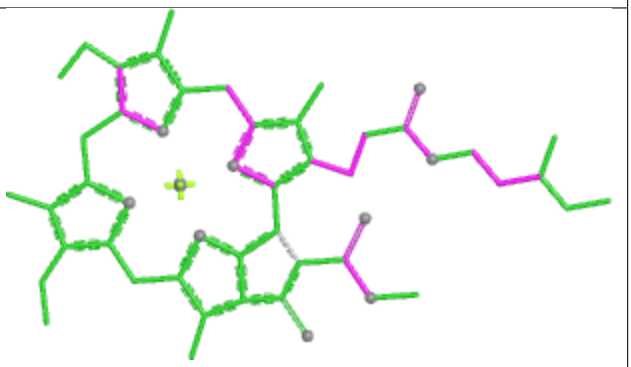


Rings

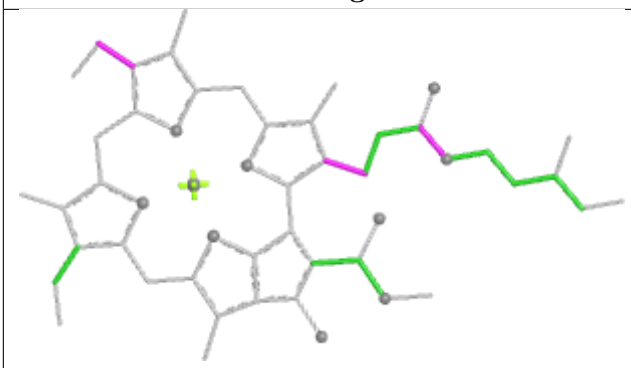
Ligand CLA n 606



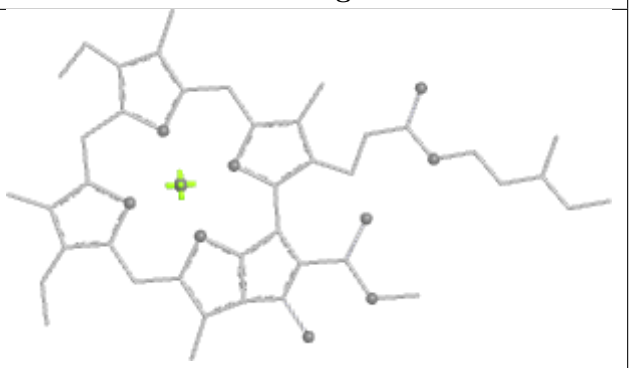
Bond lengths



Bond angles

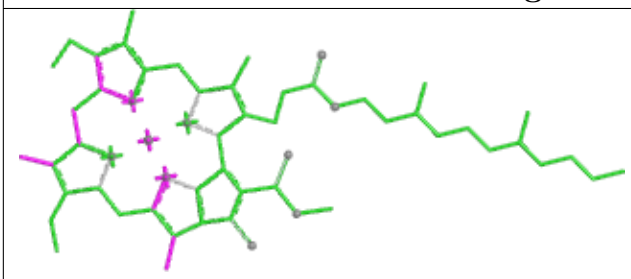


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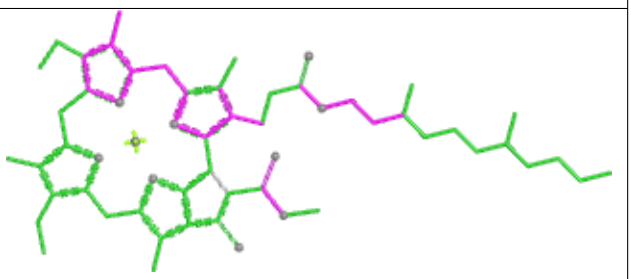


Rings

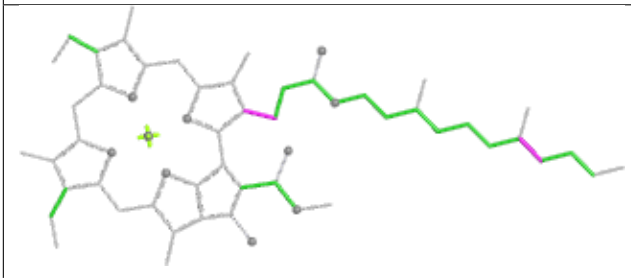
Ligand CLA B 832



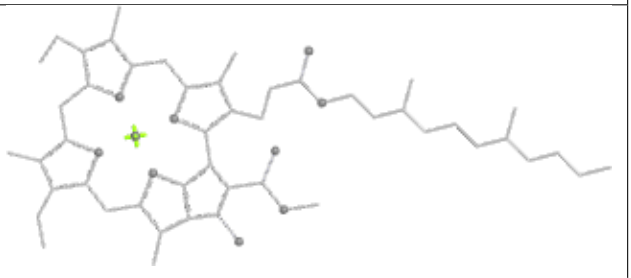
Bond lengths



Bond angles

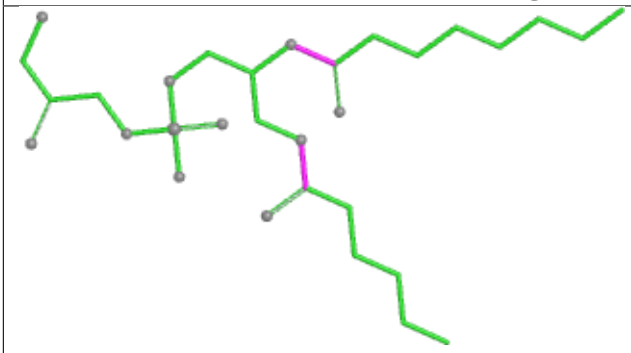


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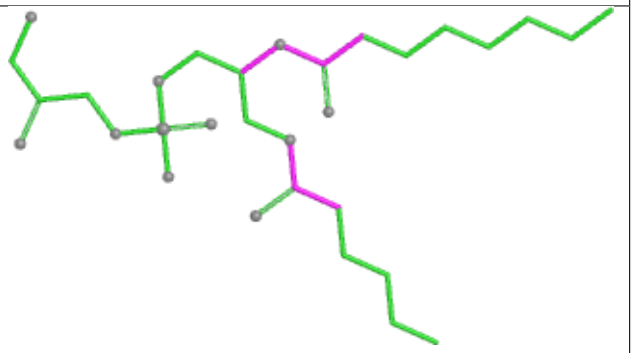


Rings

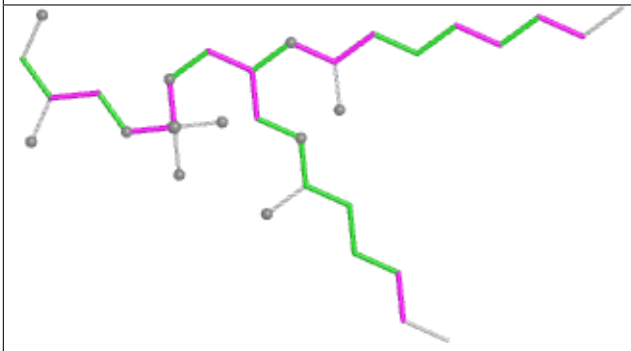
Ligand LHG b 620



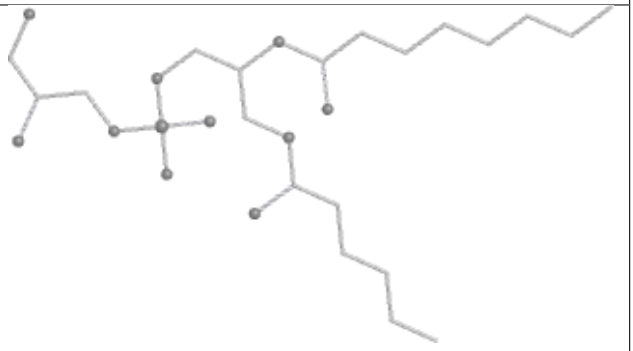
Bond lengths



Bond angles

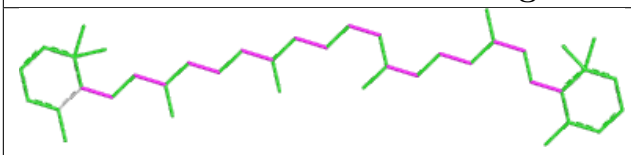


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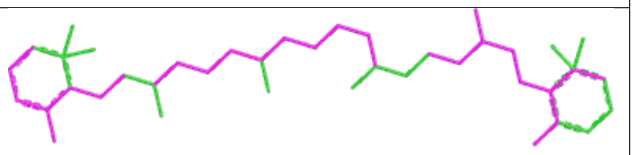


Rings

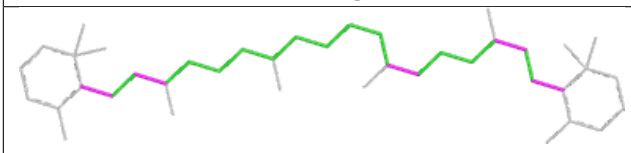
Ligand WVN J 102



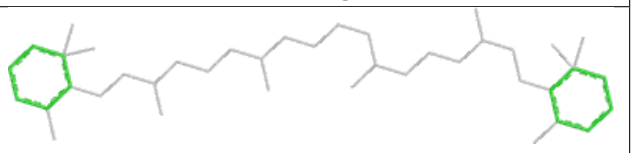
Bond lengths



Bond angles

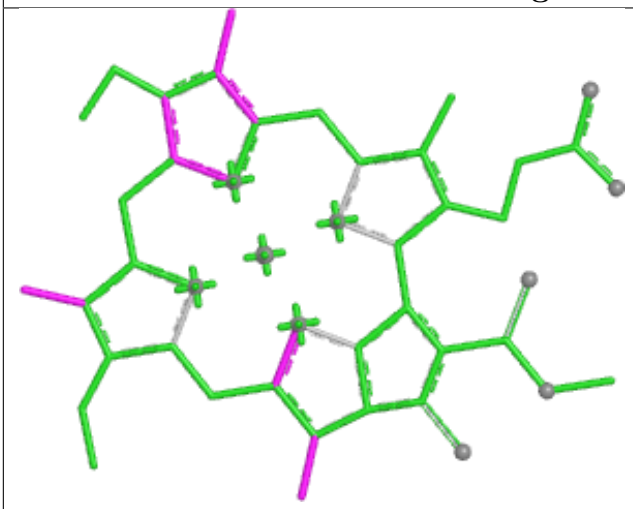


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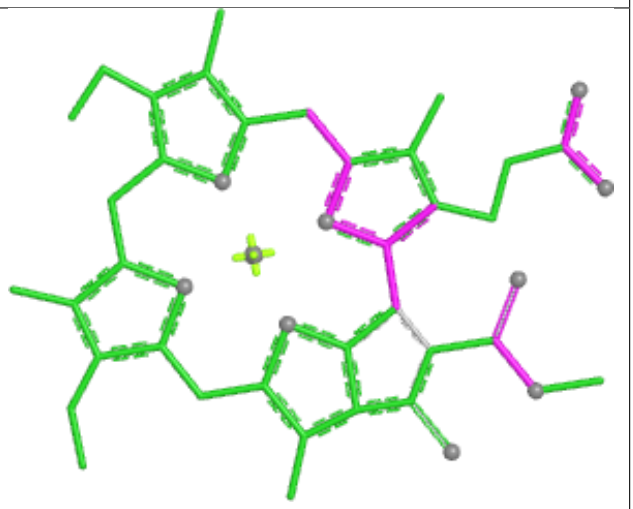


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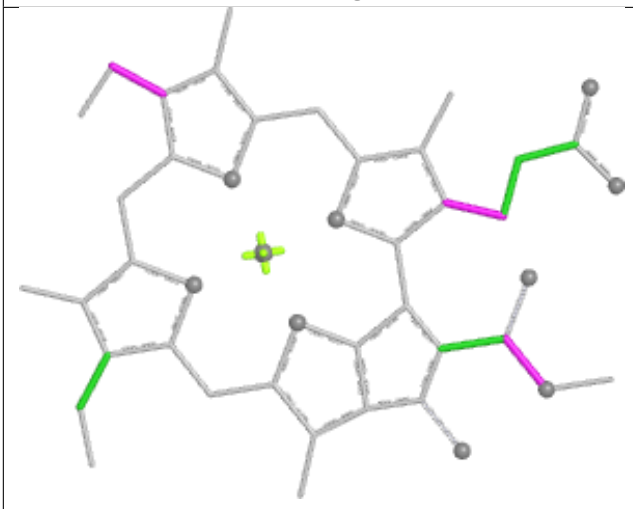
Ligand CLA f 605



Bond lengths



Bond angles

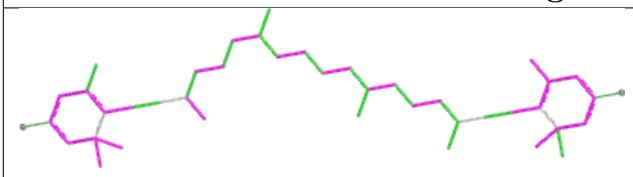


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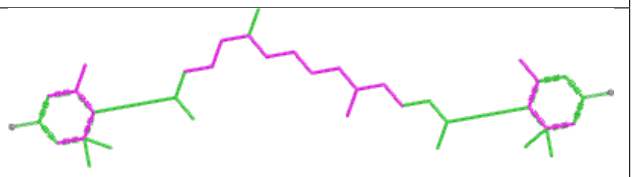


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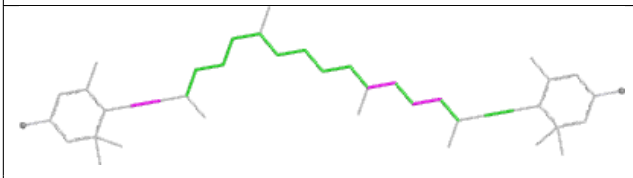
Ligand II0 l 312



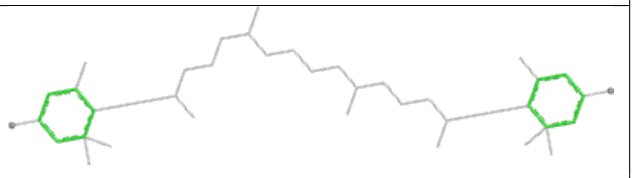
Bond lengths



Bond angles

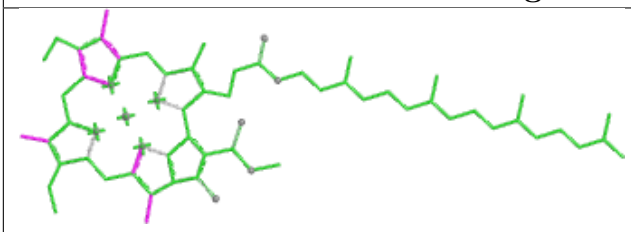


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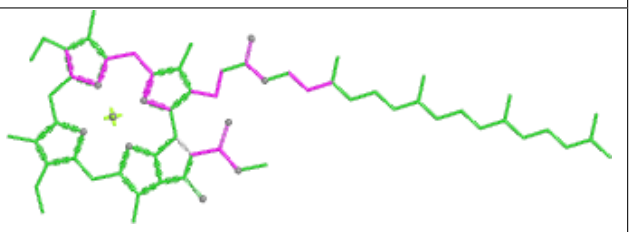


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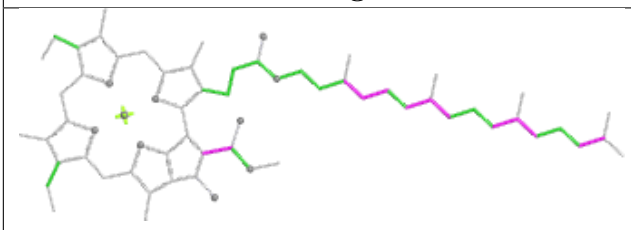
Ligand CLA B 807



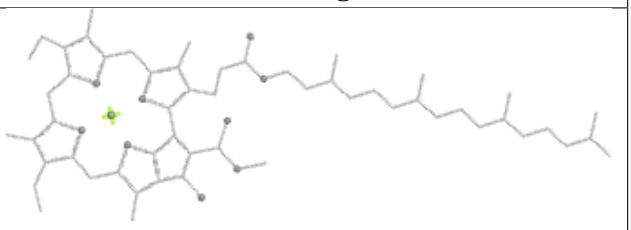
Bond lengths



Bond angles

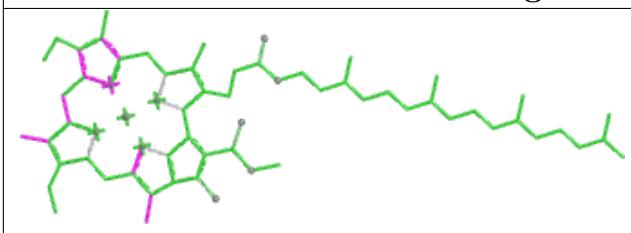


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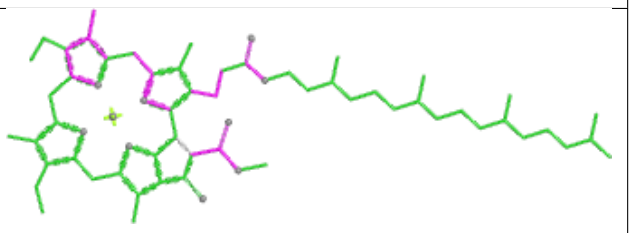


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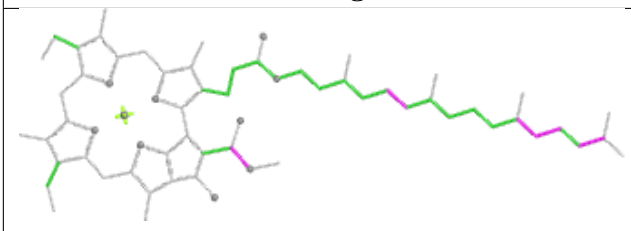
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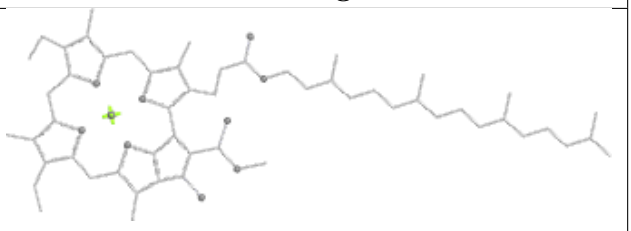
Bond lengths



Bond angles

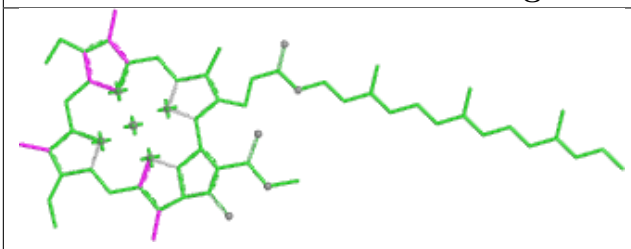


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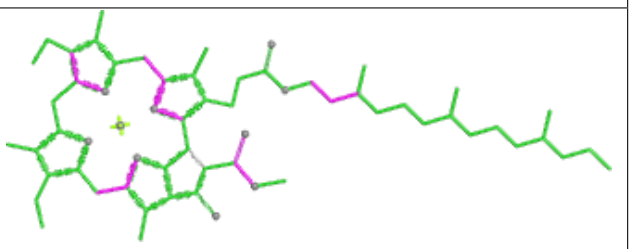


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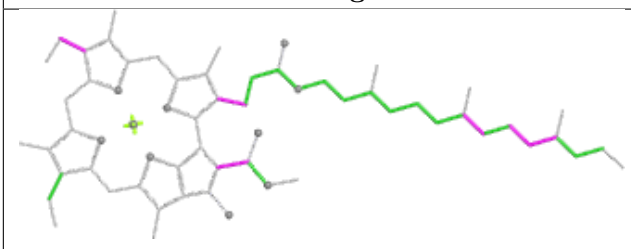
Ligand CLA A 810



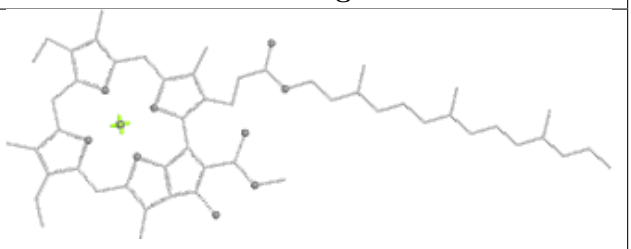
Bond lengths



Bond angles

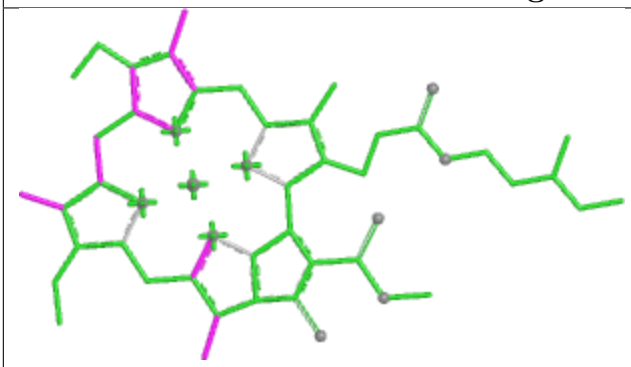


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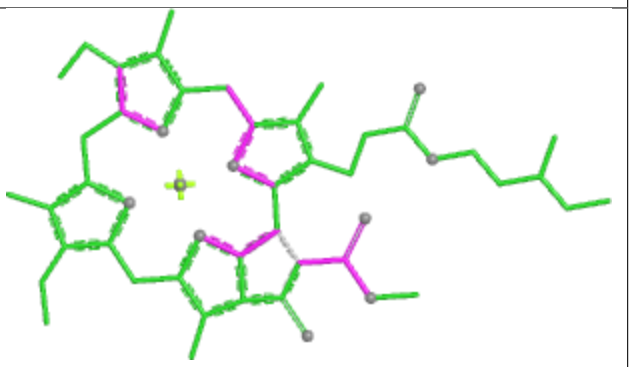


Rings

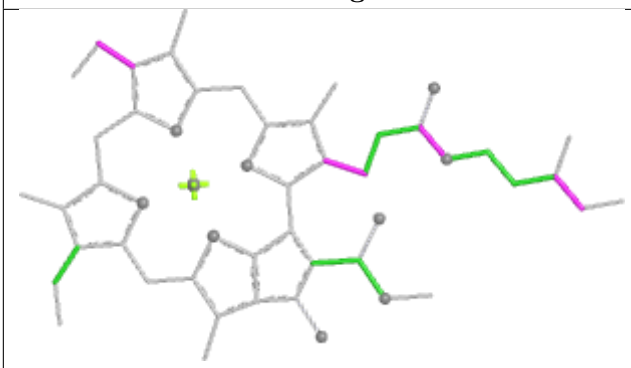
Ligand CLA n 608



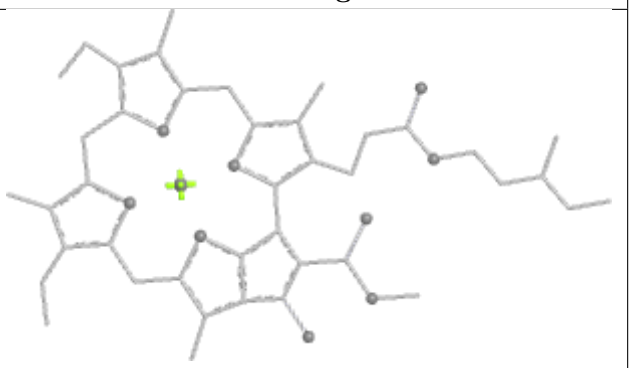
Bond lengths



Bond angles

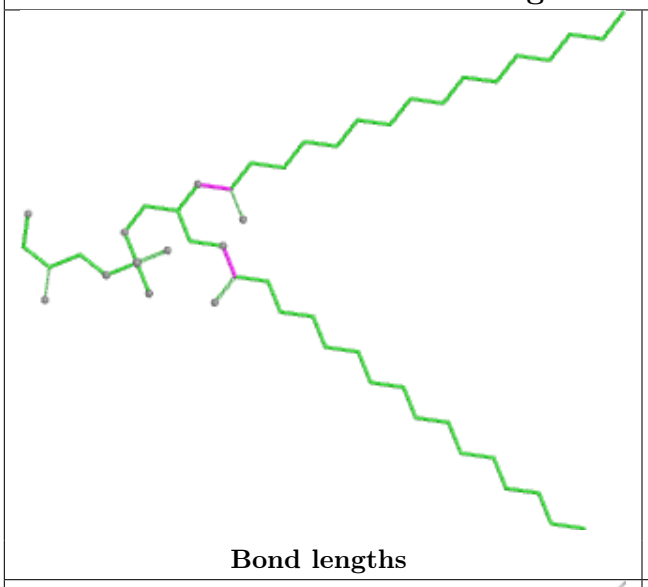


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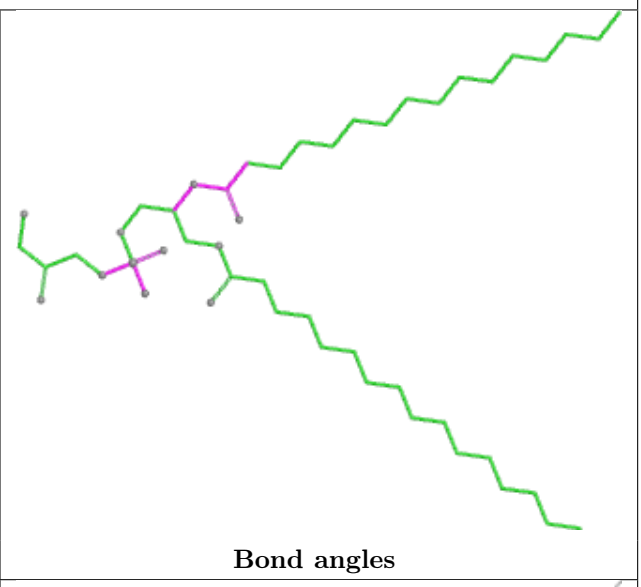


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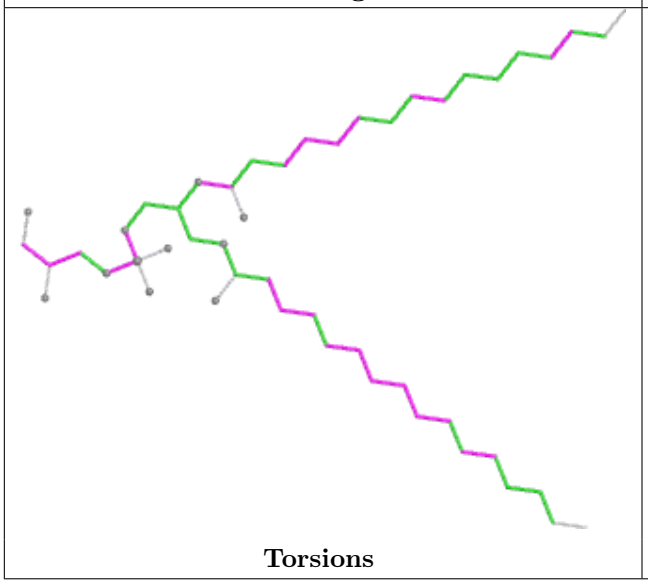
Ligand LHG b 619



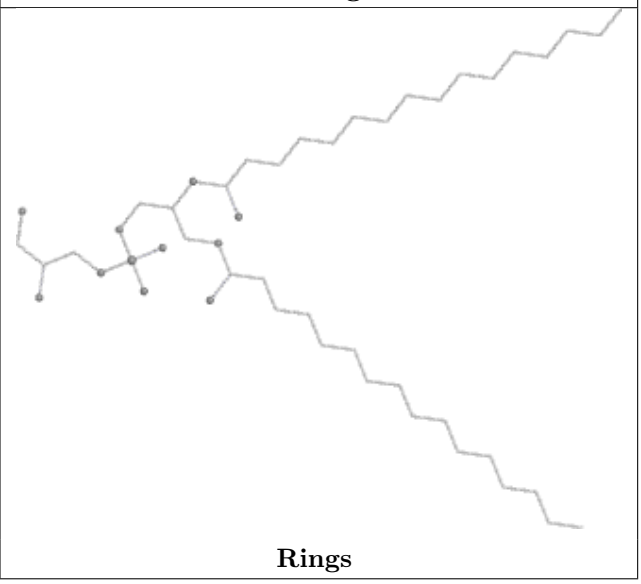
Bond lengths



Bond angles

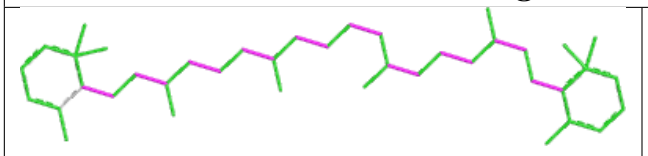


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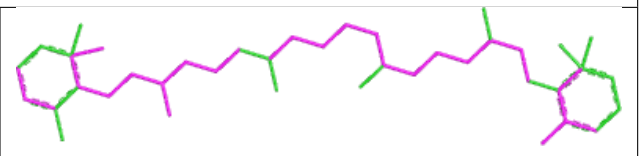


Rings

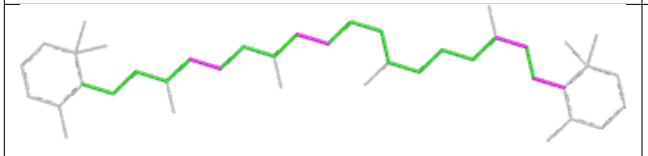
Ligand WVN K 104



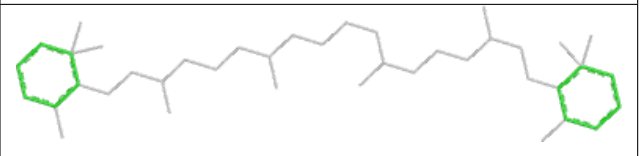
Bond lengths



Bond angles

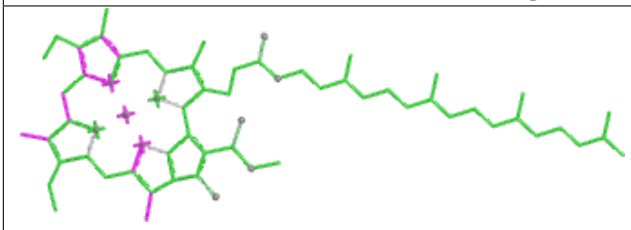


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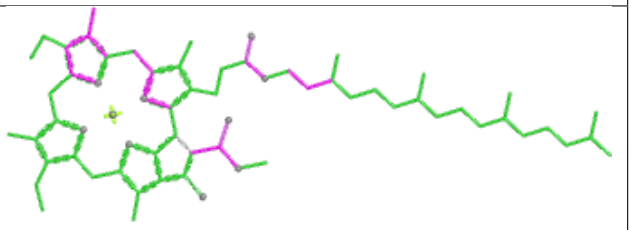


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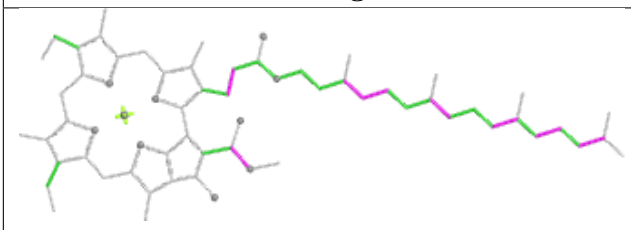
Ligand CLA B 801



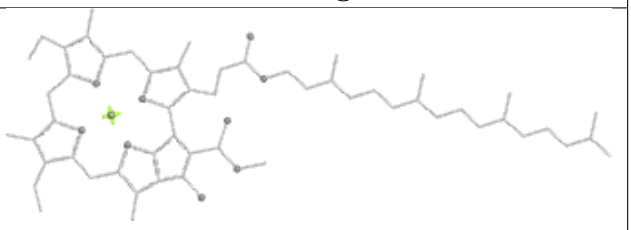
Bond lengths



Bond angles

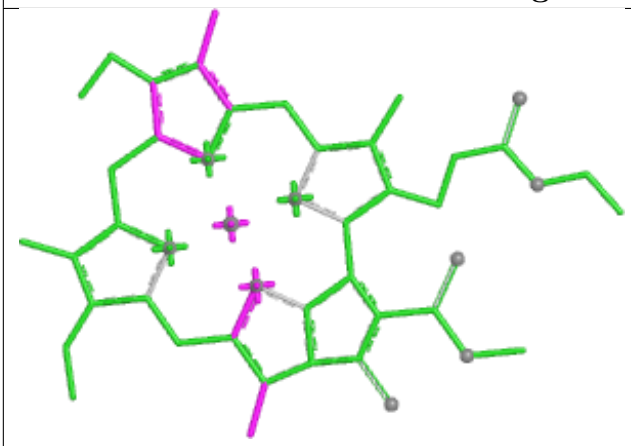


Torsions

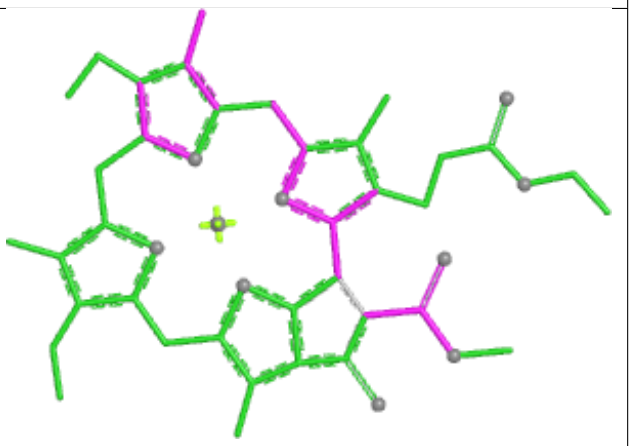


Rings

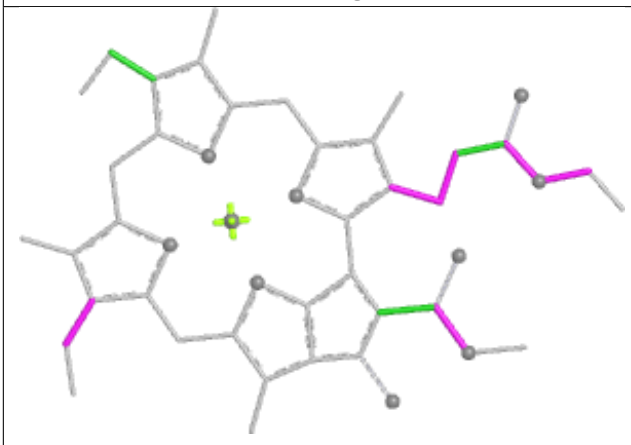
Ligand CLA f 601



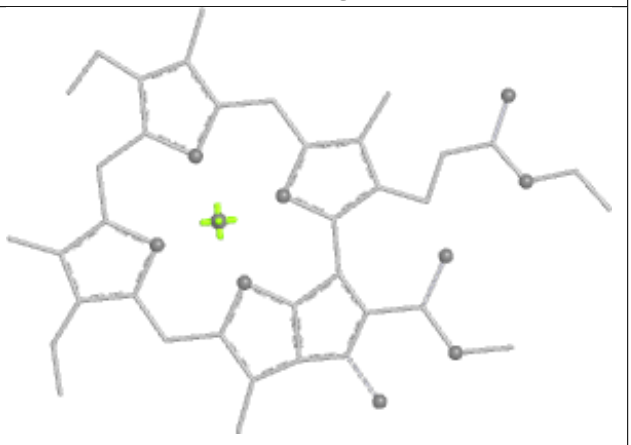
Bond lengths



Bond angles

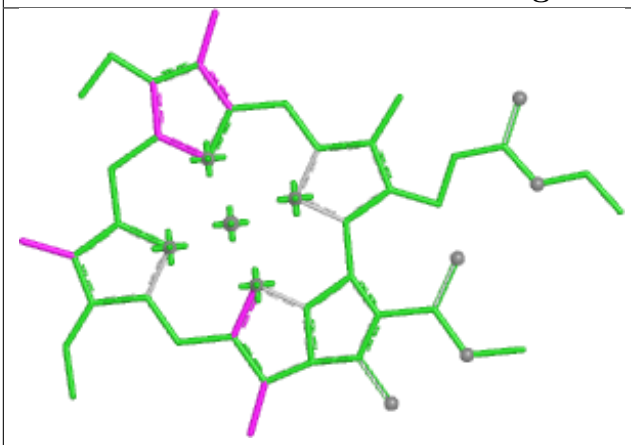


Torsions

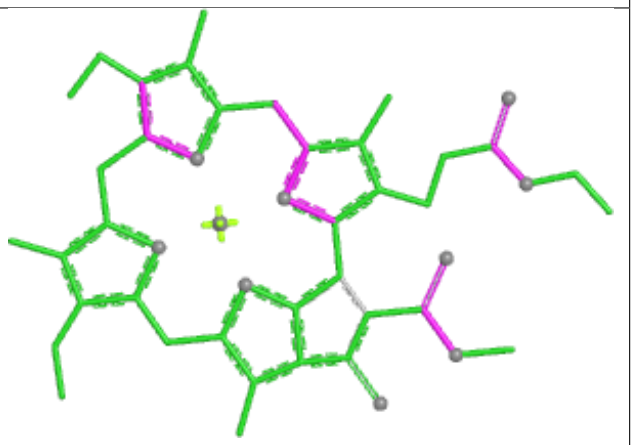


Rings

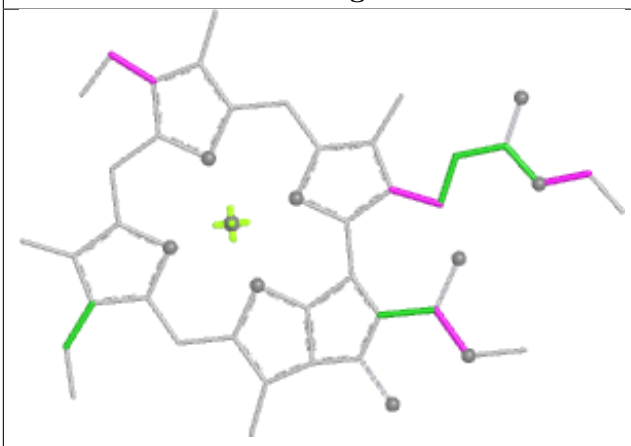
Ligand CLA l 302



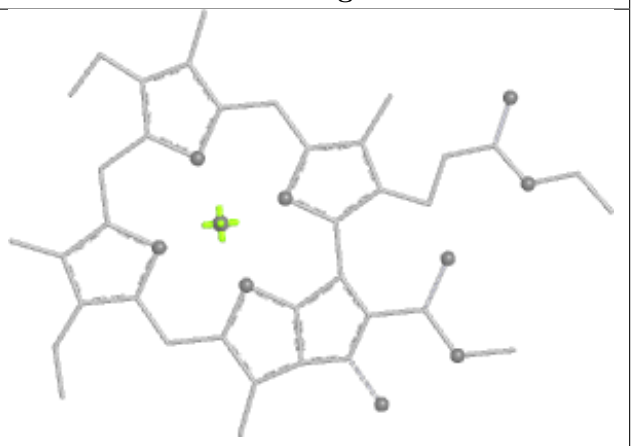
Bond lengths



Bond angles

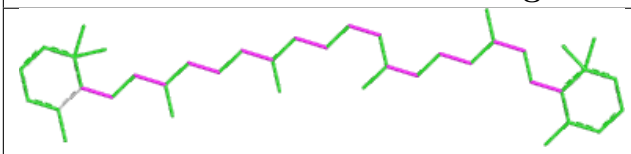


Torsions

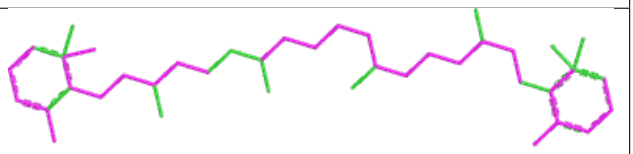


Rings

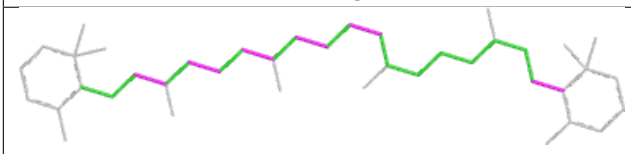
Ligand WVN l 315



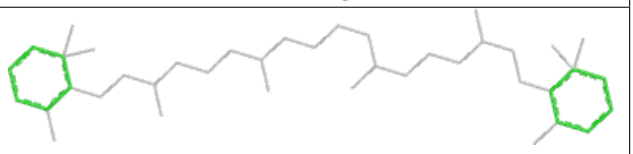
Bond lengths



Bond angles

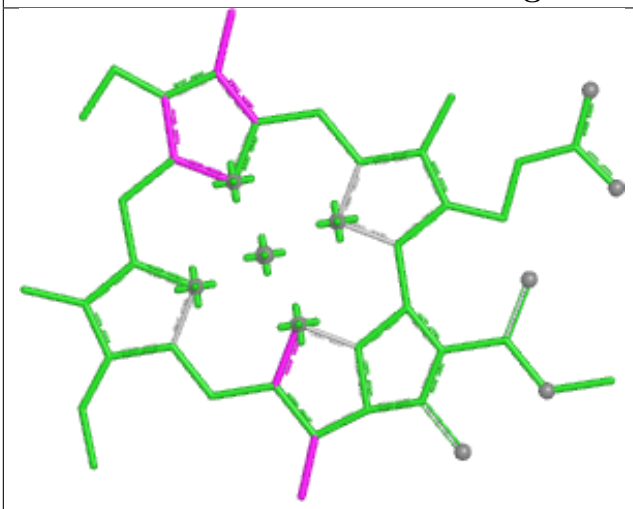


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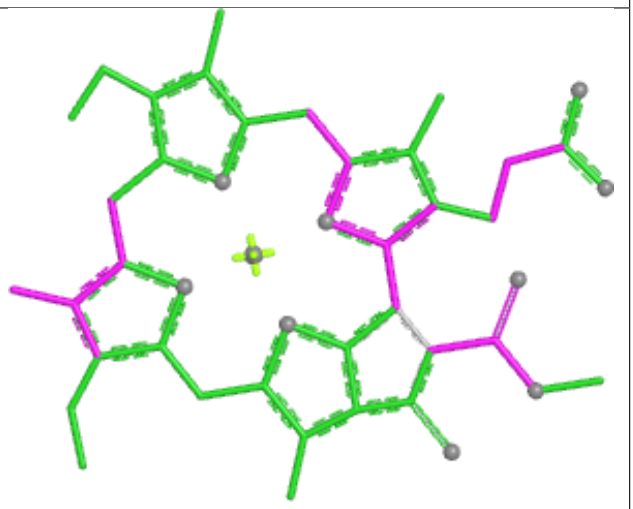


Rings

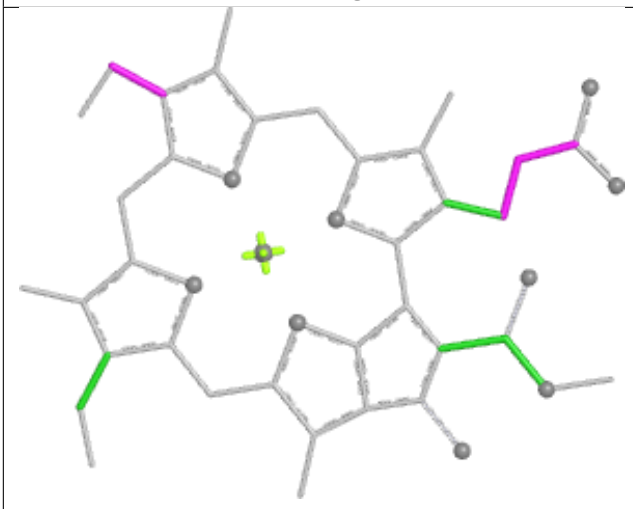
Ligand CLA A 819



Bond lengths



Bond angles

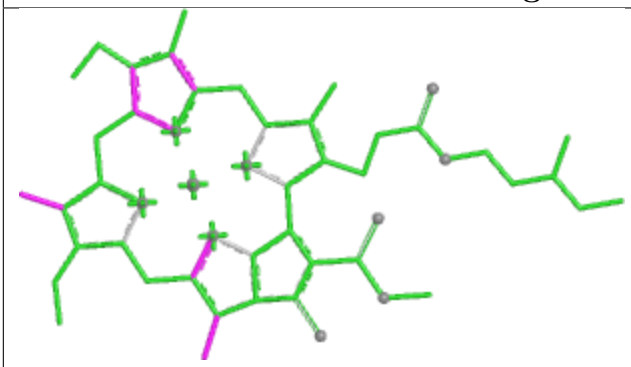


Torsions

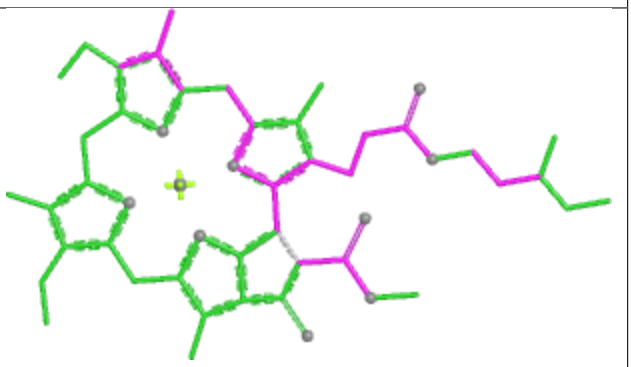


Rings

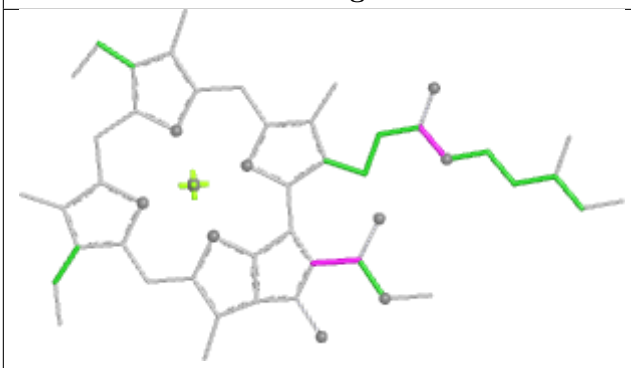
Ligand CLA K 101



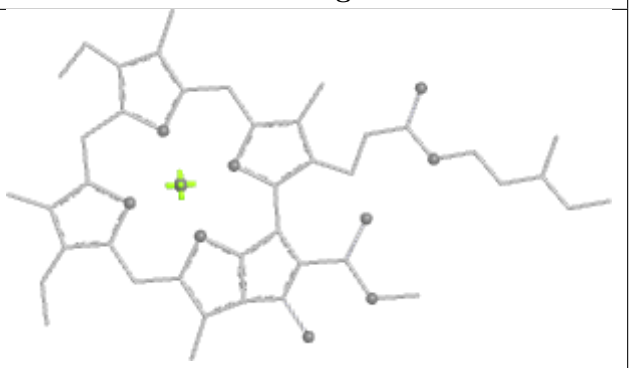
Bond lengths



Bond angles

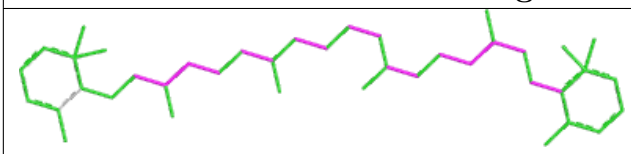


Torsions

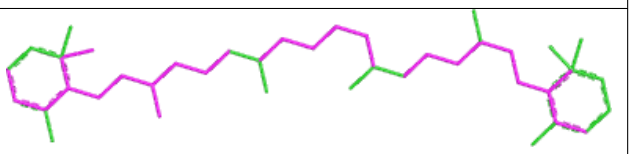


Rings

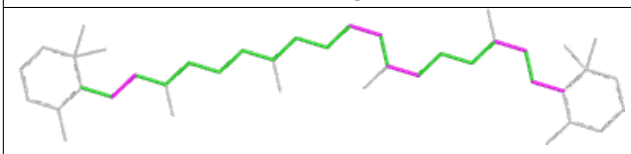
Ligand WVN B 844



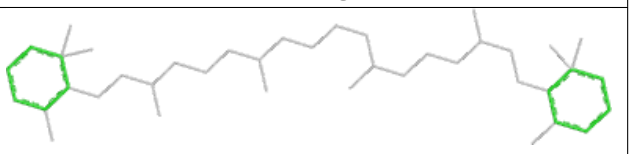
Bond lengths



Bond angles

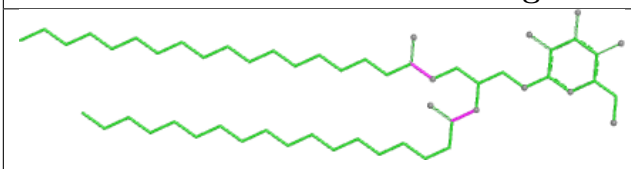


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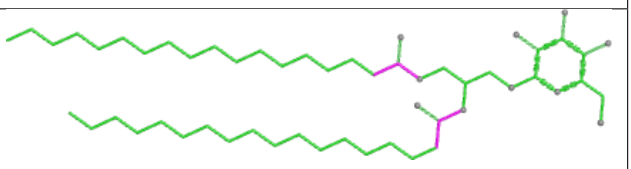


Rings

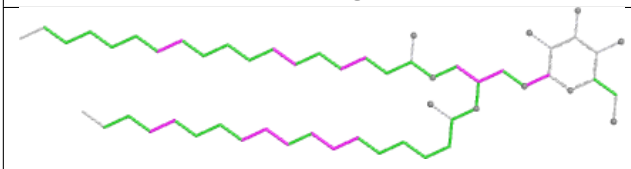
Ligand LMG n 620



Bond lengths



Bond angles

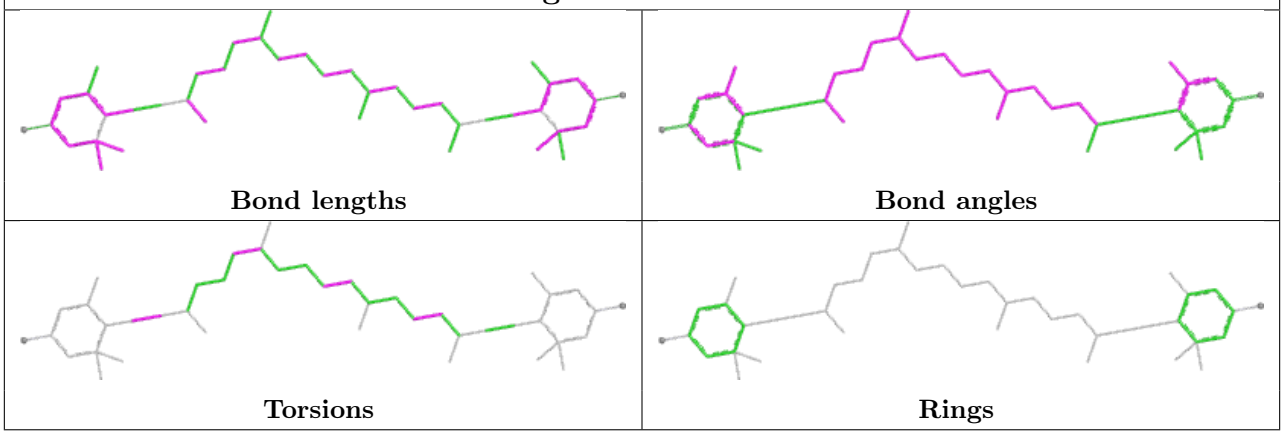


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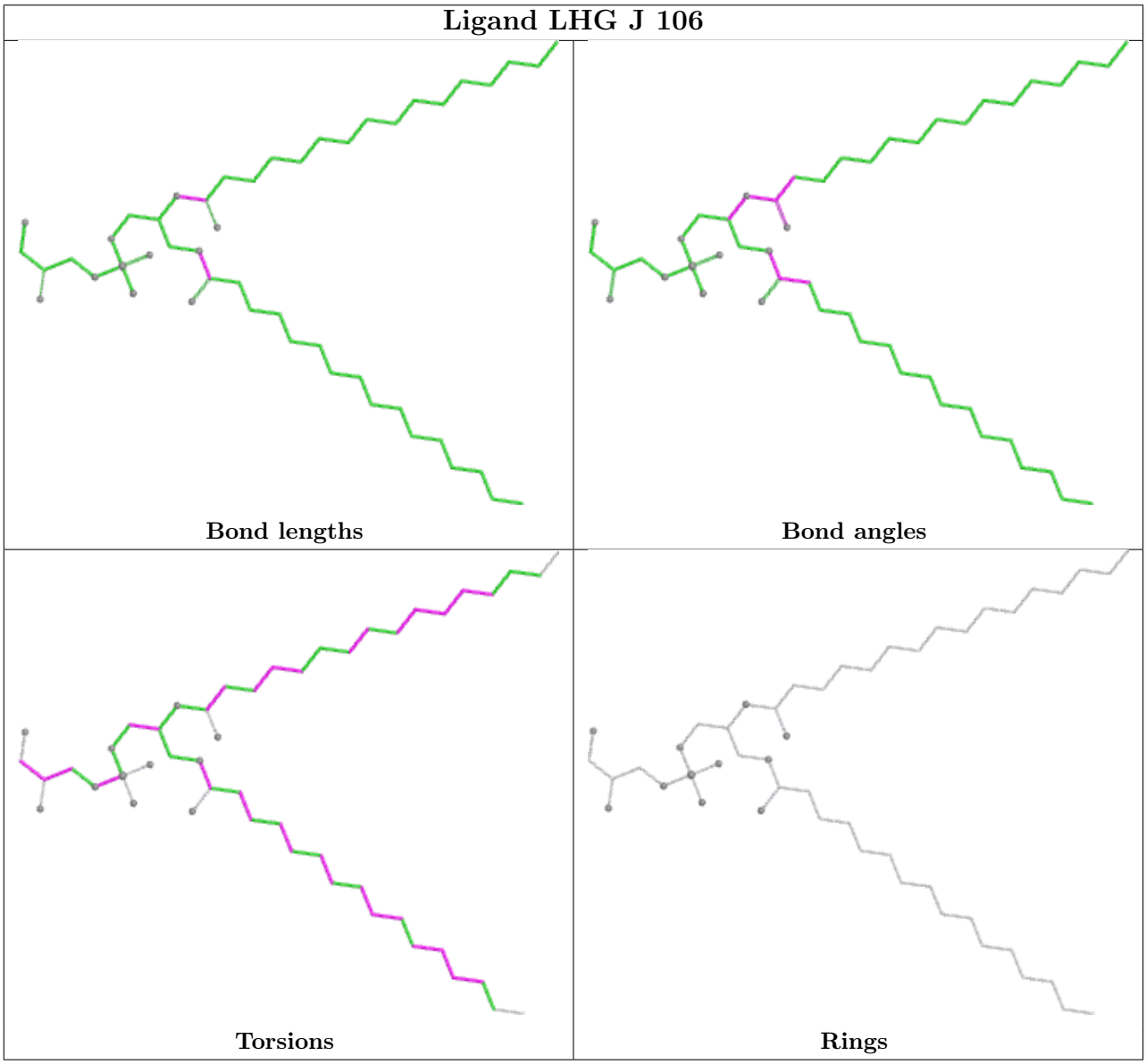


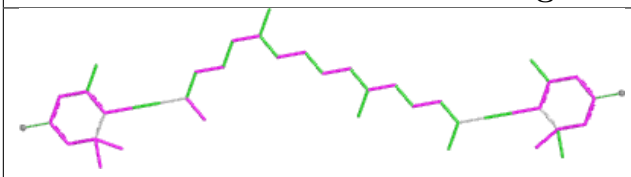
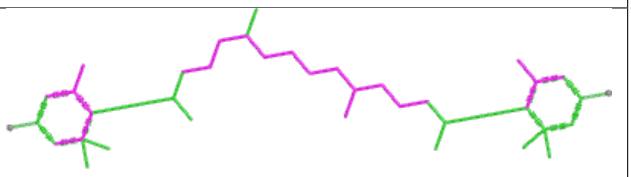
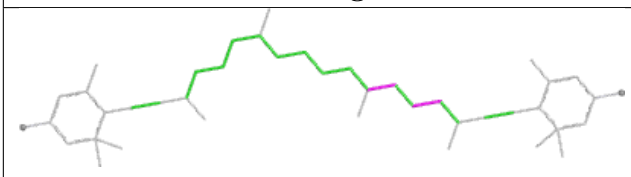
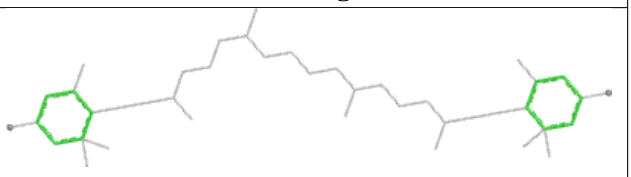
Rings

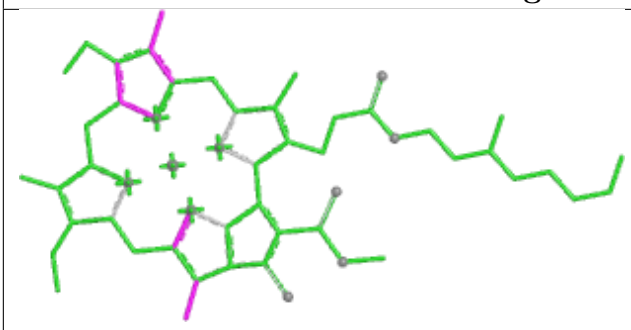
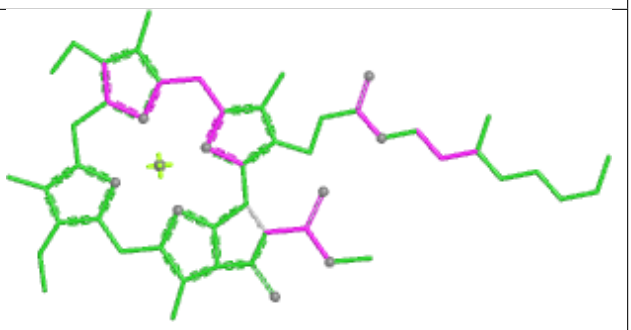
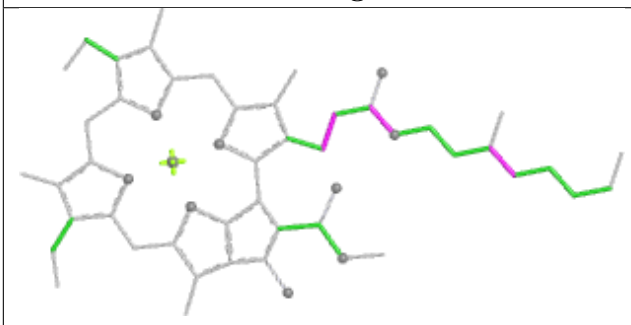
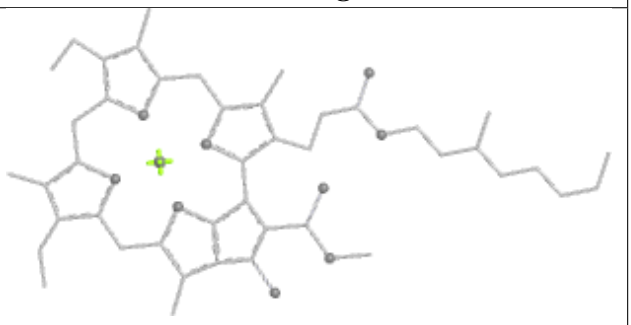
Ligand II0 d 315

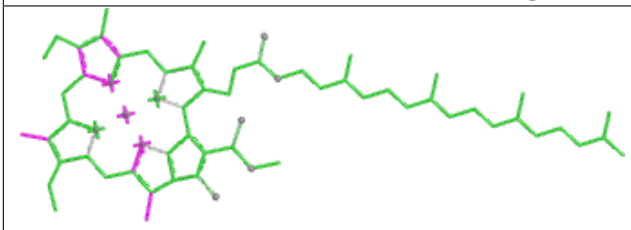
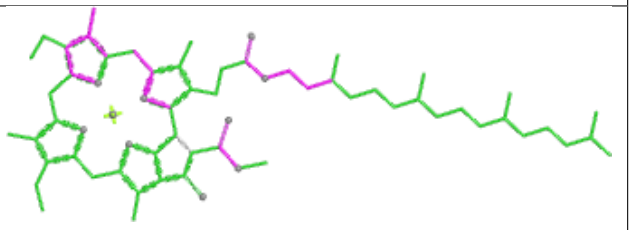
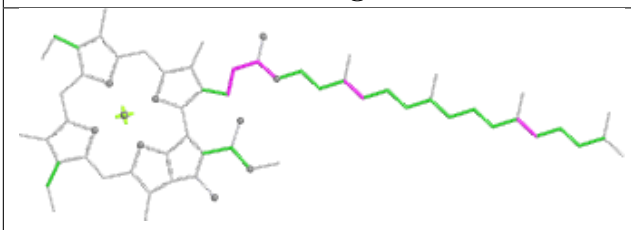
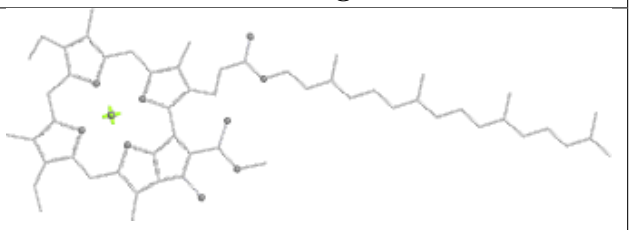


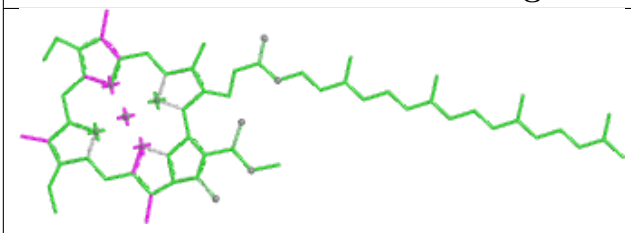
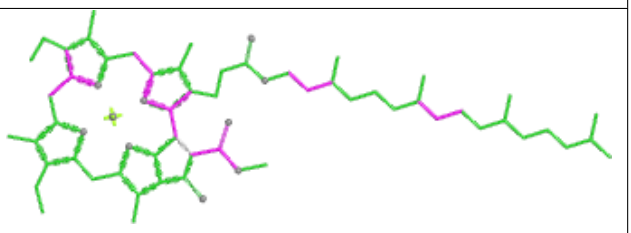
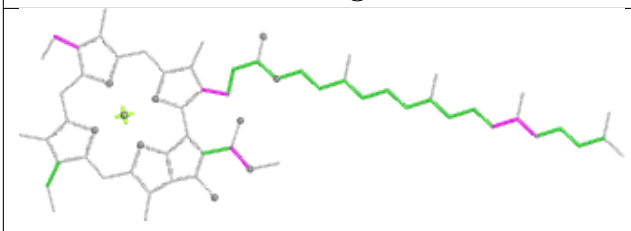
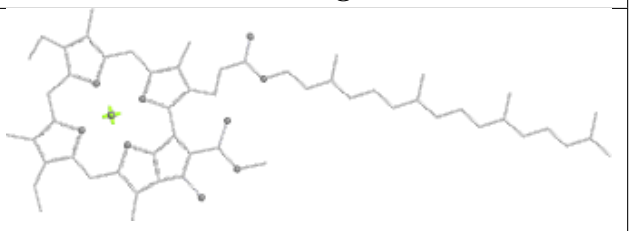
Ligand LHG J 106



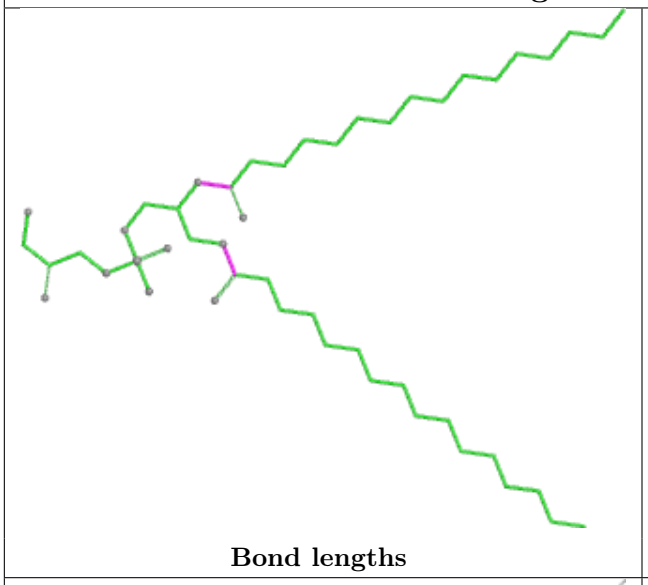
Ligand II0 m 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

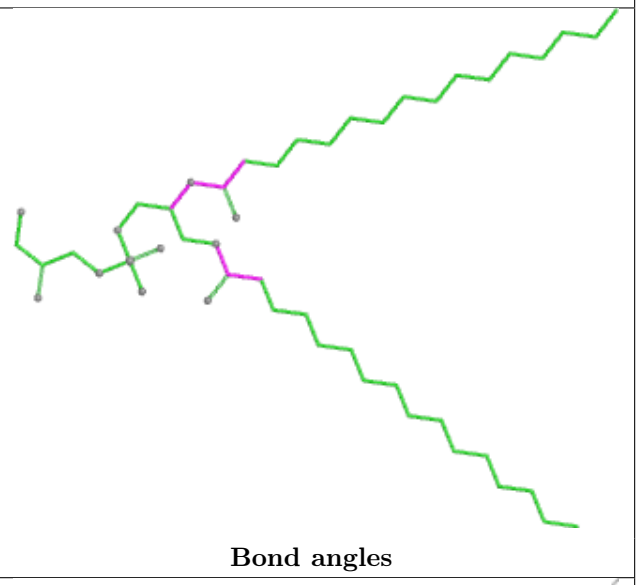
Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

