Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID	:	8WMV / pdb_00008wmv
EMDB ID	:	EMD-37659
Title	:	The structure of PSI-14CAC complex at stationary growth phase
Authors	:	Zhang, S.M.; Si, L.; Li, M.
Deposited on	:	2023-10-04
Resolution	:	2.94 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:

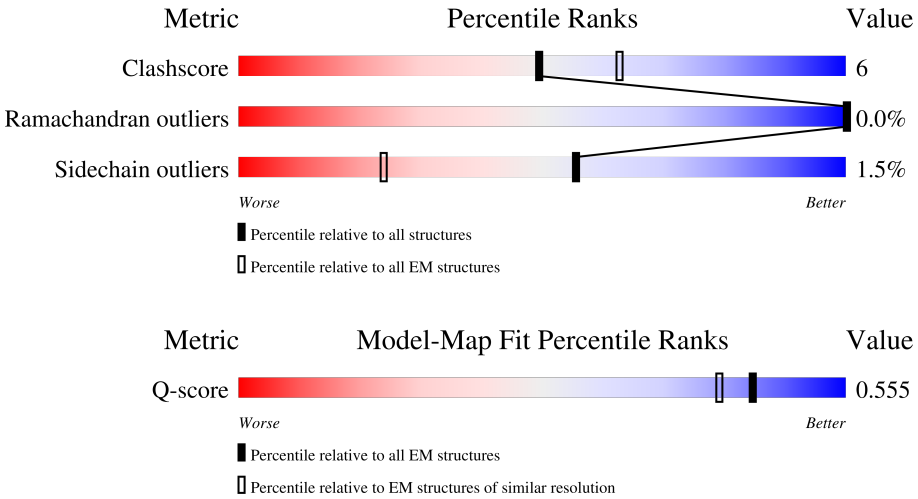
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	92% 7%
2	B	734	91% 8%
3	C	81	94% 5%
4	D	141	87% 12%

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Mol	Chain	Length	Quality of chain
5	E	64	78% 16% 6%
6	F	188	79% 7% 14%
7	I	36	69% 25% 6%
8	J	42	90% 10%
9	L	153	91% 7%
10	M	30	87% 7% 7%
11	O	146	5% 60% 10% 29%
12	K	87	71% 8% 21%
13	s	269	52% 6% 43%
14	c	216	70% 9% 21%
15	a	216	79% 19%
16	b	223	76% 10% 13%
17	h	225	65% 7% 28%
18	f	212	8% 72% 9% 18%
18	j	212	71% 9% 19%
18	m	212	73% 8% 18%
19	e	203	8% 73% 10% 17%
20	l	238	65% 8% 26%
21	k	241	8% 53% 13% 34%
22	i	218	27% 69% 11% 20%
23	d	213	10% 53% 7% 39%
24	g	255	11% 74% 12% 14%
25	R	129	64% 5% 30%
26	n	219	15% 69% 11% 17%

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
27	CLA	A	801	X	-	-	-
27	CLA	A	802	X	-	-	-
27	CLA	A	803	X	-	-	-
27	CLA	A	804	X	-	-	-
27	CLA	A	805	X	-	-	-
27	CLA	A	807	X	-	-	-
27	CLA	A	808	X	-	-	-
27	CLA	A	809	X	-	-	-
27	CLA	A	810	X	-	-	-
27	CLA	A	812	X	-	-	-
27	CLA	A	813	X	-	-	-
27	CLA	A	814	X	-	-	-
27	CLA	A	815	X	-	-	-
27	CLA	A	816	X	-	-	-
27	CLA	A	817	X	-	-	-
27	CLA	A	818	X	-	-	-
27	CLA	A	819	X	-	-	-
27	CLA	A	820	X	-	-	-
27	CLA	A	822	X	-	-	-
27	CLA	A	823	X	-	-	-
27	CLA	A	824	X	-	-	-
27	CLA	A	826	X	-	-	-
27	CLA	A	827	X	-	-	-
27	CLA	A	828	X	-	-	-
27	CLA	A	829	X	-	-	-
27	CLA	A	831	X	-	-	-
27	CLA	A	832	X	-	-	-
27	CLA	A	833	X	-	-	-
27	CLA	A	834	X	-	-	-
27	CLA	A	835	X	-	-	-
27	CLA	A	837	X	-	-	-
27	CLA	A	838	X	-	-	-
27	CLA	A	839	X	-	-	-
27	CLA	A	841	X	-	-	-
27	CLA	A	842	X	-	-	-
27	CLA	A	852	X	-	-	-
27	CLA	A	853	X	-	-	-
27	CLA	A	855	X	-	-	-
27	CLA	A	856	X	-	-	-
27	CLA	B	801	X	-	-	-
27	CLA	B	802	X	-	-	-
27	CLA	B	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	804	X	-	-	-
27	CLA	B	805	X	-	-	-
27	CLA	B	806	X	-	-	-
27	CLA	B	807	X	-	-	-
27	CLA	B	808	X	-	-	-
27	CLA	B	809	X	-	-	-
27	CLA	B	810	X	-	-	-
27	CLA	B	811	X	-	-	-
27	CLA	B	812	X	-	-	-
27	CLA	B	813	X	-	-	-
27	CLA	B	814	X	-	-	-
27	CLA	B	816	X	-	-	-
27	CLA	B	818	X	-	-	-
27	CLA	B	819	X	-	-	-
27	CLA	B	820	X	-	-	-
27	CLA	B	821	X	-	-	-
27	CLA	B	822	X	-	-	-
27	CLA	B	823	X	-	-	-
27	CLA	B	824	X	-	-	-
27	CLA	B	825	X	-	-	-
27	CLA	B	826	X	-	-	-
27	CLA	B	827	X	-	-	-
27	CLA	B	828	X	-	-	-
27	CLA	B	829	X	-	-	-
27	CLA	B	830	X	-	-	-
27	CLA	B	831	X	-	-	-
27	CLA	B	832	X	-	-	-
27	CLA	B	833	X	-	-	-
27	CLA	B	834	X	-	-	-
27	CLA	B	835	X	-	-	-
27	CLA	B	836	X	-	-	-
27	CLA	B	837	X	-	-	-
27	CLA	B	838	X	-	-	-
27	CLA	B	839	X	-	-	-
27	CLA	B	840	X	-	-	-
27	CLA	F	201	X	-	-	-
27	CLA	F	202	X	-	-	-
27	CLA	F	203	X	-	-	-
27	CLA	J	103	X	-	-	-
27	CLA	J	105	X	-	-	-
27	CLA	K	101	X	-	-	-
27	CLA	K	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	L	202	X	-	-	-
27	CLA	L	204	X	-	-	-
27	CLA	L	206	X	-	-	-
27	CLA	O	202	X	-	-	-
27	CLA	O	206	X	-	-	-
27	CLA	R	203	X	-	-	-
27	CLA	a	303	X	-	-	-
27	CLA	a	304	X	-	-	-
27	CLA	a	305	X	-	-	-
27	CLA	a	306	X	-	-	-
27	CLA	a	308	X	-	-	-
27	CLA	a	309	X	-	-	-
27	CLA	a	310	X	-	-	-
27	CLA	a	311	X	-	-	-
27	CLA	a	313	X	-	-	-
27	CLA	b	601	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	c	601	X	-	-	-
27	CLA	c	602	X	-	-	-
27	CLA	c	603	X	-	-	-
27	CLA	c	605	X	-	-	-
27	CLA	c	607	X	-	-	-
27	CLA	c	608	X	-	-	-
27	CLA	c	609	X	-	-	-
27	CLA	c	612	X	-	-	-
27	CLA	d	301	X	-	-	-
27	CLA	d	302	X	-	-	-
27	CLA	d	303	X	-	-	-
27	CLA	d	305	X	-	-	-
27	CLA	d	306	X	-	-	-
27	CLA	d	308	X	-	-	-
27	CLA	e	601	X	-	-	-
27	CLA	e	602	X	-	-	-
27	CLA	e	603	X	-	-	-
27	CLA	e	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	e	607	X	-	-	-
27	CLA	e	608	X	-	-	-
27	CLA	e	610	X	-	-	-
27	CLA	f	601	X	-	-	-
27	CLA	f	602	X	-	-	-
27	CLA	f	603	X	-	-	-
27	CLA	f	604	X	-	-	-
27	CLA	f	607	X	-	-	-
27	CLA	f	608	X	-	-	-
27	CLA	f	609	X	-	-	-
27	CLA	f	610	X	-	-	-
27	CLA	f	612	X	-	-	-
27	CLA	g	302	X	-	-	-
27	CLA	g	303	X	-	-	-
27	CLA	g	304	X	-	-	-
27	CLA	g	305	X	-	-	-
27	CLA	g	306	X	-	-	-
27	CLA	g	308	X	-	-	-
27	CLA	g	309	X	-	-	-
27	CLA	g	310	X	-	-	-
27	CLA	g	311	X	-	-	-
27	CLA	g	322	X	-	-	-
27	CLA	h	301	X	-	-	-
27	CLA	h	302	X	-	-	-
27	CLA	h	303	X	-	-	-
27	CLA	h	304	X	-	-	-
27	CLA	h	305	X	-	-	-
27	CLA	h	306	X	-	-	-
27	CLA	h	307	X	-	-	-
27	CLA	h	308	X	-	-	-
27	CLA	h	313	X	-	-	-
27	CLA	i	302	X	-	-	-
27	CLA	i	303	X	-	-	-
27	CLA	i	304	X	-	-	-
27	CLA	i	305	X	-	-	-
27	CLA	i	306	X	-	-	-
27	CLA	i	307	X	-	-	-
27	CLA	i	308	X	-	-	-
27	CLA	i	309	X	-	-	-
27	CLA	i	311	X	-	-	-
27	CLA	i	312	X	-	-	-
27	CLA	j	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	j	602	X	-	-	-
27	CLA	j	603	X	-	-	-
27	CLA	j	604	X	-	-	-
27	CLA	j	607	X	-	-	-
27	CLA	j	608	X	-	-	-
27	CLA	j	609	X	-	-	-
27	CLA	j	611	X	-	-	-
27	CLA	j	612	X	-	-	-
27	CLA	k	301	X	-	-	-
27	CLA	k	302	X	-	-	-
27	CLA	k	303	X	-	-	-
27	CLA	k	304	X	-	-	-
27	CLA	k	305	X	-	-	-
27	CLA	k	306	X	-	-	-
27	CLA	k	307	X	-	-	-
27	CLA	k	308	X	-	-	-
27	CLA	k	309	X	-	-	-
27	CLA	k	313	X	-	-	-
27	CLA	l	303	X	-	-	-
27	CLA	l	304	X	-	-	-
27	CLA	l	305	X	-	-	-
27	CLA	l	307	X	-	-	-
27	CLA	l	308	X	-	-	-
27	CLA	l	309	X	-	-	-
27	CLA	l	310	X	-	-	-
27	CLA	l	312	X	-	-	-
27	CLA	m	601	X	-	-	-
27	CLA	m	602	X	-	-	-
27	CLA	m	603	X	-	-	-
27	CLA	m	605	X	-	-	-
27	CLA	m	606	X	-	-	-
27	CLA	m	607	X	-	-	-
27	CLA	m	608	X	-	-	-
27	CLA	m	609	X	-	-	-
27	CLA	m	611	X	-	-	-
27	CLA	m	612	X	-	-	-
27	CLA	n	601	X	-	-	-
27	CLA	n	602	X	-	-	-
27	CLA	n	603	X	-	-	-
27	CLA	n	604	X	-	-	-
27	CLA	n	605	X	-	-	-
27	CLA	n	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	n	607	X	-	-	-
27	CLA	n	608	X	-	-	-
27	CLA	n	609	X	-	-	-
27	CLA	n	610	X	-	-	-
27	CLA	n	613	X	-	-	-
27	CLA	s	202	X	-	-	-
27	CLA	s	206	X	-	-	-
27	CLA	s	209	X	-	-	-
32	SF4	A	854	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 59342 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	1083	692	186	202	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	485	309	84	92	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-m, 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	160	Total	C	N	O	S	0	0
			1196	774	199	213	10		

- 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		

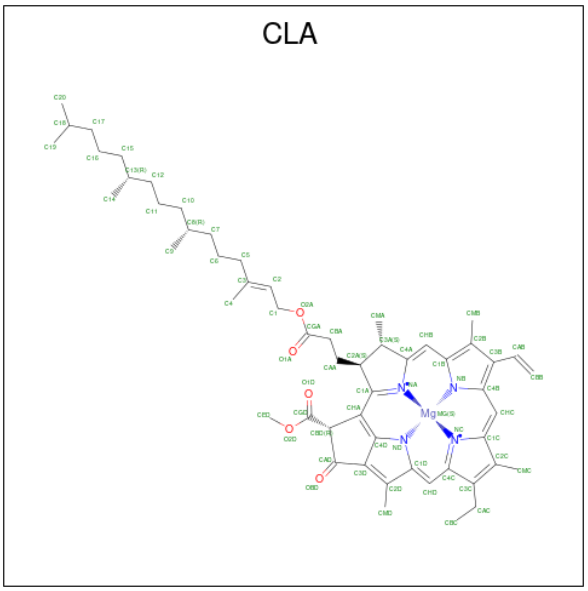
- Molecule 25 is a protein called PsaR.

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



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

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

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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

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Mol	Chain	Residues	Atoms					AltConf
27	K	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	s	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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

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

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

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

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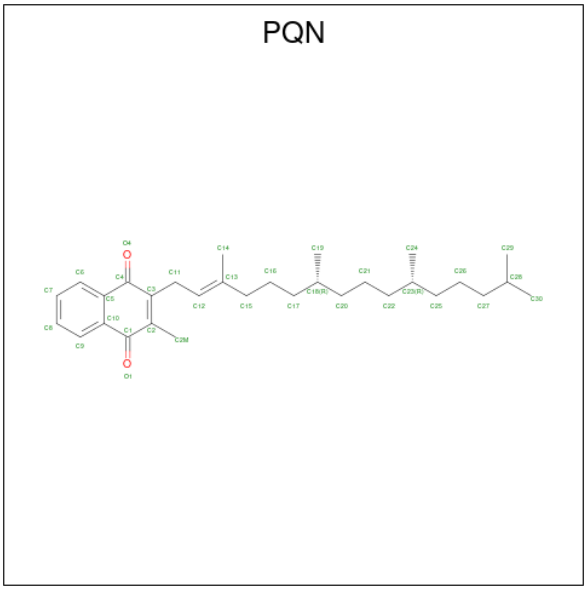
Mol	Chain	Residues	Atoms					AltConf
27	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	d	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	d	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	g	1	Total	C	Mg	N	O	0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

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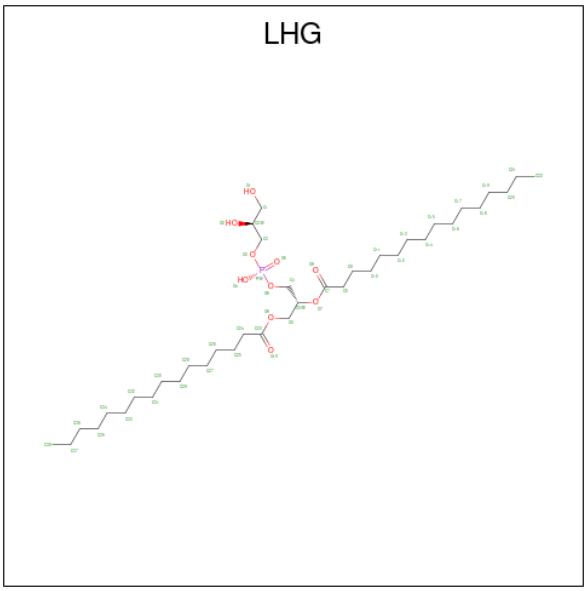
Mol	Chain	Residues	Atoms					AltConf
27	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

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



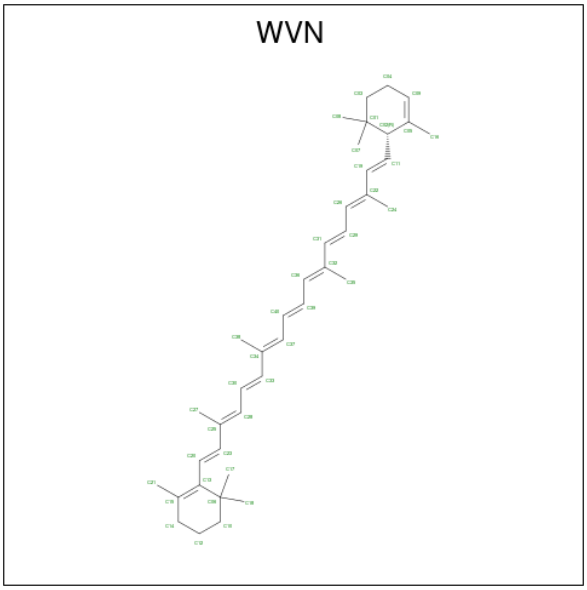
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total 48	C 37	O 10	P 1	0
29	A	1	Total 27	C 16	O 10	P 1	0
29	A	1	Total 38	C 27	O 10	P 1	0
29	J	1	Total 49	C 38	O 10	P 1	0
29	L	1	Total 49	C 38	O 10	P 1	0
29	c	1	Total 37	C 26	O 10	P 1	0
29	c	1	Total 37	C 26	O 10	P 1	0
29	a	1	Total 49	C 38	O 10	P 1	0
29	a	1	Total 49	C 38	O 10	P 1	0
29	b	1	Total 49	C 38	O 10	P 1	0
29	b	1	Total 31	C 20	O 10	P 1	0
29	m	1	Total 37	C 26	O 10	P 1	0
29	e	1	Total 37	C 26	O 10	P 1	0
29	l	1	Total 32	C 21	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	k	1	Total	C	O	P	0
			37	26	10	1	
29	f	1	Total	C	O	P	0
			49	38	10	1	
29	i	1	Total	C	O	P	0
			37	26	10	1	
29	j	1	Total	C	O	P	0
			30	19	10	1	
29	d	1	Total	C	O	P	0
			37	26	10	1	
29	g	1	Total	C	O	P	0
			37	26	10	1	
29	g	1	Total	C	O	P	0
			37	26	10	1	
29	n	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 30 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: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	C	0
			40	40	
30	A	1	Total	C	0
			40	40	

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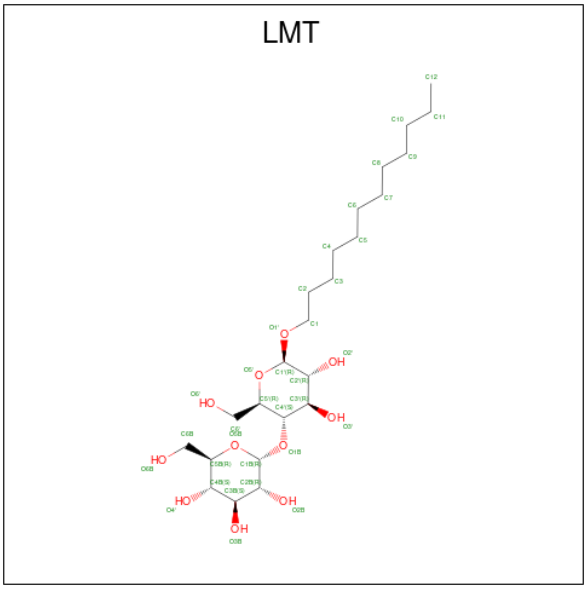
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	I	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	M	1	Total C 40 40	0
30	O	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	s	1	Total C 40 40	0
30	s	1	Total C 40 40	0
30	h	1	Total C 40 40	0

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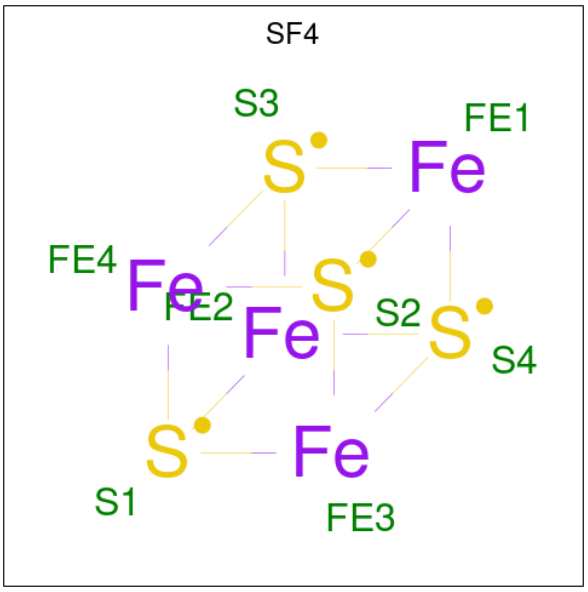
Mol	Chain	Residues	Atoms	AltConf
30	e	1	Total C 40 40	0
30	l	1	Total C 40 40	0
30	l	1	Total C 40 40	0
30	i	1	Total C 40 40	0
30	R	1	Total C 40 40	0
30	R	1	Total C 40 40	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



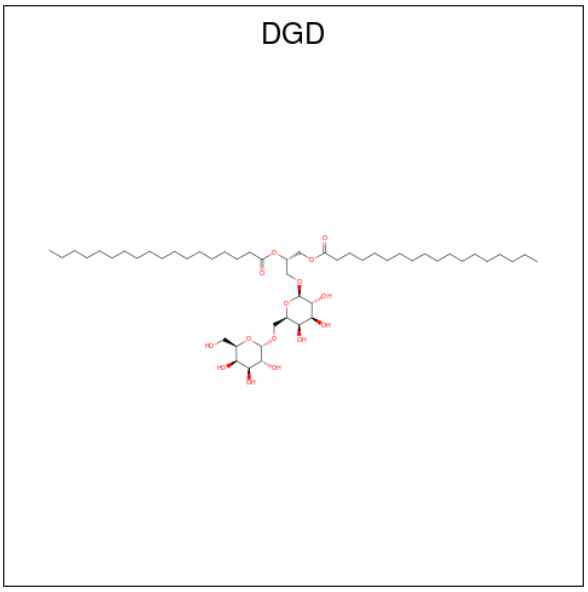
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 35 24 11	0
31	a	1	Total C O 24 18 6	0
31	a	1	Total C O 35 24 11	0
31	b	1	Total C O 24 18 6	0

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



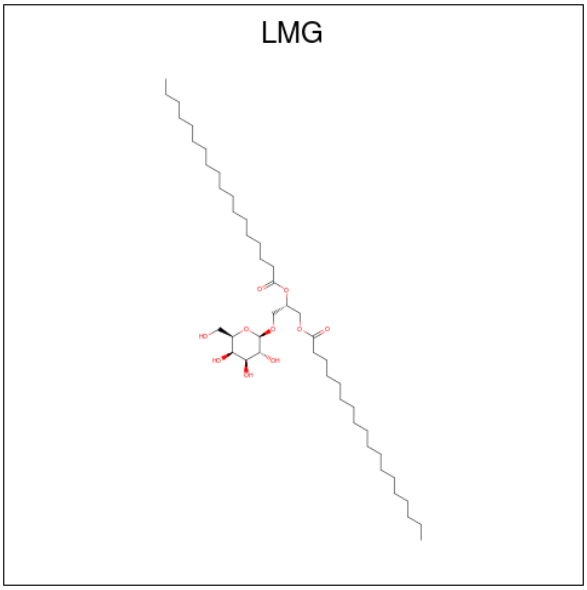
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Fe S 8 4 4	0
32	C	1	Total Fe S 8 4 4	0
32	C	1	Total Fe S 8 4 4	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



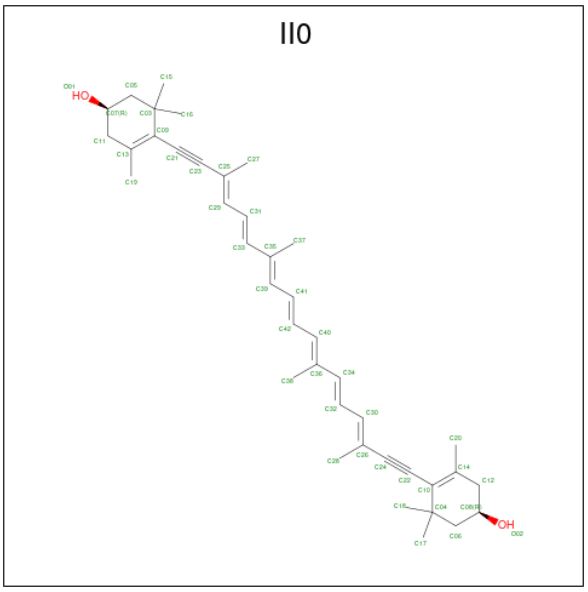
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			60	45	15	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 35 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: $C_{40}H_{52}O_2$).



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

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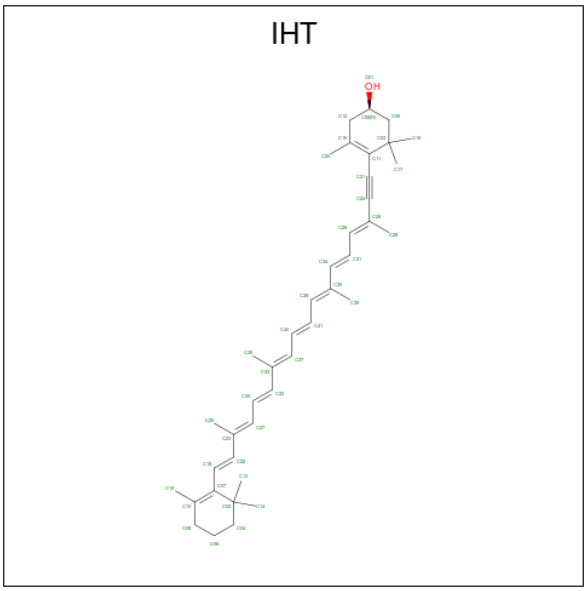
Mol	Chain	Residues	Atoms			AltConf
35	h	1	Total	C	O	0
			42	40	2	
35	h	1	Total	C	O	0
			42	40	2	
35	m	1	Total	C	O	0
			42	40	2	
35	m	1	Total	C	O	0
			42	40	2	
35	m	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0
			42	40	2	
35	e	1	Total	C	O	0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

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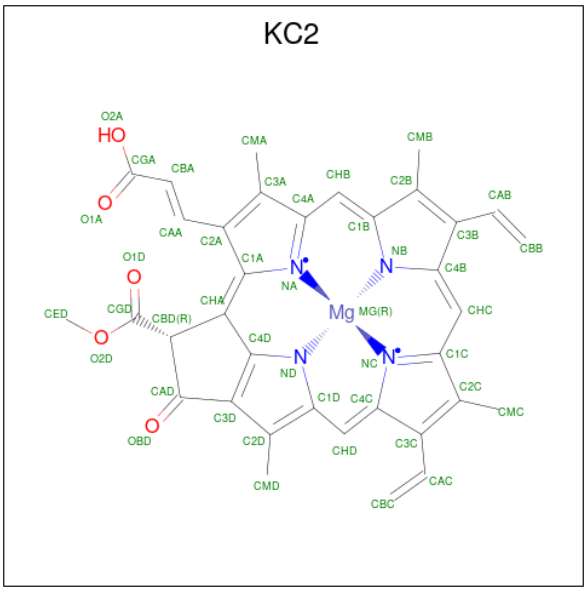
Mol	Chain	Residues	Atoms			AltConf
35	f	1	Total	C	O	0
			42	40	2	
35	i	1	Total	C	O	0
			42	40	2	
35	i	1	Total	C	O	0
			42	40	2	
35	i	1	Total	C	O	0
			42	40	2	
35	j	1	Total	C	O	0
			42	40	2	
35	j	1	Total	C	O	0
			42	40	2	
35	j	1	Total	C	O	0
			42	40	2	
35	d	1	Total	C	O	0
			42	40	2	
35	d	1	Total	C	O	0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

- Molecule 36 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
36	O	1	Total C O 41 40 1	0
36	c	1	Total C O 41 40 1	0
36	c	1	Total C O 41 40 1	0
36	a	1	Total C O 41 40 1	0
36	b	1	Total C O 41 40 1	0
36	m	1	Total C O 41 40 1	0
36	k	1	Total C O 41 40 1	0
36	f	1	Total C O 41 40 1	0
36	j	1	Total C O 41 40 1	0
36	g	1	Total C O 41 40 1	0
36	R	1	Total C O 41 40 1	0
36	n	1	Total C O 41 40 1	0

- Molecule 37 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



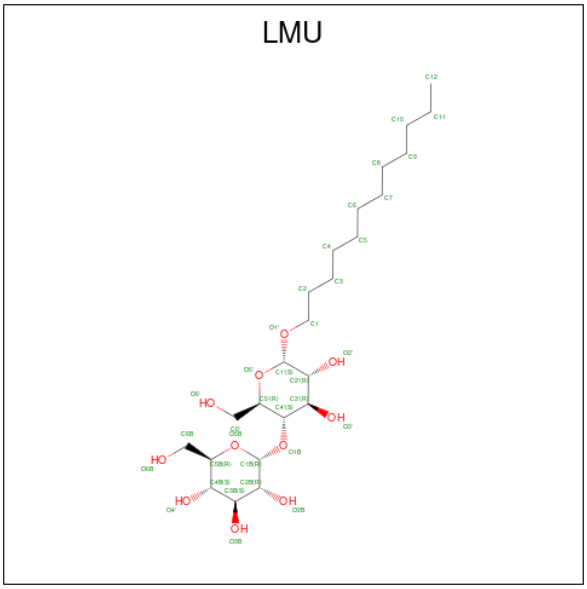
Mol	Chain	Residues	Atoms					AltConf
37	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	m	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	k	1	Total	C	Mg	N	O	0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

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

- Molecule 38 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	49	Total	O	0
			49	49	
39	B	58	Total	O	0
			58	58	

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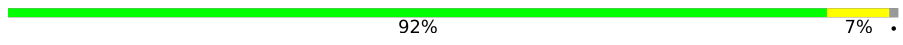
Mol	Chain	Residues	Atoms	AltConf
39	C	7	Total O 7 7	0
39	D	1	Total O 1 1	0
39	F	4	Total O 4 4	0
39	I	1	Total O 1 1	0
39	J	1	Total O 1 1	0
39	L	1	Total O 1 1	0
39	O	1	Total O 1 1	0
39	K	1	Total O 1 1	0
39	a	3	Total O 3 3	0
39	b	2	Total O 2 2	0
39	h	1	Total O 1 1	0
39	m	1	Total O 1 1	0
39	e	4	Total O 4 4	0
39	n	2	Total O 2 2	0

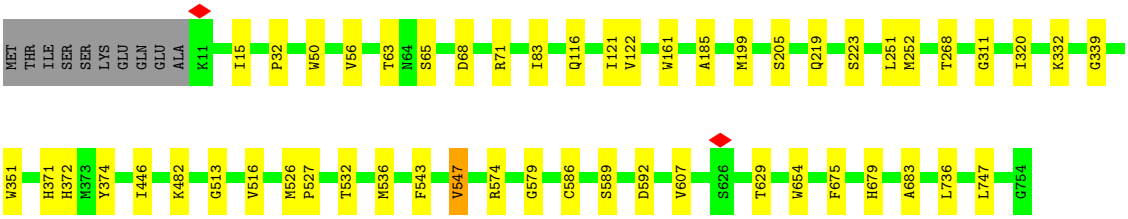
3 Residue-property plots (i)

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:

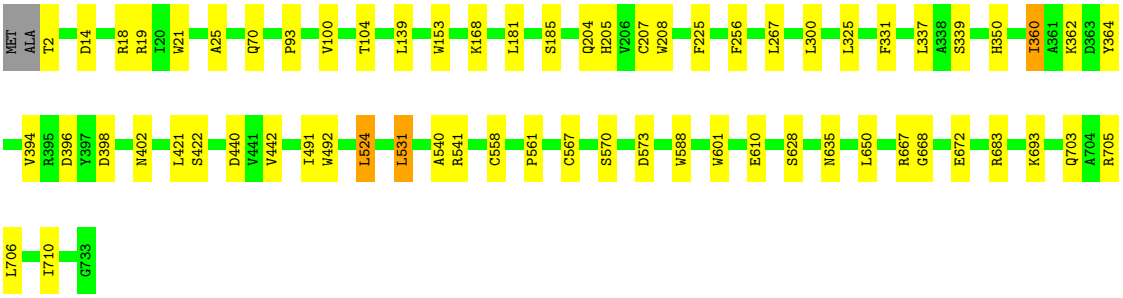




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

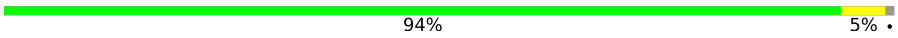
Chain B:

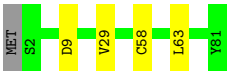




• Molecule 3: Photosystem I iron-sulfur center

Chain C:

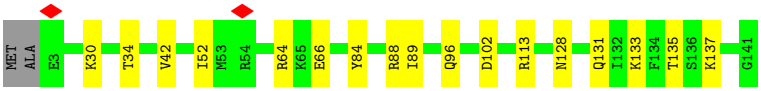




• Molecule 4: Photosystem I reaction center subunit II

Chain D:

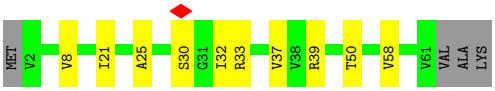




• Molecule 5: Photosystem I reaction center subunit IV

Chain E:

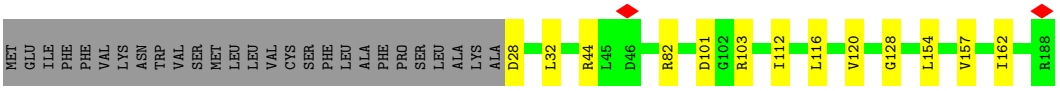




• Molecule 6: Photosystem I reaction center subunit III

Chain F:

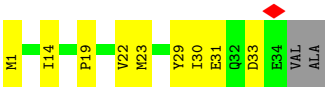




• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:

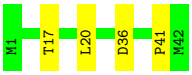




• Molecule 8: Photosystem I reaction center subunit IX

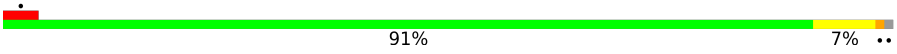
Chain J:

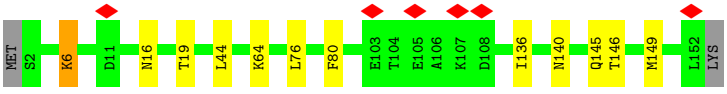




• Molecule 9: Photosystem I reaction center subunit XI

Chain L:

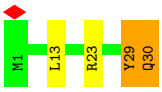




• Molecule 10: Photosystem I reaction center subunit XII

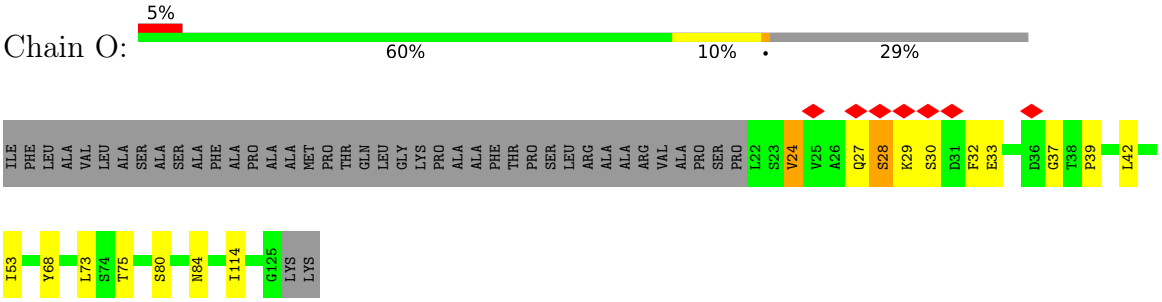
Chain M:





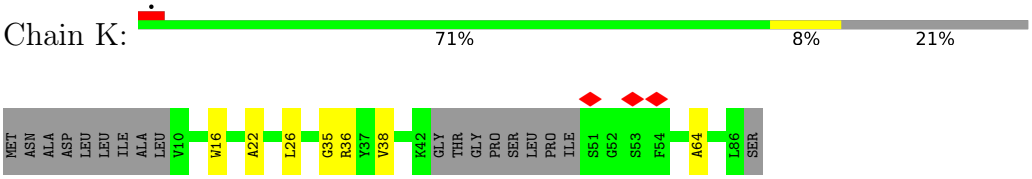
• Molecule 11: PsaO

Chain O:



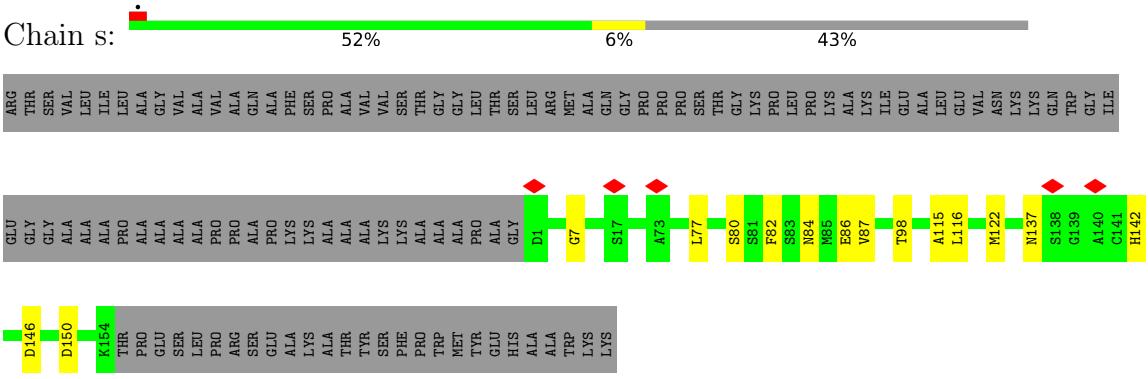
• Molecule 12: Photosystem I reaction center subunit PsaK

Chain K:



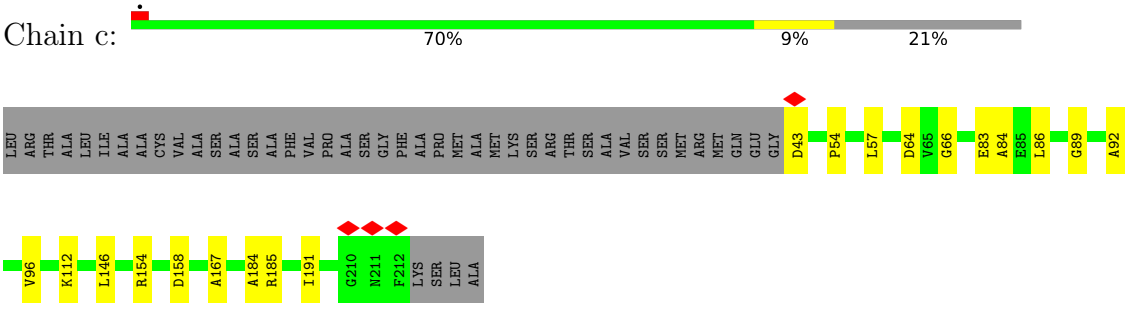
• Molecule 13: chain s

Chain s:



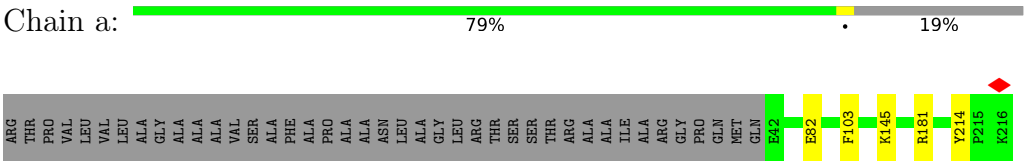
• Molecule 14: CAC-c

Chain c:



• Molecule 15: CAC-a

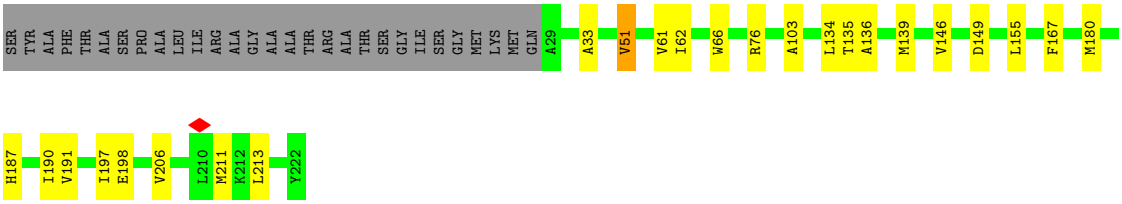
Chain a:



• Molecule 16: CAC-b

Chain b:

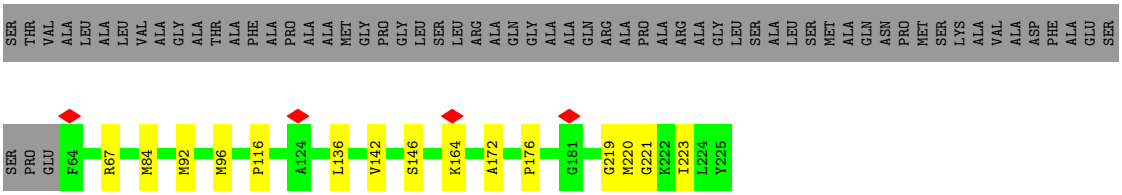




• Molecule 17: CAC-h

Chain h:

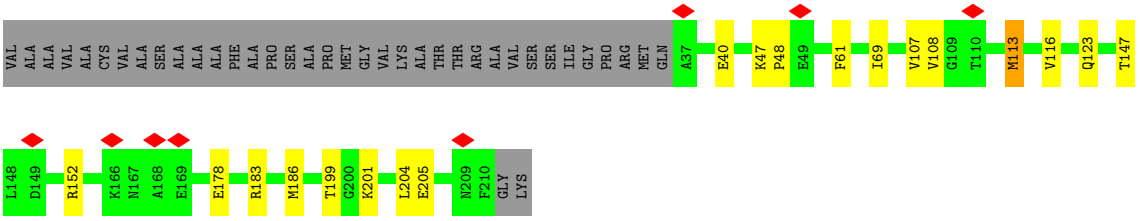




• Molecule 18: CAC-m, CAC-f

Chain m:

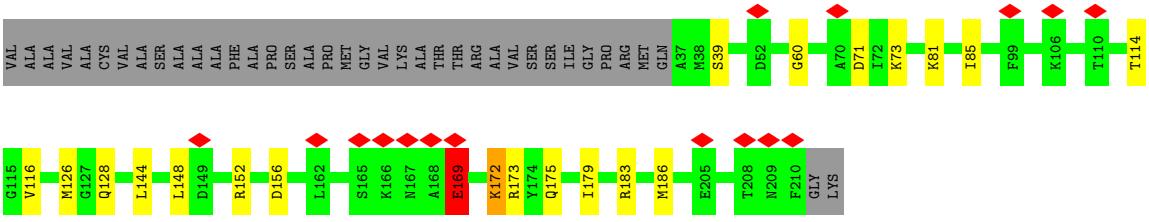




• Molecule 18: CAC-m, CAC-f

Chain f:

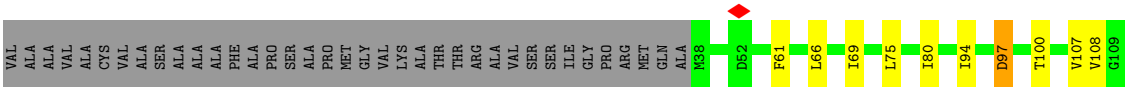


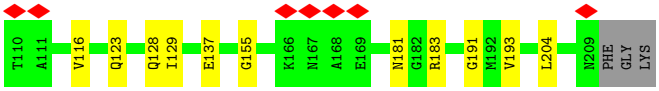


• Molecule 18: CAC-m, CAC-f

Chain j:



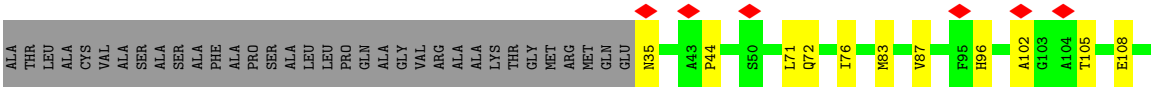


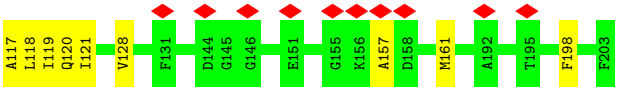


• Molecule 19: CAC-e

Chain e:







• Molecule 20: CAC-l

Chain l:





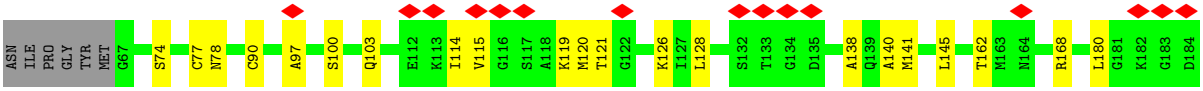


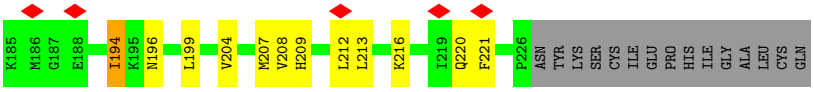
• Molecule 21: CAC-k

Chain k:





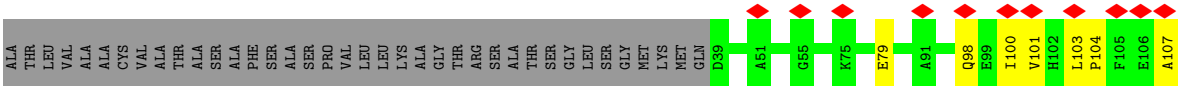


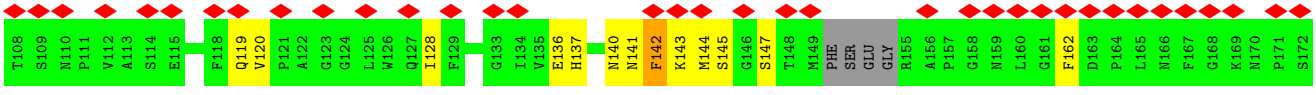


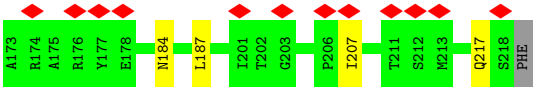
• Molecule 22: CAC-i

Chain i:

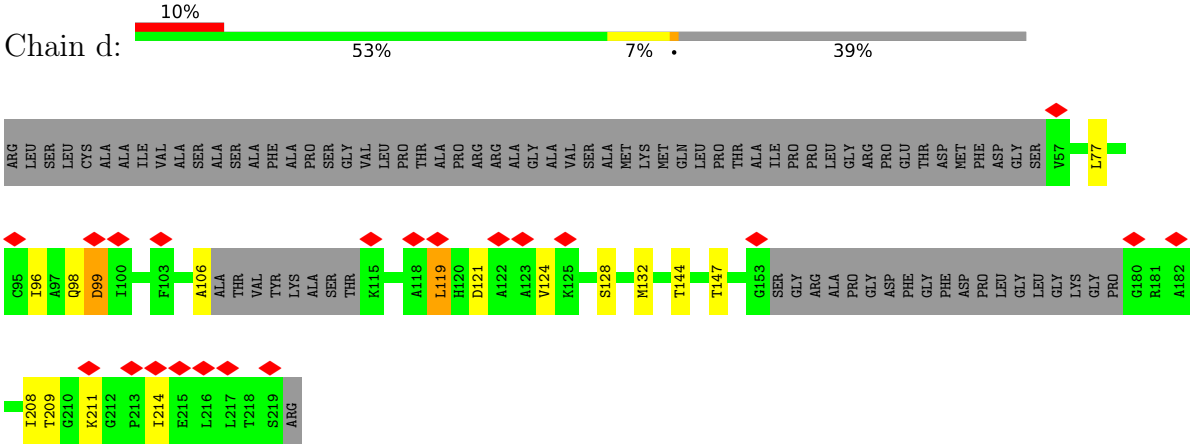




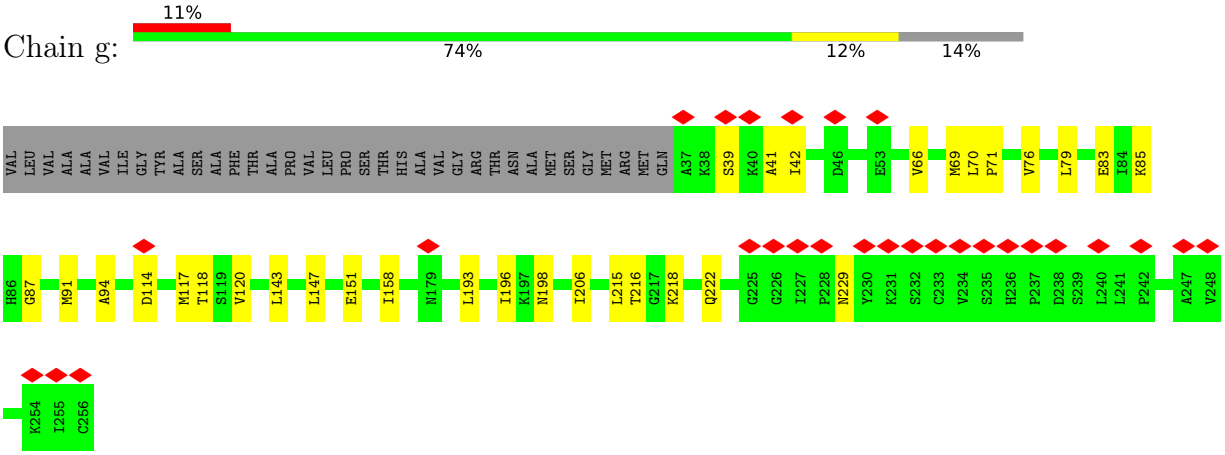




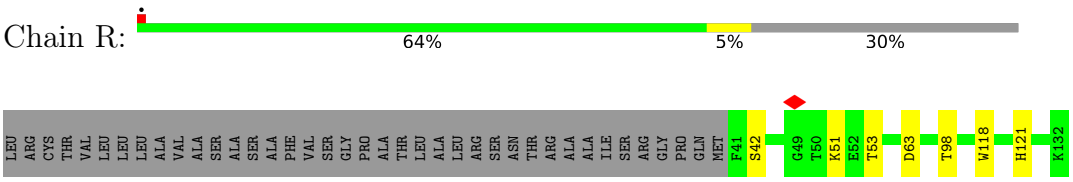
• Molecule 23: CAC-d



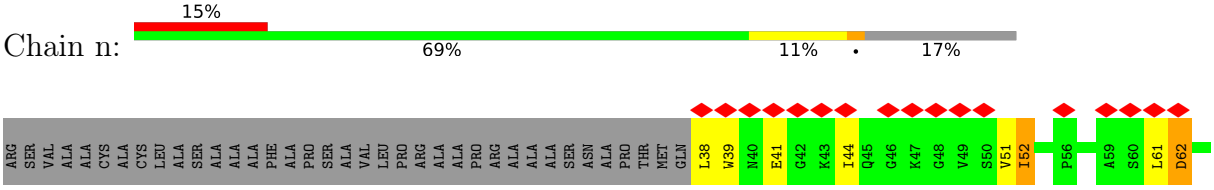
• Molecule 24: CAC-g

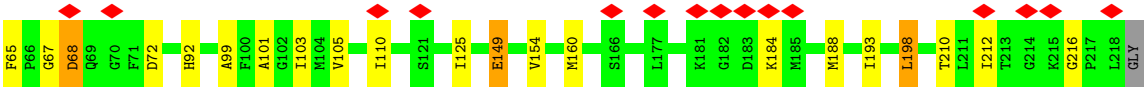


• Molecule 25: PsaR



• Molecule 26: CAC-n




F65
P66
G67
D68
Q69
G70
F71
D72
H92
A99
F100
A101
G102
I103
M104
V105
I110
S121
I125
E149
V154
M160
S166
L177
K181
G182
D183
K184
M185
M188
I193
L198
T210
L211
I212
T213
G214
K215
G216
P217
L218
GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42423	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)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.52	0/6019	0.76	0/8204
2	B	0.54	1/6045 (0.0%)	0.80	3/8254 (0.0%)
3	C	0.43	0/601	0.82	0/813
4	D	0.50	0/1108	0.79	0/1499
5	E	0.48	0/493	0.77	0/667
6	F	0.55	0/1287	0.83	0/1747
7	I	0.60	0/271	0.81	0/370
8	J	0.45	0/364	0.77	0/495
9	L	0.48	0/1175	0.80	0/1599
10	M	0.48	0/233	0.90	2/315 (0.6%)
11	O	0.59	0/799	0.85	0/1094
12	K	0.48	0/495	0.86	0/672
13	s	0.55	0/1170	0.85	0/1580
14	c	0.57	0/1396	0.88	0/1889
15	a	0.50	0/1406	0.81	0/1903
16	b	0.57	0/1469	0.91	0/1983
17	h	0.56	0/1226	0.94	0/1667
18	f	0.51	0/1328	0.87	1/1790 (0.1%)
18	j	0.61	0/1318	0.94	2/1775 (0.1%)
18	m	0.52	0/1335	0.85	1/1798 (0.1%)
19	e	0.54	0/1324	0.88	0/1795
20	l	0.52	0/1379	0.83	0/1863
21	k	0.61	0/1223	0.95	0/1651
22	i	0.55	0/1359	0.91	0/1835
23	d	0.50	0/993	0.87	1/1335 (0.1%)
24	g	0.57	0/1673	0.90	0/2264
25	R	0.45	0/686	0.79	1/940 (0.1%)
26	n	0.63	0/1383	0.94	1/1867 (0.1%)
All	All	0.54	1/39558 (0.0%)	0.84	12/53664 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	635	ASN	C-N	5.04	1.39	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	362	LYS	N-CA-C	-7.16	104.69	113.50
18	m	113	MET	CB-CA-C	-5.95	109.72	116.63
2	B	667	ARG	N-CA-C	5.81	117.61	111.28
18	j	191	GLY	CA-C-N	5.80	128.33	120.44
18	j	191	GLY	C-N-CA	5.80	128.33	120.44
10	M	29	TYR	CA-C-N	5.80	132.15	121.70
10	M	29	TYR	C-N-CA	5.80	132.15	121.70
26	n	198	LEU	CD1-CG-CD2	-5.43	98.85	110.80
18	f	169	GLU	N-CA-C	-5.14	105.76	111.36
25	R	53	THR	OG1-CB-CG2	-5.07	99.17	109.30
23	d	98	GLN	CB-CG-CD	5.04	121.16	112.60
2	B	360	ILE	CA-C-O	-5.02	115.91	121.98

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	5678	37	0
2	B	5826	0	5642	50	0
3	C	592	0	567	3	0
4	D	1083	0	1077	11	0
5	E	485	0	489	5	0
6	F	1254	0	1264	13	0
7	I	264	0	276	7	0
8	J	351	0	344	4	0
9	L	1146	0	1160	14	0
10	M	232	0	265	4	0
11	O	773	0	765	31	0
12	K	488	0	516	6	0
13	s	1140	0	1099	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	c	1357	0	1337	14	0
15	a	1361	0	1305	4	0
16	b	1439	0	1456	18	0
17	h	1200	0	1228	10	0
18	f	1302	0	1320	30	0
18	j	1293	0	1321	17	0
18	m	1309	0	1335	11	0
19	e	1286	0	1262	15	0
20	l	1344	0	1315	14	0
21	k	1196	0	1204	26	0
22	i	1324	0	1297	18	0
23	d	974	0	978	10	0
24	g	1630	0	1644	20	0
25	R	664	0	647	3	0
26	n	1350	0	1348	22	0
27	A	2758	0	2820	78	0
27	B	2440	0	2452	46	0
27	F	182	0	187	7	0
27	J	93	0	72	2	0
27	K	93	0	72	0	0
27	L	215	0	191	5	0
27	O	130	0	144	2	0
27	R	51	0	41	0	0
27	a	619	0	588	11	0
27	b	673	0	696	22	0
27	c	586	0	520	9	0
27	d	447	0	366	6	0
27	e	582	0	578	23	0
27	f	700	0	695	25	0
27	g	661	0	611	14	0
27	h	505	0	470	11	0
27	i	528	0	451	11	0
27	j	586	0	515	16	0
27	k	545	0	493	14	0
27	l	535	0	538	12	0
27	m	600	0	565	21	0
27	n	605	0	552	14	0
27	s	297	0	298	8	0
28	A	33	0	46	2	0
28	B	33	0	46	1	0
29	A	113	0	142	4	0
29	J	49	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	L	49	0	74	2	0
29	a	98	0	148	2	0
29	b	80	0	106	6	0
29	c	74	0	88	6	0
29	d	37	0	44	0	0
29	e	37	0	44	1	0
29	f	49	0	74	3	0
29	g	74	0	88	4	0
29	i	37	0	44	1	0
29	j	30	0	30	2	0
29	k	37	0	44	0	0
29	l	32	0	34	2	0
29	m	37	0	44	0	0
29	n	43	0	59	1	0
30	A	160	0	0	0	0
30	B	240	0	0	0	0
30	F	80	0	0	0	0
30	I	40	0	0	0	0
30	J	80	0	0	0	0
30	K	40	0	0	0	0
30	L	80	0	0	0	0
30	M	40	0	0	0	0
30	O	40	0	0	0	0
30	R	80	0	0	0	0
30	e	40	0	0	0	0
30	h	40	0	0	0	0
30	i	40	0	0	0	0
30	l	80	0	0	0	0
30	s	80	0	0	1	0
31	A	35	0	44	1	0
31	a	59	0	79	1	0
31	b	24	0	34	1	0
32	A	8	0	0	5	0
32	C	16	0	0	0	0
33	B	60	0	81	2	0
34	F	48	0	69	1	0
34	J	55	0	86	3	0
34	L	55	0	86	2	0
34	O	26	0	22	0	0
34	b	49	0	71	2	0
34	c	55	0	86	3	0
34	s	55	0	86	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	J	42	0	0	0	0
35	O	42	0	0	0	0
35	a	168	0	0	0	0
35	b	126	0	0	1	0
35	c	168	0	0	0	0
35	d	126	0	0	0	0
35	e	168	0	0	0	0
35	f	168	0	0	1	0
35	g	168	0	0	0	0
35	h	112	0	0	1	0
35	i	126	0	0	1	0
35	j	126	0	0	1	0
35	k	168	0	0	1	0
35	l	210	0	0	2	0
35	m	126	0	0	1	0
35	n	168	0	0	1	0
36	O	41	0	0	0	0
36	R	41	0	0	0	0
36	a	41	0	0	0	0
36	b	41	0	0	3	0
36	c	82	0	0	1	0
36	f	41	0	0	2	0
36	g	41	0	0	1	0
36	j	41	0	0	2	0
36	k	41	0	0	0	0
36	m	41	0	0	0	0
36	n	41	0	0	0	0
37	c	45	0	0	0	0
37	d	90	0	0	0	0
37	e	45	0	0	0	0
37	f	45	0	0	2	0
37	g	135	0	0	0	0
37	i	90	0	0	1	0
37	j	45	0	0	1	0
37	k	135	0	0	4	0
37	l	45	0	0	1	0
37	m	45	0	0	7	0
37	n	90	0	0	0	0
37	s	90	0	0	0	0
38	i	35	0	46	1	0
39	A	49	0	0	0	0
39	B	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	C	7	0	0	0	0
39	D	1	0	0	0	0
39	F	4	0	0	0	0
39	I	1	0	0	0	0
39	J	1	0	0	0	0
39	K	1	0	0	0	0
39	L	1	0	0	0	0
39	O	1	0	0	0	0
39	a	3	0	0	0	0
39	b	2	0	0	0	0
39	e	4	0	0	0	0
39	h	1	0	0	0	0
39	m	1	0	0	0	0
39	n	2	0	0	0	0
All	All	59342	0	54073	645	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 6.