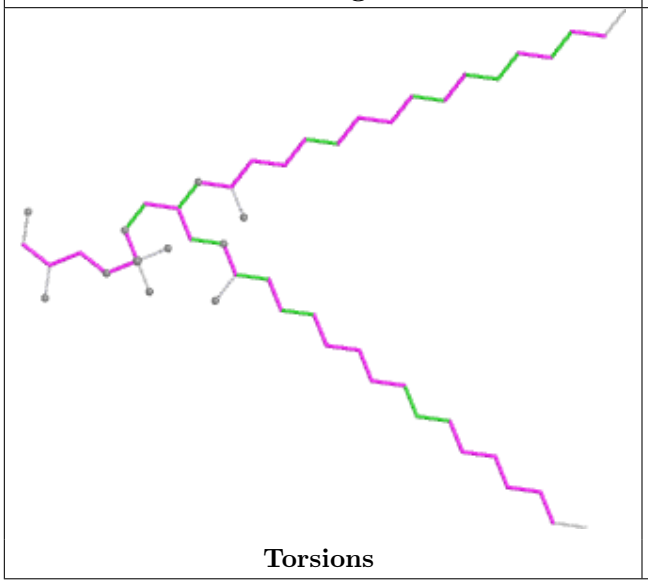
Ligand LHG f 619



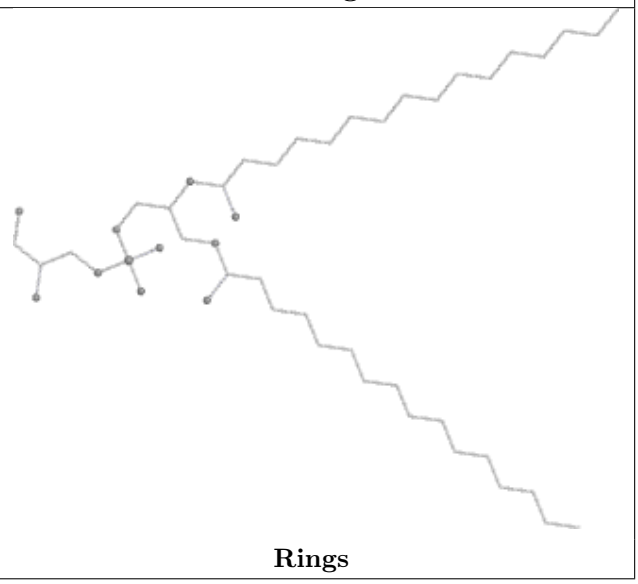
Bond lengths



Bond angles

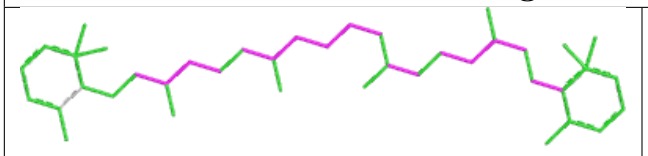


Torsions

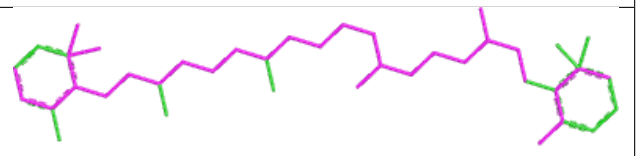


Rings

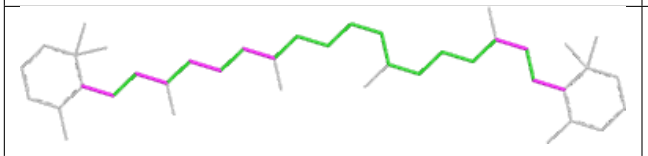
Ligand WVN L 201



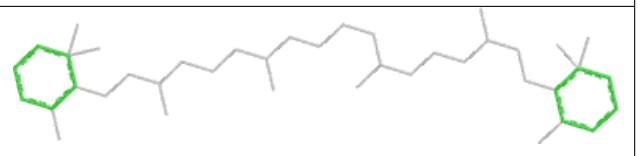
Bond lengths



Bond angles

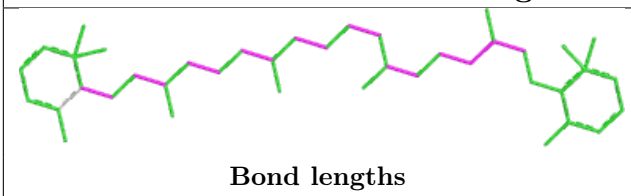


Torsions

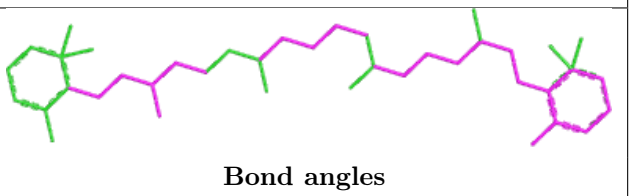


Rings

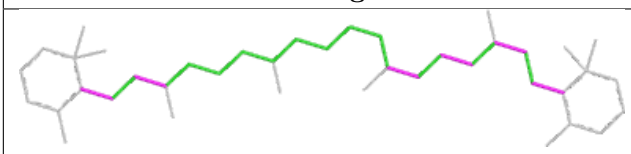
Ligand WVN A 848



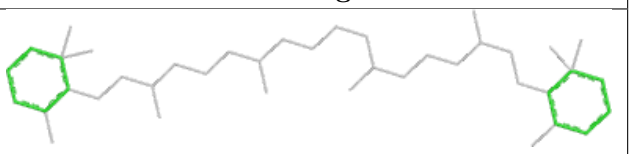
Bond lengths



Bond angles

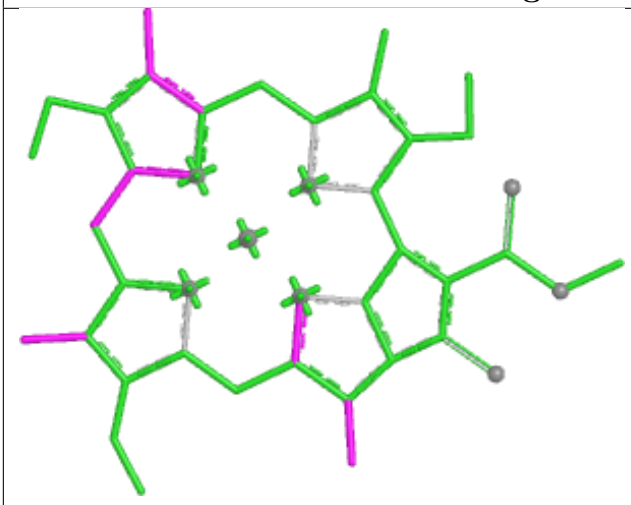


Torsions

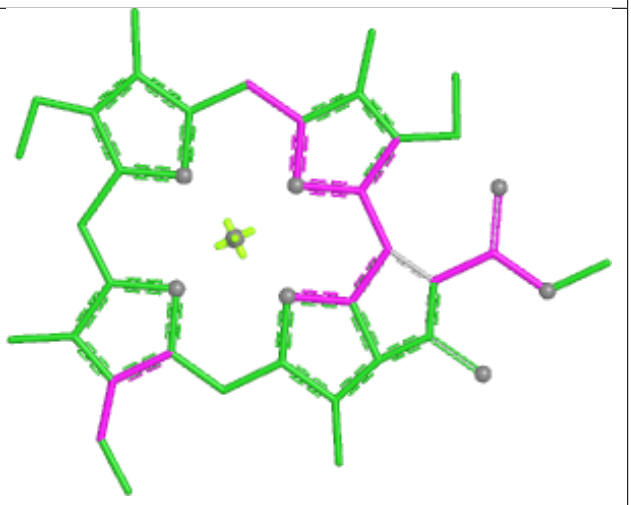


Rings

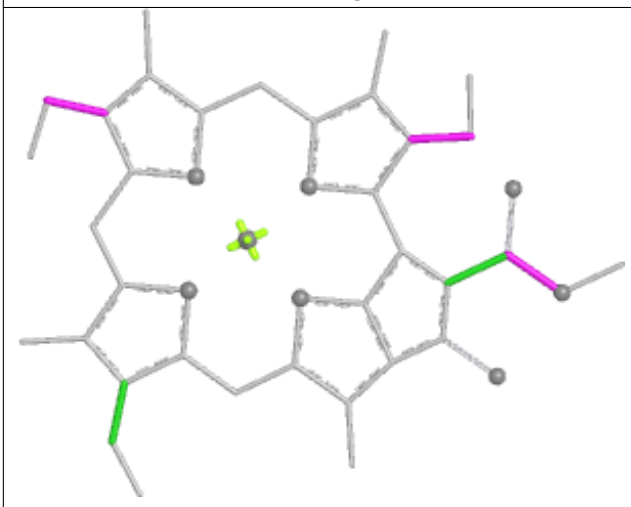
Ligand CLA K 103



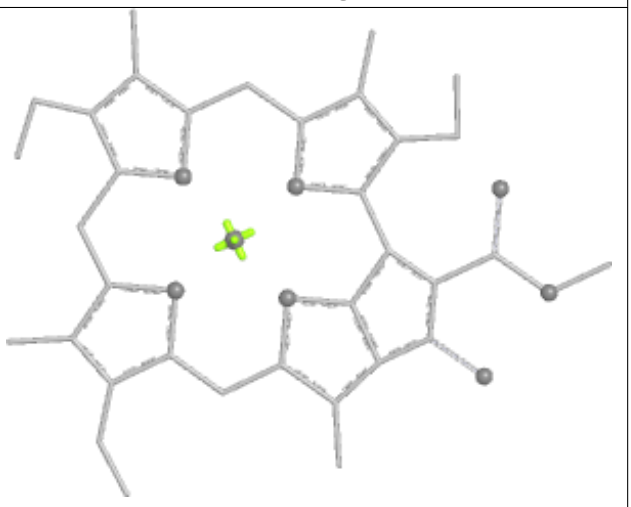
Bond lengths



Bond angles

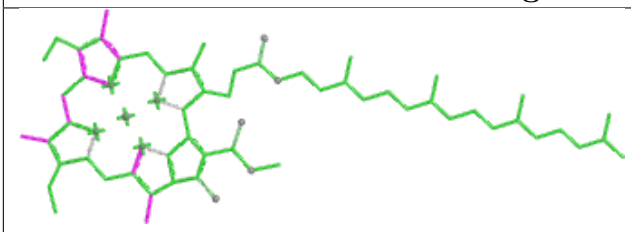


Torsions

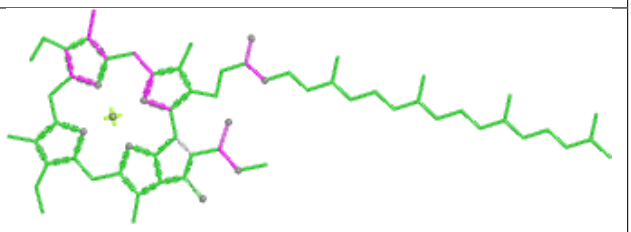


Rings

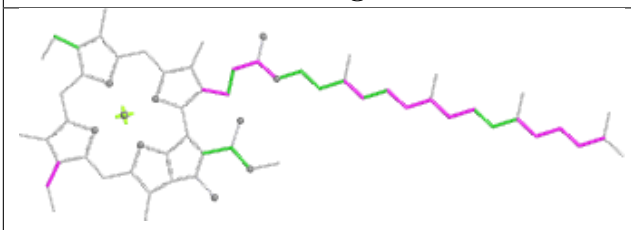
Ligand CLA m 608



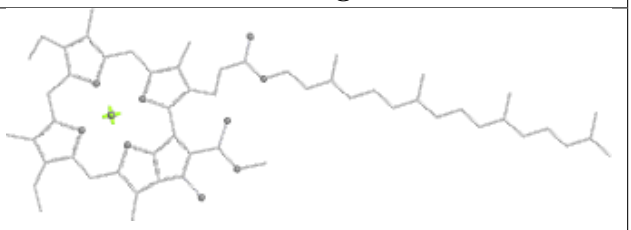
Bond lengths



Bond angles

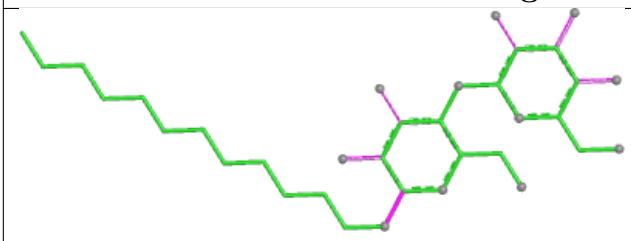


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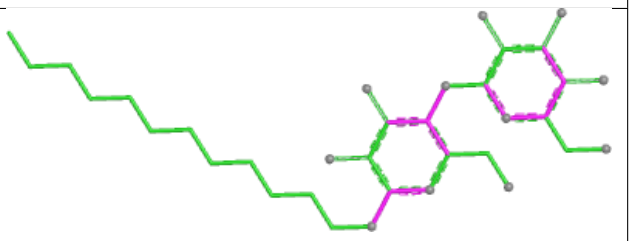


Rings

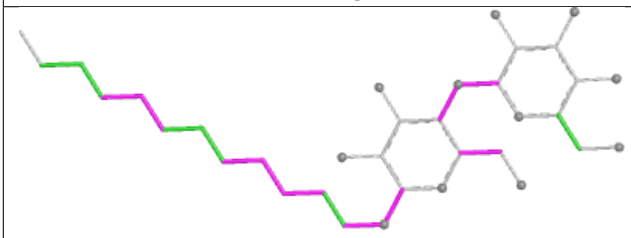
Ligand LMT A 850



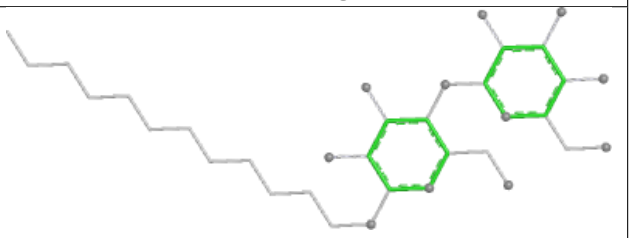
Bond lengths



Bond angles

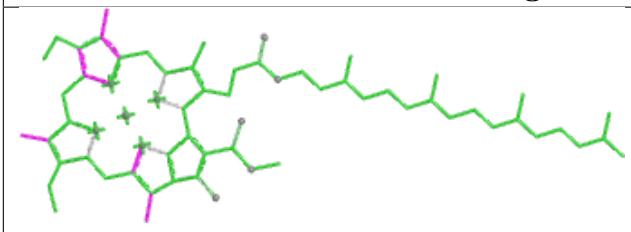


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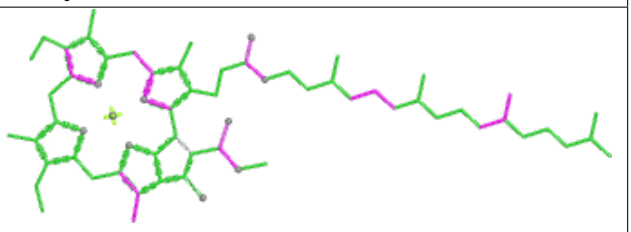


Rings

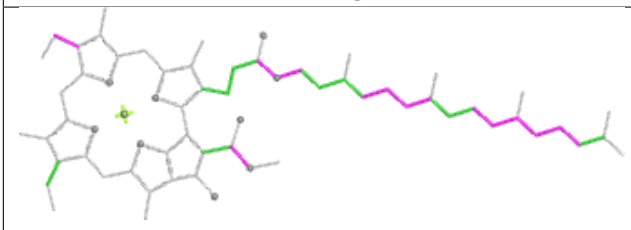
Ligand CLA Q 302



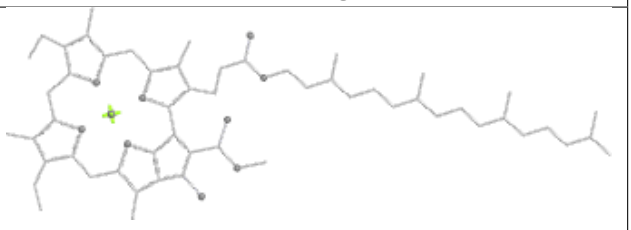
Bond lengths



Bond angles

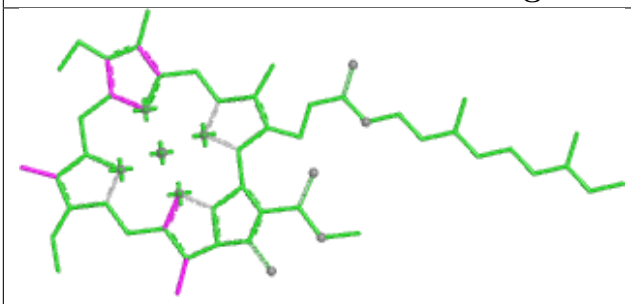


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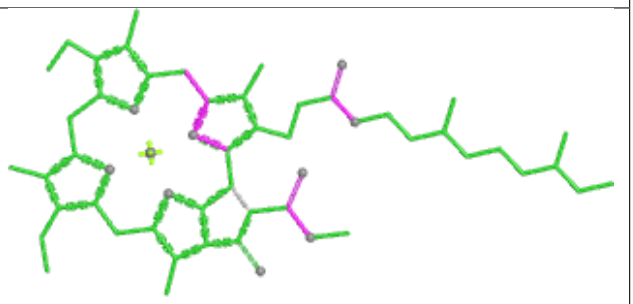


Rings

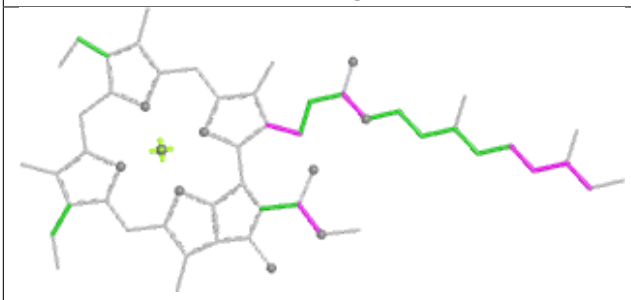
Ligand CLA A 809



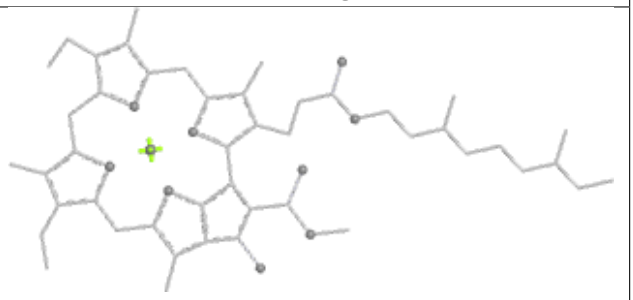
Bond lengths



Bond angles

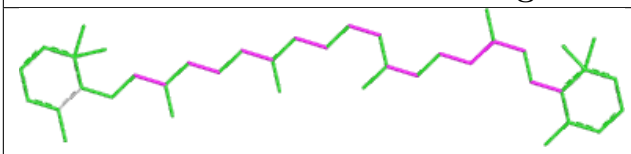


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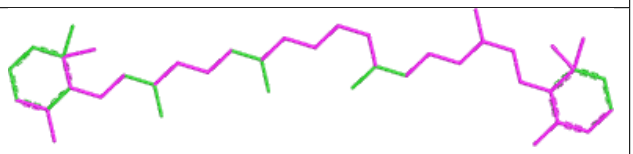


Rings

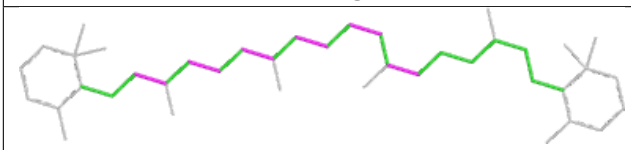
Ligand WVN F 203



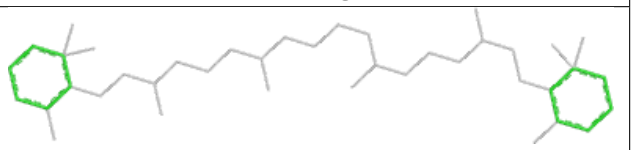
Bond lengths



Bond angles

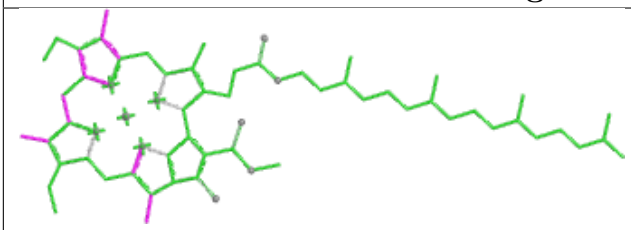


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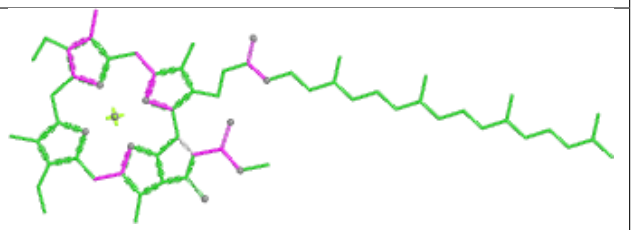


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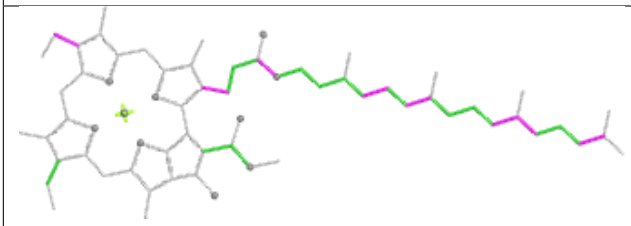
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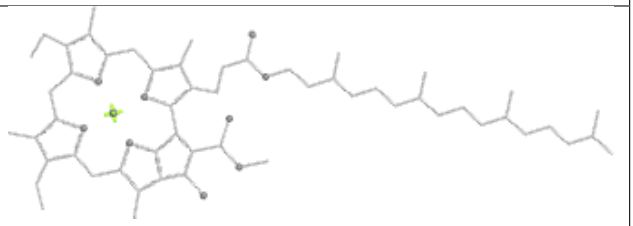
Bond lengths



Bond angles

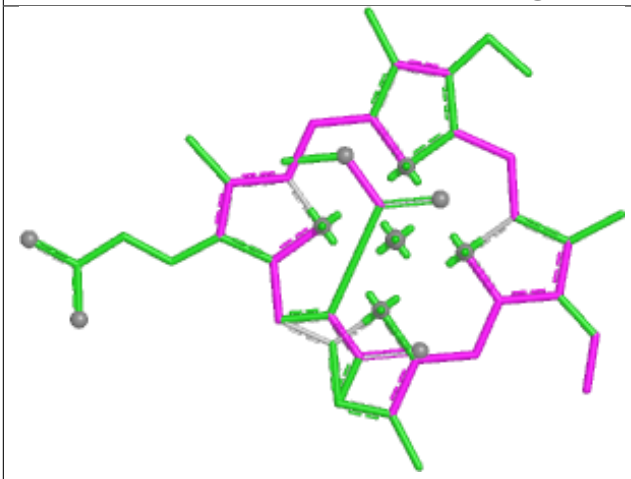


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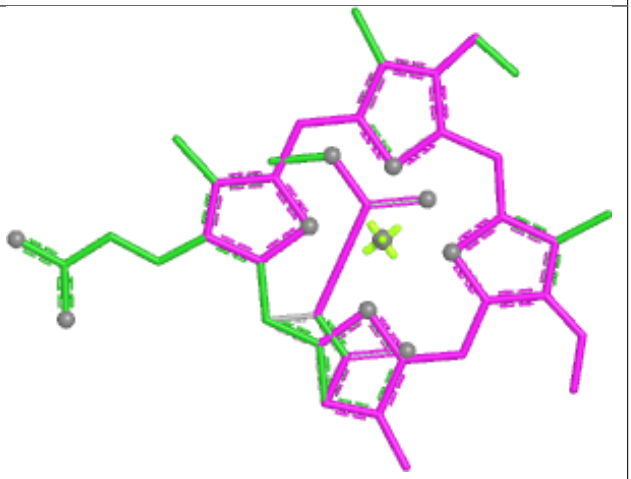


Rings

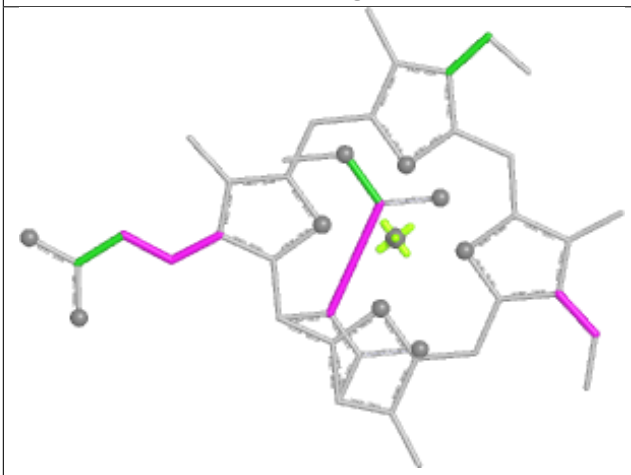
Ligand KC2 n 612



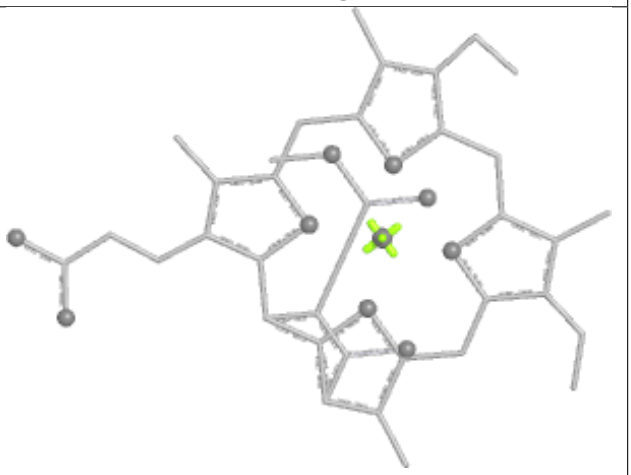
Bond lengths



Bond angles

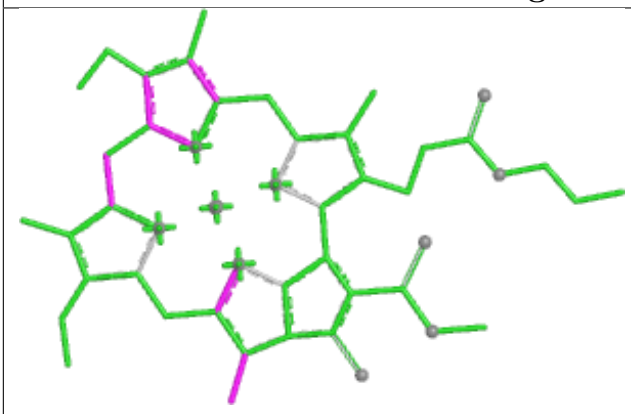


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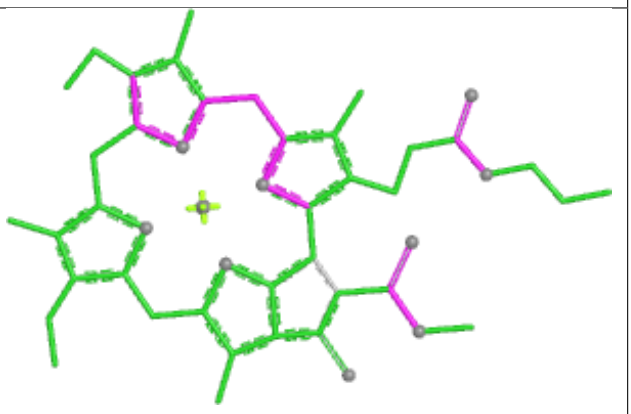


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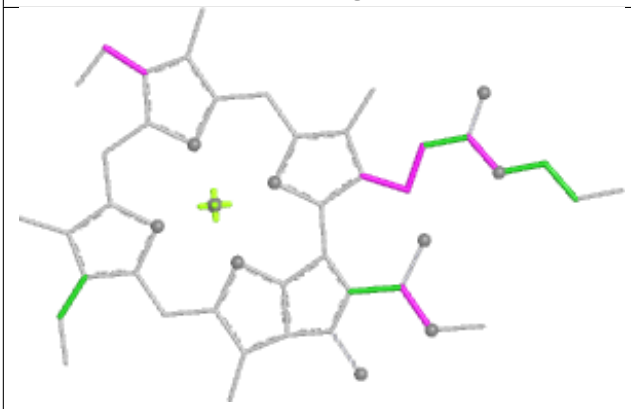
Ligand CLA a 313



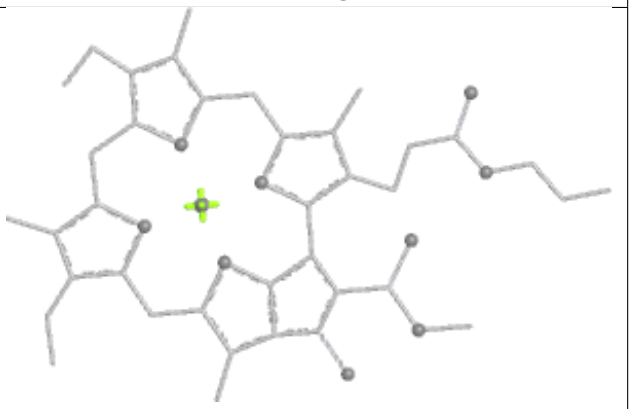
Bond lengths



Bond angles

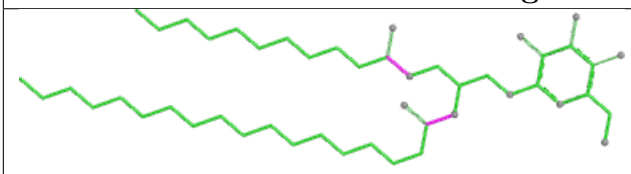


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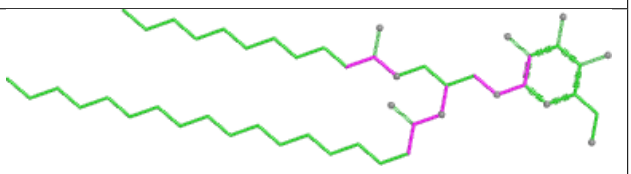


Rings

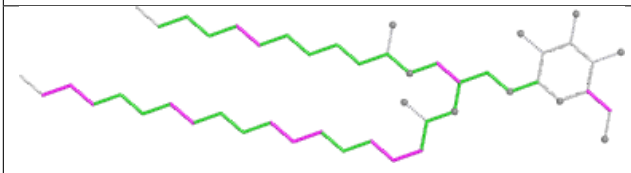
Ligand LMG F 205



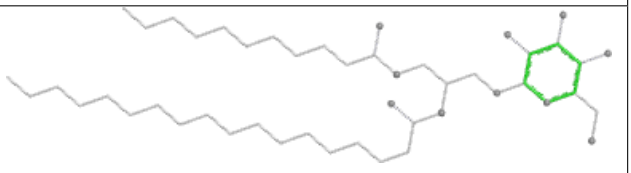
Bond lengths



Bond angles

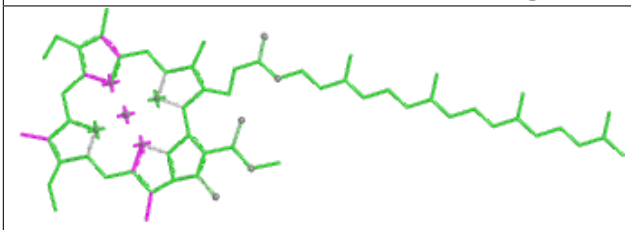


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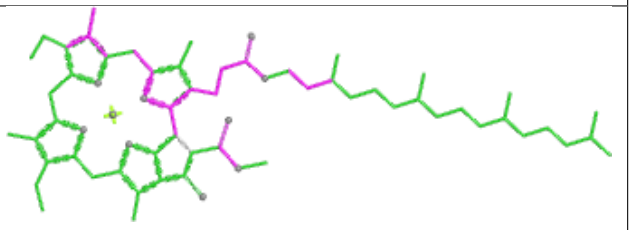


Rings

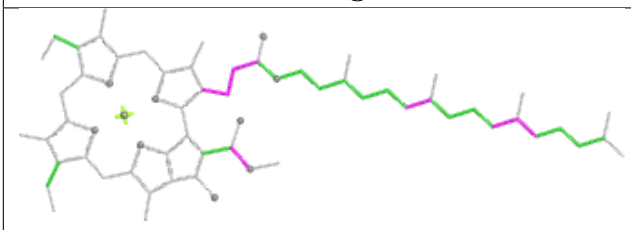
Ligand CLA A 808



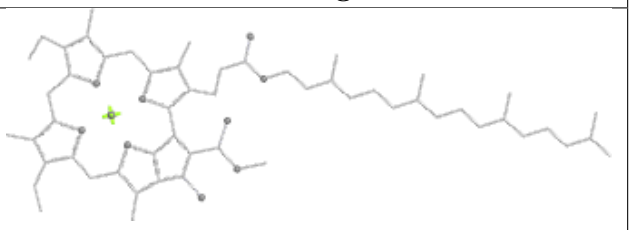
Bond lengths



Bond angles

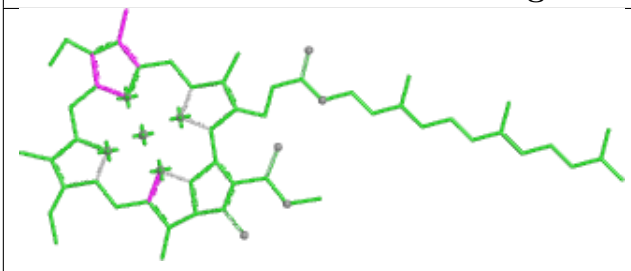


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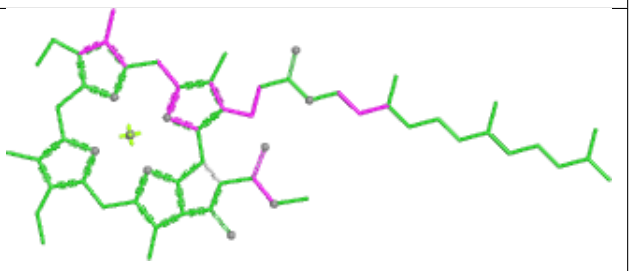


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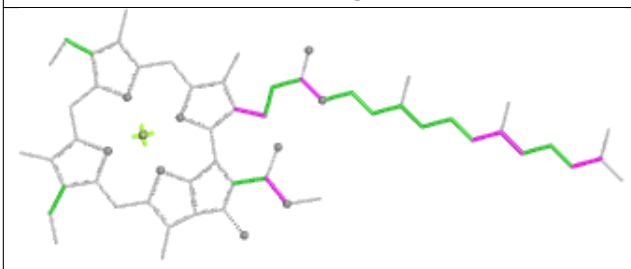
Ligand CLA n 604



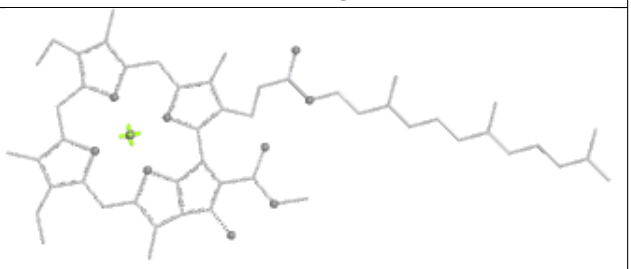
Bond lengths



Bond angles

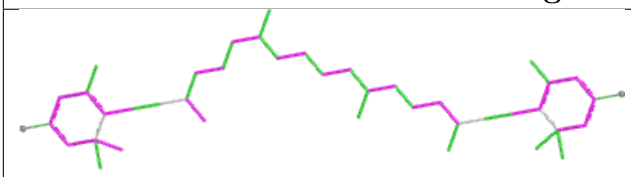


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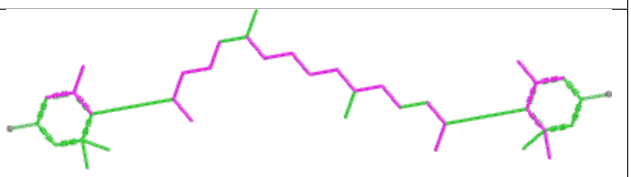


Rings

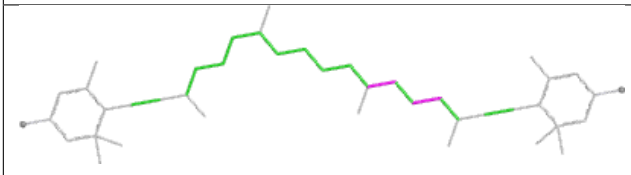
Ligand II0 c 617



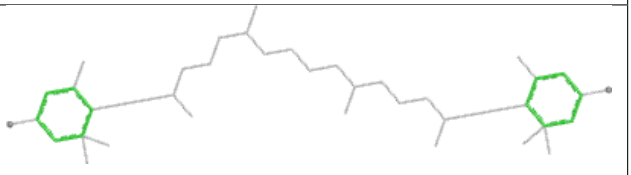
Bond lengths



Bond angles

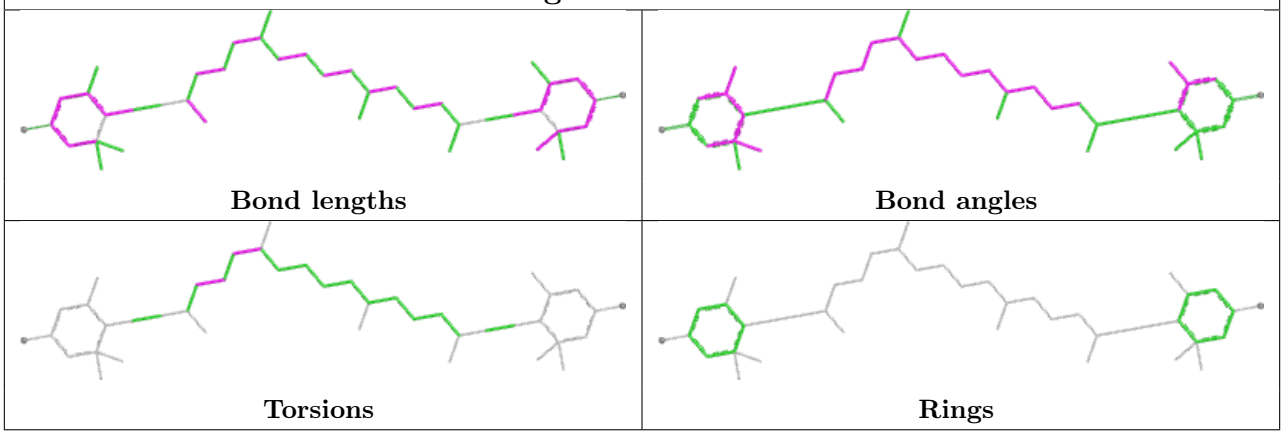


Torsions



Rings

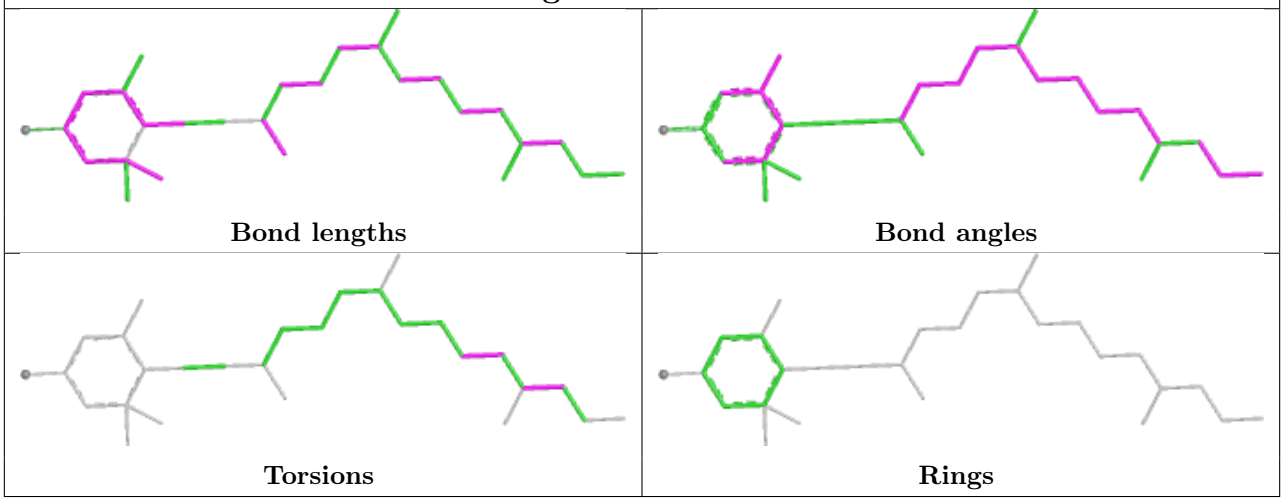
Ligand II0 a 316



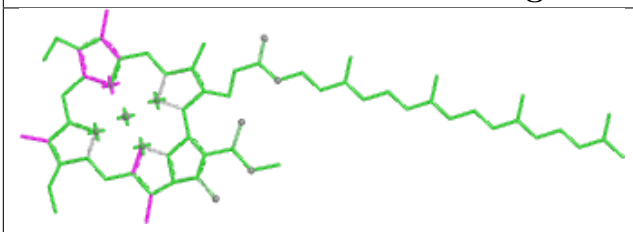
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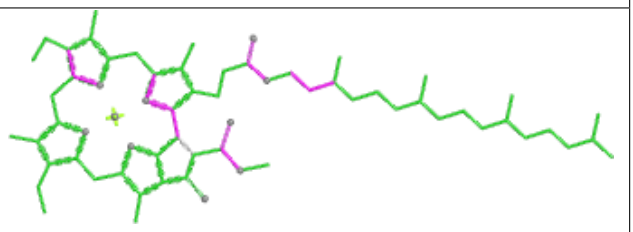
Ligand II0 h 310



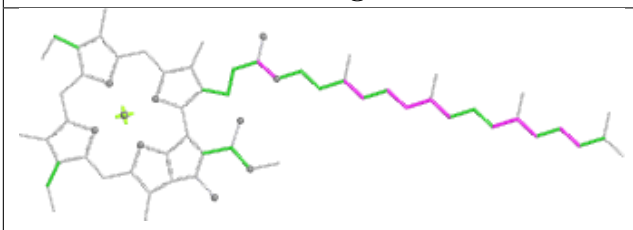
Ligand CLA F 201



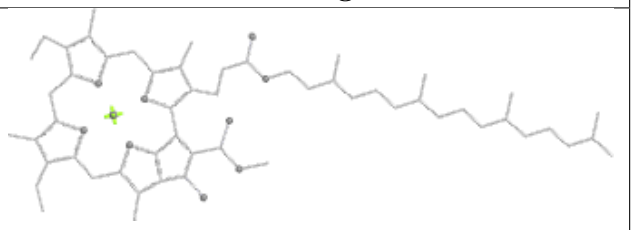
Bond lengths



Bond angles

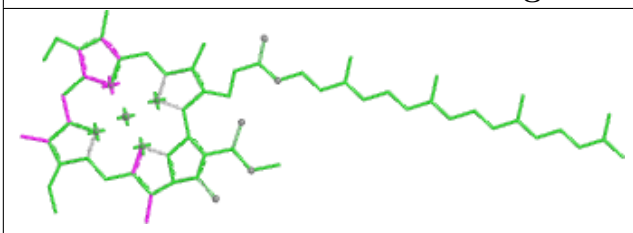


Torsions

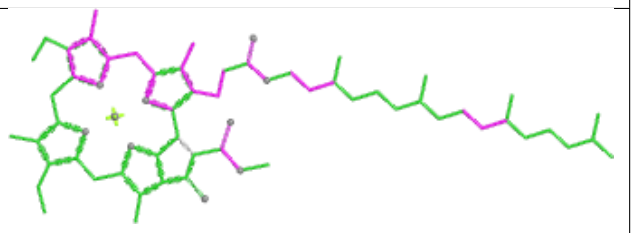


Rings

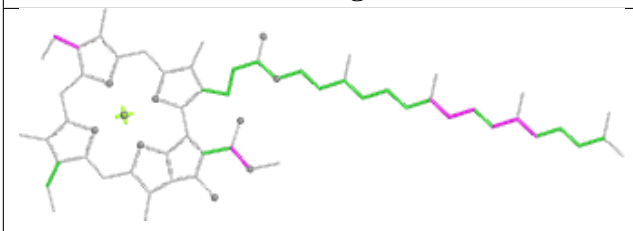
Ligand CLA A 852



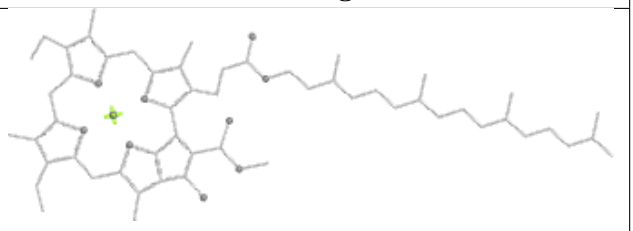
Bond lengths



Bond angles

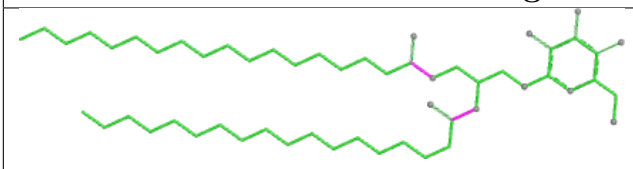


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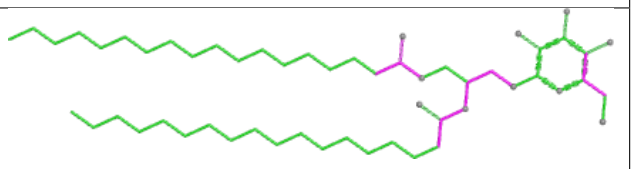


Rings

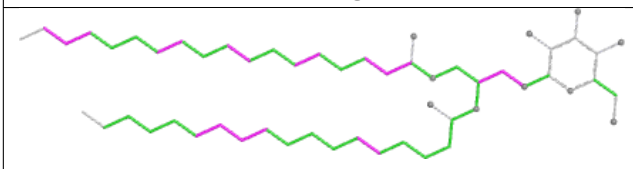
Ligand LMG J 105



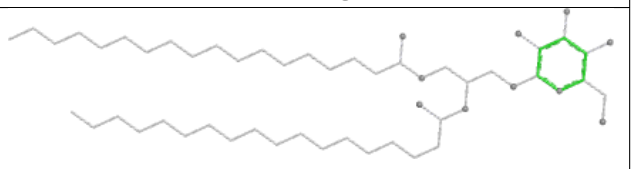
Bond lengths



Bond angles

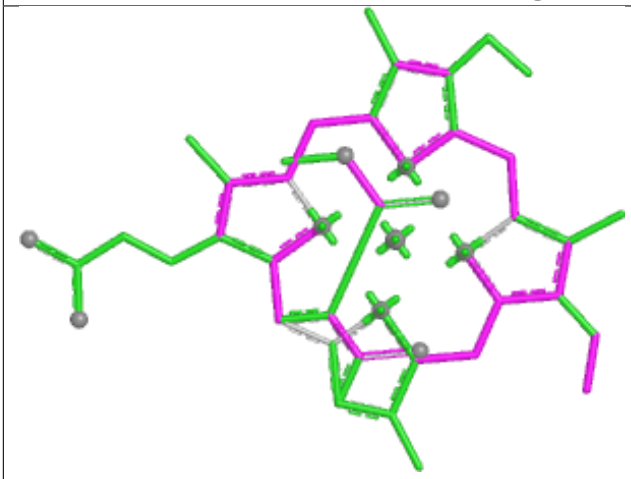


Torsions

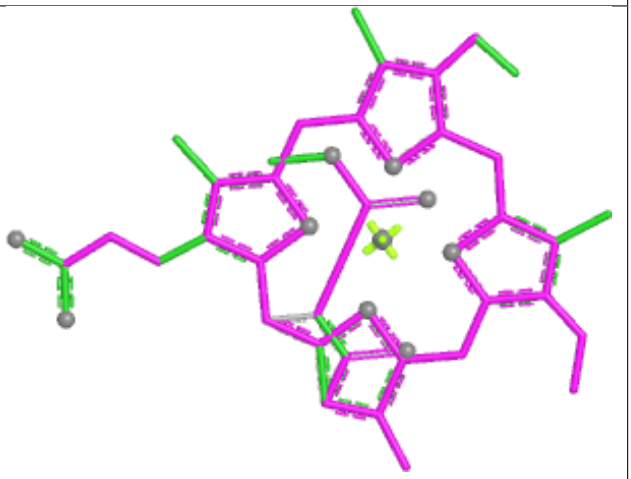


Rings

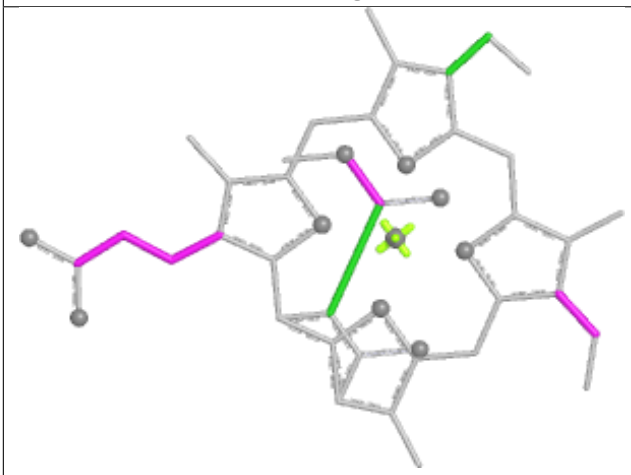
Ligand KC2 n 611



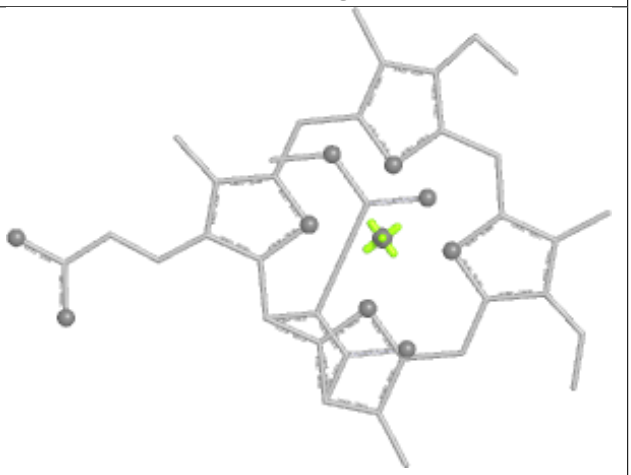
Bond lengths



Bond angles

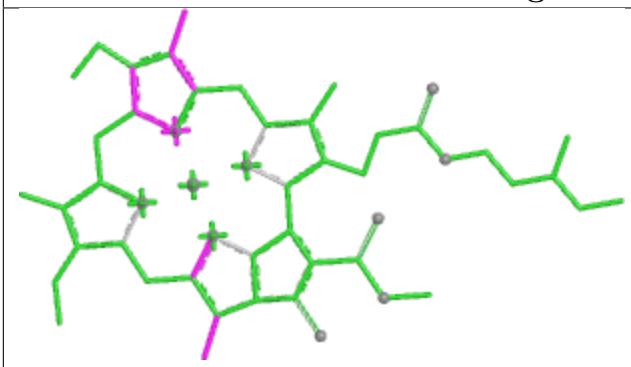


Torsions

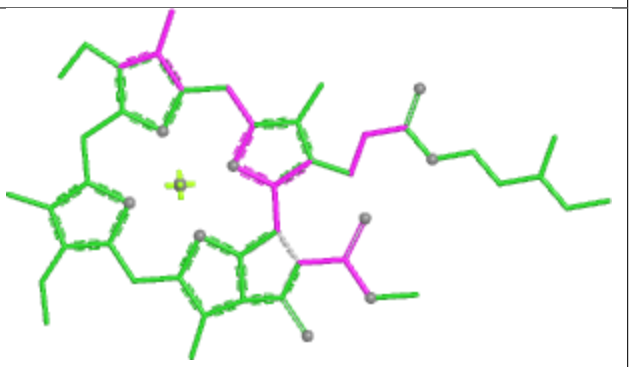


Rings

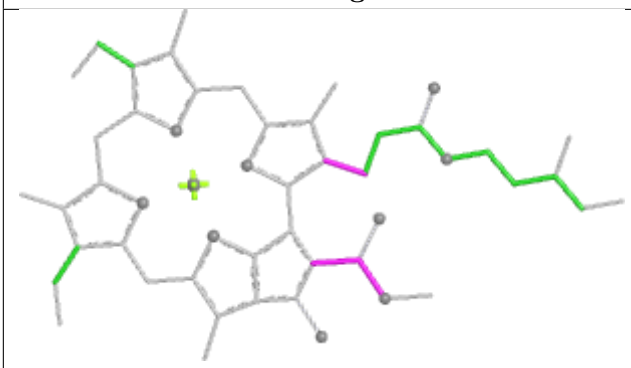
Ligand CLA h 304



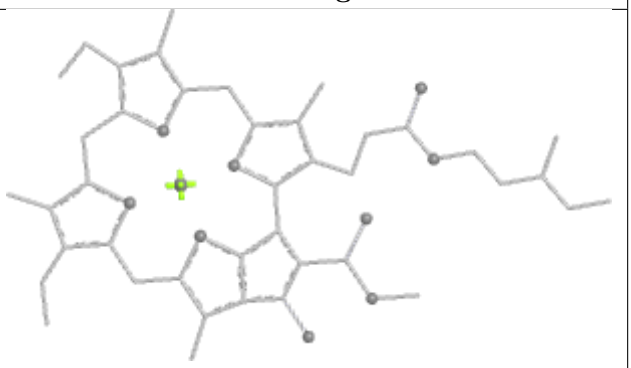
Bond lengths



Bond angles

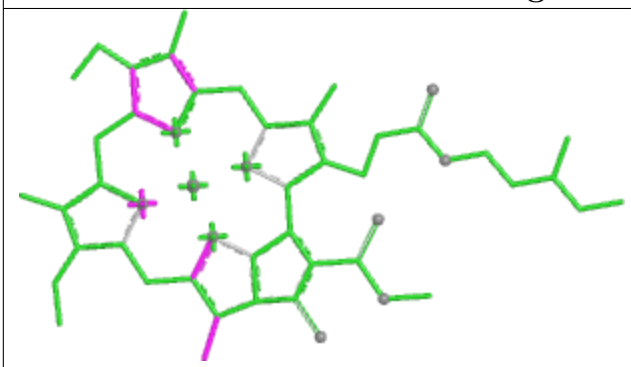


Torsions

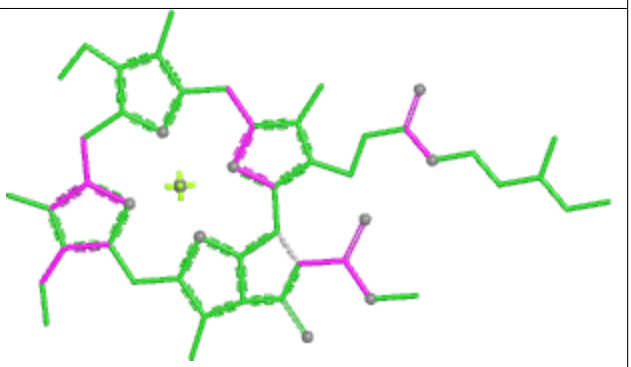


Rings

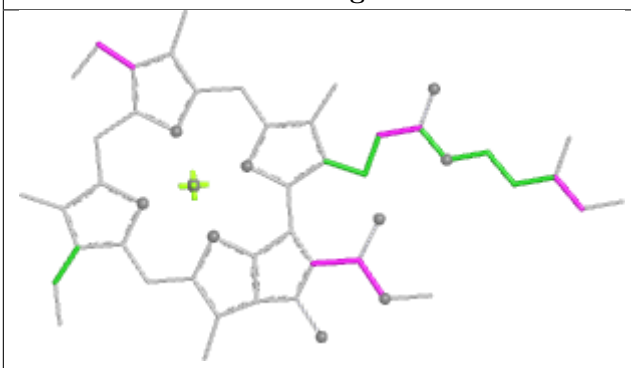
Ligand CLA d 305



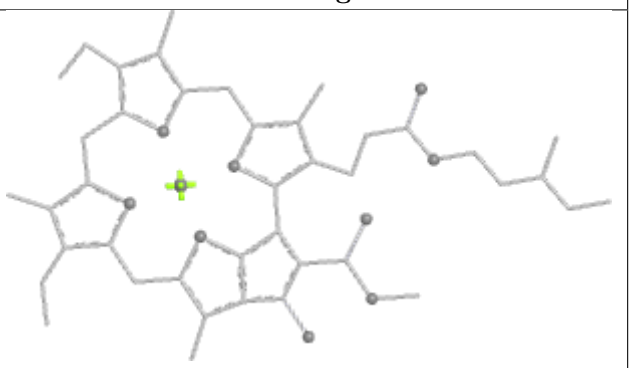
Bond lengths



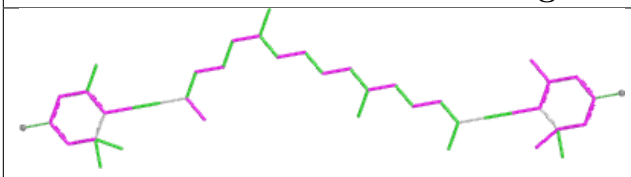
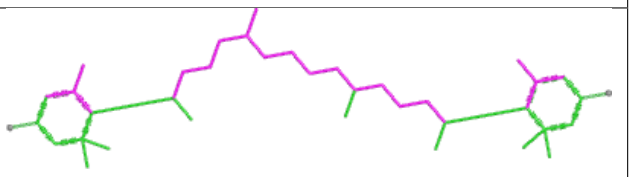
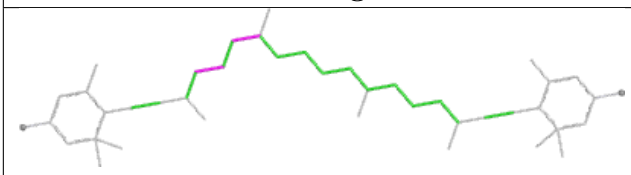
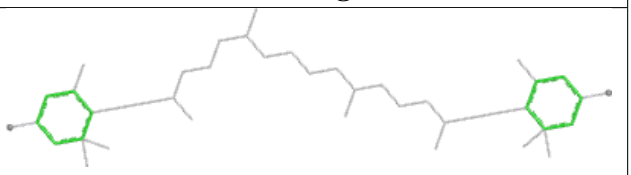
Bond angles

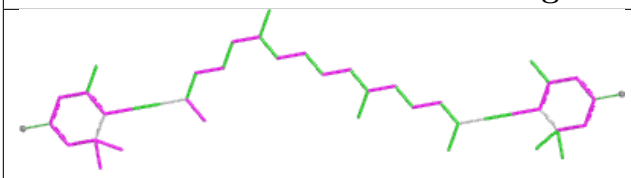
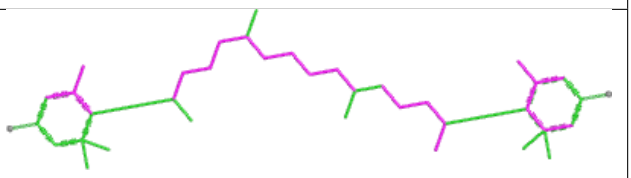
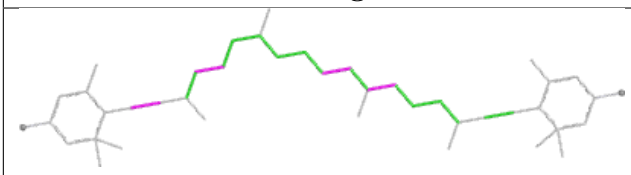
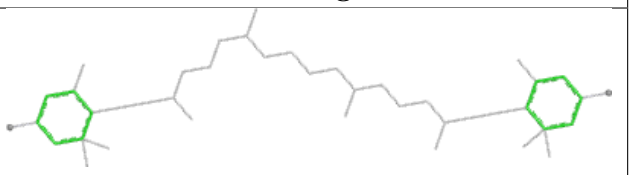


Torsions

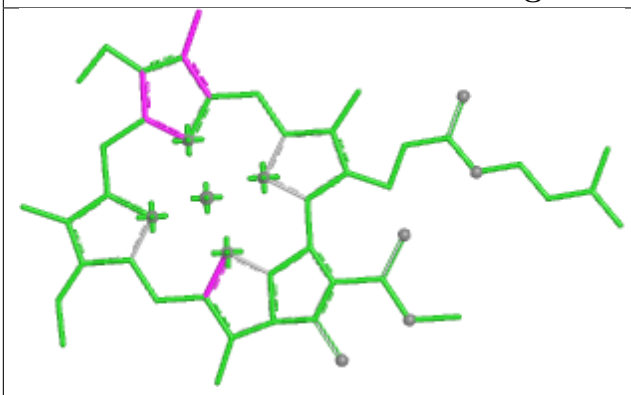


Rings

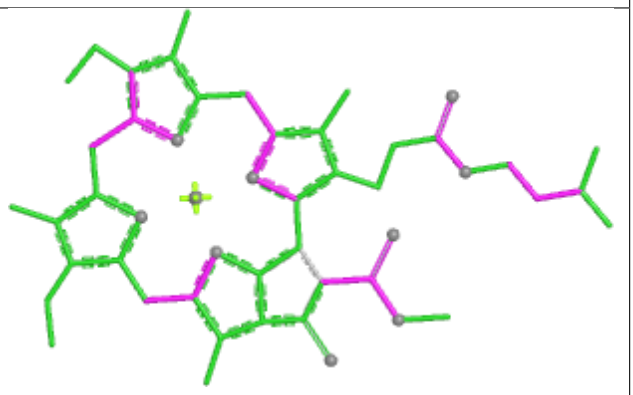
Ligand II0 O 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 d 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

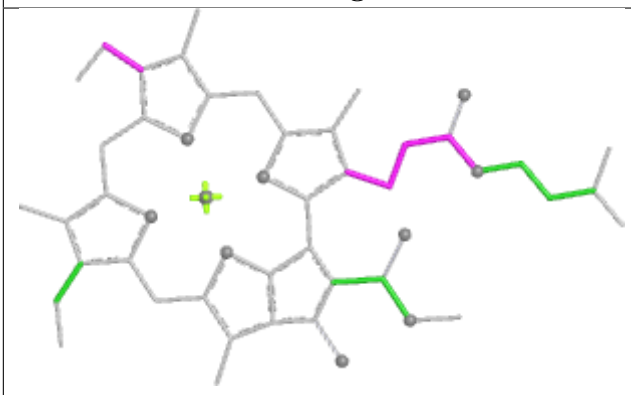
Ligand CLA B 827



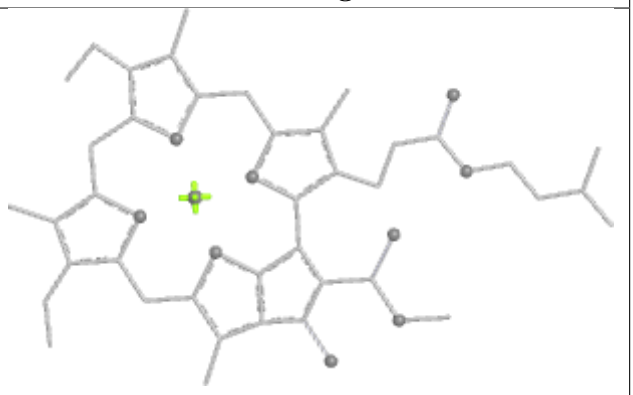
Bond lengths



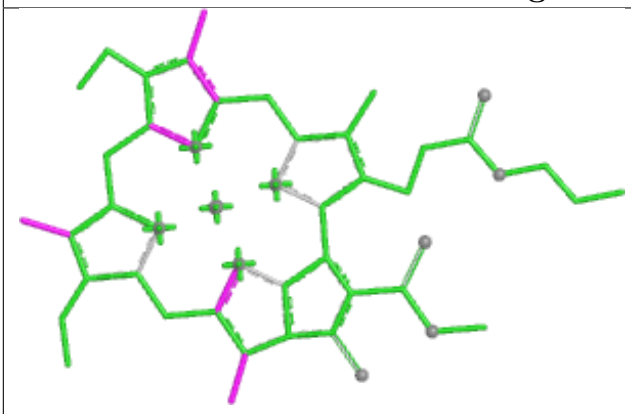
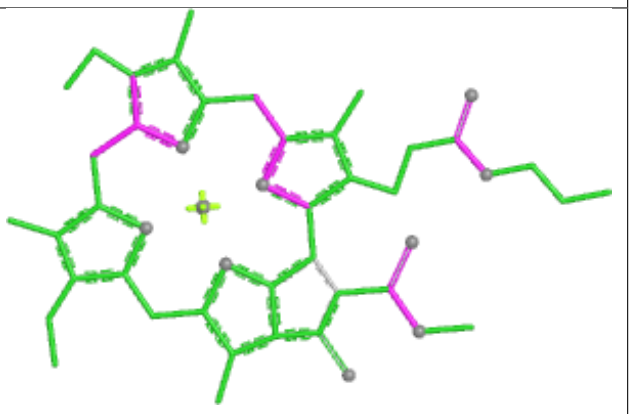
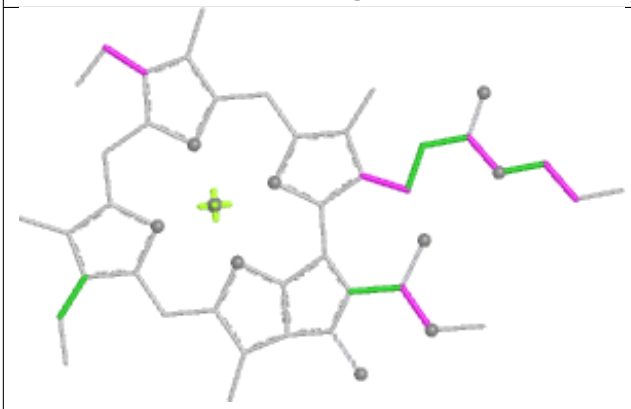
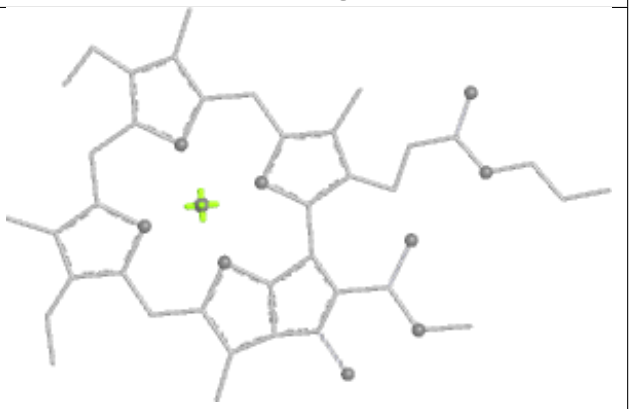
Bond angles

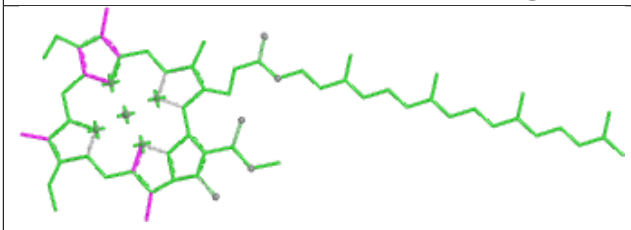
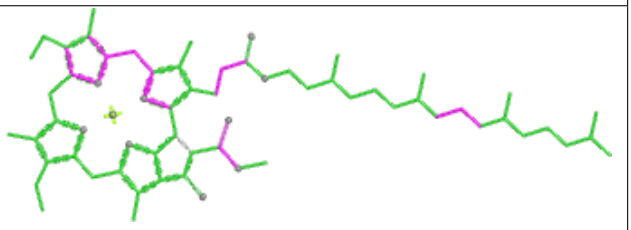
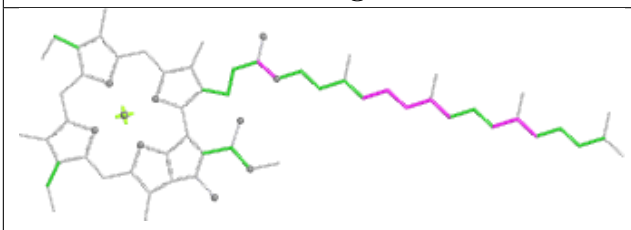
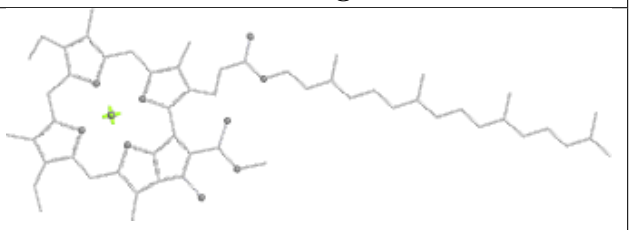


Torsions

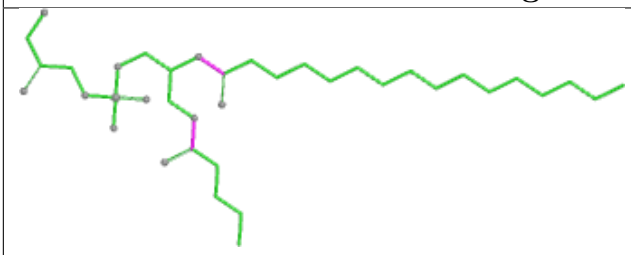


Rings

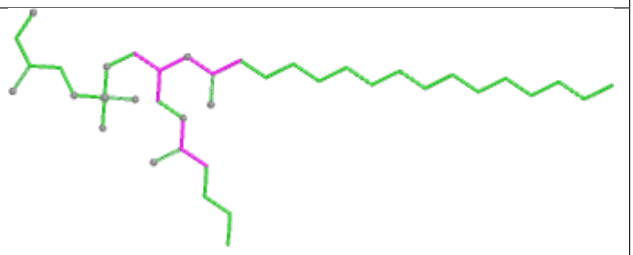
Ligand CLA a 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

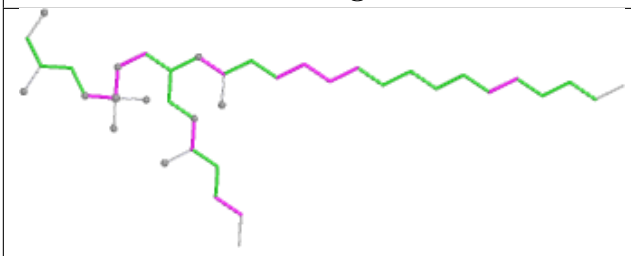
Ligand LHG A 849



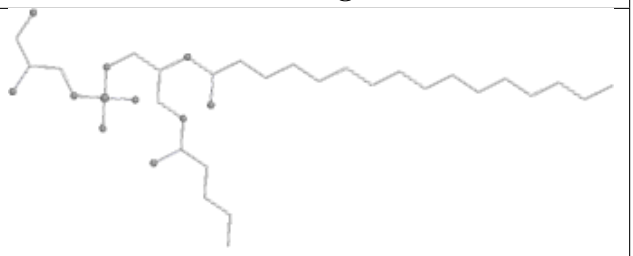
Bond lengths



Bond angles

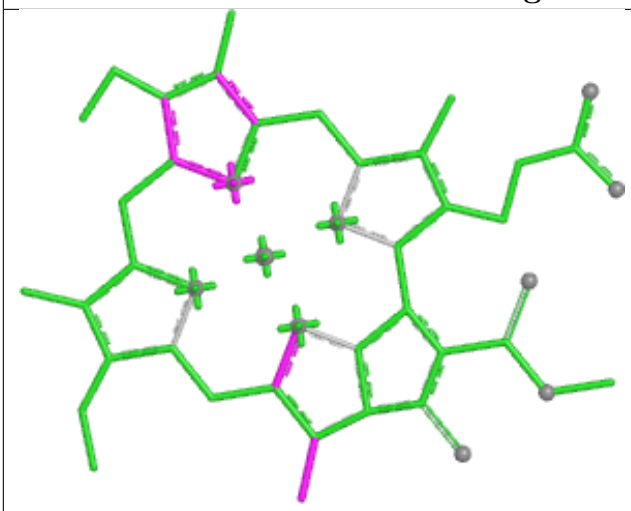


Torsions

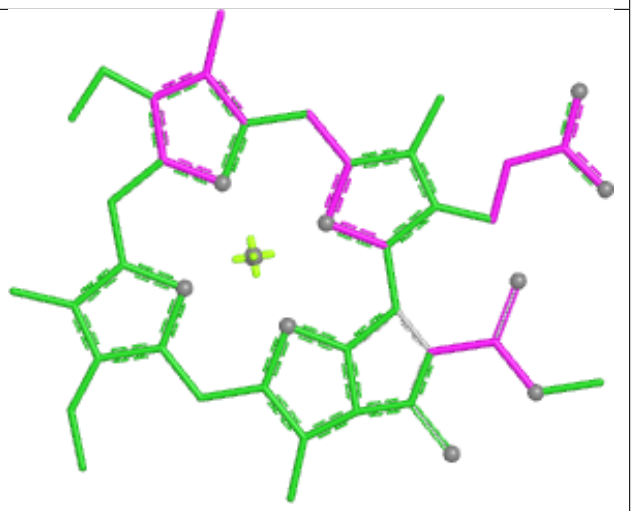


Rings

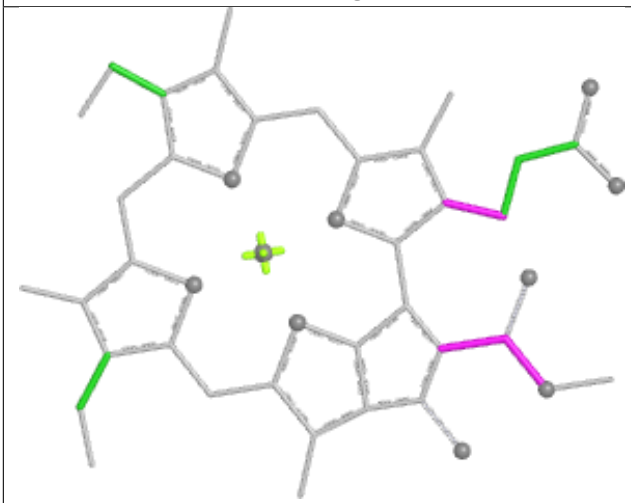
Ligand CLA A 813



Bond lengths



Bond angles

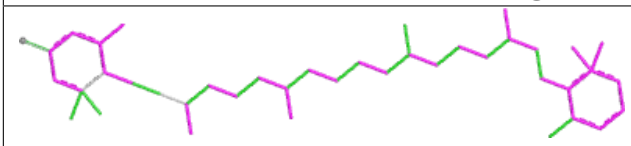


Torsions

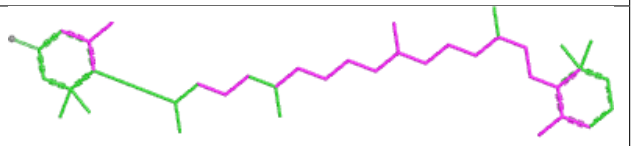


Rings

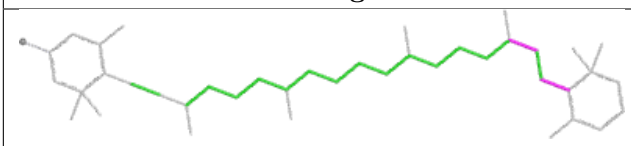
Ligand IHT R 204



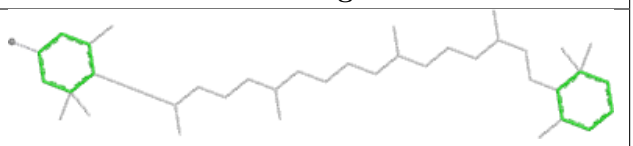
Bond lengths



Bond angles

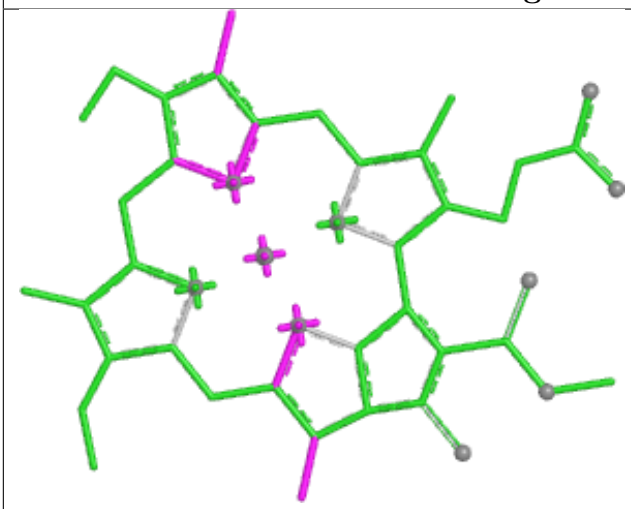


Torsions

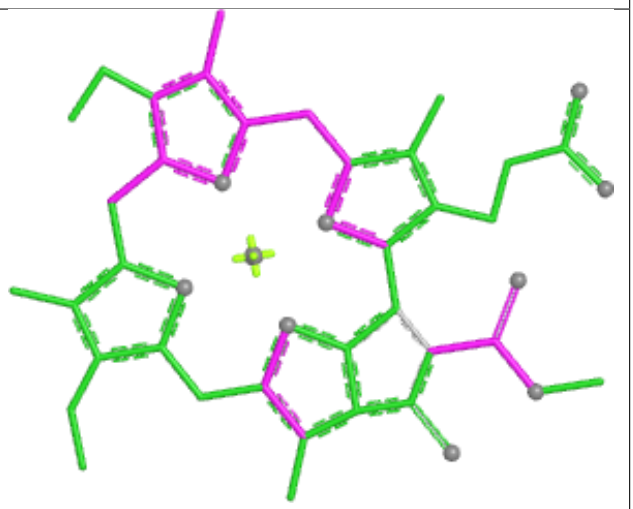


Rings

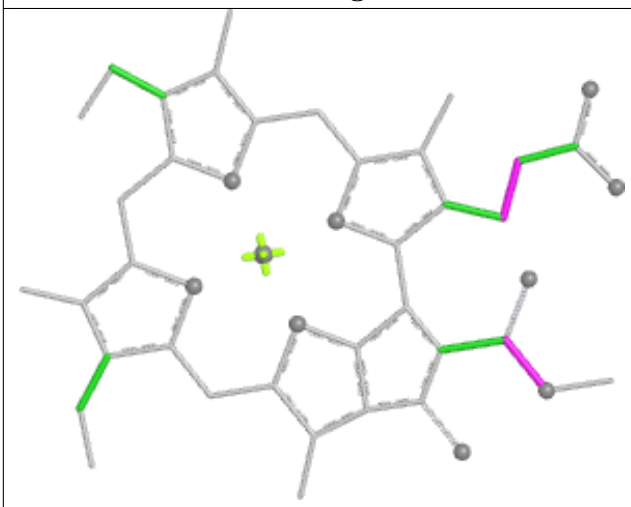
Ligand CLA A 815



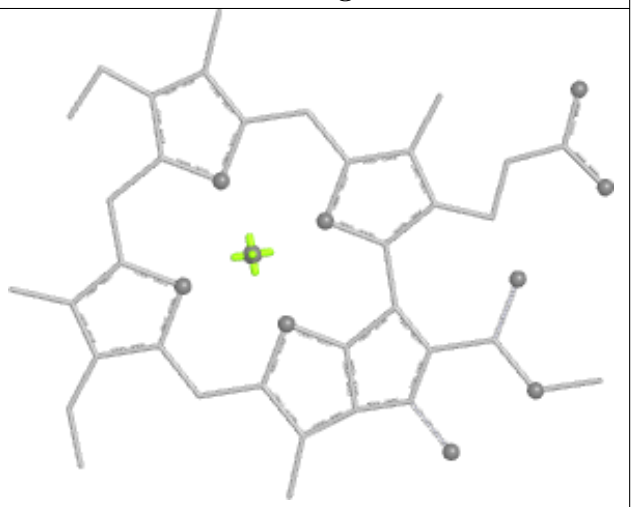
Bond lengths



Bond angles

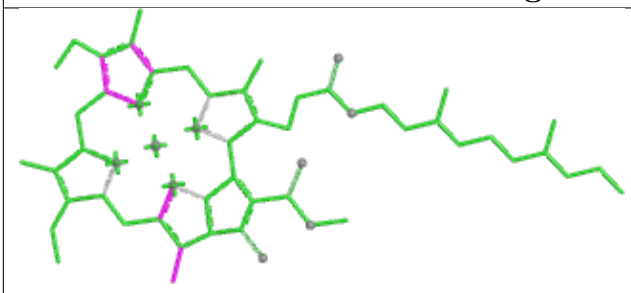


Torsions

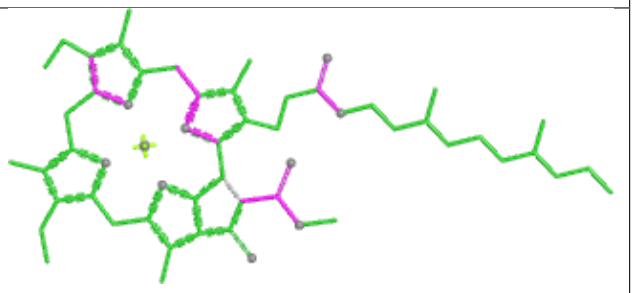


Rings

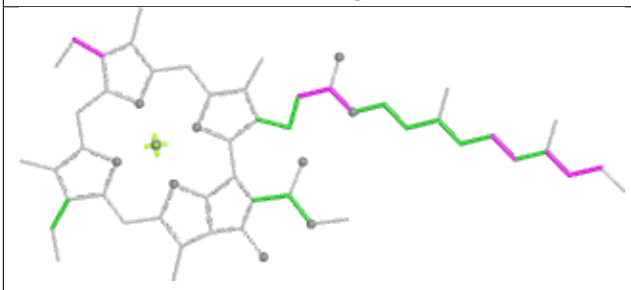
Ligand CLA B 838



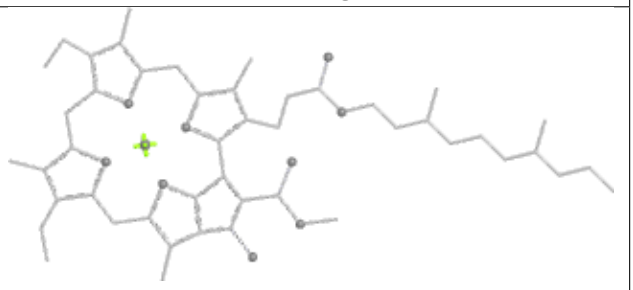
Bond lengths



Bond angles

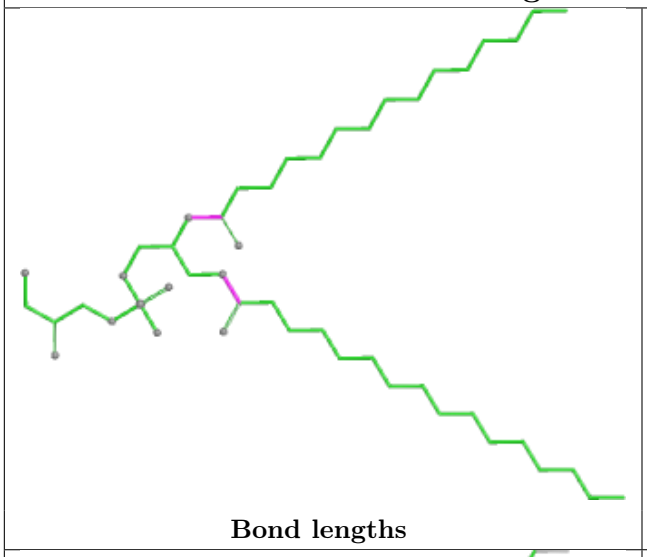


Torsions

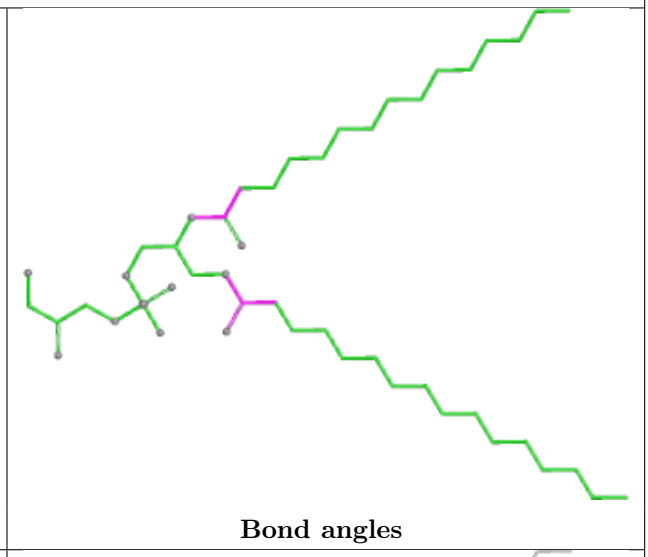


Rings

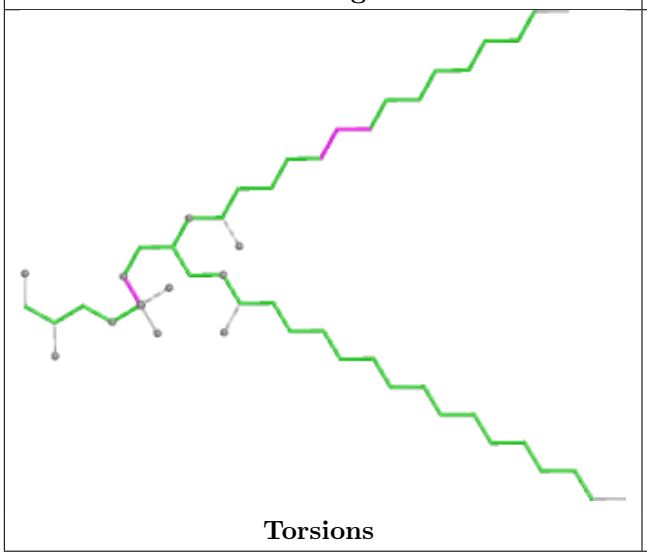
Ligand LHG A 843



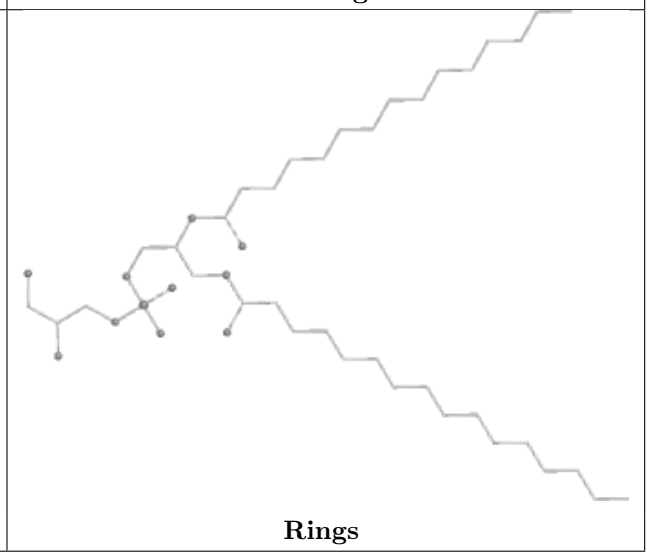
Bond lengths



Bond angles

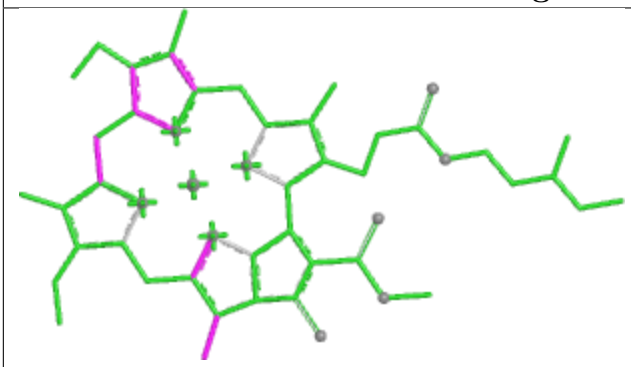


Torsions

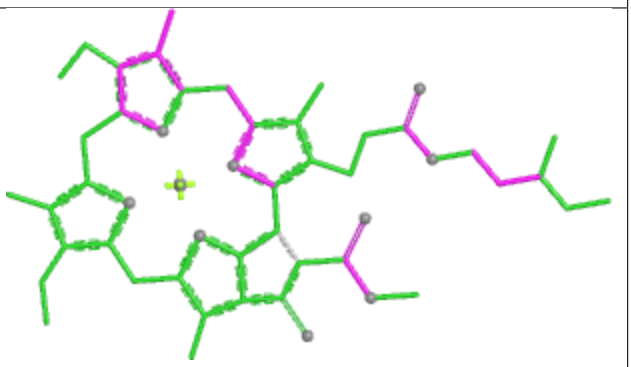


Rings

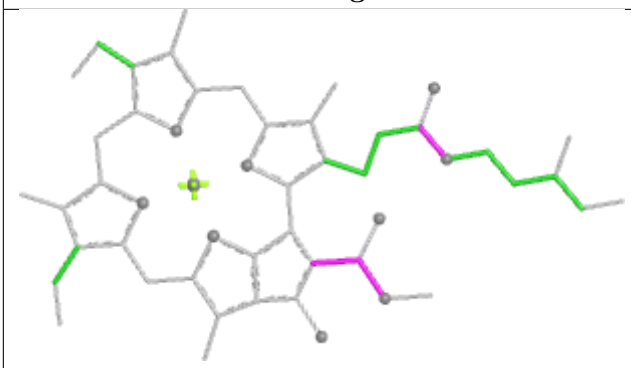
Ligand CLA i 304



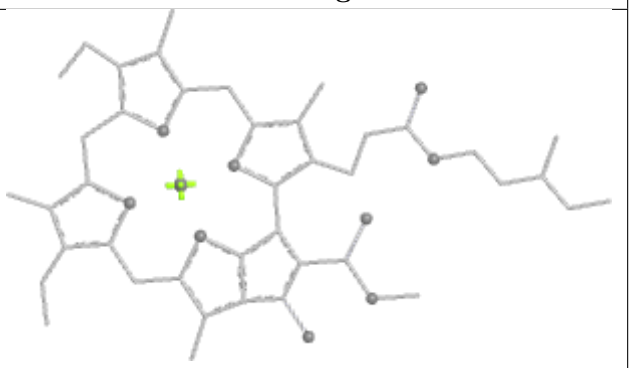
Bond lengths



Bond angles

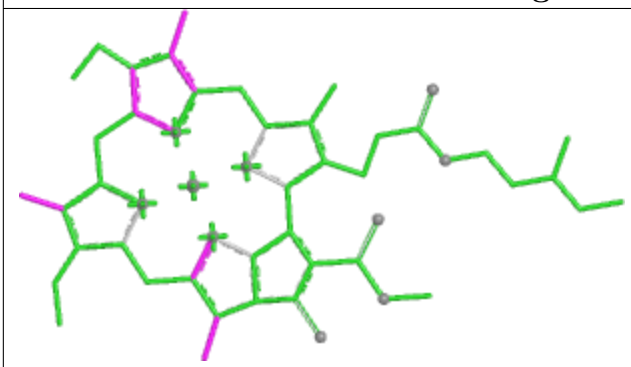


Torsions

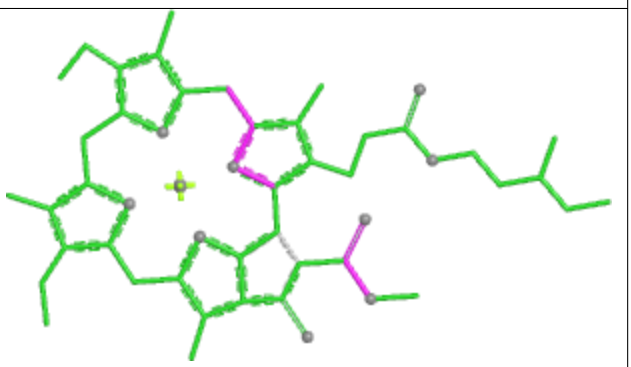


Rings

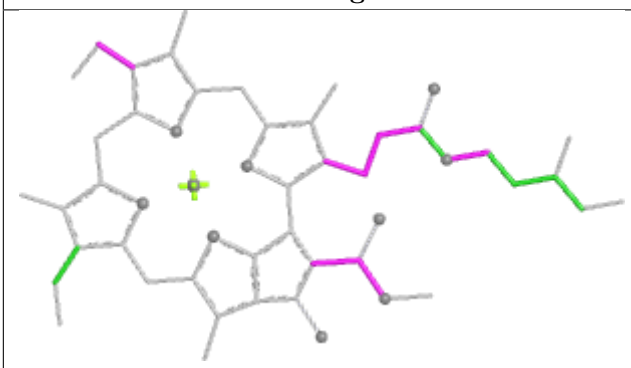
Ligand CLA i 306



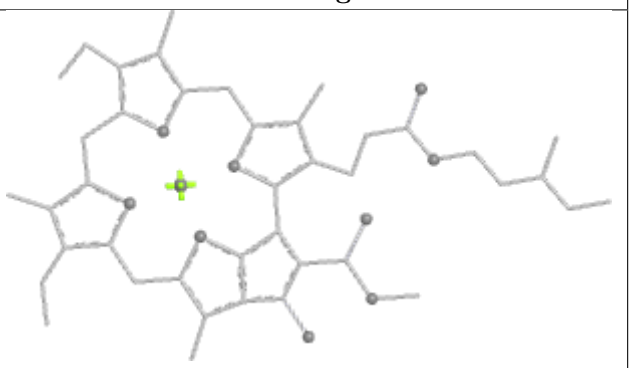
Bond lengths



Bond angles

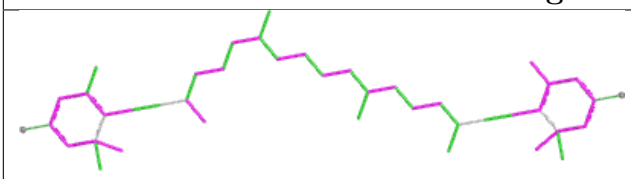


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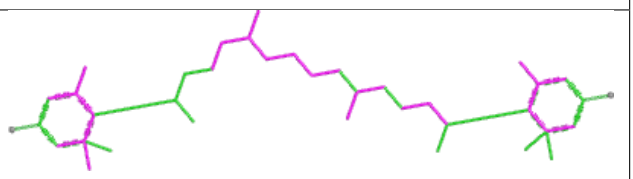


Rings

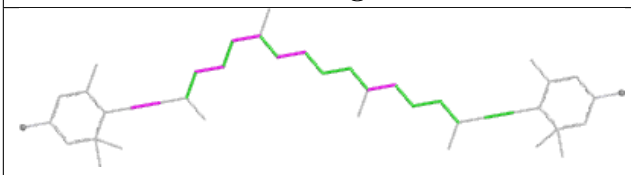
Ligand II0 f 618



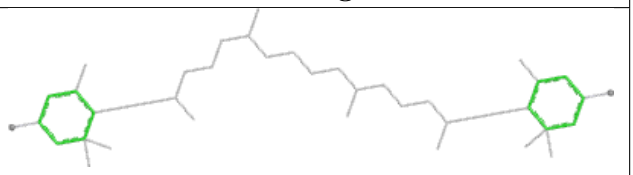
Bond lengths



Bond angles

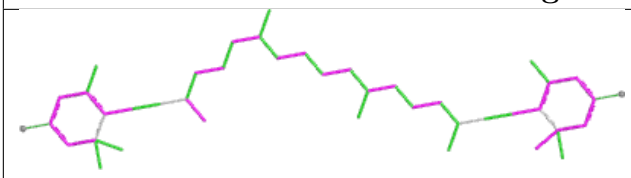


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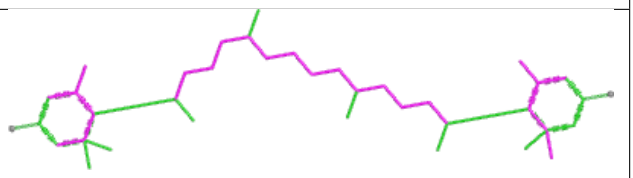


Rings

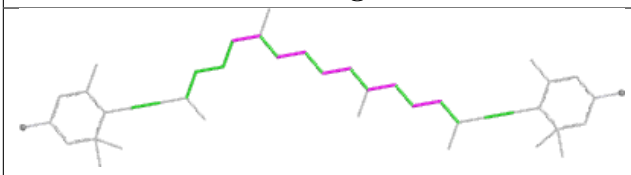
Ligand II0 h 311



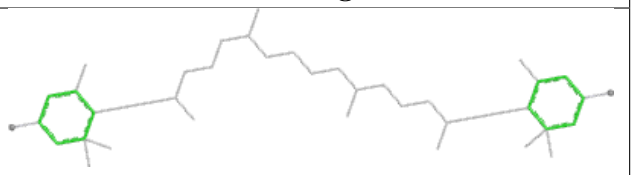
Bond lengths



Bond angles

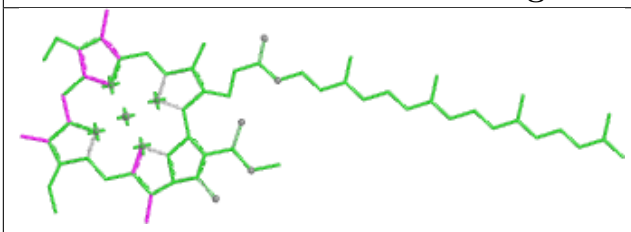


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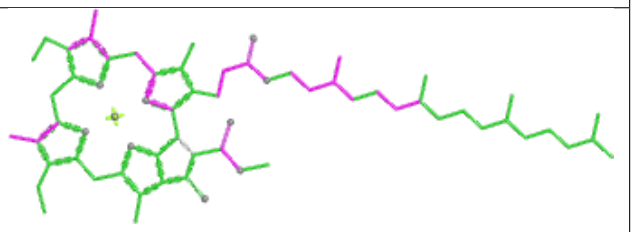


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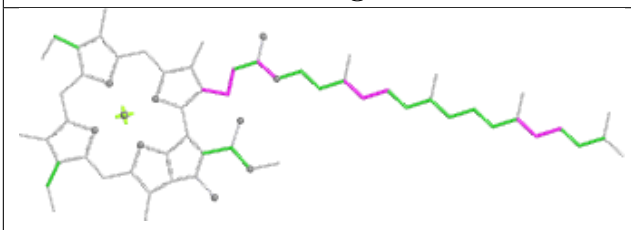
Ligand CLA n 609



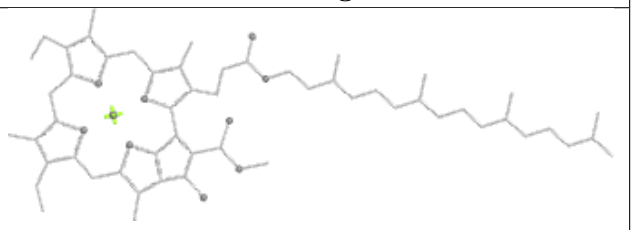
Bond lengths



Bond angles

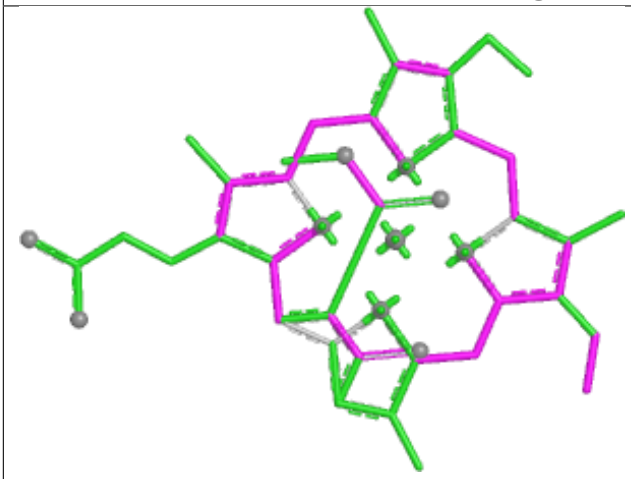


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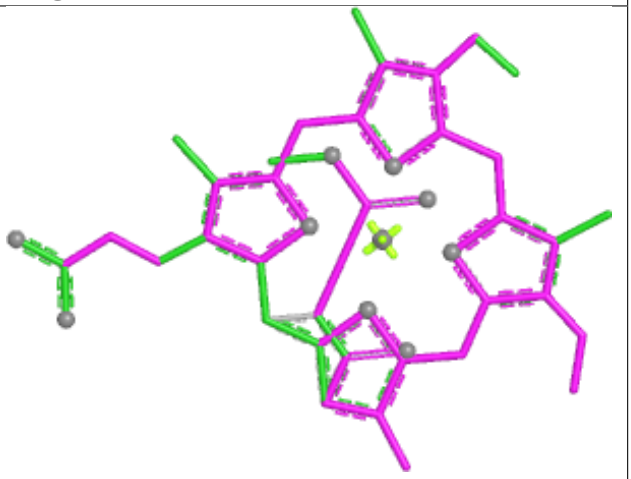


Rings

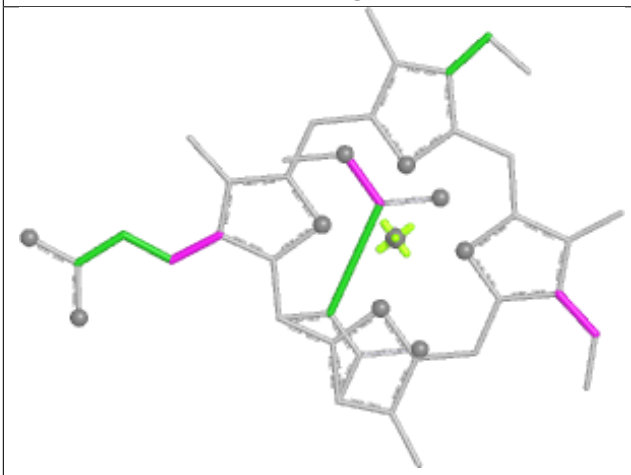
Ligand KC2 g 314



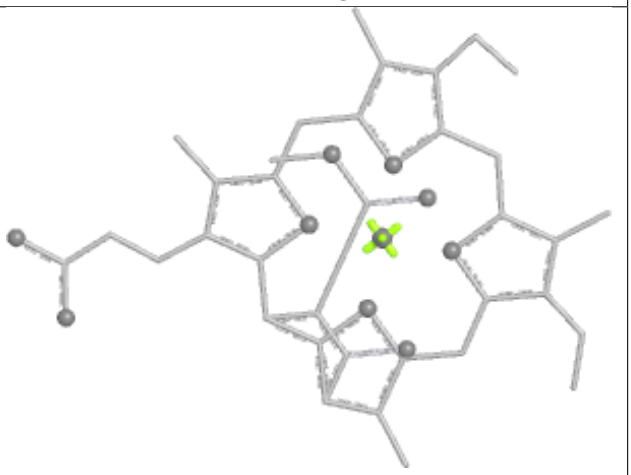
Bond lengths



Bond angles

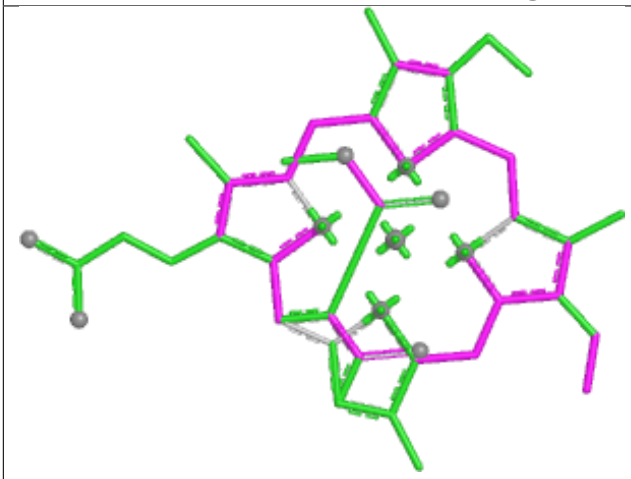


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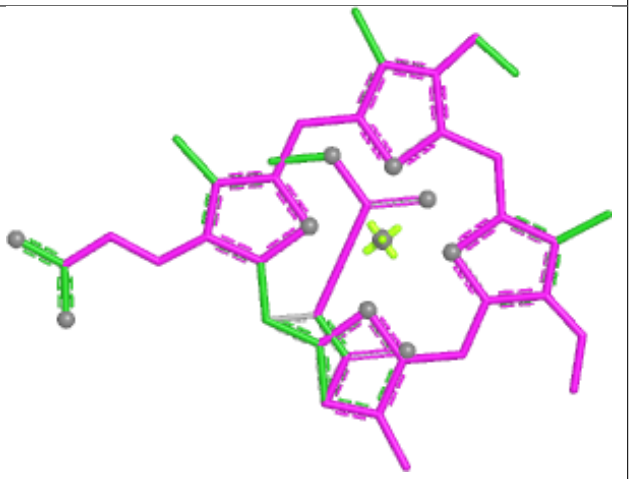


Rings

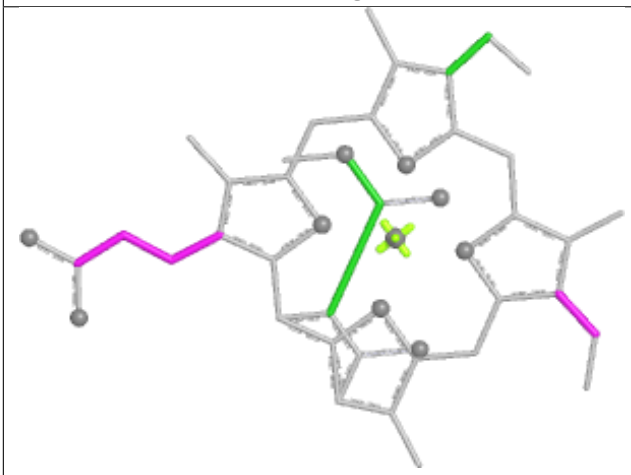
Ligand KC2 m 611



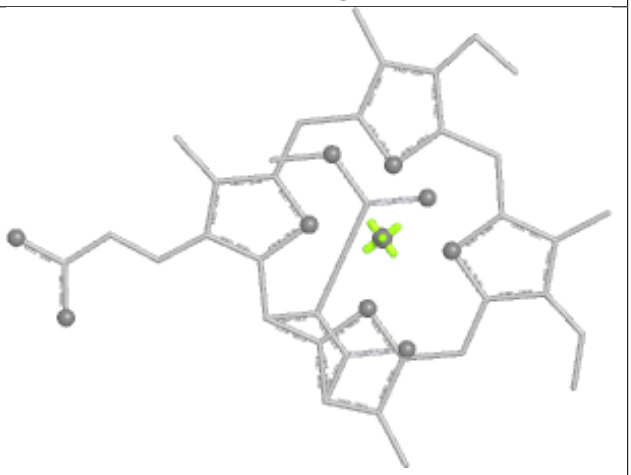
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Bond angles

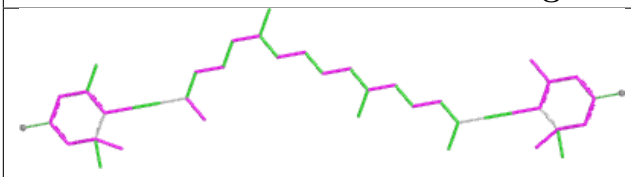


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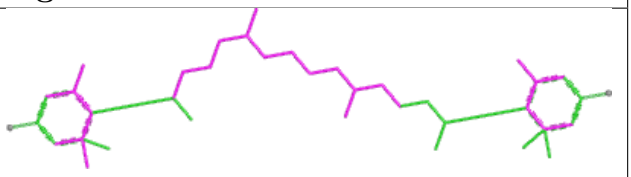


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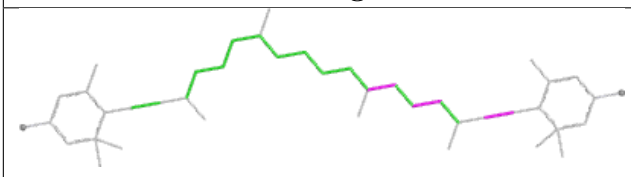
Ligand II0 g 320



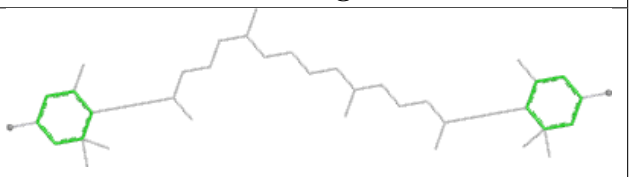
Bond lengths



Bond angles

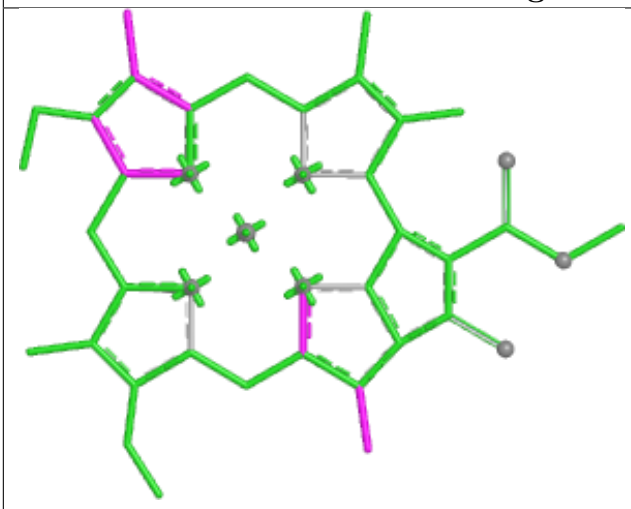


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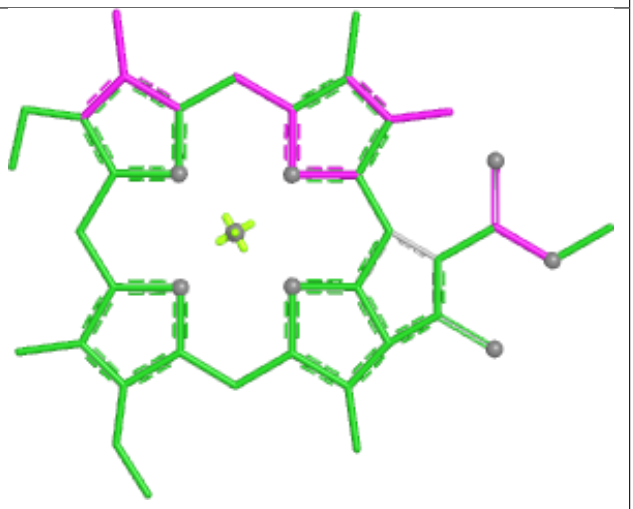


Rings

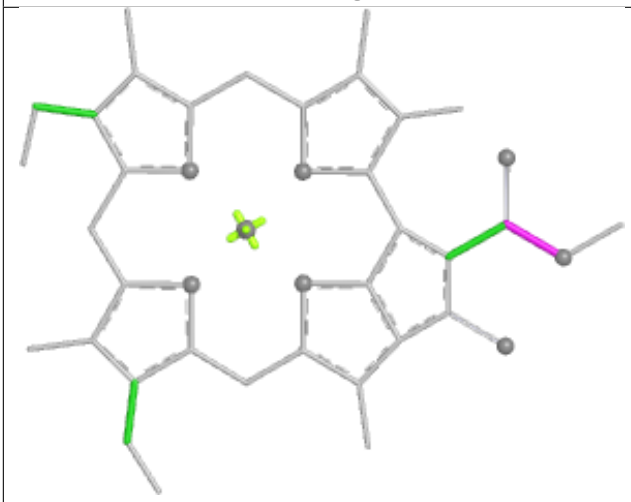
Ligand CLA d 309



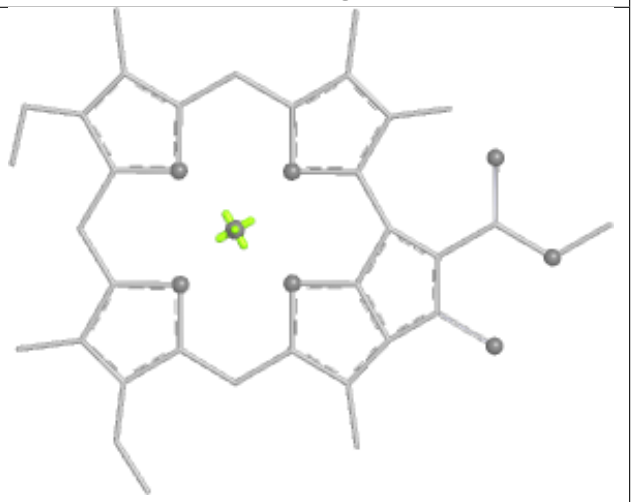
Bond lengths



Bond angles

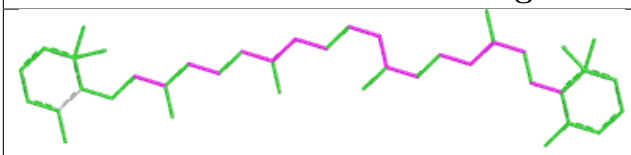


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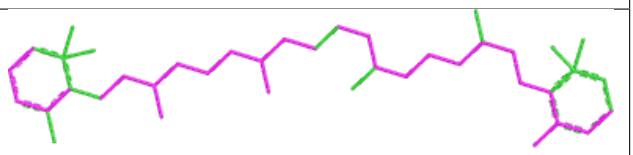


Rings

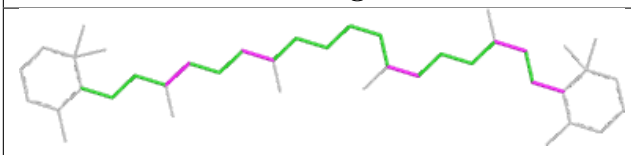
Ligand WVN A 846



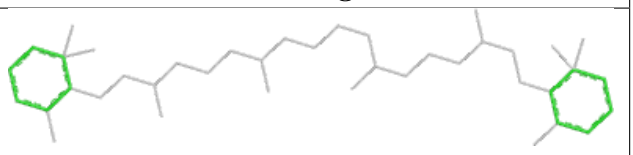
Bond lengths



Bond angles

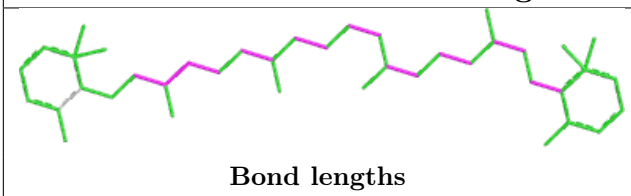


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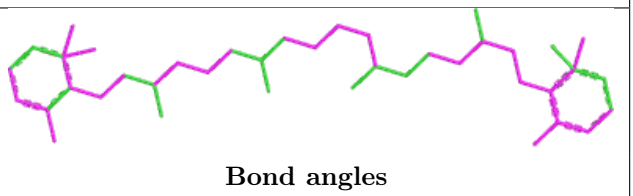


Rings

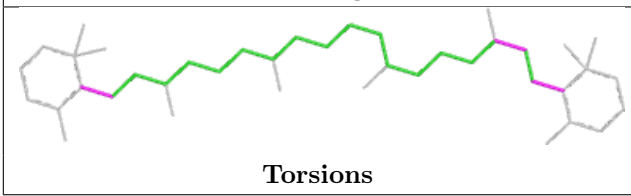
Ligand WVN R 202



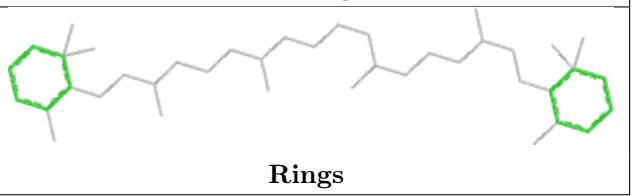
Bond lengths



Bond angles

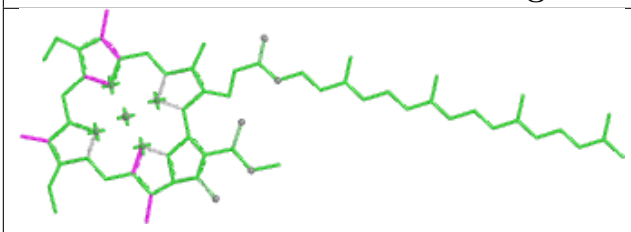


Torsions

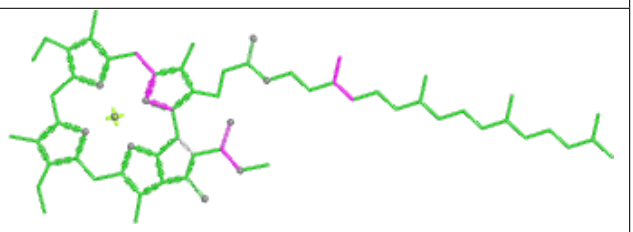


Rings

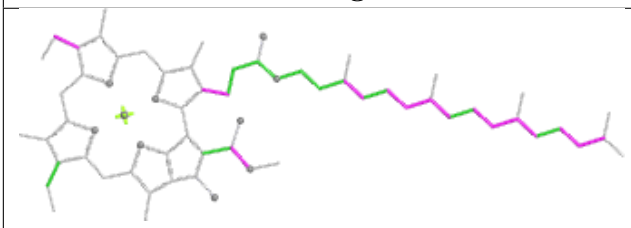
Ligand CLA b 610



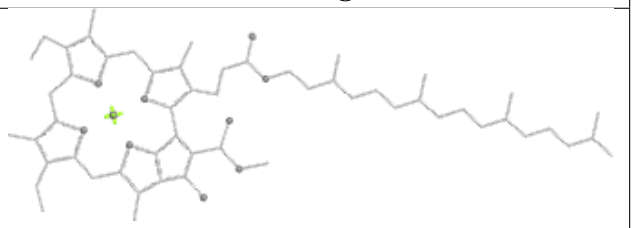
Bond lengths



Bond angles

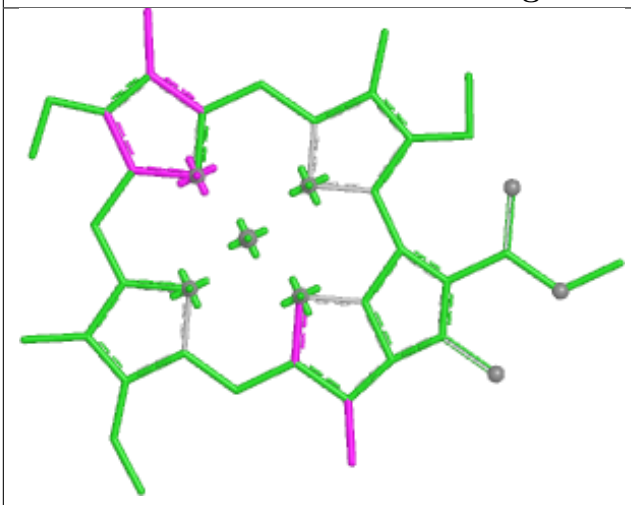


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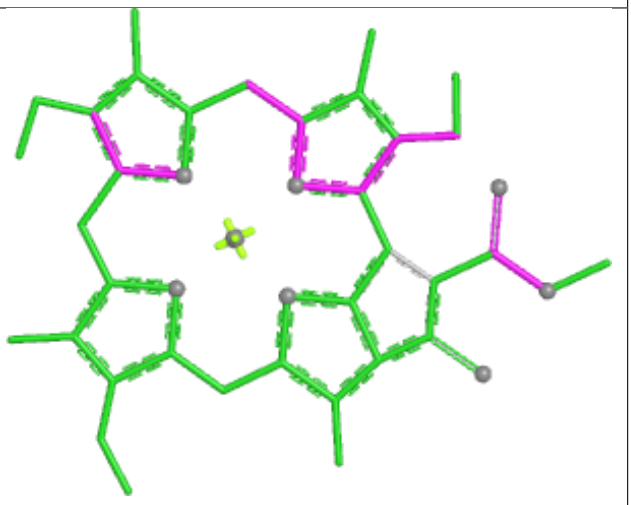


Rings

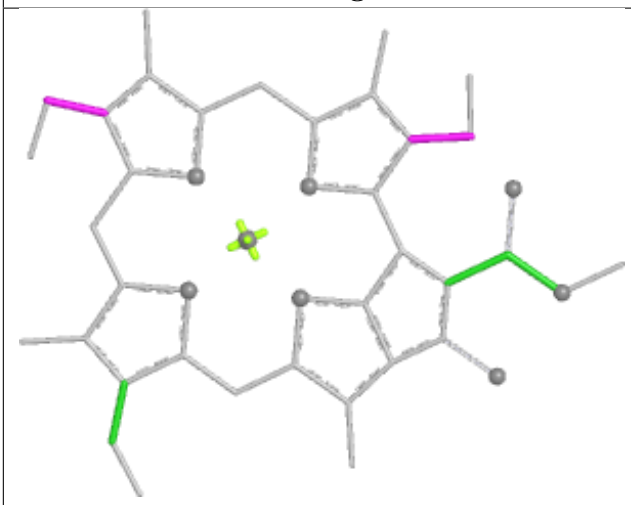
Ligand CLA m 605



Bond lengths



Bond angles

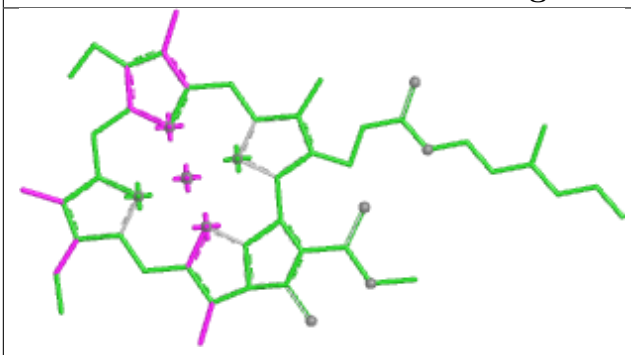


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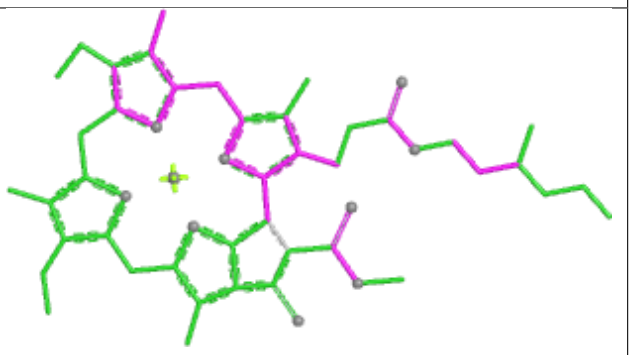


Rings

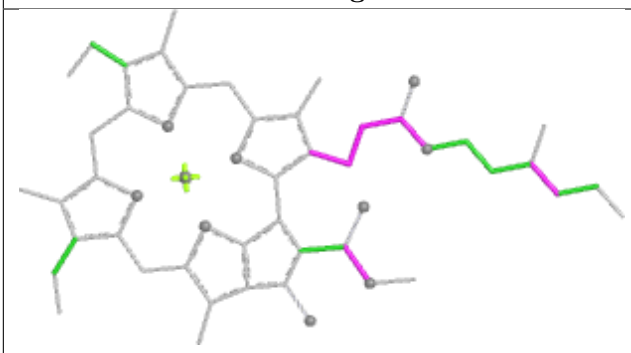
Ligand CLA c 606



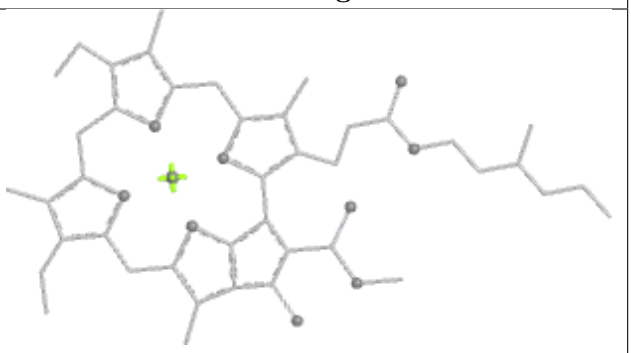
Bond lengths



Bond angles

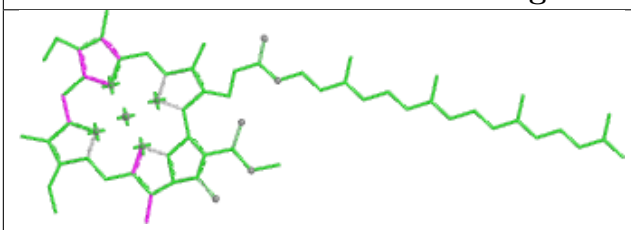


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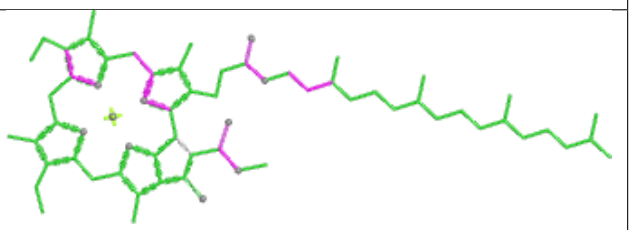


Rings

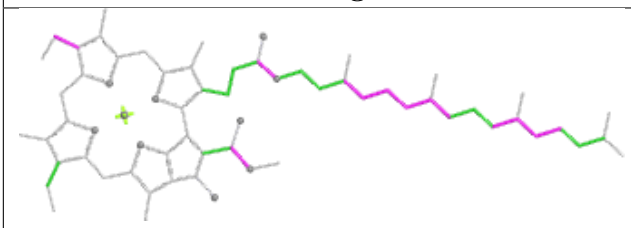
Ligand CLA e 611



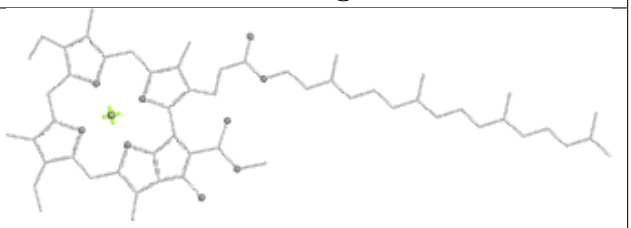
Bond lengths



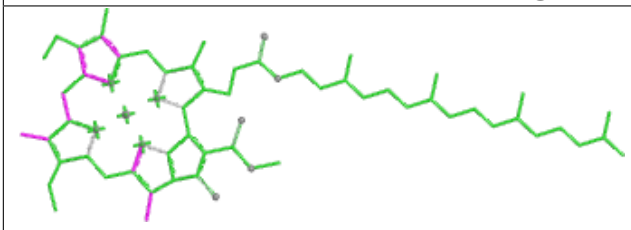
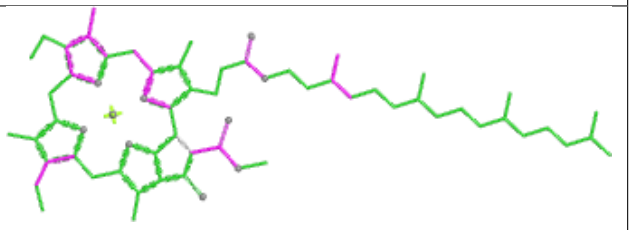
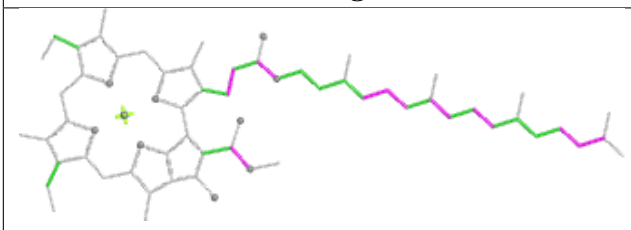
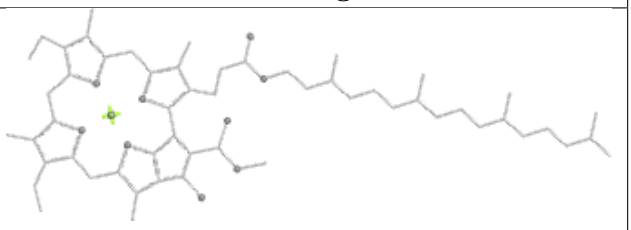
Bond angles

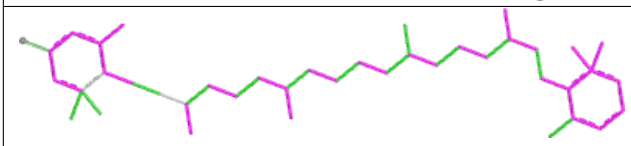
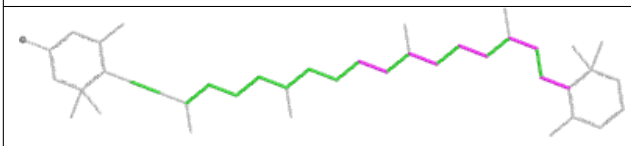
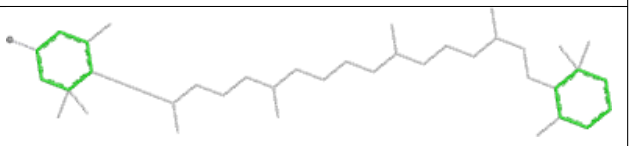


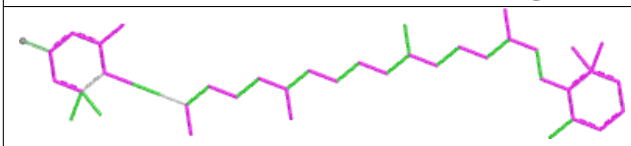
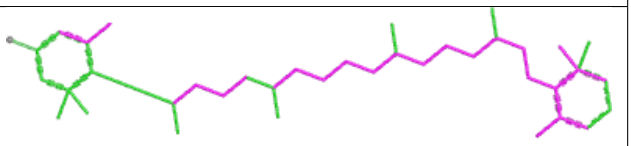
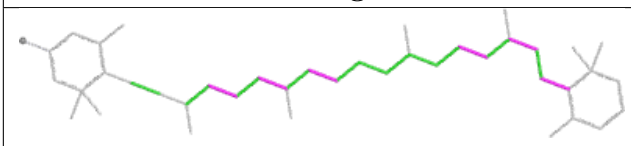
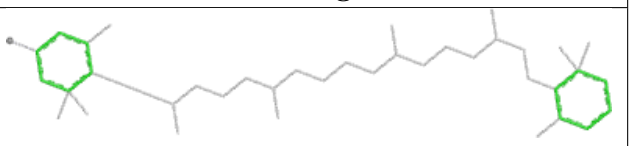
Torsions

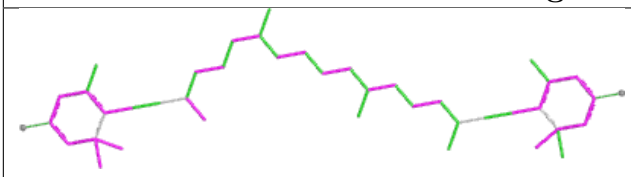
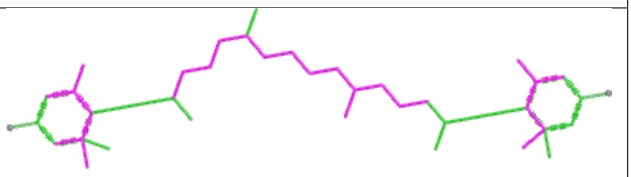
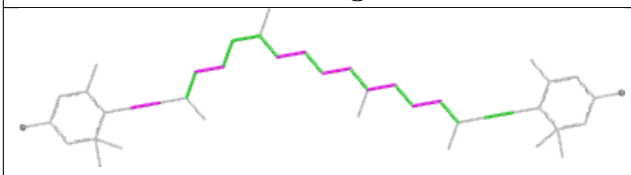
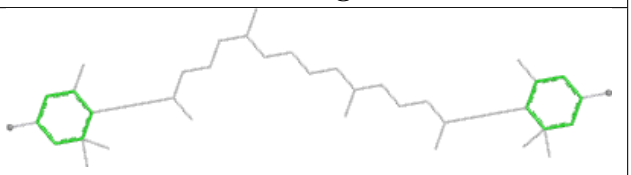


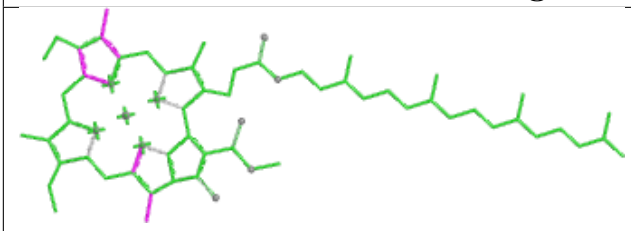
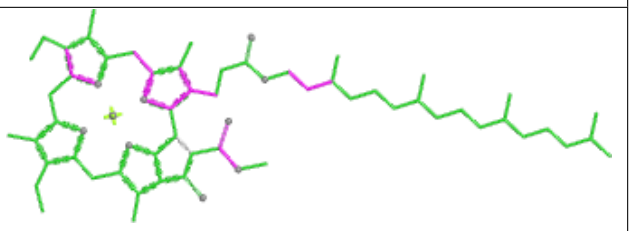
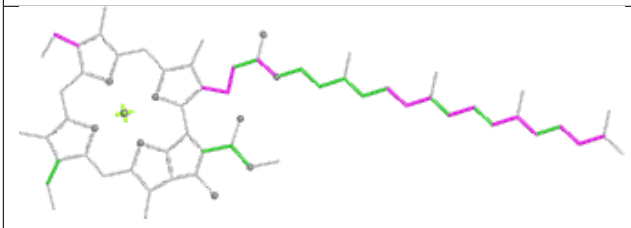
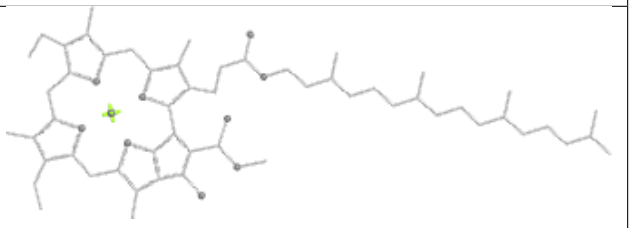
Rings

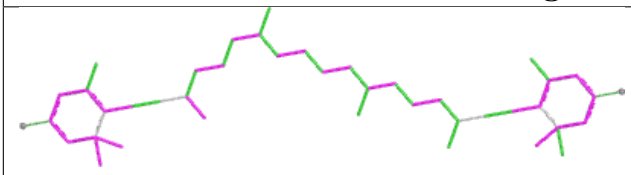
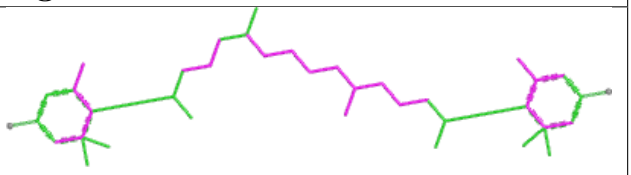
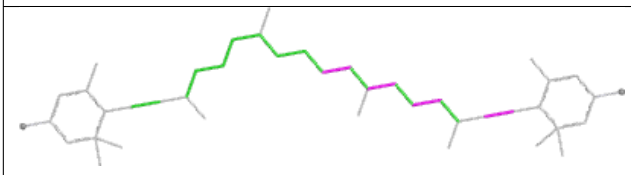
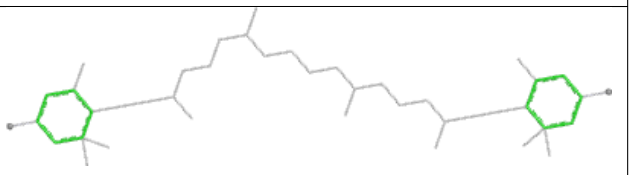
Ligand CLA f 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHT n 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

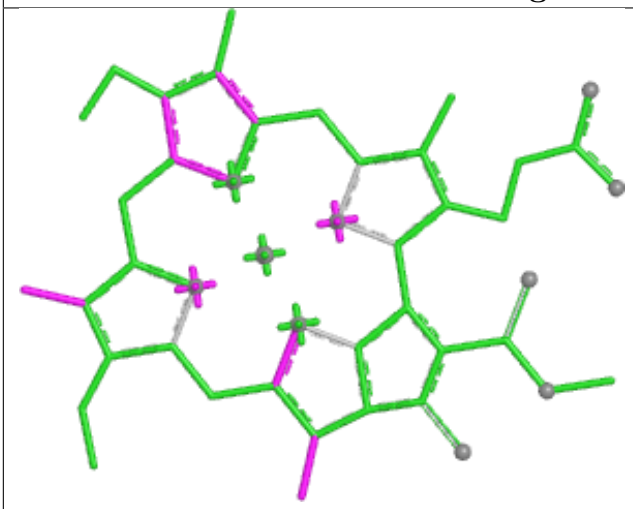
Ligand IHT O 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 i 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

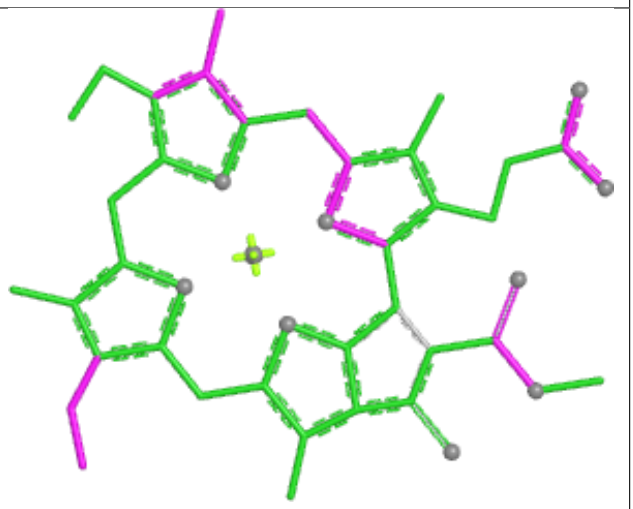
Ligand CLA a 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 g 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

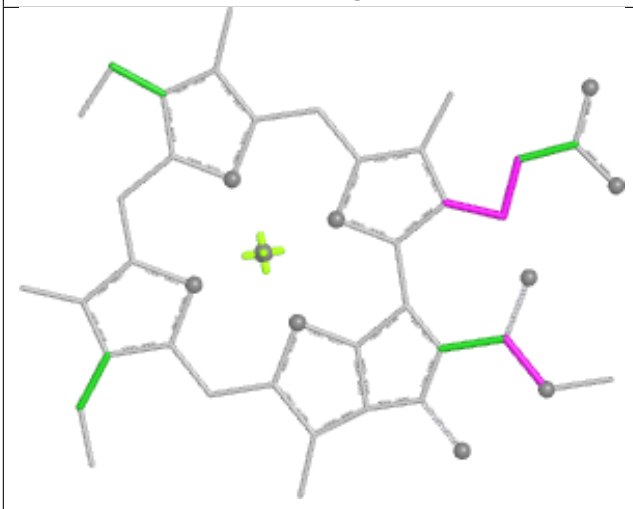
Ligand CLA c 611



Bond lengths



Bond angles

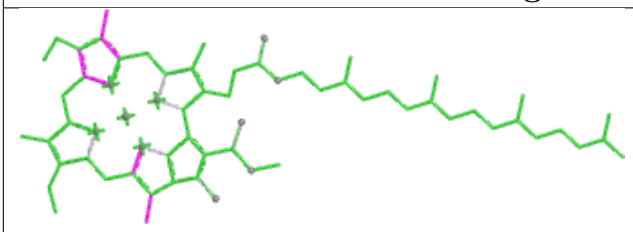


Torsions

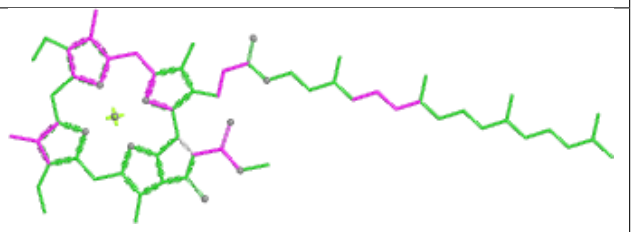


Rings

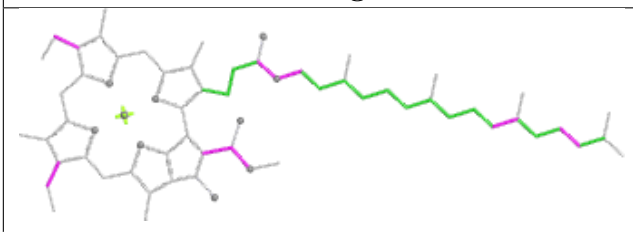
Ligand CLA A 832



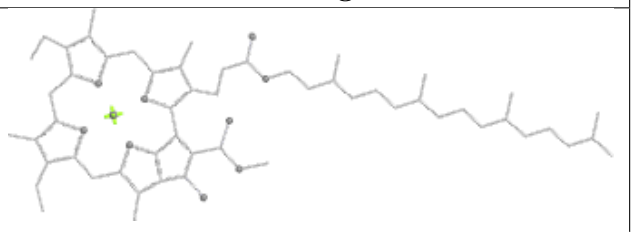
Bond lengths



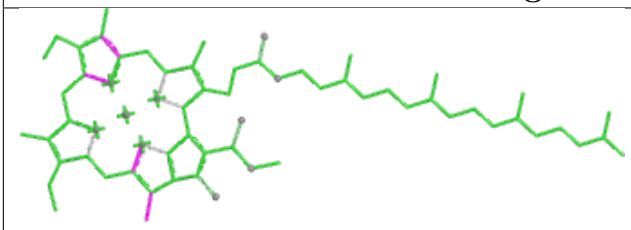
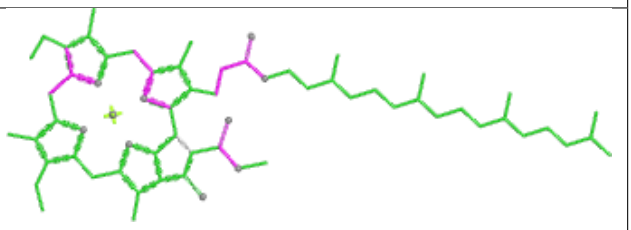
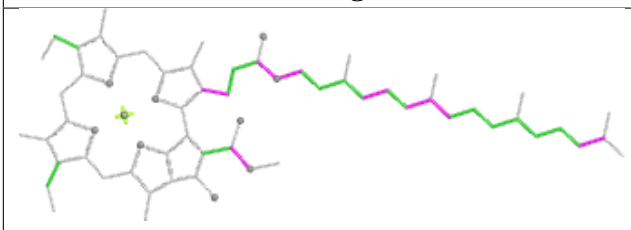
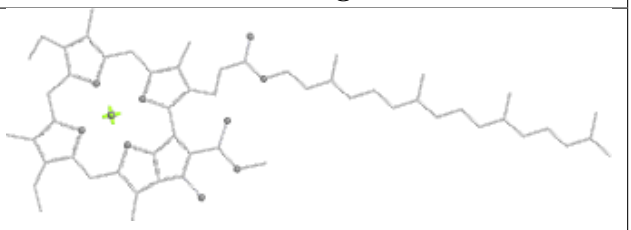
Bond angles

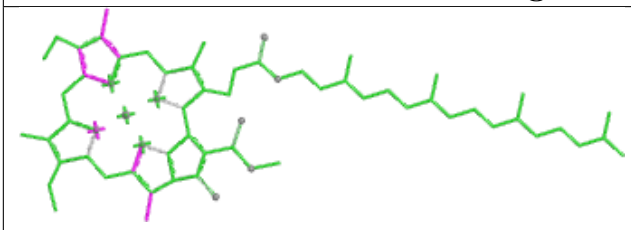
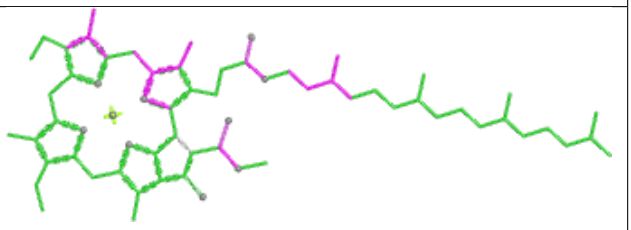
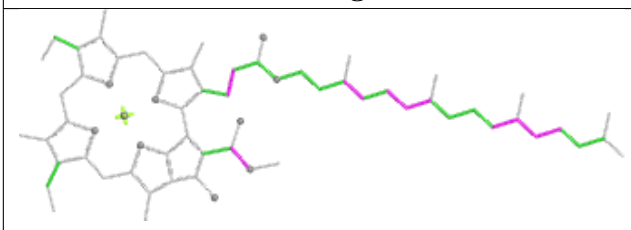
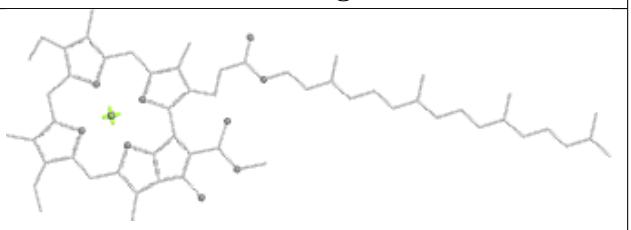


Torsions

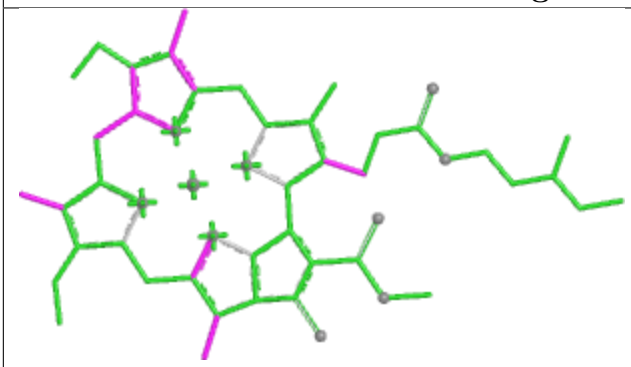


Rings

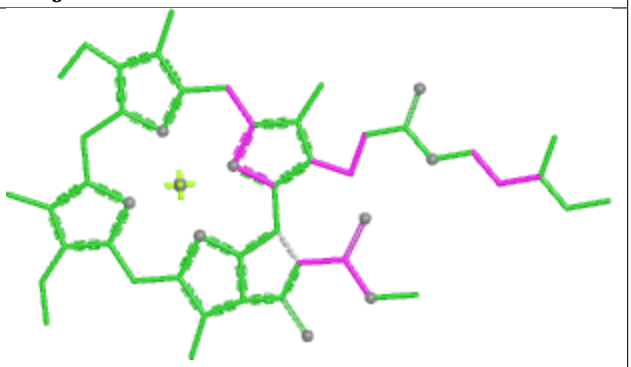
Ligand CLA B 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA k 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