All (645) 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)
11:O:27:GLN:HB2	18:f:148:LEU:O	1.49	1.12
11:O:27:GLN:OE1	18:f:148:LEU:O	1.63	1.11
11:O:27:GLN:CB	18:f:148:LEU:O	2.05	1.04
21:k:221:PHE:HE2	37:k:311:KC2:CED	1.71	1.02
26:n:67:GLY:HA3	26:n:193:ILE:HG21	1.37	1.02
16:b:206:VAL:HG11	36:b:614:IHT:C06	1.89	1.01
32:A:854:SF4:FE4	2:B:558:CYS:HG	0.73	0.95
32:A:854:SF4:FE1	2:B:567:CYS:HG	0.66	0.94
11:O:24:VAL:HG13	11:O:42:LEU:HB2	1.50	0.92
1:A:586:CYS:HG	32:A:854:SF4:FE2	0.64	0.89
21:k:221:PHE:CE2	37:k:311:KC2:CED	2.56	0.87
16:b:206:VAL:CG1	36:b:614:IHT:C06	2.52	0.87
11:O:27:GLN:HE22	18:f:73:LYS:CE	1.87	0.86
11:O:27:GLN:CB	18:f:148:LEU:C	2.50	0.85
11:O:27:GLN:HB3	18:f:148:LEU:C	2.03	0.84
26:n:210:THR:HG22	26:n:216:GLY:HA2	1.62	0.81
2:B:325:LEU:HD13	2:B:331:PHE:HD2	1.48	0.79
11:O:27:GLN:HB3	18:f:148:LEU:HB3	1.65	0.79
37:m:610:KC2:CBA	37:m:610:KC2:CGD	2.61	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:CYS:SG	32:A:854:SF4:FE2	1.73	0.77
27:k:305:CLA:HED3	27:k:305:CLA:H2A	1.67	0.77
17:h:221:GLY:HA3	27:h:308:CLA:H2A	1.68	0.76
11:O:27:GLN:CD	18:f:148:LEU:O	2.29	0.75
11:O:27:GLN:HE22	18:f:73:LYS:HE2	1.51	0.74
11:O:27:GLN:HE22	18:f:73:LYS:HE3	1.50	0.74
27:A:822:CLA:HBB2	27:A:836:CLA:H18	1.70	0.73
11:O:27:GLN:NE2	18:f:73:LYS:HE3	2.05	0.72
18:m:186:MET:HE1	27:m:602:CLA:HAB	1.72	0.71
11:O:27:GLN:HB2	18:f:148:LEU:C	2.14	0.71
27:J:105:CLA:H3A	29:b:618:LHG:HC62	1.72	0.70
26:n:184:LYS:HA	26:n:188:MET:HB2	1.73	0.70
26:n:67:GLY:HA3	26:n:193:ILE:CG2	2.17	0.69
2:B:421:LEU:HB3	2:B:531:LEU:HG	1.76	0.68
24:g:66:VAL:HG11	27:g:303:CLA:H2	1.76	0.67
6:F:120:VAL:HG13	27:F:202:CLA:HAA1	1.77	0.66
11:O:24:VAL:CG1	11:O:42:LEU:HB2	2.25	0.66
21:k:114:ILE:HG23	21:k:115:VAL:HG23	1.78	0.65
22:i:137:HIS:HB3	22:i:142:PHE:CE1	2.32	0.65
22:i:144:MET:H	22:i:147:SER:HB2	1.60	0.65
23:d:106:ALA:HB1	27:d:303:CLA:HED3	1.78	0.65
26:n:68:ASP:C	26:n:68:ASP:OD1	2.40	0.64
14:c:83:GLU:HG2	14:c:146:LEU:HD12	1.80	0.64
27:A:852:CLA:H11	2:B:650:LEU:HB3	1.80	0.64
18:m:201:LYS:HB3	18:m:205:GLU:HG3	1.79	0.63
18:j:108:VAL:HG11	18:j:116:VAL:HG12	1.80	0.63
27:B:809:CLA:HBB2	27:B:837:CLA:H8	1.80	0.63
27:A:814:CLA:H12	27:A:814:CLA:HBD	1.80	0.62
3:C:9:ASP:OD2	5:E:33:ARG:NH1	2.32	0.62
27:e:607:CLA:H3A	27:e:607:CLA:H2	1.81	0.62
27:A:831:CLA:HBA1	27:A:855:CLA:H42	1.82	0.62
7:I:29:TYR:OH	10:M:29:TYR:OH	2.17	0.62
26:n:68:ASP:HB2	27:n:602:CLA:HED2	1.82	0.62
11:O:27:GLN:NE2	18:f:73:LYS:CE	2.60	0.61
29:c:621:LHG:H101	27:b:610:CLA:H172	1.81	0.61
27:m:609:CLA:H72	37:m:610:KC2:C2D	2.29	0.61
2:B:325:LEU:HD13	2:B:331:PHE:CD2	2.31	0.61
6:F:82:ARG:HH22	8:J:36:ASP:HB2	1.66	0.61
18:j:137:GLU:HG2	27:j:607:CLA:NB	2.16	0.61
27:B:805:CLA:H12	7:I:14:ILE:HG13	1.82	0.60
26:n:184:LYS:HG3	27:n:609:CLA:HAA2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:76:ARG:HB3	27:b:607:CLA:HBC3	1.84	0.60
12:K:26:LEU:HD21	27:e:606:CLA:H121	1.83	0.60
19:e:118:LEU:HD13	27:e:611:CLA:H122	1.82	0.60
19:e:128:VAL:HG21	27:e:604:CLA:H18	1.84	0.60
1:A:205:SER:HB2	1:A:311:GLY:HA3	1.84	0.60
6:F:162:ILE:HD11	16:b:135:THR:HG22	1.82	0.60
34:L:208:LMG:H452	27:g:309:CLA:HAA1	1.83	0.59
19:e:120:GLN:OE1	27:e:605:CLA:ND	2.35	0.59
5:E:39:ARG:HG3	5:E:50:THR:HG22	1.85	0.59
16:b:33:ALA:HB2	16:b:51:VAL:HG13	1.85	0.59
27:A:842:CLA:H42	28:A:843:PQN:H191	1.82	0.59
18:f:114:THR:HB	36:f:617:IHT:C05	2.33	0.59
1:A:372:HIS:ND1	27:A:817:CLA:OBD	2.36	0.59
23:d:77:LEU:HD13	27:d:301:CLA:HBA2	1.85	0.59
27:m:609:CLA:H42	37:m:610:KC2:CED	2.33	0.58
34:s:210:LMG:H192	27:n:603:CLA:HBC1	1.85	0.58
4:D:42:VAL:HG22	4:D:52:ILE:HG12	1.86	0.58
18:m:147:THR:OG1	18:m:152:ARG:NH1	2.34	0.58
21:k:216:LYS:HD2	21:k:220:GLN:HB3	1.86	0.58
27:l:307:CLA:HMA3	27:l:307:CLA:H102	1.86	0.57
26:n:61:LEU:HD22	26:n:72:ASP:HB2	1.86	0.57
18:j:181:ASN:ND2	27:j:609:CLA:OBD	2.37	0.57
29:g:301:LHG:H312	29:g:301:LHG:H121	1.86	0.57
27:A:839:CLA:H71	29:A:850:LHG:HC12	1.85	0.57
22:i:143:LYS:HD2	22:i:147:SER:HB3	1.86	0.57
14:c:185:ARG:HB3	27:c:602:CLA:HBC2	1.85	0.57
18:f:126:MET:HE3	27:f:604:CLA:H3A	1.85	0.57
24:g:83:GLU:HG2	24:g:196:ILE:HD11	1.86	0.57
24:g:143:LEU:O	24:g:147:LEU:HB2	2.05	0.57
22:i:184:ASN:ND2	27:i:309:CLA:OBD	2.38	0.57
27:A:856:CLA:HMA1	34:c:619:LMG:HC92	1.86	0.57
4:D:64:ARG:NH2	4:D:66:GLU:OE1	2.38	0.57
21:k:145:LEU:HB2	27:k:306:CLA:HAC1	1.85	0.57
24:g:87:GLY:O	24:g:91:MET:HG3	2.05	0.57
27:B:836:CLA:H122	27:B:836:CLA:H51	1.87	0.56
27:B:838:CLA:HHC	27:B:838:CLA:HBB1	1.87	0.56
16:b:155:LEU:HD13	34:b:619:LMG:H131	1.87	0.56
27:A:820:CLA:HBC3	27:A:826:CLA:H171	1.87	0.56
19:e:87:VAL:HG11	27:e:607:CLA:H201	1.85	0.56
27:O:202:CLA:HHB	27:O:202:CLA:H42	1.86	0.56
12:K:26:LEU:HB2	27:e:611:CLA:H141	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:835:CLA:H101	7:I:23:MET:HE1	1.88	0.56
27:m:602:CLA:H93	27:m:603:CLA:H61	1.87	0.56
29:i:316:LHG:H242	29:i:316:LHG:H112	1.88	0.56
27:A:830:CLA:HMA2	9:L:19:THR:HG21	1.88	0.55
24:g:198:ASN:ND2	27:g:311:CLA:OBD	2.39	0.55
27:A:835:CLA:H191	27:L:203:CLA:H72	1.87	0.55
19:e:35:ASN:HB2	19:e:44:PRO:HD2	1.89	0.55
29:g:301:LHG:H101	29:g:301:LHG:H292	1.87	0.55
27:L:202:CLA:H41	27:g:308:CLA:H142	1.89	0.55
19:e:72:GLN:O	19:e:76:ILE:HG13	2.07	0.55
20:l:180:ARG:HA	20:l:183:MET:HE3	1.89	0.55
18:m:183:ARG:NH2	35:m:615:II0:O02	2.40	0.55
1:A:15:ILE:HD13	27:A:809:CLA:HAA2	1.88	0.55
6:F:28:ASP:N	6:F:32:LEU:O	2.40	0.55
22:i:142:PHE:HB3	37:i:317:KC2:CMC	2.36	0.55
27:A:852:CLA:H143	27:B:838:CLA:HBC3	1.89	0.54
9:L:140:ASN:HB3	27:g:308:CLA:HAA2	1.90	0.54
37:m:610:KC2:CBA	37:m:610:KC2:CBD	2.86	0.54
2:B:339:SER:HB3	27:B:820:CLA:H42	1.89	0.54
36:j:616:IHT:C06	29:j:617:LHG:H102	2.37	0.54
27:A:814:CLA:HBA2	27:d:305:CLA:HMA2	1.89	0.54
27:s:202:CLA:H61	27:s:202:CLA:H142	1.89	0.54
18:f:128:GLN:NE2	27:f:606:CLA:NA	2.56	0.54
27:i:308:CLA:H2A	27:i:308:CLA:HED2	1.90	0.54
27:j:603:CLA:H2	27:j:603:CLA:HED2	1.89	0.54
11:O:27:GLN:HB3	18:f:148:LEU:CB	2.36	0.54
13:s:7:GLY:HA2	16:b:136:ALA:O	2.07	0.54
2:B:398:ASP:OD1	4:D:131:GLN:NE2	2.41	0.53
11:O:32:PHE:CD1	11:O:32:PHE:C	2.85	0.53
2:B:18:ARG:NH1	39:B:907:HOH:O	2.41	0.53
9:L:6:LYS:HZ1	11:O:37:GLY:H	1.56	0.53
2:B:100:VAL:O	2:B:104:THR:OG1	2.27	0.53
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.91	0.53
27:g:302:CLA:HHD	36:g:319:IHT:C04	2.38	0.53
2:B:207:CYS:SG	2:B:208:TRP:N	2.82	0.53
27:B:808:CLA:HBA2	38:i:301:LMU:H41	1.90	0.53
36:c:620:IHT:O01	29:c:621:LHG:HC81	2.08	0.53
2:B:350:HIS:ND1	27:B:814:CLA:OBD	2.42	0.53
20:l:192:GLN:NE2	35:l:313:II0:O02	2.42	0.53
27:A:818:CLA:HBC2	27:A:828:CLA:H121	1.91	0.53
2:B:396:ASP:OD1	4:D:133:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:838:CLA:H41	9:L:80:PHE:HD2	1.72	0.53
27:B:803:CLA:H93	27:B:810:CLA:H2	1.91	0.52
21:k:114:ILE:HB	27:k:304:CLA:HMD2	1.91	0.52
24:g:66:VAL:HA	24:g:69:MET:HG3	1.91	0.52
27:A:837:CLA:H101	8:J:17:THR:HG23	1.90	0.52
6:F:112:ILE:HD12	29:J:107:LHG:H102	1.91	0.52
1:A:50:TRP:HE1	27:F:201:CLA:HBB1	1.75	0.52
16:b:61:VAL:HG23	16:b:62:ILE:HG13	1.92	0.52
10:M:29:TYR:O	10:M:30:GLN:NE2	2.43	0.52
18:j:94:ILE:HG23	18:j:204:LEU:HD11	1.91	0.52
18:j:137:GLU:HG2	27:j:607:CLA:C4B	2.40	0.52
23:d:208:ILE:HG22	23:d:209:THR:HG23	1.91	0.52
24:g:79:LEU:HD13	27:g:303:CLA:HBA2	1.91	0.52
29:c:621:LHG:H291	27:b:610:CLA:H93	1.91	0.52
15:a:82:GLU:OE2	15:a:145:LYS:NZ	2.36	0.52
20:l:168:LEU:HD21	20:l:172:ARG:HH21	1.73	0.52
18:j:107:VAL:HG21	27:j:605:CLA:HMB2	1.91	0.52
11:O:53:ILE:HG13	27:f:608:CLA:HMB2	1.91	0.52
18:f:126:MET:CE	27:f:604:CLA:H3A	2.40	0.52
1:A:532:THR:HG22	1:A:536:MET:HE2	1.92	0.51
1:A:268:THR:HB	12:K:16:TRP:HB2	1.93	0.51
14:c:84:ALA:HB2	27:c:607:CLA:HED2	1.93	0.51
27:A:818:CLA:H92	27:A:828:CLA:H91	1.92	0.51
3:C:29:VAL:HG12	4:D:113:ARG:HB3	1.92	0.51
29:J:107:LHG:H201	29:J:107:LHG:H141	1.93	0.51
24:g:218:LYS:HB3	24:g:222:GLN:HB2	1.92	0.51
27:A:802:CLA:HBA2	2:B:524:LEU:HD11	1.91	0.51
17:h:220:MET:HG2	17:h:223:ILE:HD12	1.93	0.51
21:k:209:HIS:HA	21:k:212:LEU:HD12	1.93	0.51
1:A:589:SER:OG	1:A:592:ASP:OD2	2.29	0.51
14:c:89:GLY:HA3	14:c:184:ALA:HB1	1.91	0.51
13:s:122:MET:HE1	27:s:208:CLA:HED2	1.92	0.51
21:k:120:MET:O	35:k:315:II0:O02	2.29	0.51
27:f:601:CLA:HHC	27:f:601:CLA:HBB1	1.92	0.51
24:g:85:LYS:NZ	24:g:158:ILE:HD11	2.25	0.51
27:A:827:CLA:H92	29:A:850:LHG:H223	1.92	0.50
11:O:24:VAL:HG13	11:O:42:LEU:CB	2.35	0.50
27:e:604:CLA:H151	27:e:607:CLA:HBC1	1.92	0.50
2:B:492:TRP:HH2	27:B:830:CLA:H2A	1.77	0.50
11:O:75:THR:HG22	29:f:619:LHG:H241	1.93	0.50
17:h:84:MET:HE1	27:h:306:CLA:CAB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:SER:OG	1:A:68:ASP:OD1	2.28	0.50
31:A:851:LMT:O2B	31:A:851:LMT:O6'	2.29	0.50
11:O:80:SER:O	11:O:84:ASN:ND2	2.45	0.50
27:m:609:CLA:H92	37:m:610:KC2:C1D	2.42	0.50
14:c:54:PRO:HG2	14:c:57:LEU:HD12	1.94	0.50
27:A:802:CLA:HBA1	27:A:839:CLA:HBB2	1.92	0.50
20:l:157:ASP:OD1	35:l:313:II0:O01	2.29	0.50
22:i:137:HIS:HB3	22:i:142:PHE:CD1	2.47	0.50
27:B:821:CLA:H52	27:B:840:CLA:H201	1.92	0.50
6:F:101:ASP:OD2	6:F:103:ARG:NH2	2.44	0.50
34:J:106:LMG:H312	31:b:616:LMT:H41	1.93	0.50
27:s:203:CLA:OBD	15:a:214:TYR:OH	2.29	0.50
1:A:121:ILE:HG13	1:A:122:VAL:HG13	1.94	0.49
2:B:204:GLN:NE2	2:B:205:HIS:O	2.44	0.49
27:B:849:CLA:HBC1	18:j:129:ILE:HB	1.93	0.49
18:f:144:LEU:HD22	27:f:608:CLA:HED2	1.93	0.49
2:B:225:PHE:O	27:B:849:CLA:H2A	2.11	0.49
21:k:140:ALA:HB2	27:k:304:CLA:HBC2	1.93	0.49
14:c:154:ARG:NH1	14:c:158:ASP:O	2.41	0.49
1:A:579:GLY:HA2	2:B:561:PRO:HD3	1.94	0.49
11:O:28:SER:O	11:O:28:SER:OG	2.27	0.49
27:f:608:CLA:HBB1	27:f:608:CLA:HMB1	1.94	0.49
18:f:116:VAL:HG11	27:f:604:CLA:HED2	1.93	0.49
23:d:144:THR:HA	23:d:147:THR:HG22	1.94	0.49
29:c:621:LHG:H252	27:b:610:CLA:H203	1.95	0.49
27:b:601:CLA:H2A	27:b:601:CLA:HED2	1.95	0.49
27:b:608:CLA:H3A	29:n:619:LHG:O9	2.13	0.49
27:b:608:CLA:H43	26:n:154:VAL:HG11	1.95	0.49
21:k:121:THR:HG21	21:k:208:VAL:HG23	1.95	0.49
34:L:208:LMG:H291	27:g:308:CLA:H2	1.95	0.49
24:g:39:SER:OG	24:g:42:ILE:O	2.26	0.49
9:L:136:ILE:HG23	29:L:207:LHG:H122	1.94	0.49
24:g:218:LYS:HD2	24:g:229:ASN:HD21	1.77	0.49
2:B:14:ASP:HB3	2:B:19:ARG:HB2	1.93	0.49
27:b:608:CLA:H122	27:b:608:CLA:H162	1.63	0.49
21:k:199:LEU:HD22	27:k:309:CLA:HMD1	1.94	0.49
23:d:121:ASP:HA	23:d:124:VAL:HG22	1.95	0.49
1:A:71:ARG:HG2	1:A:185:ALA:HB1	1.95	0.49
2:B:168:LYS:NZ	25:R:42:SER:OG	2.39	0.49
27:B:804:CLA:H151	27:B:824:CLA:HBB2	1.95	0.49
24:g:91:MET:HE3	24:g:198:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:19:PRO:HA	7:I:22:VAL:HG22	1.94	0.48
19:e:105:THR:HG23	19:e:108:GLU:H	1.78	0.48
27:A:839:CLA:O1A	27:A:839:CLA:H3A	2.13	0.48
2:B:93:PRO:HA	17:h:116:PRO:HB2	1.95	0.48
21:k:180:LEU:HD11	27:k:308:CLA:H11	1.94	0.48
6:F:116:LEU:HD23	29:J:107:LHG:H151	1.95	0.48
17:h:67:ARG:HD3	17:h:164:LYS:HB2	1.95	0.48
18:j:128:GLN:NE2	27:j:606:CLA:NA	2.61	0.48
1:A:219:GLN:HA	1:A:223:SER:HB2	1.95	0.48
16:b:66:TRP:CZ3	16:b:136:ALA:HA	2.48	0.48
27:e:602:CLA:HBA2	27:e:602:CLA:H3A	1.60	0.48
26:n:62:ASP:O	26:n:68:ASP:OD2	2.32	0.48
27:A:809:CLA:H2	27:A:811:CLA:HBC2	1.95	0.48
2:B:181:LEU:O	2:B:185:SER:OG	2.29	0.48
15:a:181:ARG:NH2	27:a:310:CLA:O1D	2.43	0.48
25:R:51:LYS:HD2	25:R:63:ASP:HB3	1.96	0.48
23:d:209:THR:HB	23:d:211:LYS:HD2	1.95	0.48
27:B:838:CLA:H141	27:B:838:CLA:H161	1.44	0.48
13:s:115:ALA:O	13:s:116:LEU:HB3	2.14	0.48
22:i:162:PHE:N	27:i:308:CLA:OBD	2.47	0.48
5:E:8:VAL:O	5:E:21:ILE:HA	2.14	0.48
27:h:305:CLA:HMA2	27:h:306:CLA:HBC1	1.96	0.48
22:i:98:GLN:HE22	27:i:305:CLA:C4D	2.27	0.48
1:A:513:GLY:HA2	1:A:527:PRO:HB3	1.95	0.47
27:A:836:CLA:H191	11:O:114:ILE:HG21	1.96	0.47
13:s:82:PHE:HB3	13:s:98:THR:HG21	1.96	0.47
2:B:706:LEU:HD23	33:B:842:DGD:HA21	1.96	0.47
27:a:308:CLA:H151	27:a:308:CLA:H111	1.47	0.47
17:h:219:GLY:O	27:h:308:CLA:ND	2.47	0.47
27:f:602:CLA:H3A	27:f:602:CLA:HBA2	1.62	0.47
1:A:543:PHE:O	1:A:547:VAL:HG12	2.14	0.47
28:B:841:PQN:H222	28:B:841:PQN:H262	1.27	0.47
27:i:303:CLA:HED2	27:i:303:CLA:H2A	1.96	0.47
26:n:92:HIS:NE2	27:n:603:CLA:NC	2.62	0.47
16:b:167:PHE:HZ	18:m:69:ILE:HD12	1.79	0.47
27:A:839:CLA:H122	29:A:850:LHG:H191	1.97	0.47
2:B:588:TRP:HE1	27:B:801:CLA:H52	1.80	0.47
27:F:202:CLA:H72	27:b:606:CLA:H11	1.96	0.47
27:f:608:CLA:H92	27:f:608:CLA:HAA1	1.96	0.47
1:A:116:GLN:NE2	27:A:808:CLA:OBD	2.46	0.47
14:c:57:LEU:HB3	14:c:64:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:e:607:CLA:H92	27:e:607:CLA:H61	1.76	0.47
1:A:574:ARG:NH2	27:A:829:CLA:O1D	2.48	0.47
11:O:27:GLN:HB3	18:f:148:LEU:CA	2.44	0.47
13:s:137:ASN:ND2	13:s:146:ASP:OD2	2.40	0.47
27:c:608:CLA:HBA2	27:c:608:CLA:H3A	1.36	0.47
18:m:183:ARG:HB3	27:m:602:CLA:HBC2	1.95	0.47
26:n:65:PHE:O	26:n:68:ASP:HB3	2.15	0.47
27:l:304:CLA:H3A	27:l:304:CLA:HBA2	1.66	0.47
27:k:308:CLA:H162	27:k:308:CLA:H122	1.62	0.47
24:g:41:ALA:O	27:g:302:CLA:NA	2.47	0.47
27:a:303:CLA:H3A	27:a:303:CLA:HBA2	1.55	0.47
27:m:606:CLA:HAC2	27:m:606:CLA:H203	1.97	0.47
27:f:610:CLA:H8	27:f:610:CLA:H52	1.54	0.47
4:D:88:ARG:HB3	4:D:96:GLN:HB3	1.97	0.46
8:J:41:PRO:HG2	27:J:105:CLA:HMD3	1.97	0.46
18:m:113:MET:O	18:m:116:VAL:HG22	2.15	0.46
22:i:136:GLU:O	22:i:140:ASN:ND2	2.48	0.46
27:a:304:CLA:HBA2	27:a:304:CLA:H3A	1.59	0.46
27:h:307:CLA:H62	27:h:307:CLA:H2	1.55	0.46
27:e:610:CLA:H161	27:e:610:CLA:H121	1.78	0.46
22:i:107:ALA:HA	22:i:119:GLN:HE22	1.80	0.46
29:j:617:LHG:H251	29:j:617:LHG:HC82	1.97	0.46
27:g:322:CLA:H62	27:g:322:CLA:H101	1.63	0.46
27:A:821:CLA:HBB1	27:O:202:CLA:H71	1.96	0.46
12:K:22:ALA:HA	19:e:119:ILE:HD11	1.98	0.46
20:l:164:ASN:HB3	20:l:167:ALA:HB3	1.97	0.46
27:g:322:CLA:H13	27:g:322:CLA:H172	1.77	0.46
26:n:160:MET:HE3	26:n:160:MET:HB3	1.86	0.46
27:B:835:CLA:H92	27:B:835:CLA:H61	1.80	0.46
18:j:116:VAL:HG11	27:j:604:CLA:HED2	1.97	0.46
11:O:27:GLN:CG	18:f:148:LEU:O	2.63	0.46
20:l:139:LEU:HB3	27:l:308:CLA:H3A	1.97	0.46
27:n:609:CLA:H41	27:n:609:CLA:H62	1.62	0.46
2:B:300:LEU:HD23	27:B:816:CLA:HED3	1.98	0.46
13:s:77:LEU:HD13	20:l:210:ILE:HG23	1.97	0.46
27:A:807:CLA:H122	27:A:807:CLA:H161	1.71	0.46
27:A:830:CLA:HBA1	27:A:830:CLA:H3A	1.76	0.46
27:f:610:CLA:H51	37:f:611:KC2:CMD	2.46	0.46
27:A:817:CLA:HBA2	27:A:817:CLA:H3A	1.67	0.46
22:i:217:GLN:O	35:i:318:II0:O02	2.34	0.46
2:B:256:PHE:HE2	2:B:492:TRP:HE3	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:683:ARG:HD2	9:L:16:ASN:HD22	1.81	0.46
27:B:804:CLA:H112	27:B:804:CLA:H152	1.73	0.46
5:E:25:ALA:HB3	5:E:37:VAL:HB	1.98	0.46
6:F:116:LEU:HG	29:J:107:LHG:H132	1.97	0.46
16:b:191:VAL:HG13	16:b:211:MET:HE3	1.98	0.46
27:s:202:CLA:H72	27:s:202:CLA:H112	1.75	0.45
29:c:621:LHG:H261	27:b:610:CLA:H171	1.98	0.45
27:k:309:CLA:H3A	27:k:309:CLA:HBA2	1.80	0.45
27:A:824:CLA:H172	27:A:824:CLA:H13	1.80	0.45
34:b:619:LMG:H142	27:m:603:CLA:H12	1.97	0.45
27:f:609:CLA:H41	27:f:609:CLA:H61	1.79	0.45
27:s:208:CLA:HMB3	27:m:612:CLA:HBC1	1.99	0.45
17:h:92:MET:O	17:h:96:MET:HB2	2.16	0.45
21:k:162:THR:HG22	21:k:168:ARG:HG3	1.99	0.45
1:A:332:LYS:HB3	1:A:339:GLY:HA3	1.98	0.45
27:B:820:CLA:H62	27:B:820:CLA:H41	1.52	0.45
29:a:319:LHG:H182	29:a:319:LHG:H212	1.76	0.45
27:b:603:CLA:H202	27:b:603:CLA:H161	1.83	0.45
2:B:398:ASP:O	2:B:402:ASN:ND2	2.39	0.45
16:b:187:HIS:HA	16:b:190:ILE:HD12	1.97	0.45
27:h:301:CLA:H52	27:h:301:CLA:H8	1.68	0.45
21:k:213:LEU:HG	37:k:311:KC2:CGA	2.46	0.45
27:f:607:CLA:H3A	27:f:607:CLA:HBA2	1.48	0.45
27:f:608:CLA:H161	27:f:608:CLA:H122	1.59	0.45
1:A:56:VAL:HG21	27:A:803:CLA:C2D	2.47	0.45
27:A:852:CLA:HBB1	27:A:852:CLA:HMB3	1.99	0.45
27:B:809:CLA:HHC	27:B:809:CLA:HBB1	1.98	0.45
11:O:33:GLU:HA	11:O:39:PRO:HA	1.98	0.45
27:e:604:CLA:H13	27:e:604:CLA:H102	1.60	0.45
27:l:303:CLA:HBA2	29:l:318:LHG:HC92	1.98	0.45
21:k:100:SER:OG	21:k:120:MET:HE2	2.17	0.45
29:f:619:LHG:H311	29:f:619:LHG:H281	1.82	0.45
24:g:85:LYS:HZ1	24:g:158:ILE:HD11	1.81	0.45
1:A:351:TRP:HB3	27:A:804:CLA:HAC1	1.99	0.45
27:A:824:CLA:H62	27:A:824:CLA:H102	1.77	0.45
27:e:606:CLA:H93	27:e:606:CLA:H62	1.89	0.45
27:A:821:CLA:HMB1	27:A:822:CLA:H12	1.97	0.45
27:B:834:CLA:H121	27:B:834:CLA:H162	1.83	0.45
9:L:64:LYS:NZ	9:L:145:GLN:O	2.50	0.45
27:c:606:CLA:HBA1	34:c:619:LMG:H441	1.98	0.45
29:f:619:LHG:H332	29:f:619:LHG:H362	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:MET:HE1	27:A:824:CLA:H151	1.99	0.45
27:A:829:CLA:H61	27:A:829:CLA:H41	1.69	0.45
27:e:601:CLA:H3A	27:e:601:CLA:HBA2	1.38	0.45
27:l:304:CLA:H202	27:l:304:CLA:H161	1.89	0.45
27:A:840:CLA:H111	27:A:840:CLA:H151	1.72	0.44
2:B:139:LEU:HD22	10:M:13:LEU:HD12	2.00	0.44
27:B:838:CLA:H111	27:B:838:CLA:H142	1.60	0.44
12:K:35:GLY:HA2	12:K:38:VAL:HG22	1.99	0.44
27:b:611:CLA:H2	27:b:611:CLA:H102	1.99	0.44
27:B:816:CLA:H102	27:B:822:CLA:H11	1.99	0.44
6:F:162:ILE:HD12	34:F:206:LMG:H111	1.99	0.44
27:F:202:CLA:H101	27:F:202:CLA:H61	1.66	0.44
34:c:619:LMG:H202	34:c:619:LMG:H171	1.75	0.44
17:h:136:LEU:HD21	27:h:301:CLA:H102	2.00	0.44
27:m:606:CLA:HBA2	27:l:312:CLA:HBD	1.99	0.44
1:A:482:LYS:HA	1:A:482:LYS:HD3	1.79	0.44
2:B:610:GLU:OE1	6:F:44:ARG:NH2	2.38	0.44
27:m:603:CLA:H92	27:m:603:CLA:H62	1.84	0.44
18:f:183:ARG:HA	18:f:186:MET:HE3	1.98	0.44
27:A:831:CLA:HBB1	27:A:832:CLA:H2	1.99	0.44
34:J:106:LMG:H452	34:J:106:LMG:H421	1.86	0.44
9:L:6:LYS:HE3	9:L:6:LYS:HB2	1.46	0.44
9:L:146:THR:HB	9:L:149:MET:HB3	2.00	0.44
27:b:606:CLA:H62	27:b:606:CLA:H41	1.81	0.44
21:k:120:MET:HE1	21:k:207:MET:HB3	2.00	0.44
27:j:609:CLA:H13	37:j:610:KC2:C4B	2.47	0.44
27:A:820:CLA:H2	27:A:820:CLA:H62	1.60	0.44
27:A:842:CLA:H112	27:A:842:CLA:H142	1.77	0.44
27:B:835:CLA:H41	27:B:835:CLA:H62	1.60	0.44
4:D:135:THR:HG22	4:D:137:LYS:H	1.82	0.44
27:F:203:CLA:HBA1	27:F:203:CLA:H3A	1.38	0.44
27:k:301:CLA:H3A	27:k:301:CLA:HBA2	1.68	0.44
18:j:61:PHE:HE1	27:j:601:CLA:HBC3	1.82	0.44
18:j:66:LEU:HA	18:j:69:ILE:HD12	1.99	0.44
26:n:103:ILE:HG23	26:n:125:ILE:HG21	1.99	0.44
2:B:573:ASP:OD1	2:B:705:ARG:NH1	2.51	0.44
27:B:803:CLA:HBA1	27:B:803:CLA:H3A	1.69	0.44
27:B:826:CLA:HBA2	27:B:826:CLA:H3A	1.51	0.44
27:B:834:CLA:H112	27:B:835:CLA:H142	1.98	0.44
16:b:103:ALA:O	35:b:613:II0:O01	2.35	0.44
27:m:603:CLA:HBA1	27:m:603:CLA:H3A	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:193:VAL:HG21	36:j:616:IHT:C31	2.48	0.44
27:A:853:CLA:H172	6:F:128:GLY:HA2	1.99	0.44
2:B:394:VAL:HG23	2:B:540:ALA:HB1	1.99	0.44
11:O:29:LYS:HD2	11:O:29:LYS:C	2.43	0.44
27:c:604:CLA:H191	27:c:608:CLA:HMD2	1.98	0.44
27:e:606:CLA:H151	27:e:606:CLA:H111	1.86	0.44
27:k:307:CLA:H122	27:k:307:CLA:H162	1.56	0.44
9:L:6:LYS:NZ	11:O:37:GLY:H	2.15	0.44
13:s:142:HIS:NE2	13:s:150:ASP:OD2	2.32	0.44
27:A:837:CLA:HBA2	27:A:837:CLA:H3A	1.60	0.44
27:B:820:CLA:H143	27:B:820:CLA:H112	1.78	0.44
27:s:206:CLA:H201	29:c:621:LHG:H271	2.00	0.44
34:s:210:LMG:H361	34:s:210:LMG:H332	1.83	0.44
19:e:83:MET:SD	27:e:607:CLA:HAB	2.58	0.44
20:l:196:THR:HB	20:l:198:GLN:HG2	2.00	0.44
27:f:601:CLA:H3A	27:f:601:CLA:HBA2	1.75	0.44
22:i:100:ILE:HD11	22:i:207:ILE:HG21	2.00	0.44
27:j:609:CLA:H12	27:j:609:CLA:H51	1.77	0.44
1:A:516:VAL:HG22	1:A:526:MET:HB2	2.00	0.43
27:A:801:CLA:HED3	27:A:801:CLA:HBD	1.65	0.43
27:F:202:CLA:HBC2	8:J:20:LEU:HD11	2.00	0.43
30:s:205:WVN:C20	27:b:605:CLA:HAB	2.48	0.43
27:m:603:CLA:HMA1	27:m:603:CLA:H2	1.99	0.43
27:m:609:CLA:H92	37:m:610:KC2:ND	2.33	0.43
27:i:302:CLA:HBA2	27:i:302:CLA:H3A	1.55	0.43
27:i:303:CLA:H3A	27:i:303:CLA:HBA2	1.44	0.43
26:n:105:VAL:HG13	26:n:110:ILE:HB	1.99	0.43
2:B:710:ILE:HD13	27:B:835:CLA:HED2	1.99	0.43
27:B:801:CLA:H62	27:B:801:CLA:H2	1.69	0.43
27:B:836:CLA:H122	27:B:836:CLA:H8	1.81	0.43
27:i:311:CLA:H3A	27:i:311:CLA:HBA2	1.67	0.43
1:A:83:ILE:HG12	27:A:808:CLA:H162	2.00	0.43
27:A:818:CLA:HBA2	27:A:818:CLA:H3A	1.74	0.43
22:i:141:ASN:O	22:i:142:PHE:HB2	2.18	0.43
2:B:668:GLY:O	2:B:672:GLU:HG3	2.18	0.43
27:a:312:CLA:HBA2	27:a:312:CLA:H11	1.62	0.43
27:b:606:CLA:H91	27:b:606:CLA:H112	1.78	0.43
24:g:215:LEU:HD12	24:g:216:THR:HG23	2.00	0.43
27:F:202:CLA:HED3	27:b:603:CLA:H13	2.00	0.43
27:c:602:CLA:HBA2	27:c:602:CLA:H3A	1.54	0.43
27:l:309:CLA:H3A	27:l:309:CLA:HBA2	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:75:LEU:HB3	27:j:602:CLA:H3A	2.00	0.43
2:B:337:LEU:HD21	27:B:825:CLA:HAB	2.01	0.43
2:B:541:ARG:NH2	4:D:128:ASN:OD1	2.52	0.43
14:c:64:ASP:OD1	14:c:66:GLY:N	2.44	0.43
20:l:107:THR:H	20:l:110:ASP:HB2	1.84	0.43
20:l:132:PHE:CE1	20:l:139:LEU:HD11	2.53	0.43
21:k:74:SER:HB3	27:k:301:CLA:HBA1	2.01	0.43
27:k:308:CLA:HAA1	27:k:308:CLA:HED2	1.99	0.43
18:f:39:SER:OG	18:f:60:GLY:O	2.28	0.43
27:f:602:CLA:H62	27:f:602:CLA:H101	1.83	0.43
27:f:610:CLA:H202	27:f:610:CLA:H161	1.88	0.43
1:A:63:THR:HG21	1:A:68:ASP:HB2	2.00	0.43
2:B:21:TRP:CG	2:B:703:GLN:HE22	2.36	0.43
4:D:102:ASP:OD1	4:D:102:ASP:N	2.49	0.43
6:F:112:ILE:HG23	29:J:107:LHG:H102	2.01	0.43
18:j:97:ASP:HB2	18:j:204:LEU:HD12	2.00	0.43
27:j:609:CLA:H3A	27:j:609:CLA:HBA2	1.63	0.43
23:d:99:ASP:HB2	23:d:214:ILE:HD11	2.00	0.43
27:A:811:CLA:H12	27:A:811:CLA:HBA2	1.87	0.43
27:c:601:CLA:H12	27:c:601:CLA:NA	2.34	0.43
27:b:611:CLA:H142	27:b:611:CLA:H111	1.85	0.43
27:m:609:CLA:H12	27:m:609:CLA:H51	1.81	0.43
27:l:307:CLA:H11	27:l:307:CLA:HBA1	1.84	0.43
21:k:126:LYS:HD2	21:k:126:LYS:HA	1.81	0.43
27:j:606:CLA:HBA2	27:j:606:CLA:HED2	2.01	0.43
27:n:610:CLA:H3A	27:n:610:CLA:HBA2	1.56	0.43
2:B:2:THR:HB	7:I:33:ASP:HA	2.00	0.43
11:O:29:LYS:HE2	18:f:71:ASP:HB2	2.01	0.43
27:c:603:CLA:H3A	27:c:603:CLA:HBA1	1.72	0.43
27:A:806:CLA:OBD	27:A:856:CLA:HHD	2.19	0.42
27:A:842:CLA:H141	27:A:842:CLA:H161	1.83	0.42
11:O:68:TYR:CZ	11:O:73:LEU:HB2	2.53	0.42
27:b:610:CLA:H152	27:b:610:CLA:H18	1.61	0.42
18:m:61:PHE:HE1	27:m:601:CLA:HBC3	1.83	0.42
27:e:611:CLA:H72	27:e:611:CLA:H112	1.57	0.42
29:l:318:LHG:H241	29:l:318:LHG:H271	1.60	0.42
21:k:119:LYS:HA	21:k:119:LYS:HD3	1.63	0.42
27:f:608:CLA:H62	27:f:608:CLA:H101	1.83	0.42
1:A:251:LEU:HD12	1:A:252:MET:N	2.34	0.42
27:A:839:CLA:H51	29:A:850:LHG:HC31	2.00	0.42
27:A:855:CLA:H61	27:A:855:CLA:H41	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:e:604:CLA:H3A	27:e:604:CLA:HBA2	1.79	0.42
26:n:149:GLU:HG2	27:n:608:CLA:NB	2.33	0.42
2:B:267:LEU:HD13	27:B:814:CLA:HMA2	2.01	0.42
9:L:44:LEU:HD23	24:g:70:LEU:HD23	2.01	0.42
18:m:47:LYS:HA	18:m:48:PRO:HD3	1.87	0.42
18:m:116:VAL:HG11	27:m:604:CLA:HED2	2.01	0.42
21:k:138:ALA:HA	27:k:304:CLA:HBC1	2.00	0.42
27:i:302:CLA:HHC	27:i:302:CLA:HBB1	2.02	0.42
24:g:147:LEU:O	24:g:151:GLU:HB2	2.19	0.42
28:A:843:PQN:H222	28:A:843:PQN:H262	1.25	0.42
2:B:422:SER:HA	2:B:531:LEU:HD11	2.01	0.42
27:l:310:CLA:H102	37:l:311:KC2:ND	2.33	0.42
27:n:610:CLA:H111	27:n:610:CLA:H72	1.74	0.42
2:B:70:GLN:HG2	7:I:1:MET:HE2	2.02	0.42
27:a:306:CLA:H143	27:a:306:CLA:H111	1.83	0.42
27:A:802:CLA:CBA	27:A:839:CLA:HBB2	2.50	0.42
27:A:804:CLA:HBA1	27:A:804:CLA:H3A	1.69	0.42
27:A:855:CLA:H111	27:B:834:CLA:H62	2.00	0.42
2:B:693:LYS:HE3	2:B:693:LYS:HB3	1.83	0.42
27:B:815:CLA:H61	27:B:815:CLA:H102	1.65	0.42
27:B:836:CLA:H51	27:B:836:CLA:H8	1.82	0.42
13:s:80:SER:OG	13:s:84:ASN:ND2	2.49	0.42
14:c:43:ASP:OD1	14:c:43:ASP:N	2.53	0.42
27:m:609:CLA:H72	37:m:610:KC2:C1D	2.50	0.42
18:f:172:LYS:HA	18:f:172:LYS:HD2	1.65	0.42
23:d:119:LEU:HD21	27:d:303:CLA:HED2	2.02	0.42
27:A:852:CLA:H151	27:B:802:CLA:H202	2.01	0.42
2:B:25:ALA:HB2	33:B:842:DGD:HA62	2.02	0.42
27:a:312:CLA:H143	27:a:312:CLA:H112	1.67	0.42
19:e:119:ILE:HD13	19:e:119:ILE:HA	1.79	0.42
27:L:203:CLA:H162	27:L:203:CLA:H121	1.94	0.42
21:k:120:MET:HG3	21:k:121:THR:HG23	2.01	0.42
6:F:154:LEU:HA	6:F:157:VAL:HG22	2.01	0.42
27:e:606:CLA:H161	27:e:606:CLA:H141	1.82	0.42
20:l:134:SER:HB2	20:l:154:PHE:CD1	2.55	0.42
22:i:144:MET:HG2	22:i:145:SER:H	1.84	0.42
23:d:128:SER:OG	27:d:304:CLA:OBD	2.35	0.42
23:d:132:MET:HE3	27:d:305:CLA:HAC1	2.01	0.42
24:g:94:ALA:HA	24:g:206:ILE:HD13	2.01	0.42
27:A:853:CLA:H62	27:A:853:CLA:H102	1.86	0.42
2:B:364:TYR:HB3	2:B:601:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:312:CLA:H61	27:a:312:CLA:H102	1.51	0.42
17:h:172:ALA:HB1	17:h:176:PRO:HG3	2.02	0.42
18:f:85:ILE:HD12	27:f:608:CLA:HMD3	2.00	0.42
18:j:80:ILE:HG21	18:j:155:GLY:HA3	2.02	0.42
1:A:747:LEU:HD23	1:A:747:LEU:HA	1.81	0.41
27:A:839:CLA:HMB3	27:A:839:CLA:HBB1	2.02	0.41
4:D:30:LYS:HG2	4:D:89:ILE:HB	2.02	0.41
27:b:608:CLA:H62	27:b:608:CLA:H41	1.86	0.41
27:h:306:CLA:H101	27:h:306:CLA:H61	1.62	0.41
27:m:603:CLA:H62	27:m:603:CLA:H41	1.80	0.41
22:i:103:LEU:HA	22:i:104:PRO:HD3	1.92	0.41
1:A:32:PRO:HB3	27:A:842:CLA:HAC1	2.01	0.41
27:B:829:CLA:H2	27:B:829:CLA:H61	1.67	0.41
29:a:301:LHG:H162	29:a:301:LHG:H191	1.91	0.41
16:b:66:TRP:CZ3	16:b:139:MET:HE2	2.56	0.41
27:e:610:CLA:CAD	27:f:606:CLA:H3A	2.50	0.41
18:j:183:ARG:NH2	35:j:615:II0:O01	2.44	0.41
27:j:602:CLA:HAB	27:j:602:CLA:HHC	1.84	0.41
27:A:802:CLA:HBA1	27:A:802:CLA:H11	1.67	0.41
27:A:839:CLA:H41	27:A:839:CLA:H61	1.77	0.41
27:A:856:CLA:NA	29:b:617:LHG:O4	2.53	0.41
2:B:256:PHE:CE2	2:B:492:TRP:HB3	2.55	0.41
9:L:76:LEU:HD21	35:h:312:II0:C24	2.50	0.41
14:c:86:LEU:HD23	14:c:86:LEU:HA	1.90	0.41
14:c:167:ALA:HB2	27:c:608:CLA:HBA1	2.01	0.41
27:a:303:CLA:H41	27:a:303:CLA:H61	1.80	0.41
27:a:311:CLA:H111	27:a:311:CLA:H152	1.84	0.41
21:k:128:LEU:HG	21:k:141:MET:HG3	2.01	0.41
22:i:187:LEU:HD12	27:i:309:CLA:HHD	2.02	0.41
27:j:607:CLA:HMB1	27:j:607:CLA:HBB1	2.01	0.41
29:J:107:LHG:H201	29:J:107:LHG:H171	1.75	0.41
13:s:7:GLY:HA3	16:b:139:MET:O	2.20	0.41
14:c:112:LYS:HA	14:c:112:LYS:HD2	1.94	0.41
21:k:97:ALA:HB2	21:k:204:VAL:HG23	2.02	0.41
22:i:128:ILE:HG12	27:i:306:CLA:HBC3	2.02	0.41
27:n:607:CLA:H111	27:n:607:CLA:H151	1.55	0.41
29:e:617:LHG:H262	29:e:617:LHG:H292	1.89	0.41
21:k:194:ILE:HD13	21:k:194:ILE:HA	1.88	0.41
27:f:610:CLA:HBD	37:f:611:KC2:CAD	2.50	0.41
35:f:616:II0:C21	29:g:301:LHG:HC61	2.50	0.41
1:A:607:VAL:HG21	27:A:801:CLA:H202	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ALA:HB3	27:A:802:CLA:HBB2	2.01	0.41
27:A:802:CLA:HMB3	27:A:802:CLA:HHB	1.83	0.41
27:A:838:CLA:H62	27:A:838:CLA:H41	1.91	0.41
16:b:211:MET:HE2	16:b:211:MET:HB2	1.99	0.41
17:h:142:VAL:O	17:h:146:SER:OG	2.34	0.41
27:h:306:CLA:H91	27:h:306:CLA:H111	1.81	0.41
27:e:605:CLA:H151	27:e:605:CLA:H18	1.86	0.41
22:i:137:HIS:CB	22:i:142:PHE:CE1	3.03	0.41
26:n:198:LEU:HD12	27:n:610:CLA:HAC2	2.03	0.41
27:A:841:CLA:H112	27:A:841:CLA:H151	1.76	0.41
27:L:202:CLA:H3A	27:L:202:CLA:HBA2	1.68	0.41
21:k:77:CYS:SG	21:k:78:ASN:N	2.94	0.41
18:f:169:GLU:H	18:f:169:GLU:HG3	1.67	0.41
27:n:610:CLA:H201	35:n:614:II0:C23	2.51	0.41
1:A:446:ILE:HD13	1:A:446:ILE:HA	1.91	0.41
2:B:256:PHE:CE2	2:B:492:TRP:HE3	2.39	0.41
2:B:570:SER:OG	2:B:573:ASP:OD2	2.30	0.41
27:B:812:CLA:H12	27:B:812:CLA:H52	1.69	0.41
29:b:617:LHG:H132	29:b:617:LHG:H101	1.68	0.41
18:m:40:GLU:HG2	27:m:601:CLA:HED1	2.02	0.41
27:g:311:CLA:H2A	27:g:311:CLA:HED3	2.03	0.41
26:n:99:ALA:O	26:n:103:ILE:HG12	2.21	0.41
1:A:320:ILE:HD13	12:K:64:ALA:HB2	2.03	0.41
1:A:371:HIS:HA	1:A:374:TYR:CE2	2.56	0.41
1:A:675:PHE:CZ	1:A:679:HIS:HE1	2.39	0.41
27:A:837:CLA:H91	27:A:837:CLA:H111	1.92	0.41
27:A:855:CLA:H13	27:A:855:CLA:H101	1.84	0.41
7:I:30:ILE:HG13	7:I:31:GLU:HG3	2.02	0.41
9:L:44:LEU:HD23	24:g:71:PRO:HD3	2.02	0.41
27:s:202:CLA:HAB	15:a:103:PHE:HZ	1.86	0.41
34:s:210:LMG:H362	34:s:210:LMG:H391	1.89	0.41
31:a:320:LMT:H81	31:a:320:LMT:H111	1.49	0.41
27:h:306:CLA:H62	27:h:306:CLA:H2	1.81	0.41
19:e:157:ALA:HB1	19:e:161:MET:HB3	2.02	0.41
27:e:611:CLA:H93	27:e:611:CLA:H111	1.92	0.41
27:l:308:CLA:HHC	27:l:308:CLA:HAB	1.87	0.41
36:f:617:IHT:C19	29:g:301:LHG:H281	2.51	0.41
26:n:38:LEU:HB3	26:n:39:TRP:H	1.71	0.41
26:n:101:ALA:HB1	27:n:604:CLA:HBC2	2.02	0.41
32:A:854:SF4:FE1	2:B:567:CYS:SG	1.84	0.41
14:c:92:ALA:O	14:c:96:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:m:602:CLA:HBA2	27:m:602:CLA:H3A	1.77	0.41
19:e:71:LEU:HD23	19:e:71:LEU:HA	1.95	0.41
18:j:61:PHE:CE1	27:j:601:CLA:HBC3	2.56	0.41
25:R:118:TRP:CD1	25:R:121:HIS:HE1	2.38	0.41
26:n:212:ILE:HG22	27:n:613:CLA:HED3	2.03	0.41
1:A:654:TRP:CZ2	2:B:628:SER:HB3	2.57	0.40
27:A:809:CLA:HBB2	27:A:812:CLA:HMA2	2.03	0.40
2:B:153:TRP:CD1	10:M:23:ARG:HG2	2.56	0.40
27:B:831:CLA:H51	27:B:831:CLA:H11	1.75	0.40
20:l:73:LEU:HB3	27:l:304:CLA:H3A	2.03	0.40
18:f:152:ARG:NE	18:f:156:ASP:O	2.53	0.40
27:g:322:CLA:H91	27:g:322:CLA:H112	1.78	0.40
27:A:816:CLA:H122	27:A:816:CLA:H8	1.94	0.40
27:A:827:CLA:H152	27:A:837:CLA:H42	2.02	0.40
27:A:838:CLA:HHC	27:A:838:CLA:HAB	1.89	0.40
27:B:836:CLA:H52	27:B:836:CLA:H11	1.71	0.40
27:L:206:CLA:HBB1	27:g:322:CLA:H143	2.02	0.40
27:b:603:CLA:H61	27:b:603:CLA:H41	1.61	0.40
27:h:306:CLA:H192	27:h:306:CLA:H161	1.90	0.40
19:e:198:PHE:HZ	27:e:610:CLA:H2A	1.86	0.40
27:k:307:CLA:H91	27:k:307:CLA:H111	1.87	0.40
27:f:604:CLA:H91	27:f:604:CLA:H111	1.88	0.40
27:n:604:CLA:H61	27:n:604:CLA:H41	1.88	0.40
1:A:161:TRP:CE2	27:A:815:CLA:HAA2	2.56	0.40
27:A:823:CLA:H61	27:A:823:CLA:H41	1.81	0.40
27:A:826:CLA:H61	27:A:826:CLA:H2	1.63	0.40
27:B:804:CLA:H61	27:B:804:CLA:H2	1.84	0.40
27:b:611:CLA:H3A	29:b:617:LHG:H312	2.03	0.40
27:f:602:CLA:H143	27:f:602:CLA:H162	1.88	0.40
27:B:802:CLA:H72	27:B:802:CLA:H112	1.88	0.40
5:E:30:SER:HB2	5:E:32:ILE:HG12	2.03	0.40
34:J:106:LMG:H191	34:J:106:LMG:H162	1.89	0.40
9:L:136:ILE:HG12	29:L:207:LHG:H101	2.03	0.40
14:c:191:ILE:HD12	14:c:191:ILE:HA	1.95	0.40
16:b:180:MET:HG3	36:b:614:IHT:C29	2.51	0.40
29:b:617:LHG:H131	29:b:617:LHG:H212	2.04	0.40
20:l:139:LEU:HB3	27:l:308:CLA:CMA	2.51	0.40
20:l:195:LEU:HD21	20:l:210:ILE:HD11	2.03	0.40
18:f:175:GLN:O	18:f:179:ILE:HG12	2.22	0.40
24:g:193:LEU:HA	24:g:196:ILE:HG22	2.04	0.40
27:A:802:CLA:H91	27:A:802:CLA:H111	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:840:CLA:HHC	27:A:840:CLA:HBB1	2.03	0.40
4:D:34:THR:O	4:D:84:TYR:HA	2.21	0.40
27:s:206:CLA:H143	27:b:608:CLA:HAC2	2.03	0.40
27:a:308:CLA:H111	27:a:308:CLA:H91	1.86	0.40
16:b:146:VAL:HB	16:b:149:ASP:HB3	2.03	0.40
29:b:617:LHG:H211	29:b:617:LHG:H182	1.89	0.40
19:e:96:HIS:CG	19:e:102:ALA:HB2	2.57	0.40
19:e:117:ALA:O	19:e:121:ILE:HG12	2.21	0.40
21:k:196:ASN:HD21	37:k:310:KC2:CHA	2.34	0.40
27:f:607:CLA:H202	27:f:607:CLA:H161	1.90	0.40
26:n:51:VAL:HG23	26:n:52:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	720 (97%)	20 (3%)	0	100	100
2	B	731/734 (100%)	705 (96%)	26 (4%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/141 (97%)	133 (97%)	4 (3%)	0	100	100
5	E	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
6	F	159/188 (85%)	156 (98%)	3 (2%)	0	100	100
7	I	32/36 (89%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
9	L	149/153 (97%)	148 (99%)	1 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	102/146 (70%)	94 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	s	152/269 (56%)	145 (95%)	7 (5%)	0	100	100
14	c	168/216 (78%)	162 (96%)	6 (4%)	0	100	100
15	a	173/216 (80%)	166 (96%)	7 (4%)	0	100	100
16	b	192/223 (86%)	188 (98%)	4 (2%)	0	100	100
17	h	160/225 (71%)	156 (98%)	4 (2%)	0	100	100
18	f	172/212 (81%)	166 (96%)	6 (4%)	0	100	100
18	j	170/212 (80%)	163 (96%)	7 (4%)	0	100	100
18	m	172/212 (81%)	164 (95%)	8 (5%)	0	100	100
19	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
20	l	173/238 (73%)	169 (98%)	4 (2%)	0	100	100
21	k	158/241 (66%)	151 (96%)	7 (4%)	0	100	100
22	i	171/218 (78%)	161 (94%)	9 (5%)	1 (1%)	21	45
23	d	123/213 (58%)	122 (99%)	1 (1%)	0	100	100
24	g	217/255 (85%)	202 (93%)	15 (7%)	0	100	100
25	R	88/129 (68%)	85 (97%)	3 (3%)	0	100	100
26	n	179/219 (82%)	172 (96%)	7 (4%)	0	100	100
All	All	4954/5955 (83%)	4788 (97%)	165 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	i	142	PHE