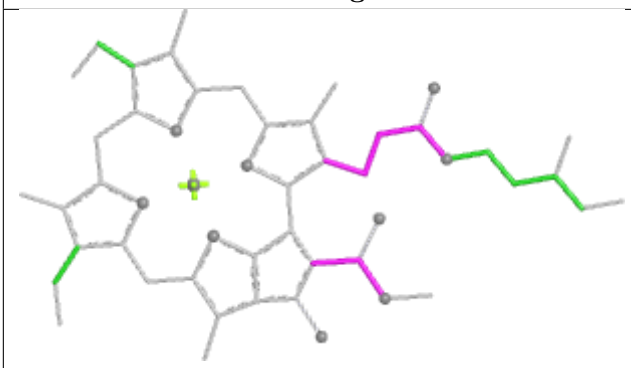
Ligand CLA j 606



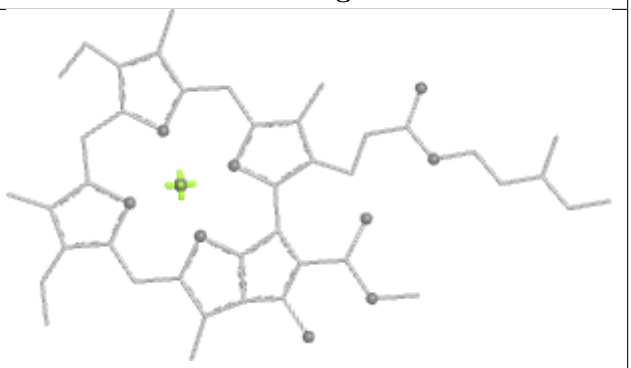
Bond lengths



Bond angles

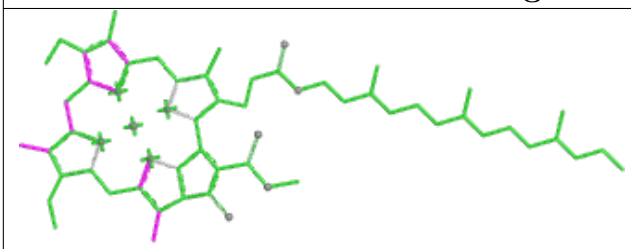


Torsions

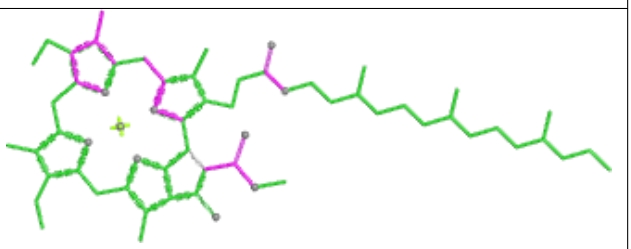


Rings

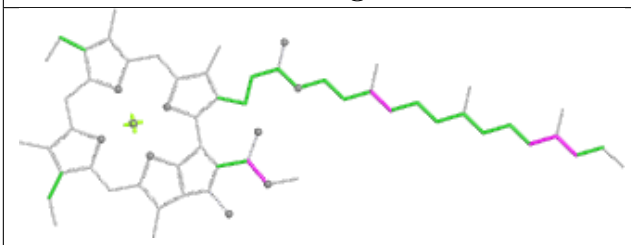
Ligand CLA A 827



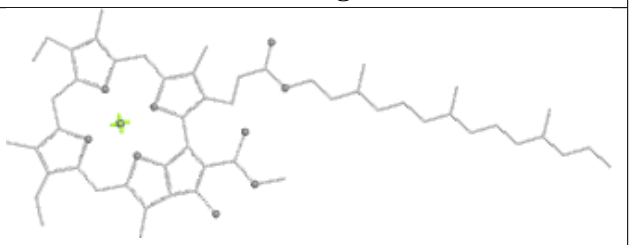
Bond lengths



Bond angles

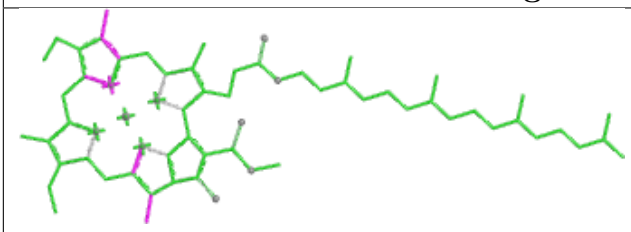


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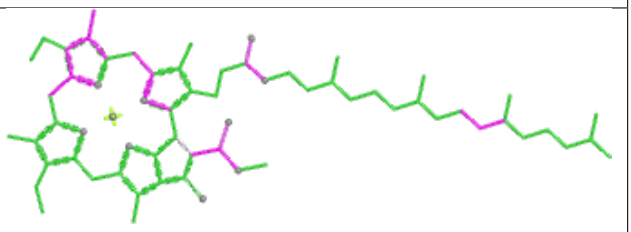


Rings

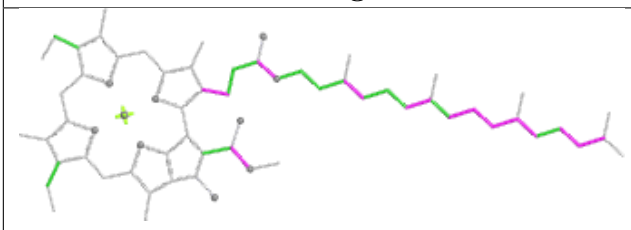
Ligand CLA A 840



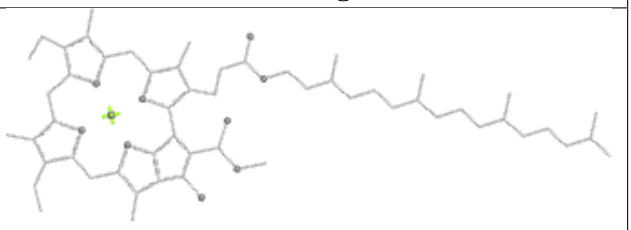
Bond lengths



Bond angles

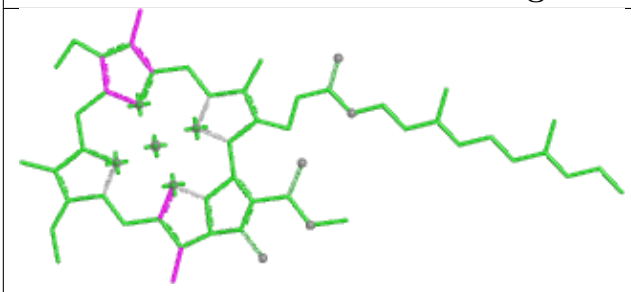


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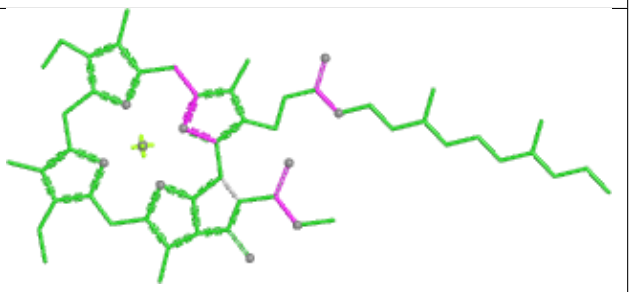


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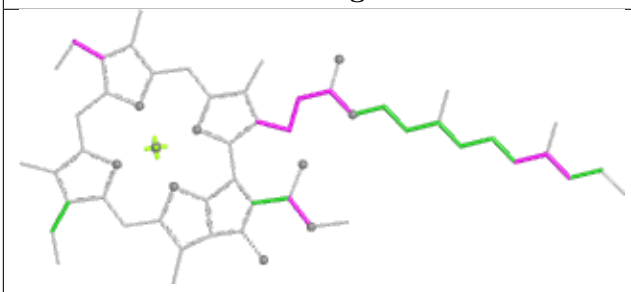
Ligand CLA h 307



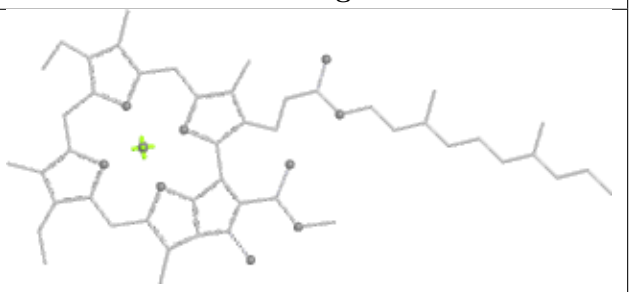
Bond lengths



Bond angles

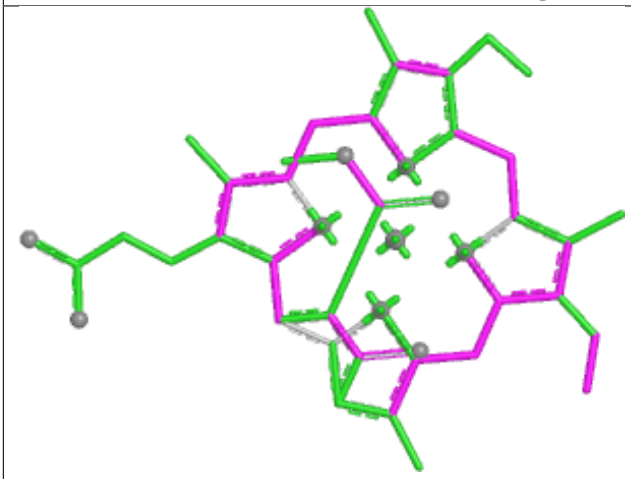


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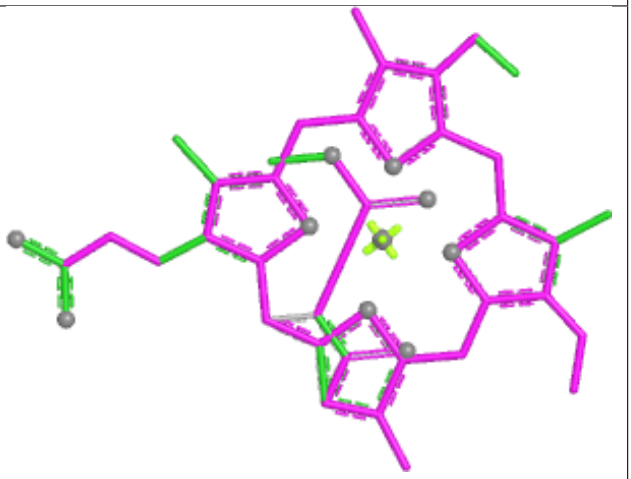


Rings

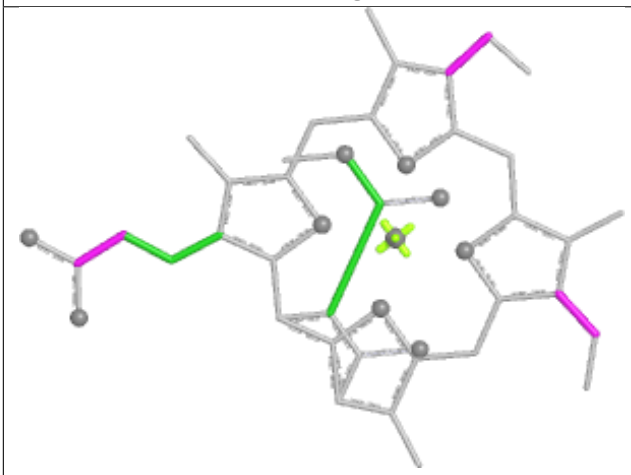
Ligand KC2 i 319



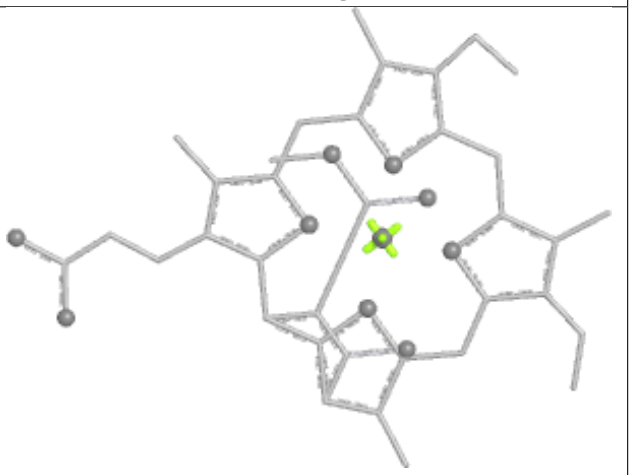
Bond lengths



Bond angles

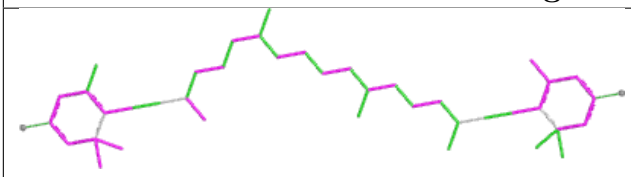


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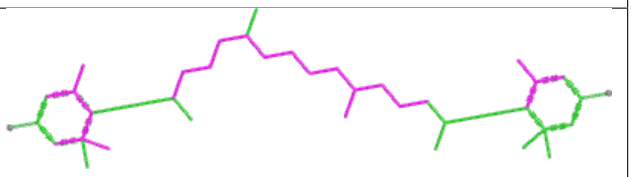


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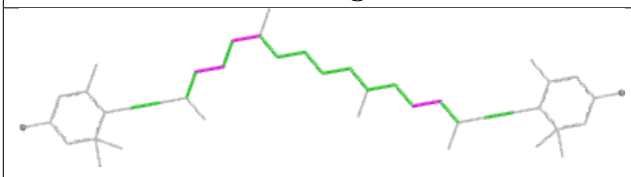
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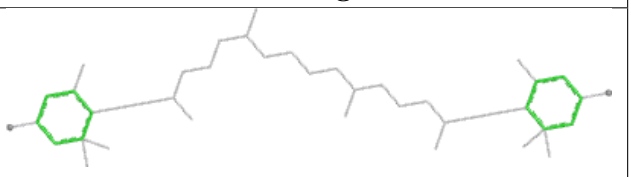
Bond lengths



Bond angles

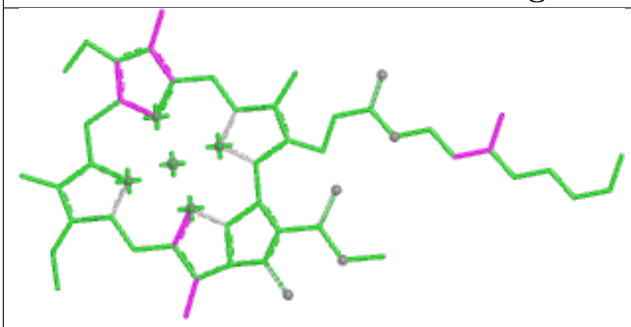


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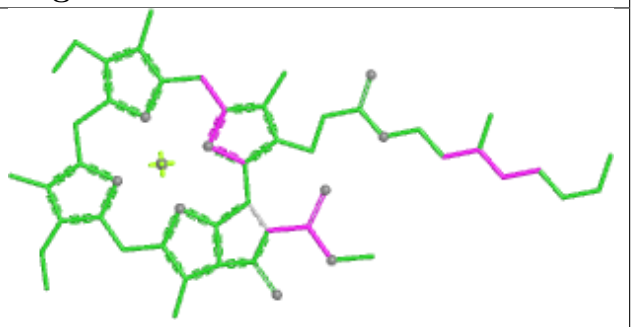


Rings

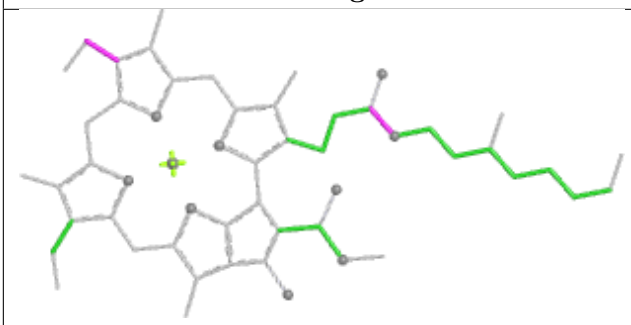
Ligand CLA g 311



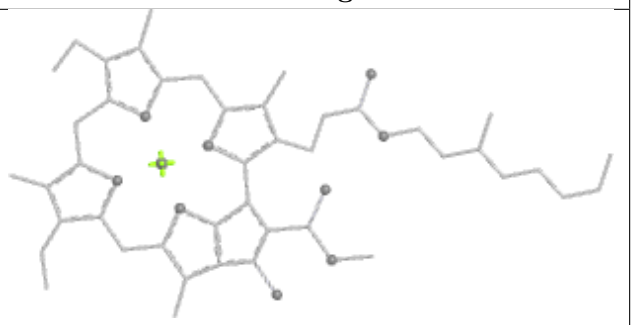
Bond lengths



Bond angles

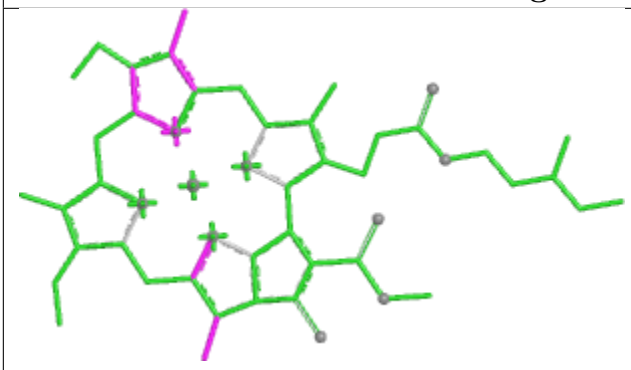


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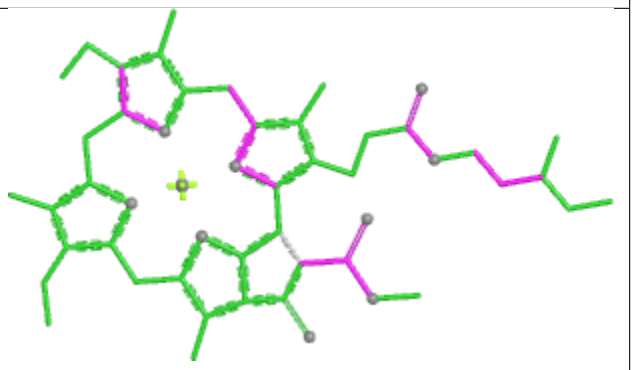


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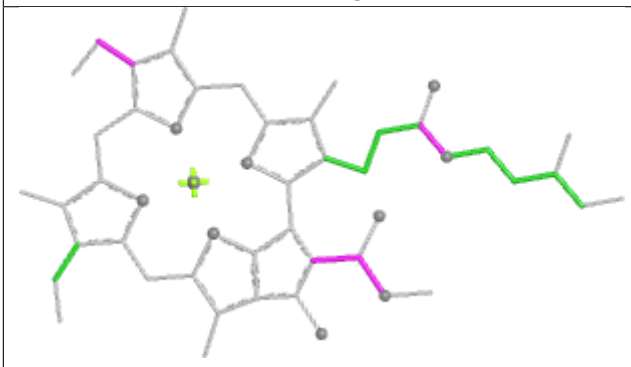
Ligand CLA s 208



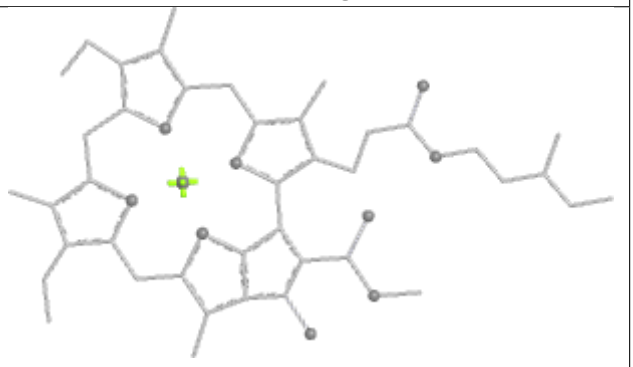
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Bond angles

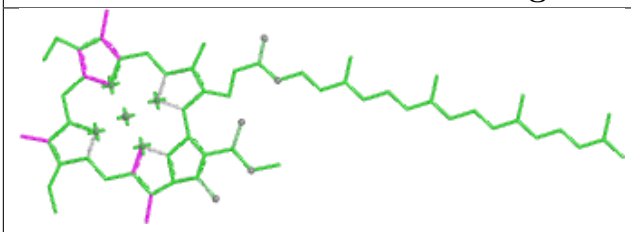


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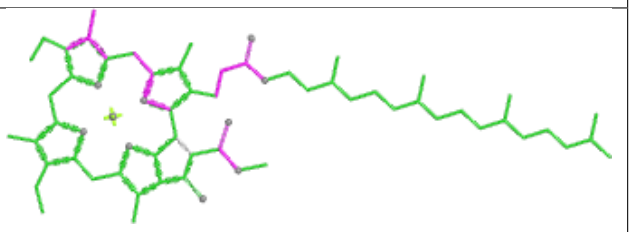


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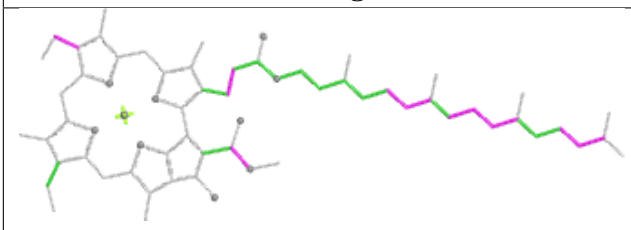
Ligand CLA e 610



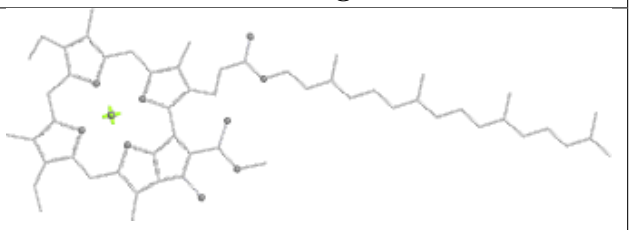
Bond lengths



Bond angles

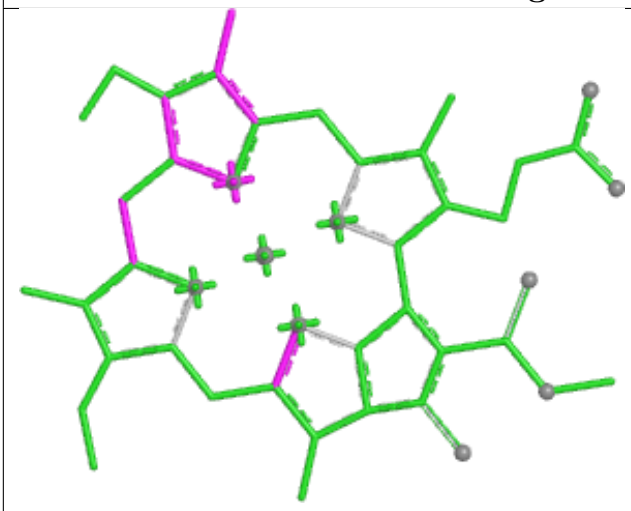


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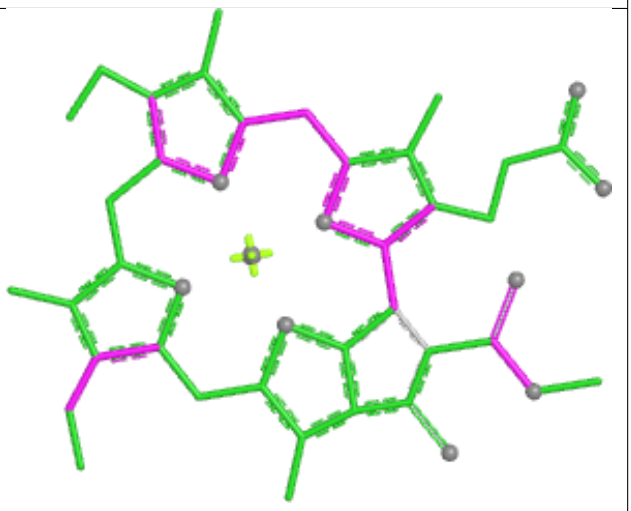


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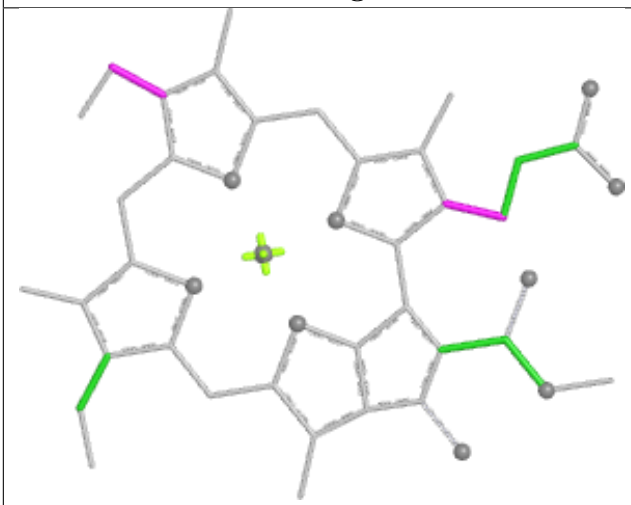
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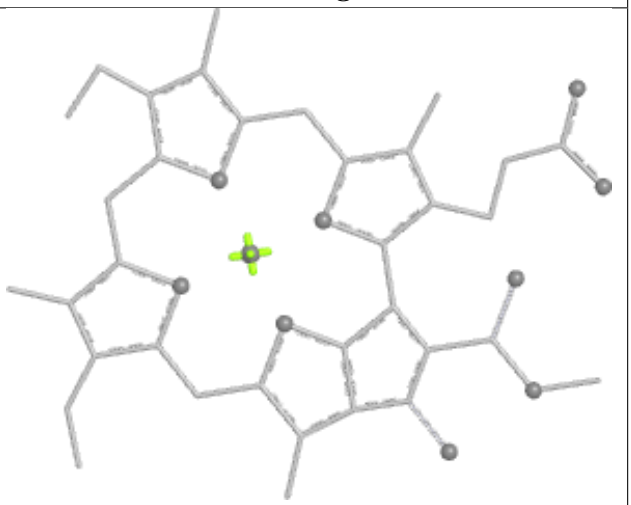
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Bond angles

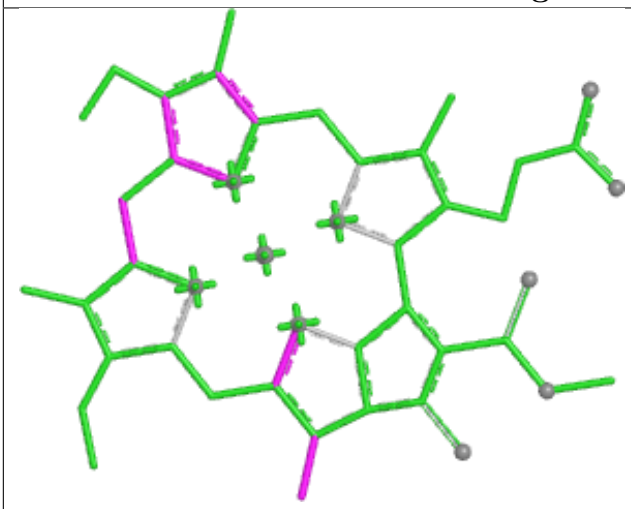


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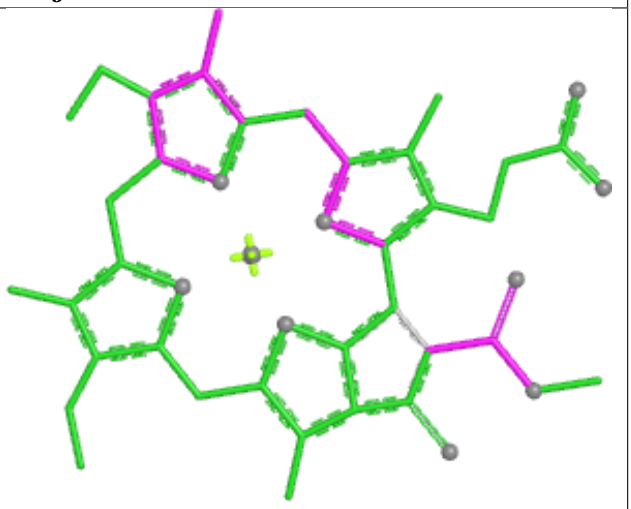


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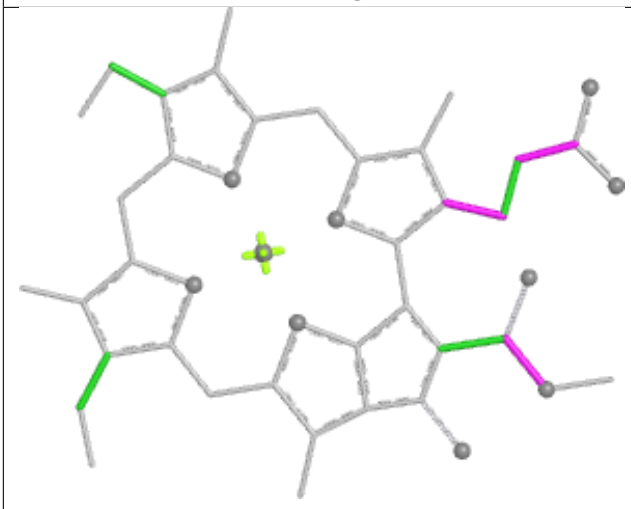
Ligand CLA j 608



Bond lengths



Bond angles

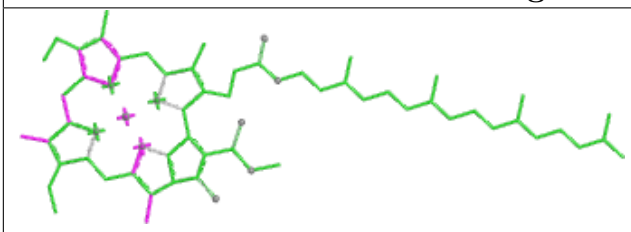


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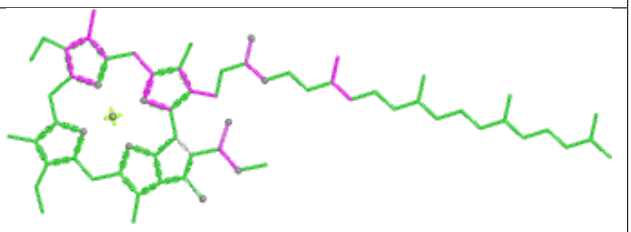


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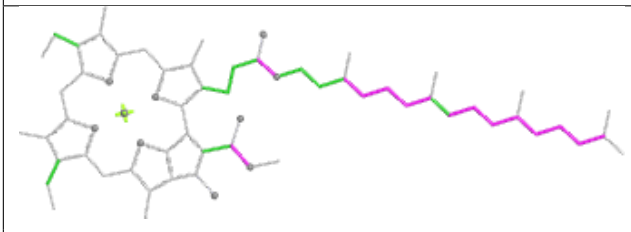
Ligand CLA b 603



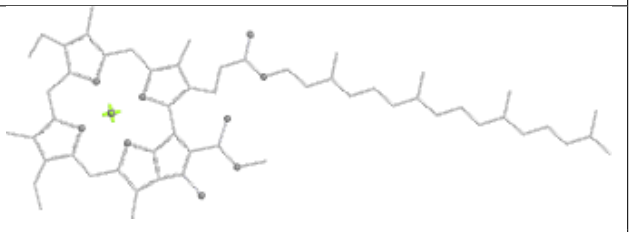
Bond lengths



Bond angles

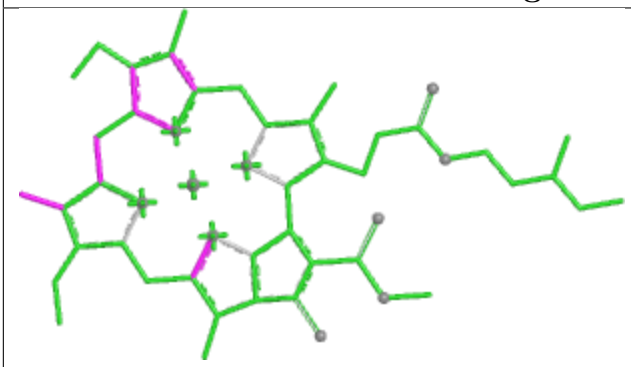


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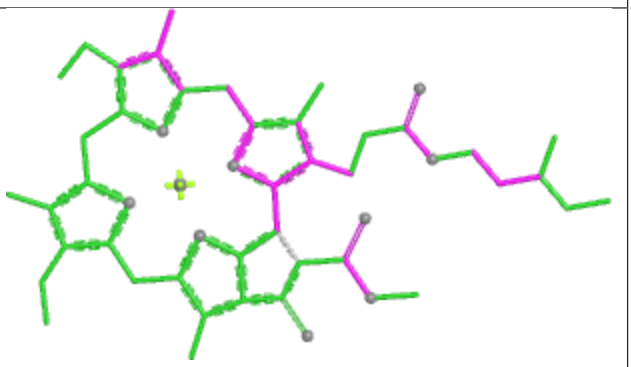


Rings

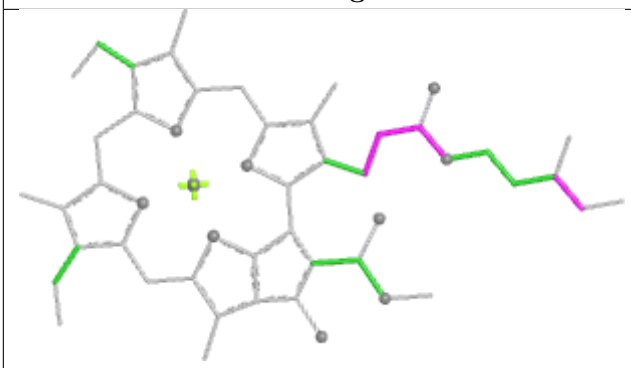
Ligand CLA R 203



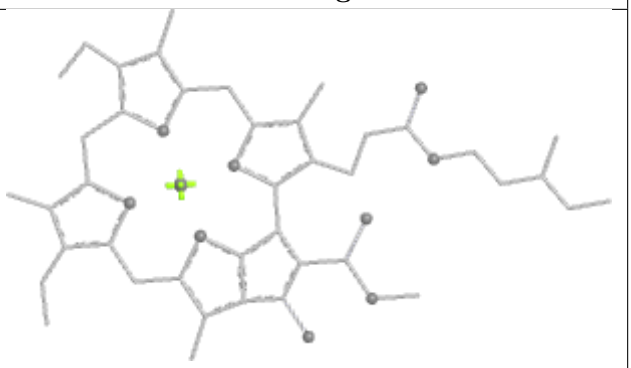
Bond lengths



Bond angles

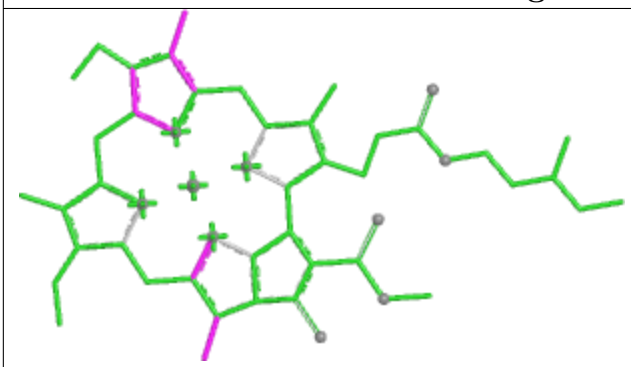


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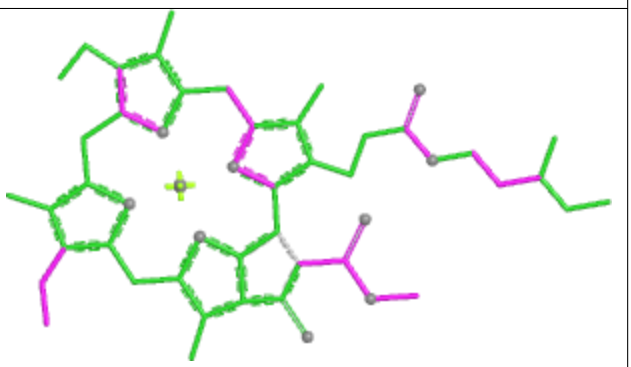


Rings

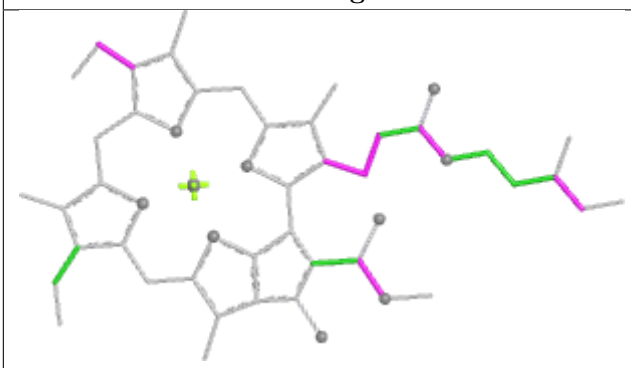
Ligand CLA k 607



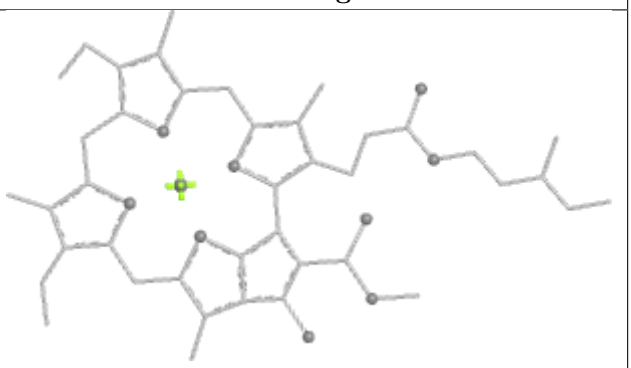
Bond lengths



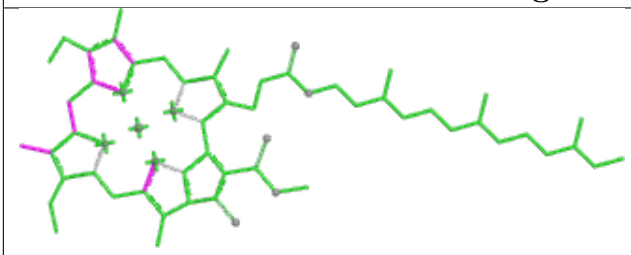
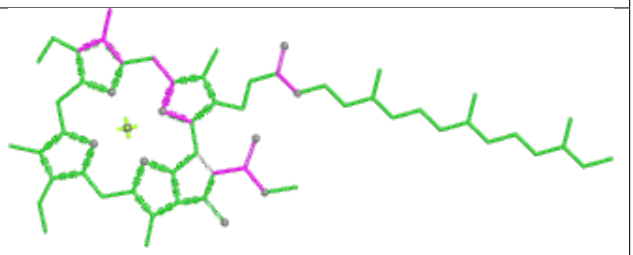
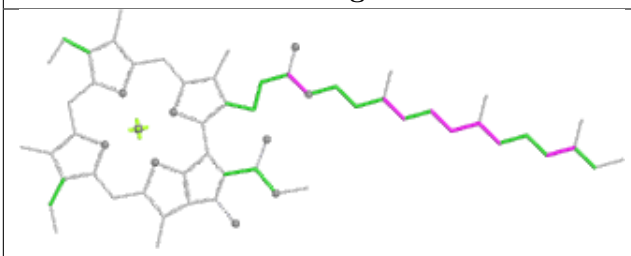
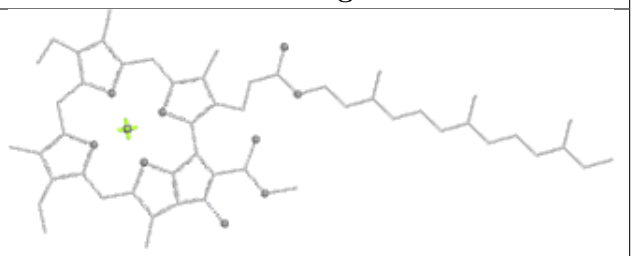
Bond angles

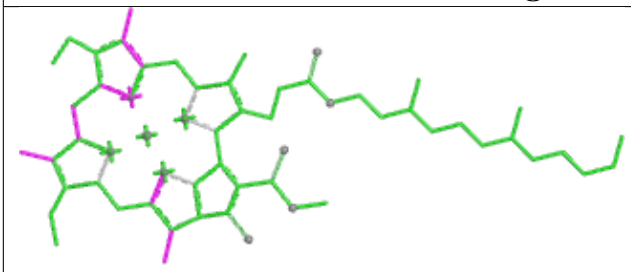
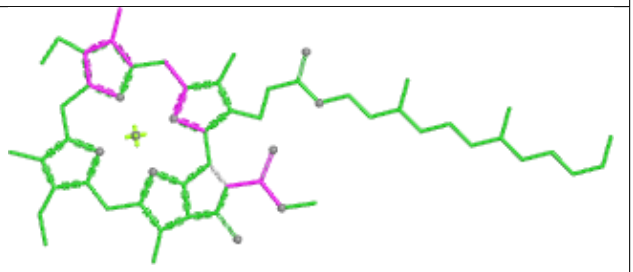
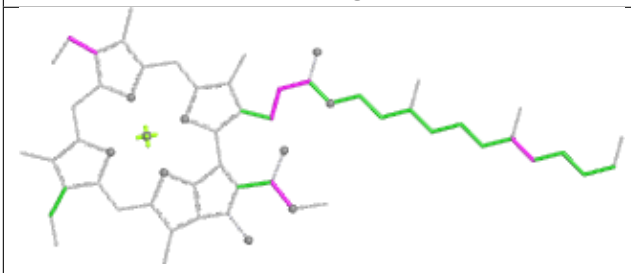
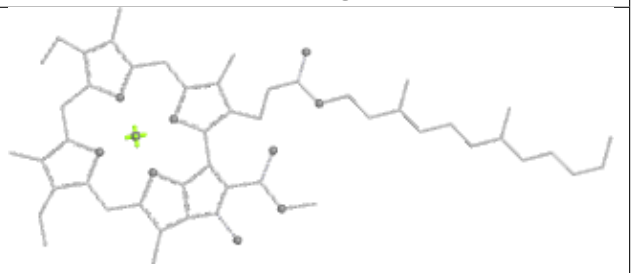


Torsions

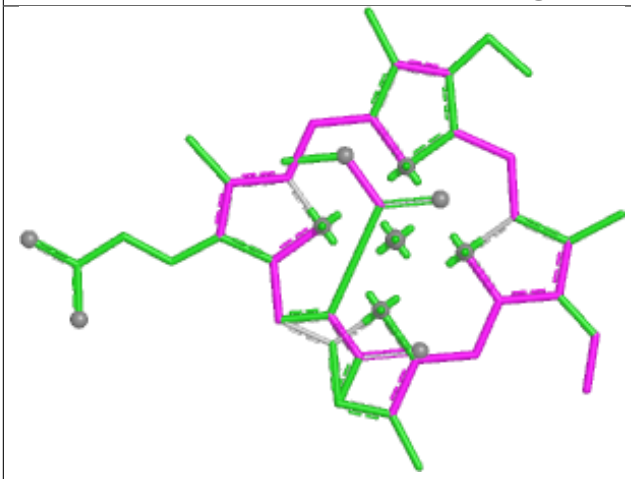


Rings

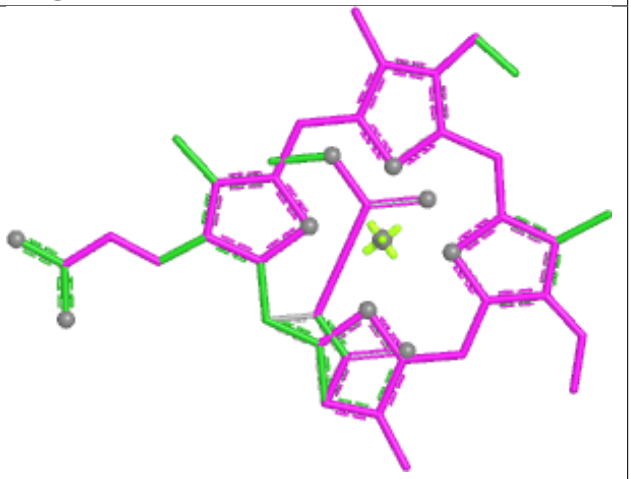
Ligand CLA i 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

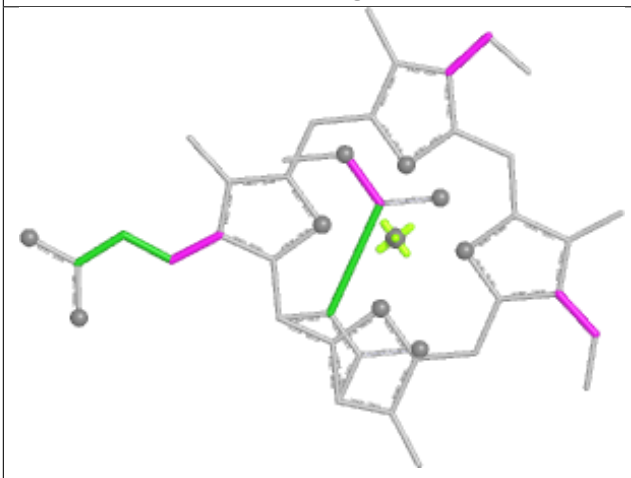
Ligand KC2 g 312



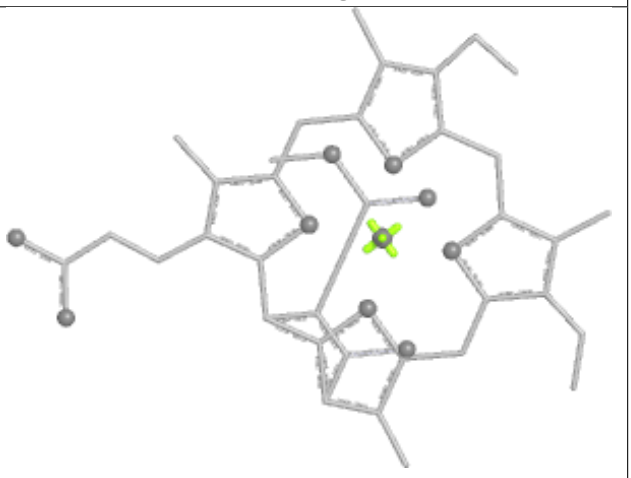
Bond lengths



Bond angles

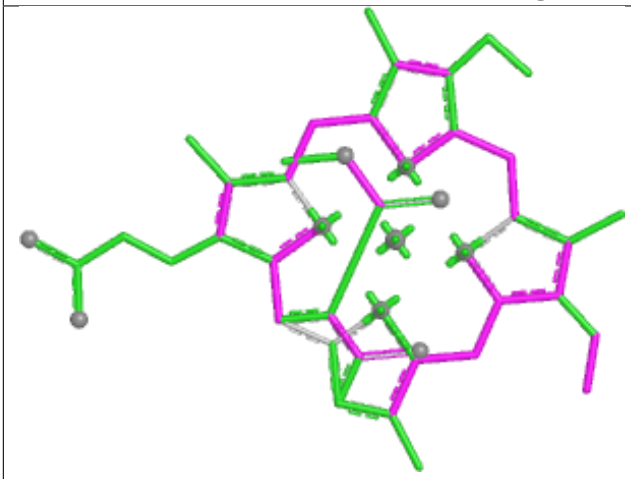


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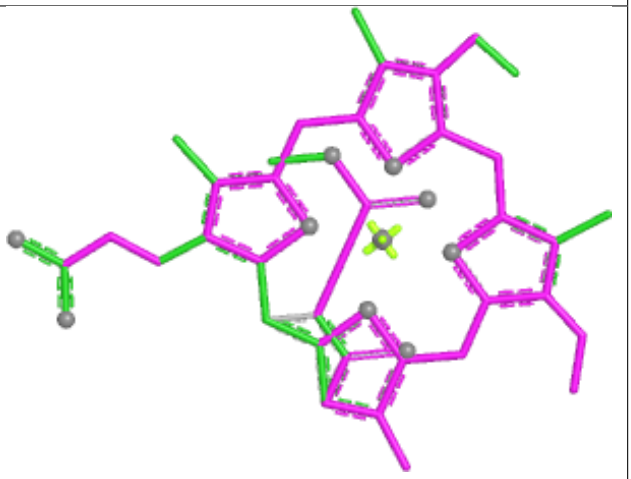


Rings

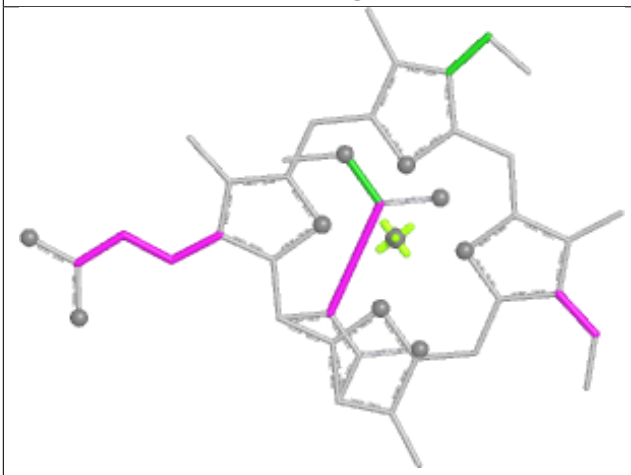
Ligand KC2 s 201



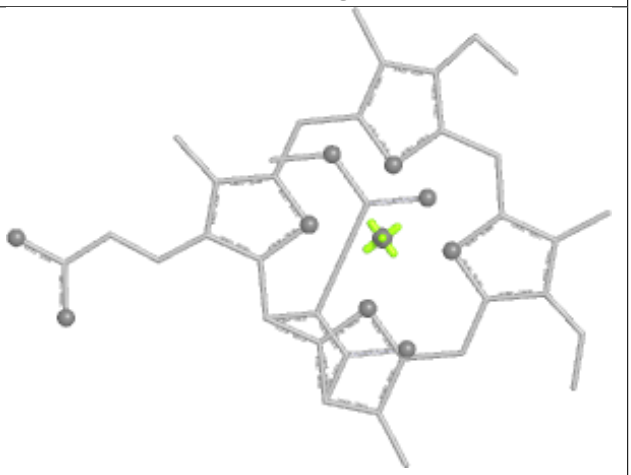
Bond lengths



Bond angles

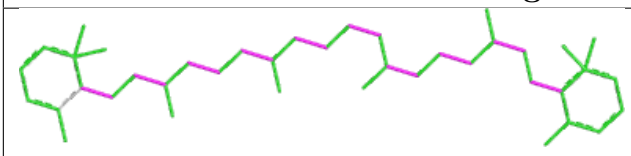


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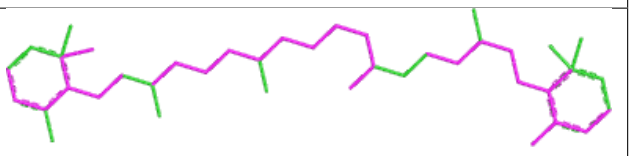


Rings

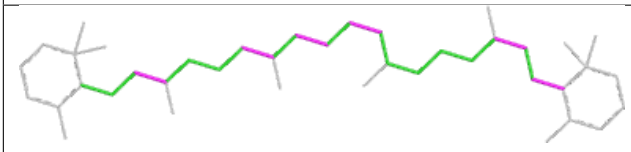
Ligand WVN i 316



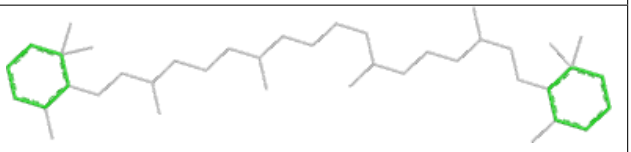
Bond lengths



Bond angles

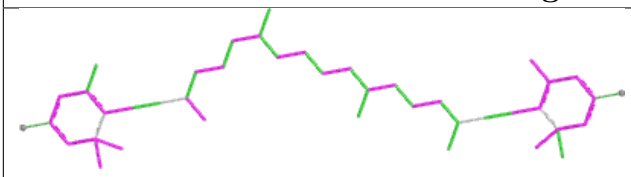


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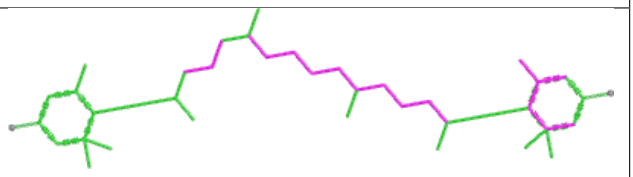


Rings

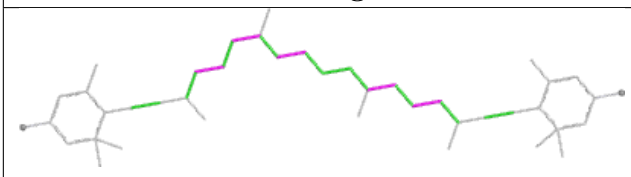
Ligand II0 b 614



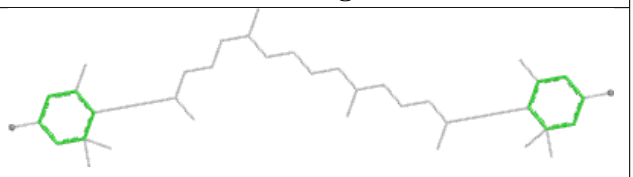
Bond lengths



Bond angles

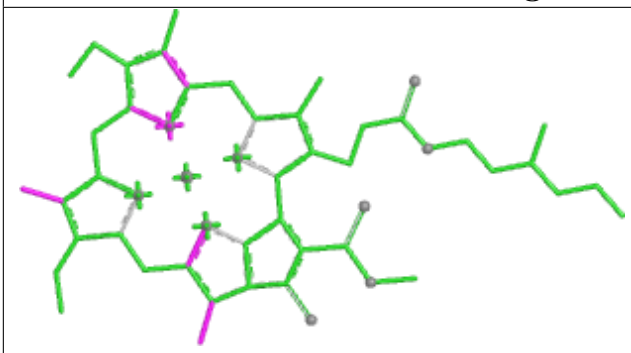


Torsions

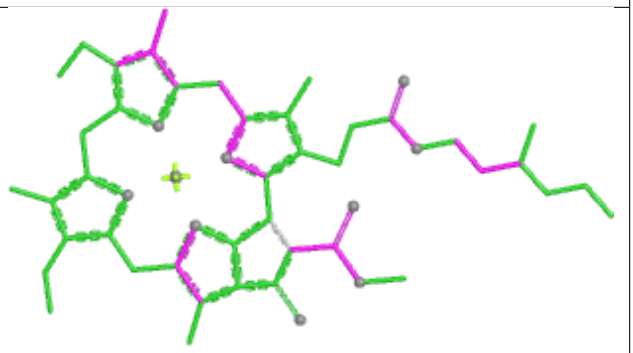


Rings

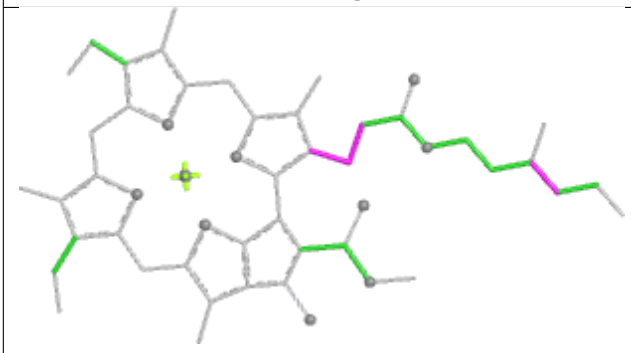
Ligand CLA O 201



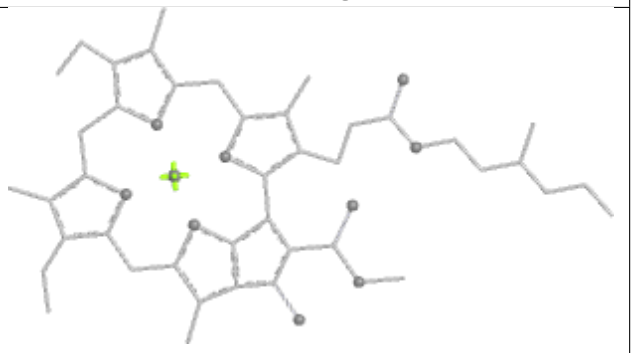
Bond lengths



Bond angles

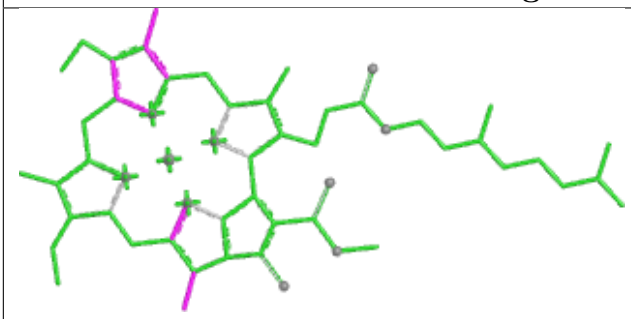


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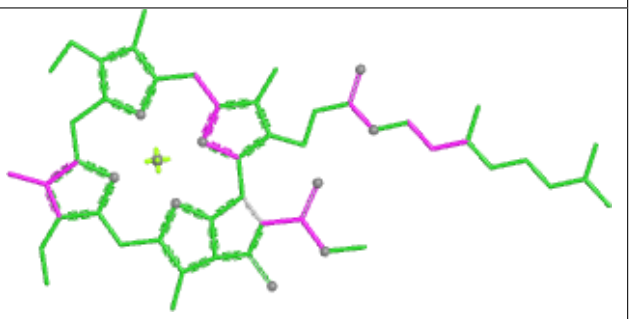


Rings

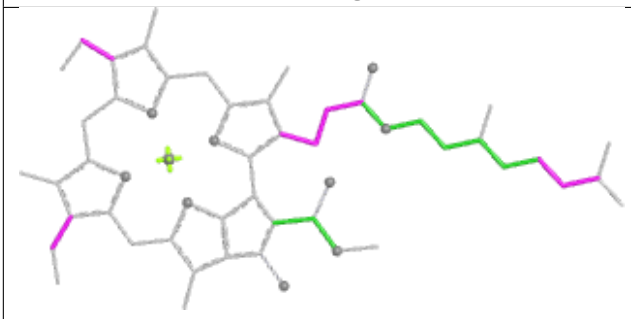
Ligand CLA m 610



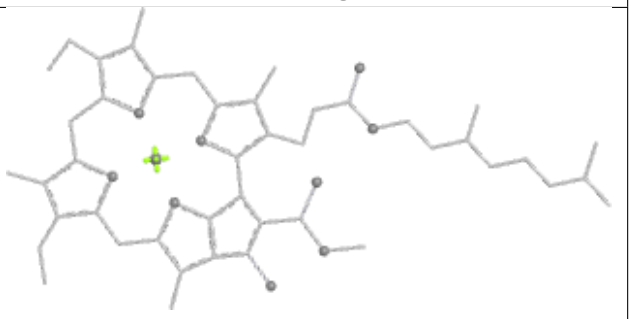
Bond lengths



Bond angles

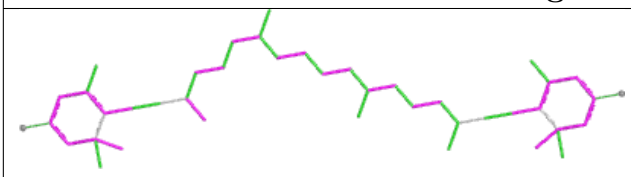


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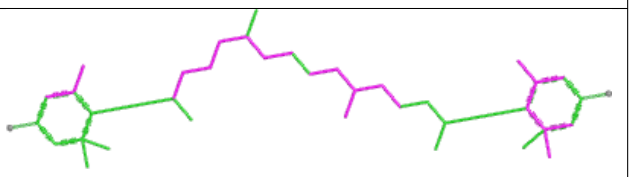


Rings

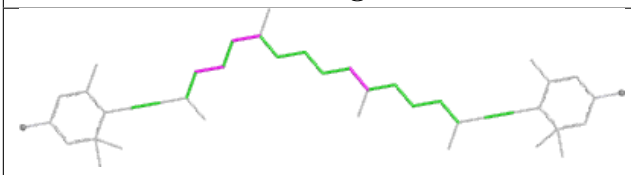
Ligand II0 l 313



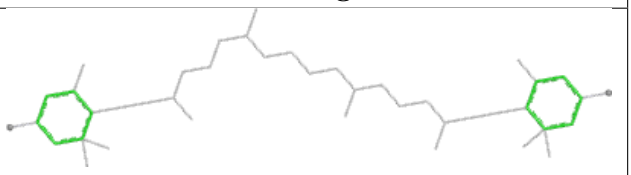
Bond lengths



Bond angles

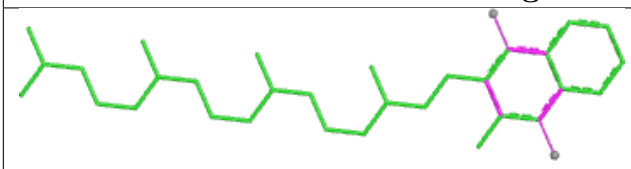


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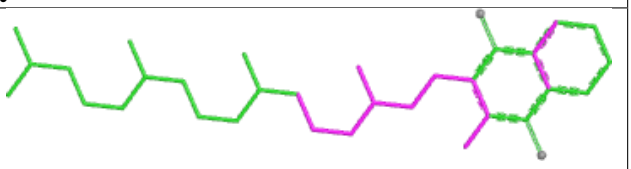


Rings

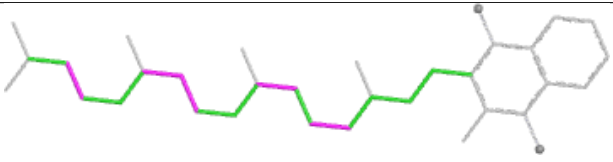
Ligand PQN B 842



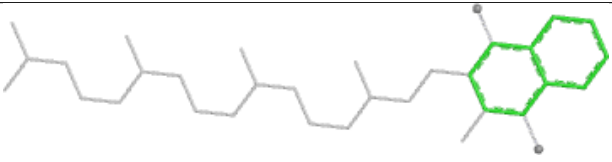
Bond lengths



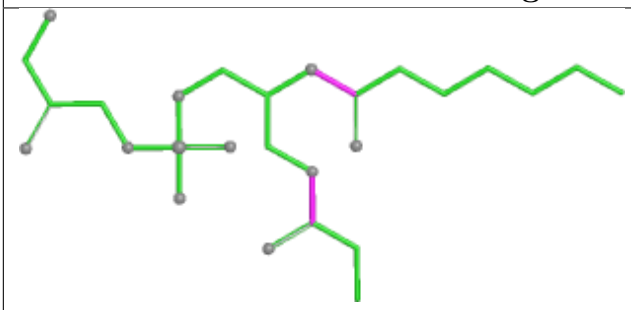
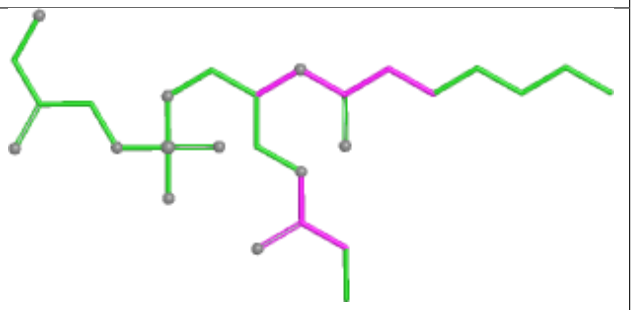
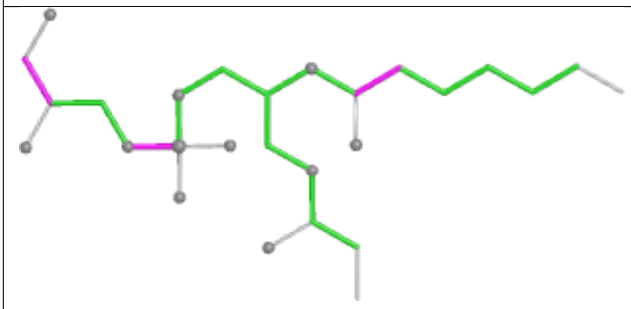
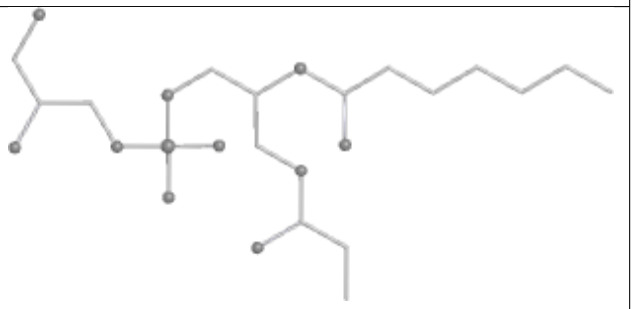
Bond angles

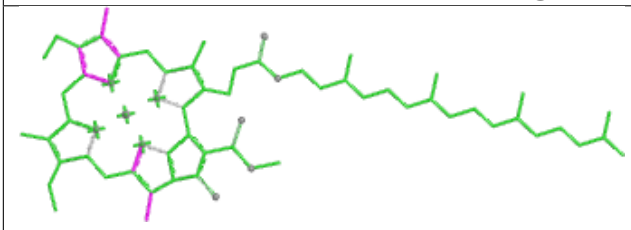
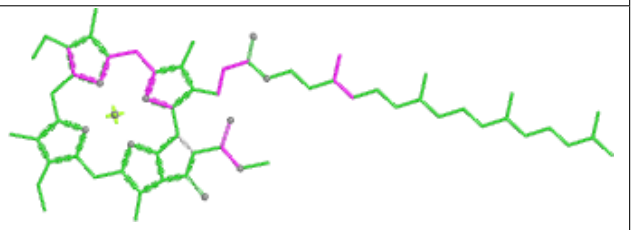
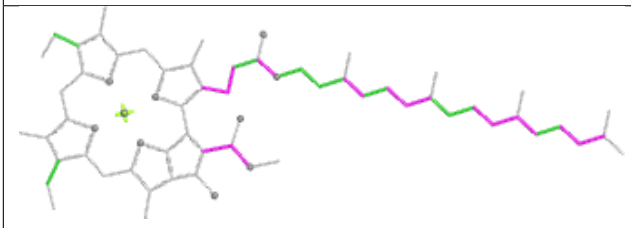
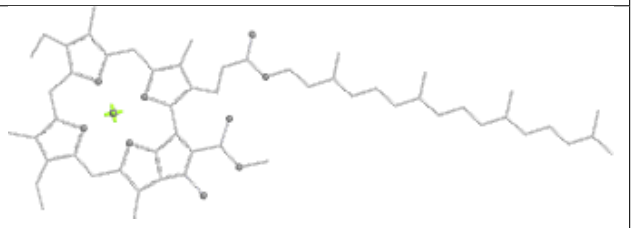


Torsions

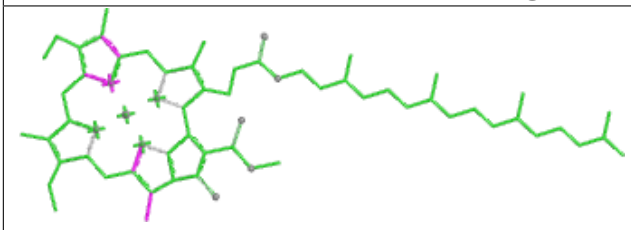


Rings

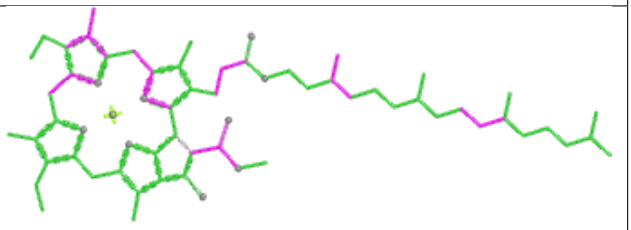
Ligand LHG A 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

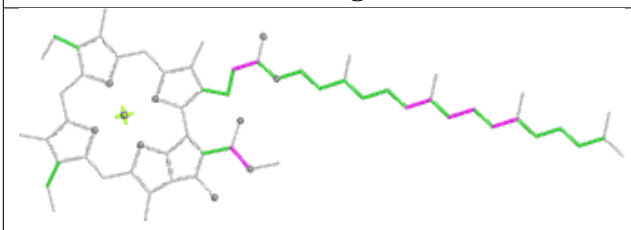
Ligand CLA A 836



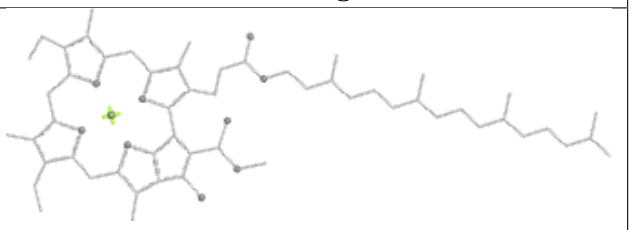
Bond lengths



Bond angles

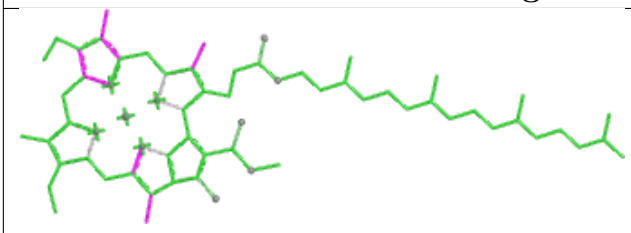


Torsions

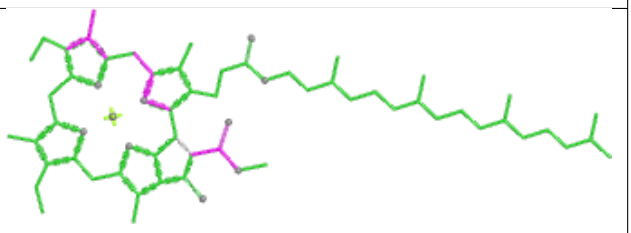


Rings

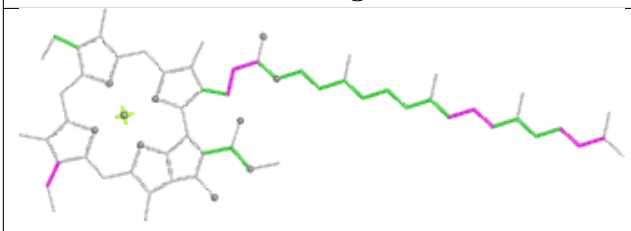
Ligand CLA m 604



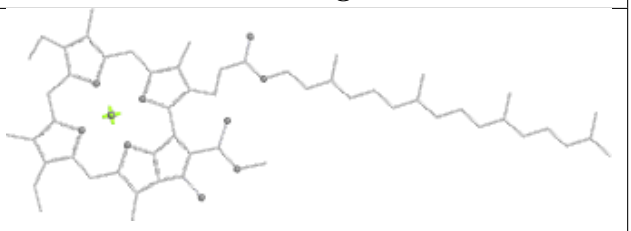
Bond lengths



Bond angles

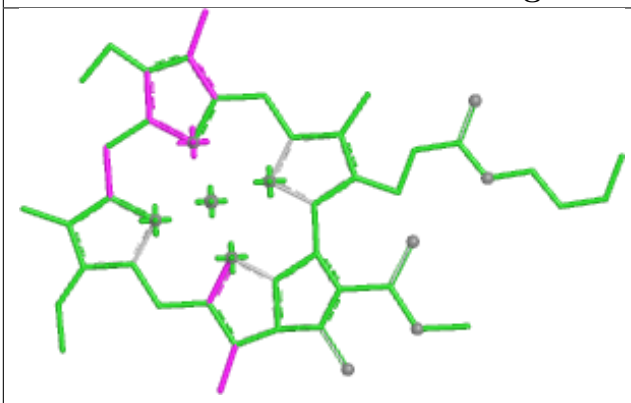


Torsions

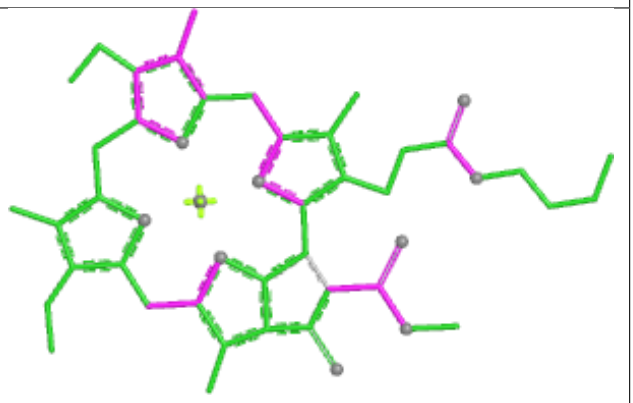


Rings

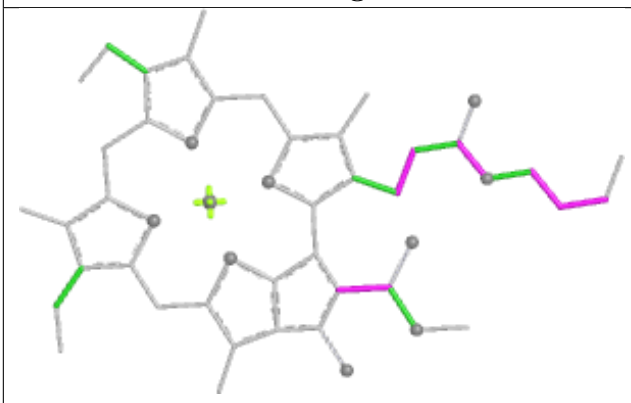
Ligand CLA A 821



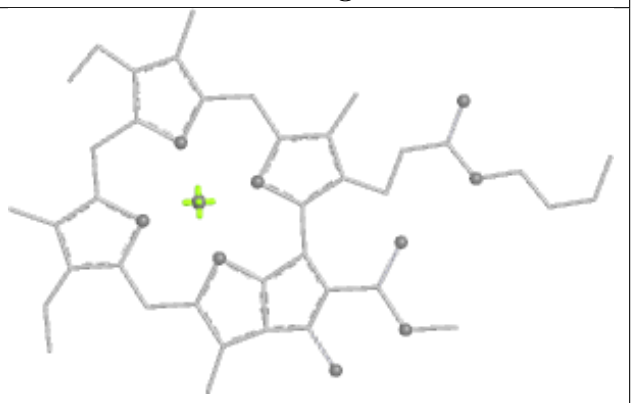
Bond lengths



Bond angles

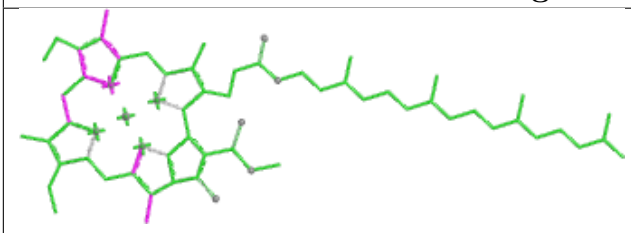


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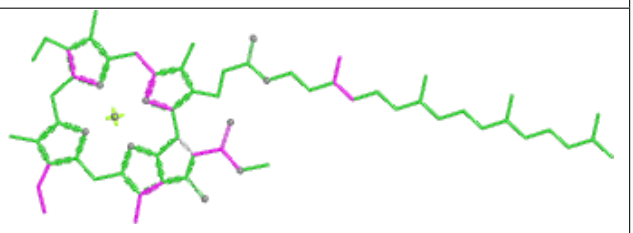