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	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	593/593 (100%)	587 (99%)	6 (1%)	68 81
3	C	67/68 (98%)	67 (100%)	0	100 100
4	D	115/117 (98%)	115 (100%)	0	100 100
5	E	55/58 (95%)	54 (98%)	1 (2%)	51 72
6	F	133/157 (85%)	133 (100%)	0	100 100
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 84
10	M	25/25 (100%)	24 (96%)	1 (4%)	28 53
11	O	81/110 (74%)	78 (96%)	3 (4%)	30 55
12	K	52/66 (79%)	51 (98%)	1 (2%)	50 71
13	s	116/195 (60%)	114 (98%)	2 (2%)	53 73
14	c	138/171 (81%)	138 (100%)	0	100 100
15	a	139/165 (84%)	139 (100%)	0	100 100
16	b	149/168 (89%)	144 (97%)	5 (3%)	32 58
17	h	123/162 (76%)	123 (100%)	0	100 100
18	f	135/161 (84%)	131 (97%)	4 (3%)	36 61
18	j	136/161 (84%)	133 (98%)	3 (2%)	45 69
18	m	137/161 (85%)	131 (96%)	6 (4%)	25 50
19	e	130/155 (84%)	130 (100%)	0	100 100
20	l	137/191 (72%)	136 (99%)	1 (1%)	76 86
21	k	122/186 (66%)	119 (98%)	3 (2%)	42 66
22	i	138/168 (82%)	135 (98%)	3 (2%)	45 69
23	d	97/157 (62%)	94 (97%)	3 (3%)	35 60
24	g	171/199 (86%)	166 (97%)	5 (3%)	37 62
25	R	69/98 (70%)	68 (99%)	1 (1%)	59 76
26	n	140/163 (86%)	134 (96%)	6 (4%)	26 51
All	All	3996/4665 (86%)	3938 (98%)	58 (2%)	55 75

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	VAL

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Mol	Chain	Res	Type
1	A	629	THR
1	A	736	LEU
2	B	360	ILE
2	B	440	ASP
2	B	442	VAL
2	B	491	ILE
2	B	524	LEU
2	B	531	LEU
5	E	58	VAL
9	L	6	LYS
10	M	30	GLN
11	O	24	VAL
11	O	28	SER
11	O	30	SER
12	K	36	ARG
13	s	86	GLU
13	s	87	VAL
16	b	51	VAL
16	b	134	LEU
16	b	197	ILE
16	b	198	GLU
16	b	213	LEU
18	m	107	VAL
18	m	108	VAL
18	m	123	GLN
18	m	178	GLU
18	m	199	THR
18	m	204	LEU
20	l	149	ARG
21	k	90	CYS
21	k	103	GLN
21	k	194	ILE
18	f	81	LYS
18	f	169	GLU
18	f	172	LYS
18	f	173	ARG
22	i	79	GLU
22	i	101	VAL
22	i	120	VAL
18	j	97	ASP
18	j	100	THR
18	j	123	GLN

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Mol	Chain	Res	Type
23	d	96	ILE
23	d	99	ASP
23	d	119	LEU
24	g	76	VAL
24	g	114	ASP
24	g	117	MET
24	g	118	THR
24	g	120	VAL
25	R	98	THR
26	n	41	GLU
26	n	44	ILE
26	n	52	ILE
26	n	62	ASP
26	n	68	ASP
26	n	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	ASN
1	A	717	GLN
2	B	75	GLN
2	B	113	ASN
2	B	438	HIS
2	B	632	ASN
2	B	635	ASN
4	D	8	GLN
4	D	140	ASN
9	L	3	GLN
10	M	6	GLN
10	M	30	GLN
19	e	78	ASN
20	l	66	ASN
18	f	76	GLN
22	i	217	GLN
24	g	100	GLN
26	n	129	HIS
26	n	179	GLN
26	n	189	GLN
26	n	208	HIS