Rings

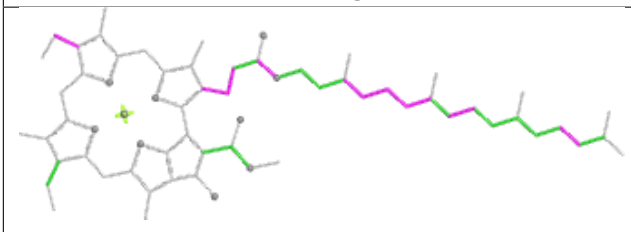
Ligand CLA f 610



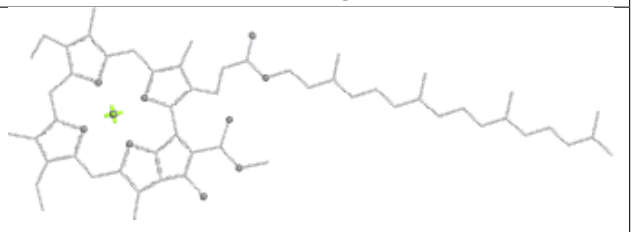
Bond lengths



Bond angles

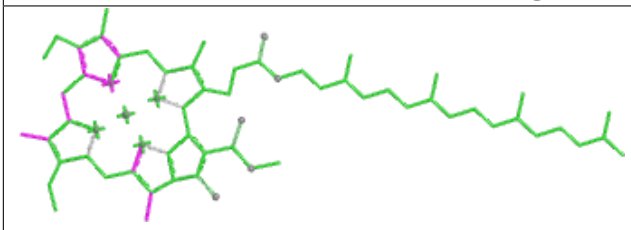


Torsions

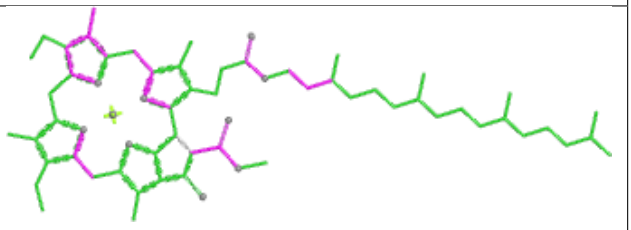


Rings

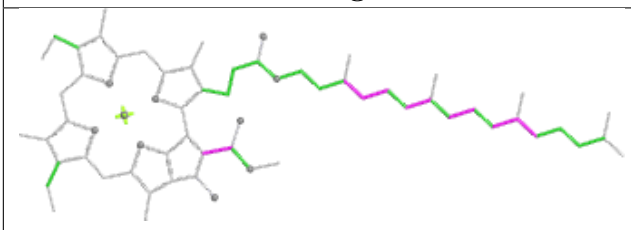
Ligand CLA a 309



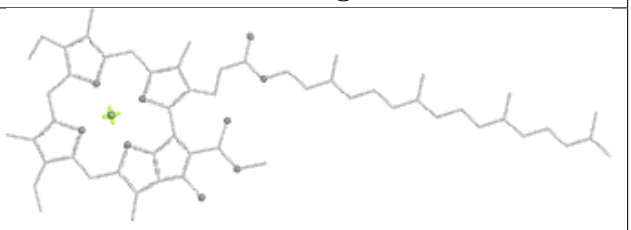
Bond lengths



Bond angles

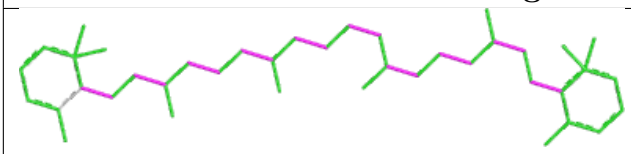


Torsions

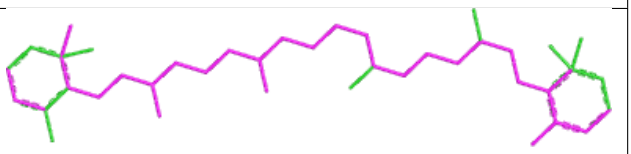


Rings

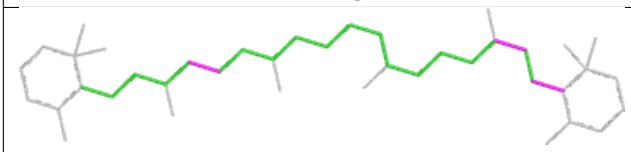
Ligand WVN l 301



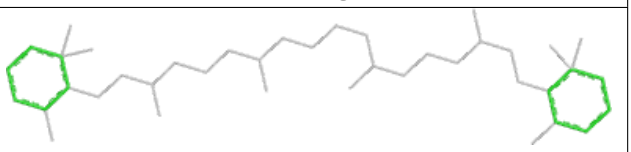
Bond lengths



Bond angles

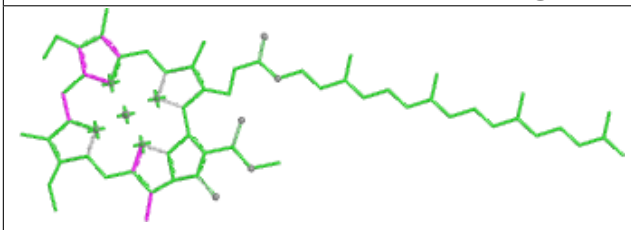


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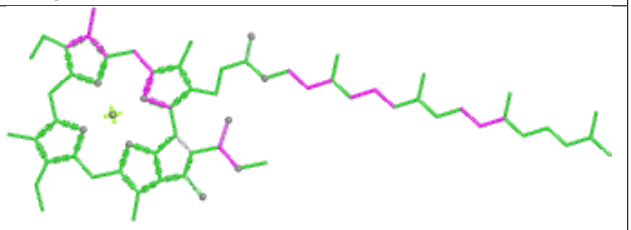


Rings

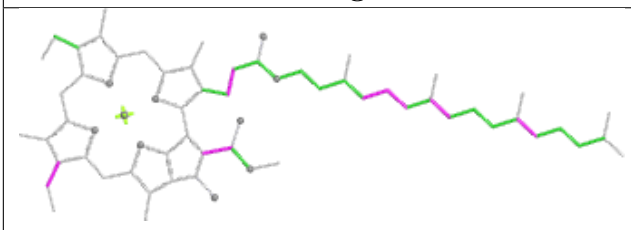
Ligand CLA j 604



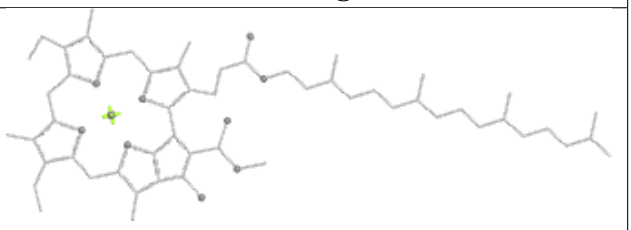
Bond lengths



Bond angles

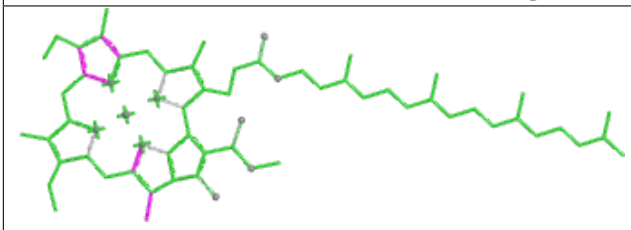


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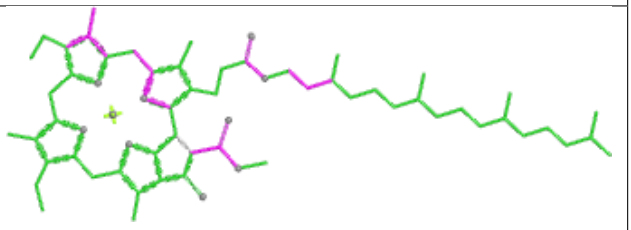


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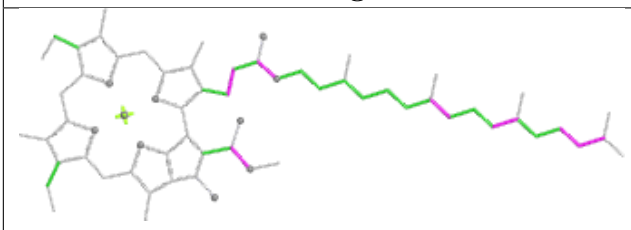
Ligand CLA B 837



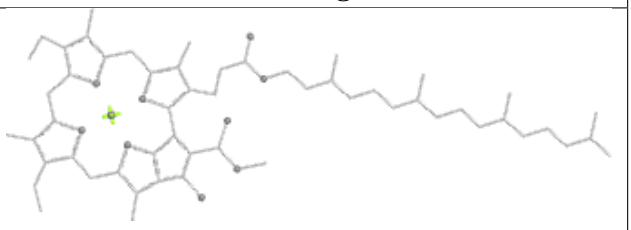
Bond lengths



Bond angles

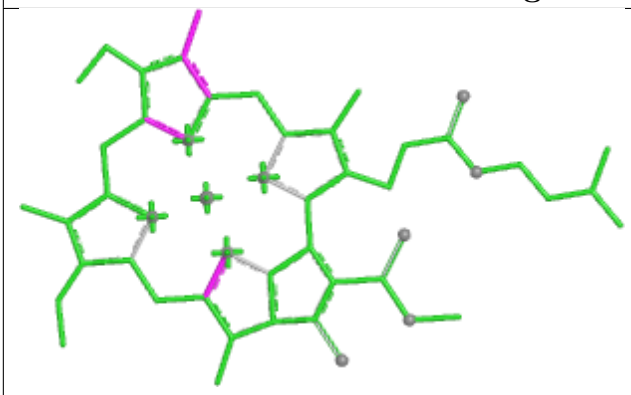


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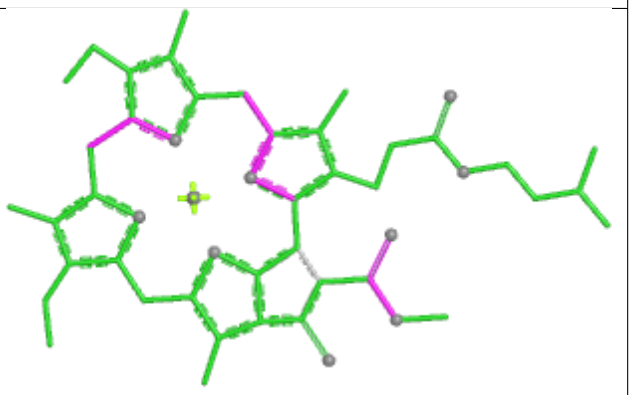


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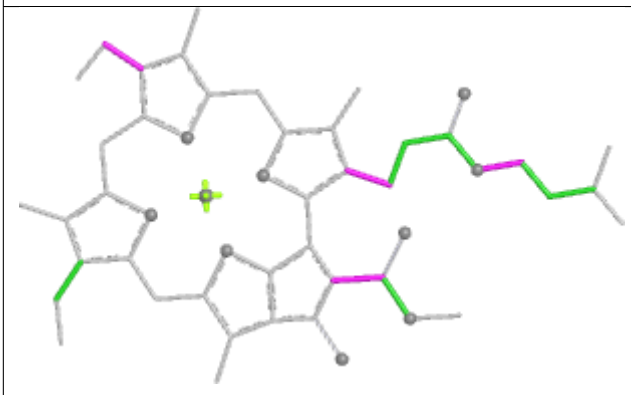
Ligand CLA A 833



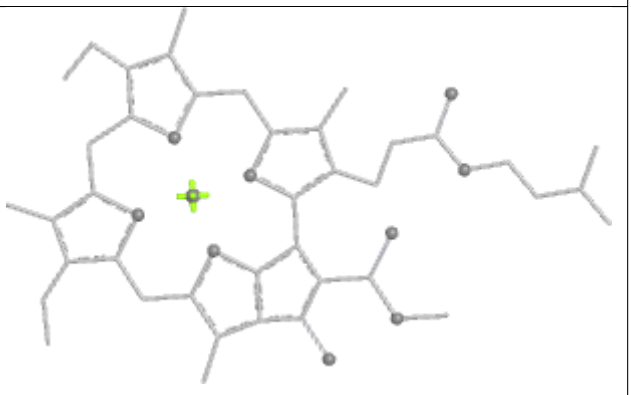
Bond lengths



Bond angles

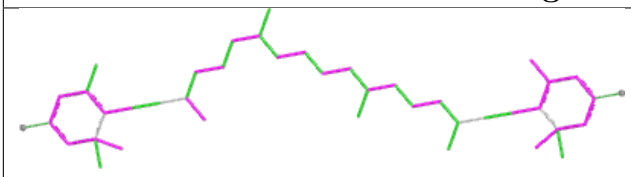


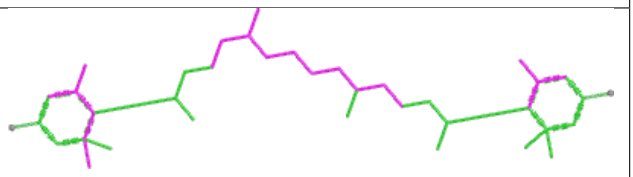
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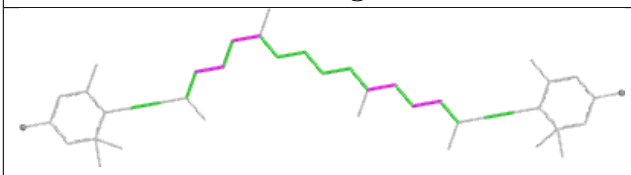


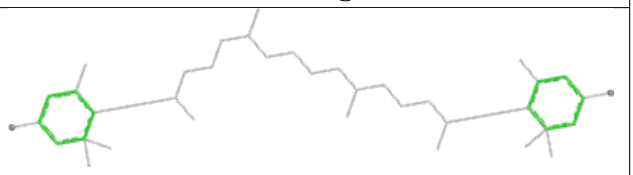
Rings

Ligand II0 J 104

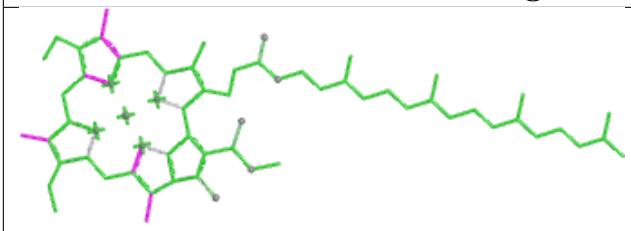

Bond lengths

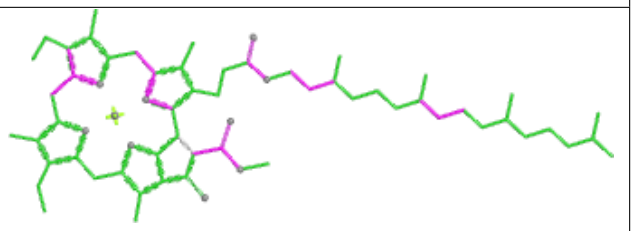

Bond angles

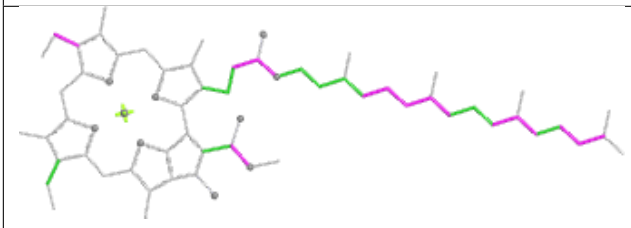

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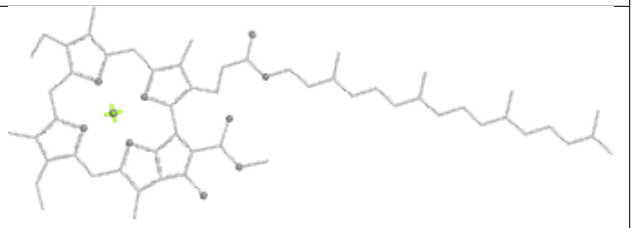

Rings

Ligand CLA B 802

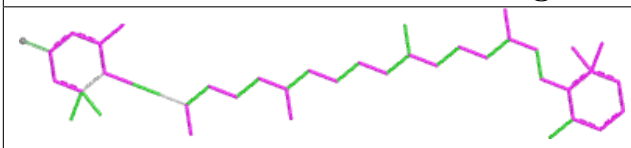

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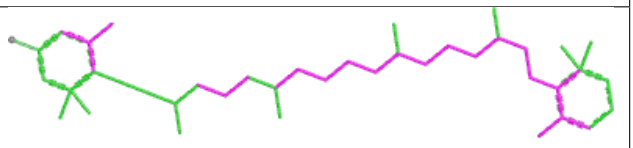

Bond angles

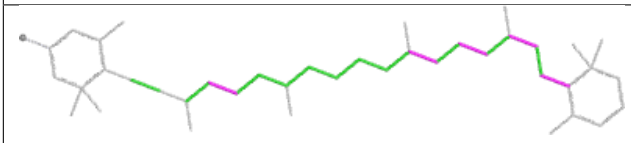

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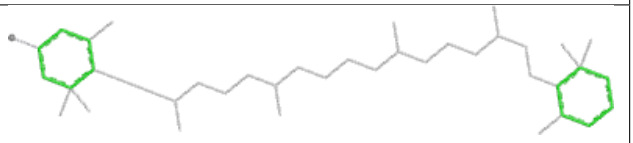

Rings

Ligand IHT a 317

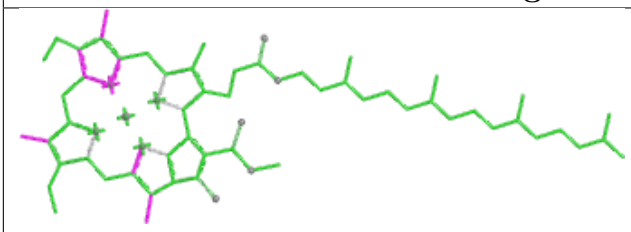

Bond lengths


Bond angles

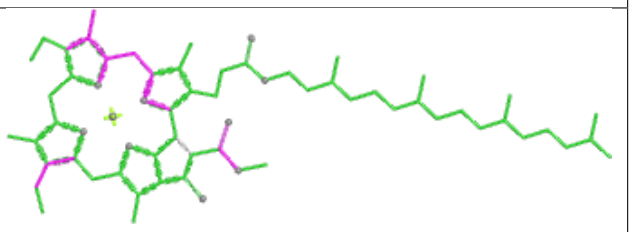

Torsions


Rings

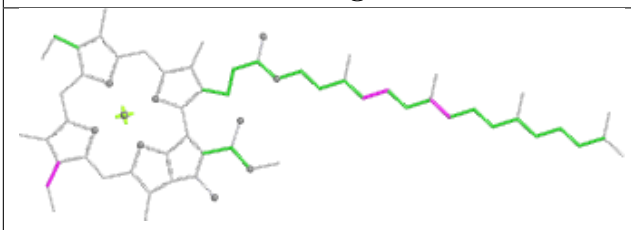
Ligand CLA A 820



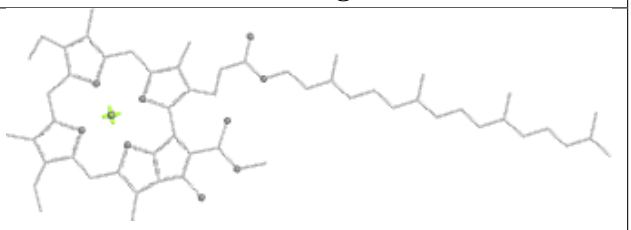
Bond lengths



Bond angles

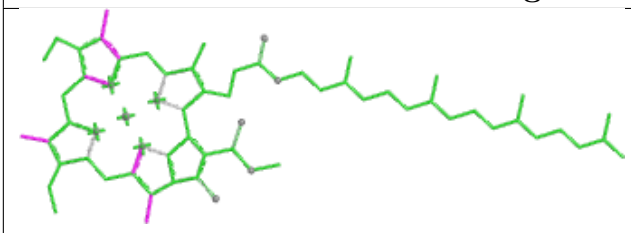


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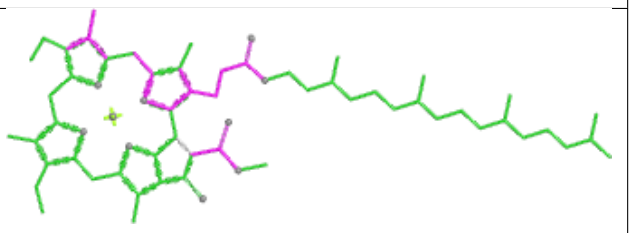


Rings

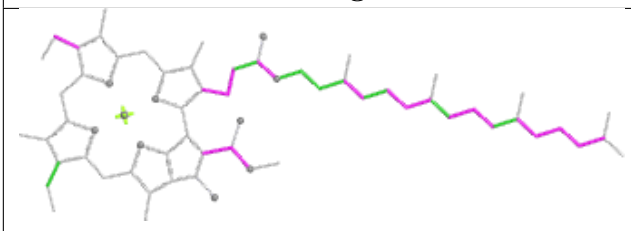
Ligand CLA A 841



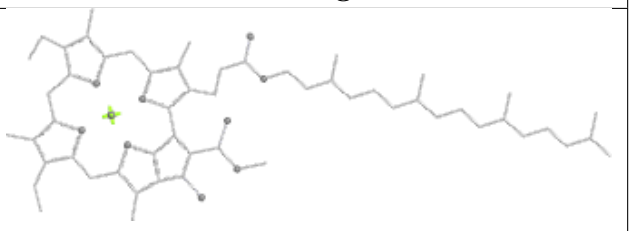
Bond lengths



Bond angles

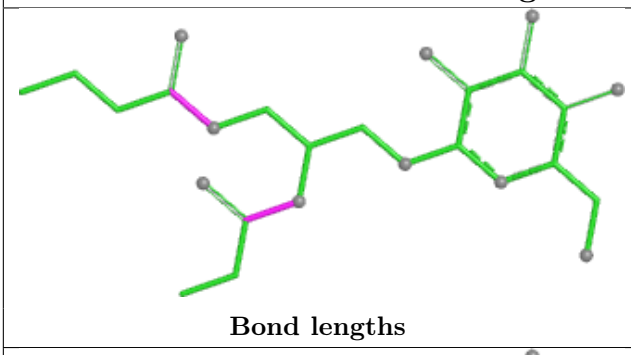


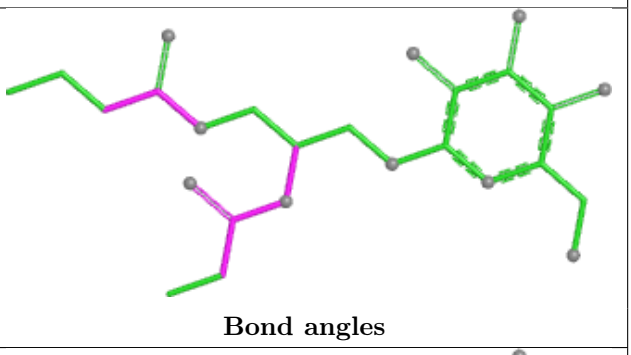
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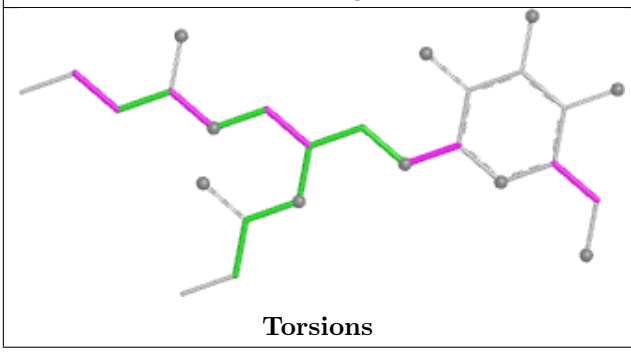


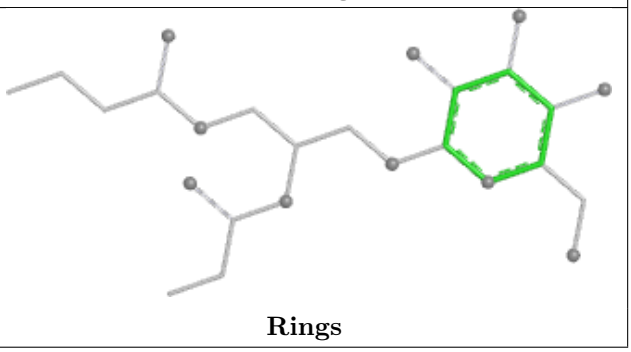
Rings

Ligand LMG O 205

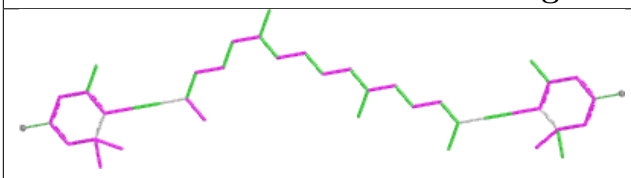

Bond lengths

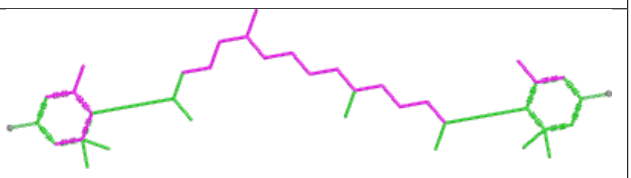

Bond angles

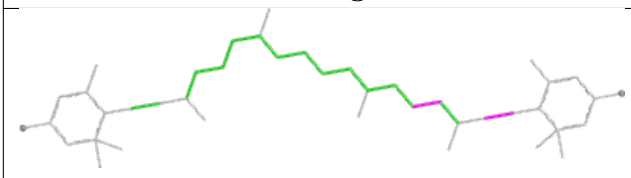

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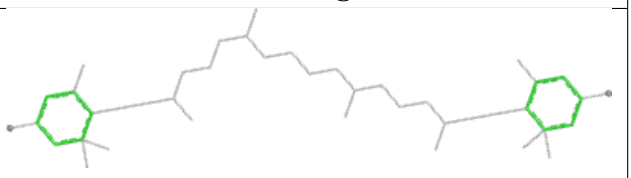

Rings

Ligand II0 b 613

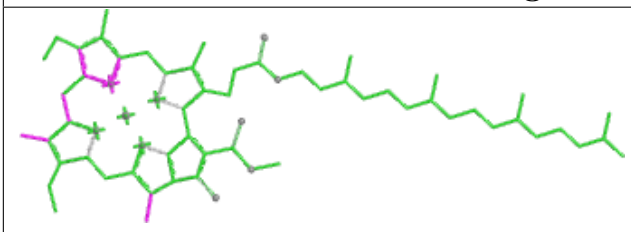

Bond lengths

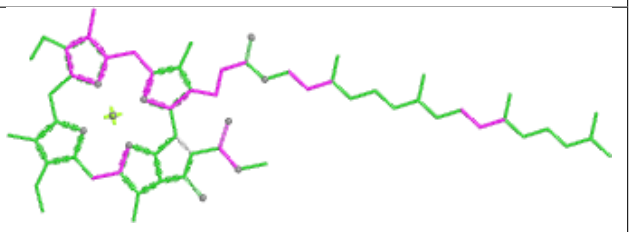

Bond angles

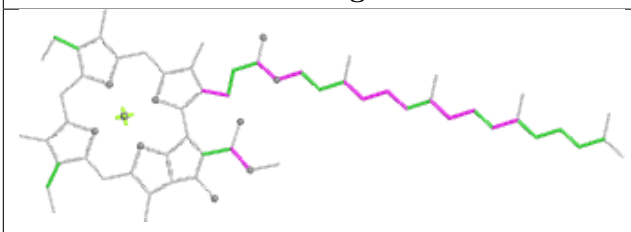

Torsions

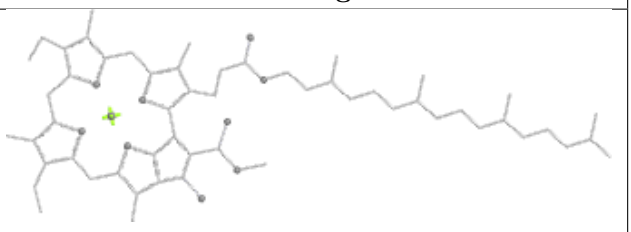

Rings

Ligand CLA A 802

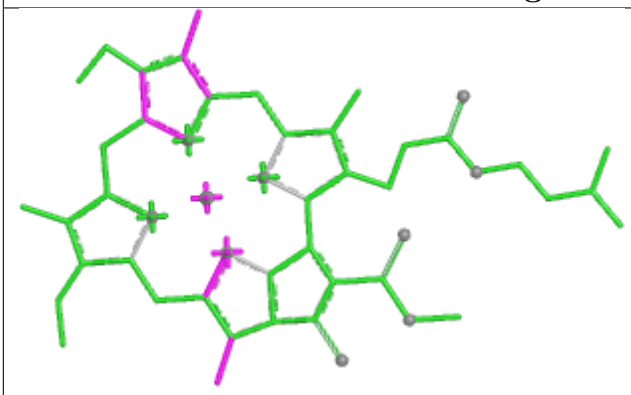

Bond lengths


Bond angles

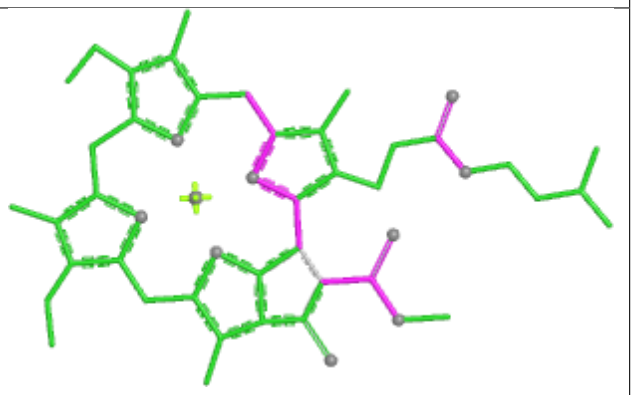

Torsions


Rings

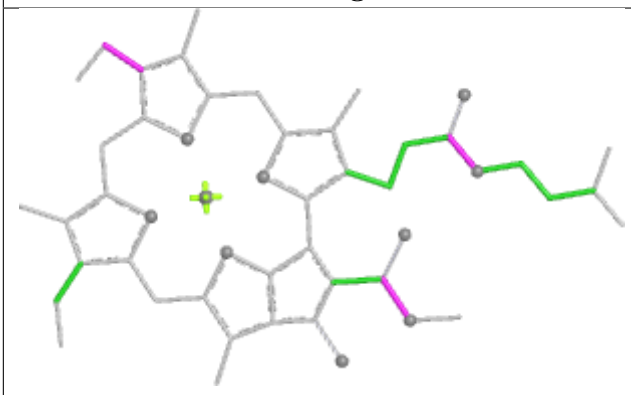
Ligand CLA B 829



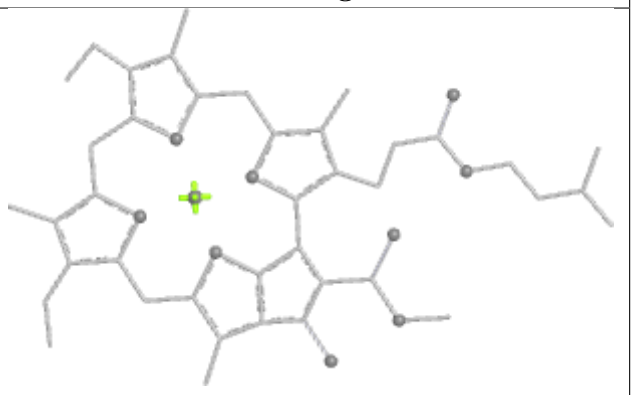
Bond lengths



Bond angles

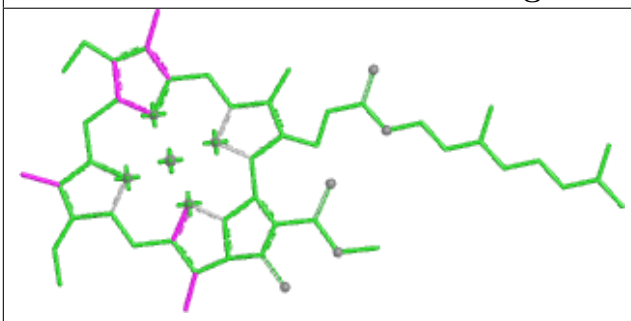


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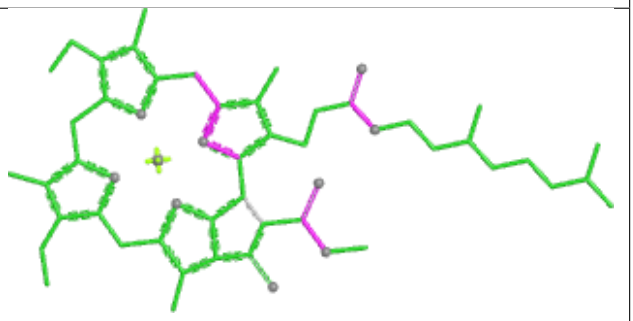


Rings

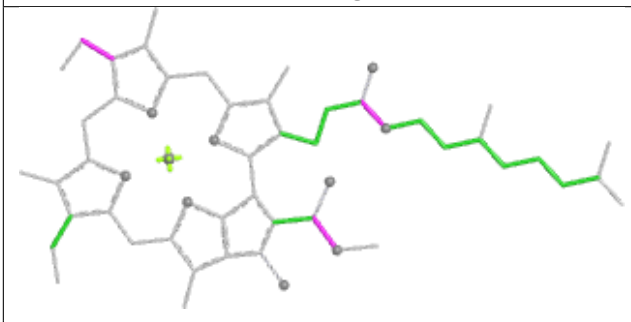
Ligand CLA A 823



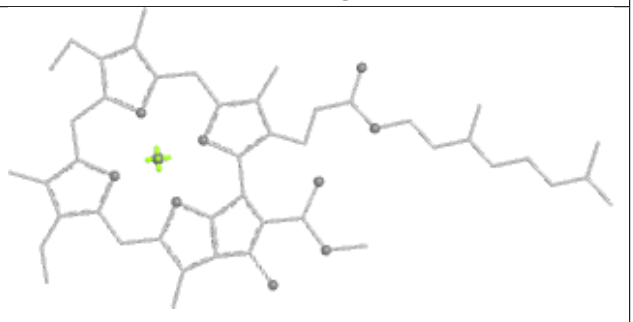
Bond lengths



Bond angles

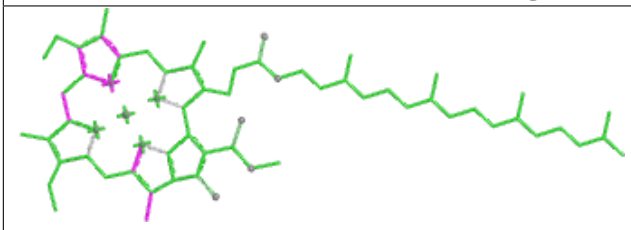


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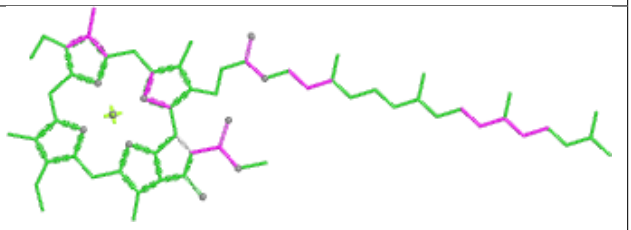


Rings

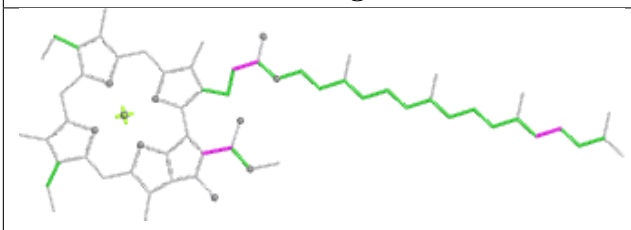
Ligand CLA B 841



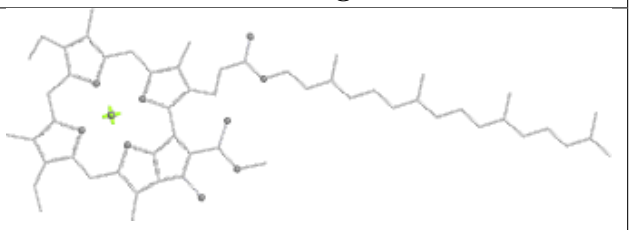
Bond lengths



Bond angles

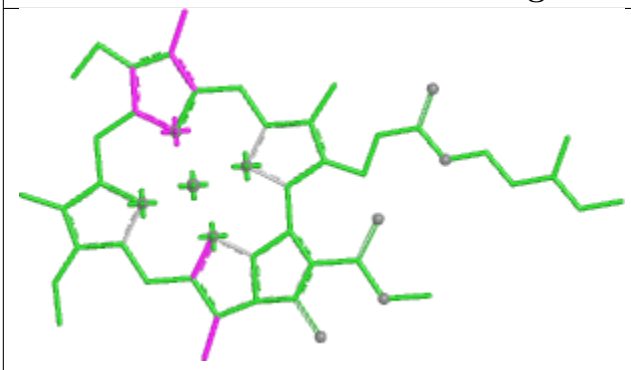


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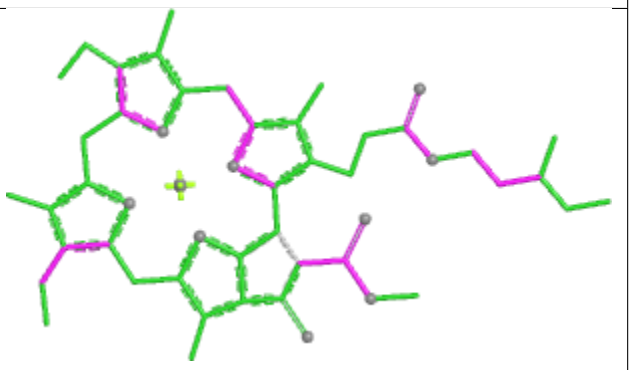


Rings

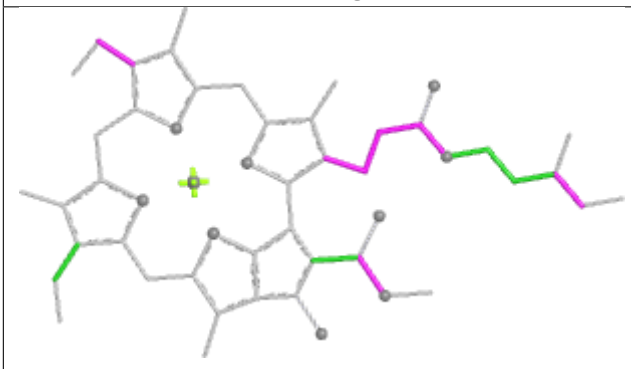
Ligand CLA k 601



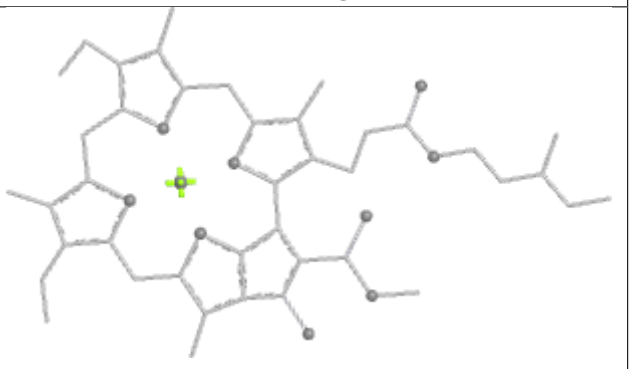
Bond lengths



Bond angles

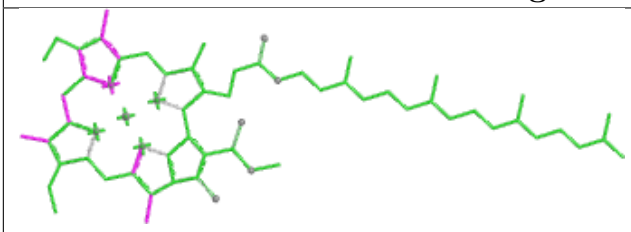


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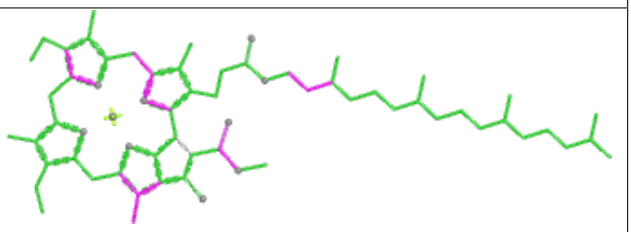


Rings

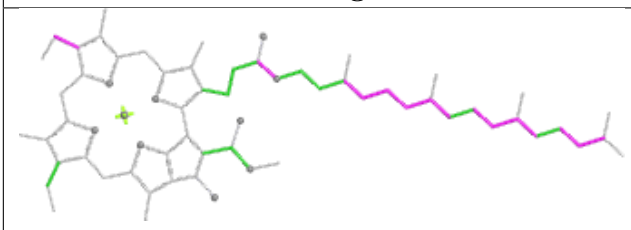
Ligand CLA e 605



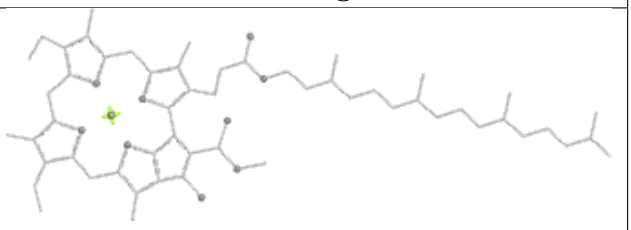
Bond lengths



Bond angles

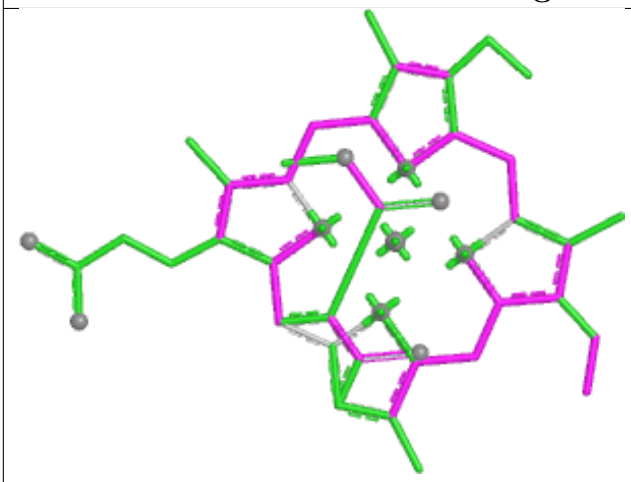


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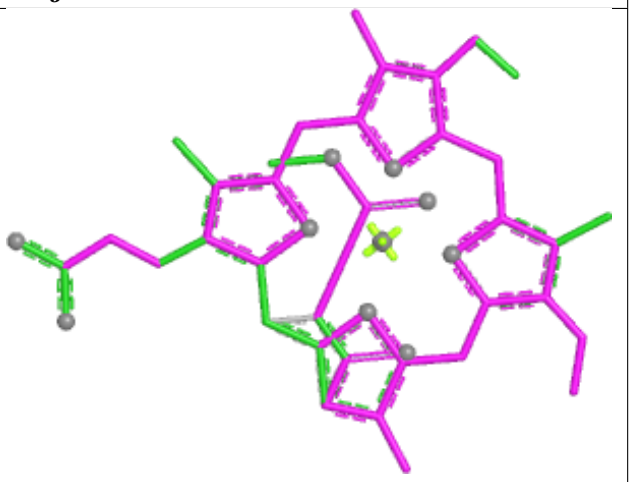


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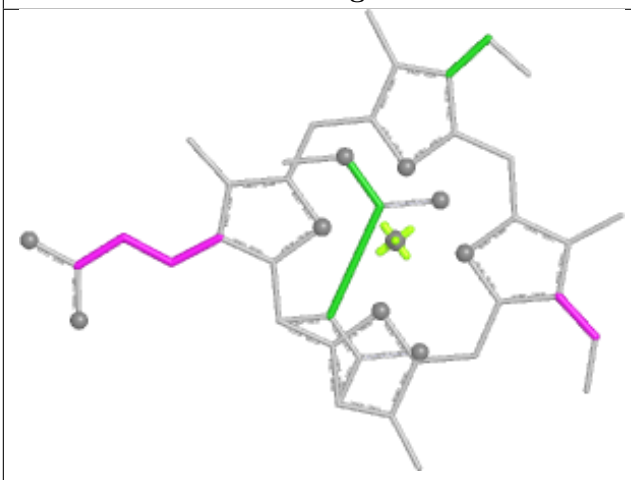
Ligand KC2 j 611



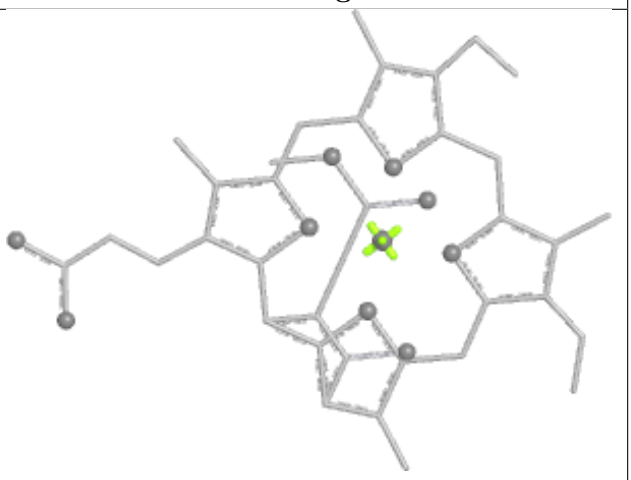
Bond lengths



Bond angles

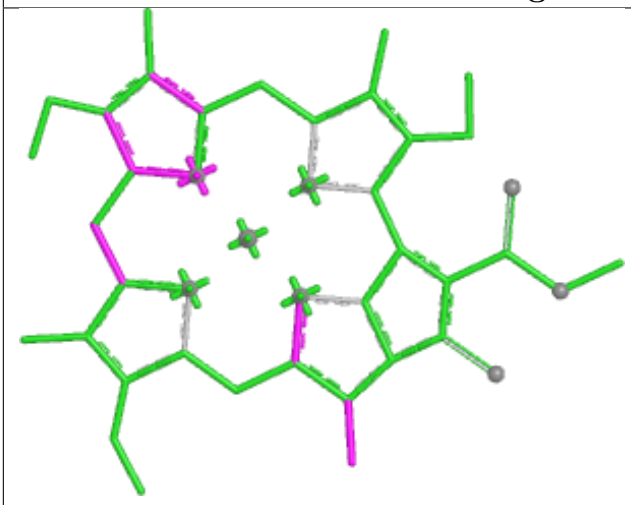


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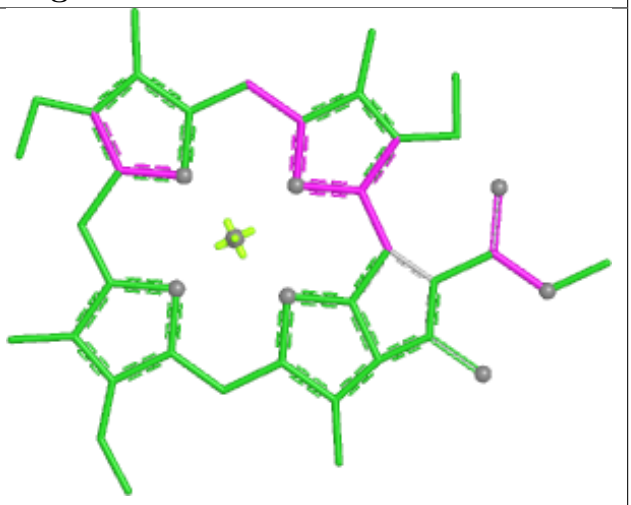


Rings

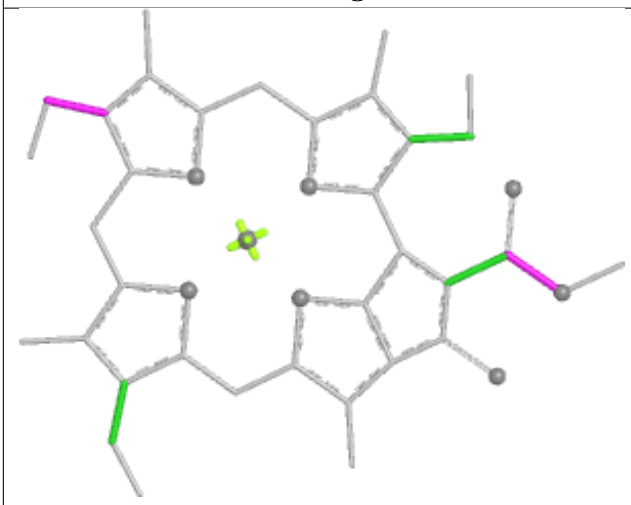
Ligand CLA g 302



Bond lengths



Bond angles

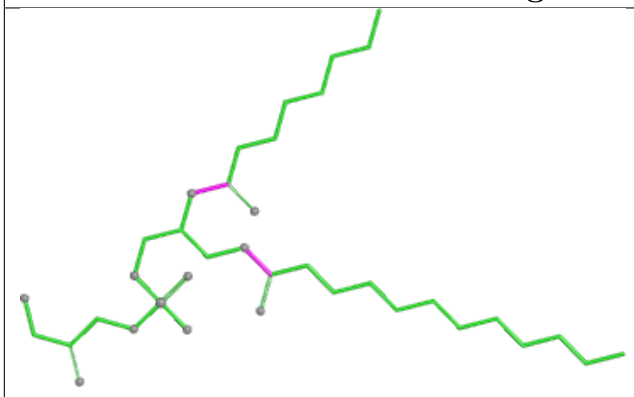


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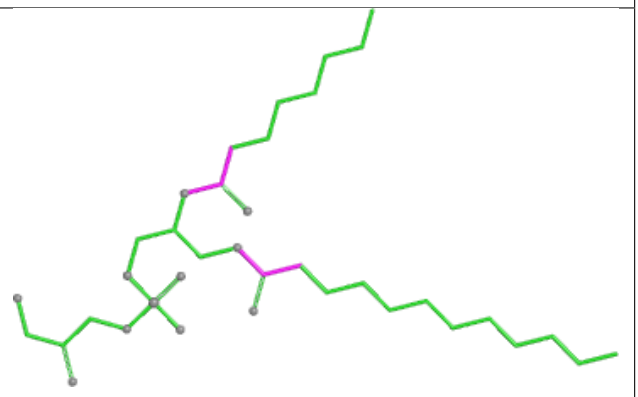


Rings

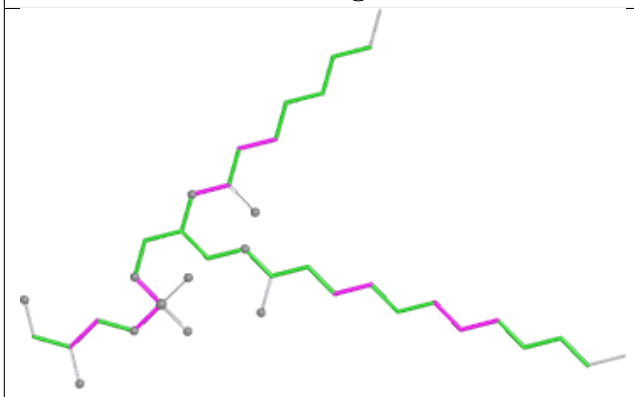
Ligand LHG d 317



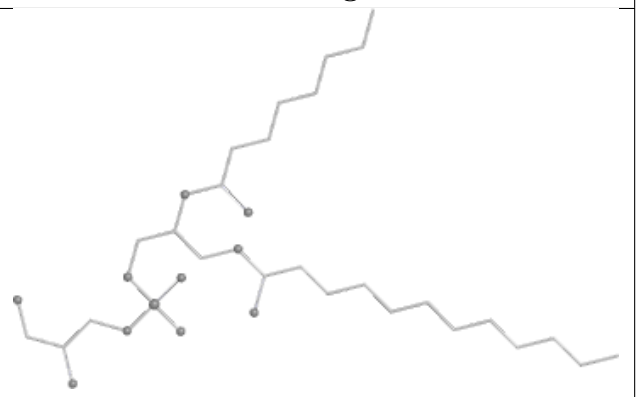
Bond lengths



Bond angles

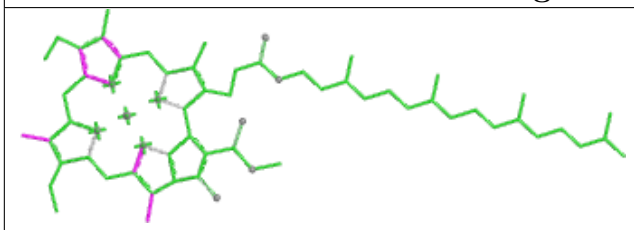


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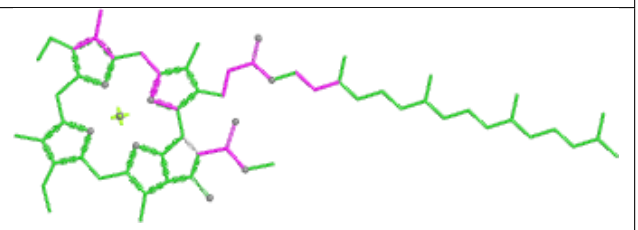


Rings

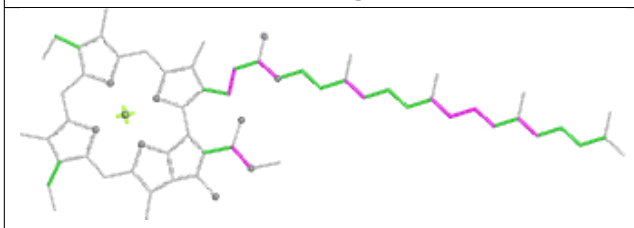
Ligand CLA l 305



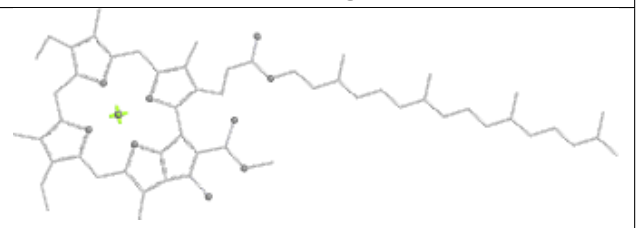
Bond lengths



Bond angles

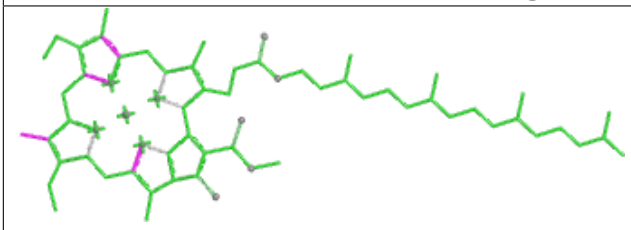


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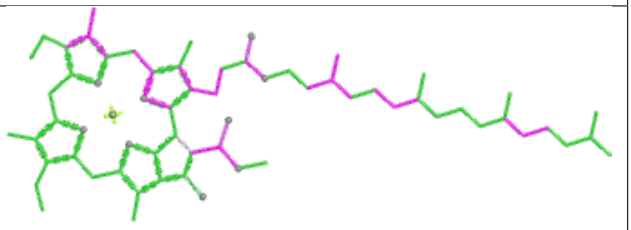


Rings

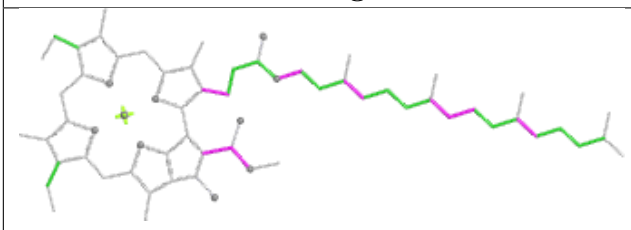
Ligand CLA A 816



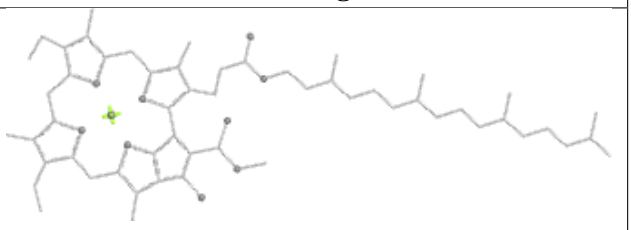
Bond lengths



Bond angles

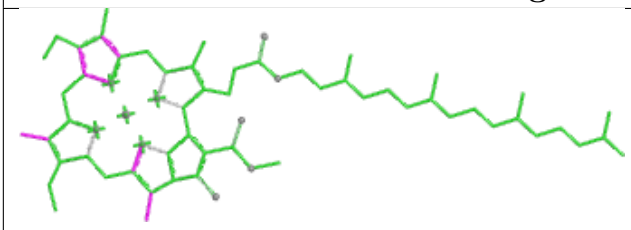


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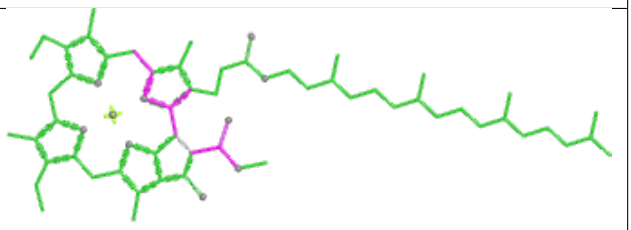


Rings

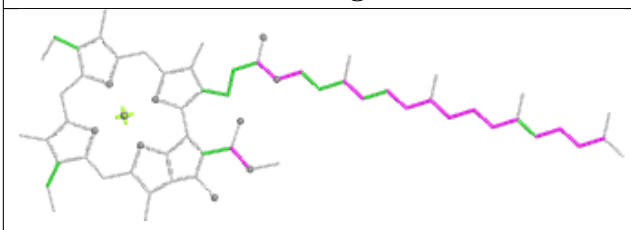
Ligand CLA e 606



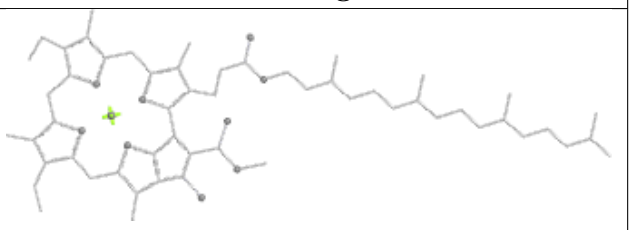
Bond lengths



Bond angles

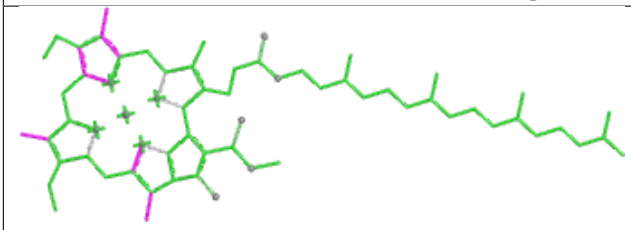


Torsions

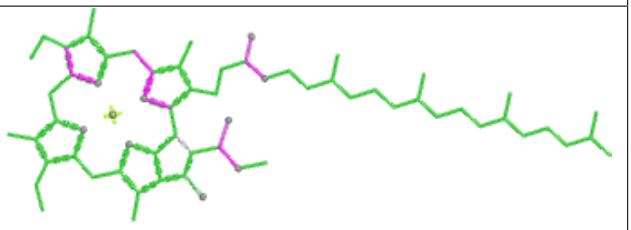


Rings

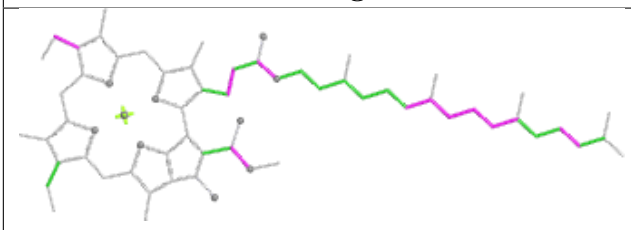
Ligand CLA B 835



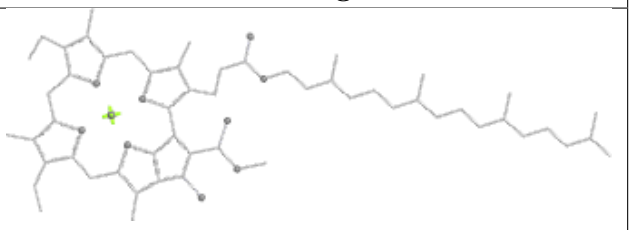
Bond lengths



Bond angles

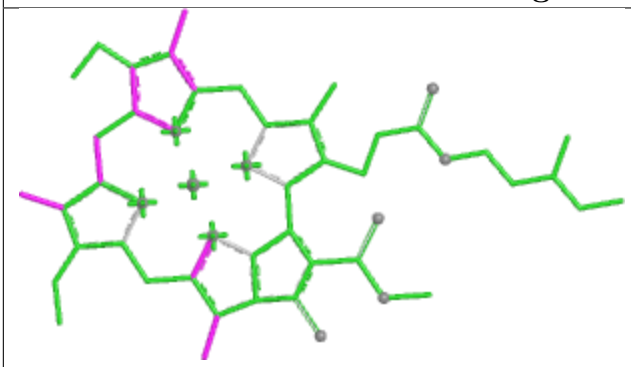


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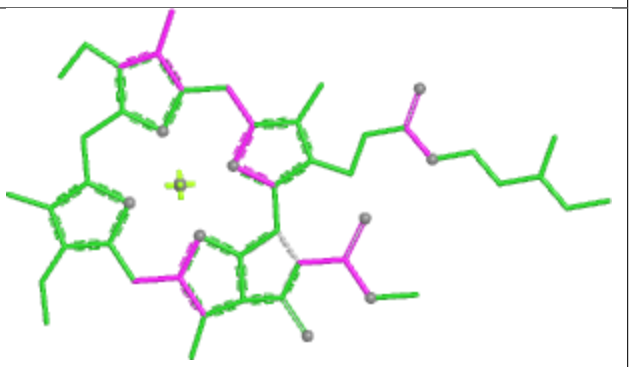


Rings

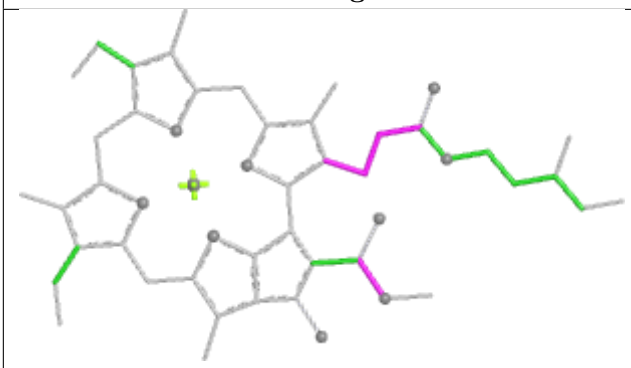
Ligand CLA l 308



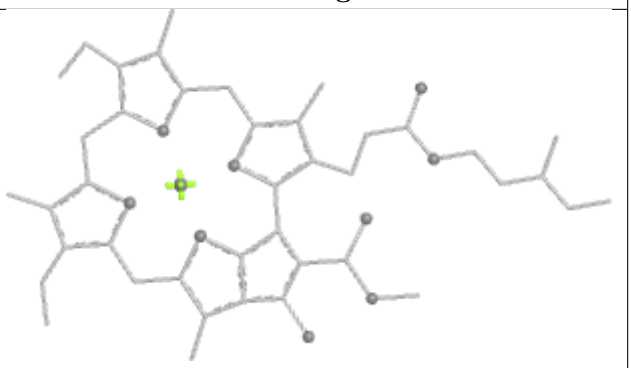
Bond lengths



Bond angles

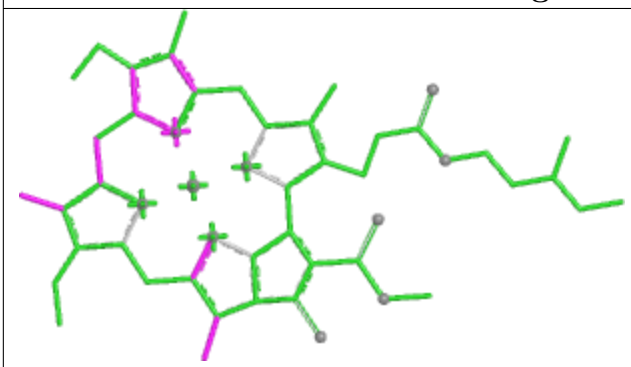


Torsions

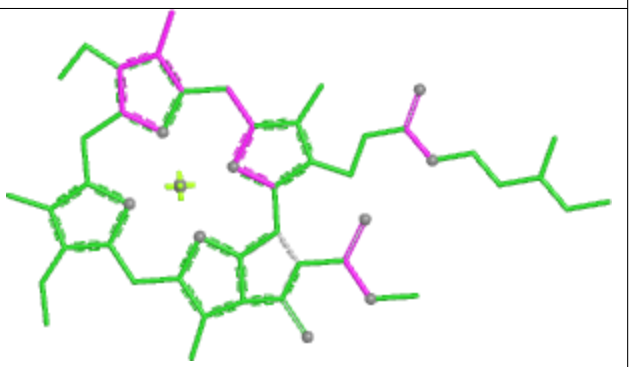


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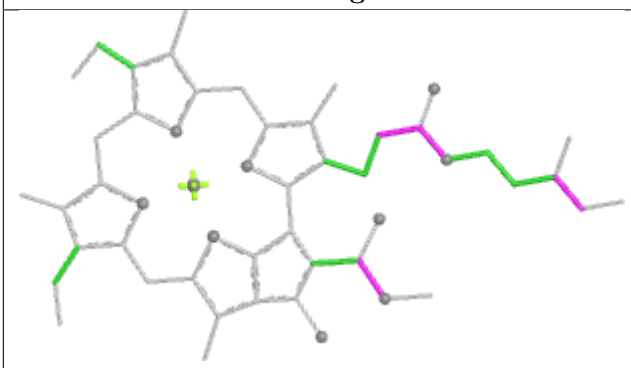
Ligand CLA f 603



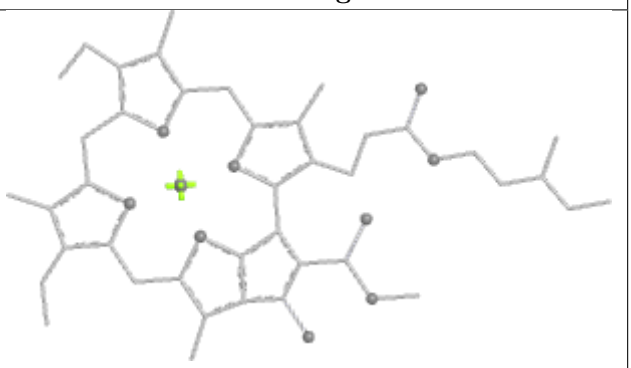
Bond lengths



Bond angles

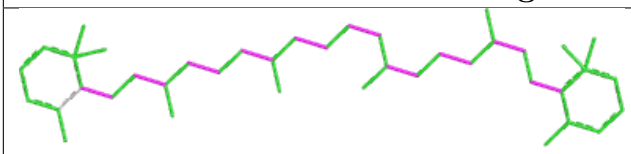


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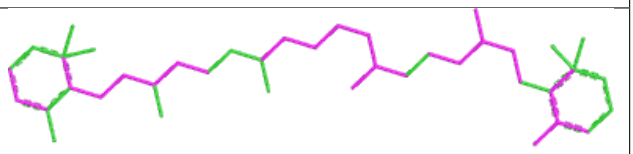


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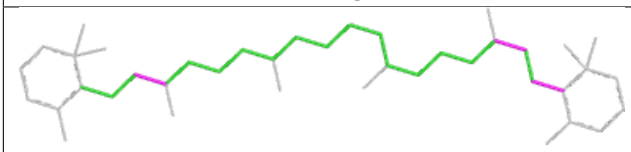
Ligand WVN L 205



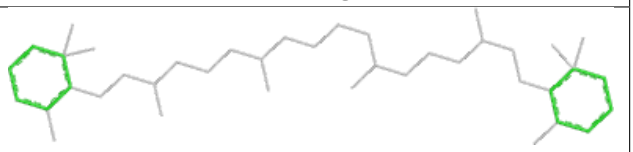
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Bond angles

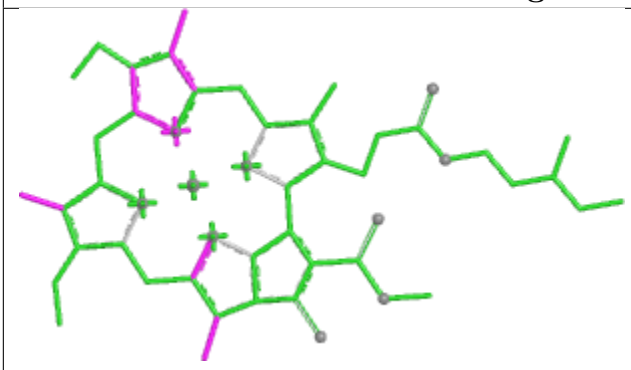


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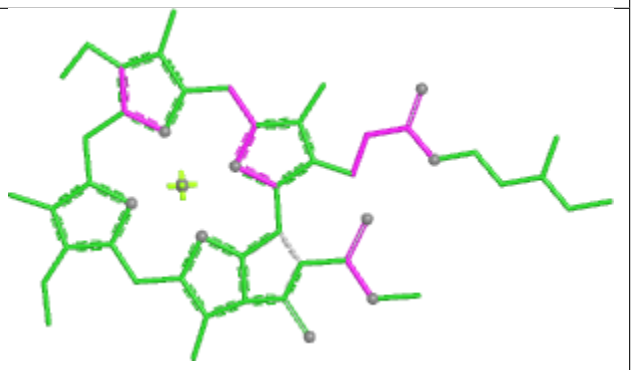