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

407 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	$\#\|Z\| > 2$
35	II0	n	614	-	39,43,43	6.72	21 (53%)	48,60,60	2.20	14 (29%)
27	CLA	e	603	19	55,59,73	1.31	6 (10%)	64,96,113	1.44	8 (12%)
37	KC2	f	611	18	49,53,53	2.75	19 (38%)	60,89,89	3.79	32 (53%)
30	WVN	B	843	-	40,41,41	1.73	11 (27%)	51,56,56	2.49	21 (41%)
27	CLA	B	813	-	59,63,73	1.20	7 (11%)	70,101,113	1.39	9 (12%)
35	II0	j	614	-	39,43,43	6.77	22 (56%)	48,60,60	2.07	15 (31%)
27	CLA	A	819	-	49,53,73	1.41	7 (14%)	58,89,113	1.72	10 (17%)
27	CLA	B	806	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	9 (10%)
27	CLA	f	604	18	69,73,73	1.13	7 (10%)	82,113,113	1.36	8 (9%)
27	CLA	g	306	24	55,59,73	1.31	5 (9%)	64,96,113	1.39	7 (10%)
30	WVN	F	205	-	40,41,41	1.79	13 (32%)	51,56,56	2.90	18 (35%)
27	CLA	B	824	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
27	CLA	g	305	24	69,73,73	1.18	8 (11%)	82,113,113	1.43	10 (12%)
27	CLA	B	833	-	51,55,73	1.29	7 (13%)	60,91,113	1.85	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	l	310	29	65,69,73	1.19	7 (10%)	77,108,113	1.24	4 (5%)
27	CLA	a	310	29	52,56,73	1.27	6 (11%)	61,92,113	1.42	8 (13%)
30	WVN	l	316	-	40,41,41	1.79	10 (25%)	51,56,56	2.51	19 (37%)
36	IHT	f	617	-	40,42,42	6.23	26 (65%)	52,58,58	2.21	14 (26%)
27	CLA	A	856	29	45,49,73	1.48	11 (24%)	54,84,113	2.24	9 (16%)
30	WVN	J	101	-	40,41,41	1.68	10 (25%)	51,56,56	2.26	18 (35%)
27	CLA	a	313	-	52,56,73	1.30	7 (13%)	61,92,113	1.20	7 (11%)
27	CLA	A	821	-	53,57,73	1.28	9 (16%)	61,93,113	1.53	8 (13%)
27	CLA	c	611	14	49,53,73	1.40	8 (16%)	58,89,113	1.45	10 (17%)
30	WVN	i	315	-	40,41,41	1.78	10 (25%)	51,56,56	2.39	16 (31%)
27	CLA	B	826	-	54,58,73	1.27	7 (12%)	64,95,113	1.35	6 (9%)
27	CLA	m	605	18	46,50,73	1.37	8 (17%)	53,85,113	1.62	13 (24%)
36	IHT	c	620	-	40,42,42	6.21	25 (62%)	52,58,58	2.21	20 (38%)
35	II0	m	615	-	39,43,43	6.66	22 (56%)	48,60,60	1.78	10 (20%)
27	CLA	B	810	-	69,73,73	1.17	8 (11%)	82,113,113	1.54	14 (17%)
37	KC2	d	309	23	49,53,53	2.77	20 (40%)	60,89,89	3.78	33 (55%)
27	CLA	g	309	-	69,73,73	1.19	8 (11%)	82,113,113	1.60	10 (12%)
27	CLA	g	302	24	46,50,73	1.37	7 (15%)	53,85,113	1.83	8 (15%)
27	CLA	B	822	-	69,73,73	1.19	8 (11%)	82,113,113	1.50	16 (19%)
30	WVN	s	207	-	40,41,41	1.74	11 (27%)	51,56,56	2.40	15 (29%)
27	CLA	A	832	-	69,73,73	1.15	5 (7%)	82,113,113	1.62	13 (15%)
27	CLA	B	825	-	55,59,73	1.32	8 (14%)	64,96,113	1.40	9 (14%)
27	CLA	n	603	-	55,59,73	1.34	7 (12%)	64,96,113	1.45	10 (15%)
27	CLA	g	308	-	69,73,73	1.18	7 (10%)	82,113,113	1.54	11 (13%)
37	KC2	l	311	20	49,53,53	2.74	20 (40%)	60,89,89	3.85	33 (55%)
30	WVN	F	204	-	40,41,41	1.67	11 (27%)	51,56,56	2.54	20 (39%)
27	CLA	f	610	29	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
27	CLA	B	827	-	53,57,73	1.27	7 (13%)	61,93,113	1.45	9 (14%)
35	II0	b	613	-	39,43,43	6.69	24 (61%)	48,60,60	1.90	11 (22%)
32	SF4	C	102	3	0,12,12	-	-	-		
35	II0	m	613	-	39,43,43	6.61	20 (51%)	48,60,60	1.77	13 (27%)
35	II0	f	616	-	39,43,43	6.58	20 (51%)	48,60,60	1.98	14 (29%)
37	KC2	e	609	19	49,53,53	2.77	20 (40%)	60,89,89	3.78	33 (55%)
29	LHG	g	301	27	36,36,48	1.14	2 (5%)	39,42,54	1.45	6 (15%)
35	II0	c	614	-	39,43,43	6.68	21 (53%)	48,60,60	2.18	16 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	LMU	i	301	-	36,36,36	1.22	3 (8%)	47,47,47	1.47	7 (14%)
27	CLA	i	304	-	55,59,73	1.30	7 (12%)	64,96,113	1.38	9 (14%)
35	II0	a	318	-	39,43,43	6.87	21 (53%)	48,60,60	2.60	16 (33%)
27	CLA	A	812	-	69,73,73	1.16	9 (13%)	82,113,113	1.51	13 (15%)
35	II0	d	313	-	39,43,43	6.86	21 (53%)	48,60,60	1.66	14 (29%)
33	DGD	B	842	-	61,61,67	0.90	2 (3%)	75,75,81	1.10	3 (4%)
37	KC2	c	610	-	49,53,53	2.76	20 (40%)	60,89,89	3.72	31 (51%)
27	CLA	L	202	9	53,57,73	1.32	8 (15%)	61,93,113	1.44	7 (11%)
29	LHG	c	621	27	36,36,48	1.09	2 (5%)	39,42,54	1.27	3 (7%)
27	CLA	d	302	-	55,59,73	1.26	6 (10%)	64,96,113	1.34	9 (14%)
27	CLA	A	833	-	54,58,73	1.27	6 (11%)	64,95,113	1.33	6 (9%)
35	II0	c	613	-	39,43,43	6.71	22 (56%)	48,60,60	2.08	14 (29%)
27	CLA	A	825	39	69,73,73	1.16	9 (13%)	82,113,113	1.26	8 (9%)
35	II0	i	318	-	39,43,43	6.60	22 (56%)	48,60,60	1.78	8 (16%)
30	WVN	K	103	-	40,41,41	1.71	10 (25%)	51,56,56	1.99	17 (33%)
32	SF4	C	101	3	0,12,12	-	-	-		
29	LHG	A	850	-	37,37,48	1.05	2 (5%)	40,43,54	1.20	3 (7%)
27	CLA	A	838	29	56,60,73	1.26	7 (12%)	65,97,113	1.50	7 (10%)
35	II0	i	314	-	39,43,43	6.61	22 (56%)	48,60,60	1.92	14 (29%)
30	WVN	B	844	-	40,41,41	1.58	13 (32%)	51,56,56	2.56	24 (47%)
27	CLA	A	824	39	69,73,73	1.16	8 (11%)	82,113,113	1.45	11 (13%)
27	CLA	A	828	-	69,73,73	1.17	10 (14%)	82,113,113	1.38	10 (12%)
27	CLA	L	204	39	54,58,73	1.40	10 (18%)	64,95,113	1.44	9 (14%)
35	II0	c	617	-	39,43,43	6.66	21 (53%)	48,60,60	2.12	15 (31%)
35	II0	a	316	-	39,43,43	6.79	21 (53%)	48,60,60	1.90	13 (27%)
27	CLA	m	609	29	59,63,73	1.28	5 (8%)	70,101,113	1.52	11 (15%)
35	II0	n	615	-	39,43,43	6.74	23 (58%)	48,60,60	1.92	13 (27%)
27	CLA	d	306	23	50,54,73	1.34	7 (14%)	59,90,113	1.35	6 (10%)
35	II0	g	318	-	39,43,43	6.54	19 (48%)	48,60,60	2.06	15 (31%)
27	CLA	d	305	-	55,59,73	1.28	6 (10%)	64,96,113	1.54	9 (14%)
37	KC2	n	611	26	49,53,53	2.71	19 (38%)	60,89,89	3.87	33 (55%)
27	CLA	h	306	17	69,73,73	1.17	7 (10%)	82,113,113	1.28	11 (13%)
36	IHT	g	319	-	40,42,42	6.20	25 (62%)	52,58,58	2.25	17 (32%)
27	CLA	h	305	-	55,59,73	1.26	8 (14%)	64,96,113	1.40	8 (12%)
27	CLA	B	840	29	69,73,73	1.16	8 (11%)	82,113,113	1.33	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	IHT	R	204	-	40,42,42	6.31	26 (65%)	52,58,58	2.23	16 (30%)
27	CLA	f	612	18	55,59,73	1.34	8 (14%)	64,96,113	1.51	15 (23%)
27	CLA	A	807	1	69,73,73	1.15	7 (10%)	82,113,113	1.31	5 (6%)
27	CLA	A	822	-	55,59,73	1.31	8 (14%)	64,96,113	1.43	6 (9%)
27	CLA	i	312	-	55,59,73	1.28	5 (9%)	64,96,113	1.43	9 (14%)
27	CLA	j	606	18	55,59,73	1.32	6 (10%)	64,96,113	1.73	10 (15%)
27	CLA	g	303	24	54,58,73	1.23	6 (11%)	64,95,113	1.44	8 (12%)
27	CLA	A	808	1	69,73,73	1.12	5 (7%)	82,113,113	1.38	12 (14%)
27	CLA	d	311	-	55,59,73	1.29	6 (10%)	64,96,113	1.50	11 (17%)
37	KC2	g	312	24	49,53,53	2.75	20 (40%)	60,89,89	3.74	33 (55%)
27	CLA	j	608	18	55,59,73	1.28	6 (10%)	64,96,113	1.41	12 (18%)
31	LMT	a	320	-	36,36,36	0.40	0	47,47,47	1.06	4 (8%)
36	IHT	n	617	-	40,42,42	6.28	26 (65%)	52,58,58	2.36	16 (30%)
27	CLA	k	307	21	69,73,73	1.19	7 (10%)	82,113,113	1.30	5 (6%)
27	CLA	i	302	22	55,59,73	1.30	5 (9%)	64,96,113	1.35	4 (6%)
37	KC2	i	310	22	49,53,53	2.76	20 (40%)	60,89,89	3.69	32 (53%)
35	II0	l	317	-	39,43,43	6.84	21 (53%)	48,60,60	1.86	12 (25%)
27	CLA	A	801	-	69,73,73	1.16	6 (8%)	82,113,113	1.15	8 (9%)
27	CLA	d	301	23	54,58,73	1.28	8 (14%)	64,95,113	1.43	9 (14%)
35	II0	e	616	-	39,43,43	6.73	21 (53%)	48,60,60	1.72	11 (22%)
27	CLA	a	311	15	69,73,73	1.13	7 (10%)	82,113,113	1.52	10 (12%)
27	CLA	A	815	39	49,53,73	1.39	7 (14%)	58,89,113	1.77	8 (13%)
35	II0	l	314	-	39,43,43	6.70	23 (58%)	48,60,60	2.18	13 (27%)
29	LHG	a	319	27	48,48,48	0.91	2 (4%)	51,54,54	1.25	5 (9%)
27	CLA	m	601	18	46,50,73	1.41	6 (13%)	53,85,113	1.24	4 (7%)
27	CLA	m	606	18	69,73,73	1.15	8 (11%)	82,113,113	1.33	7 (8%)
27	CLA	a	309	15	69,73,73	1.17	9 (13%)	82,113,113	1.38	7 (8%)
27	CLA	k	302	-	55,59,73	1.28	7 (12%)	64,96,113	1.47	12 (18%)
27	CLA	F	201	39	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
27	CLA	B	821	39	68,72,73	1.14	8 (11%)	80,111,113	1.26	8 (10%)
35	II0	k	316	-	39,43,43	6.89	20 (51%)	48,60,60	1.86	12 (25%)
35	II0	j	613	-	39,43,43	6.69	21 (53%)	48,60,60	2.50	20 (41%)
27	CLA	b	608	29	69,73,73	1.13	6 (8%)	82,113,113	1.31	10 (12%)
27	CLA	a	308	15	69,73,73	1.15	6 (8%)	82,113,113	1.30	10 (12%)
27	CLA	c	605	-	55,59,73	1.32	5 (9%)	64,96,113	1.27	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	k	304	21	49,53,73	1.39	8 (16%)	58,89,113	1.84	16 (27%)
27	CLA	i	306	-	55,59,73	1.29	6 (10%)	64,96,113	1.37	7 (10%)
27	CLA	s	206	-	69,73,73	1.17	7 (10%)	82,113,113	1.36	10 (12%)
35	II0	l	313	-	39,43,43	6.77	20 (51%)	48,60,60	1.82	13 (27%)
27	CLA	c	609	29	49,53,73	1.36	8 (16%)	58,89,113	1.39	10 (17%)
27	CLA	c	604	14	69,73,73	1.17	7 (10%)	82,113,113	1.35	5 (6%)
36	IHT	m	616	-	40,42,42	6.22	25 (62%)	52,58,58	2.08	16 (30%)
27	CLA	j	607	18	49,53,73	1.38	6 (12%)	58,89,113	1.27	5 (8%)
27	CLA	A	826	-	69,73,73	1.21	8 (11%)	82,113,113	1.62	15 (18%)
27	CLA	c	608	14	69,73,73	1.18	7 (10%)	82,113,113	1.52	10 (12%)
27	CLA	B	802	-	69,73,73	1.13	7 (10%)	82,113,113	1.75	12 (14%)
27	CLA	i	311	22	55,59,73	1.37	9 (16%)	64,96,113	1.59	12 (18%)
35	II0	f	618	-	39,43,43	6.70	20 (51%)	48,60,60	2.08	17 (35%)
34	LMG	s	210	-	55,55,55	0.87	2 (3%)	63,63,63	0.99	3 (4%)
27	CLA	l	312	20	69,73,73	1.16	7 (10%)	82,113,113	1.41	13 (15%)
37	KC2	d	310	-	49,53,53	2.73	20 (40%)	60,89,89	3.63	32 (53%)
27	CLA	B	811	-	64,68,73	1.20	8 (12%)	76,107,113	1.37	9 (11%)
27	CLA	b	606	16	65,69,73	1.20	8 (12%)	77,108,113	1.38	11 (14%)
30	WVN	A	849	-	40,41,41	1.68	11 (27%)	51,56,56	2.06	13 (25%)
27	CLA	A	841	-	69,73,73	1.13	9 (13%)	82,113,113	1.29	9 (10%)
27	CLA	n	601	26	49,53,73	1.38	7 (14%)	58,89,113	1.32	5 (8%)
27	CLA	e	605	19	69,73,73	1.14	7 (10%)	82,113,113	1.43	9 (10%)
30	WVN	L	201	-	40,41,41	1.69	14 (35%)	51,56,56	2.61	17 (33%)
27	CLA	f	607	-	69,73,73	1.21	7 (10%)	82,113,113	1.37	10 (12%)
29	LHG	k	319	27	36,36,48	1.13	2 (5%)	39,42,54	1.18	5 (12%)
30	WVN	J	102	-	40,41,41	1.78	11 (27%)	51,56,56	2.08	17 (33%)
27	CLA	k	309	29	55,59,73	1.40	6 (10%)	64,96,113	1.88	18 (28%)
27	CLA	e	604	39	69,73,73	1.15	7 (10%)	82,113,113	1.59	11 (13%)
27	CLA	e	610	39	69,73,73	1.19	8 (11%)	82,113,113	1.18	7 (8%)
34	LMG	O	205	-	26,26,55	1.30	2 (7%)	34,34,63	1.28	4 (11%)
27	CLA	A	811	-	58,62,73	1.26	7 (12%)	68,99,113	1.41	8 (11%)
27	CLA	g	310	24	55,59,73	1.32	7 (12%)	64,96,113	1.58	14 (21%)
27	CLA	F	203	6	56,60,73	1.26	8 (14%)	65,97,113	1.46	6 (9%)
27	CLA	A	820	39	69,73,73	1.18	9 (13%)	82,113,113	1.41	11 (13%)
27	CLA	B	803	-	69,73,73	1.12	8 (11%)	82,113,113	1.47	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	b	603	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	9 (10%)
35	II0	e	613	-	39,43,43	6.81	23 (58%)	48,60,60	1.85	13 (27%)
27	CLA	h	303	17	54,58,73	1.28	8 (14%)	64,95,113	1.49	9 (14%)
27	CLA	n	610	39	69,73,73	1.23	9 (13%)	82,113,113	1.25	8 (9%)
27	CLA	R	203	-	55,59,73	1.30	7 (12%)	64,96,113	1.57	11 (17%)
27	CLA	B	818	-	59,63,73	1.30	9 (15%)	70,101,113	1.35	9 (12%)
27	CLA	h	301	39	69,73,73	1.20	9 (13%)	82,113,113	1.44	14 (17%)
27	CLA	h	304	-	55,59,73	1.31	10 (18%)	64,96,113	1.64	11 (17%)
29	LHG	f	619	-	48,48,48	0.91	2 (4%)	51,54,54	1.04	3 (5%)
27	CLA	s	208	-	55,59,73	1.31	8 (14%)	64,96,113	1.67	18 (28%)
27	CLA	b	610	16	69,73,73	1.13	6 (8%)	82,113,113	1.31	7 (8%)
27	CLA	g	304	-	55,59,73	1.32	10 (18%)	64,96,113	1.47	14 (21%)
27	CLA	a	304	15	54,58,73	1.29	7 (12%)	64,95,113	1.40	8 (12%)
27	CLA	B	838	-	69,73,73	1.17	7 (10%)	82,113,113	1.41	7 (8%)
27	CLA	O	206	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	9 (10%)
27	CLA	b	604	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
27	CLA	A	827	-	66,70,73	1.16	7 (10%)	78,109,113	1.35	13 (16%)
28	PQN	B	841	-	34,34,34	1.88	5 (14%)	43,45,45	1.30	4 (9%)
27	CLA	f	613	-	69,73,73	1.20	6 (8%)	82,113,113	1.42	10 (12%)
27	CLA	a	303	15	56,60,73	1.36	10 (17%)	65,97,113	1.63	13 (20%)
37	KC2	k	312	-	49,53,53	2.79	20 (40%)	60,89,89	3.73	33 (55%)
29	LHG	a	301	27	48,48,48	0.91	2 (4%)	51,54,54	1.15	5 (9%)
27	CLA	m	611	39	55,59,73	1.31	10 (18%)	64,96,113	1.53	13 (20%)
35	II0	b	612	-	39,43,43	6.44	21 (53%)	48,60,60	2.17	16 (33%)
27	CLA	B	849	-	55,59,73	1.24	7 (12%)	64,96,113	1.43	9 (14%)
35	II0	n	618	-	39,43,43	6.83	21 (53%)	48,60,60	1.85	15 (31%)
31	LMT	b	616	-	24,24,36	1.14	3 (12%)	29,29,47	1.24	3 (10%)
27	CLA	B	804	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	8 (9%)
27	CLA	B	839	-	69,73,73	1.22	10 (14%)	82,113,113	1.44	14 (17%)
27	CLA	A	830	-	54,58,73	1.28	10 (18%)	64,95,113	1.49	10 (15%)
27	CLA	K	101	39	55,59,73	1.31	8 (14%)	64,96,113	1.59	10 (15%)
34	LMG	L	208	-	55,55,55	0.88	2 (3%)	63,63,63	1.55	9 (14%)
35	II0	n	616	-	39,43,43	6.86	21 (53%)	48,60,60	1.79	13 (27%)
30	WVN	B	846	-	40,41,41	1.75	10 (25%)	51,56,56	2.51	19 (37%)
27	CLA	A	853	-	69,73,73	1.12	6 (8%)	82,113,113	1.33	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	m	607	18	69,73,73	1.17	8 (11%)	82,113,113	1.26	10 (12%)
27	CLA	B	837	-	61,65,73	1.23	7 (11%)	72,103,113	1.46	11 (15%)
27	CLA	f	601	18	51,55,73	1.35	7 (13%)	60,91,113	1.29	6 (10%)
29	LHG	J	107	27	48,48,48	0.93	2 (4%)	51,54,54	0.92	3 (5%)
27	CLA	h	307	17	61,65,73	1.23	6 (9%)	72,103,113	1.17	4 (5%)
27	CLA	s	209	-	55,59,73	1.30	6 (10%)	64,96,113	1.29	5 (7%)
30	WVN	h	309	-	40,41,41	1.73	9 (22%)	51,56,56	2.62	22 (43%)
35	II0	k	315	-	39,43,43	6.50	23 (58%)	48,60,60	2.15	16 (33%)
35	II0	a	314	-	39,43,43	6.49	22 (56%)	48,60,60	2.08	19 (39%)
27	CLA	A	809	-	60,64,73	1.26	8 (13%)	71,102,113	1.39	7 (9%)
35	II0	m	614	-	39,43,43	6.64	22 (56%)	48,60,60	2.03	14 (29%)
27	CLA	A	803	-	59,63,73	1.24	8 (13%)	70,101,113	1.50	9 (12%)
27	CLA	e	607	19	69,73,73	1.14	7 (10%)	82,113,113	1.29	9 (10%)
27	CLA	d	308	29	45,49,73	1.42	5 (11%)	54,84,113	1.54	9 (16%)
27	CLA	j	604	18	69,73,73	1.18	7 (10%)	82,113,113	1.62	18 (21%)
27	CLA	f	605	18	49,53,73	1.41	7 (14%)	58,89,113	1.46	6 (10%)
30	WVN	A	846	-	40,41,41	1.74	10 (25%)	51,56,56	2.39	13 (25%)
27	CLA	B	816	39	69,73,73	1.25	8 (11%)	82,113,113	1.53	8 (9%)
27	CLA	A	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.45	11 (13%)
37	KC2	s	204	-	49,53,53	2.70	21 (42%)	60,89,89	3.78	35 (58%)
27	CLA	B	807	2	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
36	IHT	j	616	-	40,42,42	6.23	26 (65%)	52,58,58	2.26	16 (30%)
35	II0	f	614	-	39,43,43	6.68	21 (53%)	48,60,60	1.94	15 (31%)
27	CLA	B	801	-	69,73,73	1.15	7 (10%)	82,113,113	1.21	7 (8%)
27	CLA	h	308	17	55,59,73	1.34	8 (14%)	64,96,113	1.71	9 (14%)
29	LHG	b	617	27	48,48,48	0.89	4 (8%)	51,54,54	1.20	4 (7%)
37	KC2	k	311	-	49,53,53	2.73	20 (40%)	60,89,89	3.77	36 (60%)
27	CLA	b	601	16	55,59,73	1.30	7 (12%)	64,96,113	1.43	7 (10%)
27	CLA	A	814	-	54,58,73	1.28	7 (12%)	64,95,113	1.37	7 (10%)
37	KC2	j	610	18	49,53,53	2.75	19 (38%)	60,89,89	3.76	31 (51%)
27	CLA	B	817	-	50,54,73	1.34	7 (14%)	59,90,113	1.59	8 (13%)
30	WVN	e	615	-	40,41,41	1.72	10 (25%)	51,56,56	2.25	15 (29%)
27	CLA	L	203	-	69,73,73	1.13	8 (11%)	82,113,113	1.19	7 (8%)
35	II0	i	313	-	39,43,43	6.81	23 (58%)	48,60,60	1.77	11 (22%)
27	CLA	A	806	-	69,73,73	1.18	7 (10%)	82,113,113	1.36	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	A	834	-	55,59,73	1.33	7 (12%)	64,96,113	1.55	12 (18%)
27	CLA	j	603	-	55,59,73	1.31	8 (14%)	64,96,113	1.51	11 (17%)
27	CLA	e	608	29	50,54,73	1.34	7 (14%)	59,90,113	1.59	8 (13%)
37	KC2	n	612	-	49,53,53	2.71	19 (38%)	60,89,89	3.86	32 (53%)
27	CLA	A	829	-	69,73,73	1.17	7 (10%)	82,113,113	1.37	10 (12%)
27	CLA	B	815	-	61,65,73	1.20	6 (9%)	72,103,113	1.37	9 (12%)
27	CLA	c	601	14	55,59,73	1.27	6 (10%)	64,96,113	1.40	9 (14%)
35	II0	k	314	-	39,43,43	6.67	20 (51%)	48,60,60	1.79	12 (25%)
27	CLA	b	611	-	69,73,73	1.14	7 (10%)	82,113,113	1.16	6 (7%)
30	WVN	O	201	-	40,41,41	1.64	9 (22%)	51,56,56	2.02	14 (27%)
34	LMG	b	619	-	49,49,55	1.01	3 (6%)	57,57,63	1.17	5 (8%)
27	CLA	l	309	20	55,59,73	1.34	9 (16%)	64,96,113	1.44	11 (17%)
27	CLA	g	322	-	69,73,73	1.20	6 (8%)	82,113,113	1.43	9 (10%)
27	CLA	j	602	18	54,58,73	1.25	8 (14%)	64,95,113	1.55	10 (15%)
27	CLA	n	609	26	69,73,73	1.18	8 (11%)	82,113,113	1.49	13 (15%)
30	WVN	A	847	-	40,41,41	1.73	10 (25%)	51,56,56	2.63	18 (35%)
27	CLA	n	605	26	55,59,73	1.35	7 (12%)	64,96,113	1.81	14 (21%)
27	CLA	s	202	13	69,73,73	1.21	8 (11%)	82,113,113	1.40	13 (15%)
30	WVN	l	301	-	40,41,41	1.68	10 (25%)	51,56,56	2.24	15 (29%)
34	LMG	c	619	-	55,55,55	0.99	2 (3%)	63,63,63	1.50	12 (19%)
27	CLA	n	608	26	55,59,73	1.28	8 (14%)	64,96,113	1.32	7 (10%)
27	CLA	j	612	-	69,73,73	1.14	6 (8%)	82,113,113	1.18	8 (9%)
35	II0	l	315	-	39,43,43	6.60	21 (53%)	48,60,60	2.02	14 (29%)
27	CLA	i	305	22	69,73,73	1.16	7 (10%)	82,113,113	1.19	7 (8%)
27	CLA	A	835	-	69,73,73	1.14	7 (10%)	82,113,113	1.30	9 (10%)
27	CLA	A	855	39	69,73,73	1.22	10 (14%)	82,113,113	1.64	18 (21%)
27	CLA	f	609	18	69,73,73	1.14	8 (11%)	82,113,113	1.22	8 (9%)
27	CLA	b	602	16	59,63,73	1.22	7 (11%)	70,101,113	1.49	11 (15%)
27	CLA	F	202	39	69,73,73	1.18	6 (8%)	82,113,113	1.18	7 (8%)
30	WVN	L	205	-	40,41,41	1.77	10 (25%)	51,56,56	2.06	14 (27%)
27	CLA	c	603	-	55,59,73	1.27	8 (14%)	64,96,113	1.56	8 (12%)
27	CLA	k	305	21	55,59,73	1.31	11 (20%)	64,96,113	1.52	9 (14%)
27	CLA	f	608	18	69,73,73	1.17	7 (10%)	82,113,113	1.14	5 (6%)
27	CLA	k	303	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	10 (12%)
27	CLA	n	613	-	55,59,73	1.28	6 (10%)	64,96,113	1.21	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	A	831	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	6 (7%)
27	CLA	k	301	21	54,58,73	1.33	7 (12%)	64,95,113	1.29	6 (9%)
27	CLA	j	611	-	55,59,73	1.28	6 (10%)	64,96,113	1.43	8 (12%)
27	CLA	m	604	18	69,73,73	1.22	7 (10%)	82,113,113	1.52	14 (17%)
37	KC2	i	317	-	49,53,53	2.91	22 (44%)	60,89,89	3.41	32 (53%)
30	WVN	I	101	-	40,41,41	1.70	11 (27%)	51,56,56	2.06	14 (27%)
27	CLA	b	607	16	69,73,73	1.15	5 (7%)	82,113,113	1.62	14 (17%)
27	CLA	B	812	-	63,67,73	1.20	8 (12%)	74,105,113	1.47	9 (12%)
27	CLA	c	602	14	54,58,73	1.31	9 (16%)	64,95,113	1.75	13 (20%)
35	II0	g	316	-	39,43,43	6.66	22 (56%)	48,60,60	2.02	13 (27%)
29	LHG	b	618	-	30,30,48	1.22	2 (6%)	33,36,54	1.24	3 (9%)
27	CLA	m	608	18	55,59,73	1.29	6 (10%)	64,96,113	1.32	8 (12%)
27	CLA	d	307	23	45,49,73	1.44	7 (15%)	54,84,113	1.56	8 (14%)
30	WVN	s	205	-	40,41,41	1.70	12 (30%)	51,56,56	2.45	20 (39%)
27	CLA	f	606	18	55,59,73	1.31	7 (12%)	64,96,113	1.49	7 (10%)
27	CLA	g	307	24	55,59,73	1.28	6 (10%)	64,96,113	1.41	7 (10%)
27	CLA	g	315	-	55,59,73	1.31	5 (9%)	64,96,113	1.39	11 (17%)
27	CLA	a	312	-	69,73,73	1.16	9 (13%)	82,113,113	1.48	8 (9%)
27	CLA	a	306	39	69,73,73	1.13	7 (10%)	82,113,113	1.40	9 (10%)
27	CLA	a	305	-	55,59,73	1.31	9 (16%)	64,96,113	1.40	7 (10%)
27	CLA	c	607	14	50,54,73	1.35	6 (12%)	59,90,113	1.24	7 (11%)
27	CLA	O	202	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
35	II0	b	615	-	39,43,43	6.48	20 (51%)	48,60,60	2.32	17 (35%)
27	CLA	A	805	1	69,73,73	1.16	9 (13%)	82,113,113	1.47	10 (12%)
35	II0	d	312	-	39,43,43	6.69	23 (58%)	48,60,60	1.99	14 (29%)
29	LHG	c	618	27	36,36,48	1.14	2 (5%)	39,42,54	1.32	3 (7%)
27	CLA	i	303	22	54,58,73	1.30	8 (14%)	64,95,113	1.52	12 (18%)
27	CLA	l	303	20	51,55,73	1.34	7 (13%)	60,91,113	1.43	4 (6%)
27	CLA	e	601	19	49,53,73	1.37	8 (16%)	58,89,113	1.68	5 (8%)
30	WVN	R	202	-	40,41,41	1.67	12 (30%)	51,56,56	2.72	22 (43%)
27	CLA	B	831	-	62,66,73	1.23	8 (12%)	73,104,113	1.48	14 (19%)
27	CLA	n	607	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	13 (15%)
27	CLA	A	816	-	69,73,73	1.10	6 (8%)	82,113,113	1.47	14 (17%)
27	CLA	B	814	-	63,67,73	1.21	8 (12%)	74,105,113	1.30	6 (8%)
27	CLA	B	830	39	49,53,73	1.39	9 (18%)	58,89,113	1.57	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	II0	k	318	-	39,43,43	6.51	19 (48%)	48,60,60	2.17	20 (41%)
27	CLA	l	304	20	69,73,73	1.14	8 (11%)	82,113,113	1.48	11 (13%)
32	SF4	A	854	1,2	0,12,12	-	-	-		
27	CLA	j	605	18	49,53,73	1.40	6 (12%)	58,89,113	1.59	8 (13%)
27	CLA	A	852	-	69,73,73	1.16	7 (10%)	82,113,113	1.10	4 (4%)
27	CLA	A	837	-	69,73,73	1.13	6 (8%)	82,113,113	1.45	10 (12%)
35	II0	d	314	-	39,43,43	6.86	22 (56%)	48,60,60	2.18	13 (27%)
35	II0	j	615	-	39,43,43	6.78	20 (51%)	48,60,60	1.85	11 (22%)
27	CLA	B	834	39	69,73,73	1.20	8 (11%)	82,113,113	1.21	10 (12%)
27	CLA	A	802	-	69,73,73	1.14	9 (13%)	82,113,113	1.49	14 (17%)
27	CLA	B	836	-	69,73,73	1.09	4 (5%)	82,113,113	1.47	11 (13%)
27	CLA	B	808	-	58,62,73	1.37	8 (13%)	71,100,113	1.18	4 (5%)
35	II0	O	203	-	39,43,43	6.68	20 (51%)	48,60,60	1.97	11 (22%)
37	KC2	k	310	21	49,53,53	2.77	19 (38%)	60,89,89	3.83	33 (55%)
27	CLA	l	307	20	69,73,73	1.20	9 (13%)	82,113,113	1.60	13 (15%)
28	PQN	A	843	-	34,34,34	1.89	5 (14%)	43,45,45	1.31	4 (9%)
29	LHG	A	845	27	26,26,48	1.25	3 (11%)	29,32,54	1.51	5 (17%)
27	CLA	B	809	-	59,63,73	1.24	8 (13%)	70,101,113	1.48	14 (20%)
27	CLA	s	203	13,27	69,73,73	1.16	6 (8%)	82,113,113	1.44	7 (8%)
27	CLA	b	605	39,27	69,73,73	1.16	9 (13%)	82,113,113	1.39	7 (8%)
35	II0	e	612	-	39,43,43	6.93	23 (58%)	48,60,60	1.84	11 (22%)
27	CLA	m	612	-	47,51,73	1.39	8 (17%)	55,86,113	1.60	14 (25%)
27	CLA	B	829	39	69,73,73	1.14	7 (10%)	82,113,113	1.35	13 (15%)
27	CLA	k	306	-	55,59,73	1.34	6 (10%)	64,96,113	1.44	11 (17%)
29	LHG	A	844	-	47,47,48	0.97	2 (4%)	50,53,54	1.17	3 (6%)
30	WVN	M	101	-	40,41,41	1.68	11 (27%)	51,56,56	2.34	19 (37%)
30	WVN	B	847	-	40,41,41	1.72	11 (27%)	51,56,56	2.07	13 (25%)
30	WVN	R	201	-	40,41,41	1.69	10 (25%)	51,56,56	2.32	19 (37%)
27	CLA	J	105	29	55,59,73	1.35	8 (14%)	64,96,113	1.74	13 (20%)
35	II0	h	311	-	39,43,43	6.51	22 (56%)	48,60,60	2.18	18 (37%)
36	IHT	a	317	-	40,42,42	6.24	26 (65%)	52,58,58	2.08	14 (26%)
27	CLA	B	823	-	69,73,73	1.16	9 (13%)	82,113,113	1.38	11 (13%)
34	LMG	F	206	-	48,48,55	0.98	2 (4%)	56,56,63	1.25	5 (8%)
30	WVN	B	845	-	40,41,41	1.70	11 (27%)	51,56,56	2.52	19 (37%)