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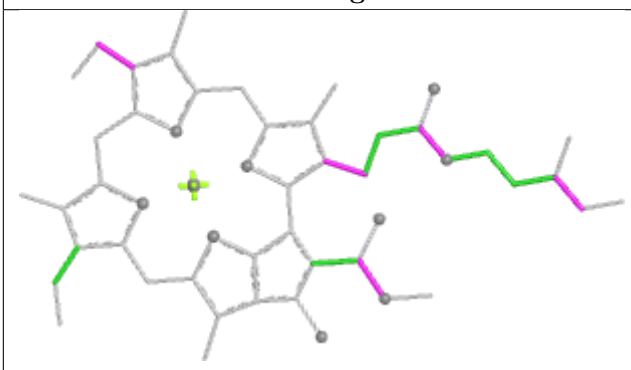
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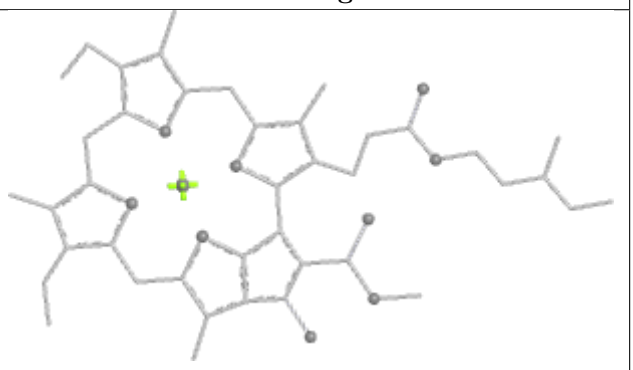
Bond lengths



Bond angles

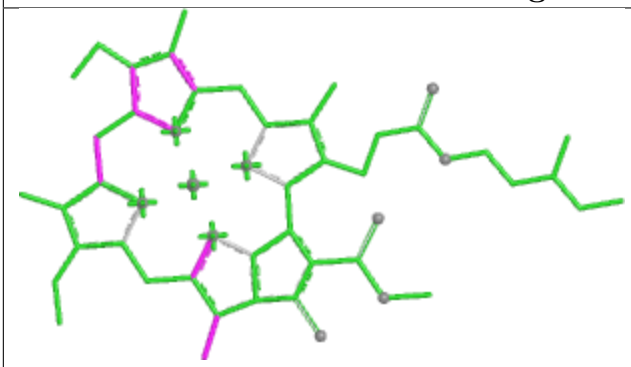


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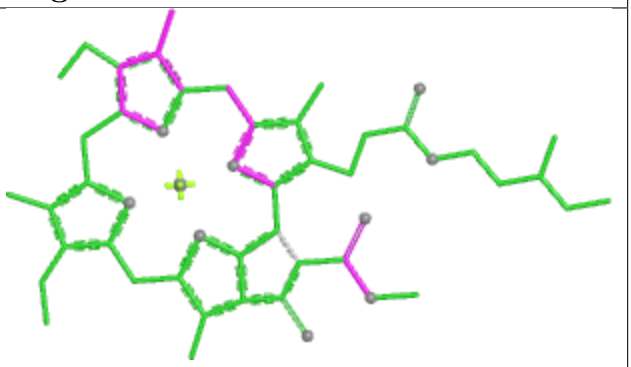


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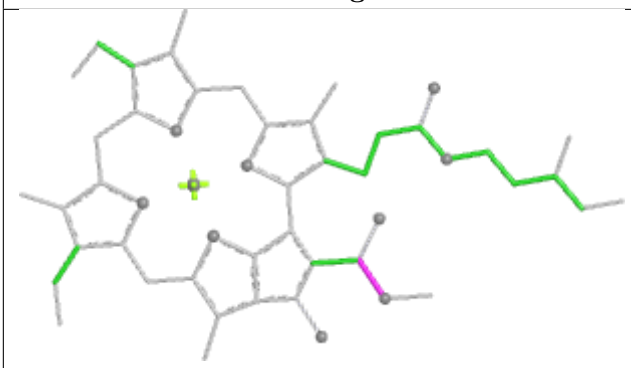
Ligand CLA g 304



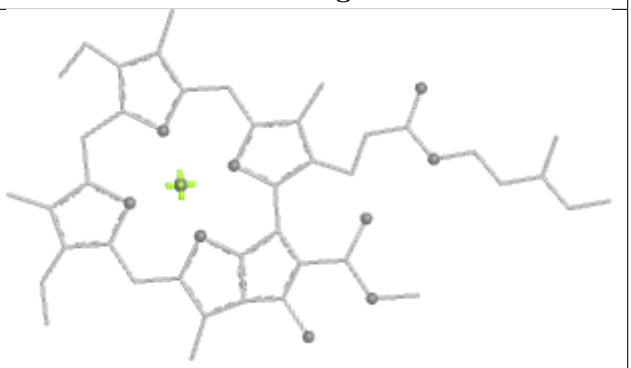
Bond lengths



Bond angles

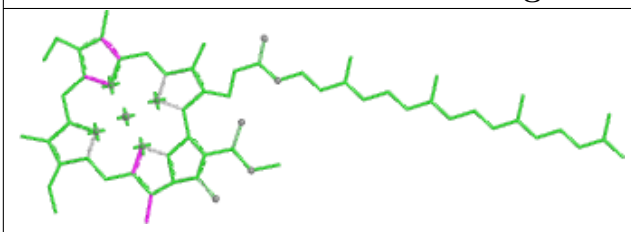


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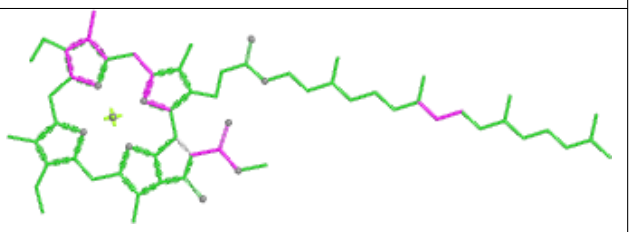


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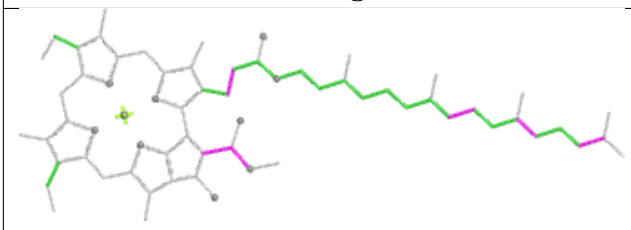
Ligand CLA A 807



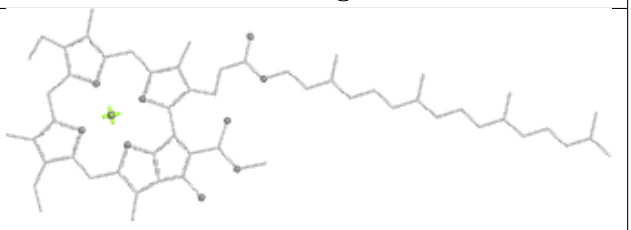
Bond lengths



Bond angles

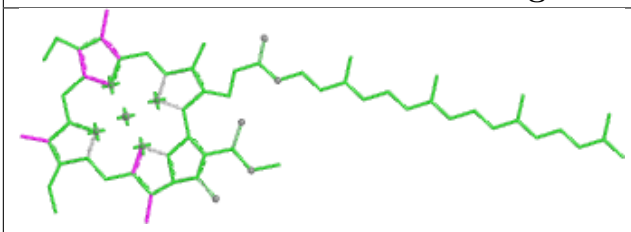


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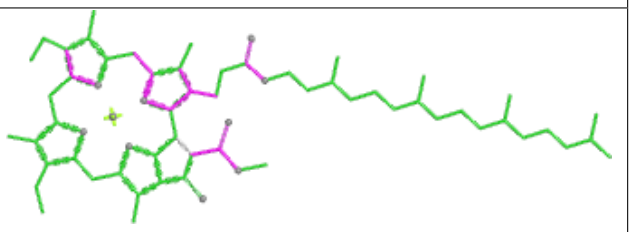


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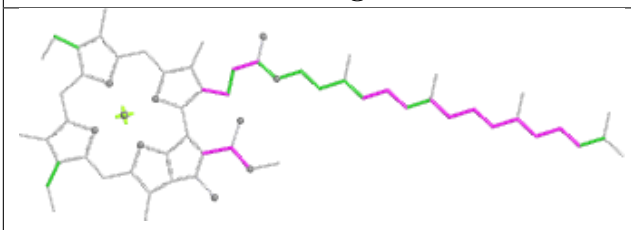
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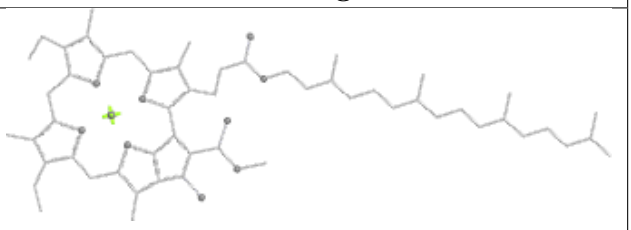
Bond lengths



Bond angles

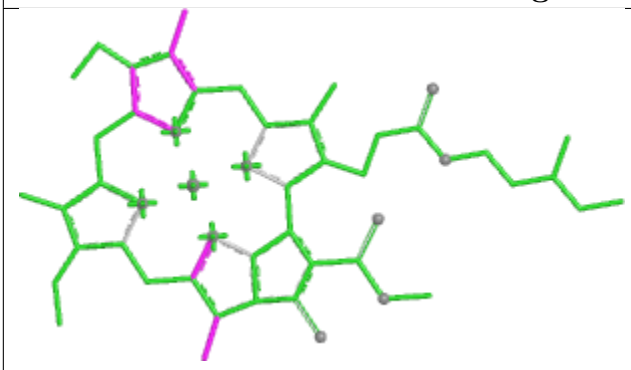


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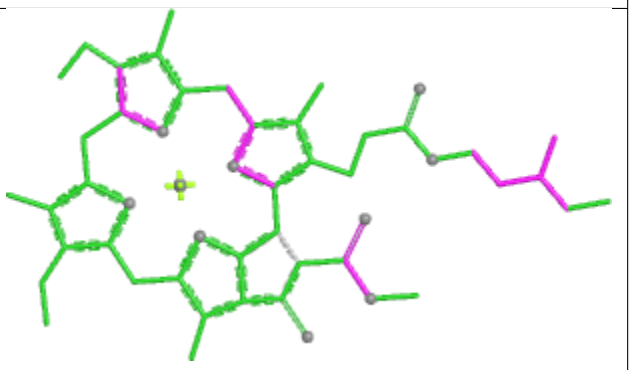


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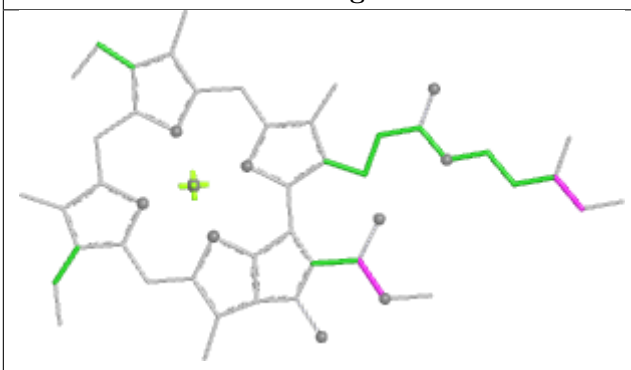
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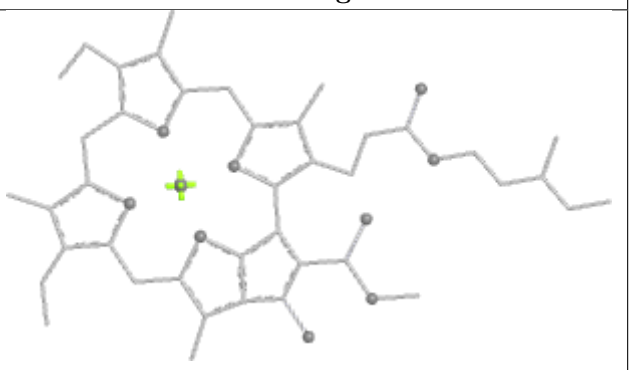
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Bond angles

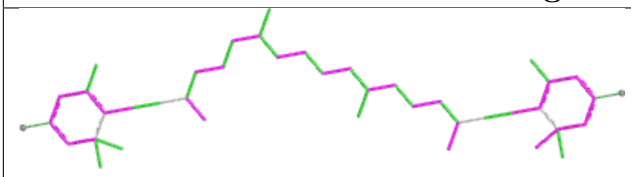


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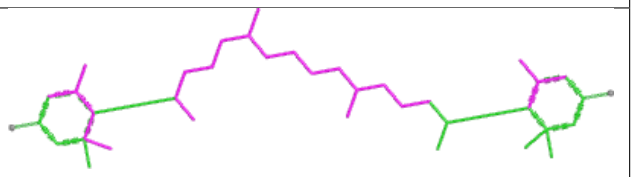


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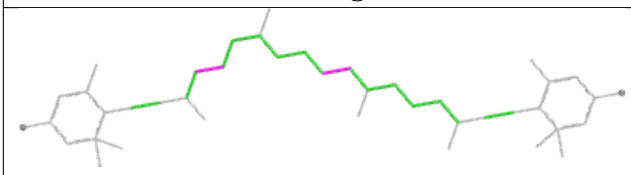
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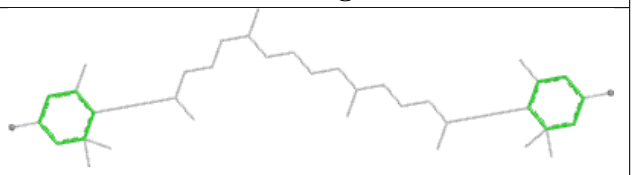
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Bond angles

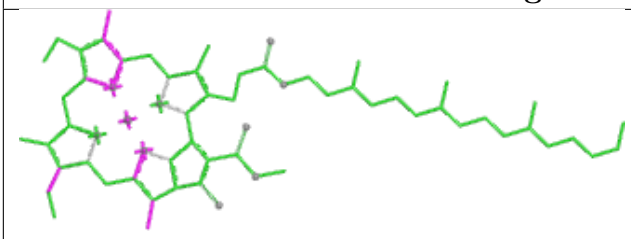


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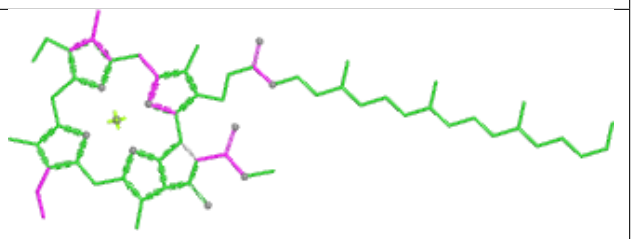


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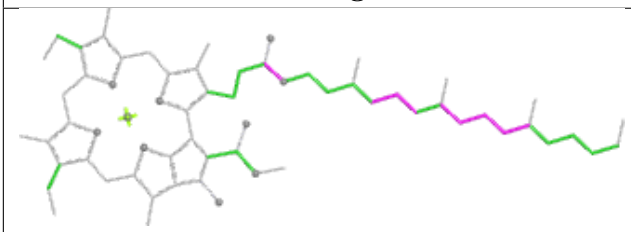
Ligand CLA B 822



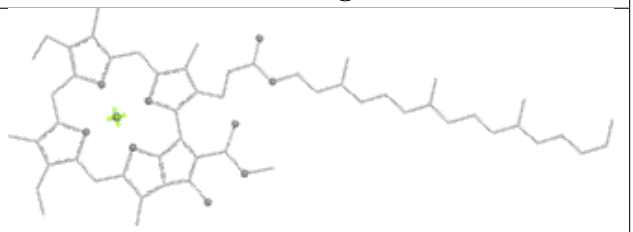
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Bond angles

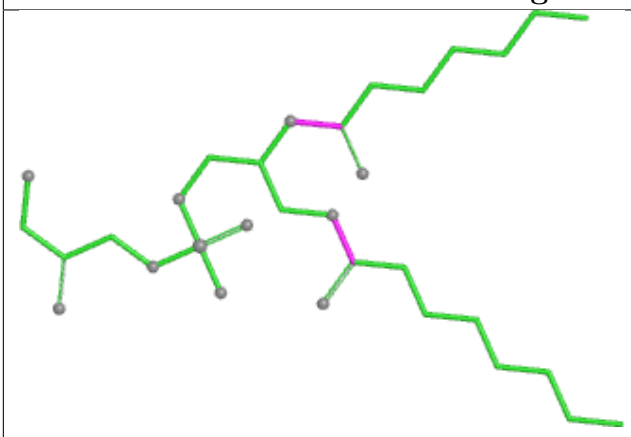


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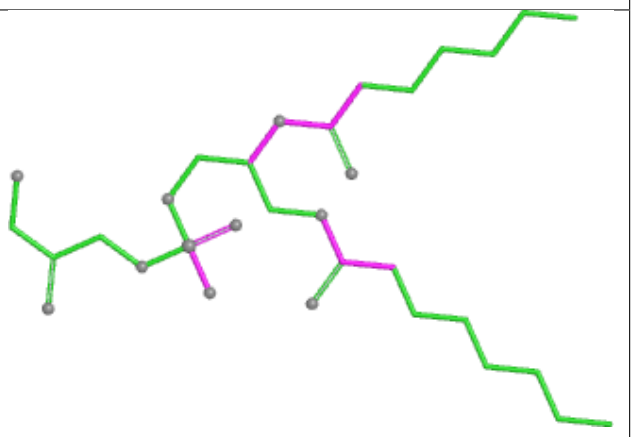


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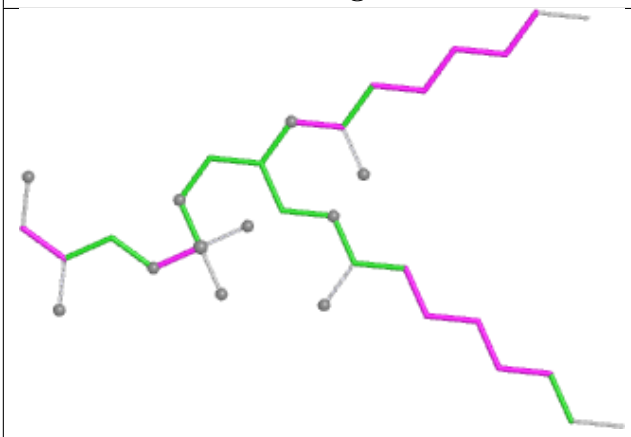
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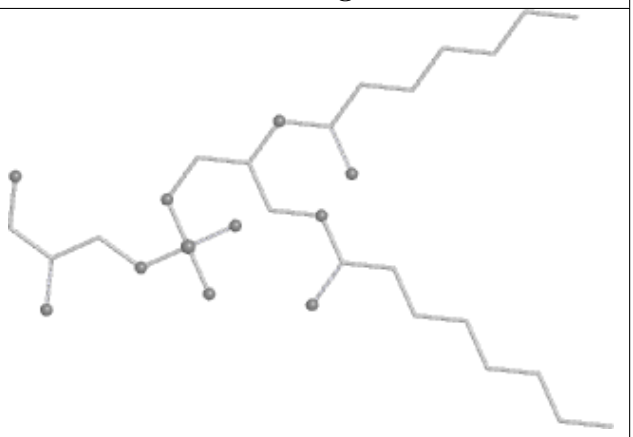
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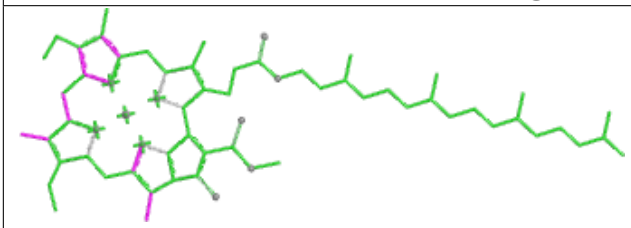


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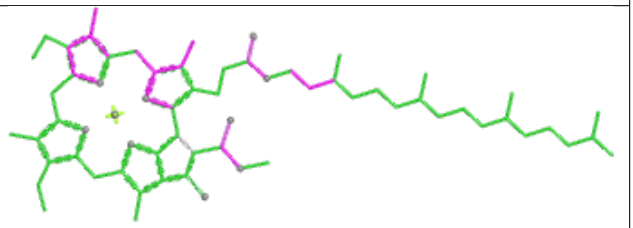


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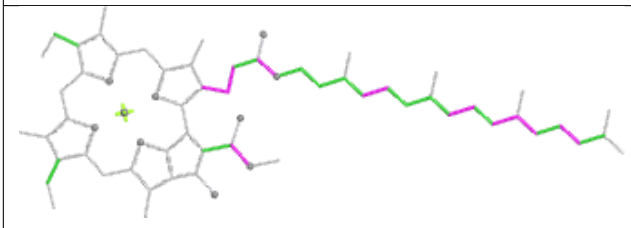
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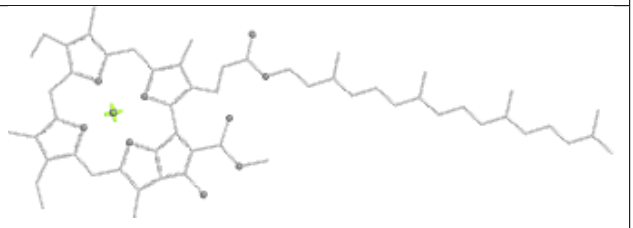
Bond lengths



Bond angles

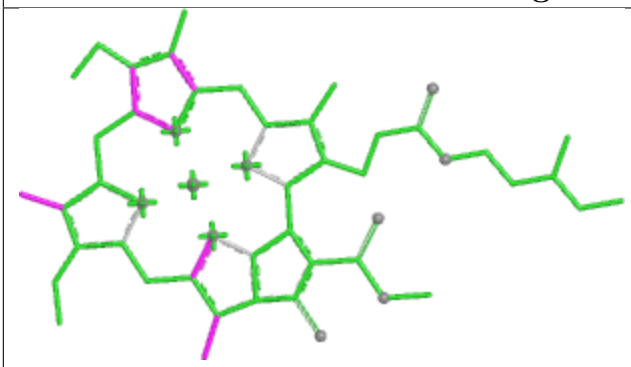


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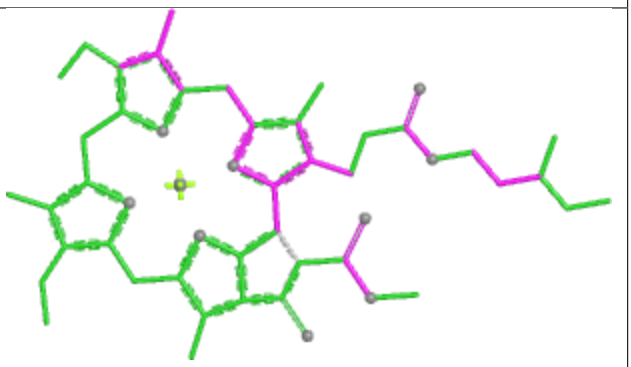


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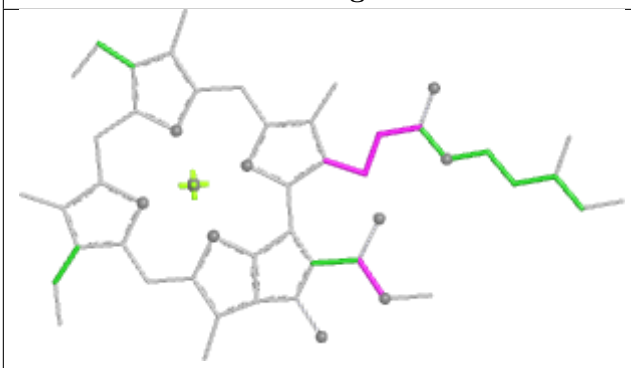
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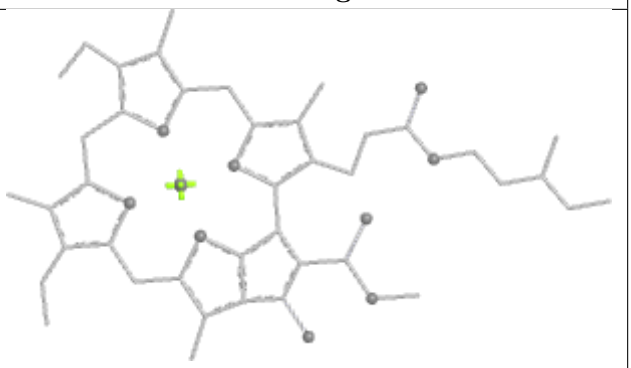
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Bond angles

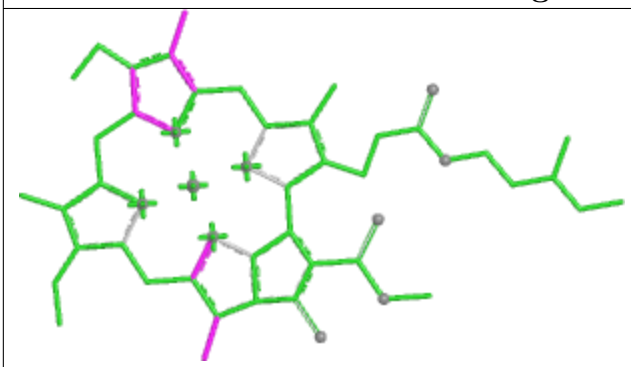


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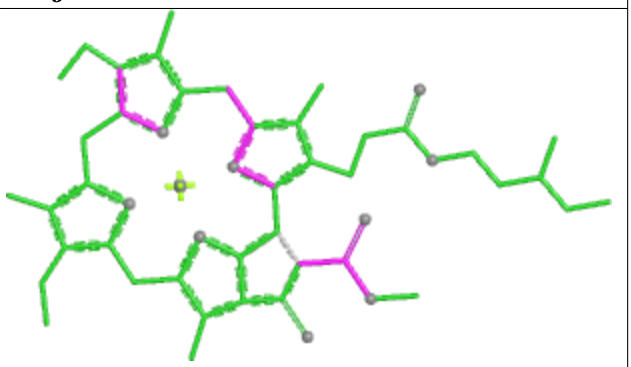


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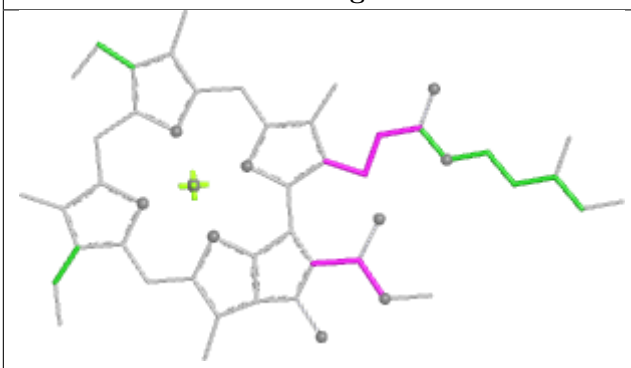
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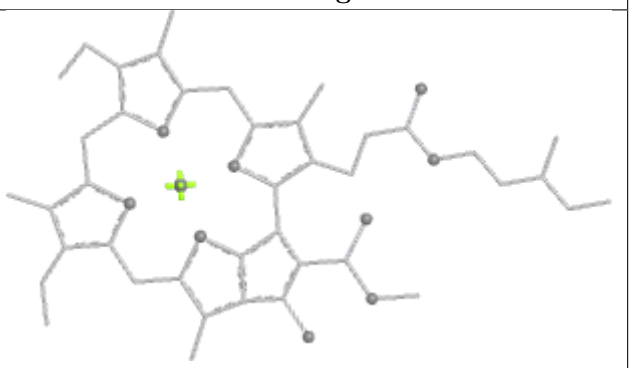
Bond lengths



Bond angles

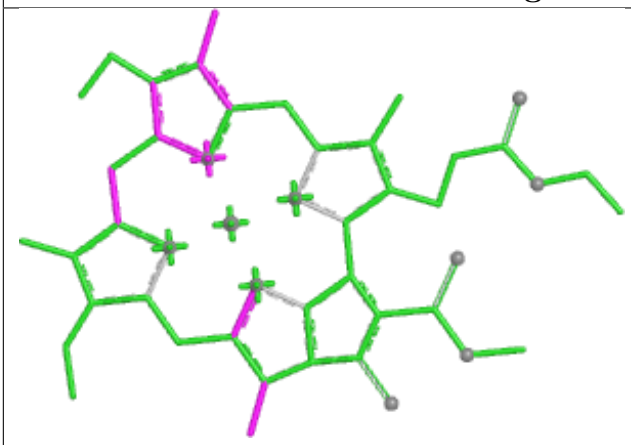


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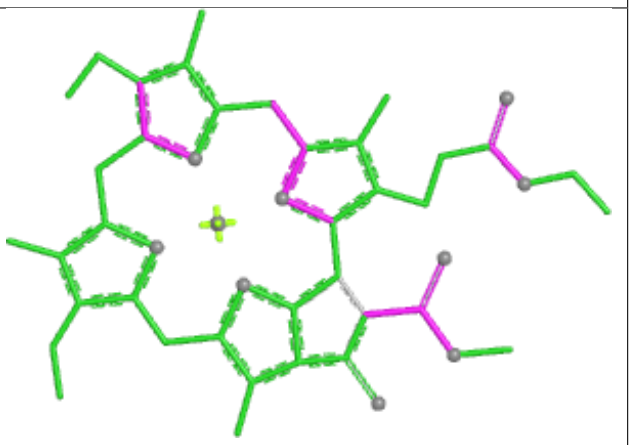


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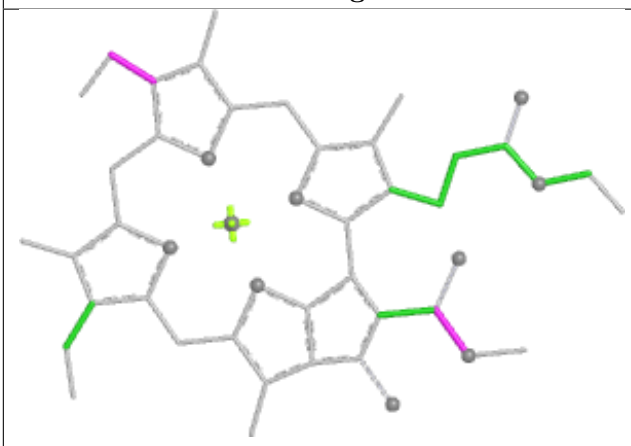
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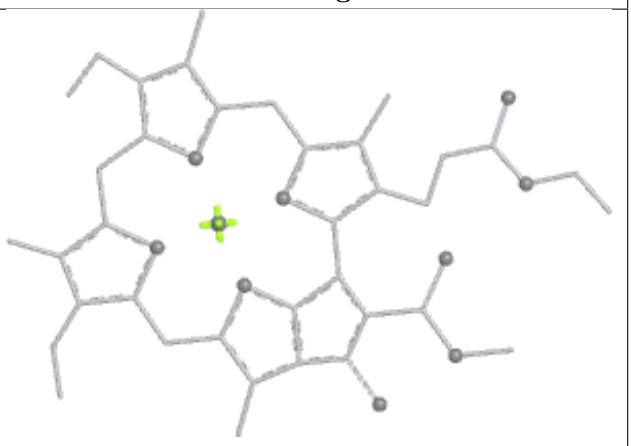
Bond lengths



Bond angles

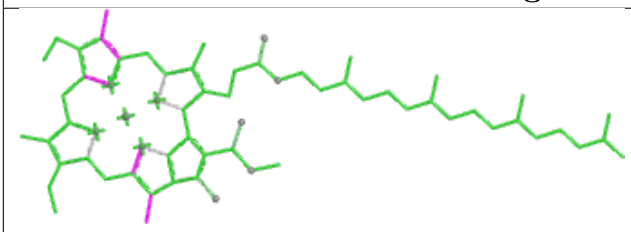


Torsions

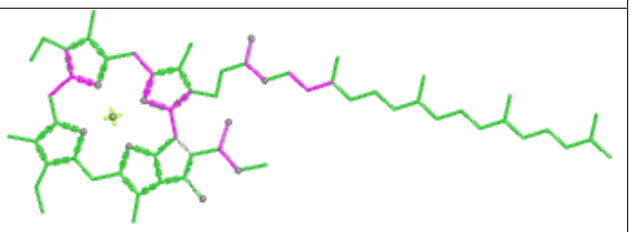


Rings

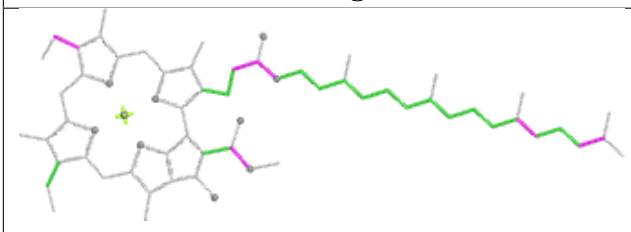
Ligand CLA A 801



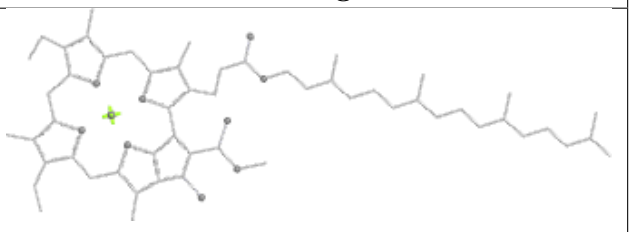
Bond lengths



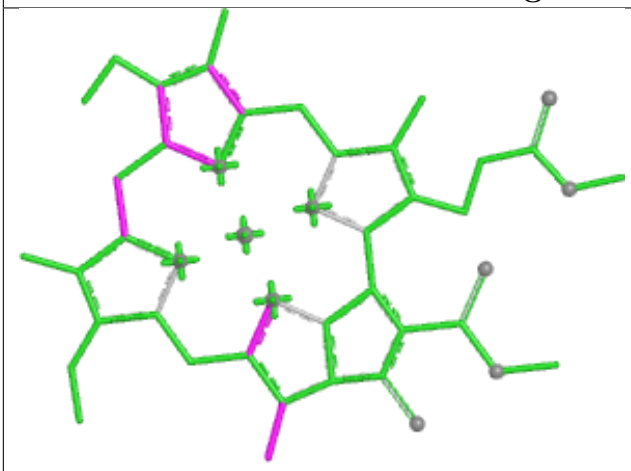
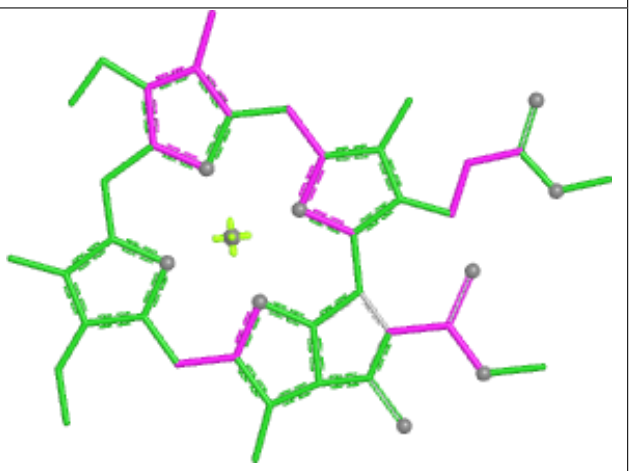
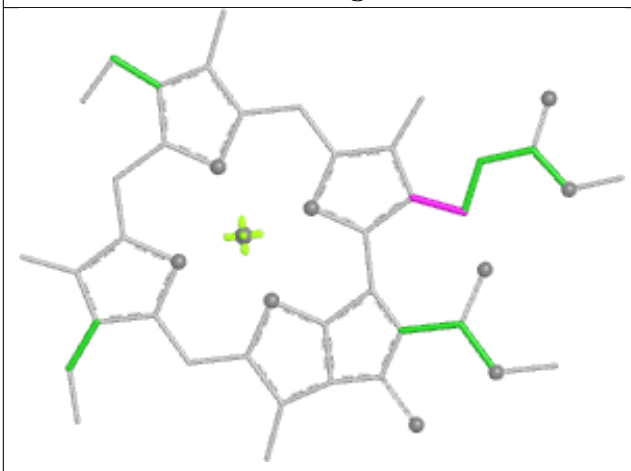
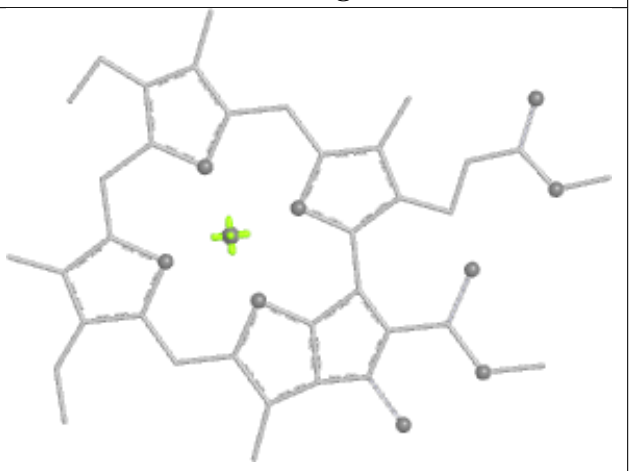
Bond angles



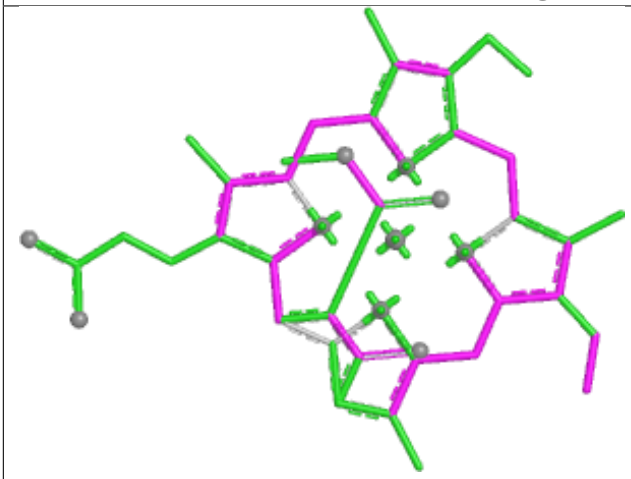
Torsions



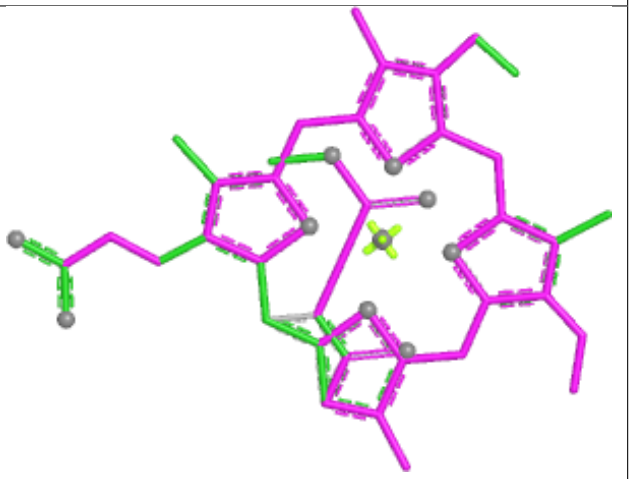
Rings

Ligand CLA B 818	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

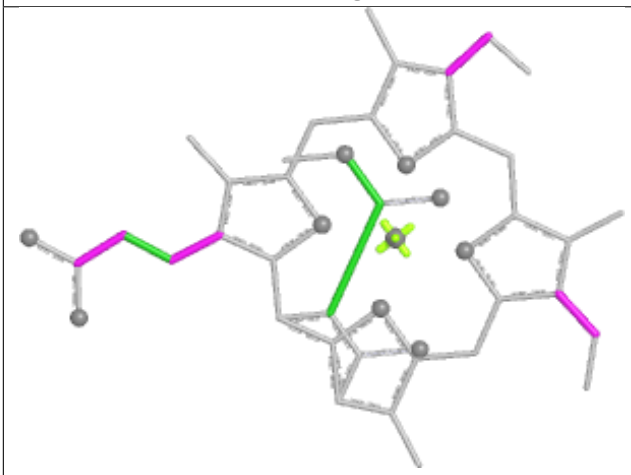
Ligand KC2 i 310



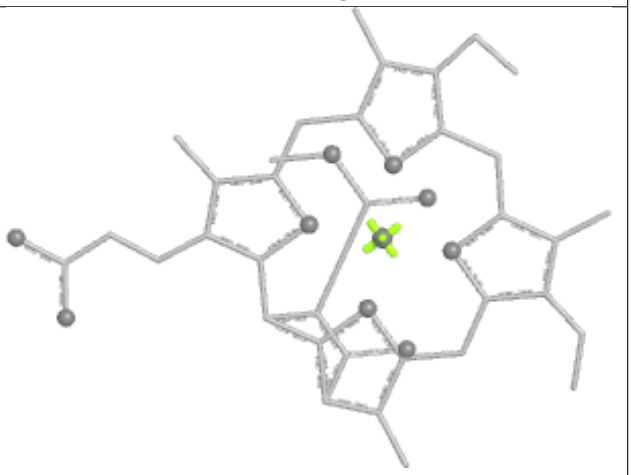
Bond lengths



Bond angles

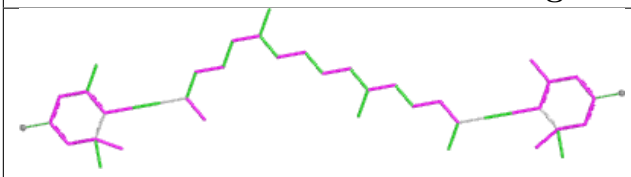


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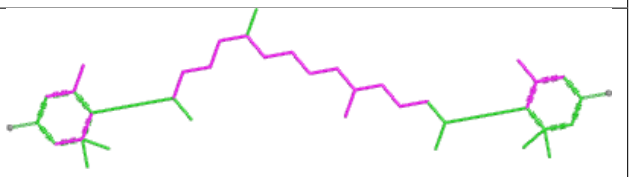


Rings

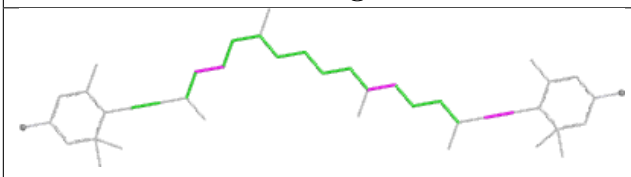
Ligand II0 f 615



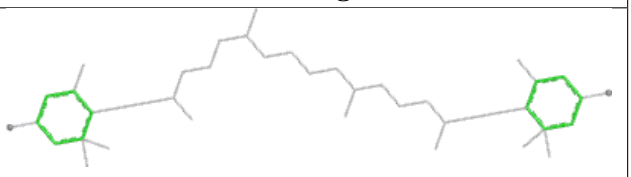
Bond lengths



Bond angles

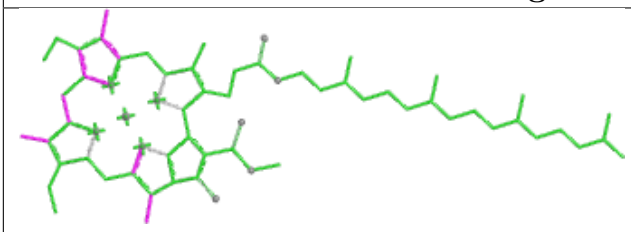


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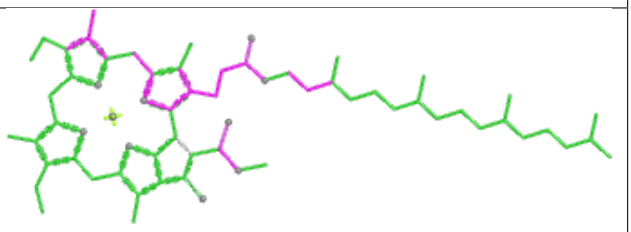


Rings

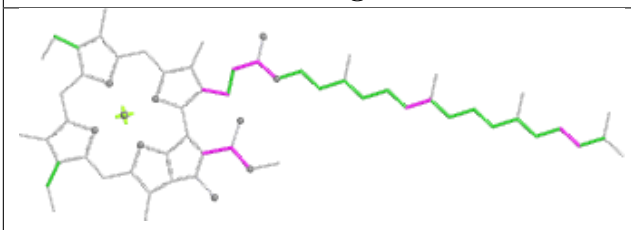
Ligand CLA a 311



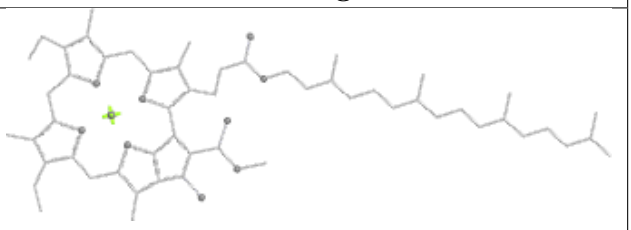
Bond lengths



Bond angles

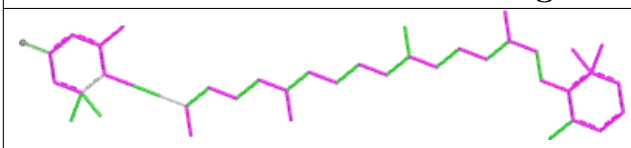


Torsions



Rings

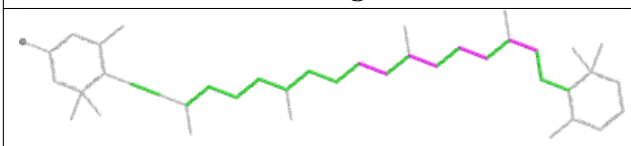
Ligand IHT f 617



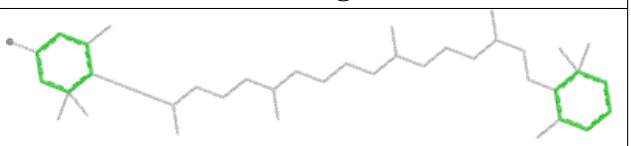
Bond lengths



Bond angles

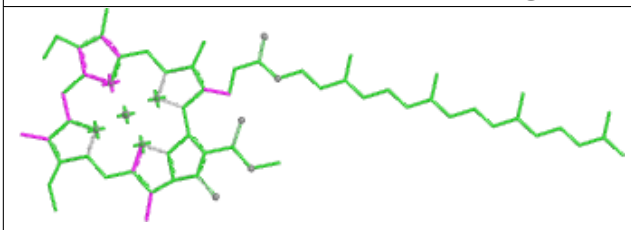


Torsions

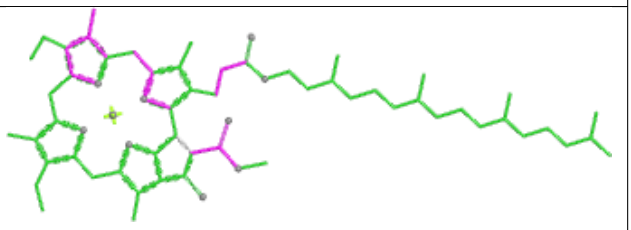


Rings

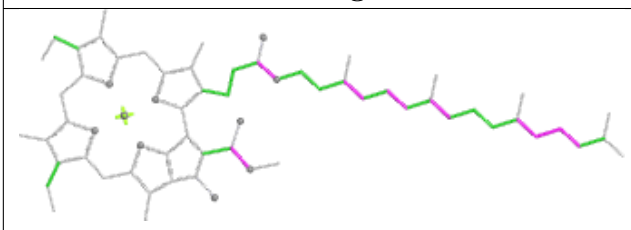
Ligand CLA m 603



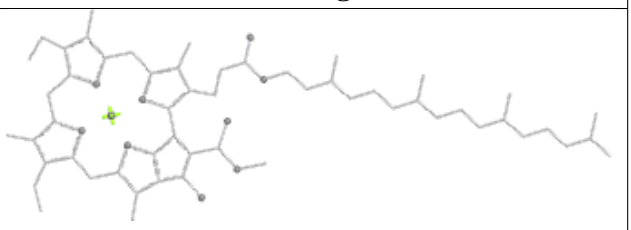
Bond lengths



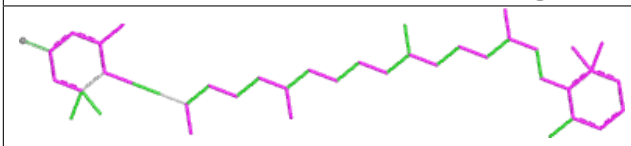
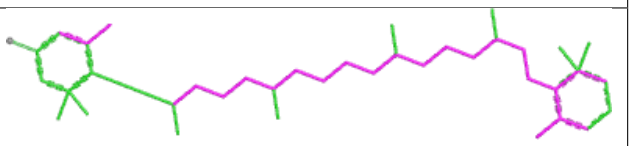
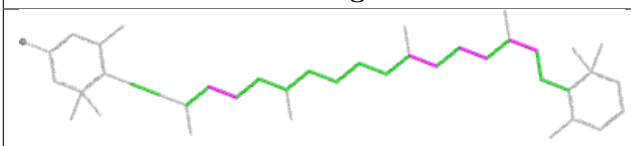
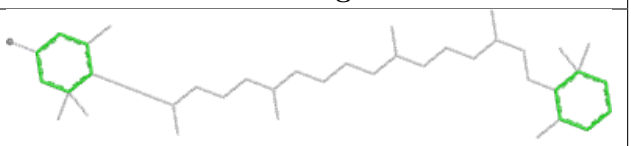
Bond angles

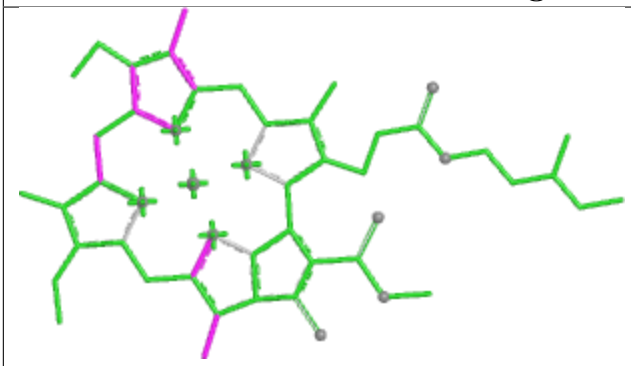
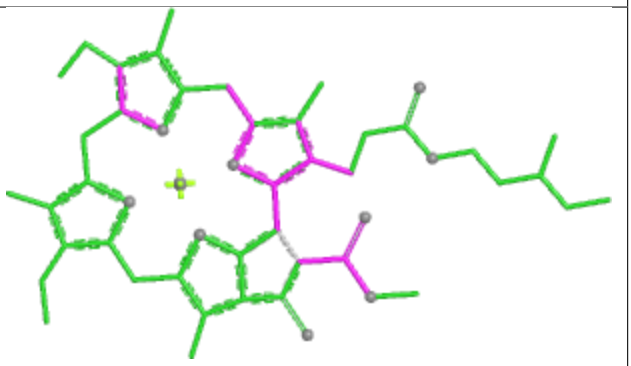
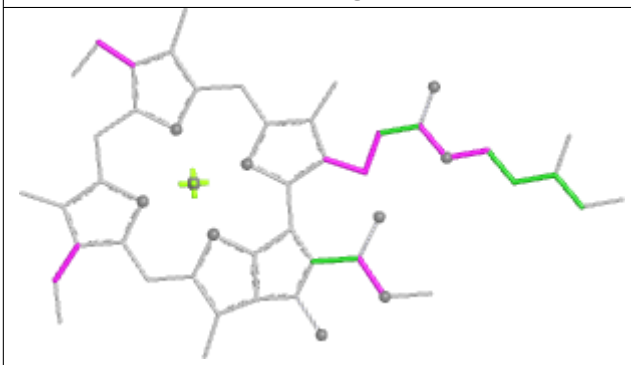
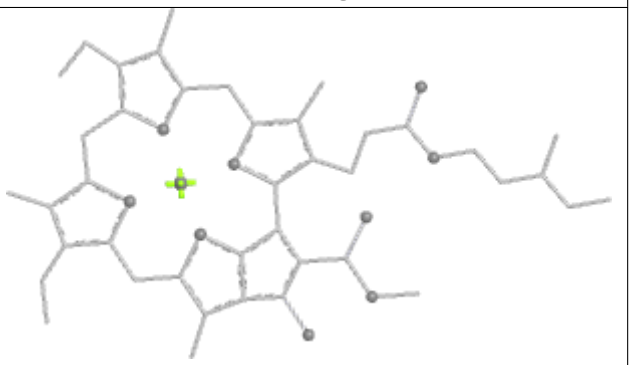


Torsions

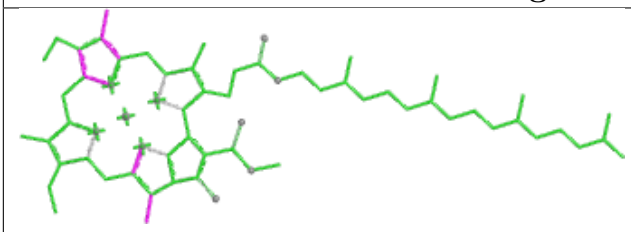


Rings

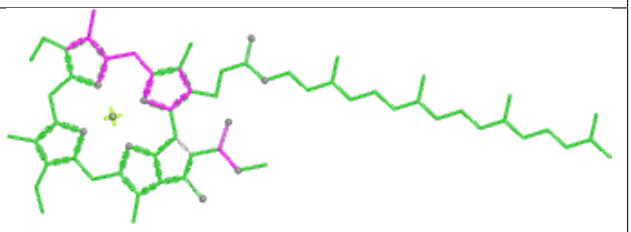
Ligand IHT b 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

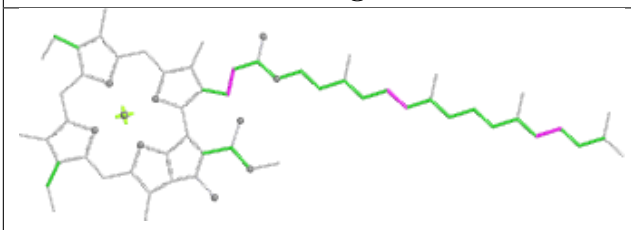
Ligand CLA c 604



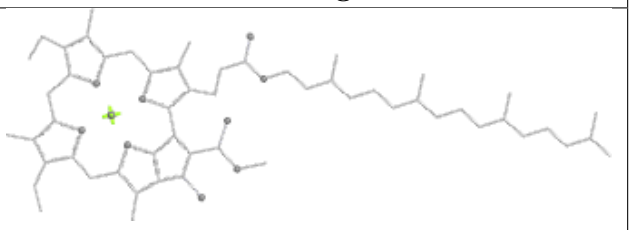
Bond lengths



Bond angles

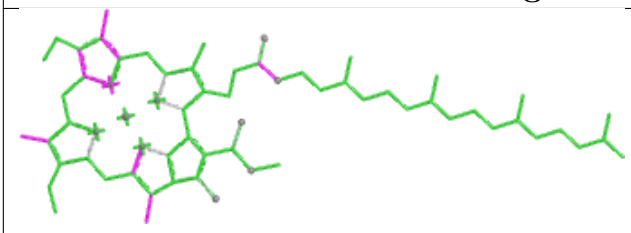


Torsions

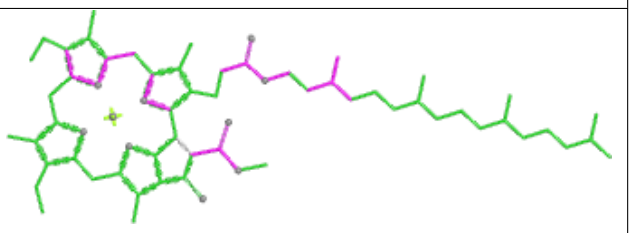


Rings

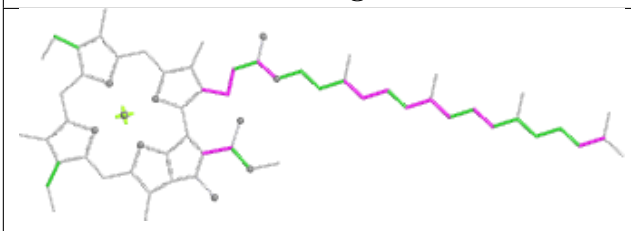
Ligand CLA A 854



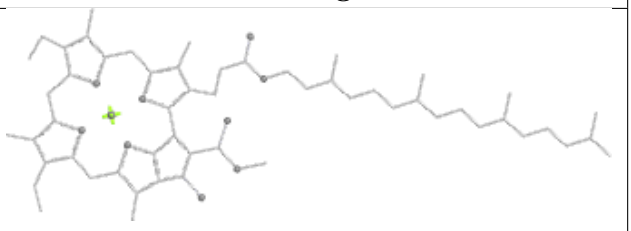
Bond lengths



Bond angles

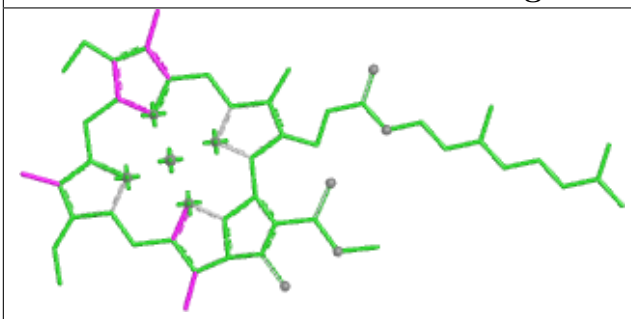


Torsions

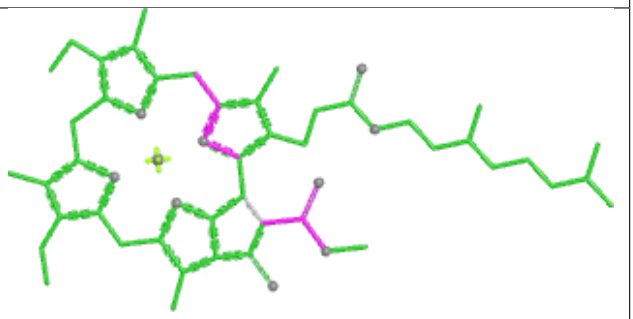


Rings

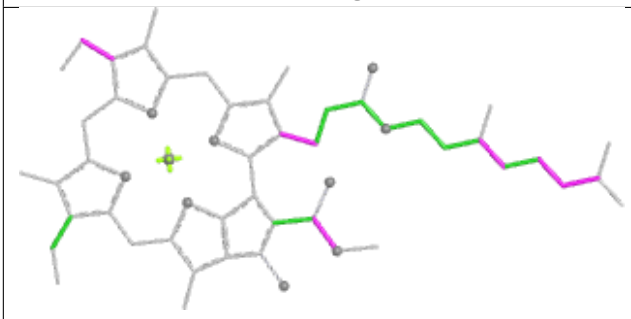
Ligand CLA B 819



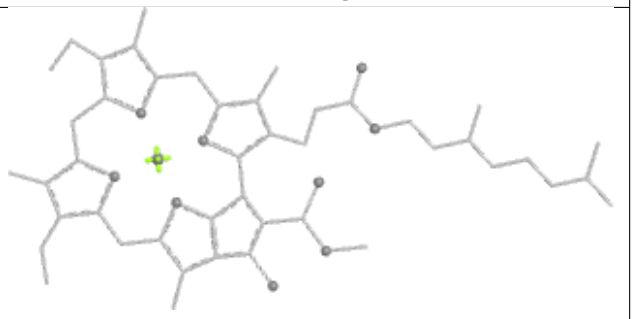
Bond lengths



Bond angles

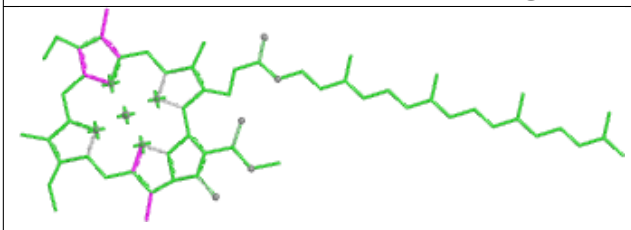


Torsions

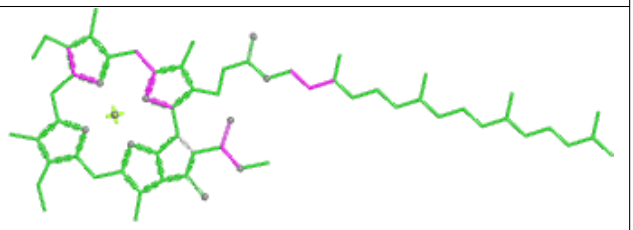


Rings

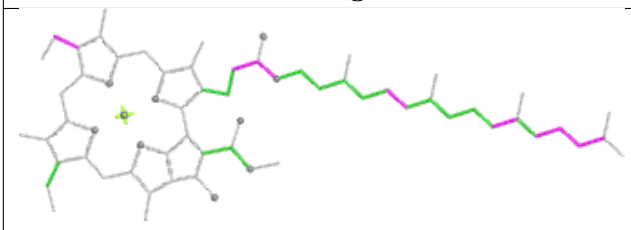
Ligand CLA m 606



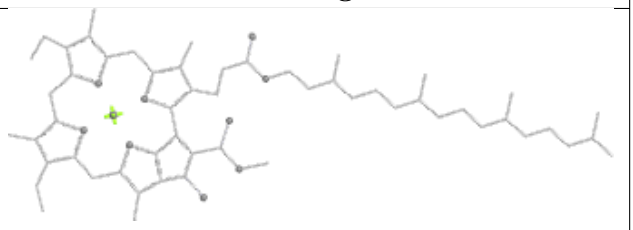
Bond lengths



Bond angles

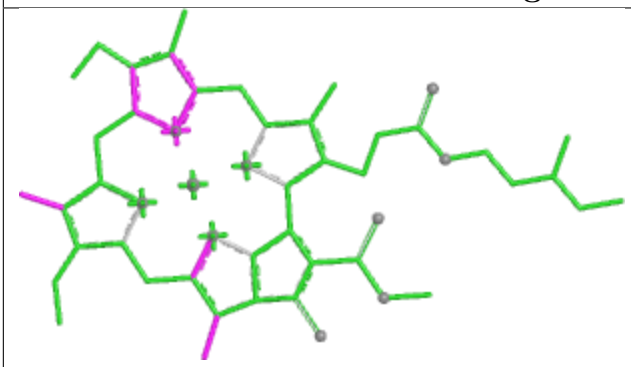


Torsions

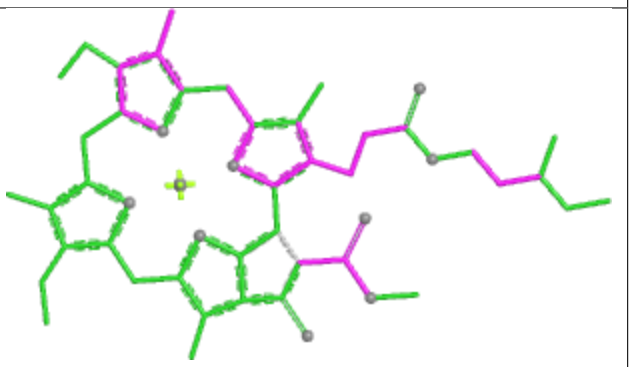


Rings

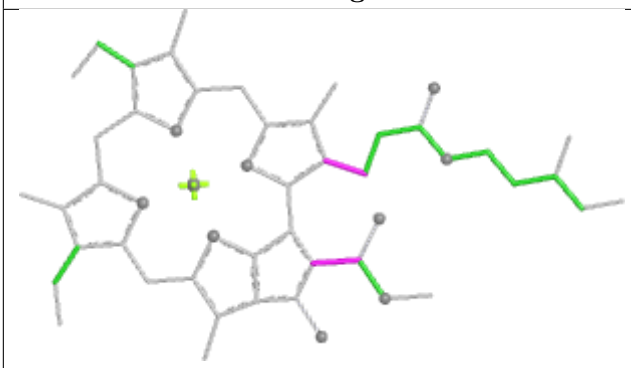
Ligand CLA A 834



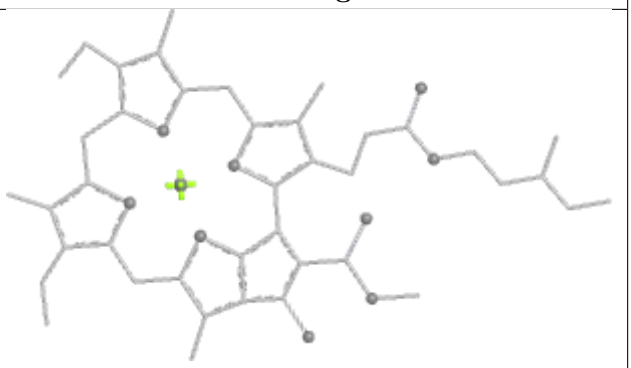
Bond lengths



Bond angles

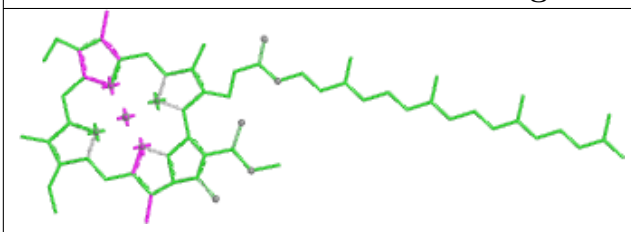


Torsions

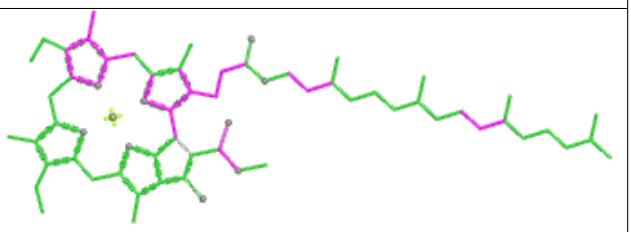


Rings

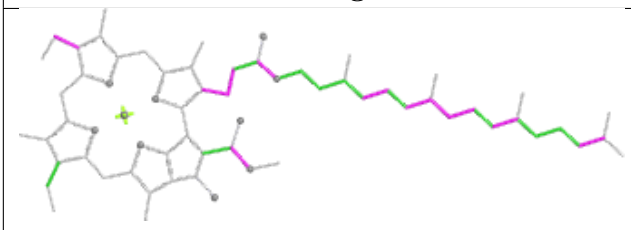
Ligand CLA s 202



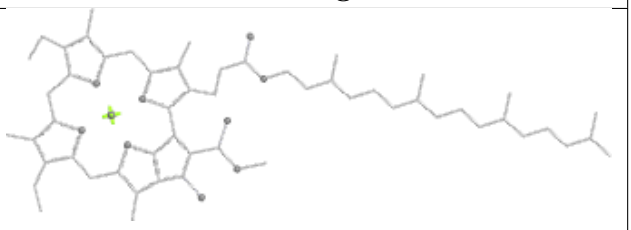
Bond lengths



Bond angles

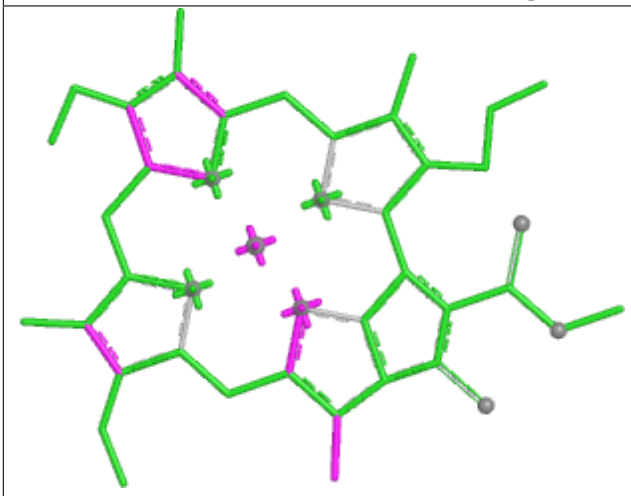


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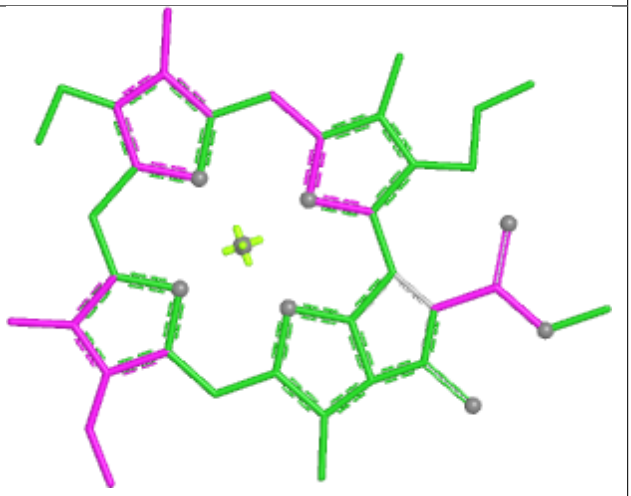


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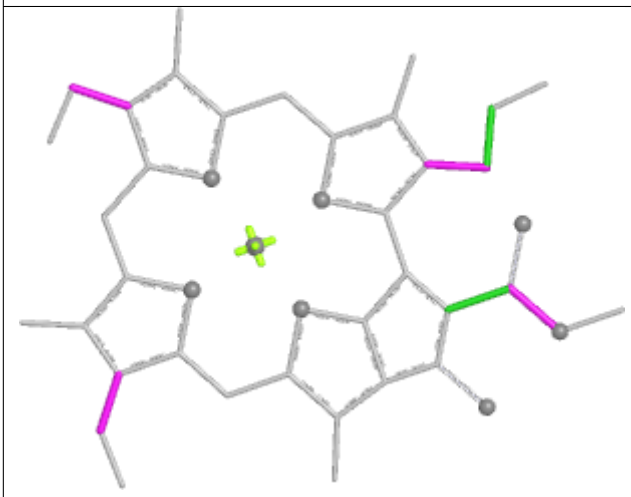
Ligand CLA m 613



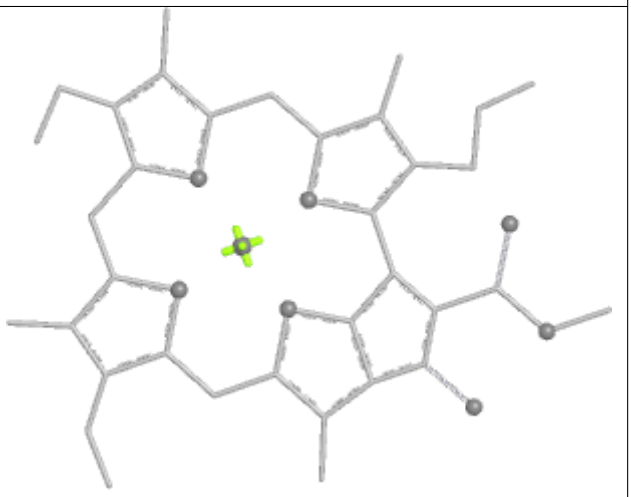
Bond lengths



Bond angles

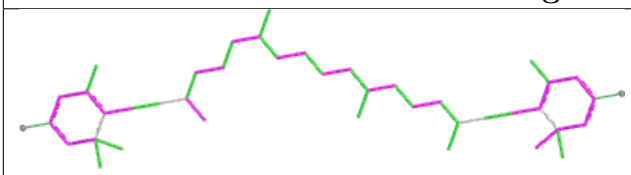


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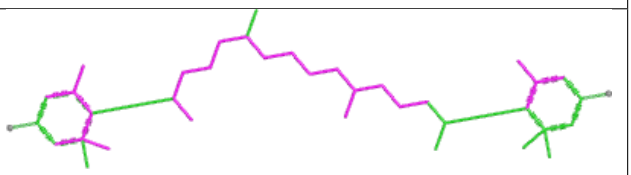