29	LHG	d	315	27	36,36,48	1.11	2 (5%)	39,42,54	1.09	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	II0	e	614	-	39,43,43	6.69	20 (51%)	48,60,60	2.03	14 (29%)
37	KC2	s	201	13	49,53,53	2.59	20 (40%)	60,89,89	3.77	34 (56%)
27	CLA	d	304	-	55,59,73	1.31	7 (12%)	64,96,113	1.35	7 (10%)
27	CLA	A	813	-	49,53,73	1.44	7 (14%)	58,89,113	2.29	12 (20%)
29	LHG	g	321	27	36,36,48	1.12	2 (5%)	39,42,54	1.52	8 (20%)
29	LHG	l	318	27	31,31,48	1.17	2 (6%)	34,37,54	1.27	4 (11%)
27	CLA	A	818	-	69,73,73	1.19	7 (10%)	82,113,113	1.57	12 (14%)
27	CLA	a	307	15	49,53,73	1.39	9 (18%)	58,89,113	1.74	12 (20%)
36	IHT	O	204	-	40,42,42	6.17	26 (65%)	52,58,58	2.27	20 (38%)
27	CLA	e	611	-	69,73,73	1.18	9 (13%)	82,113,113	1.46	12 (14%)
27	CLA	d	303	23	69,73,73	1.17	6 (8%)	82,113,113	1.18	4 (4%)
29	LHG	j	617	27	29,29,48	1.22	2 (6%)	32,35,54	1.52	6 (18%)
37	KC2	m	610	18	49,53,53	2.78	20 (40%)	60,89,89	3.78	33 (55%)
37	KC2	g	314	37	49,53,53	2.77	20 (40%)	60,89,89	3.74	33 (55%)
27	CLA	A	810	-	66,70,73	1.15	7 (10%)	78,109,113	1.15	5 (6%)
29	LHG	L	207	-	48,48,48	0.90	2 (4%)	51,54,54	1.06	2 (3%)
27	CLA	L	206	39	55,59,73	1.26	7 (12%)	64,96,113	1.37	6 (9%)
36	IHT	c	616	-	40,42,42	6.30	25 (62%)	52,58,58	2.57	14 (26%)
27	CLA	A	840	1	69,73,73	1.23	9 (13%)	82,113,113	1.49	8 (9%)
27	CLA	A	836	-	69,73,73	1.18	7 (10%)	82,113,113	1.51	12 (14%)
27	CLA	B	805	-	69,73,73	1.11	6 (8%)	82,113,113	1.45	6 (7%)
29	LHG	i	316	27	36,36,48	1.16	2 (5%)	39,42,54	1.56	6 (15%)
27	CLA	j	609	29	65,69,73	1.22	9 (13%)	77,108,113	1.58	13 (16%)
27	CLA	m	603	-	69,73,73	1.13	7 (10%)	82,113,113	1.46	11 (13%)
27	CLA	A	804	-	69,73,73	1.17	9 (13%)	82,113,113	1.58	9 (10%)
27	CLA	m	602	18	60,64,73	1.22	8 (13%)	71,102,113	1.43	10 (14%)
27	CLA	A	839	39	69,73,73	1.17	7 (10%)	82,113,113	1.12	8 (9%)
27	CLA	c	612	-	69,73,73	1.13	5 (7%)	82,113,113	1.33	8 (9%)
35	II0	J	104	-	39,43,43	6.69	22 (56%)	48,60,60	1.92	11 (22%)
27	CLA	n	604	26	64,68,73	1.28	10 (15%)	76,107,113	1.38	9 (11%)
27	CLA	B	835	-	69,73,73	1.16	7 (10%)	82,113,113	1.57	11 (13%)
37	KC2	g	313	37	49,53,53	2.76	20 (40%)	60,89,89	3.78	32 (53%)
36	IHT	k	317	-	40,42,42	6.20	26 (65%)	52,58,58	2.18	18 (34%)
27	CLA	c	606	-	56,60,73	1.34	7 (12%)	65,97,113	1.61	12 (18%)
31	LMT	A	851	-	36,36,36	1.23	5 (13%)	47,47,47	1.43	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	i	308	22	55,59,73	1.28	6 (10%)	64,96,113	1.66	17 (26%)
27	CLA	e	602	19	54,58,73	1.32	8 (14%)	64,95,113	1.57	9 (14%)
29	LHG	n	619	-	42,42,48	0.96	2 (4%)	45,48,54	1.38	4 (8%)
30	WVN	B	848	-	40,41,41	1.68	11 (27%)	51,56,56	2.71	23 (45%)
35	II0	h	312	-	39,43,43	6.76	22 (56%)	48,60,60	2.31	16 (33%)
27	CLA	k	313	-	55,59,73	1.33	6 (10%)	64,96,113	1.35	10 (15%)
35	II0	g	317	-	39,43,43	6.67	22 (56%)	48,60,60	2.15	13 (27%)
27	CLA	A	823	-	59,63,73	1.25	7 (11%)	70,101,113	1.34	8 (11%)
27	CLA	f	602	18	69,73,73	1.14	6 (8%)	82,113,113	1.39	12 (14%)
29	LHG	m	617	27	36,36,48	1.07	2 (5%)	39,42,54	1.26	4 (10%)
27	CLA	B	819	-	57,61,73	1.29	9 (15%)	67,98,113	1.27	6 (8%)
27	CLA	n	606	26	55,59,73	1.32	7 (12%)	64,96,113	1.52	8 (12%)
35	II0	a	315	-	39,43,43	6.76	24 (61%)	48,60,60	1.88	17 (35%)
35	II0	g	320	-	39,43,43	6.68	22 (56%)	48,60,60	1.97	13 (27%)
27	CLA	h	302	17	54,58,73	1.28	7 (12%)	64,95,113	1.41	8 (12%)
36	IHT	b	614	-	40,42,42	6.35	25 (62%)	52,58,58	2.24	16 (30%)
27	CLA	B	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	10 (12%)
27	CLA	j	601	18	55,59,73	1.32	6 (10%)	64,96,113	1.28	5 (7%)
27	CLA	b	609	-	55,59,73	1.29	9 (16%)	64,96,113	1.59	9 (14%)
30	WVN	A	848	-	40,41,41	1.71	12 (30%)	51,56,56	2.61	22 (43%)
27	CLA	i	307	22	65,69,73	1.22	7 (10%)	77,108,113	1.24	6 (7%)
34	LMG	J	106	-	55,55,55	0.86	3 (5%)	63,63,63	0.99	3 (4%)
29	LHG	e	617	27	36,36,48	1.10	2 (5%)	39,42,54	1.43	4 (10%)
35	II0	f	615	-	39,43,43	6.63	23 (58%)	48,60,60	2.21	18 (37%)
27	CLA	f	603	-	55,59,73	1.28	6 (10%)	64,96,113	1.40	9 (14%)
27	CLA	n	602	26	54,58,73	1.29	7 (12%)	64,95,113	1.52	10 (15%)
27	CLA	i	309	29	50,54,73	1.35	8 (16%)	59,90,113	1.59	11 (18%)
27	CLA	k	308	21	69,73,73	1.23	6 (8%)	82,113,113	1.49	17 (20%)
27	CLA	l	305	-	55,59,73	1.27	9 (16%)	64,96,113	1.40	8 (12%)
35	II0	l	302	-	39,43,43	6.78	21 (53%)	48,60,60	2.23	16 (33%)
35	II0	h	310	-	26,28,43	6.04	12 (46%)	30,37,60	2.33	11 (36%)
27	CLA	A	817	-	69,73,73	1.18	10 (14%)	82,113,113	1.33	11 (13%)
27	CLA	J	103	8	46,50,73	1.33	7 (15%)	53,85,113	1.47	6 (11%)
27	CLA	B	828	-	54,58,73	1.32	8 (14%)	64,95,113	1.48	10 (15%)
27	CLA	K	102	-	46,50,73	1.38	7 (15%)	53,85,113	1.53	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	g	311	29	58,62,73	1.28	8 (13%)	68,99,113	1.45	6 (8%)
31	LMT	a	302	-	24,24,36	1.18	3 (12%)	29,29,47	0.97	0
27	CLA	l	308	20	69,73,73	1.14	6 (8%)	82,113,113	1.27	7 (8%)
27	CLA	e	606	19	69,73,73	1.18	9 (13%)	82,113,113	1.25	7 (8%)
27	CLA	B	820	39	69,73,73	1.19	8 (11%)	82,113,113	1.41	10 (12%)
27	CLA	h	313	39	69,73,73	1.14	7 (10%)	82,113,113	1.29	6 (7%)
35	II0	c	615	-	39,43,43	6.75	20 (51%)	48,60,60	2.24	17 (35%)
27	CLA	l	306	20	69,73,73	1.16	8 (11%)	82,113,113	1.56	13 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	II0	n	614	-	-	1/21/67/67	0/2/2/2
27	CLA	e	603	19	1/1/12/20	2/23/99/115	-
37	KC2	f	611	18	-	5/15/71/71	-
30	WVN	B	843	-	-	10/29/63/63	0/2/2/2
27	CLA	B	813	-	1/1/13/20	5/27/103/115	-
35	II0	j	614	-	-	2/21/67/67	0/2/2/2
27	CLA	A	819	-	1/1/11/20	3/15/91/115	-
27	CLA	B	806	-	1/1/15/20	9/39/115/115	-
27	CLA	f	604	18	1/1/15/20	10/39/115/115	-
27	CLA	g	306	24	1/1/12/20	8/23/99/115	-
30	WVN	F	205	-	-	12/29/63/63	0/2/2/2
27	CLA	B	824	-	1/1/15/20	7/39/115/115	-
27	CLA	g	305	24	1/1/15/20	13/39/115/115	-
27	CLA	B	833	-	1/1/11/20	2/18/94/115	-
27	CLA	l	310	29	1/1/14/20	13/35/111/115	-
27	CLA	a	310	29	1/1/11/20	6/19/95/115	-
30	WVN	l	316	-	-	9/29/63/63	0/2/2/2
36	IHT	f	617	-	-	7/25/65/65	0/2/2/2
27	CLA	A	856	29	1/1/10/20	4/10/86/115	-
30	WVN	J	101	-	-	8/29/63/63	0/2/2/2
27	CLA	a	313	-	1/1/11/20	11/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	821	-	-	5/20/96/115	-
27	CLA	c	611	14	-	5/15/91/115	-
30	WVN	i	315	-	-	9/29/63/63	0/2/2/2
27	CLA	B	826	-	1/1/12/20	9/21/97/115	-
27	CLA	m	605	18	1/1/10/20	6/12/88/115	-
36	IHT	c	620	-	-	11/25/65/65	0/2/2/2
35	II0	m	615	-	-	3/21/67/67	0/2/2/2
27	CLA	B	810	-	1/1/15/20	12/39/115/115	-
37	KC2	d	309	23	-	7/15/71/71	-
27	CLA	g	309	-	1/1/15/20	10/39/115/115	-
27	CLA	g	302	24	1/1/10/20	4/12/88/115	-
27	CLA	B	822	-	1/1/15/20	4/39/115/115	-
30	WVN	s	207	-	-	6/29/63/63	0/2/2/2
27	CLA	A	832	-	1/1/15/20	12/39/115/115	-
27	CLA	B	825	-	1/1/12/20	3/23/99/115	-
27	CLA	n	603	-	1/1/12/20	9/23/99/115	-
27	CLA	g	308	-	1/1/15/20	16/39/115/115	-
37	KC2	l	311	20	-	5/15/71/71	-
30	WVN	F	204	-	-	9/29/63/63	0/2/2/2
27	CLA	f	610	29	1/1/15/20	16/39/115/115	-
27	CLA	B	827	-	1/1/11/20	5/20/96/115	-
35	II0	b	613	-	-	8/21/67/67	0/2/2/2
32	SF4	C	102	3	-	-	0/6/5/5
35	II0	m	613	-	-	4/21/67/67	0/2/2/2
35	II0	f	616	-	-	3/21/67/67	0/2/2/2
37	KC2	e	609	19	-	7/15/71/71	-
29	LHG	g	301	27	-	20/41/41/53	-
35	II0	c	614	-	-	1/21/67/67	0/2/2/2
38	LMU	i	301	-	-	8/21/61/61	0/2/2/2
27	CLA	i	304	-	1/1/12/20	3/23/99/115	-
35	II0	a	318	-	-	8/21/67/67	0/2/2/2
27	CLA	A	812	-	1/1/15/20	20/39/115/115	-
35	II0	d	313	-	-	6/21/67/67	0/2/2/2
33	DGD	B	842	-	-	5/49/89/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC2	c	610	-	-	8/15/71/71	-
27	CLA	L	202	9	1/1/11/20	9/20/96/115	-
29	LHG	c	621	27	-	23/41/41/53	-
27	CLA	d	302	-	1/1/12/20	7/23/99/115	-
27	CLA	A	833	-	1/1/12/20	5/21/97/115	-
35	II0	c	613	-	-	4/21/67/67	0/2/2/2
27	CLA	A	825	39	-	7/39/115/115	-
35	II0	i	318	-	-	5/21/67/67	0/2/2/2
30	WVN	K	103	-	-	5/29/63/63	0/2/2/2
32	SF4	C	101	3	-	-	0/6/5/5
29	LHG	A	850	-	-	15/42/42/53	-
27	CLA	A	838	29	1/1/12/20	7/24/100/115	-
35	II0	i	314	-	-	3/21/67/67	0/2/2/2
30	WVN	B	844	-	-	0/29/63/63	0/2/2/2
27	CLA	A	824	39	1/1/15/20	7/39/115/115	-
27	CLA	A	828	-	1/1/15/20	9/39/115/115	-
27	CLA	L	204	39	1/1/12/20	5/21/97/115	-
35	II0	c	617	-	-	5/21/67/67	0/2/2/2
35	II0	a	316	-	-	2/21/67/67	0/2/2/2
27	CLA	m	609	29	1/1/13/20	13/27/103/115	-
35	II0	n	615	-	-	3/21/67/67	0/2/2/2
27	CLA	d	306	23	1/1/11/20	5/17/93/115	-
35	II0	g	318	-	-	3/21/67/67	0/2/2/2
27	CLA	d	305	-	1/1/12/20	9/23/99/115	-
37	KC2	n	611	26	-	4/15/71/71	-
27	CLA	h	306	17	1/1/15/20	19/39/115/115	-
36	IHT	g	319	-	-	5/25/65/65	0/2/2/2
27	CLA	h	305	-	1/1/12/20	6/23/99/115	-
27	CLA	B	840	29	1/1/15/20	4/39/115/115	-
36	IHT	R	204	-	-	2/25/65/65	0/2/2/2
27	CLA	f	612	18	1/1/12/20	8/23/99/115	-
27	CLA	A	807	1	1/1/15/20	7/39/115/115	-
27	CLA	A	822	-	1/1/12/20	8/23/99/115	-
27	CLA	i	312	-	1/1/12/20	5/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	j	606	18	-	10/23/99/115	-
27	CLA	g	303	24	1/1/12/20	4/21/97/115	-
27	CLA	A	808	1	1/1/15/20	8/39/115/115	-
27	CLA	d	311	-	-	7/23/99/115	-
37	KC2	g	312	24	-	10/15/71/71	-
27	CLA	j	608	18	1/1/12/20	2/23/99/115	-
31	LMT	a	320	-	-	13/21/61/61	0/2/2/2
36	IHT	n	617	-	-	8/25/65/65	0/2/2/2
27	CLA	k	307	21	1/1/15/20	16/39/115/115	-
27	CLA	i	302	22	1/1/12/20	7/23/99/115	-
37	KC2	i	310	22	-	9/15/71/71	-
35	II0	l	317	-	-	4/21/67/67	0/2/2/2
27	CLA	A	801	-	1/1/15/20	9/39/115/115	-
27	CLA	d	301	23	1/1/12/20	4/21/97/115	-
35	II0	e	616	-	-	4/21/67/67	0/2/2/2
27	CLA	a	311	15	1/1/15/20	13/39/115/115	-
27	CLA	A	815	39	1/1/11/20	4/15/91/115	-
35	II0	l	314	-	-	5/21/67/67	0/2/2/2
29	LHG	a	319	27	-	14/53/53/53	-
27	CLA	m	601	18	1/1/10/20	1/12/88/115	-
27	CLA	m	606	18	1/1/15/20	13/39/115/115	-
27	CLA	a	309	15	1/1/15/20	10/39/115/115	-
27	CLA	k	302	-	1/1/12/20	2/23/99/115	-
27	CLA	F	201	39	1/1/15/20	16/39/115/115	-
27	CLA	B	821	39	1/1/14/20	8/38/114/115	-
35	II0	k	316	-	-	1/21/67/67	0/2/2/2
35	II0	j	613	-	-	5/21/67/67	0/2/2/2
27	CLA	b	608	29	1/1/15/20	10/39/115/115	-
27	CLA	a	308	15	1/1/15/20	20/39/115/115	-
27	CLA	c	605	-	1/1/12/20	9/23/99/115	-
27	CLA	k	304	21	1/1/11/20	4/15/91/115	-
27	CLA	i	306	-	1/1/12/20	2/23/99/115	-
27	CLA	s	206	-	1/1/15/20	11/39/115/115	-
35	II0	l	313	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	c	609	29	1/1/11/20	5/15/91/115	-
27	CLA	c	604	14	-	9/39/115/115	-
36	IHT	m	616	-	-	4/25/65/65	0/2/2/2
27	CLA	j	607	18	1/1/11/20	4/15/91/115	-
27	CLA	A	826	-	1/1/15/20	8/39/115/115	-
27	CLA	c	608	14	1/1/15/20	16/39/115/115	-
27	CLA	B	802	-	1/1/15/20	7/39/115/115	-
27	CLA	i	311	22	1/1/12/20	7/23/99/115	-
35	II0	f	618	-	-	7/21/67/67	0/2/2/2
34	LMG	s	210	-	-	12/50/70/70	0/1/1/1
27	CLA	l	312	20	1/1/15/20	14/39/115/115	-
37	KC2	d	310	-	-	6/15/71/71	-
27	CLA	B	811	-	1/1/14/20	11/33/109/115	-
27	CLA	b	606	16	1/1/14/20	14/35/111/115	-
30	WVN	A	849	-	-	13/29/63/63	0/2/2/2
27	CLA	A	841	-	1/1/15/20	15/39/115/115	-
27	CLA	n	601	26	1/1/11/20	9/15/91/115	-
27	CLA	e	605	19	-	17/39/115/115	-
30	WVN	L	201	-	-	9/29/63/63	0/2/2/2
27	CLA	f	607	-	1/1/15/20	18/39/115/115	-
29	LHG	k	319	27	-	12/41/41/53	-
30	WVN	J	102	-	-	8/29/63/63	0/2/2/2
27	CLA	k	309	29	1/1/12/20	11/23/99/115	-
27	CLA	e	604	39	-	21/39/115/115	-
27	CLA	e	610	39	1/1/15/20	14/39/115/115	-
34	LMG	O	205	-	-	6/21/41/70	0/1/1/1
27	CLA	A	811	-	-	7/26/102/115	-
27	CLA	g	310	24	1/1/12/20	6/23/99/115	-
27	CLA	F	203	6	1/1/12/20	13/24/100/115	-
27	CLA	A	820	39	1/1/15/20	3/39/115/115	-
27	CLA	B	803	-	1/1/15/20	12/39/115/115	-
27	CLA	b	603	-	1/1/15/20	15/39/115/115	-
35	II0	e	613	-	-	5/21/67/67	0/2/2/2
27	CLA	h	303	17	1/1/12/20	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	n	610	39	1/1/15/20	16/39/115/115	-
27	CLA	R	203	-	1/1/12/20	5/23/99/115	-
27	CLA	B	818	-	1/1/13/20	10/27/103/115	-
27	CLA	h	301	39	1/1/15/20	13/39/115/115	-
27	CLA	h	304	-	1/1/12/20	4/23/99/115	-
29	LHG	f	619	-	-	35/53/53/53	-
27	CLA	b	610	16	1/1/15/20	20/39/115/115	-
27	CLA	s	208	-	-	5/23/99/115	-
27	CLA	g	304	-	1/1/12/20	3/23/99/115	-
27	CLA	a	304	15	1/1/12/20	5/21/97/115	-
27	CLA	B	838	-	1/1/15/20	18/39/115/115	-
27	CLA	O	206	-	1/1/15/20	17/39/115/115	-
27	CLA	b	604	-	-	15/39/115/115	-
27	CLA	A	827	-	1/1/14/20	7/36/112/115	-
28	PQN	B	841	-	-	10/23/43/43	0/2/2/2
27	CLA	f	613	-	-	20/39/115/115	-
27	CLA	a	303	15	1/1/12/20	7/24/100/115	-
37	KC2	k	312	-	-	9/15/71/71	-
29	LHG	a	301	27	-	13/53/53/53	-
27	CLA	m	611	39	1/1/12/20	12/23/99/115	-
35	II0	b	612	-	-	1/21/67/67	0/2/2/2
27	CLA	B	849	-	-	10/23/99/115	-
35	II0	n	618	-	-	5/21/67/67	0/2/2/2
31	LMT	b	616	-	-	9/15/35/61	0/1/1/2
27	CLA	B	804	-	1/1/15/20	14/39/115/115	-
27	CLA	B	839	-	1/1/15/20	8/39/115/115	-
27	CLA	A	830	-	-	5/21/97/115	-
27	CLA	K	101	39	1/1/12/20	8/23/99/115	-
34	LMG	L	208	-	-	19/50/70/70	0/1/1/1
35	II0	n	616	-	-	3/21/67/67	0/2/2/2
30	WVN	B	846	-	-	7/29/63/63	0/2/2/2
27	CLA	A	853	-	1/1/15/20	9/39/115/115	-
27	CLA	m	607	18	1/1/15/20	9/39/115/115	-
27	CLA	B	837	-	1/1/13/20	8/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	f	601	18	1/1/11/20	5/18/94/115	-
29	LHG	J	107	27	-	28/53/53/53	-
27	CLA	h	307	17	1/1/13/20	14/30/106/115	-
27	CLA	s	209	-	1/1/12/20	6/23/99/115	-
30	WVN	h	309	-	-	8/29/63/63	0/2/2/2
35	II0	k	315	-	-	8/21/67/67	0/2/2/2
35	II0	a	314	-	-	5/21/67/67	0/2/2/2
27	CLA	A	809	-	1/1/13/20	9/29/105/115	-
35	II0	m	614	-	-	8/21/67/67	0/2/2/2
27	CLA	A	803	-	1/1/13/20	6/27/103/115	-
27	CLA	e	607	19	1/1/15/20	22/39/115/115	-
27	CLA	d	308	29	1/1/10/20	2/10/86/115	-
27	CLA	j	604	18	1/1/15/20	16/39/115/115	-
27	CLA	f	605	18	-	6/15/91/115	-
30	WVN	A	846	-	-	8/29/63/63	0/2/2/2
27	CLA	B	816	39	1/1/15/20	9/39/115/115	-
27	CLA	A	842	-	1/1/15/20	15/39/115/115	-
37	KC2	s	204	-	-	6/15/71/71	-
27	CLA	B	807	2	1/1/15/20	11/39/115/115	-
36	IHT	j	616	-	-	6/25/65/65	0/2/2/2
35	II0	f	614	-	-	5/21/67/67	0/2/2/2
27	CLA	B	801	-	1/1/15/20	20/39/115/115	-
27	CLA	h	308	17	1/1/12/20	10/23/99/115	-
29	LHG	b	617	27	-	20/53/53/53	-
37	KC2	k	311	-	-	8/15/71/71	-
27	CLA	b	601	16	1/1/12/20	10/23/99/115	-
27	CLA	A	814	-	1/1/12/20	8/21/97/115	-
37	KC2	j	610	18	-	5/15/71/71	-
27	CLA	B	817	-	-	4/17/93/115	-
30	WVN	e	615	-	-	11/29/63/63	0/2/2/2
27	CLA	L	203	-	-	14/39/115/115	-
35	II0	i	313	-	-	4/21/67/67	0/2/2/2
27	CLA	A	806	-	-	10/39/115/115	-
27	CLA	A	834	-	1/1/12/20	2/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	j	603	-	1/1/12/20	3/23/99/115	-
27	CLA	e	608	29	1/1/11/20	6/17/93/115	-
37	KC2	n	612	-	-	7/15/71/71	-
27	CLA	A	829	-	1/1/15/20	14/39/115/115	-
27	CLA	B	815	-	-	8/30/106/115	-
27	CLA	c	601	14	1/1/12/20	10/23/99/115	-
35	II0	k	314	-	-	3/21/67/67	0/2/2/2
27	CLA	b	611	-	1/1/15/20	22/39/115/115	-
30	WVN	O	201	-	-	9/29/63/63	0/2/2/2
34	LMG	b	619	-	-	16/44/64/70	0/1/1/1
27	CLA	l	309	20	1/1/12/20	6/23/99/115	-
27	CLA	g	322	-	1/1/15/20	19/39/115/115	-
27	CLA	j	602	18	1/1/12/20	4/21/97/115	-
27	CLA	n	609	26	1/1/15/20	10/39/115/115	-
30	WVN	A	847	-	-	11/29/63/63	0/2/2/2
27	CLA	n	605	26	1/1/12/20	7/23/99/115	-
27	CLA	s	202	13	1/1/15/20	14/39/115/115	-
30	WVN	l	301	-	-	3/29/63/63	0/2/2/2
34	LMG	c	619	-	-	21/50/70/70	0/1/1/1
27	CLA	n	608	26	1/1/12/20	7/23/99/115	-
27	CLA	j	612	-	1/1/15/20	16/39/115/115	-
35	II0	l	315	-	-	5/21/67/67	0/2/2/2
27	CLA	i	305	22	1/1/15/20	10/39/115/115	-
27	CLA	A	835	-	1/1/15/20	14/39/115/115	-
27	CLA	A	855	39	1/1/15/20	15/39/115/115	-
27	CLA	f	609	18	1/1/15/20	7/39/115/115	-
27	CLA	b	602	16	1/1/13/20	10/27/103/115	-
27	CLA	F	202	39	1/1/15/20	13/39/115/115	-
30	WVN	L	205	-	-	6/29/63/63	0/2/2/2
27	CLA	c	603	-	1/1/12/20	2/23/99/115	-
27	CLA	k	305	21	1/1/12/20	12/23/99/115	-
27	CLA	f	608	18	1/1/15/20	6/39/115/115	-
27	CLA	k	303	-	1/1/15/20	11/39/115/115	-
27	CLA	n	613	-	1/1/12/20	9/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	831	-	1/1/15/20	8/39/115/115	-
27	CLA	k	301	21	1/1/12/20	5/21/97/115	-
27	CLA	j	611	-	1/1/12/20	8/23/99/115	-
27	CLA	m	604	18	-	14/39/115/115	-
37	KC2	i	317	-	-	8/15/71/71	-
30	WVN	I	101	-	-	9/29/63/63	0/2/2/2
27	CLA	b	607	16	1/1/15/20	17/39/115/115	-
27	CLA	B	812	-	1/1/13/20	11/32/108/115	-
27	CLA	c	602	14	1/1/12/20	10/21/97/115	-
35	II0	g	316	-	-	4/21/67/67	0/2/2/2
29	LHG	b	618	-	-	15/35/35/53	-
27	CLA	m	608	18	1/1/12/20	4/23/99/115	-
27	CLA	d	307	23	-	2/10/86/115	-
30	WVN	s	205	-	-	4/29/63/63	0/2/2/2
27	CLA	f	606	18	-	4/23/99/115	-
27	CLA	g	307	24	-	8/23/99/115	-
27	CLA	g	315	-	-	9/23/99/115	-
27	CLA	a	312	-	-	19/39/115/115	-
27	CLA	a	306	39	1/1/15/20	14/39/115/115	-
27	CLA	a	305	-	1/1/12/20	6/23/99/115	-
27	CLA	c	607	14	1/1/11/20	5/17/93/115	-
27	CLA	O	202	-	1/1/15/20	14/39/115/115	-
35	II0	b	615	-	-	2/21/67/67	0/2/2/2
27	CLA	A	805	1	1/1/15/20	9/39/115/115	-
35	II0	d	312	-	-	5/21/67/67	0/2/2/2
29	LHG	c	618	27	-	13/41/41/53	-
27	CLA	i	303	22	1/1/12/20	9/21/97/115	-
27	CLA	l	303	20	1/1/11/20	5/18/94/115	-
27	CLA	e	601	19	1/1/11/20	7/15/91/115	-
30	WVN	R	202	-	-	10/29/63/63	0/2/2/2
27	CLA	B	831	-	1/1/13/20	6/31/107/115	-
27	CLA	n	607	-	1/1/15/20	13/39/115/115	-
27	CLA	A	816	-	1/1/15/20	17/39/115/115	-
27	CLA	B	814	-	1/1/13/20	5/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	830	39	1/1/11/20	6/15/91/115	-
35	II0	k	318	-	-	6/21/67/67	0/2/2/2
27	CLA	l	304	20	1/1/15/20	21/39/115/115	-
32	SF4	A	854	1,2	-	-	0/6/5/5
27	CLA	j	605	18	-	5/15/91/115	-
27	CLA	A	852	-	1/1/15/20	7/39/115/115	-
27	CLA	A	837	-	1/1/15/20	10/39/115/115	-
35	II0	d	314	-	-	5/21/67/67	0/2/2/2
35	II0	j	615	-	-	9/21/67/67	0/2/2/2
27	CLA	B	834	39	1/1/15/20	15/39/115/115	-
27	CLA	A	802	-	1/1/15/20	14/39/115/115	-
27	CLA	B	836	-	1/1/15/20	12/39/115/115	-
27	CLA	B	808	-	1/1/13/20	2/25/101/115	-
35	II0	O	203	-	-	4/21/67/67	0/2/2/2
37	KC2	k	310	21	-	8/15/71/71	-
27	CLA	l	307	20	1/1/15/20	15/39/115/115	-
28	PQN	A	843	-	-	12/23/43/43	0/2/2/2
29	LHG	A	845	27	-	5/31/31/53	-
27	CLA	B	809	-	1/1/13/20	5/27/103/115	-
27	CLA	s	203	13,27	-	19/39/115/115	-
27	CLA	b	605	39,27	1/1/15/20	13/39/115/115	-
35	II0	e	612	-	-	4/21/67/67	0/2/2/2
27	CLA	m	612	-	1/1/10/20	8/13/89/115	-
27	CLA	B	829	39	1/1/15/20	11/39/115/115	-
27	CLA	k	306	-	1/1/12/20	11/23/99/115	-
29	LHG	A	844	-	-	4/52/52/53	-
30	WVN	M	101	-	-	7/29/63/63	0/2/2/2
30	WVN	B	847	-	-	12/29/63/63	0/2/2/2
30	WVN	R	201	-	-	6/29/63/63	0/2/2/2
27	CLA	J	105	29	1/1/12/20	9/23/99/115	-
35	II0	h	311	-	-	8/21/67/67	0/2/2/2
36	IHT	a	317	-	-	4/25/65/65	0/2/2/2
27	CLA	B	823	-	1/1/15/20	13/39/115/115	-
34	LMG	F	206	-	-	11/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	WVN	B	845	-	-	10/29/63/63	0/2/2/2
29	LHG	d	315	27	-	15/41/41/53	-
35	II0	e	614	-	-	5/21/67/67	0/2/2/2
37	KC2	s	201	13	-	7/15/71/71	-
27	CLA	d	304	-	-	7/23/99/115	-
27	CLA	A	813	-	1/1/11/20	6/15/91/115	-
29	LHG	g	321	27	-	13/41/41/53	-
29	LHG	l	318	27	-	14/36/36/53	-
27	CLA	A	818	-	1/1/15/20	16/39/115/115	-
27	CLA	a	307	15	-	6/15/91/115	-
36	IHT	O	204	-	-	10/25/65/65	0/2/2/2
27	CLA	e	611	-	-	14/39/115/115	-
27	CLA	d	303	23	1/1/15/20	23/39/115/115	-
29	LHG	j	617	27	-	4/34/34/53	-
37	KC2	m	610	18	-	5/15/71/71	-
37	KC2	g	314	37	-	5/15/71/71	-
27	CLA	A	810	-	1/1/14/20	11/36/112/115	-
29	LHG	L	207	-	-	20/53/53/53	-
27	CLA	L	206	39	1/1/12/20	5/23/99/115	-
36	IHT	c	616	-	-	8/25/65/65	0/2/2/2
27	CLA	A	840	1	-	15/39/115/115	-
27	CLA	A	836	-	-	6/39/115/115	-
27	CLA	B	805	-	1/1/15/20	10/39/115/115	-
29	LHG	i	316	27	-	11/41/41/53	-
27	CLA	j	609	29	1/1/14/20	18/35/111/115	-
27	CLA	m	603	-	1/1/15/20	9/39/115/115	-
27	CLA	A	804	-	1/1/15/20	6/39/115/115	-
27	CLA	m	602	18	1/1/13/20	10/29/105/115	-
27	CLA	A	839	39	1/1/15/20	13/39/115/115	-
27	CLA	c	612	-	1/1/15/20	14/39/115/115	-
35	II0	J	104	-	-	7/21/67/67	0/2/2/2
27	CLA	n	604	26	1/1/14/20	10/33/109/115	-
27	CLA	B	835	-	1/1/15/20	23/39/115/115	-
37	KC2	g	313	37	-	3/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	IHT	k	317	-	-	7/25/65/65	0/2/2/2
27	CLA	c	606	-	-	11/24/100/115	-
31	LMT	A	851	-	-	13/21/61/61	0/2/2/2
27	CLA	i	308	22	1/1/12/20	4/23/99/115	-
27	CLA	e	602	19	1/1/12/20	11/21/97/115	-
29	LHG	n	619	-	-	16/47/47/53	-
30	WVN	B	848	-	-	7/29/63/63	0/2/2/2
35	II0	h	312	-	-	5/21/67/67	0/2/2/2
27	CLA	k	313	-	1/1/12/20	11/23/99/115	-
35	II0	g	317	-	-	3/21/67/67	0/2/2/2
27	CLA	A	823	-	1/1/13/20	4/27/103/115	-
27	CLA	f	602	18	1/1/15/20	15/39/115/115	-
29	LHG	m	617	27	-	16/41/41/53	-
27	CLA	B	819	-	1/1/12/20	6/25/101/115	-
27	CLA	n	606	26	1/1/12/20	6/23/99/115	-
35	II0	a	315	-	-	4/21/67/67	0/2/2/2
35	II0	g	320	-	-	3/21/67/67	0/2/2/2
27	CLA	h	302	17	1/1/12/20	7/21/97/115	-
36	IHT	b	614	-	-	5/25/65/65	0/2/2/2
27	CLA	B	832	-	1/1/15/20	8/39/115/115	-
27	CLA	j	601	18	1/1/12/20	5/23/99/115	-
27	CLA	b	609	-	-	5/23/99/115	-
30	WVN	A	848	-	-	8/29/63/63	0/2/2/2
27	CLA	i	307	22	1/1/14/20	11/35/111/115	-
34	LMG	J	106	-	-	14/50/70/70	0/1/1/1
29	LHG	e	617	27	-	26/41/41/53	-
35	II0	f	615	-	-	5/21/67/67	0/2/2/2
27	CLA	f	603	-	1/1/12/20	7/23/99/115	-
27	CLA	n	602	26	1/1/12/20	2/21/97/115	-
27	CLA	i	309	29	1/1/11/20	5/17/93/115	-
27	CLA	k	308	21	1/1/15/20	12/39/115/115	-
27	CLA	l	305	-	1/1/12/20	4/23/99/115	-
35	II0	l	302	-	-	6/21/67/67	0/2/2/2
35	II0	h	310	-	-	3/17/40/67	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	817	-	1/1/15/20	15/39/115/115	-
27	CLA	J	103	8	1/1/10/20	4/12/88/115	-
27	CLA	B	828	-	1/1/12/20	5/21/97/115	-
27	CLA	K	102	-	1/1/10/20	5/12/88/115	-
27	CLA	g	311	29	1/1/12/20	8/26/102/115	-
31	LMT	a	302	-	-	6/15/35/61	0/1/1/2
27	CLA	l	308	20	1/1/15/20	10/39/115/115	-
27	CLA	e	606	19	1/1/15/20	20/39/115/115	-
27	CLA	B	820	39	1/1/15/20	13/39/115/115	-
27	CLA	h	313	39	1/1/15/20	7/39/115/115	-
35	II0	c	615	-	-	2/21/67/67	0/2/2/2
27	CLA	l	306	20	-	15/39/115/115	-

All (4103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	204	IHT	C15-C11	25.57	1.63	1.35
36	c	616	IHT	C15-C11	25.37	1.63	1.35
36	n	617	IHT	C15-C11	25.20	1.62	1.35
36	j	616	IHT	C15-C11	25.05	1.62	1.35
36	m	616	IHT	C15-C11	25.02	1.62	1.35
36	a	317	IHT	C15-C11	25.01	1.62	1.35
36	c	620	IHT	C15-C11	24.89	1.62	1.35
36	g	319	IHT	C15-C11	24.85	1.62	1.35
36	f	617	IHT	C15-C11	24.79	1.62	1.35
36	b	614	IHT	C15-C11	24.74	1.62	1.35
36	k	317	IHT	C15-C11	24.51	1.62	1.35
36	O	204	IHT	C15-C11	24.29	1.61	1.35
35	l	317	II0	C14-C10	24.01	1.61	1.35
35	c	615	II0	C14-C10	23.85	1.61	1.35
35	a	315	II0	C14-C10	23.80	1.61	1.35
35	j	613	II0	C13-C09	23.77	1.61	1.35
35	n	616	II0	C13-C09	23.68	1.61	1.35
35	n	618	II0	C13-C09	23.68	1.61	1.35
35	j	615	II0	C14-C10	23.62	1.61	1.35
35	d	313	II0	C14-C10	23.60	1.61	1.35
35	c	613	II0	C14-C10	23.58	1.61	1.35
35	a	318	II0	C13-C09	23.58	1.61	1.35
35	a	316	II0	C14-C10	23.57	1.61	1.35
35	l	302	II0	C13-C09	23.54	1.61	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	j	614	II0	C14-C10	23.54	1.61	1.35
35	i	313	II0	C14-C10	23.46	1.61	1.35
35	n	615	II0	C13-C09	23.38	1.60	1.35
35	J	104	II0	C14-C10	23.37	1.60	1.35
35	e	613	II0	C13-C09	23.28	1.60	1.35
35	d	314	II0	C14-C10	23.25	1.60	1.35
35	d	314	II0	C13-C09	23.20	1.60	1.35
35	g	317	II0	C14-C10	23.19	1.60	1.35
35	e	612	II0	C14-C10	23.18	1.60	1.35
35	h	312	II0	C13-C09	23.15	1.60	1.35
35	a	318	II0	C14-C10	23.13	1.60	1.35
35	n	614	II0	C13-C09	23.12	1.60	1.35
35	e	613	II0	C14-C10	23.11	1.60	1.35
35	k	316	II0	C13-C09	23.11	1.60	1.35
35	g	316	II0	C13-C09	23.08	1.60	1.35
35	n	618	II0	C14-C10	23.07	1.60	1.35
35	e	616	II0	C13-C09	23.05	1.60	1.35
35	m	615	II0	C14-C10	23.00	1.60	1.35
35	l	302	II0	C14-C10	22.99	1.60	1.35
35	k	316	II0	C14-C10	22.98	1.60	1.35
35	e	614	II0	C14-C10	22.97	1.60	1.35
35	i	314	II0	C14-C10	22.97	1.60	1.35
35	i	318	II0	C13-C09	22.94	1.60	1.35
35	n	616	II0	C14-C10	22.94	1.60	1.35
35	d	312	II0	C14-C10	22.91	1.60	1.35
35	m	614	II0	C14-C10	22.86	1.60	1.35
35	g	316	II0	C14-C10	22.85	1.60	1.35
35	l	313	II0	C14-C10	22.85	1.60	1.35
35	b	615	II0	C13-C09	22.84	1.60	1.35
35	d	313	II0	C13-C09	22.82	1.60	1.35
35	h	310	II0	C13-C09	22.81	1.60	1.35
35	k	314	II0	C14-C10	22.78	1.60	1.35
35	e	616	II0	C14-C10	22.78	1.60	1.35
35	j	614	II0	C13-C09	22.77	1.60	1.35
35	c	614	II0	C13-C09	22.75	1.60	1.35
35	i	313	II0	C13-C09	22.75	1.60	1.35
35	h	312	II0	C14-C10	22.72	1.60	1.35
35	l	317	II0	C13-C09	22.70	1.60	1.35
35	l	314	II0	C14-C10	22.69	1.60	1.35
35	n	614	II0	C14-C10	22.69	1.60	1.35
35	f	614	II0	C14-C10	22.68	1.60	1.35
35	b	613	II0	C14-C10	22.61	1.60	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	618	II0	C13-C09	22.61	1.60	1.35
35	m	613	II0	C14-C10	22.59	1.60	1.35
35	c	617	II0	C13-C09	22.59	1.60	1.35
35	b	613	II0	C13-C09	22.57	1.60	1.35
35	f	615	II0	C14-C10	22.57	1.60	1.35
35	j	613	II0	C14-C10	22.50	1.59	1.35
35	g	317	II0	C13-C09	22.48	1.59	1.35
35	c	617	II0	C14-C10	22.48	1.59	1.35
35	e	614	II0	C13-C09	22.48	1.59	1.35
35	O	203	II0	C14-C10	22.47	1.59	1.35
35	g	320	II0	C14-C10	22.47	1.59	1.35
35	a	316	II0	C13-C09	22.47	1.59	1.35
35	g	318	II0	C14-C10	22.46	1.59	1.35
35	f	616	II0	C13-C09	22.44	1.59	1.35
35	O	203	II0	C13-C09	22.42	1.59	1.35
35	m	615	II0	C13-C09	22.41	1.59	1.35
35	l	315	II0	C14-C10	22.36	1.59	1.35
35	f	618	II0	C14-C10	22.36	1.59	1.35
35	f	615	II0	C13-C09	22.35	1.59	1.35
35	d	312	II0	C13-C09	22.34	1.59	1.35
35	m	614	II0	C13-C09	22.33	1.59	1.35
35	n	615	II0	C14-C10	22.32	1.59	1.35
35	J	104	II0	C13-C09	22.30	1.59	1.35
35	k	315	II0	C14-C10	22.29	1.59	1.35
35	c	615	II0	C13-C09	22.28	1.59	1.35
35	h	311	II0	C13-C09	22.27	1.59	1.35
35	l	314	II0	C13-C09	22.26	1.59	1.35
35	e	612	II0	C13-C09	22.25	1.59	1.35
35	f	614	II0	C13-C09	22.24	1.59	1.35
35	a	314	II0	C14-C10	22.23	1.59	1.35
35	g	320	II0	C13-C09	22.23	1.59	1.35
35	l	313	II0	C13-C09	22.20	1.59	1.35
35	j	615	II0	C13-C09	22.14	1.59	1.35
35	c	613	II0	C13-C09	22.07	1.59	1.35
35	a	315	II0	C13-C09	22.07	1.59	1.35
35	m	613	II0	C13-C09	22.04	1.59	1.35
35	i	318	II0	C14-C10	22.03	1.59	1.35
35	l	315	II0	C13-C09	22.02	1.59	1.35
35	k	318	II0	C14-C10	21.96	1.59	1.35
35	k	314	II0	C13-C09	21.94	1.59	1.35
35	k	315	II0	C13-C09	21.90	1.59	1.35
35	c	614	II0	C14-C10	21.88	1.59	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	616	II0	C14-C10	21.73	1.59	1.35
35	a	314	II0	C13-C09	21.72	1.59	1.35
35	b	612	II0	C14-C10	21.65	1.59	1.35
35	b	612	II0	C13-C09	21.62	1.59	1.35
35	i	314	II0	C13-C09	21.59	1.58	1.35
35	g	318	II0	C13-C09	21.50	1.58	1.35
35	k	318	II0	C13-C09	21.37	1.58	1.35
35	h	311	II0	C14-C10	21.34	1.58	1.35
35	b	615	II0	C14-C10	20.72	1.58	1.35
36	b	614	IHT	C10-C07	15.59	1.60	1.34
36	O	204	IHT	C10-C07	15.50	1.60	1.34
36	k	317	IHT	C10-C07	15.36	1.60	1.34
36	c	620	IHT	C10-C07	15.35	1.60	1.34
36	a	317	IHT	C10-C07	15.31	1.60	1.34
36	n	617	IHT	C10-C07	15.29	1.60	1.34
36	m	616	IHT	C10-C07	15.22	1.60	1.34
36	R	204	IHT	C10-C07	15.21	1.60	1.34
36	g	319	IHT	C10-C07	15.17	1.59	1.34
36	c	616	IHT	C10-C07	15.17	1.59	1.34
36	f	617	IHT	C10-C07	15.02	1.59	1.34
36	j	616	IHT	C10-C07	14.89	1.59	1.34
36	c	616	IHT	C05-C08	-12.26	1.34	1.52
35	J	104	II0	C05-C07	-12.16	1.35	1.52
35	k	316	II0	C05-C07	-12.11	1.35	1.52
35	c	613	II0	C05-C07	-12.11	1.35	1.52
35	n	615	II0	C05-C07	-12.01	1.35	1.52
35	h	311	II0	C05-C07	-11.99	1.35	1.52
35	e	612	II0	C27-C25	11.95	1.58	1.50
36	c	620	IHT	C05-C08	-11.92	1.35	1.52
35	c	614	II0	C06-C08	-11.81	1.35	1.52
35	i	314	II0	C05-C07	-11.79	1.35	1.52
35	a	316	II0	C05-C07	-11.79	1.35	1.52
35	f	615	II0	C05-C07	-11.73	1.35	1.52
35	l	313	II0	C05-C07	-11.73	1.35	1.52
35	c	614	II0	C05-C07	-11.72	1.35	1.52
36	g	319	IHT	C05-C08	-11.71	1.35	1.52
36	R	204	IHT	C05-C08	-11.68	1.35	1.52
35	a	315	II0	C05-C07	-11.64	1.35	1.52
35	j	614	II0	C06-C08	-11.62	1.35	1.52
35	c	617	II0	C05-C07	-11.61	1.35	1.52
35	b	613	II0	C05-C07	-11.60	1.35	1.52
36	b	614	IHT	C05-C08	-11.57	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	614	II0	C05-C07	-11.55	1.35	1.52
35	m	613	II0	C05-C07	-11.55	1.35	1.52
36	m	616	IHT	C05-C08	-11.54	1.36	1.52
36	a	317	IHT	C05-C08	-11.54	1.36	1.52
35	n	618	II0	C05-C07	-11.54	1.36	1.52
35	l	314	II0	C06-C08	-11.53	1.36	1.52
35	j	615	II0	C05-C07	-11.51	1.36	1.52
35	i	313	II0	C05-C07	-11.50	1.36	1.52
35	l	302	II0	C06-C08	-11.50	1.36	1.52
36	k	317	IHT	C05-C08	-11.49	1.36	1.52
35	b	615	II0	C05-C07	-11.49	1.36	1.52
35	c	615	II0	C05-C07	-11.49	1.36	1.52
35	g	320	II0	C05-C07	-11.47	1.36	1.52
35	j	613	II0	C05-C07	-11.45	1.36	1.52
35	f	616	II0	C05-C07	-11.43	1.36	1.52
35	e	614	II0	C05-C07	-11.41	1.36	1.52
35	n	616	II0	C05-C07	-11.40	1.36	1.52
35	e	613	II0	C05-C07	-11.39	1.36	1.52
35	a	318	II0	C05-C07	-11.38	1.36	1.52
35	n	614	II0	C05-C07	-11.37	1.36	1.52
36	O	204	IHT	C05-C08	-11.35	1.36	1.52
35	h	312	II0	C05-C07	-11.34	1.36	1.52
36	j	616	IHT	C05-C08	-11.31	1.36	1.52
35	O	203	II0	C05-C07	-11.28	1.36	1.52
35	a	314	II0	C05-C07	-11.28	1.36	1.52
36	f	617	IHT	C05-C08	-11.27	1.36	1.52
35	l	314	II0	C05-C07	-11.25	1.36	1.52
35	k	314	II0	C06-C08	-11.25	1.36	1.52
35	l	317	II0	C05-C07	-11.24	1.36	1.52
36	n	617	IHT	C05-C08	-11.22	1.36	1.52
35	n	616	II0	C06-C08	-11.22	1.36	1.52
35	e	616	II0	C11-C07	11.21	1.71	1.52
35	a	315	II0	C06-C08	-11.20	1.36	1.52
36	f	617	IHT	C12-C08	11.20	1.71	1.52
35	d	314	II0	C11-C07	11.20	1.71	1.52
35	g	317	II0	C11-C07	11.15	1.71	1.52
35	b	612	II0	C05-C07	-11.14	1.36	1.52
35	l	302	II0	C05-C07	-11.14	1.36	1.52
35	n	618	II0	C11-C07	11.09	1.71	1.52
35	j	614	II0	C05-C07	-11.07	1.36	1.52
35	h	310	II0	C05-C07	-11.05	1.36	1.52
35	n	616	II0	C11-C07	11.05	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	315	II0	C05-C07	-11.03	1.36	1.52
36	n	617	IHT	C12-C08	11.03	1.71	1.52
35	f	618	II0	C06-C08	-10.99	1.36	1.52
35	g	316	II0	C05-C07	-10.98	1.36	1.52
36	R	204	IHT	C12-C08	10.98	1.71	1.52
35	m	614	II0	C05-C07	-10.97	1.36	1.52
35	g	318	II0	C05-C07	-10.97	1.36	1.52
36	O	204	IHT	C12-C08	10.95	1.71	1.52
35	g	320	II0	C06-C08	-10.95	1.36	1.52
35	J	104	II0	C06-C08	-10.94	1.36	1.52
35	m	615	II0	C05-C07	-10.92	1.36	1.52
35	f	618	II0	C11-C07	10.92	1.71	1.52
35	c	617	II0	C11-C07	10.90	1.71	1.52
36	j	616	IHT	C12-C08	10.88	1.71	1.52
35	j	615	II0	C11-C07	10.87	1.71	1.52
35	e	612	II0	C11-C07	10.85	1.71	1.52
35	k	318	II0	C11-C07	10.85	1.71	1.52
36	k	317	IHT	C12-C08	10.85	1.71	1.52
35	k	314	II0	C05-C07	-10.83	1.37	1.52
35	g	317	II0	C05-C07	-10.82	1.37	1.52
36	b	614	IHT	C12-C08	10.82	1.71	1.52
35	O	203	II0	C11-C07	10.81	1.71	1.52
35	d	312	II0	C06-C08	-10.80	1.37	1.52
35	O	203	II0	C06-C08	-10.80	1.37	1.52
36	c	616	IHT	C12-C08	10.77	1.71	1.52
35	m	614	II0	C06-C08	-10.77	1.37	1.52
35	f	615	II0	C06-C08	-10.76	1.37	1.52
35	m	615	II0	C11-C07	10.76	1.71	1.52
35	f	615	II0	C11-C07	10.74	1.71	1.52
35	d	313	II0	C05-C07	-10.73	1.37	1.52
36	a	317	IHT	C12-C08	10.73	1.71	1.52
35	h	310	II0	C11-C07	10.72	1.71	1.52
35	l	313	II0	C06-C08	-10.72	1.37	1.52
35	b	613	II0	C06-C08	-10.71	1.37	1.52
35	g	317	II0	C06-C08	-10.69	1.37	1.52
35	k	318	II0	C06-C08	-10.69	1.37	1.52
35	e	616	II0	C05-C07	-10.65	1.37	1.52
35	a	316	II0	C06-C08	-10.64	1.37	1.52
35	l	315	II0	C11-C07	10.63	1.70	1.52
35	a	314	II0	C06-C08	-10.62	1.37	1.52
35	f	618	II0	C05-C07	-10.60	1.37	1.52
35	i	314	II0	C11-C07	10.60	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	m	616	IHT	C12-C08	10.58	1.70	1.52
35	k	318	II0	C05-C07	-10.57	1.37	1.52
35	d	312	II0	C05-C07	-10.56	1.37	1.52
36	c	620	IHT	C12-C08	10.55	1.70	1.52
35	g	318	II0	C11-C07	10.55	1.70	1.52
35	i	313	II0	C06-C08	-10.55	1.37	1.52
35	d	312	II0	C11-C07	10.54	1.70	1.52
35	e	612	II0	C06-C08	-10.53	1.37	1.52
35	a	318	II0	C11-C07	10.53	1.70	1.52
35	h	311	II0	C06-C08	-10.51	1.37	1.52
35	i	318	II0	C05-C07	-10.51	1.37	1.52
35	i	313	II0	C11-C07	10.49	1.70	1.52
36	g	319	IHT	C12-C08	10.48	1.70	1.52
35	i	318	II0	C11-C07	10.47	1.70	1.52
35	b	612	II0	C06-C08	-10.47	1.37	1.52
35	d	314	II0	C06-C08	-10.47	1.37	1.52
35	l	317	II0	C11-C07	10.46	1.70	1.52
35	h	312	II0	C11-C07	10.46	1.70	1.52
35	n	615	II0	C06-C08	-10.45	1.37	1.52
35	c	614	II0	C11-C07	10.44	1.70	1.52
35	a	316	II0	C11-C07	10.44	1.70	1.52
35	m	613	II0	C11-C07	10.44	1.70	1.52
35	m	615	II0	C06-C08	-10.44	1.37	1.52
35	l	317	II0	C06-C08	-10.43	1.37	1.52
35	e	614	II0	C11-C07	10.41	1.70	1.52
35	m	614	II0	C11-C07	10.40	1.70	1.52
35	n	614	II0	C11-C07	10.40	1.70	1.52
35	l	302	II0	C11-C07	10.39	1.70	1.52
35	b	615	II0	C11-C07	10.37	1.70	1.52
35	b	615	II0	C06-C08	-10.37	1.37	1.52
35	d	313	II0	C11-C07	10.36	1.70	1.52
35	g	320	II0	C11-C07	10.35	1.70	1.52
35	j	615	II0	C06-C08	-10.35	1.37	1.52
35	c	613	II0	C11-C07	10.33	1.70	1.52
35	j	613	II0	C11-C07	10.30	1.70	1.52
35	k	315	II0	C06-C08	-10.27	1.37	1.52
35	g	316	II0	C11-C07	10.26	1.70	1.52
35	m	613	II0	C06-C08	-10.25	1.37	1.52
35	k	315	II0	C05-C07	-10.25	1.37	1.52
35	h	311	II0	C11-C07	10.24	1.70	1.52
35	k	316	II0	C11-C07	10.22	1.70	1.52
35	f	614	II0	C06-C08	-10.19	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	312	II0	C06-C08	-10.17	1.37	1.52
35	d	314	II0	C05-C07	-10.17	1.37	1.52
35	c	617	II0	C06-C08	-10.17	1.37	1.52
35	n	615	II0	C11-C07	10.16	1.70	1.52
35	e	614	II0	C06-C08	-10.16	1.37	1.52
35	e	612	II0	C05-C07	-10.16	1.37	1.52
35	l	314	II0	C11-C07	10.13	1.70	1.52
35	k	314	II0	C11-C07	10.10	1.70	1.52
35	e	613	II0	C06-C08	-10.10	1.38	1.52
35	j	614	II0	C11-C07	10.09	1.69	1.52
35	n	614	II0	C06-C08	-10.08	1.38	1.52
35	b	612	II0	C11-C07	10.08	1.69	1.52
35	k	315	II0	C11-C07	10.04	1.69	1.52
35	k	316	II0	C06-C08	-10.03	1.38	1.52
35	f	614	II0	C11-C07	10.02	1.69	1.52
35	a	315	II0	C11-C07	9.98	1.69	1.52
35	a	314	II0	C11-C07	9.96	1.69	1.52
35	e	613	II0	C11-C07	9.95	1.69	1.52
35	l	315	II0	C06-C08	-9.93	1.38	1.52
35	g	318	II0	C06-C08	-9.92	1.38	1.52
35	d	313	II0	C06-C08	-9.87	1.38	1.52
35	c	613	II0	C06-C08	-9.87	1.38	1.52
35	c	615	II0	C11-C07	9.80	1.69	1.52
35	g	316	II0	C06-C08	-9.77	1.38	1.52
35	c	615	II0	C06-C08	-9.73	1.38	1.52
35	J	104	II0	C11-C07	9.71	1.69	1.52
35	n	618	II0	C06-C08	-9.65	1.38	1.52
35	l	313	II0	C11-C07	9.62	1.69	1.52
35	f	616	II0	C11-C07	9.60	1.69	1.52
35	b	613	II0	C11-C07	9.57	1.69	1.52
35	e	616	II0	C06-C08	-9.57	1.38	1.52
35	j	613	II0	C06-C08	-9.52	1.38	1.52
35	a	318	II0	C06-C08	-9.45	1.38	1.52
35	i	314	II0	C06-C08	-9.29	1.39	1.52
35	f	616	II0	C06-C08	-9.29	1.39	1.52
35	i	318	II0	C06-C08	-9.24	1.39	1.52
35	f	616	II0	C12-C08	9.08	1.68	1.52
35	l	313	II0	C27-C25	9.03	1.56	1.50
35	g	320	II0	C12-C08	8.91	1.67	1.52
35	c	615	II0	C12-C08	8.83	1.67	1.52
35	n	618	II0	C12-C08	8.76	1.67	1.52
35	b	615	II0	C12-C08	8.74	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	615	II0	C12-C08	8.73	1.67	1.52
35	a	316	II0	C12-C08	8.72	1.67	1.52
35	i	314	II0	C12-C08	8.72	1.67	1.52
35	n	614	II0	C12-C08	8.70	1.67	1.52
35	j	614	II0	C12-C08	8.66	1.67	1.52
35	k	316	II0	C12-C08	8.64	1.67	1.52
35	g	316	II0	C12-C08	8.62	1.67	1.52
35	a	318	II0	C12-C08	8.59	1.67	1.52
35	m	614	II0	C12-C08	8.59	1.67	1.52
35	g	318	II0	C12-C08	8.53	1.67	1.52
35	d	313	II0	C12-C08	8.52	1.67	1.52
35	e	613	II0	C12-C08	8.52	1.67	1.52
35	i	318	II0	C12-C08	8.51	1.67	1.52
35	k	316	II0	C21-C09	8.49	1.58	1.42
35	l	317	II0	C12-C08	8.49	1.67	1.52
35	l	317	II0	C22-C10	8.46	1.58	1.42
35	l	313	II0	C12-C08	8.45	1.67	1.52
35	c	613	II0	C12-C08	8.43	1.67	1.52
35	j	615	II0	C12-C08	8.41	1.67	1.52
35	f	614	II0	C12-C08	8.38	1.66	1.52
35	l	314	II0	C12-C08	8.37	1.66	1.52
35	g	317	II0	C12-C08	8.36	1.66	1.52
35	J	104	II0	C12-C08	8.31	1.66	1.52
35	m	615	II0	C12-C08	8.30	1.66	1.52
35	k	315	II0	C12-C08	8.27	1.66	1.52
35	e	612	II0	C12-C08	8.26	1.66	1.52
35	d	314	II0	C12-C08	8.21	1.66	1.52
35	l	315	II0	C12-C08	8.20	1.66	1.52
35	d	312	II0	C12-C08	8.19	1.66	1.52
35	c	614	II0	C12-C08	8.19	1.66	1.52
35	l	302	II0	C12-C08	8.19	1.66	1.52
35	f	618	II0	C12-C08	8.18	1.66	1.52
35	O	203	II0	C12-C08	8.17	1.66	1.52
35	e	616	II0	C12-C08	8.17	1.66	1.52
35	j	613	II0	C12-C08	8.17	1.66	1.52
35	n	615	II0	C12-C08	8.13	1.66	1.52
35	k	318	II0	C12-C08	8.13	1.66	1.52
35	e	614	II0	C12-C08	8.12	1.66	1.52
35	n	616	II0	C12-C08	8.11	1.66	1.52
35	m	613	II0	C12-C08	8.09	1.66	1.52
35	b	612	II0	C12-C08	8.04	1.66	1.52
35	a	318	II0	C22-C10	8.03	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	315	II0	C12-C08	7.98	1.66	1.52
35	h	312	II0	C12-C08	7.94	1.66	1.52
35	d	313	II0	C21-C09	7.92	1.57	1.42
35	a	314	II0	C12-C08	7.92	1.66	1.52
35	n	618	II0	C22-C10	7.88	1.57	1.42
35	b	613	II0	C12-C08	7.87	1.66	1.52
35	l	302	II0	C21-C09	7.87	1.57	1.42
35	c	615	II0	C21-C09	7.85	1.57	1.42
35	d	313	II0	C22-C10	7.82	1.57	1.42
35	k	314	II0	C12-C08	7.77	1.65	1.52
35	j	613	II0	C21-C09	7.77	1.57	1.42
35	j	615	II0	C21-C09	7.76	1.57	1.42
35	l	315	II0	C21-C09	7.75	1.57	1.42
35	a	318	II0	C21-C09	7.67	1.57	1.42
35	c	617	II0	C12-C08	7.67	1.65	1.52
35	j	615	II0	C22-C10	7.66	1.57	1.42
35	f	616	II0	C21-C09	7.66	1.57	1.42
35	e	614	II0	C22-C10	7.63	1.56	1.42
35	g	318	II0	C21-C09	7.61	1.56	1.42
35	i	313	II0	C12-C08	7.60	1.65	1.52
35	f	618	II0	C22-C10	7.60	1.56	1.42
28	A	843	PQN	C3-C2	7.57	1.48	1.35
35	d	314	II0	C22-C10	7.55	1.56	1.42
35	i	318	II0	C21-C09	7.55	1.56	1.42
35	O	203	II0	C22-C10	7.52	1.56	1.42
35	k	316	II0	C22-C10	7.52	1.56	1.42
28	B	841	PQN	C3-C2	7.51	1.48	1.35
35	d	312	II0	C22-C10	7.50	1.56	1.42
35	c	614	II0	C22-C10	7.49	1.56	1.42
35	m	613	II0	C21-C09	7.48	1.56	1.42
35	l	315	II0	C22-C10	7.44	1.56	1.42
35	n	616	II0	C21-C09	7.44	1.56	1.42
35	i	314	II0	C22-C10	7.43	1.56	1.42
35	k	314	II0	C22-C10	7.42	1.56	1.42
35	c	613	II0	C22-C10	7.42	1.56	1.42
35	i	314	II0	C21-C09	7.40	1.56	1.42
35	c	617	II0	C22-C10	7.40	1.56	1.42
35	n	615	II0	C21-C09	7.39	1.56	1.42
35	e	612	II0	C21-C09	7.38	1.56	1.42
35	m	615	II0	C22-C10	7.37	1.56	1.42
35	h	311	II0	C12-C08	7.37	1.65	1.52
35	d	314	II0	C21-C09	7.37	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	616	II0	C22-C10	7.34	1.56	1.42
35	c	615	II0	C22-C10	7.32	1.56	1.42
35	j	614	II0	C21-C09	7.31	1.56	1.42
35	c	617	II0	C21-C09	7.31	1.56	1.42
35	l	314	II0	C22-C10	7.30	1.56	1.42
36	g	319	IHT	C02-C07	-7.29	1.44	1.53
37	g	313	KC2	C4C-NC	7.27	1.49	1.37
35	e	616	II0	C21-C09	7.26	1.56	1.42
36	c	620	IHT	C04-C06	-7.26	1.35	1.52
36	b	614	IHT	C22-C23	7.26	1.61	1.46
36	j	616	IHT	C04-C06	-7.25	1.35	1.52
35	d	312	II0	C21-C09	7.24	1.56	1.42
35	b	615	II0	C22-C10	7.24	1.56	1.42
36	j	616	IHT	C02-C07	-7.24	1.44	1.53
35	a	316	II0	C22-C10	7.23	1.56	1.42
35	k	315	II0	C21-C09	7.22	1.56	1.42
35	e	613	II0	C22-C10	7.21	1.56	1.42
36	k	317	IHT	C04-C06	-7.21	1.35	1.52
35	n	616	II0	C22-C10	7.20	1.56	1.42
35	O	203	II0	C21-C09	7.19	1.56	1.42
35	k	318	II0	C21-C09	7.19	1.56	1.42
36	m	616	IHT	C04-C06	-7.19	1.35	1.52
37	m	610	KC2	C4C-NC	7.19	1.49	1.37
35	a	314	II0	C21-C09	7.18	1.56	1.42
37	k	310	KC2	C4C-NC	7.17	1.49	1.37
37	k	312	KC2	C4C-NC	7.16	1.49	1.37
35	f	616	II0	C22-C10	7.16	1.56	1.42
36	c	616	IHT	C04-C06	-7.16	1.35	1.52
35	h	312	II0	C21-C09	7.15	1.56	1.42
35	e	613	II0	C21-C09	7.14	1.56	1.42
36	O	204	IHT	C04-C06	-7.14	1.35	1.52
37	f	611	KC2	C4C-NC	7.13	1.49	1.37
36	R	204	IHT	C04-C06	-7.12	1.35	1.52
35	e	614	II0	C21-C09	7.12	1.55	1.42
35	c	613	II0	C21-C09	7.11	1.55	1.42
37	g	314	KC2	C4C-NC	7.10	1.49	1.37
36	g	319	IHT	C04-C06	-7.10	1.35	1.52
37	d	309	KC2	C4C-NC	7.10	1.49	1.37
35	l	317	II0	C21-C09	7.10	1.55	1.42
35	e	612	II0	C22-C10	7.09	1.55	1.42
36	a	317	IHT	C04-C06	-7.09	1.35	1.52
35	f	614	II0	C21-C09	7.07	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	e	609	KC2	C4C-NC	7.07	1.49	1.37
36	f	617	IHT	C04-C06	-7.06	1.35	1.52
37	i	310	KC2	C4C-NC	7.06	1.49	1.37
35	a	315	II0	C22-C10	7.06	1.55	1.42
35	m	613	II0	C22-C10	7.05	1.55	1.42
35	i	313	II0	C22-C10	7.05	1.55	1.42
37	c	610	KC2	C4C-NC	7.04	1.49	1.37
36	n	617	IHT	C04-C06	-7.04	1.35	1.52
37	g	312	KC2	C4C-NC	7.04	1.49	1.37
35	m	614	II0	C21-C09	7.03	1.55	1.42
35	f	614	II0	C22-C10	7.02	1.55	1.42
35	f	618	II0	C21-C09	7.02	1.55	1.42
35	n	618	II0	C21-C09	7.01	1.55	1.42
35	f	615	II0	C21-C09	7.01	1.55	1.42
37	j	610	KC2	C4C-NC	7.01	1.49	1.37
37	l	311	KC2	C4C-NC	6.99	1.49	1.37
35	l	313	II0	C22-C10	6.99	1.55	1.42
35	i	313	II0	C21-C09	6.98	1.55	1.42
37	n	611	KC2	C4C-NC	6.98	1.49	1.37
35	a	316	II0	C21-C09	6.97	1.55	1.42
35	l	314	II0	C21-C09	6.97	1.55	1.42
35	g	316	II0	C22-C10	6.95	1.55	1.42
35	g	317	II0	C21-C09	6.94	1.55	1.42
35	k	318	II0	C22-C10	6.93	1.55	1.42
37	i	317	KC2	C4C-NC	6.92	1.49	1.37
36	f	617	IHT	C21-C11	6.91	1.55	1.42
35	b	612	II0	C21-C09	6.90	1.55	1.42
36	R	204	IHT	C21-C11	6.90	1.55	1.42
37	k	311	KC2	C4C-NC	6.90	1.49	1.37
35	g	320	II0	C22-C10	6.90	1.55	1.42
35	c	614	II0	C21-C09	6.90	1.55	1.42
35	b	613	II0	C22-C10	6.88	1.55	1.42
35	h	311	II0	C22-C10	6.87	1.55	1.42
36	b	614	IHT	C34-C35	6.87	1.60	1.46
35	l	313	II0	C21-C09	6.87	1.55	1.42
36	a	317	IHT	C21-C11	6.86	1.55	1.42
37	n	612	KC2	C4C-NC	6.85	1.48	1.37
37	s	204	KC2	C4C-NC	6.83	1.48	1.37
35	a	315	II0	C21-C09	6.82	1.55	1.42
35	d	314	II0	C27-C25	6.81	1.55	1.50
35	g	318	II0	C22-C10	6.81	1.55	1.42
35	J	104	II0	C21-C09	6.81	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	317	IHT	C02-C07	-6.79	1.45	1.53
35	n	614	II0	C21-C09	6.79	1.55	1.42
36	n	617	IHT	C21-C11	6.79	1.55	1.42
37	s	201	KC2	C4C-NC	6.78	1.48	1.37
36	c	616	IHT	C21-C11	6.78	1.55	1.42
35	e	613	II0	C27-C25	6.76	1.55	1.50
35	g	320	II0	C21-C09	6.74	1.55	1.42
37	d	310	KC2	C4C-NC	6.73	1.48	1.37
35	m	615	II0	C21-C09	6.72	1.55	1.42
36	j	616	IHT	C21-C11	6.72	1.55	1.42
36	R	204	IHT	C02-C07	-6.71	1.45	1.53
35	n	615	II0	C22-C10	6.69	1.55	1.42
36	c	616	IHT	C02-C07	-6.68	1.45	1.53
35	n	614	II0	C22-C10	6.66	1.55	1.42
36	b	614	IHT	C04-C06	-6.64	1.36	1.52
35	h	312	II0	C22-C10	6.62	1.55	1.42
35	h	310	II0	C21-C09	6.62	1.55	1.42
35	h	311	II0	C21-C09	6.60	1.54	1.42
36	f	617	IHT	C02-C07	-6.60	1.45	1.53
36	b	614	IHT	C02-C07	-6.59	1.45	1.53
36	m	616	IHT	C21-C11	6.58	1.54	1.42
35	b	615	II0	C21-C09	6.58	1.54	1.42
35	k	314	II0	C21-C09	6.57	1.54	1.42
36	n	617	IHT	C02-C07	-6.55	1.45	1.53
36	k	317	IHT	C21-C11	6.54	1.54	1.42
35	b	612	II0	C11-C13	-6.51	1.40	1.51
35	b	613	II0	C21-C09	6.50	1.54	1.42
35	b	612	II0	C22-C10	6.49	1.54	1.42
35	J	104	II0	C22-C10	6.49	1.54	1.42
35	g	317	II0	C22-C10	6.44	1.54	1.42
36	O	204	IHT	C02-C07	-6.42	1.45	1.53
36	k	317	IHT	C02-C07	-6.41	1.45	1.53
35	l	302	II0	C22-C10	6.40	1.54	1.42
36	c	620	IHT	C21-C11	6.40	1.54	1.42
35	j	614	II0	C22-C10	6.39	1.54	1.42
36	g	319	IHT	C21-C11	6.39	1.54	1.42
36	k	317	IHT	C12-C15	-6.32	1.41	1.51
36	c	620	IHT	C02-C07	-6.29	1.45	1.53
35	i	313	II0	C27-C25	6.26	1.55	1.50
35	j	613	II0	C22-C10	6.24	1.54	1.42
36	O	204	IHT	C21-C11	6.20	1.54	1.42
36	g	319	IHT	C12-C15	-6.20	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	616	II0	C11-C13	-6.18	1.41	1.51
36	O	204	IHT	C22-C23	6.17	1.59	1.46
36	O	204	IHT	C12-C15	-6.17	1.41	1.51
36	m	616	IHT	C02-C07	-6.12	1.45	1.53
35	g	316	II0	C21-C09	6.08	1.53	1.42
36	n	617	IHT	C22-C23	6.06	1.58	1.46
36	c	620	IHT	C22-C23	6.05	1.58	1.46
37	d	310	KC2	C2A-C3A	6.01	1.49	1.37
36	j	616	IHT	C12-C15	-6.01	1.41	1.51
35	m	614	II0	C22-C10	6.00	1.53	1.42
35	k	315	II0	C22-C10	6.00	1.53	1.42
35	b	613	II0	C28-C26	6.00	1.54	1.50
36	c	620	IHT	C12-C15	-5.97	1.41	1.51
35	k	314	II0	C11-C13	-5.95	1.41	1.51
36	m	616	IHT	C22-C23	5.94	1.58	1.46
36	a	317	IHT	C22-C23	5.92	1.58	1.46
36	R	204	IHT	C22-C23	5.91	1.58	1.46
36	m	616	IHT	C12-C15	-5.91	1.41	1.51
35	f	615	II0	C22-C10	5.90	1.53	1.42
36	f	617	IHT	C22-C23	5.89	1.58	1.46
36	k	317	IHT	C22-C23	5.88	1.58	1.46
36	b	614	IHT	C04-C02	5.86	1.67	1.54
35	a	314	II0	C22-C10	5.86	1.53	1.42
35	f	614	II0	C11-C13	-5.85	1.41	1.51
35	J	104	II0	C11-C13	-5.84	1.41	1.51
35	a	315	II0	C11-C13	-5.84	1.41	1.51
35	b	613	II0	C11-C13	-5.82	1.42	1.51
36	c	616	IHT	C22-C23	5.82	1.58	1.46
37	e	609	KC2	C2A-C3A	5.81	1.49	1.37
35	d	313	II0	C27-C25	5.80	1.54	1.50
35	e	613	II0	C11-C13	-5.78	1.42	1.51
35	h	311	II0	C11-C13	-5.77	1.42	1.51
36	b	614	IHT	C12-C15	-5.76	1.42	1.51
35	k	316	II0	C27-C25	5.76	1.54	1.50
37	k	311	KC2	C2A-C3A	5.76	1.48	1.37
37	g	313	KC2	C2A-C3A	5.75	1.48	1.37
36	a	317	IHT	C12-C15	-5.75	1.42	1.51
36	b	614	IHT	C21-C11	5.74	1.53	1.42
35	g	320	II0	C11-C13	-5.71	1.42	1.51
36	n	617	IHT	C12-C15	-5.70	1.42	1.51
35	i	318	II0	C11-C13	-5.69	1.42	1.51
37	k	310	KC2	C2A-C3A	5.69	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	319	IHT	C22-C23	5.67	1.58	1.46
37	l	311	KC2	C2A-C3A	5.66	1.48	1.37
35	k	315	II0	C11-C13	-5.65	1.42	1.51
36	j	616	IHT	C22-C23	5.65	1.58	1.46
35	a	314	II0	C11-C13	-5.65	1.42	1.51
35	d	312	II0	C11-C13	-5.63	1.42	1.51
37	k	312	KC2	C2A-C3A	5.63	1.48	1.37
35	c	614	II0	C11-C13	-5.62	1.42	1.51
37	c	610	KC2	C2A-C3A	5.62	1.48	1.37
35	c	613	II0	C11-C13	-5.60	1.42	1.51
37	f	611	KC2	C2A-C3A	5.60	1.48	1.37
37	d	309	KC2	C2A-C3A	5.59	1.48	1.37
35	h	312	II0	C28-C26	5.57	1.54	1.50
36	f	617	IHT	C12-C15	-5.57	1.42	1.51
37	s	204	KC2	CHD-C4C	5.57	1.49	1.38
37	g	314	KC2	C2A-C3A	5.56	1.48	1.37
37	m	610	KC2	C2A-C3A	5.56	1.48	1.37
35	a	316	II0	C11-C13	-5.55	1.42	1.51
37	i	310	KC2	C2A-C3A	5.54	1.48	1.37
35	f	618	II0	C11-C13	-5.54	1.42	1.51
36	f	617	IHT	C34-C35	5.53	1.57	1.46
37	i	317	KC2	C2A-C3A	5.52	1.48	1.37
36	c	616	IHT	C34-C35	5.51	1.57	1.46
35	l	317	II0	C11-C13	-5.50	1.42	1.51
37	j	610	KC2	C2A-C3A	5.49	1.48	1.37
37	g	312	KC2	C2A-C3A	5.49	1.48	1.37
35	k	318	II0	C11-C13	-5.47	1.42	1.51
35	e	616	II0	C11-C13	-5.47	1.42	1.51
35	n	615	II0	C11-C13	-5.47	1.42	1.51
35	l	314	II0	C11-C13	-5.46	1.42	1.51
35	j	613	II0	C11-C13	-5.45	1.42	1.51
37	n	612	KC2	CHD-C4C	5.45	1.49	1.38
35	h	310	II0	C11-C13	-5.45	1.42	1.51
36	n	617	IHT	C34-C35	5.44	1.57	1.46
35	k	316	II0	C11-C13	-5.43	1.42	1.51
37	n	611	KC2	C2A-C3A	5.43	1.48	1.37
36	R	204	IHT	C34-C35	5.42	1.57	1.46
36	m	616	IHT	C34-C35	5.42	1.57	1.46
37	i	317	KC2	C3B-C2B	5.42	1.48	1.37
37	i	317	KC2	CHD-C4C	5.41	1.49	1.38
36	b	614	IHT	C30-C27	5.40	1.59	1.43
35	n	614	II0	C11-C13	-5.40	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	s	201	KC2	CHD-C4C	5.39	1.49	1.38
35	e	614	II0	C11-C13	-5.39	1.42	1.51
35	g	317	II0	C11-C13	-5.36	1.42	1.51
37	m	610	KC2	CHD-C4C	5.36	1.49	1.38
35	m	615	II0	C11-C13	-5.36	1.42	1.51
35	m	614	II0	C11-C13	-5.35	1.42	1.51
36	R	204	IHT	C12-C15	-5.34	1.42	1.51
37	k	310	KC2	C3C-C2C	5.34	1.48	1.37
35	g	316	II0	C11-C13	-5.33	1.42	1.51
37	i	317	KC2	CHB-C1B	5.33	1.48	1.38
35	g	318	II0	C11-C13	-5.33	1.42	1.51
37	d	309	KC2	CHD-C4C	5.32	1.49	1.38
35	h	312	II0	C11-C13	-5.32	1.42	1.51
37	k	312	KC2	CHD-C4C	5.32	1.49	1.38
35	j	614	II0	C11-C13	-5.31	1.42	1.51
37	e	609	KC2	CHD-C4C	5.31	1.49	1.38
37	n	612	KC2	C2A-C3A	5.29	1.47	1.37
37	c	610	KC2	CHD-C4C	5.28	1.49	1.38
37	s	204	KC2	C3C-C2C	5.28	1.47	1.37
37	i	310	KC2	CHD-C4C	5.28	1.49	1.38
35	l	302	II0	C11-C13	-5.27	1.42	1.51
35	c	615	II0	C11-C13	-5.27	1.42	1.51
37	g	314	KC2	C3C-C2C	5.27	1.47	1.37
35	d	314	II0	C11-C13	-5.27	1.42	1.51
37	l	311	KC2	C3C-C2C	5.27	1.47	1.37
37	d	309	KC2	C3C-C2C	5.26	1.47	1.37
35	a	316	II0	C27-C25	5.26	1.54	1.50
37	m	610	KC2	C3C-C2C	5.25	1.47	1.37
35	l	313	II0	C11-C13	-5.25	1.42	1.51
37	e	609	KC2	C3C-C2C	5.25	1.47	1.37
35	d	313	II0	C11-C13	-5.24	1.42	1.51
37	g	312	KC2	CHD-C4C	5.24	1.49	1.38
35	l	315	II0	C11-C13	-5.23	1.42	1.51
35	O	203	II0	C11-C13	-5.23	1.42	1.51
37	j	610	KC2	C3C-C2C	5.23	1.47	1.37
35	m	613	II0	C11-C13	-5.22	1.42	1.51
37	k	311	KC2	C1A-NA	5.22	1.48	1.38
36	c	620	IHT	C04-C02	5.22	1.66	1.54
35	a	318	II0	C11-C13	-5.22	1.42	1.51
35	i	313	II0	C11-C13	-5.21	1.42	1.51
37	g	314	KC2	CHD-C4C	5.20	1.48	1.38
37	i	310	KC2	C3C-C2C	5.19	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	m	616	IHT	C04-C02	5.19	1.66	1.54
37	k	310	KC2	CHD-C4C	5.18	1.48	1.38
36	j	616	IHT	C34-C35	5.18	1.57	1.46
37	k	312	KC2	C3C-C2C	5.18	1.47	1.37
35	i	318	II0	C27-C25	5.17	1.54	1.50
37	g	313	KC2	CHD-C4C	5.17	1.48	1.38
36	f	617	IHT	C04-C02	5.16	1.65	1.54
37	n	612	KC2	C3C-C2C	5.15	1.47	1.37
37	s	201	KC2	C3C-C2C	5.15	1.47	1.37
36	O	204	IHT	C04-C02	5.14	1.65	1.54
36	n	617	IHT	C04-C02	5.14	1.65	1.54
35	b	615	II0	C11-C13	-5.14	1.43	1.51
36	g	319	IHT	C34-C35	5.14	1.56	1.46
36	a	317	IHT	C34-C35	5.13	1.56	1.46
37	f	611	KC2	CHD-C4C	5.13	1.48	1.38
37	c	610	KC2	C3C-C2C	5.13	1.47	1.37
35	f	614	II0	C27-C25	5.12	1.54	1.50
36	k	317	IHT	C34-C35	5.12	1.56	1.46
37	k	311	KC2	C3C-C2C	5.11	1.47	1.37
37	g	313	KC2	C3C-C2C	5.10	1.47	1.37
37	k	312	KC2	C3B-C2B	5.10	1.47	1.37
37	f	611	KC2	C3C-C2C	5.10	1.47	1.37
37	i	317	KC2	C3C-C2C	5.10	1.47	1.37
35	i	314	II0	C11-C13	-5.09	1.43	1.51
37	j	610	KC2	CHD-C4C	5.09	1.48	1.38
36	c	616	IHT	C04-C02	5.08	1.65	1.54
37	c	610	KC2	C3B-C2B	5.08	1.47	1.37
36	c	616	IHT	C12-C15	-5.07	1.43	1.51
36	O	204	IHT	C34-C35	5.06	1.56	1.46
37	d	310	KC2	C3C-C2C	5.06	1.47	1.37
37	k	311	KC2	CHD-C4C	5.06	1.48	1.38
37	l	311	KC2	CHD-C4C	5.06	1.48	1.38
37	g	312	KC2	C3C-C2C	5.06	1.47	1.37
37	f	611	KC2	C3B-C2B	5.06	1.47	1.37
37	i	310	KC2	C1A-NA	5.05	1.48	1.38
37	j	610	KC2	C3B-C2B	5.05	1.47	1.37
37	g	314	KC2	C3B-C2B	5.04	1.47	1.37
37	g	312	KC2	C1A-NA	5.03	1.48	1.38
35	e	612	II0	C11-C13	-5.02	1.43	1.51
36	R	204	IHT	C04-C02	5.02	1.65	1.54
37	n	611	KC2	C3B-C2B	5.02	1.47	1.37
37	m	610	KC2	C3B-C2B	5.02	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	d	309	KC2	C3B-C2B	5.01	1.47	1.37
37	g	313	KC2	C3B-C2B	5.01	1.47	1.37
37	d	310	KC2	CHD-C4C	5.01	1.48	1.38
37	n	611	KC2	C1A-NA	5.00	1.48	1.38
37	g	314	KC2	C1A-NA	5.00	1.48	1.38
36	j	616	IHT	C04-C02	4.98	1.65	1.54
37	e	609	KC2	C3B-C2B	4.98	1.47	1.37
37	g	312	KC2	C3B-C2B	4.98	1.47	1.37
35	j	615	II0	C11-C13	-4.98	1.43	1.51
37	g	313	KC2	C1A-NA	4.98	1.48	1.38
36	c	620	IHT	C34-C35	4.97	1.56	1.46