Rings

Ligand II0 k 617



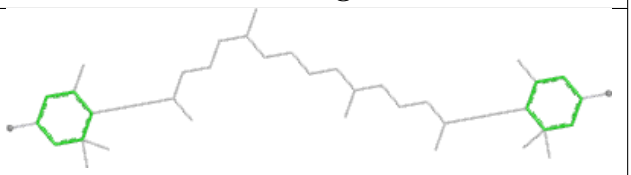
Bond lengths



Bond angles

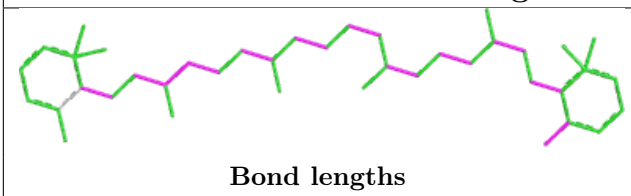


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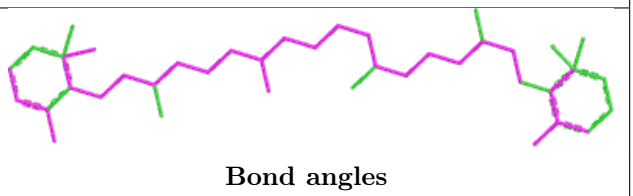


Rings

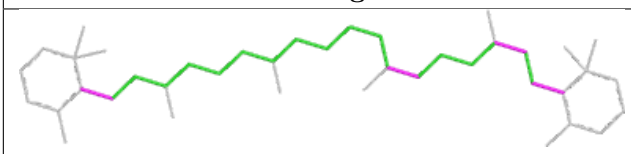
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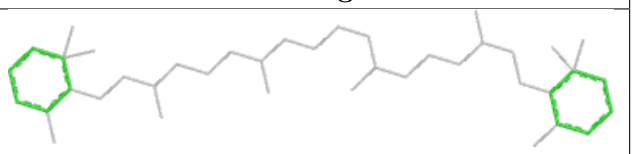
Bond lengths



Bond angles

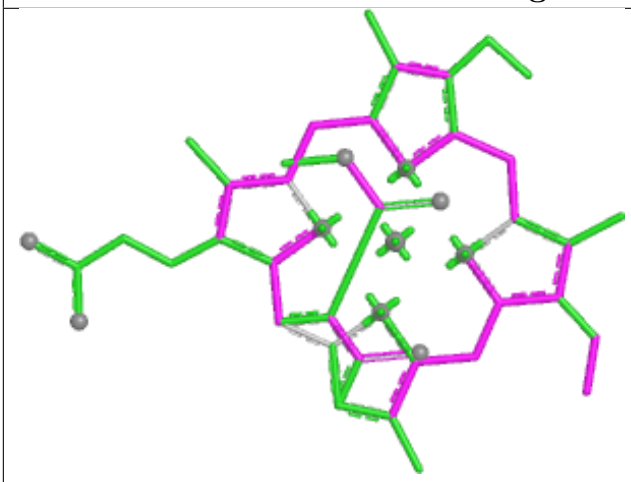


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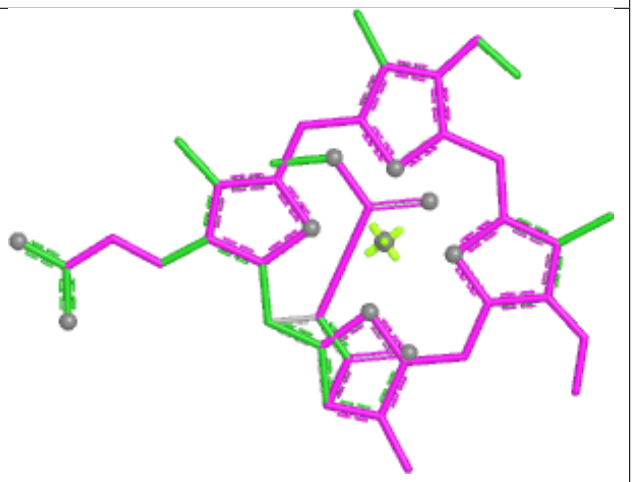


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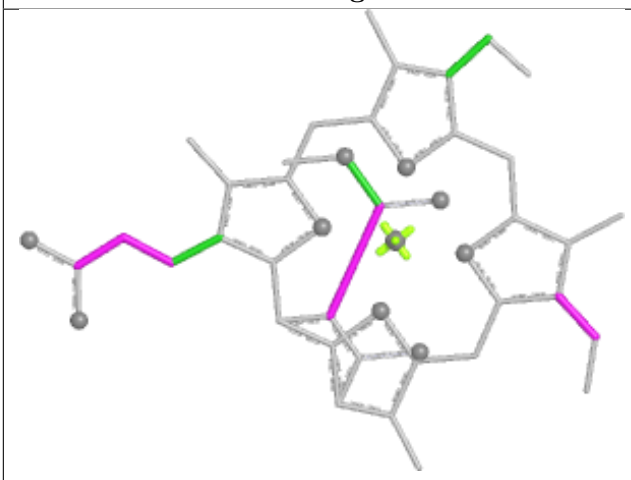
Ligand KC2 d 310



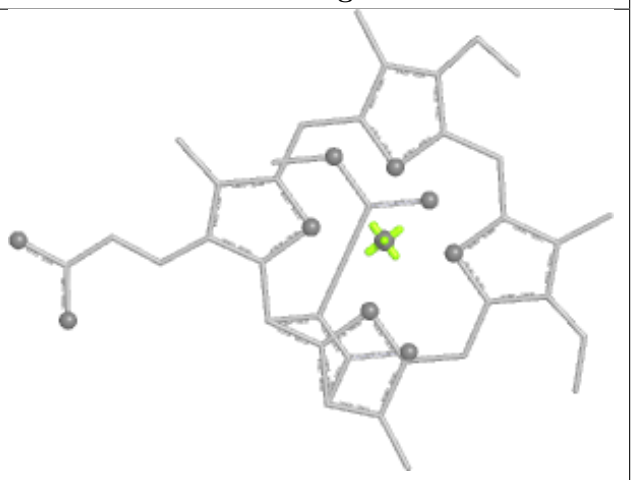
Bond lengths



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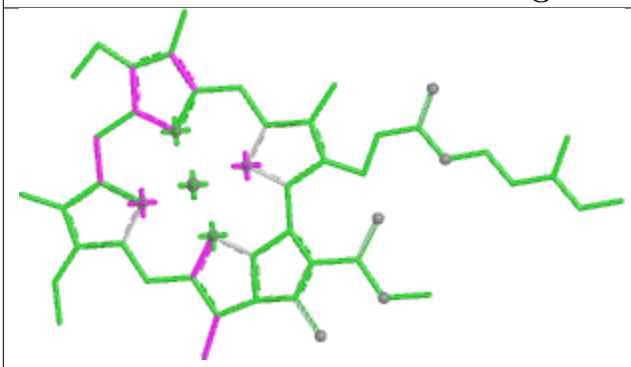


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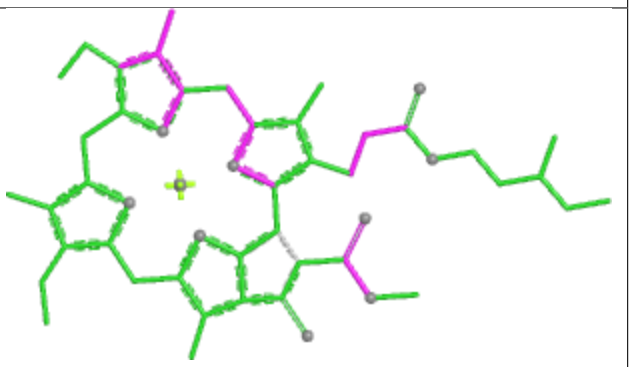


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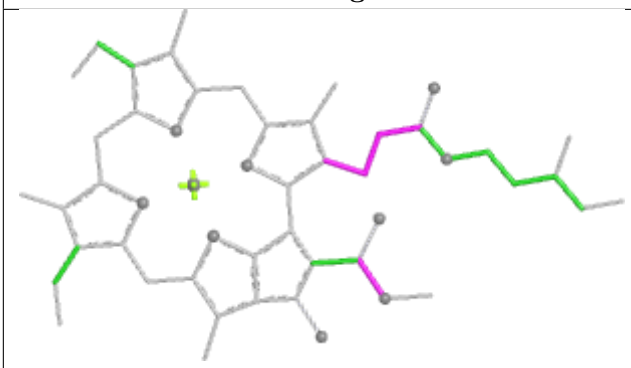
Ligand CLA i 311



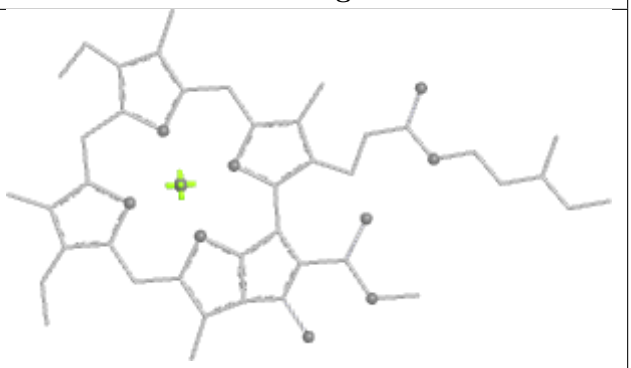
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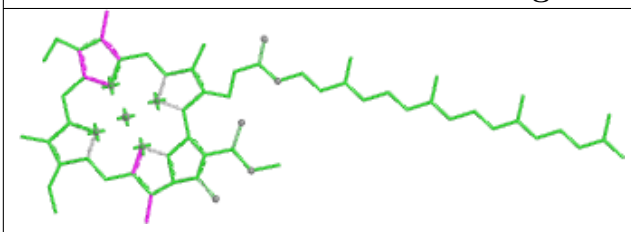


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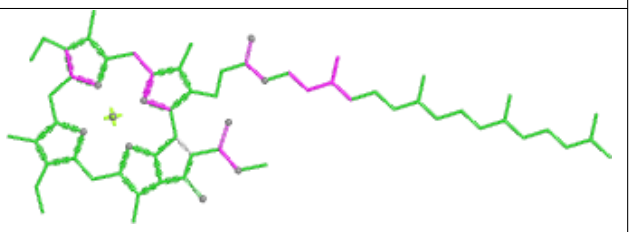


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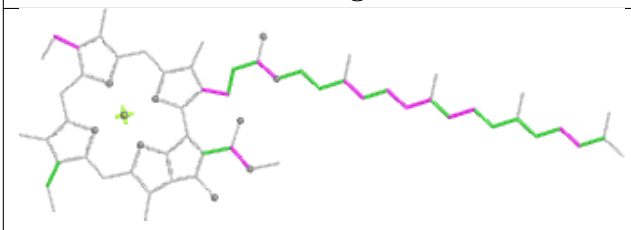
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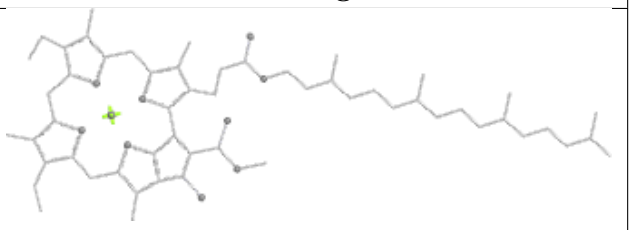
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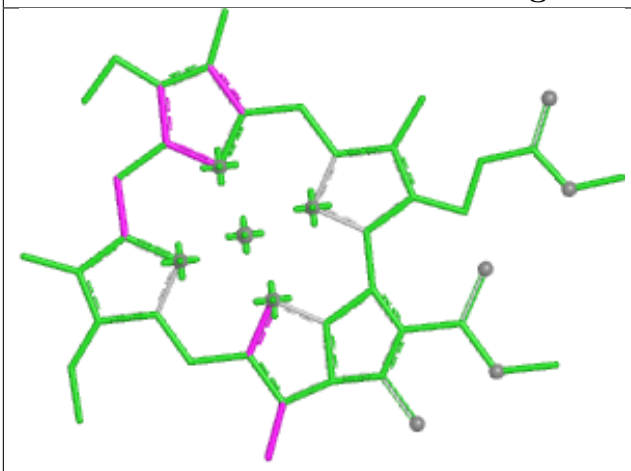


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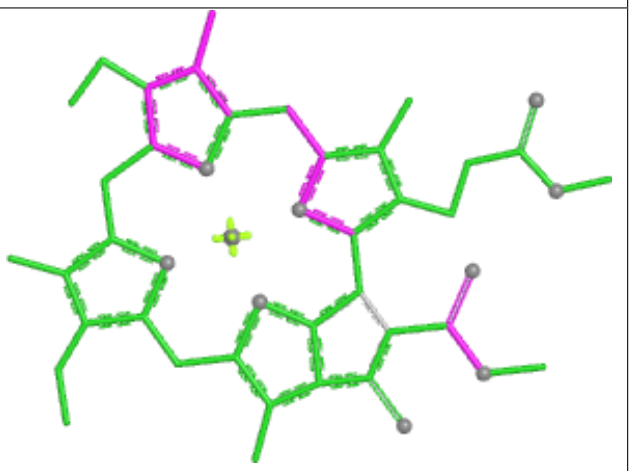


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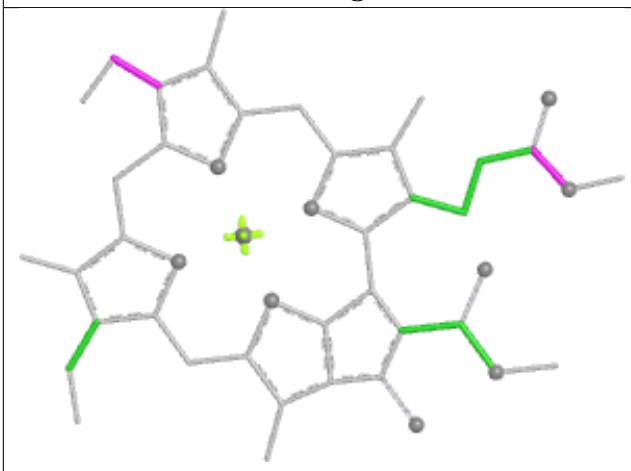
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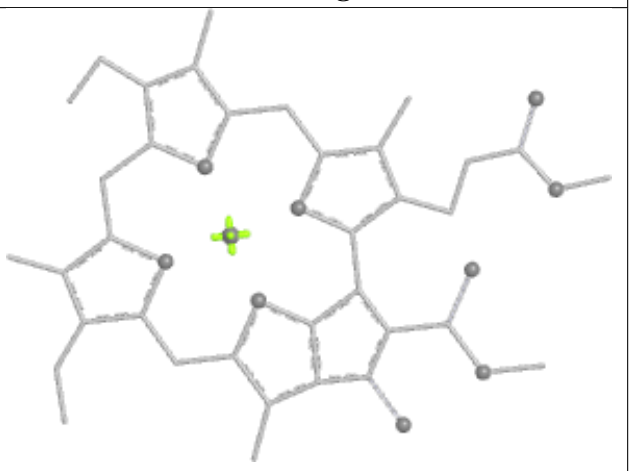
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Bond angles

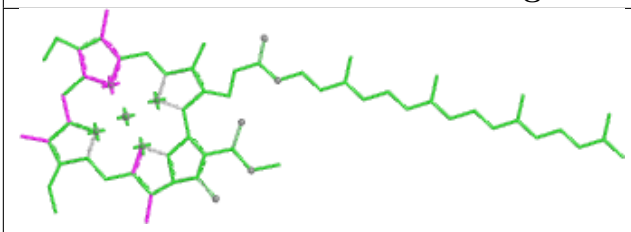


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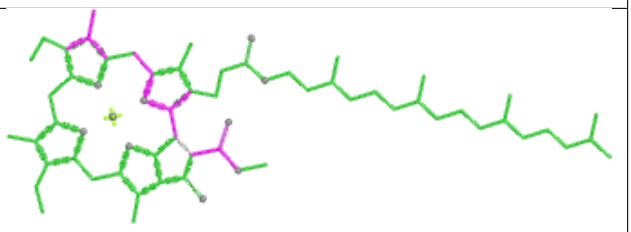


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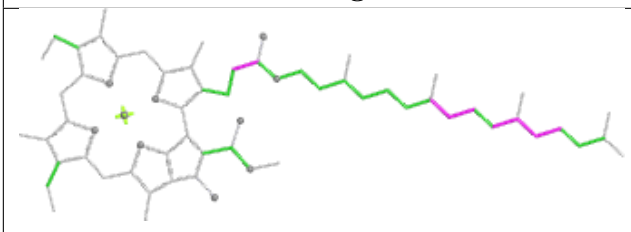
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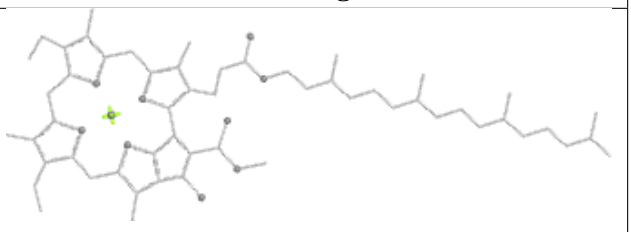
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Bond angles

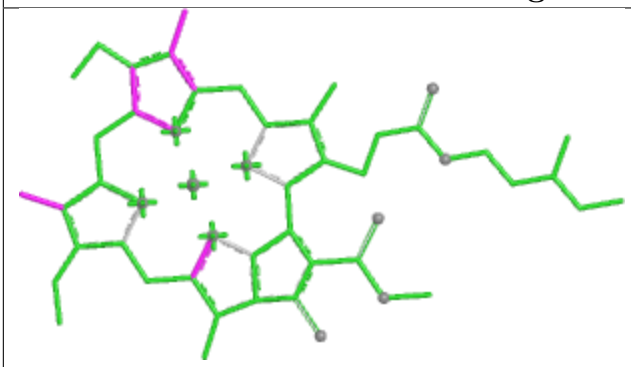


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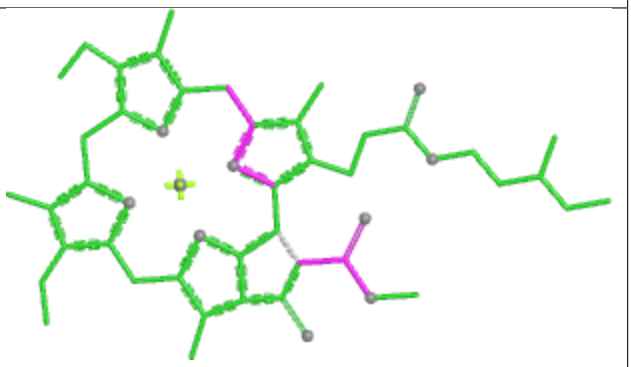


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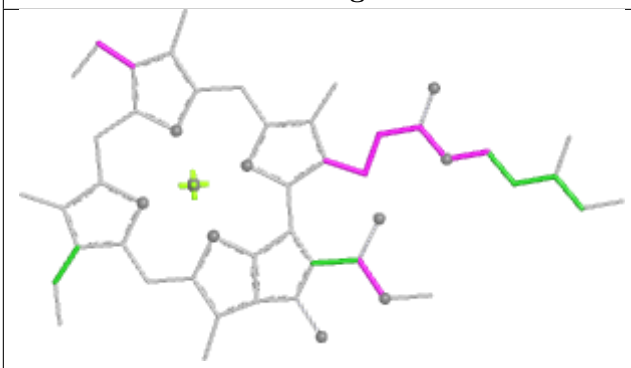
Ligand CLA k 610



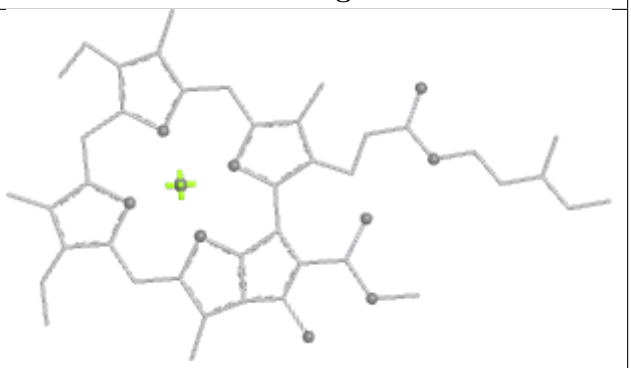
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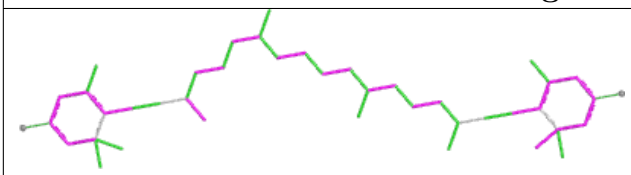


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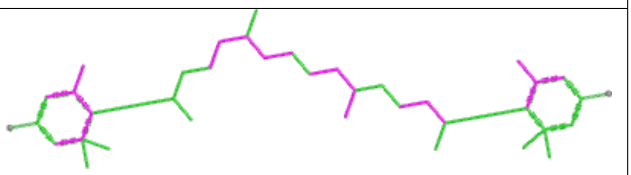


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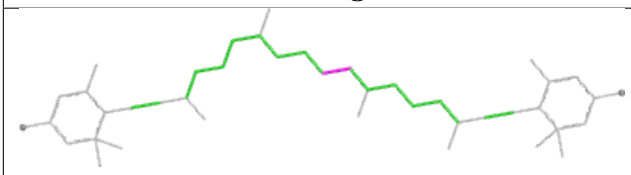
Ligand II0 d 314



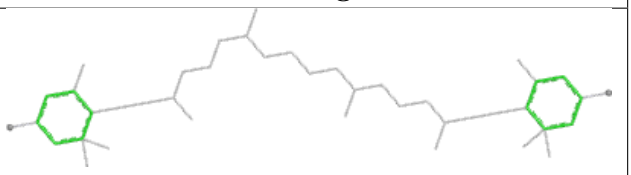
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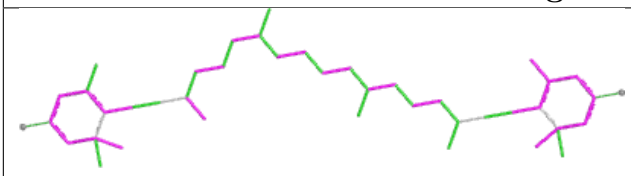


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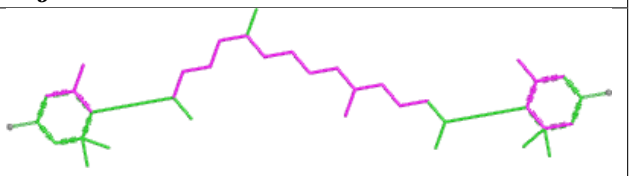


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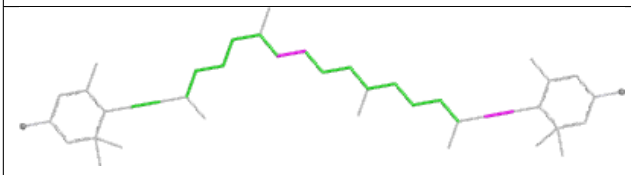
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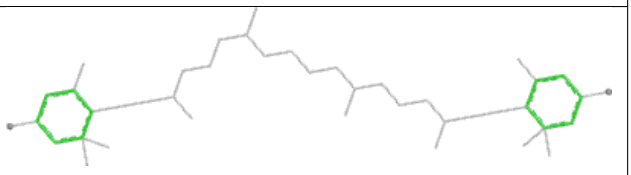
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Bond angles

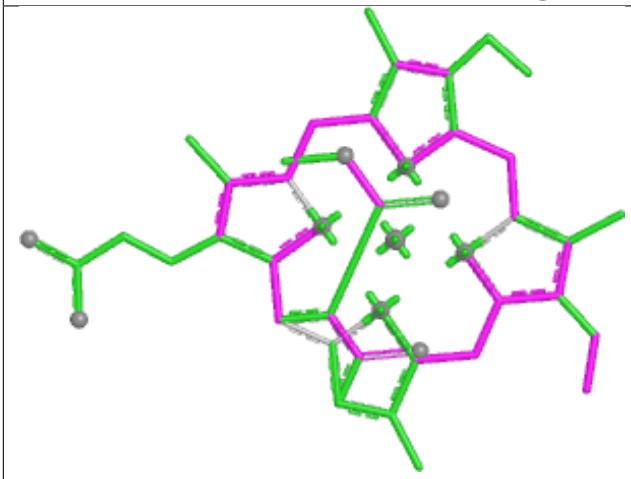


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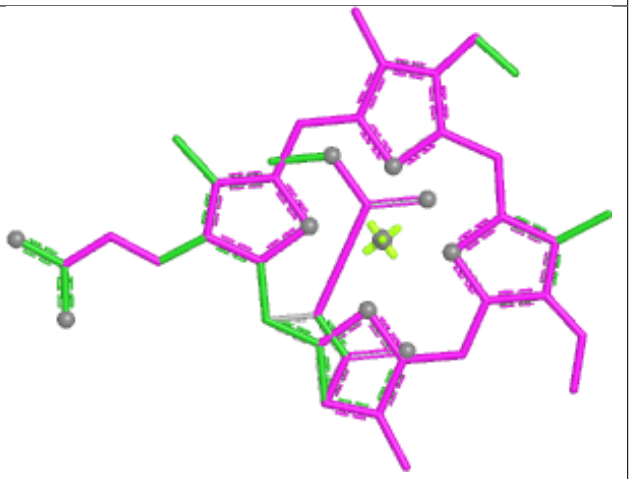


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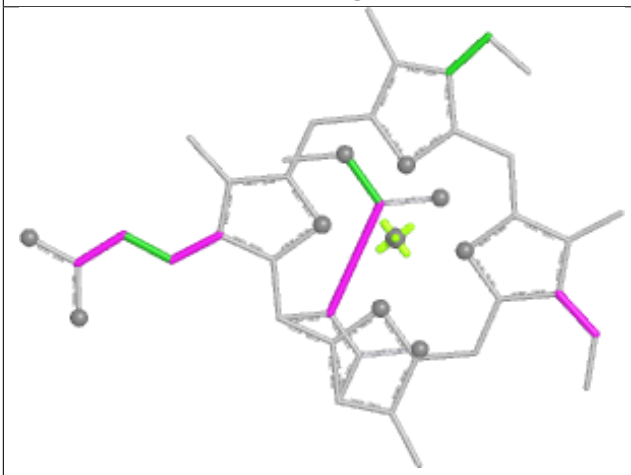
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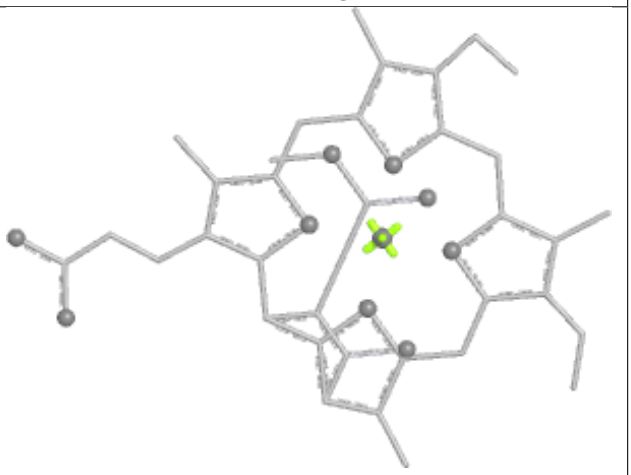
Bond lengths



Bond angles

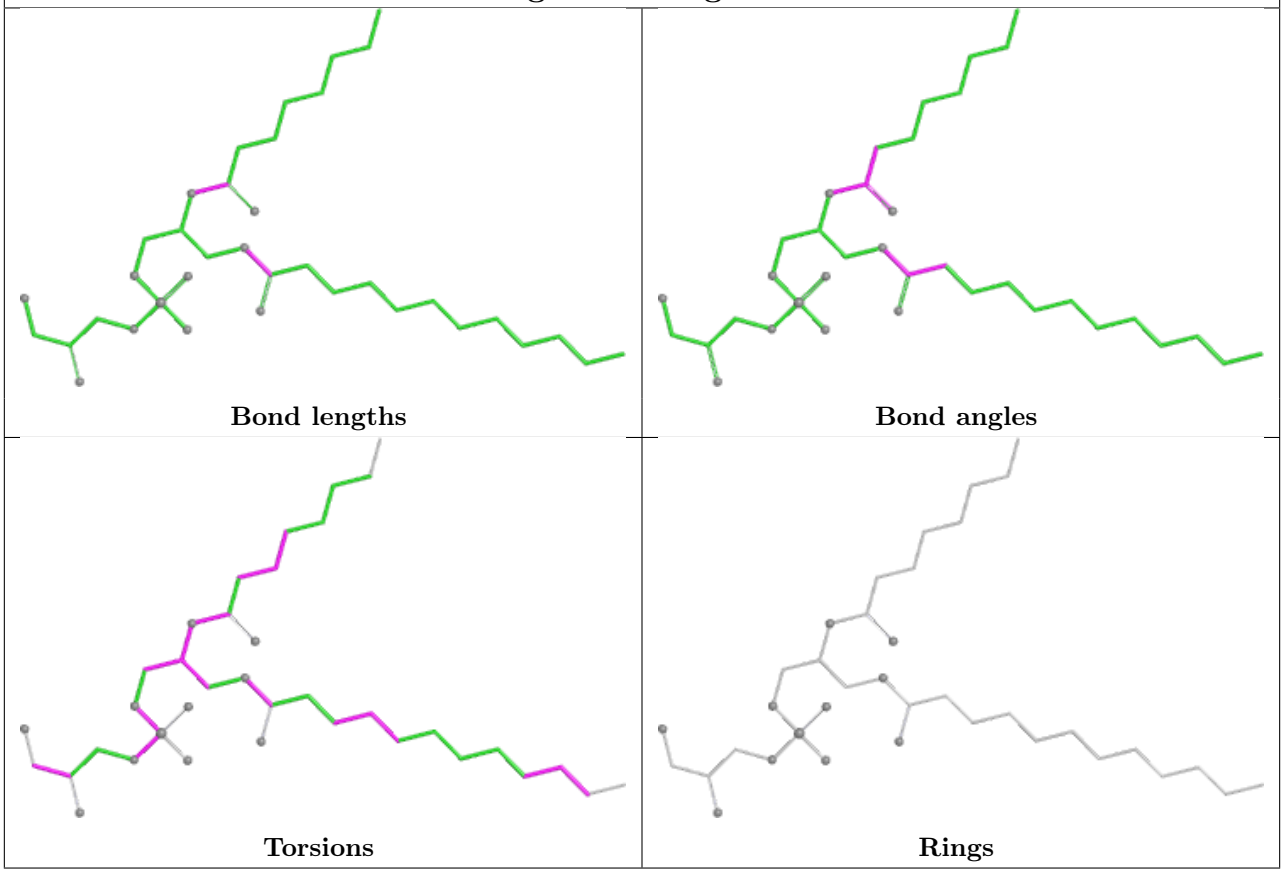


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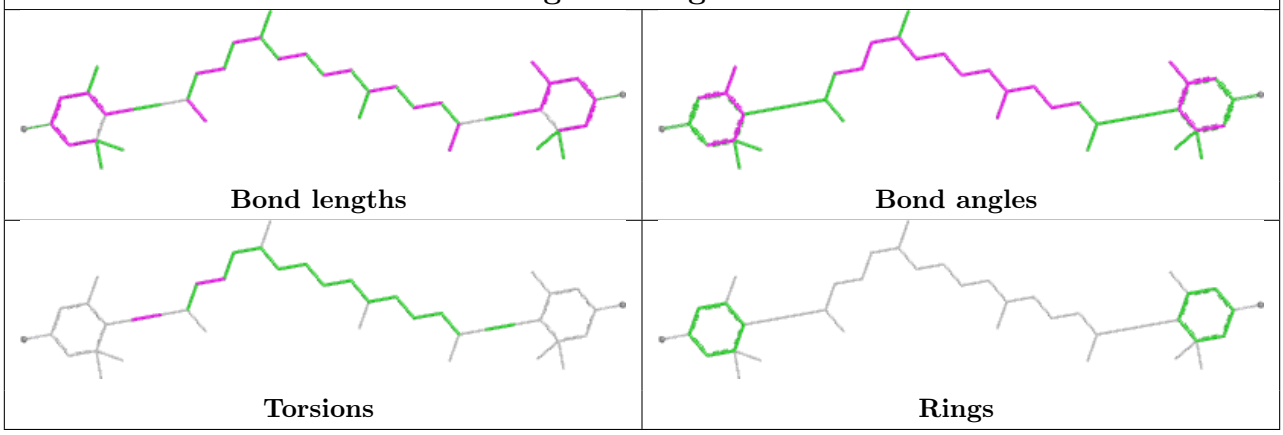


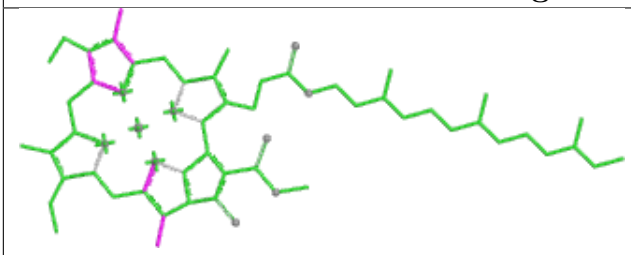
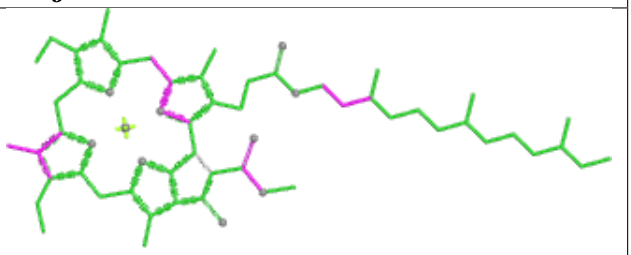
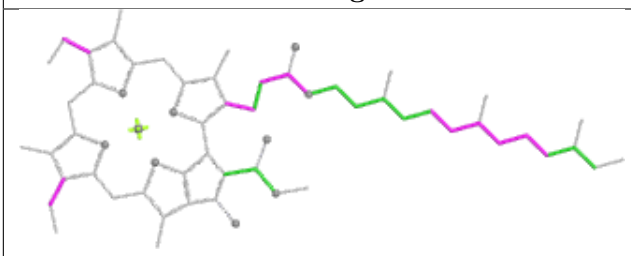
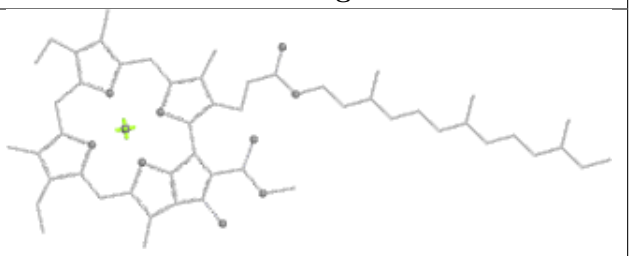
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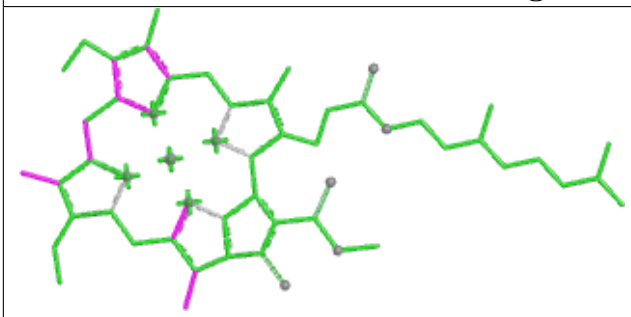
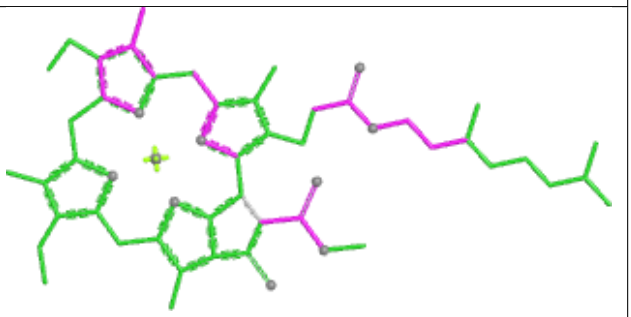
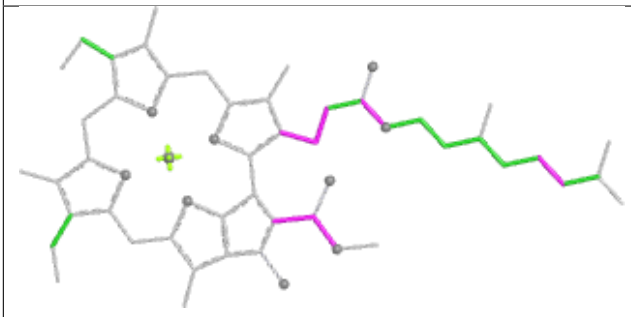
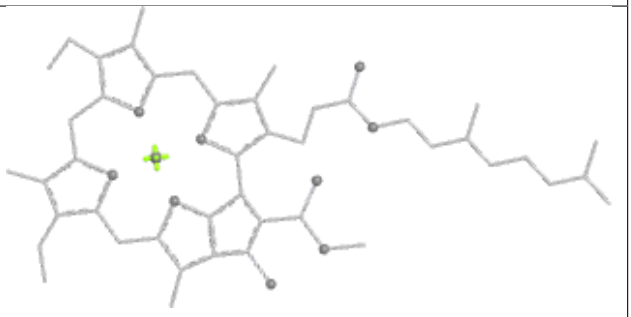
Ligand LHG g 301



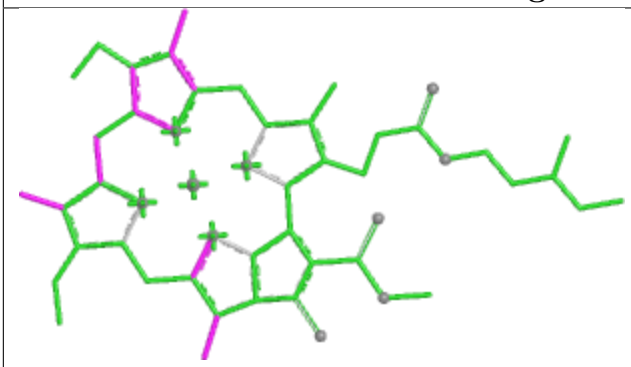
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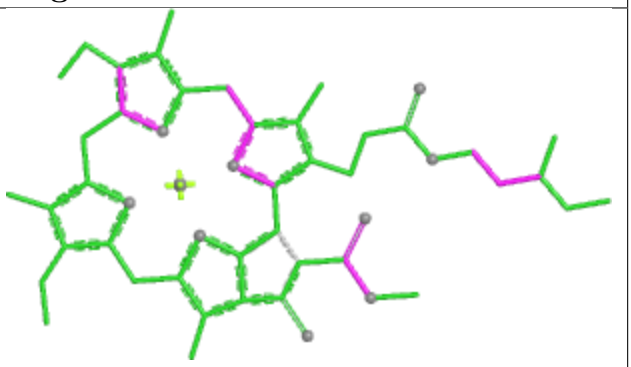
Ligand CLA j 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

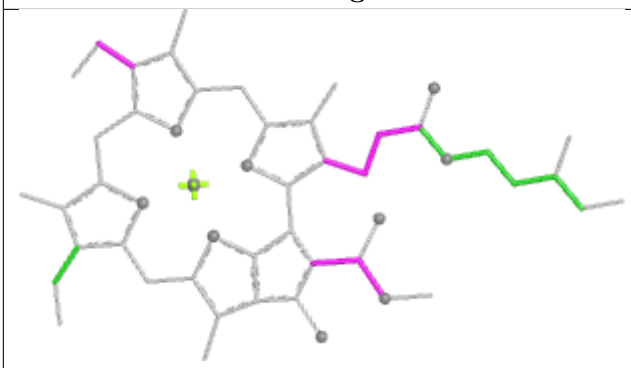
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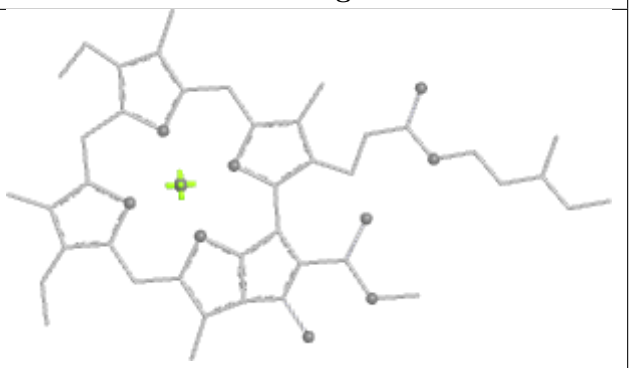
Bond lengths



Bond angles

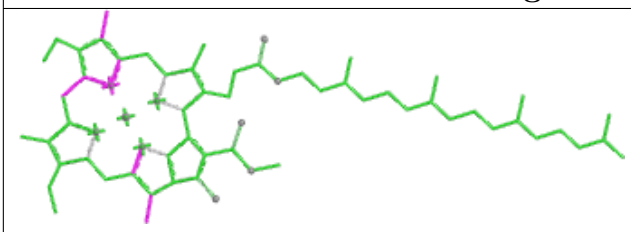


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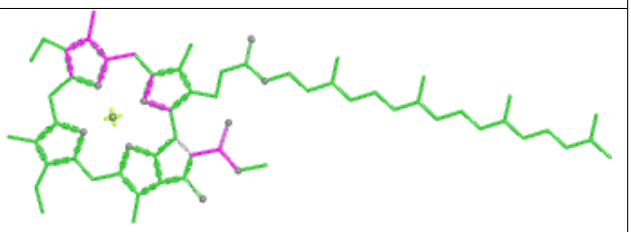


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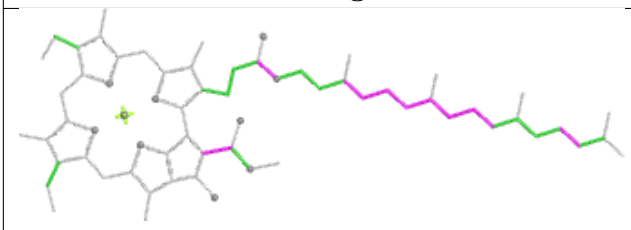
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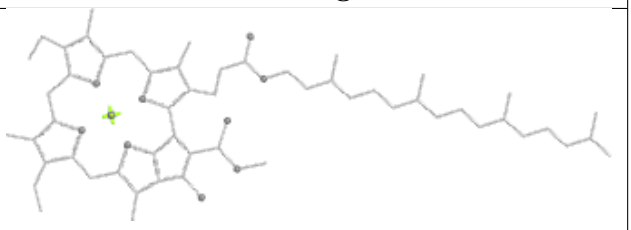
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Bond angles

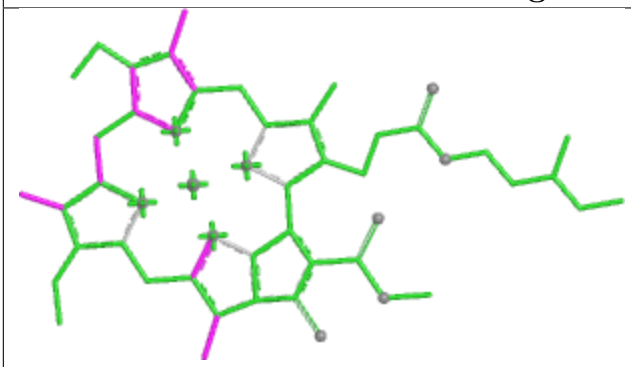


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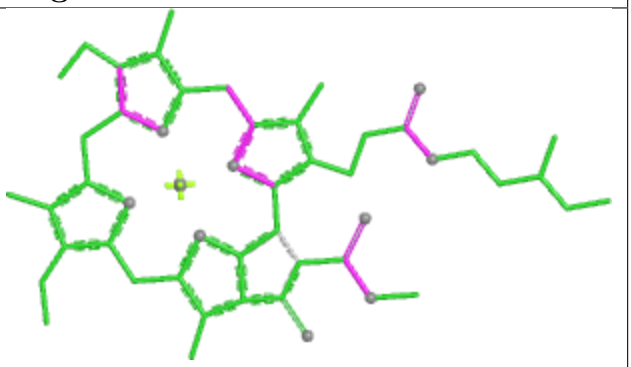


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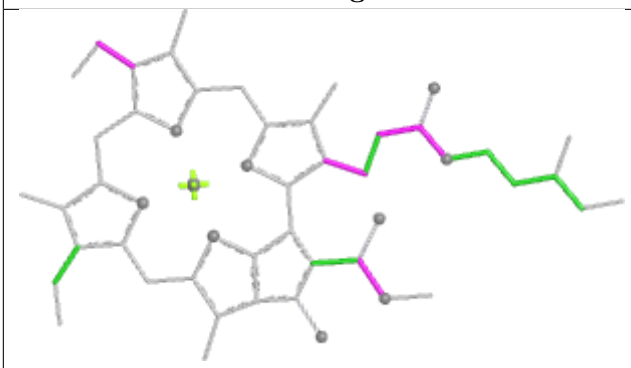
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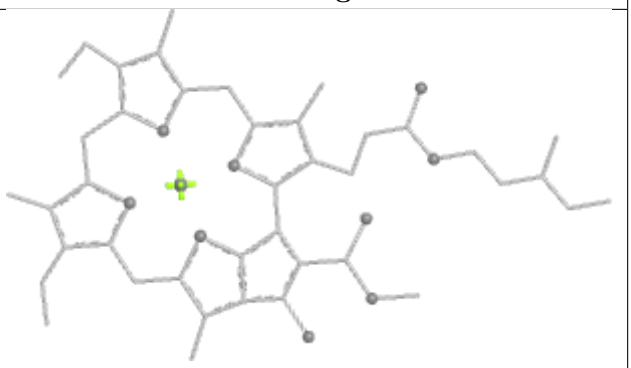
Bond lengths



Bond angles

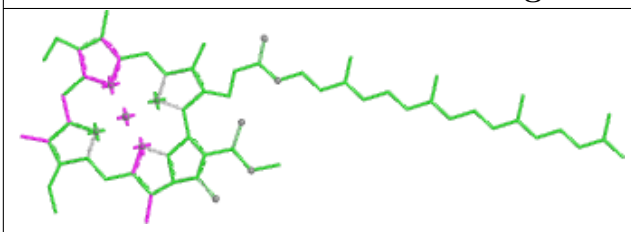


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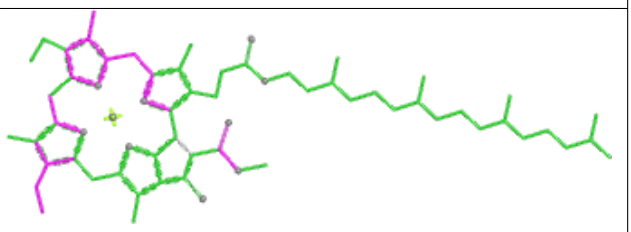


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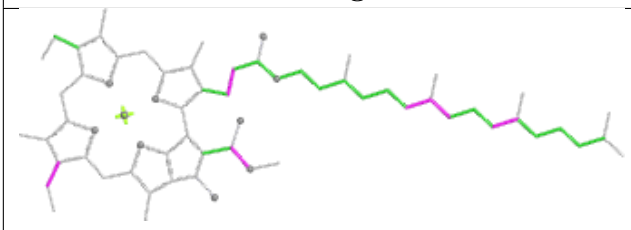
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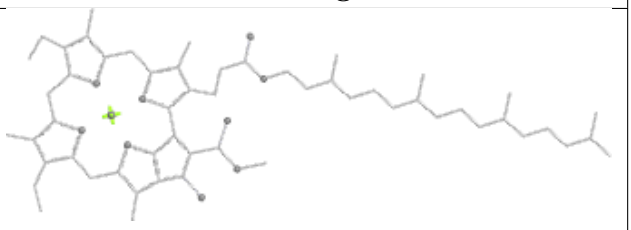
Bond lengths



Bond angles

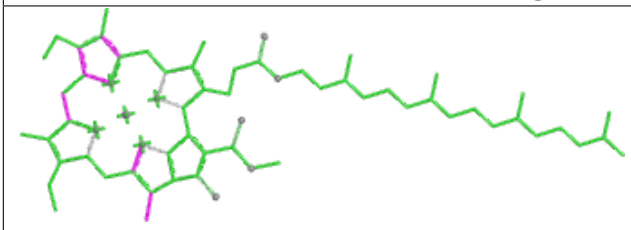


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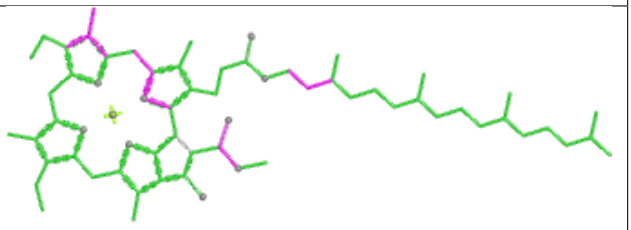


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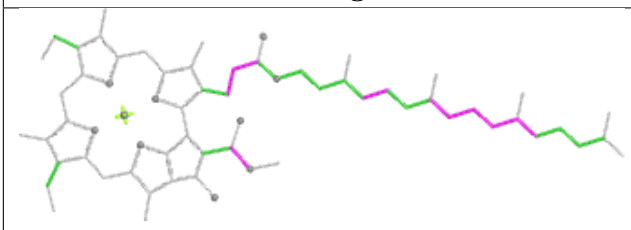
Ligand CLA c 612



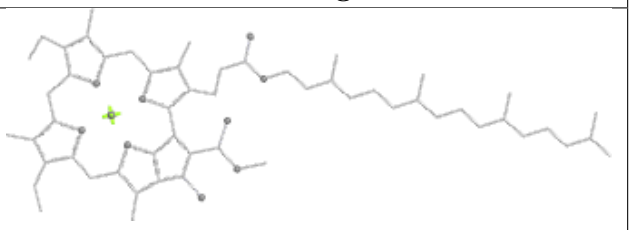
Bond lengths



Bond angles

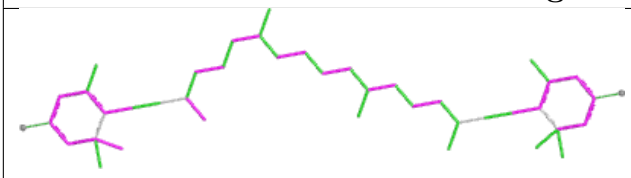


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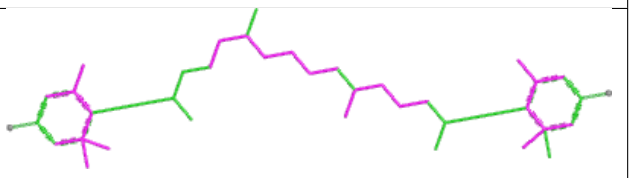


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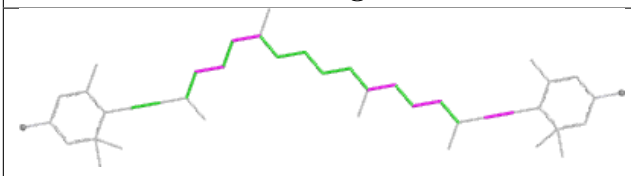
Ligand II0 i 317



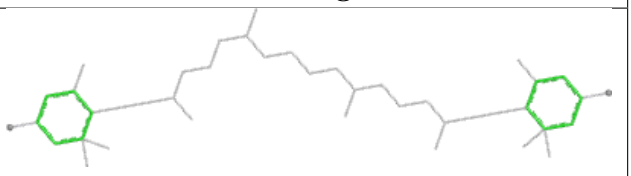
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Bond angles

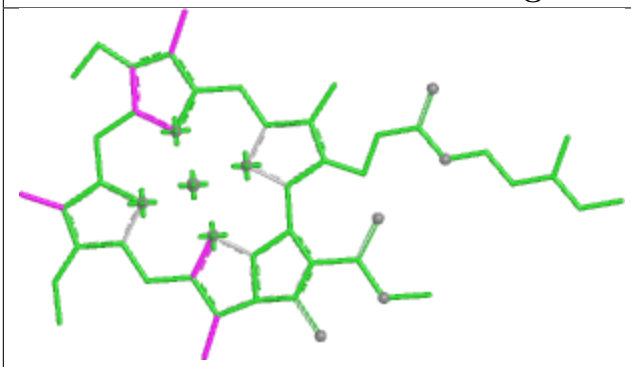


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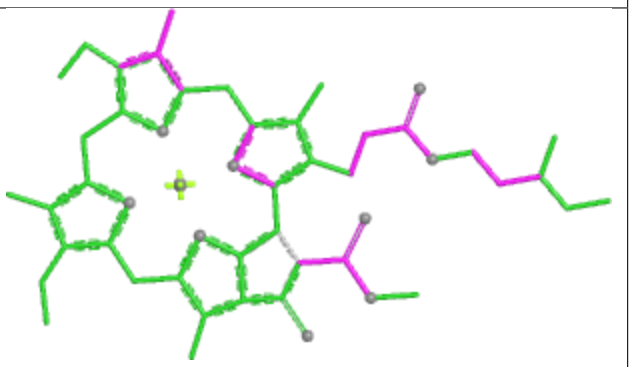


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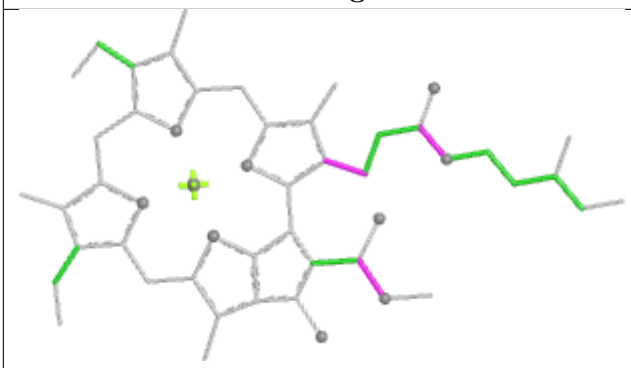
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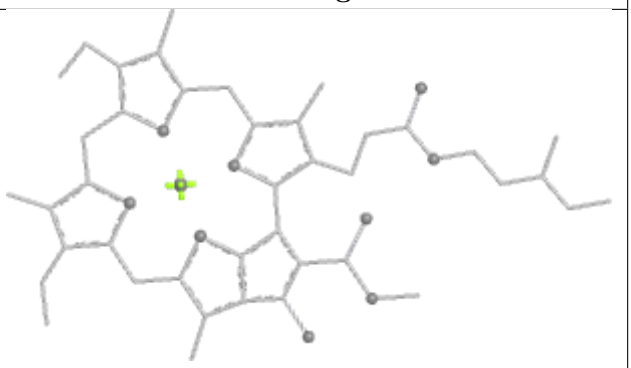
Bond lengths



Bond angles

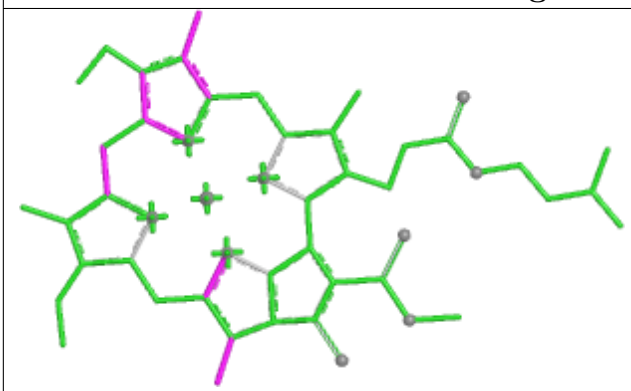


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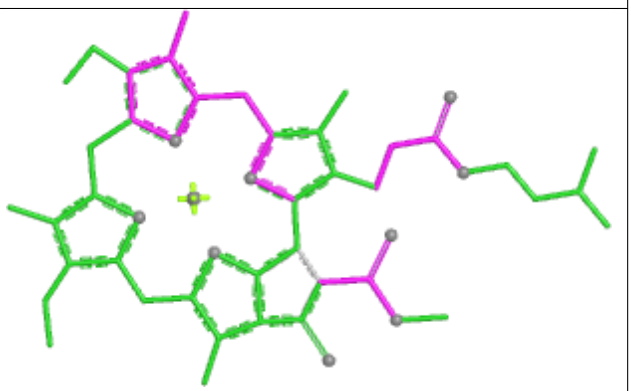


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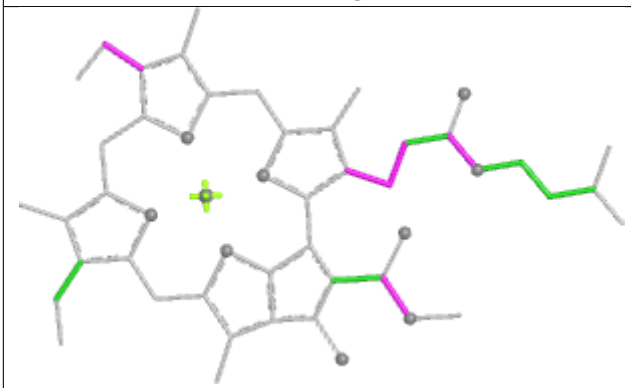
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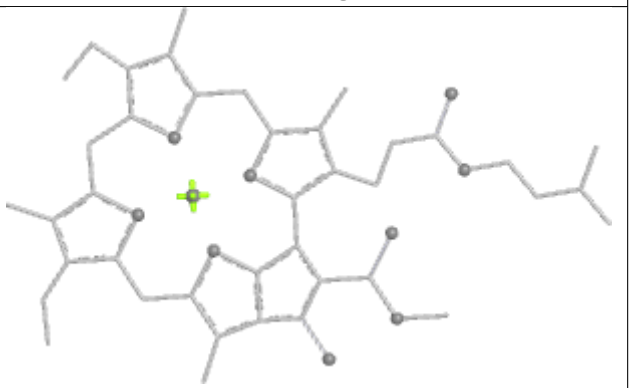
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Bond angles

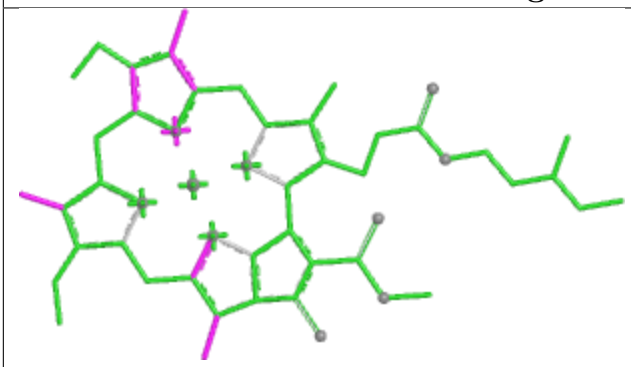


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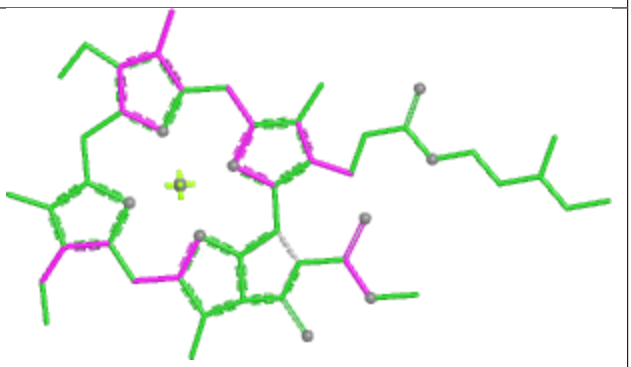


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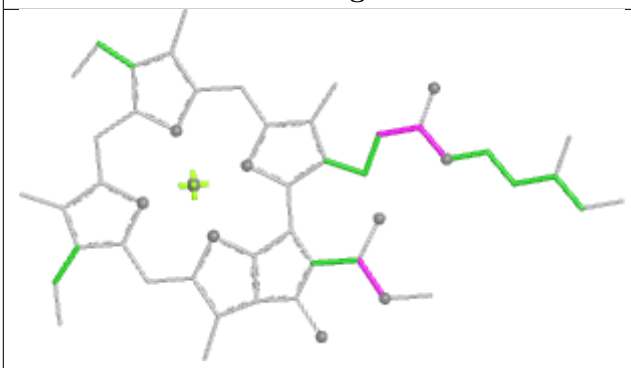
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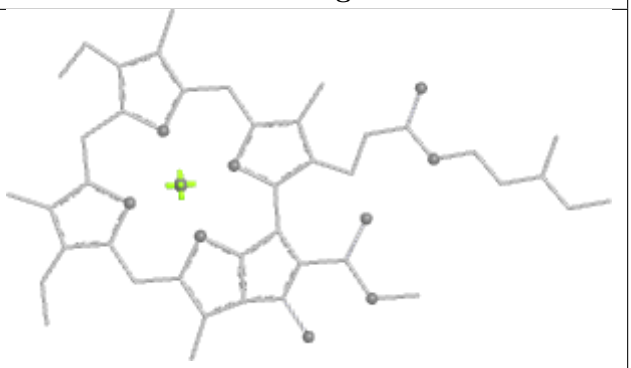
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Bond angles

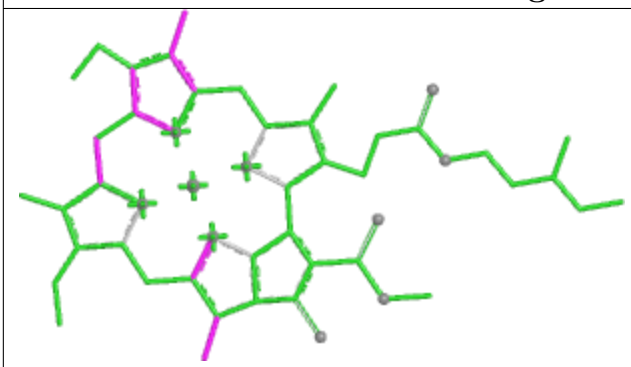


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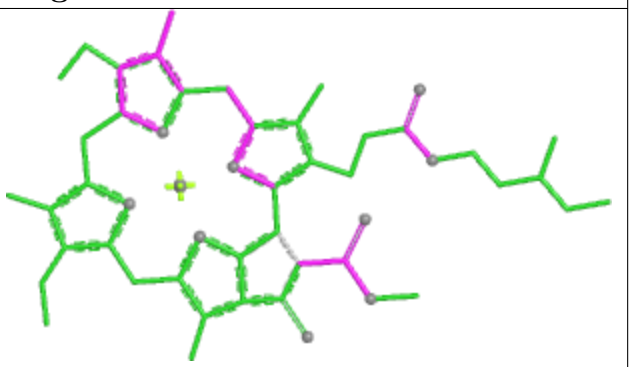


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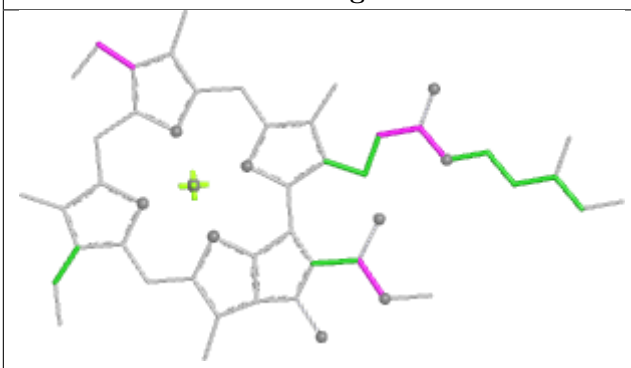
Ligand CLA g 307



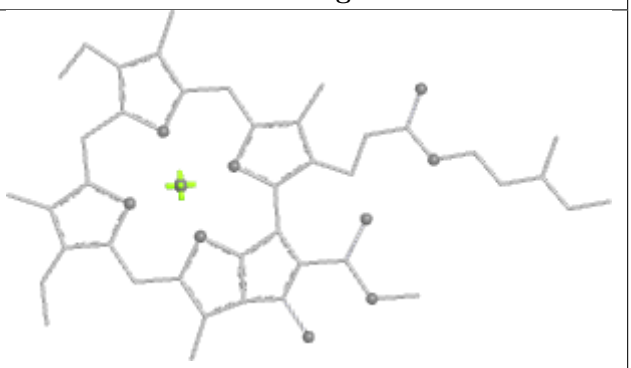
Bond lengths



Bond angles

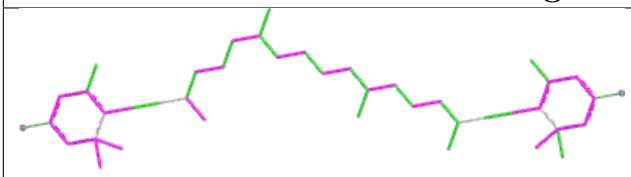


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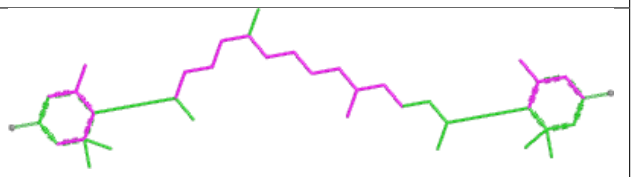


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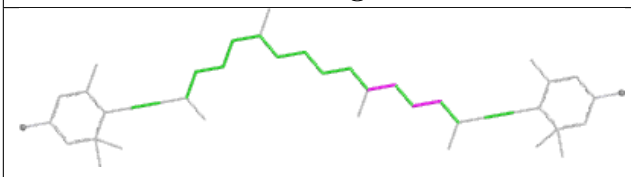
Ligand II0 c 613



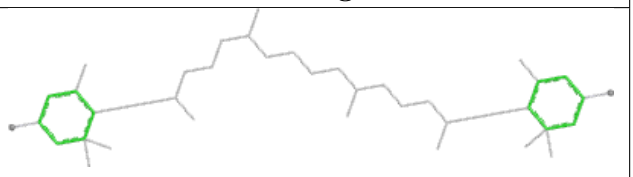
Bond lengths



Bond angles

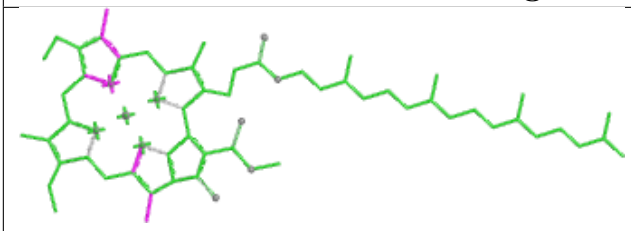


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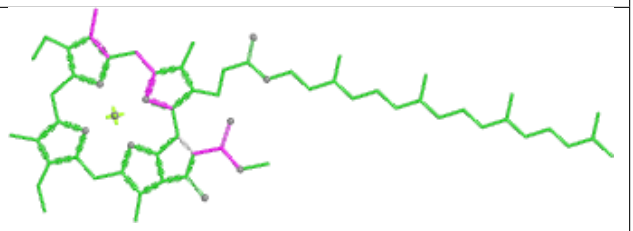


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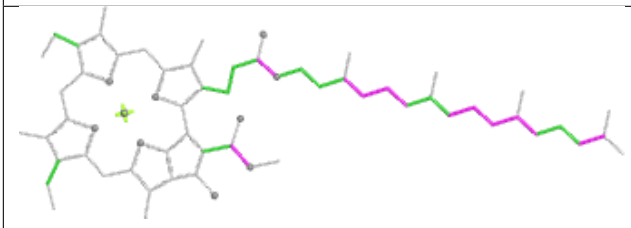
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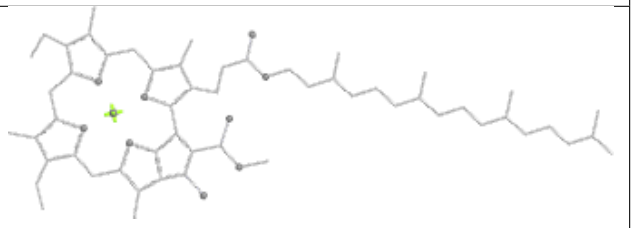
Bond lengths



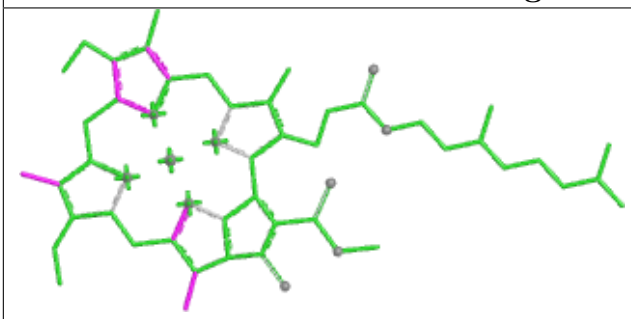
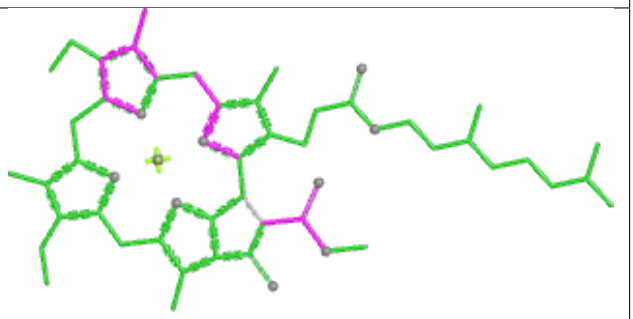
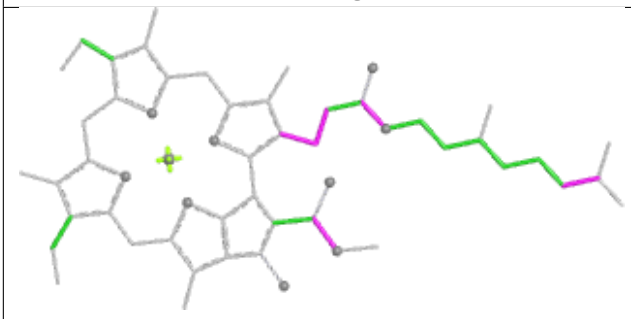
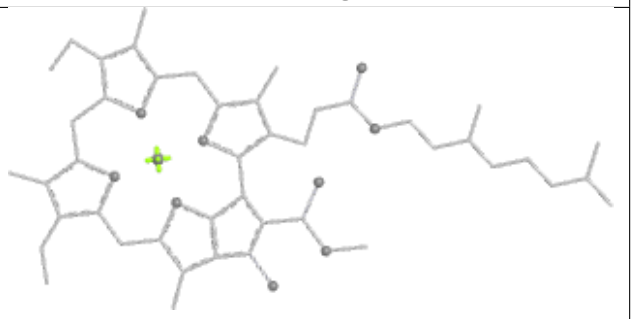
Bond angles

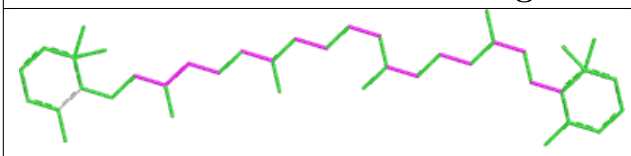
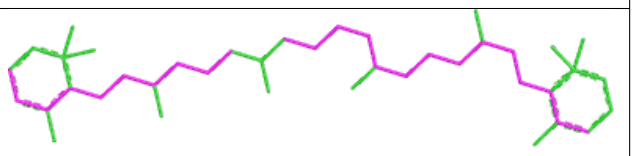
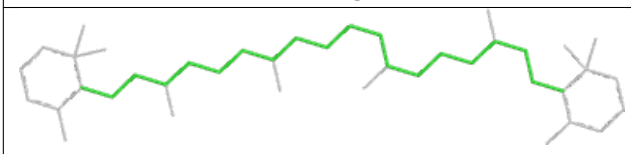
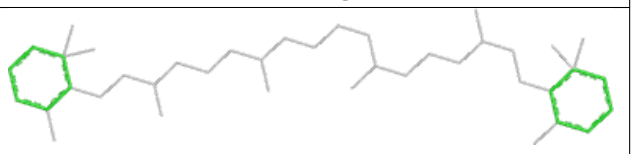


Torsions

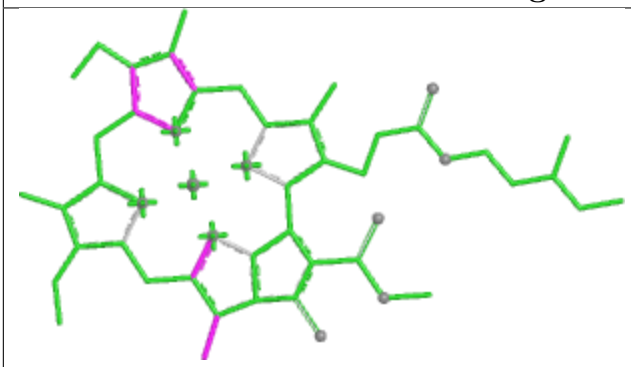


Rings

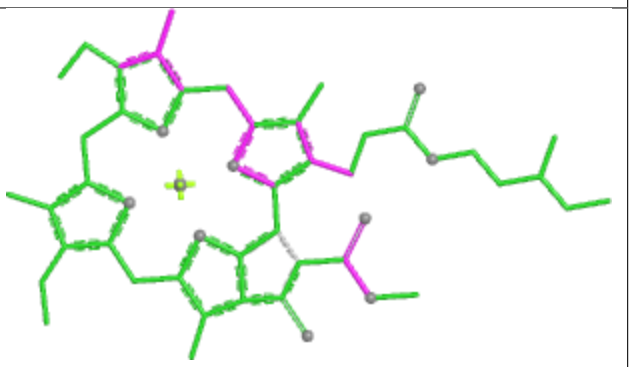
Ligand CLA B 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WVN B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

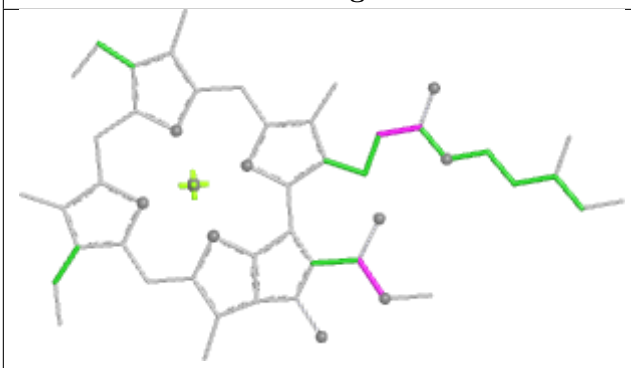
Ligand CLA e 603



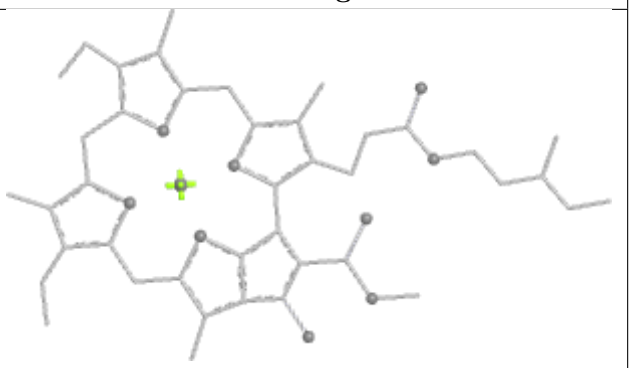
Bond lengths



Bond angles

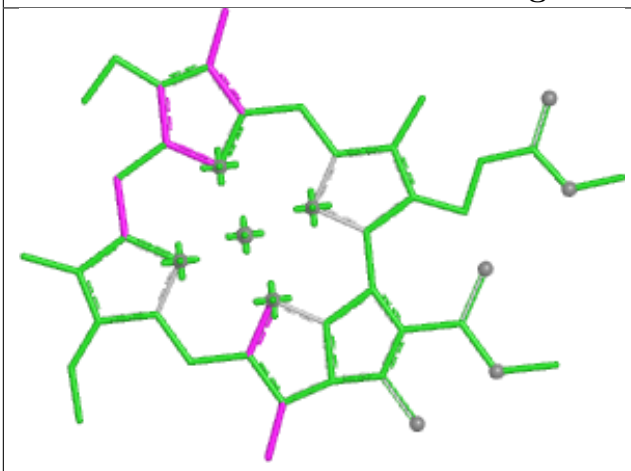


Torsions

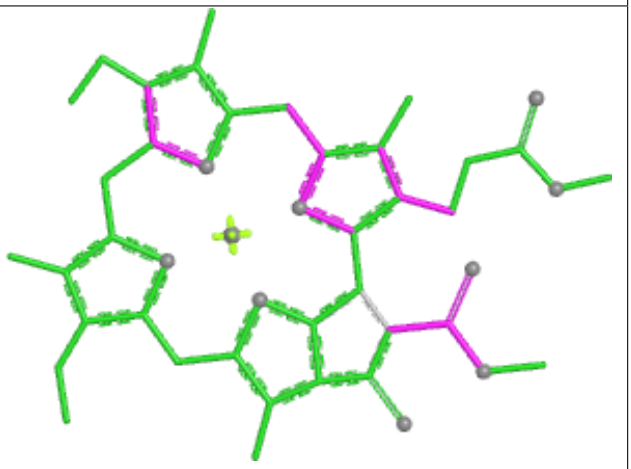


Rings

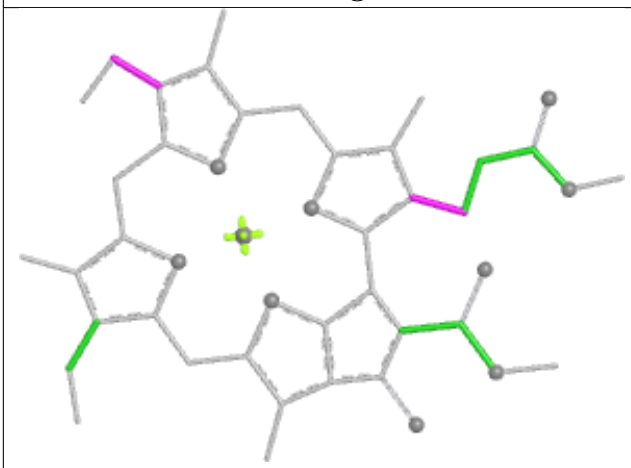
Ligand CLA e 608



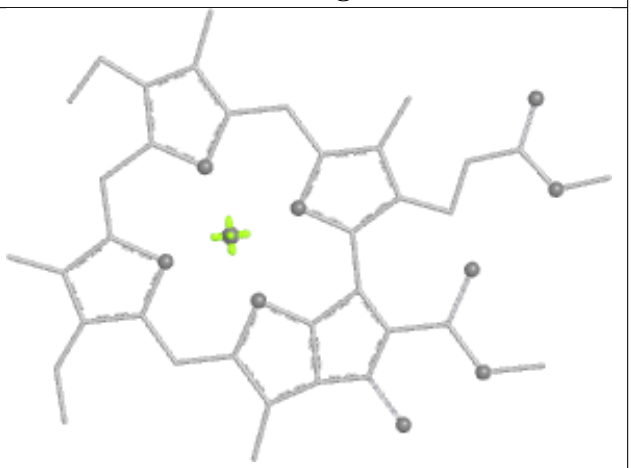
Bond lengths



Bond angles

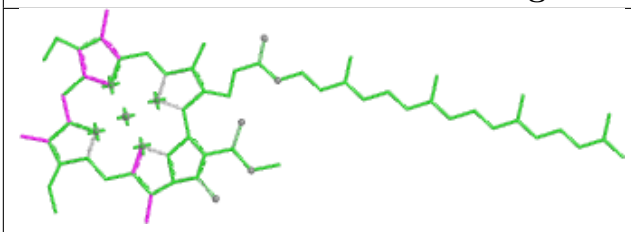


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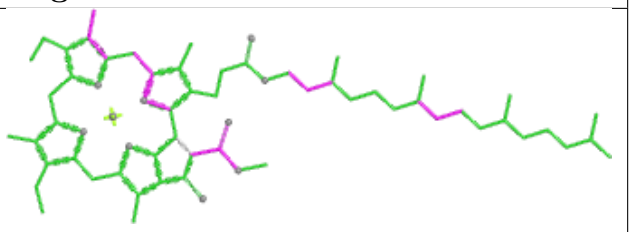


Rings

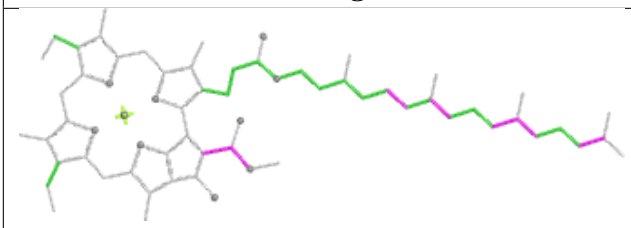
Ligand CLA g 309



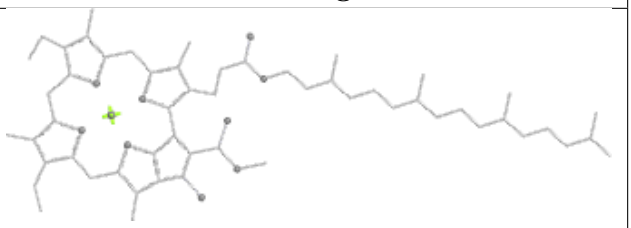
Bond lengths



Bond angles

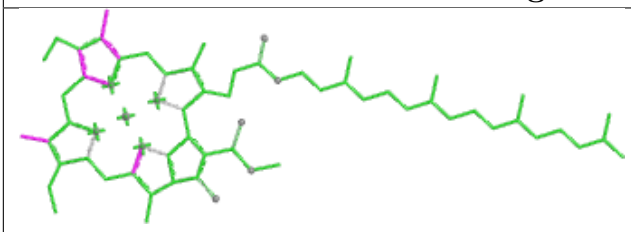


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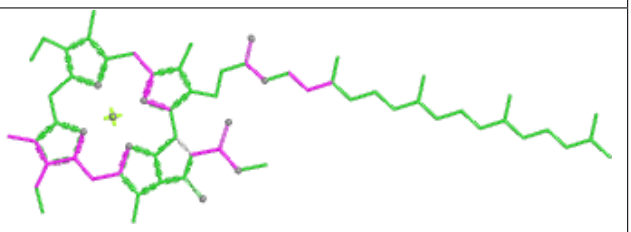


Rings

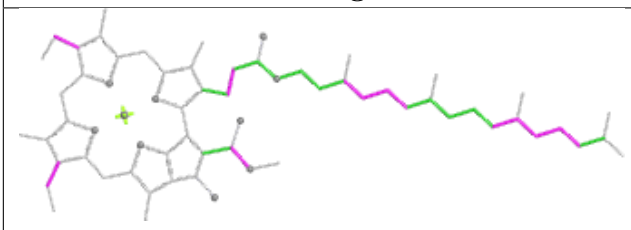
Ligand CLA b 607



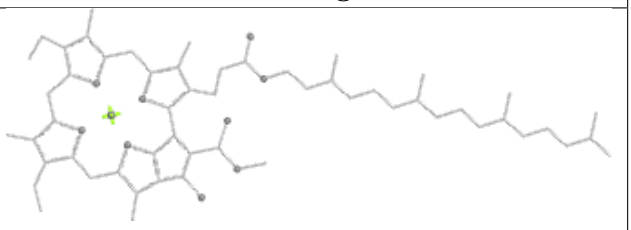
Bond lengths



Bond angles

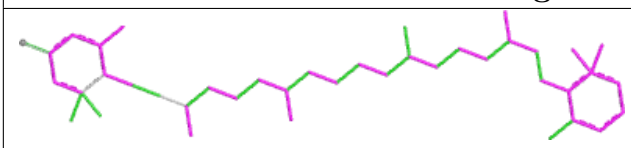


Torsions



Rings

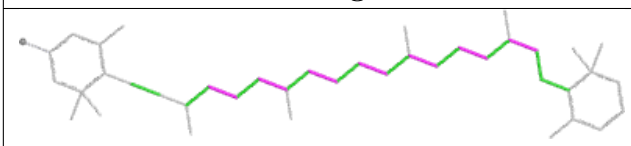
Ligand IHT c 616



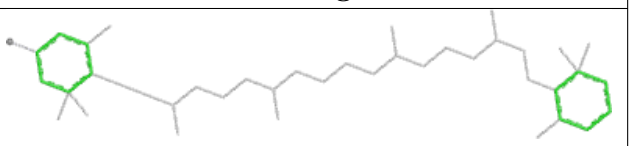
Bond lengths



Bond angles

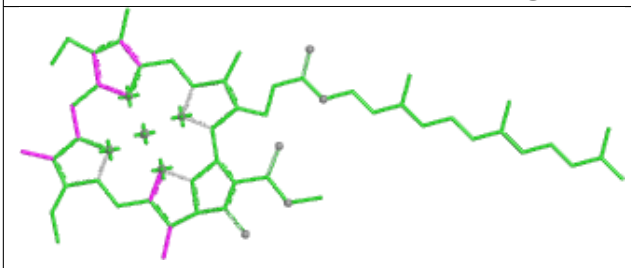


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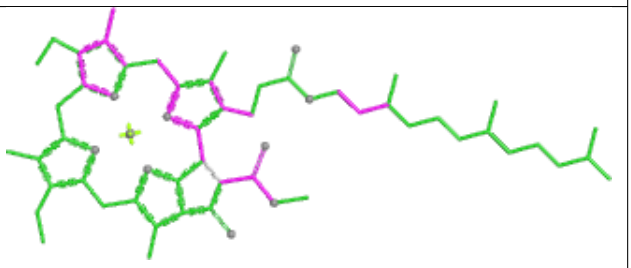


Rings

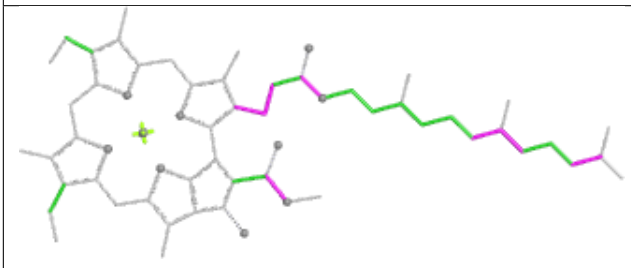
Ligand CLA B 812



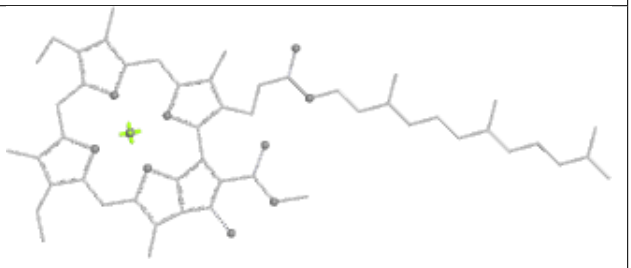
Bond lengths



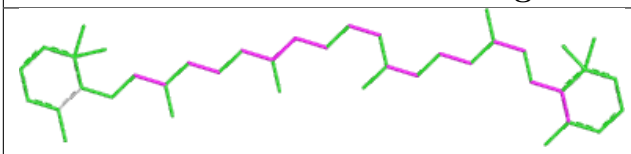
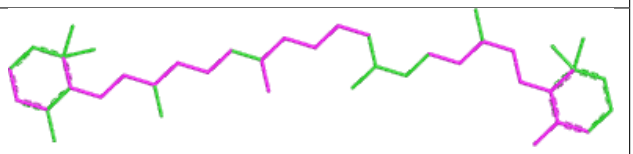
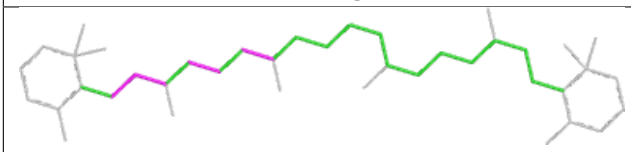
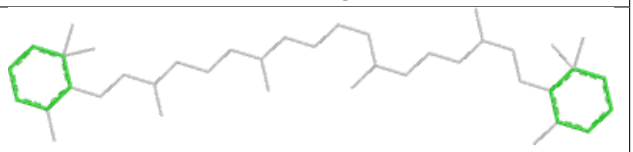
Bond angles

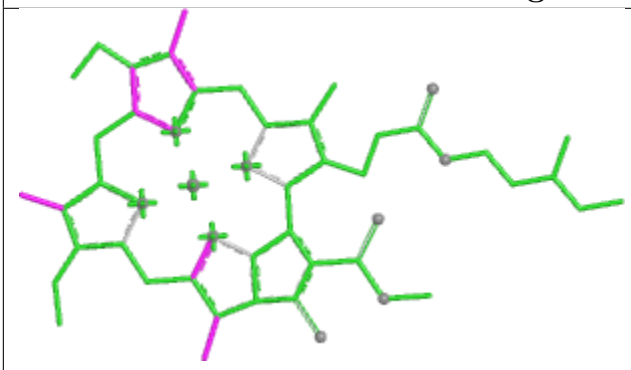
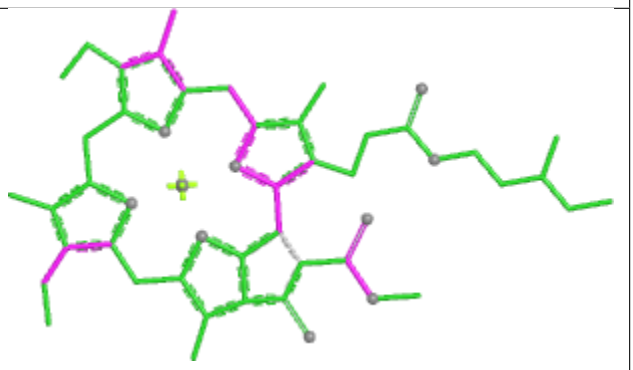
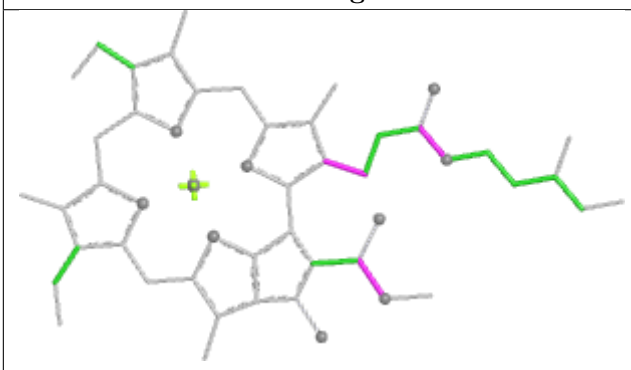
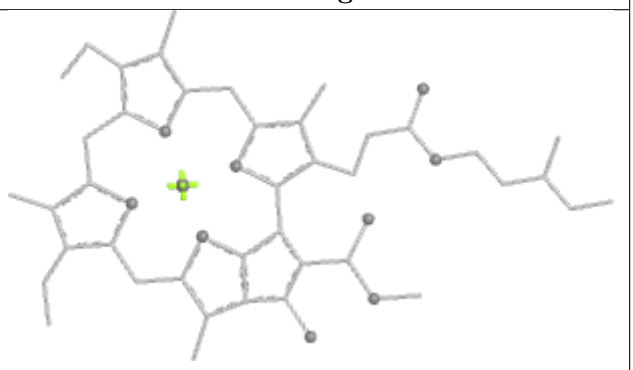


Torsions

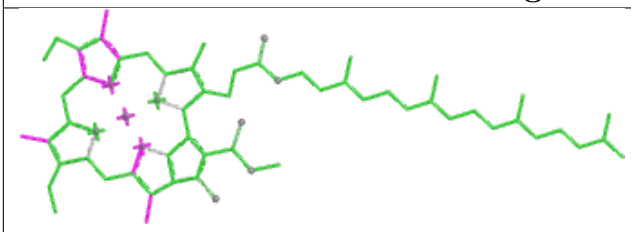


Rings

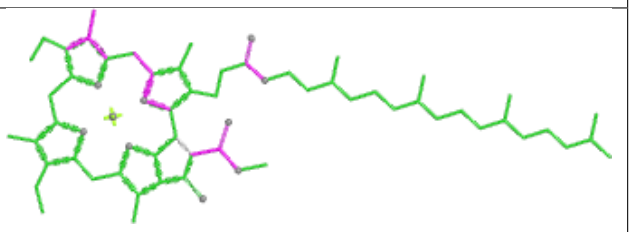
Ligand WVN K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

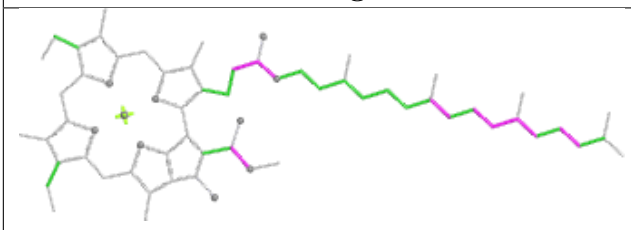
Ligand CLA B 805



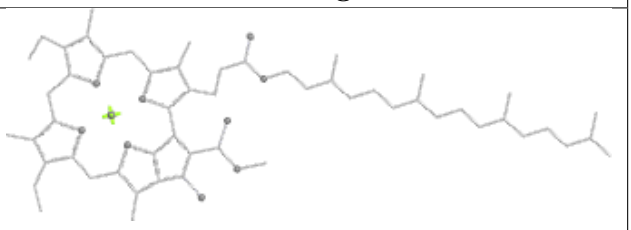
Bond lengths



Bond angles

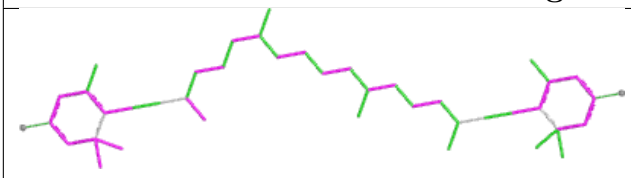


Torsions

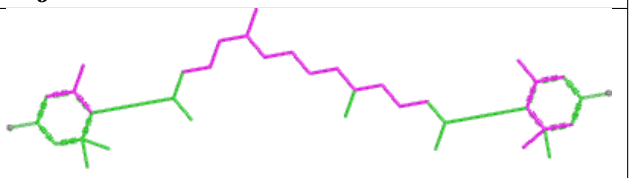


Rings

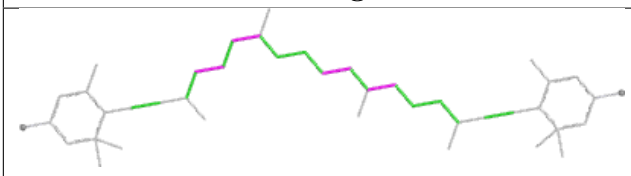
Ligand II0 j 614



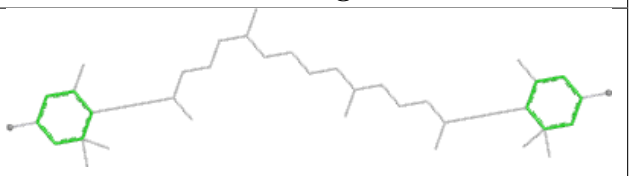
Bond lengths



Bond angles

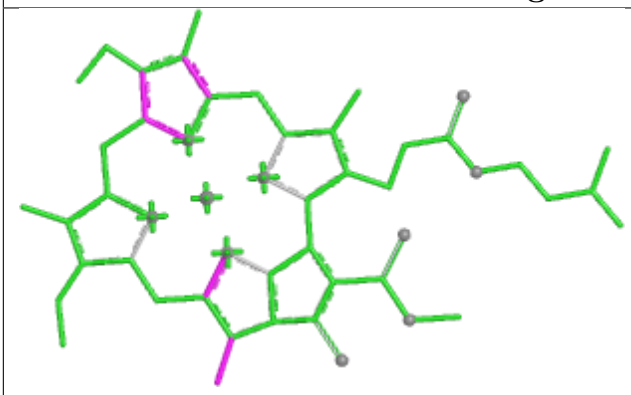


Torsions

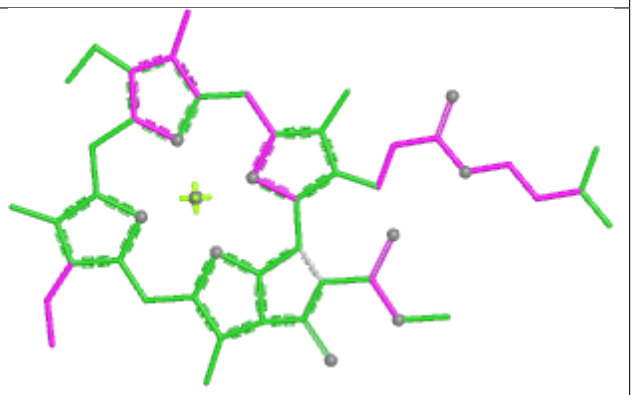


Rings

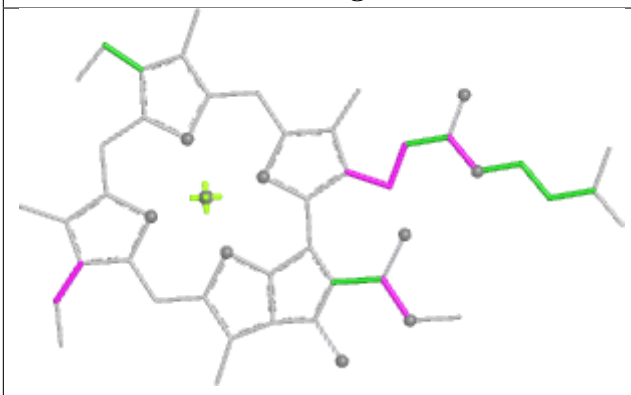
Ligand CLA k 602



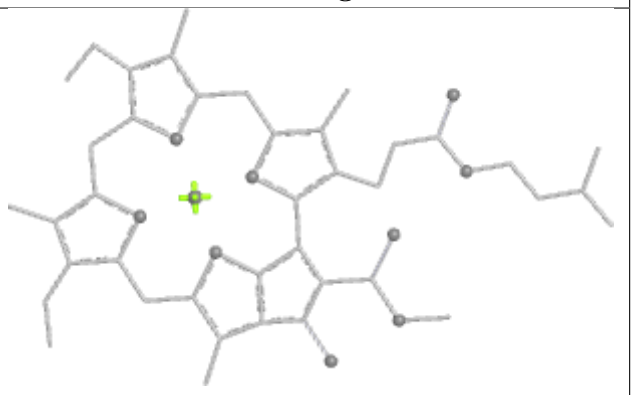
Bond lengths



Bond angles

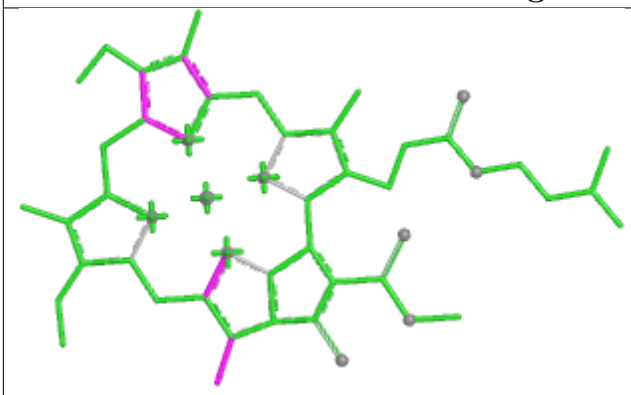


Torsions

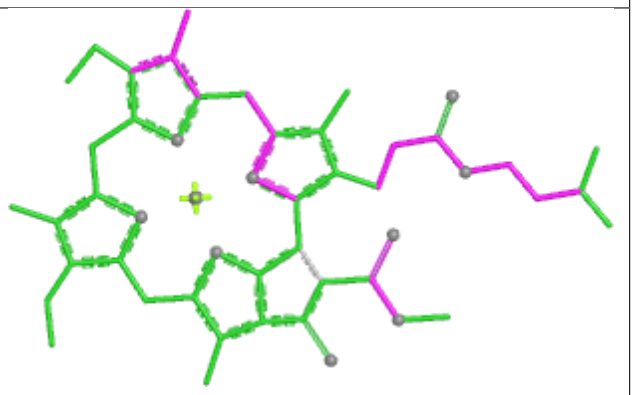


Rings

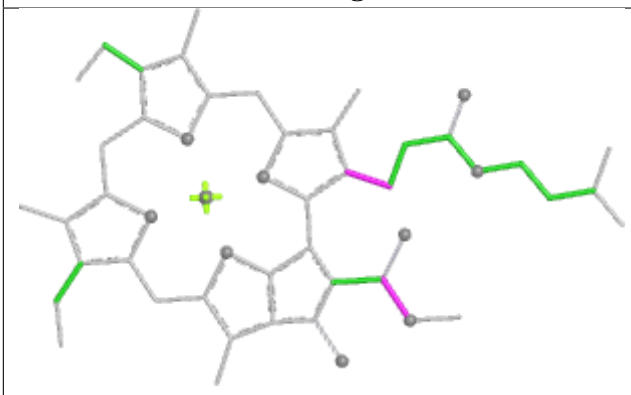
Ligand CLA d 301



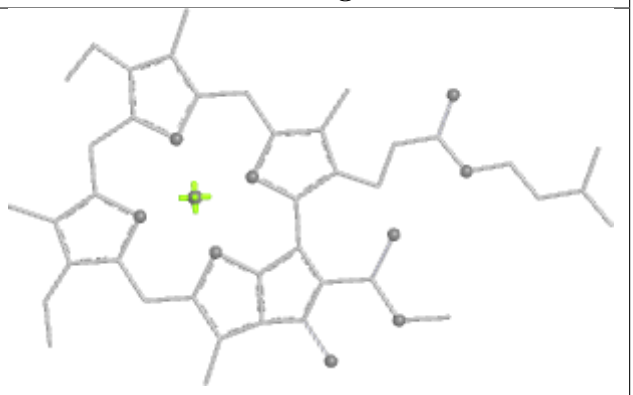
Bond lengths



Bond angles

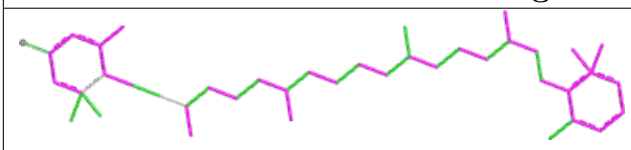


Torsions

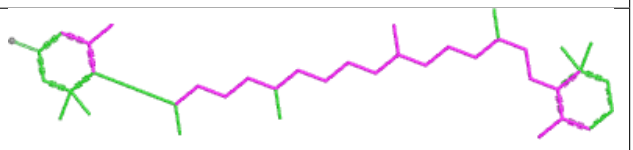


Rings

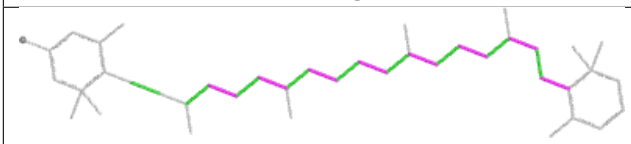
Ligand IHT k 618



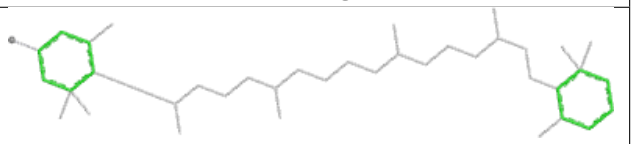
Bond lengths



Bond angles

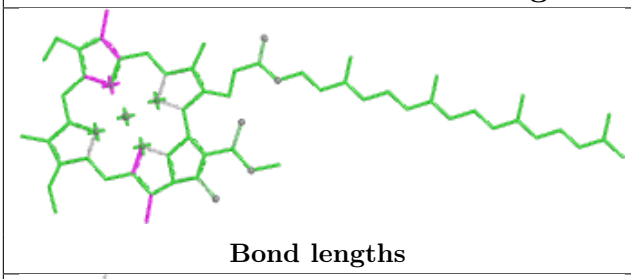


Torsions

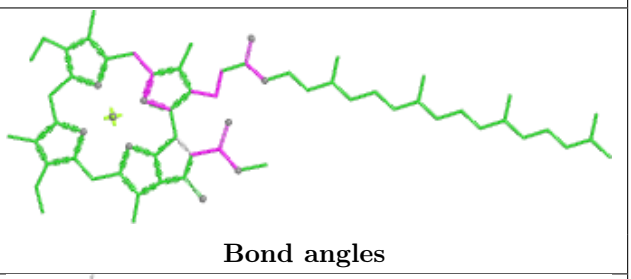


Rings

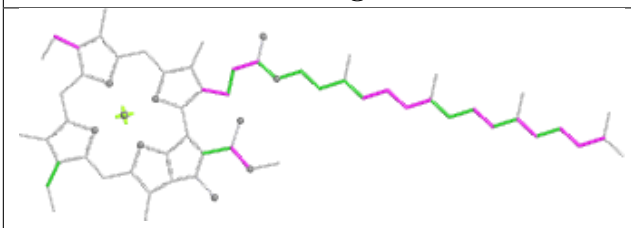
Ligand CLA s 203



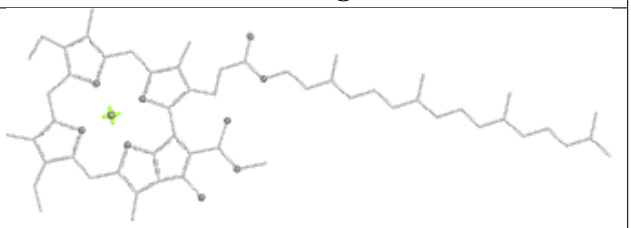
Bond lengths



Bond angles



Torsions

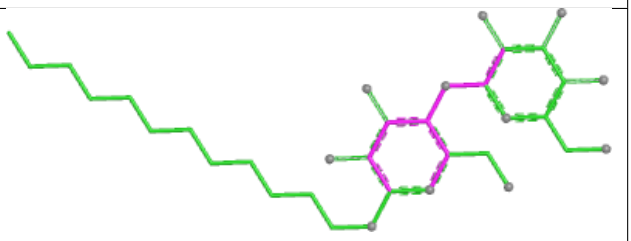


Rings

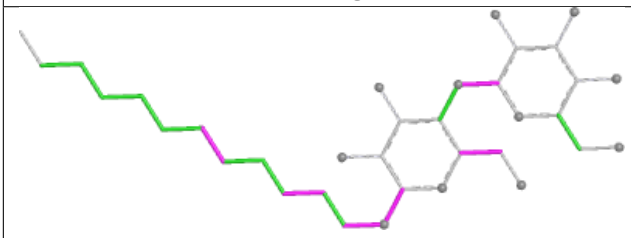
Ligand LMU i 301



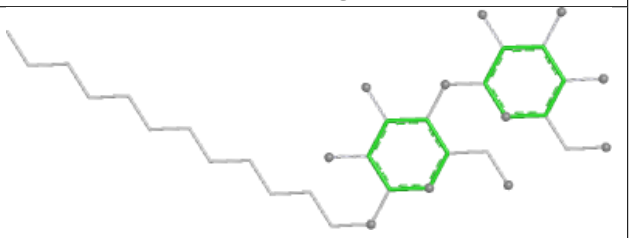
Bond lengths



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.

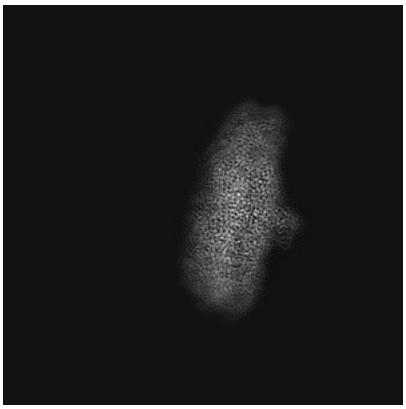
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37642. These allow visual inspection of the internal detail of the map and identification of artifacts.

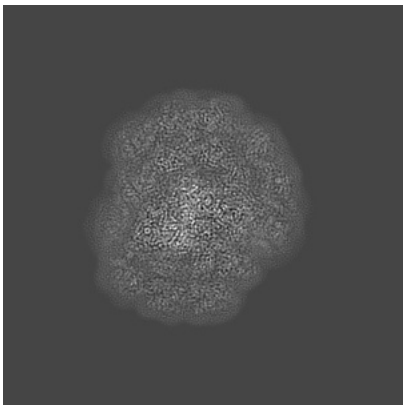
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

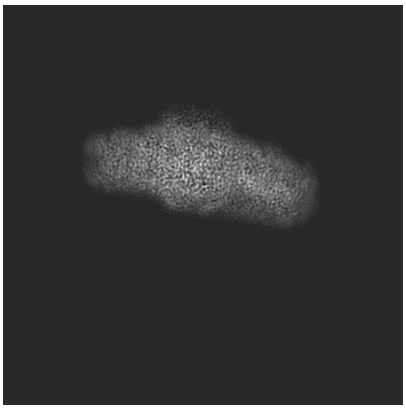
6.1.1 Primary map



X

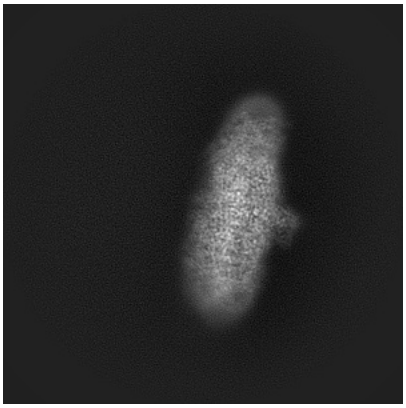


Y

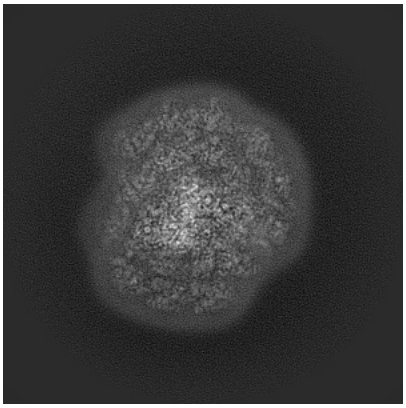


Z

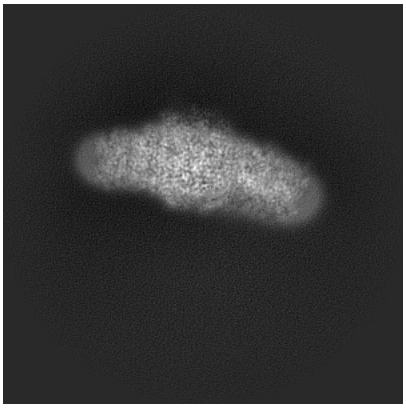
6.1.2 Raw map



X



Y

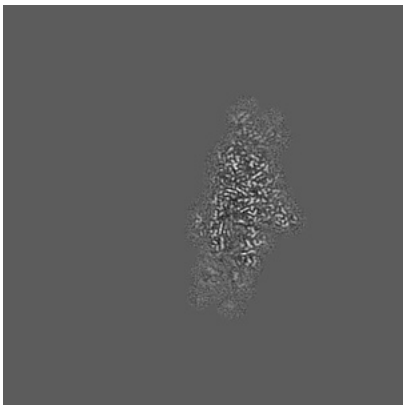


Z

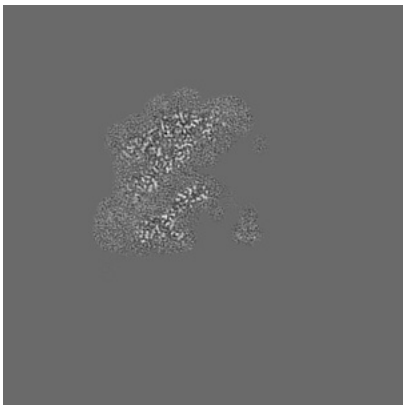
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 180

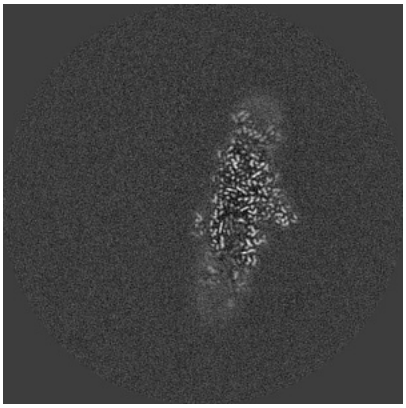


Y Index: 180

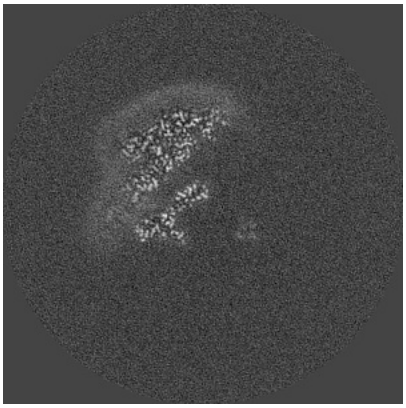


Z Index: 180

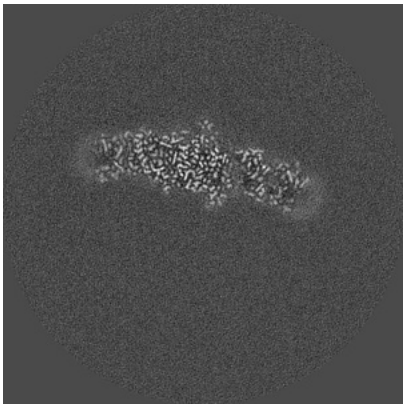
6.2.2 Raw map



X Index: 180



Y Index: 180

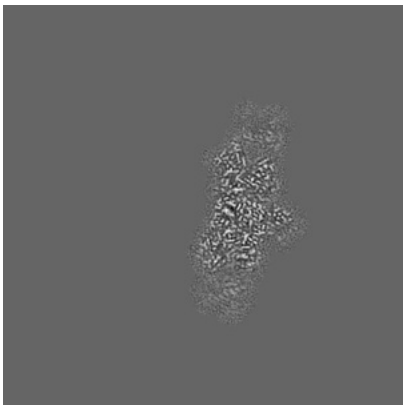


Z Index: 180

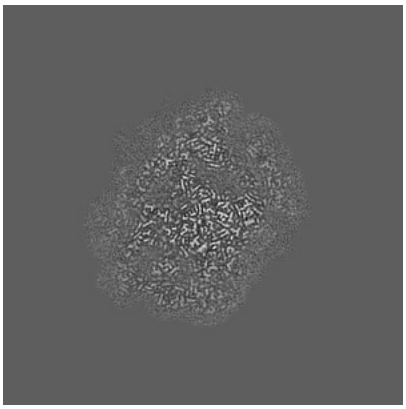
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

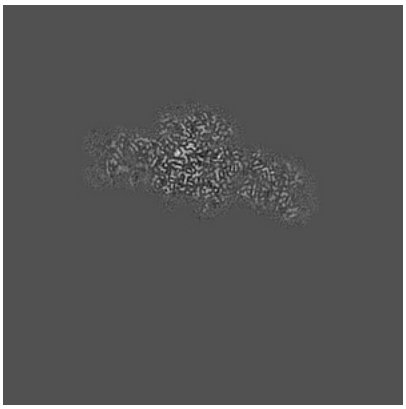
6.3.1 Primary map



X Index: 165

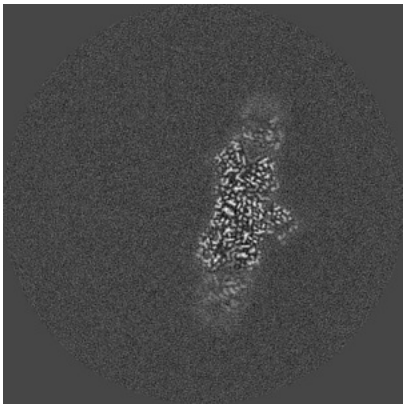


Y Index: 211

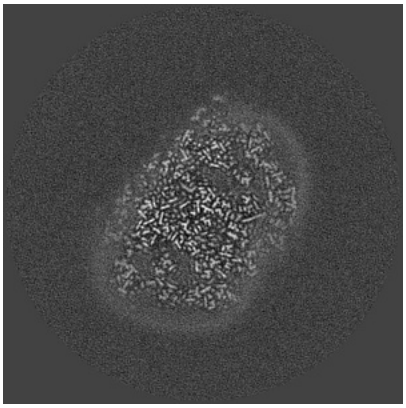


Z Index: 170

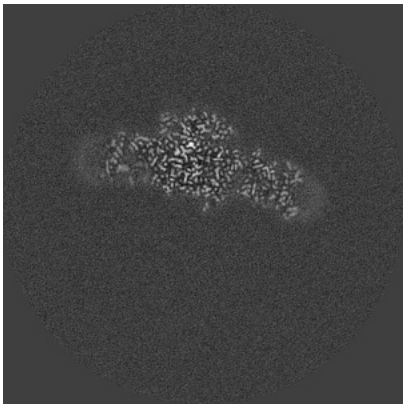
6.3.2 Raw map



X Index: 165



Y Index: 216

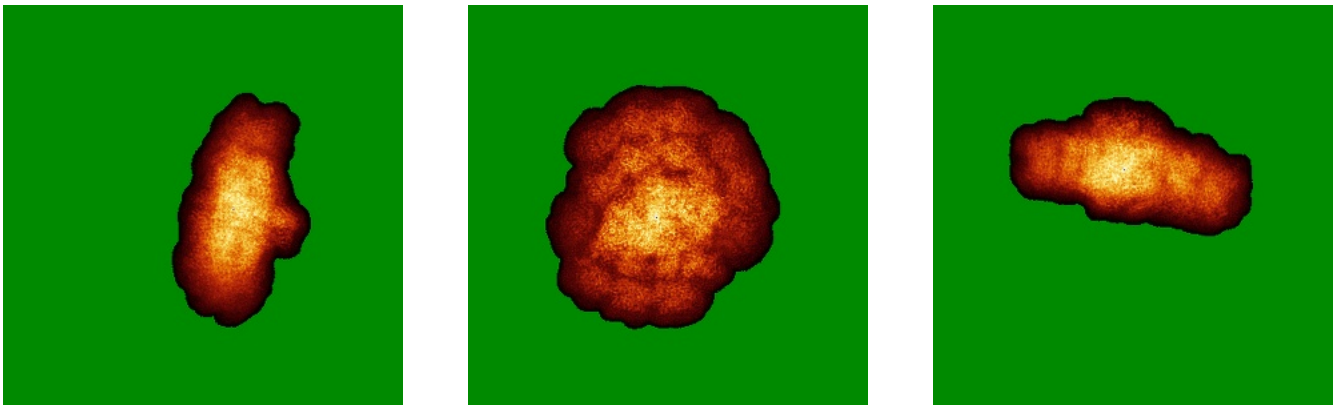


Z Index: 170

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

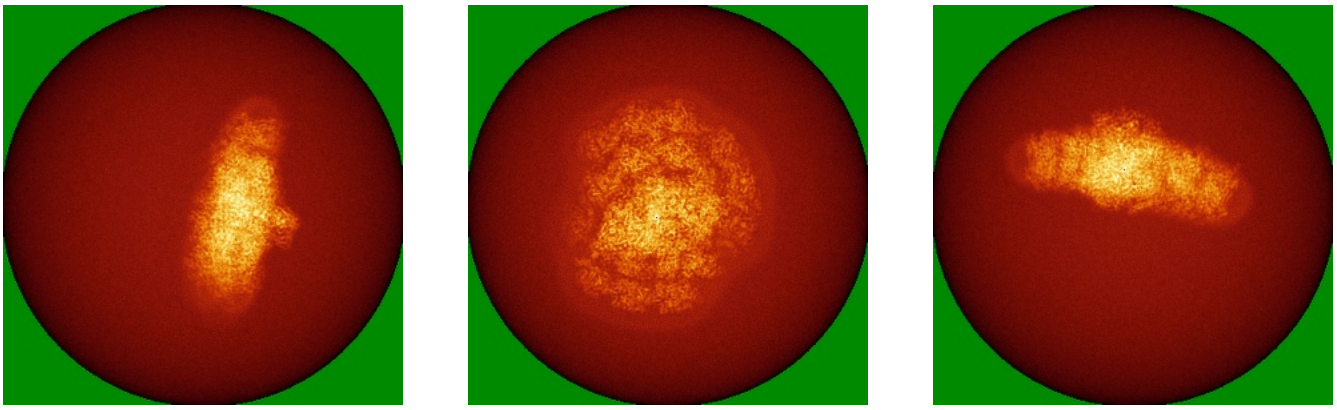
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

6.5 Orthogonal surface views (i)

This section was not generated.

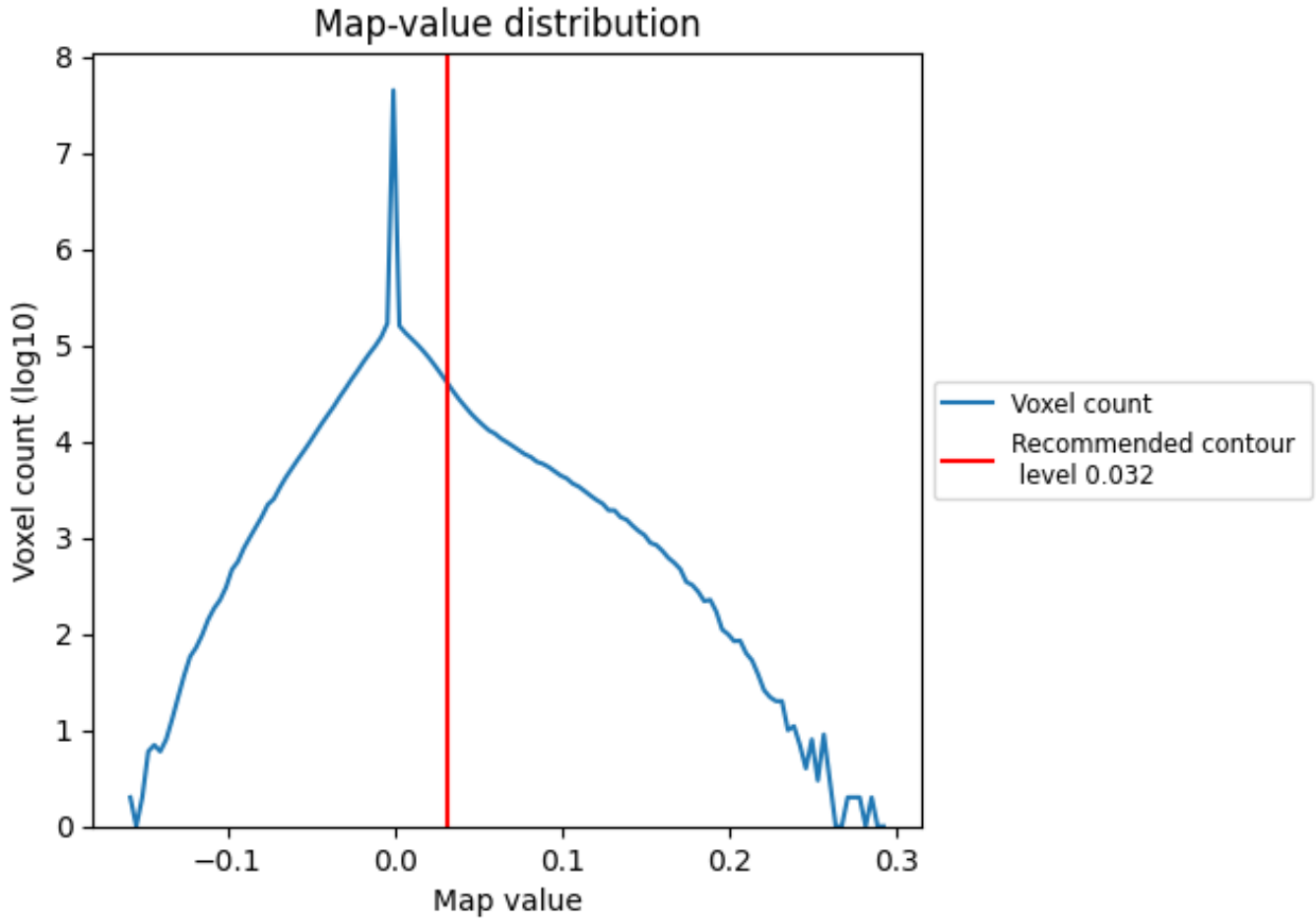
6.6 Mask visualisation (i)

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

7 Map analysis

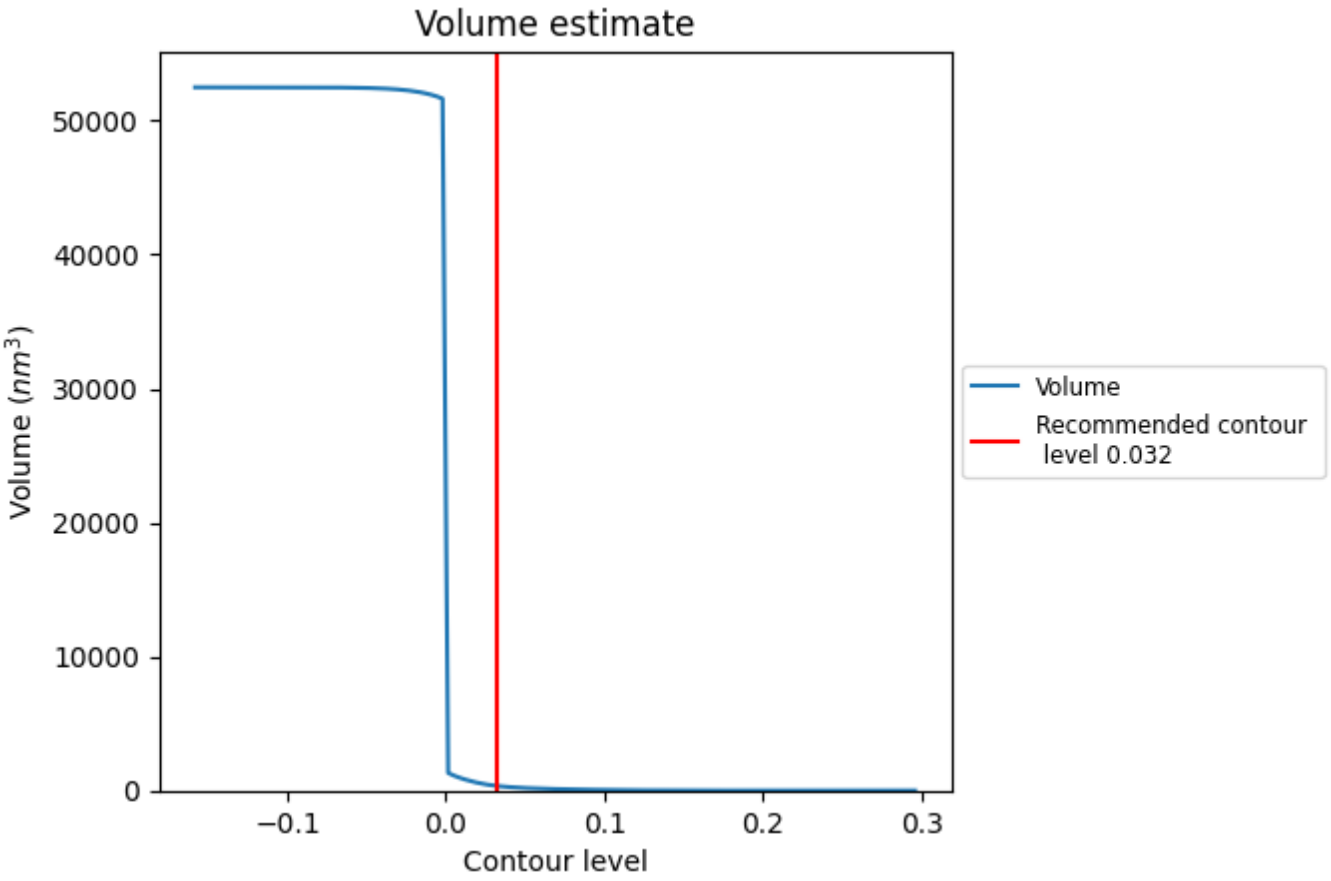
This section contains the results of statistical analysis of the map.

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.

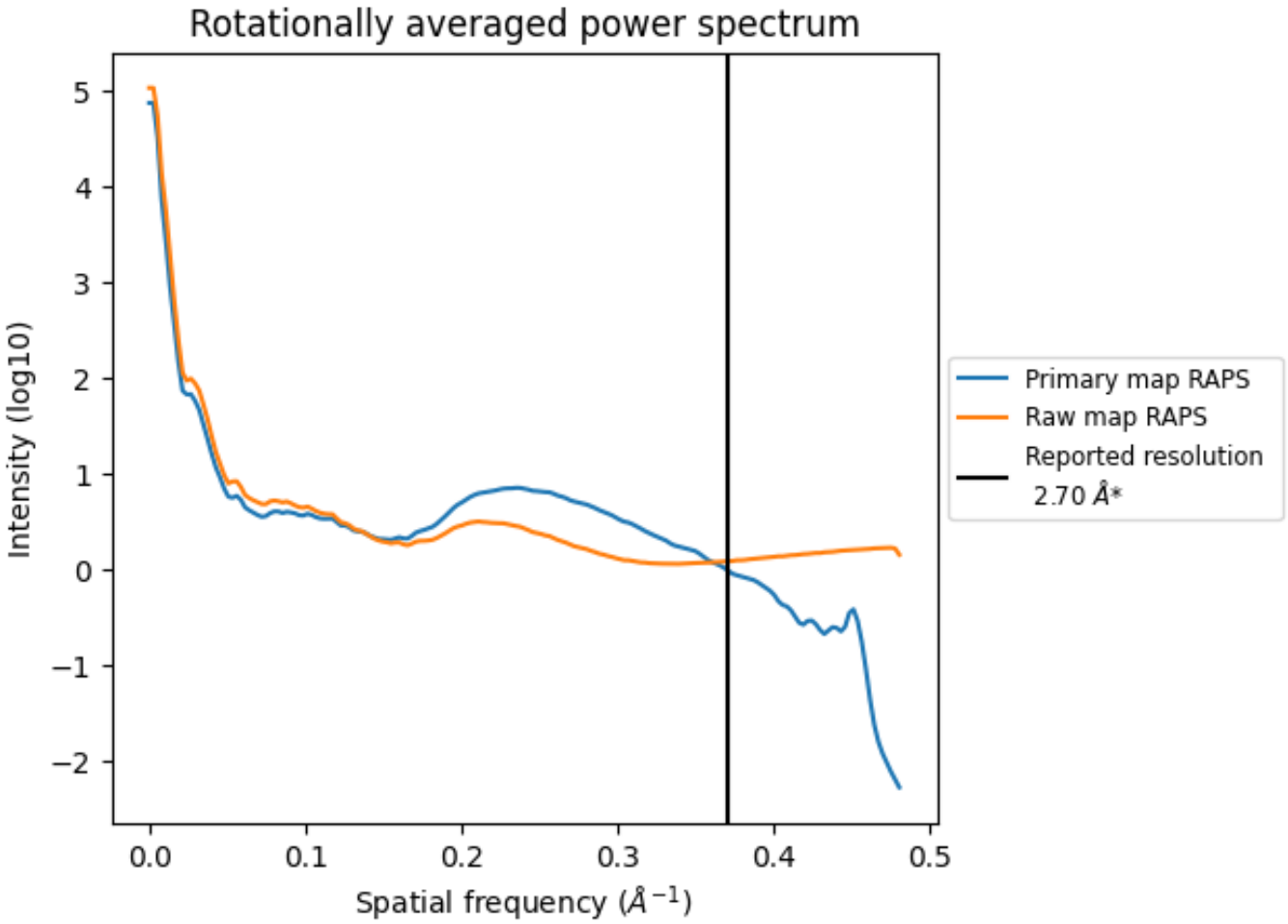
7.2 Volume estimate



The volume at the recommended contour level is 349 nm^3; this corresponds to an approximate mass of 315 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)

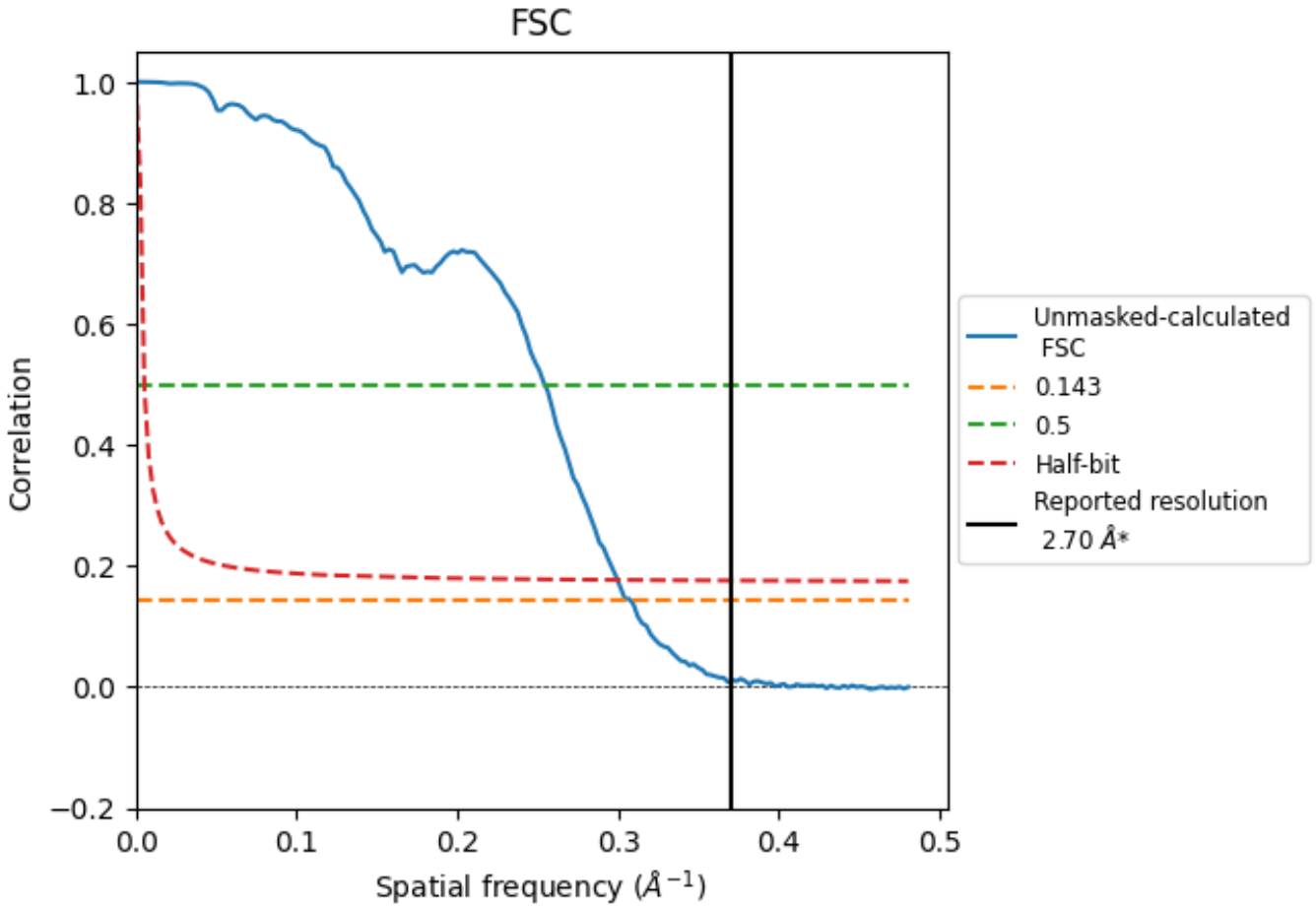


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

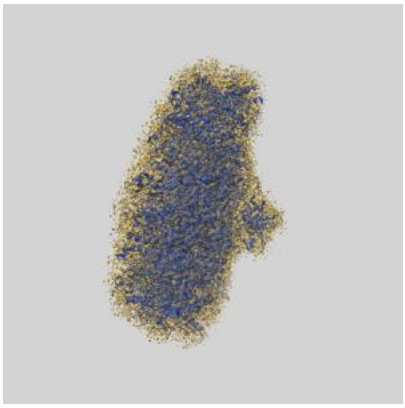
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.25	3.93	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.7 by more than 10 %

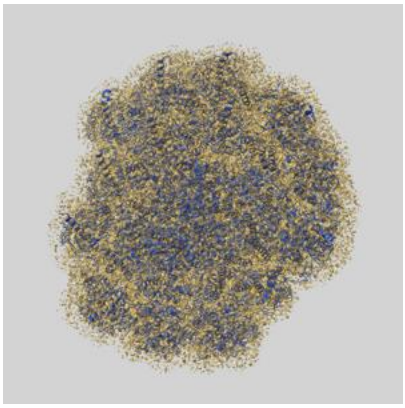
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37642 and PDB model 8WM6. Per-residue inclusion information can be found in section 3 on page 41.

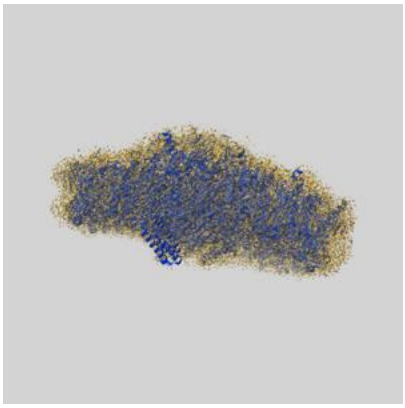
9.1 Map-model overlay



X



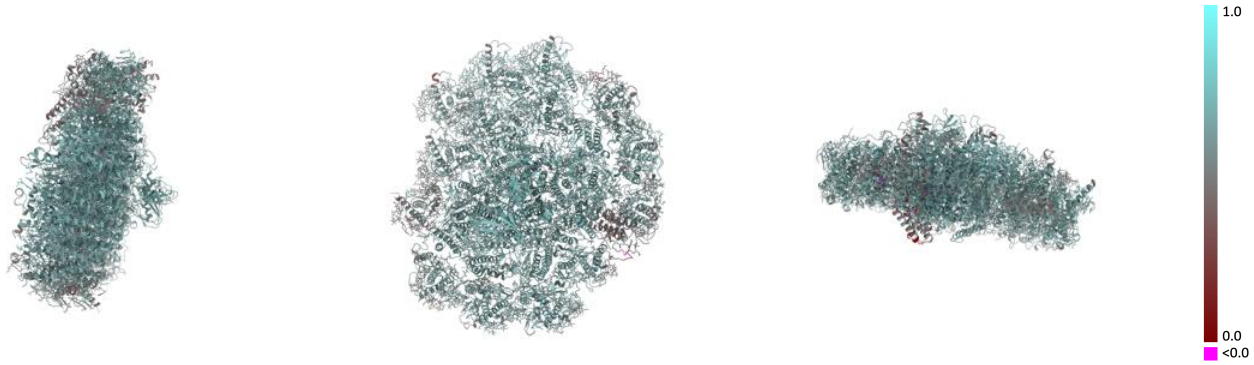
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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)



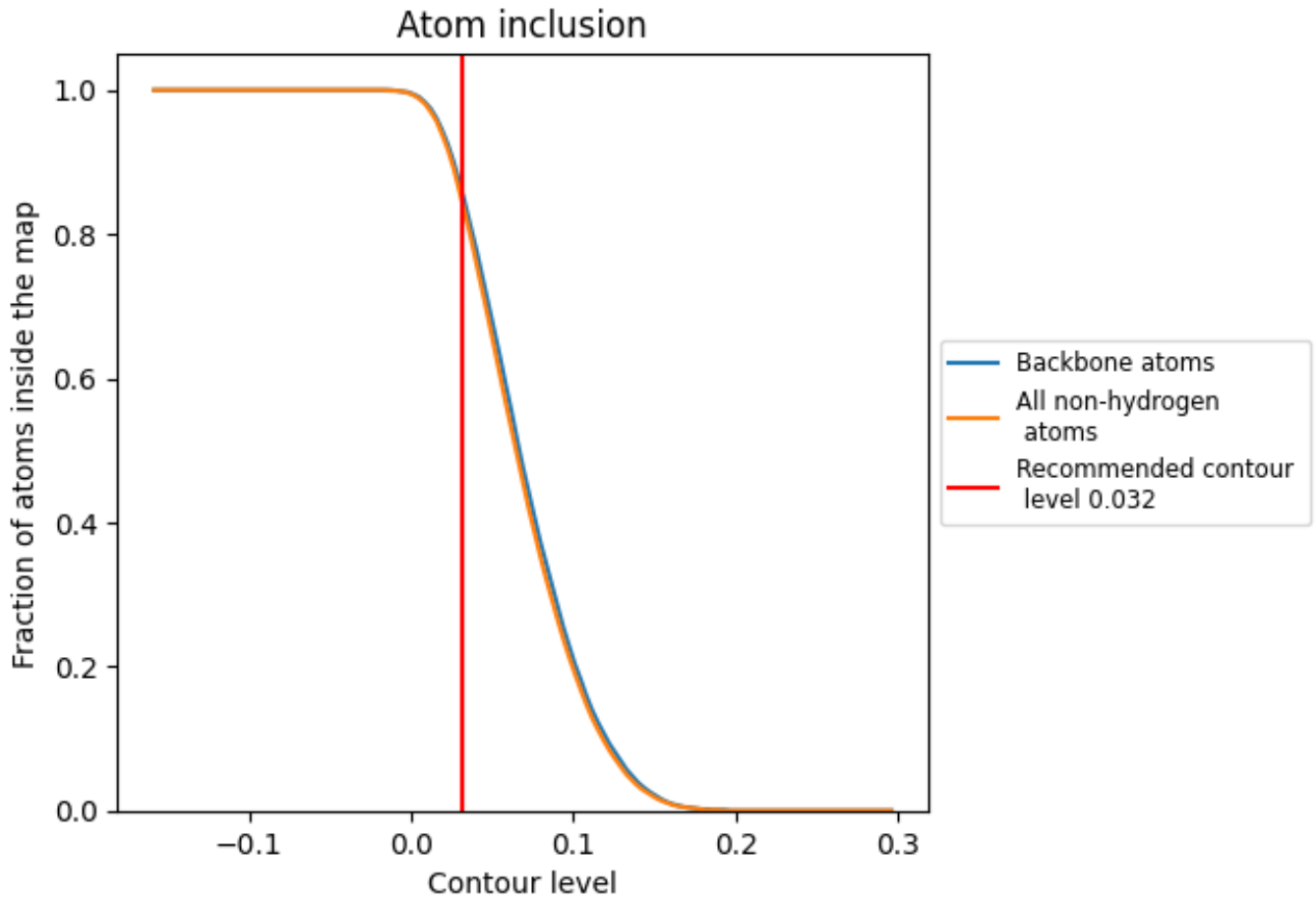
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.6190
A	0.9560	0.6740
B	0.9620	0.6780
C	0.9610	0.6650
D	0.8910	0.6380
E	0.8590	0.6300
F	0.9250	0.6600
I	0.9570	0.6610
J	0.9210	0.6630
K	0.8700	0.6330
L	0.9100	0.6530
M	0.9480	0.6580
O	0.8770	0.6260
Q	0.2720	0.3930
R	0.9240	0.6520
a	0.9190	0.6430
b	0.8960	0.6360
c	0.7960	0.5960
d	0.5010	0.4930
e	0.7280	0.5650
f	0.8040	0.6020
g	0.7870	0.6040
h	0.8440	0.6090
i	0.6260	0.5310
j	0.8130	0.6040
k	0.7010	0.5440
l	0.8460	0.6150
m	0.8580	0.6220
n	0.7180	0.5690
s	0.8770	0.6320