37	n	611	KC2	C3C-C2C	4.96	1.47	1.37
37	l	311	KC2	C3B-C2B	4.96	1.47	1.37
35	i	318	II0	C22-C10	4.96	1.51	1.42
36	b	614	IHT	C06-C09	4.96	1.68	1.52
37	j	610	KC2	C1A-NA	4.95	1.48	1.38
37	d	310	KC2	C3B-C2B	4.95	1.47	1.37
29	g	301	LHG	O7-C7	4.95	1.48	1.34
36	k	317	IHT	C04-C02	4.94	1.65	1.54
37	n	612	KC2	C3B-C2B	4.93	1.47	1.37
36	g	319	IHT	C04-C02	4.93	1.65	1.54
36	a	317	IHT	C04-C02	4.92	1.65	1.54
37	k	310	KC2	C3B-C2B	4.92	1.47	1.37
35	f	615	II0	C11-C13	-4.91	1.43	1.51
37	f	611	KC2	C1A-NA	4.91	1.48	1.38
37	n	611	KC2	CHD-C4C	4.91	1.48	1.38
37	e	609	KC2	C1A-NA	4.91	1.48	1.38
35	k	316	II0	C31-C29	4.89	1.58	1.43
37	k	312	KC2	C1A-NA	4.88	1.48	1.38
37	s	201	KC2	C2A-C3A	4.88	1.47	1.37
37	c	610	KC2	C1A-NA	4.86	1.48	1.38
37	l	311	KC2	C1A-NA	4.86	1.48	1.38
35	l	315	II0	C31-C29	4.86	1.58	1.43
35	n	616	II0	C11-C13	-4.86	1.43	1.51
37	i	310	KC2	C3B-C2B	4.85	1.47	1.37
37	k	310	KC2	C1A-NA	4.84	1.48	1.38
37	m	610	KC2	C1A-NA	4.84	1.48	1.38
35	c	617	II0	C11-C13	-4.84	1.43	1.51
35	h	310	II0	C27-C25	4.79	1.54	1.50
36	R	204	IHT	C06-C09	4.77	1.67	1.52
36	a	317	IHT	C06-C09	4.77	1.67	1.52
35	h	312	II0	C27-C25	4.76	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	d	309	KC2	C1A-NA	4.76	1.47	1.38
37	k	311	KC2	C3B-C2B	4.75	1.46	1.37
36	b	614	IHT	C41-C38	4.75	1.57	1.43
36	O	204	IHT	C06-C09	4.74	1.67	1.52
37	s	204	KC2	C3B-C2B	4.74	1.46	1.37
37	s	201	KC2	C3B-C2B	4.73	1.46	1.37
36	n	617	IHT	C06-C09	4.73	1.67	1.52
37	k	310	KC2	O2D-CGD	4.73	1.44	1.33
36	k	317	IHT	C06-C09	4.73	1.67	1.52
37	n	612	KC2	O2D-CGD	4.69	1.44	1.33
35	k	314	II0	C42-C40	4.69	1.57	1.43
36	c	616	IHT	C06-C09	4.69	1.67	1.52
34	c	619	LMG	O7-C10	4.68	1.47	1.34
37	i	317	KC2	O2D-CGD	4.68	1.44	1.33
35	n	614	II0	C31-C29	4.68	1.57	1.43
35	n	618	II0	C11-C13	-4.68	1.43	1.51
37	s	204	KC2	C2A-C3A	4.66	1.46	1.37
36	j	616	IHT	C06-C09	4.66	1.67	1.52
36	b	614	IHT	C32-C33	4.65	1.55	1.46
29	i	316	LHG	O8-C23	4.65	1.46	1.33
35	e	616	II0	C42-C40	4.65	1.57	1.43
37	d	309	KC2	O2D-CGD	4.64	1.44	1.33
35	d	313	II0	C32-C30	4.64	1.57	1.43
36	f	617	IHT	C06-C09	4.64	1.67	1.52
35	l	317	II0	C32-C30	4.63	1.57	1.43
37	i	317	KC2	C1A-NA	4.61	1.47	1.38
35	f	616	II0	C27-C25	4.61	1.54	1.50
35	a	318	II0	C31-C29	4.61	1.57	1.43
37	m	610	KC2	O2D-CGD	4.60	1.44	1.33
35	i	318	II0	C42-C40	4.60	1.57	1.43
37	s	204	KC2	C1A-NA	4.59	1.47	1.38
35	g	320	II0	C32-C30	4.59	1.57	1.43
37	k	312	KC2	O2D-CGD	4.58	1.44	1.33
36	m	616	IHT	C06-C09	4.58	1.66	1.52
36	c	620	IHT	C06-C09	4.57	1.66	1.52
35	k	314	II0	C32-C30	4.57	1.57	1.43
36	n	617	IHT	C30-C27	4.57	1.57	1.43
35	a	318	II0	C32-C30	4.57	1.57	1.43
37	e	609	KC2	O2D-CGD	4.57	1.44	1.33
35	l	317	II0	C42-C40	4.56	1.57	1.43
37	g	314	KC2	O2D-CGD	4.56	1.44	1.33
35	c	615	II0	C27-C25	4.56	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	843	PQN	C10-C1	4.56	1.57	1.48
35	k	316	II0	C42-C40	4.55	1.57	1.43
36	O	204	IHT	C30-C27	4.55	1.57	1.43
37	k	311	KC2	O2D-CGD	4.55	1.44	1.33
36	a	317	IHT	C30-C27	4.55	1.57	1.43
37	g	312	KC2	O2D-CGD	4.55	1.44	1.33
37	l	311	KC2	O2D-CGD	4.55	1.44	1.33
37	j	610	KC2	O2D-CGD	4.55	1.44	1.33
35	n	615	II0	C27-C25	4.54	1.53	1.50
37	i	310	KC2	O2D-CGD	4.54	1.44	1.33
36	g	319	IHT	C06-C09	4.54	1.66	1.52
35	d	313	II0	C42-C40	4.54	1.57	1.43
37	c	610	KC2	O2D-CGD	4.54	1.44	1.33
29	c	618	LHG	O8-C23	4.54	1.46	1.33
35	m	613	II0	C31-C29	4.53	1.57	1.43
37	n	612	KC2	C1A-NA	4.53	1.47	1.38
28	B	841	PQN	C10-C1	4.53	1.56	1.48
37	i	317	KC2	CHC-C4B	4.52	1.47	1.38
37	d	310	KC2	C1A-NA	4.52	1.47	1.38
35	m	614	II0	C27-C25	4.52	1.53	1.50
35	a	315	II0	C27-C25	4.51	1.53	1.50
35	a	318	II0	C42-C40	4.51	1.57	1.43
37	n	611	KC2	O2D-CGD	4.51	1.44	1.33
29	g	321	LHG	O7-C7	4.51	1.47	1.34
37	d	310	KC2	O2D-CGD	4.51	1.44	1.33
35	n	618	II0	C32-C30	4.50	1.57	1.43
37	g	313	KC2	O2D-CGD	4.50	1.44	1.33
28	A	843	PQN	C5-C4	4.49	1.56	1.48
35	k	314	II0	C41-C39	4.49	1.57	1.43
35	i	318	II0	C12-C14	-4.48	1.44	1.51
29	j	617	LHG	O7-C7	4.48	1.46	1.34
36	f	617	IHT	C30-C27	4.48	1.57	1.43
35	f	618	II0	C32-C30	4.48	1.57	1.43
37	f	611	KC2	O2D-CGD	4.48	1.44	1.33
35	e	612	II0	C32-C30	4.47	1.57	1.43
36	c	616	IHT	C30-C27	4.45	1.57	1.43
36	b	614	IHT	C40-C37	4.45	1.57	1.43
35	j	615	II0	C42-C40	4.45	1.57	1.43
35	k	314	II0	C12-C14	-4.45	1.44	1.51
36	j	616	IHT	C30-C27	4.45	1.57	1.43
36	R	204	IHT	C30-C27	4.44	1.57	1.43
35	d	313	II0	C31-C29	4.44	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	315	LHG	O7-C7	4.43	1.46	1.34
35	k	318	II0	C31-C29	4.43	1.56	1.43
36	k	317	IHT	C30-C27	4.43	1.56	1.43
35	O	203	II0	C31-C29	4.43	1.56	1.43
35	e	616	II0	C41-C39	4.43	1.56	1.43
35	j	615	II0	C31-C29	4.42	1.56	1.43
28	B	841	PQN	C5-C4	4.42	1.56	1.48
35	i	314	II0	C42-C40	4.42	1.56	1.43
35	h	310	II0	C42-C40	4.40	1.56	1.43
35	n	614	II0	C27-C25	4.40	1.53	1.50
29	k	319	LHG	O7-C7	4.40	1.46	1.34
36	m	616	IHT	C30-C27	4.40	1.56	1.43
35	k	316	II0	C32-C30	4.39	1.56	1.43
35	n	616	II0	C31-C29	4.39	1.56	1.43
33	B	842	DGD	O2G-C1B	4.39	1.46	1.34
35	j	615	II0	C32-C30	4.38	1.56	1.43
35	l	317	II0	C31-C29	4.37	1.56	1.43
35	m	615	II0	C32-C30	4.37	1.56	1.43
35	k	314	II0	C34-C36	4.37	1.55	1.46
35	a	318	II0	C06-C04	4.37	1.67	1.54
35	d	314	II0	C42-C40	4.37	1.56	1.43
29	b	618	LHG	O7-C7	4.36	1.46	1.34
37	n	612	KC2	OBD-CAD	4.35	1.30	1.22
35	d	313	II0	C06-C04	4.35	1.67	1.54
35	l	315	II0	C42-C40	4.35	1.56	1.43
29	e	617	LHG	O7-C7	4.35	1.46	1.34
35	g	318	II0	C31-C29	4.34	1.56	1.43
35	c	617	II0	C31-C29	4.34	1.56	1.43
35	e	616	II0	C31-C29	4.34	1.56	1.43
35	l	313	II0	C31-C29	4.33	1.56	1.43
35	d	313	II0	C34-C36	4.33	1.55	1.46
35	k	316	II0	C06-C04	4.33	1.67	1.54
35	e	612	II0	C31-C29	4.32	1.56	1.43
35	f	618	II0	C42-C40	4.32	1.56	1.43
35	n	615	II0	C31-C29	4.32	1.56	1.43
37	d	310	KC2	CHB-C1B	4.32	1.46	1.38
35	n	616	II0	C42-C40	4.32	1.56	1.43
35	f	618	II0	C27-C25	4.32	1.53	1.50
37	d	310	KC2	OBD-CAD	4.32	1.29	1.22
35	e	612	II0	C42-C40	4.31	1.56	1.43
36	g	319	IHT	C30-C27	4.31	1.56	1.43
35	b	615	II0	C06-C04	4.31	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	320	II0	C42-C40	4.31	1.56	1.43
29	A	844	LHG	O7-C7	4.31	1.46	1.34
35	f	614	II0	C06-C04	4.30	1.67	1.54
35	j	613	II0	C06-C04	4.30	1.67	1.54
35	h	311	II0	C27-C25	4.30	1.53	1.50
35	d	314	II0	C31-C29	4.30	1.56	1.43
35	k	318	II0	C42-C40	4.30	1.56	1.43
35	i	314	II0	C32-C30	4.30	1.56	1.43
35	d	314	II0	C32-C30	4.29	1.56	1.43
35	i	314	II0	C06-C04	4.29	1.67	1.54
35	k	315	II0	C27-C25	4.29	1.53	1.50
35	e	616	II0	C06-C04	4.29	1.67	1.54
37	g	312	KC2	CBC-CAC	4.28	1.51	1.30
37	k	311	KC2	OBD-CAD	4.28	1.29	1.22
35	f	614	II0	C42-C40	4.28	1.56	1.43
37	i	310	KC2	CBC-CAC	4.28	1.51	1.30
34	F	206	LMG	O7-C10	4.28	1.46	1.34
35	J	104	II0	C31-C29	4.28	1.56	1.43
37	k	311	KC2	CBC-CAC	4.28	1.50	1.30
35	f	618	II0	C31-C29	4.28	1.56	1.43
35	c	615	II0	C06-C04	4.27	1.67	1.54
35	h	312	II0	C06-C04	4.27	1.67	1.54
35	i	313	II0	C42-C40	4.27	1.56	1.43
35	c	617	II0	C06-C04	4.27	1.67	1.54
35	n	614	II0	C06-C04	4.27	1.67	1.54
37	f	611	KC2	CBC-CAC	4.27	1.50	1.30
29	A	844	LHG	O8-C23	4.27	1.45	1.33
35	i	313	II0	C31-C29	4.26	1.56	1.43
35	g	320	II0	C27-C25	4.26	1.53	1.50
37	k	312	KC2	CBC-CAC	4.26	1.50	1.30
29	a	319	LHG	O8-C23	4.26	1.45	1.33
35	n	618	II0	C27-C25	4.25	1.53	1.50
35	f	618	II0	C06-C04	4.25	1.67	1.54
35	k	318	II0	C06-C04	4.25	1.67	1.54
35	f	614	II0	C32-C30	4.25	1.56	1.43
29	c	618	LHG	O7-C7	4.25	1.46	1.34
35	e	614	II0	C06-C04	4.25	1.67	1.54
37	s	201	KC2	CBC-CAC	4.24	1.50	1.30
35	n	618	II0	C42-C40	4.24	1.56	1.43
35	d	313	II0	C41-C39	4.24	1.56	1.43
37	k	312	KC2	OBD-CAD	4.24	1.29	1.22
37	k	310	KC2	CBC-CAC	4.24	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	312	II0	C31-C29	4.24	1.56	1.43
34	b	619	LMG	O7-C10	4.24	1.46	1.34
35	m	613	II0	C42-C40	4.24	1.56	1.43
34	O	205	LMG	O8-C28	4.23	1.45	1.33
37	c	610	KC2	CBC-CAC	4.23	1.50	1.30
37	e	609	KC2	CBC-CAC	4.23	1.50	1.30
35	g	320	II0	C31-C29	4.23	1.56	1.43
37	m	610	KC2	CBC-CAC	4.23	1.50	1.30
35	f	616	II0	C42-C40	4.23	1.56	1.43
37	s	204	KC2	CHD-C1D	4.23	1.48	1.39
29	i	316	LHG	O7-C7	4.23	1.46	1.34
29	b	618	LHG	O8-C23	4.22	1.45	1.33
35	a	318	II0	C41-C39	4.22	1.56	1.43
29	j	617	LHG	O8-C23	4.22	1.45	1.33
35	d	312	II0	C32-C30	4.22	1.56	1.43
35	l	314	II0	C42-C40	4.22	1.56	1.43
35	e	614	II0	C27-C25	4.21	1.53	1.50
35	a	316	II0	C31-C29	4.21	1.56	1.43
37	j	610	KC2	CBC-CAC	4.21	1.50	1.30
35	l	315	II0	C06-C04	4.21	1.67	1.54
37	i	317	KC2	CBC-CAC	4.21	1.50	1.30
37	l	311	KC2	CBC-CAC	4.21	1.50	1.30
37	g	314	KC2	CBC-CAC	4.21	1.50	1.30
35	d	312	II0	C27-C25	4.20	1.53	1.50
35	l	314	II0	C31-C29	4.20	1.56	1.43
35	O	203	II0	C32-C30	4.20	1.56	1.43
35	d	312	II0	C42-C40	4.20	1.56	1.43
35	k	316	II0	C41-C39	4.20	1.56	1.43
34	O	205	LMG	O7-C10	4.20	1.46	1.34
35	k	318	II0	C27-C25	4.19	1.53	1.50
37	d	309	KC2	CBC-CAC	4.19	1.50	1.30
37	s	204	KC2	CBC-CAC	4.19	1.50	1.30
29	c	621	LHG	O7-C7	4.18	1.46	1.34
35	g	318	II0	C06-C04	4.18	1.67	1.54
29	g	321	LHG	O8-C23	4.18	1.45	1.33
37	g	313	KC2	CBC-CAC	4.18	1.50	1.30
35	i	318	II0	C32-C30	4.18	1.56	1.43
29	k	319	LHG	O8-C23	4.18	1.45	1.33
35	c	613	II0	C32-C30	4.18	1.56	1.43
35	m	614	II0	C31-C29	4.17	1.56	1.43
29	A	850	LHG	O8-C23	4.17	1.45	1.33
37	k	310	KC2	OBD-CAD	4.17	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	j	616	IHT	C09-C10	-4.17	1.43	1.51
37	s	201	KC2	O2D-CGD	4.17	1.43	1.33
37	m	610	KC2	OBD-CAD	4.17	1.29	1.22
37	e	609	KC2	CHB-C1B	4.17	1.46	1.38
35	e	616	II0	C32-C30	4.17	1.56	1.43
36	m	616	IHT	C09-C10	-4.16	1.43	1.51
37	i	317	KC2	OBD-CAD	4.16	1.29	1.22
35	c	617	II0	C32-C30	4.16	1.56	1.43
35	c	617	II0	C42-C40	4.16	1.56	1.43
37	i	317	KC2	CHC-C1C	4.16	1.48	1.39
37	g	314	KC2	OBD-CAD	4.16	1.29	1.22
35	j	614	II0	C42-C40	4.16	1.56	1.43
35	m	613	II0	C41-C39	4.15	1.56	1.43
37	n	611	KC2	CBC-CAC	4.15	1.50	1.30
35	c	615	II0	C31-C29	4.15	1.56	1.43
35	i	318	II0	C41-C39	4.15	1.56	1.43
35	n	616	II0	C27-C25	4.15	1.53	1.50
37	d	310	KC2	CBC-CAC	4.15	1.50	1.30
35	f	614	II0	C31-C29	4.14	1.56	1.43
29	n	619	LHG	O7-C7	4.14	1.46	1.34
37	d	309	KC2	OBD-CAD	4.14	1.29	1.22
35	a	316	II0	C42-C40	4.14	1.56	1.43
35	f	615	II0	C31-C29	4.14	1.56	1.43
35	d	314	II0	C06-C04	4.14	1.67	1.54
29	l	318	LHG	O8-C23	4.14	1.45	1.33
36	c	620	IHT	C09-C10	-4.13	1.43	1.51
35	O	203	II0	C42-C40	4.13	1.56	1.43
35	g	316	II0	C41-C39	4.13	1.56	1.43
35	g	316	II0	C06-C04	4.13	1.67	1.54
35	e	613	II0	C31-C29	4.13	1.56	1.43
35	n	616	II0	C32-C30	4.13	1.56	1.43
35	c	615	II0	C42-C40	4.13	1.56	1.43
35	f	614	II0	C41-C39	4.13	1.56	1.43
36	b	614	IHT	C05-C03	4.13	1.67	1.54
35	b	613	II0	C32-C30	4.13	1.56	1.43
35	f	616	II0	C31-C29	4.13	1.56	1.43
35	a	318	II0	C34-C36	4.13	1.54	1.46
35	e	614	II0	C42-C40	4.12	1.56	1.43
35	e	612	II0	C06-C04	4.12	1.67	1.54
35	k	315	II0	C12-C14	-4.12	1.44	1.51
35	c	614	II0	C32-C30	4.12	1.56	1.43
35	j	615	II0	C06-C04	4.12	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	301	LHG	O8-C23	4.12	1.45	1.33
29	d	315	LHG	O8-C23	4.12	1.45	1.33
36	j	616	IHT	C05-C03	4.12	1.67	1.54
35	l	315	II0	C32-C30	4.11	1.55	1.43
36	f	617	IHT	C09-C10	-4.11	1.43	1.51
35	l	302	II0	C31-C29	4.11	1.55	1.43
35	f	618	II0	C41-C39	4.11	1.55	1.43
35	j	614	II0	C31-C29	4.11	1.55	1.43
29	m	617	LHG	O7-C7	4.11	1.45	1.34
35	g	320	II0	C06-C04	4.11	1.67	1.54
35	g	318	II0	C42-C40	4.11	1.55	1.43
37	s	204	KC2	O2D-CGD	4.11	1.43	1.33
34	s	210	LMG	O8-C28	4.11	1.45	1.33
35	c	613	II0	C06-C04	4.11	1.67	1.54
35	n	618	II0	C06-C04	4.10	1.67	1.54
35	c	615	II0	C32-C30	4.10	1.55	1.43
29	e	617	LHG	O8-C23	4.10	1.45	1.33
35	g	316	II0	C27-C25	4.10	1.53	1.50
37	s	204	KC2	OBD-CAD	4.10	1.29	1.22
35	m	613	II0	C06-C04	4.10	1.67	1.54
37	c	610	KC2	CHB-C1B	4.10	1.46	1.38
35	g	318	II0	C32-C30	4.10	1.55	1.43
35	c	614	II0	C31-C29	4.10	1.55	1.43
36	g	319	IHT	C09-C10	-4.10	1.43	1.51
35	g	317	II0	C31-C29	4.10	1.55	1.43
34	L	208	LMG	O7-C10	4.09	1.45	1.34
35	h	311	II0	C32-C30	4.09	1.55	1.43
29	c	621	LHG	O8-C23	4.09	1.45	1.33
37	k	310	KC2	CHC-C4B	4.08	1.46	1.38
37	i	310	KC2	CHB-C1B	4.08	1.46	1.38
36	k	317	IHT	C05-C03	4.08	1.67	1.54
37	j	610	KC2	OBD-CAD	4.08	1.29	1.22
29	L	207	LHG	O8-C23	4.08	1.45	1.33
35	l	313	II0	C32-C30	4.08	1.55	1.43
37	g	313	KC2	OBD-CAD	4.08	1.29	1.22
27	A	813	CLA	C1D-ND	4.08	1.43	1.37
34	F	206	LMG	O8-C28	4.08	1.45	1.33
35	c	613	II0	C42-C40	4.07	1.55	1.43
35	k	314	II0	C06-C04	4.07	1.67	1.54
35	e	614	II0	C31-C29	4.07	1.55	1.43
37	f	611	KC2	CHB-C1B	4.07	1.46	1.38
37	l	311	KC2	OBD-CAD	4.07	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	k	312	KC2	CHB-C1B	4.07	1.46	1.38
35	n	615	II0	C42-C40	4.07	1.55	1.43
37	j	610	KC2	CHB-C1B	4.07	1.46	1.38
35	l	313	II0	C42-C40	4.06	1.55	1.43
37	i	317	KC2	CHD-C1D	4.06	1.48	1.39
34	b	619	LMG	O8-C28	4.06	1.45	1.33
35	f	616	II0	C06-C04	4.06	1.67	1.54
35	k	315	II0	C31-C29	4.06	1.55	1.43
35	c	613	II0	C31-C29	4.06	1.55	1.43
35	e	614	II0	C32-C30	4.05	1.55	1.43
37	m	610	KC2	CHB-C1B	4.05	1.46	1.38
37	g	314	KC2	CHB-C1B	4.05	1.46	1.38
35	b	613	II0	C42-C40	4.05	1.55	1.43
35	m	613	II0	C32-C30	4.05	1.55	1.43
29	l	318	LHG	O7-C7	4.04	1.45	1.34
36	n	617	IHT	C09-C10	-4.04	1.43	1.51
35	n	615	II0	C06-C04	4.04	1.66	1.54
35	i	318	II0	C31-C29	4.03	1.55	1.43
29	J	107	LHG	O8-C23	4.03	1.45	1.33
35	f	616	II0	C32-C30	4.03	1.55	1.43
37	k	310	KC2	CHB-C1B	4.03	1.46	1.38
29	A	845	LHG	O8-C23	4.03	1.45	1.33
35	a	314	II0	C31-C29	4.03	1.55	1.43
34	c	619	LMG	O8-C28	4.03	1.45	1.33
37	c	610	KC2	OBD-CAD	4.02	1.29	1.22
35	m	615	II0	C42-C40	4.02	1.55	1.43
29	f	619	LHG	O7-C7	4.02	1.45	1.34
35	b	615	II0	C31-C29	4.02	1.55	1.43
35	l	314	II0	C32-C30	4.02	1.55	1.43
35	O	203	II0	C06-C04	4.02	1.66	1.54
37	n	612	KC2	CBC-CAC	4.02	1.49	1.30
37	n	611	KC2	CHB-C1B	4.01	1.46	1.38
29	J	107	LHG	O7-C7	4.01	1.45	1.34
37	m	610	KC2	CHD-C1D	4.01	1.48	1.39
36	m	616	IHT	C05-C03	4.01	1.66	1.54
35	j	615	II0	C41-C39	4.01	1.55	1.43
35	i	314	II0	C31-C29	4.01	1.55	1.43
36	a	317	IHT	C05-C03	4.01	1.66	1.54
36	k	317	IHT	C09-C10	-4.01	1.43	1.51
36	g	319	IHT	C05-C03	4.00	1.66	1.54
37	n	611	KC2	CHC-C4B	4.00	1.46	1.38
35	a	314	II0	C27-C25	4.00	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	845	LHG	O7-C7	4.00	1.45	1.34
37	d	309	KC2	CHB-C1B	4.00	1.46	1.38
35	b	613	II0	C06-C04	4.00	1.66	1.54
37	n	611	KC2	OBD-CAD	4.00	1.29	1.22
35	i	314	II0	C41-C39	4.00	1.55	1.43
37	g	312	KC2	CHB-C1B	4.00	1.46	1.38
36	c	620	IHT	C30-C27	4.00	1.55	1.43
35	k	315	II0	C42-C40	3.99	1.55	1.43
35	d	314	II0	C41-C39	3.99	1.55	1.43
37	s	204	KC2	C1B-NB	-3.99	1.32	1.37
27	d	308	CLA	C1D-ND	3.99	1.43	1.37
36	n	617	IHT	C05-C03	3.99	1.66	1.54
35	e	612	II0	C41-C39	3.99	1.55	1.43
29	A	850	LHG	O7-C7	3.99	1.45	1.34
35	J	104	II0	C42-C40	3.99	1.55	1.43
35	i	313	II0	C32-C30	3.99	1.55	1.43
36	c	616	IHT	C09-C10	-3.99	1.43	1.51
35	c	614	II0	C42-C40	3.98	1.55	1.43
35	e	613	II0	C42-C40	3.98	1.55	1.43
37	f	611	KC2	CHC-C4B	3.98	1.46	1.38
35	n	614	II0	C33-C35	3.98	1.54	1.46
37	i	310	KC2	CHC-C4B	3.98	1.46	1.38
35	i	313	II0	C12-C14	-3.98	1.44	1.51
37	j	610	KC2	CHC-C4B	3.98	1.46	1.38
37	l	311	KC2	CHB-C1B	3.98	1.46	1.38
29	m	617	LHG	O8-C23	3.97	1.44	1.33
33	B	842	DGD	O1G-C1A	3.97	1.44	1.33
37	n	612	KC2	CHC-C4B	3.97	1.46	1.38
35	j	613	II0	C42-C40	3.97	1.55	1.43
27	k	309	CLA	CMD-C2D	-3.97	1.42	1.50
37	k	312	KC2	CHD-C1D	3.97	1.48	1.39
36	m	616	IHT	C41-C38	3.97	1.55	1.43
35	e	613	II0	C06-C04	3.97	1.66	1.54
37	m	610	KC2	CHC-C4B	3.97	1.46	1.38
37	d	309	KC2	CHD-C1D	3.97	1.48	1.39
37	g	314	KC2	CHC-C4B	3.96	1.46	1.38
35	a	315	II0	C42-C40	3.96	1.55	1.43
35	k	314	II0	C31-C29	3.96	1.55	1.43
37	i	310	KC2	OBD-CAD	3.96	1.29	1.22
35	a	315	II0	C32-C30	3.95	1.55	1.43
35	m	615	II0	C06-C04	3.95	1.66	1.54
37	g	312	KC2	OBD-CAD	3.95	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	316	II0	C42-C40	3.95	1.55	1.43
35	n	618	II0	C31-C29	3.95	1.55	1.43
35	m	615	II0	C31-C29	3.95	1.55	1.43
29	f	619	LHG	O8-C23	3.94	1.44	1.33
35	e	613	II0	C32-C30	3.94	1.55	1.43
34	L	208	LMG	O8-C28	3.94	1.44	1.33
35	a	316	II0	C32-C30	3.94	1.55	1.43
35	h	311	II0	C31-C29	3.94	1.55	1.43
36	f	617	IHT	C41-C38	3.94	1.55	1.43
35	l	314	II0	C41-C39	3.93	1.55	1.43
37	i	317	KC2	CHB-C4A	3.93	1.48	1.39
35	l	315	II0	C41-C39	3.93	1.55	1.43
37	k	312	KC2	CHC-C4B	3.93	1.46	1.38
35	h	312	II0	C31-C29	3.93	1.55	1.43
35	g	316	II0	C32-C30	3.93	1.55	1.43
35	b	613	II0	C31-C29	3.93	1.55	1.43
35	a	314	II0	C06-C04	3.93	1.66	1.54
35	g	317	II0	C42-C40	3.92	1.55	1.43
35	h	312	II0	C12-C14	-3.92	1.44	1.51
37	c	610	KC2	CHC-C4B	3.92	1.46	1.38
35	l	317	II0	C34-C36	3.92	1.54	1.46
35	b	615	II0	C42-C40	3.92	1.55	1.43
35	a	315	II0	C31-C29	3.92	1.55	1.43
36	c	616	IHT	C41-C38	3.91	1.55	1.43
37	d	310	KC2	CHC-C4B	3.91	1.46	1.38
29	g	301	LHG	O8-C23	3.91	1.44	1.33
35	b	612	II0	C42-C40	3.91	1.55	1.43
29	a	301	LHG	O7-C7	3.91	1.45	1.34
35	d	313	II0	C05-C03	3.91	1.66	1.54
35	k	315	II0	C05-C03	3.91	1.66	1.54
35	n	618	II0	C41-C39	3.91	1.55	1.43
37	e	609	KC2	OBD-CAD	3.90	1.29	1.22
34	J	106	LMG	O8-C28	3.90	1.44	1.33
35	l	314	II0	C27-C25	3.90	1.53	1.50
36	n	617	IHT	C41-C38	3.90	1.55	1.43
37	l	311	KC2	CHC-C4B	3.90	1.46	1.38
37	g	314	KC2	CHD-C1D	3.90	1.48	1.39
35	n	614	II0	C42-C40	3.89	1.55	1.43
37	e	609	KC2	CHD-C1D	3.89	1.48	1.39
35	k	318	II0	C32-C30	3.89	1.55	1.43
35	h	311	II0	C06-C04	3.89	1.66	1.54
38	i	301	LMU	O5B-C1B	3.89	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	313	II0	C06-C04	3.89	1.66	1.54
36	O	204	IHT	C05-C03	3.89	1.66	1.54
37	c	610	KC2	CHD-C1D	3.89	1.48	1.39
35	l	302	II0	C42-C40	3.89	1.55	1.43
37	g	312	KC2	CHC-C4B	3.89	1.46	1.38
37	d	309	KC2	CHC-C4B	3.89	1.46	1.38
36	R	204	IHT	C41-C38	3.88	1.55	1.43
36	R	204	IHT	C09-C10	-3.88	1.43	1.51
35	k	318	II0	C05-C03	3.88	1.66	1.54
35	j	613	II0	C12-C14	-3.88	1.45	1.51
37	i	310	KC2	CHD-C1D	3.88	1.48	1.39
36	R	204	IHT	C05-C03	3.88	1.66	1.54
35	n	616	II0	C12-C14	-3.88	1.45	1.51
35	b	612	II0	C06-C04	3.88	1.66	1.54
35	g	317	II0	C12-C14	-3.88	1.45	1.51
35	J	104	II0	C32-C30	3.88	1.55	1.43
37	e	609	KC2	CHC-C4B	3.87	1.46	1.38
35	n	616	II0	C41-C39	3.87	1.55	1.43
37	g	313	KC2	CHB-C1B	3.87	1.46	1.38
35	n	615	II0	C32-C30	3.87	1.55	1.43
36	f	617	IHT	C05-C03	3.87	1.66	1.54
35	h	311	II0	C42-C40	3.87	1.55	1.43
35	g	318	II0	C41-C39	3.87	1.55	1.43
35	f	615	II0	C42-C40	3.86	1.55	1.43
35	b	615	II0	C12-C14	-3.86	1.45	1.51
36	a	317	IHT	C09-C10	-3.86	1.43	1.51
35	m	614	II0	C32-C30	3.86	1.55	1.43
27	i	311	CLA	C1D-ND	3.86	1.42	1.37
37	n	612	KC2	CHD-C1D	3.86	1.48	1.39
35	l	317	II0	C06-C04	3.86	1.66	1.54
35	j	614	II0	C27-C25	3.86	1.53	1.50
37	s	201	KC2	C1A-NA	3.85	1.46	1.38
35	l	313	II0	C41-C39	3.85	1.55	1.43
37	k	311	KC2	CHC-C4B	3.84	1.45	1.38
35	i	313	II0	C06-C04	3.84	1.66	1.54
35	g	317	II0	C06-C04	3.84	1.66	1.54
37	k	310	KC2	CHD-C1D	3.84	1.48	1.39
35	b	612	II0	C31-C29	3.84	1.55	1.43
37	l	311	KC2	CHD-C1D	3.84	1.48	1.39
36	c	620	IHT	C28-C26	3.84	1.53	1.50
35	b	612	II0	C12-C14	-3.83	1.45	1.51
35	b	612	II0	C27-C25	3.83	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	i	307	CLA	C4B-NB	3.83	1.42	1.37
35	f	616	II0	C41-C39	3.83	1.55	1.43
36	O	204	IHT	C09-C10	-3.83	1.43	1.51
35	k	318	II0	C41-C39	3.82	1.55	1.43
35	l	302	II0	C32-C30	3.82	1.55	1.43
35	h	311	II0	C12-C14	-3.82	1.45	1.51
34	s	210	LMG	O7-C10	3.82	1.45	1.34
36	c	620	IHT	C05-C03	3.82	1.66	1.54
35	e	614	II0	C05-C03	3.82	1.66	1.54
35	l	314	II0	C06-C04	3.82	1.66	1.54
35	a	315	II0	C06-C04	3.81	1.66	1.54
37	d	310	KC2	CHD-C1D	3.81	1.48	1.39
36	c	620	IHT	C14-C02	3.80	1.60	1.53
35	b	615	II0	C32-C30	3.80	1.55	1.43
37	g	312	KC2	CHD-C1D	3.80	1.47	1.39
35	m	614	II0	C42-C40	3.80	1.55	1.43
35	n	614	II0	C12-C14	-3.80	1.45	1.51
30	B	848	WVN	C33-C34	3.80	1.54	1.46
35	i	313	II0	C41-C39	3.80	1.55	1.43
37	k	311	KC2	CHD-C1D	3.80	1.47	1.39
27	f	605	CLA	C1D-ND	3.80	1.42	1.37
35	c	613	II0	C41-C39	3.79	1.55	1.43
37	g	313	KC2	CHC-C4B	3.79	1.45	1.38
29	L	207	LHG	O7-C7	3.79	1.45	1.34
37	g	313	KC2	CHD-C1D	3.79	1.47	1.39
36	m	616	IHT	C40-C37	3.79	1.54	1.43
35	j	614	II0	C41-C39	3.79	1.54	1.43
35	g	317	II0	C32-C30	3.78	1.54	1.43
35	d	312	II0	C06-C04	3.78	1.66	1.54
35	m	614	II0	C06-C04	3.78	1.66	1.54
36	j	616	IHT	C41-C38	3.78	1.54	1.43
37	k	311	KC2	CHB-C1B	3.78	1.45	1.38
36	n	617	IHT	C14-C02	3.78	1.60	1.53
35	n	615	II0	C41-C39	3.78	1.54	1.43
35	g	320	II0	C41-C39	3.78	1.54	1.43
27	B	825	CLA	CMD-C2D	-3.78	1.43	1.50
27	d	307	CLA	C1D-ND	3.78	1.42	1.37
36	c	616	IHT	C40-C37	3.77	1.54	1.43
29	n	619	LHG	O8-C23	3.77	1.44	1.33
35	k	314	II0	C33-C35	3.77	1.54	1.46
35	f	618	II0	C12-C14	-3.77	1.45	1.51
35	l	315	II0	C12-C14	-3.77	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	618	II0	C05-C03	3.77	1.66	1.54
37	s	201	KC2	OBD-CAD	3.76	1.29	1.22
35	O	203	II0	C41-C39	3.76	1.54	1.43
29	a	319	LHG	O7-C7	3.76	1.44	1.34
35	a	316	II0	C06-C04	3.76	1.66	1.54
35	j	614	II0	C05-C03	3.76	1.66	1.54
35	f	615	II0	C32-C30	3.76	1.54	1.43
36	c	616	IHT	C14-C02	3.75	1.60	1.53
35	a	318	II0	C27-C25	3.75	1.53	1.50
36	k	317	IHT	C28-C26	3.75	1.53	1.50
37	f	611	KC2	CHD-C1D	3.75	1.47	1.39
35	h	310	II0	C41-C39	3.75	1.54	1.43
30	J	102	WVN	C02-C11	3.75	1.55	1.50
35	c	617	II0	C41-C39	3.75	1.54	1.43
36	k	317	IHT	C14-C02	3.75	1.60	1.53
35	d	312	II0	C41-C39	3.75	1.54	1.43
30	B	845	WVN	C31-C32	3.75	1.54	1.46
35	f	615	II0	C41-C39	3.74	1.54	1.43
36	f	617	IHT	C40-C37	3.74	1.54	1.43
37	f	611	KC2	OBD-CAD	3.74	1.28	1.22
35	d	314	II0	C34-C36	3.74	1.54	1.46
35	g	318	II0	C27-C25	3.74	1.53	1.50
36	n	617	IHT	C40-C37	3.73	1.54	1.43
35	i	318	II0	C06-C04	3.73	1.66	1.54
34	J	106	LMG	O7-C10	3.73	1.44	1.34
36	c	616	IHT	C31-C29	3.73	1.54	1.43
35	h	312	II0	C42-C40	3.73	1.54	1.43
35	e	614	II0	C41-C39	3.73	1.54	1.43
35	k	314	II0	C05-C03	3.73	1.66	1.54
35	a	315	II0	C41-C39	3.73	1.54	1.43
36	k	317	IHT	C41-C38	3.73	1.54	1.43
35	n	614	II0	C32-C30	3.72	1.54	1.43
35	k	316	II0	C34-C36	3.72	1.53	1.46
35	l	314	II0	C34-C36	3.72	1.53	1.46
36	f	617	IHT	C28-C26	3.71	1.53	1.50
35	a	314	II0	C32-C30	3.71	1.54	1.43
35	c	614	II0	C06-C04	3.71	1.65	1.54
36	a	317	IHT	C41-C38	3.71	1.54	1.43
35	e	616	II0	C34-C36	3.71	1.53	1.46
35	a	314	II0	C12-C14	-3.71	1.45	1.51
35	l	314	II0	C12-C14	-3.71	1.45	1.51
27	f	608	CLA	C1D-ND	3.71	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	612	II0	C05-C03	3.71	1.65	1.54
35	g	320	II0	C34-C36	3.70	1.53	1.46
36	O	204	IHT	C41-C38	3.70	1.54	1.43
35	i	313	II0	C05-C03	3.70	1.65	1.54
27	a	305	CLA	C1D-ND	3.70	1.42	1.37
35	m	614	II0	C05-C03	3.70	1.65	1.54
35	m	613	II0	C05-C03	3.70	1.65	1.54
35	h	310	II0	C31-C29	3.70	1.54	1.43
35	j	614	II0	C32-C30	3.70	1.54	1.43
27	j	603	CLA	C1D-ND	3.70	1.42	1.37
35	c	615	II0	C05-C03	3.70	1.65	1.54
37	s	201	KC2	C1B-NB	-3.69	1.33	1.37
37	j	610	KC2	CHD-C1D	3.69	1.47	1.39
35	m	615	II0	C41-C39	3.69	1.54	1.43
35	i	318	II0	C34-C36	3.69	1.53	1.46
27	B	828	CLA	C4B-NB	3.68	1.42	1.37
36	c	616	IHT	C28-C26	3.68	1.53	1.50
35	n	618	II0	C34-C36	3.68	1.53	1.46
35	d	314	II0	C05-C03	3.68	1.65	1.54
27	d	311	CLA	C1D-ND	3.68	1.42	1.37
35	a	314	II0	C05-C03	3.68	1.65	1.54
35	h	312	II0	C30-C26	-3.68	1.29	1.37
27	g	311	CLA	CMD-C2D	-3.68	1.43	1.50
35	j	613	II0	C41-C39	3.67	1.54	1.43
27	B	818	CLA	CMD-C2D	-3.67	1.43	1.50
36	g	319	IHT	C28-C26	3.67	1.53	1.50
35	n	614	II0	C05-C03	3.67	1.65	1.54
35	b	612	II0	C05-C03	3.67	1.65	1.54
35	O	203	II0	C05-C03	3.67	1.65	1.54
30	B	846	WVN	C30-C28	3.67	1.54	1.43
35	i	314	II0	C05-C03	3.67	1.65	1.54
36	g	319	IHT	C41-C38	3.67	1.54	1.43
35	n	615	II0	C12-C14	-3.66	1.45	1.51
35	g	320	II0	C12-C14	-3.66	1.45	1.51
27	i	312	CLA	C1D-ND	3.66	1.42	1.37
27	k	304	CLA	C1D-ND	3.66	1.42	1.37
27	h	308	CLA	C1D-ND	3.66	1.42	1.37
35	g	318	II0	C05-C03	3.65	1.65	1.54
37	n	612	KC2	CHB-C1B	3.65	1.45	1.38
35	O	203	II0	C27-C25	3.65	1.53	1.50
35	d	313	II0	C33-C35	3.65	1.53	1.46
37	s	201	KC2	CHD-C1D	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	b	612	II0	C32-C30	3.65	1.54	1.43
36	R	204	IHT	C14-C02	3.64	1.60	1.53
35	a	318	II0	C05-C03	3.64	1.65	1.54
36	g	319	IHT	C14-C02	3.64	1.60	1.53
35	f	614	II0	C34-C36	3.64	1.53	1.46
36	a	317	IHT	C14-C02	3.64	1.60	1.53
35	l	313	II0	C34-C36	3.64	1.53	1.46
35	j	613	II0	C32-C30	3.64	1.54	1.43
35	e	613	II0	C41-C39	3.63	1.54	1.43
35	k	315	II0	C41-C39	3.63	1.54	1.43
35	l	317	II0	C05-C03	3.62	1.65	1.54
35	l	313	II0	C05-C03	3.62	1.65	1.54
35	j	615	II0	C34-C36	3.62	1.53	1.46
35	c	614	II0	C41-C39	3.62	1.54	1.43
27	k	306	CLA	C1D-ND	3.62	1.42	1.37
35	a	316	II0	C41-C39	3.62	1.54	1.43
35	c	617	II0	C12-C14	-3.62	1.45	1.51
35	J	104	II0	C41-C39	3.62	1.54	1.43
27	c	612	CLA	C1D-ND	3.62	1.42	1.37
35	n	616	II0	C06-C04	3.62	1.65	1.54
36	a	317	IHT	C40-C37	3.61	1.54	1.43
36	c	620	IHT	C40-C37	3.61	1.54	1.43
27	n	605	CLA	C1D-ND	3.61	1.42	1.37
29	b	617	LHG	O7-C7	3.61	1.44	1.34
27	k	307	CLA	C1D-ND	3.61	1.42	1.37
27	A	801	CLA	C1D-ND	3.61	1.42	1.37
35	J	104	II0	C06-C04	3.61	1.65	1.54
35	b	613	II0	C12-C14	-3.61	1.45	1.51
35	i	318	II0	C05-C03	3.61	1.65	1.54
36	c	616	IHT	C05-C03	3.61	1.65	1.54
35	l	313	II0	C12-C14	-3.61	1.45	1.51
27	j	601	CLA	C4B-NB	3.60	1.42	1.37
35	g	316	II0	C31-C29	3.60	1.54	1.43
36	j	616	IHT	C40-C37	3.60	1.54	1.43
35	a	315	II0	C05-C03	3.60	1.65	1.54
35	h	312	II0	C05-C03	3.60	1.65	1.54
35	m	613	II0	C12-C14	-3.59	1.45	1.51
35	k	316	II0	C33-C35	3.59	1.53	1.46
35	f	616	II0	C34-C36	3.59	1.53	1.46
35	l	314	II0	C05-C03	3.59	1.65	1.54
36	f	617	IHT	C31-C29	3.59	1.54	1.43
30	L	205	WVN	C33-C34	3.59	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	317	II0	C41-C39	3.59	1.54	1.43
35	l	315	II0	C05-C03	3.58	1.65	1.54
36	R	204	IHT	C40-C37	3.58	1.54	1.43
35	l	302	II0	C06-C04	3.58	1.65	1.54
27	d	303	CLA	C4B-NB	3.58	1.42	1.37
35	h	310	II0	C34-C36	3.58	1.53	1.46
35	j	613	II0	C31-C29	3.58	1.54	1.43
35	k	315	II0	C06-C04	3.58	1.65	1.54
27	m	608	CLA	C1D-ND	3.57	1.42	1.37
27	A	809	CLA	C1D-ND	3.57	1.42	1.37
27	B	816	CLA	C4B-NB	3.56	1.42	1.37
35	f	614	II0	C05-C03	3.56	1.65	1.54
35	e	612	II0	C34-C36	3.56	1.53	1.46
36	m	616	IHT	C14-C02	3.56	1.60	1.53
36	k	317	IHT	C40-C37	3.56	1.54	1.43
27	i	306	CLA	C1D-ND	3.56	1.42	1.37
36	O	204	IHT	C40-C37	3.56	1.54	1.43
30	B	843	WVN	C19-C22	3.56	1.53	1.46
36	n	617	IHT	C28-C26	3.55	1.53	1.50
35	g	316	II0	C34-C36	3.55	1.53	1.46
36	f	617	IHT	C14-C02	3.55	1.60	1.53
35	a	314	II0	C42-C40	3.55	1.54	1.43
35	e	613	II0	C12-C14	-3.55	1.45	1.51
35	h	312	II0	C32-C30	3.54	1.54	1.43
27	l	310	CLA	C1D-ND	3.54	1.42	1.37
27	A	806	CLA	C1D-ND	3.54	1.42	1.37
35	l	302	II0	C41-C39	3.54	1.54	1.43
35	b	612	II0	C41-C39	3.54	1.54	1.43
27	A	819	CLA	C1D-ND	3.54	1.42	1.37
35	a	315	II0	C12-C14	-3.54	1.45	1.51
36	m	616	IHT	C31-C29	3.54	1.54	1.43
35	c	617	II0	C34-C36	3.54	1.53	1.46
36	n	617	IHT	C31-C29	3.53	1.54	1.43
27	i	309	CLA	CMD-C2D	-3.53	1.43	1.50
35	k	315	II0	C32-C30	3.53	1.54	1.43
35	e	614	II0	C12-C14	-3.53	1.45	1.51
27	i	311	CLA	C4B-NB	3.53	1.42	1.37
36	O	204	IHT	C14-C02	3.53	1.60	1.53
37	n	611	KC2	CHD-C1D	3.53	1.47	1.39
35	e	616	II0	C27-C25	3.52	1.53	1.50
36	R	204	IHT	C28-C26	3.52	1.53	1.50
35	m	613	II0	C34-C36	3.52	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	302	II0	C12-C14	-3.52	1.45	1.51
27	m	601	CLA	C1D-ND	3.52	1.42	1.37
27	f	607	CLA	C4B-NB	3.52	1.42	1.37
27	e	603	CLA	C1D-ND	3.52	1.42	1.37
35	a	314	II0	C41-C39	3.52	1.54	1.43
35	c	614	II0	C27-C25	3.51	1.53	1.50
27	A	813	CLA	MG-NC	3.51	2.14	2.06
35	c	615	II0	C41-C39	3.51	1.54	1.43
35	n	616	II0	C34-C36	3.51	1.53	1.46
35	l	302	II0	C05-C03	3.51	1.65	1.54
35	g	318	II0	C34-C36	3.51	1.53	1.46
27	j	607	CLA	C1D-ND	3.51	1.42	1.37
35	f	615	II0	C12-C14	-3.51	1.45	1.51
35	a	318	II0	C12-C14	-3.51	1.45	1.51
27	B	821	CLA	CMD-C2D	-3.51	1.43	1.50
27	A	826	CLA	C1D-ND	3.50	1.42	1.37
35	m	614	II0	C12-C14	-3.50	1.45	1.51
35	m	615	II0	C05-C03	3.50	1.65	1.54
36	j	616	IHT	C14-C02	3.50	1.60	1.53
35	h	310	II0	C05-C03	3.50	1.65	1.54
36	R	204	IHT	C31-C29	3.50	1.54	1.43
35	g	317	II0	C41-C39	3.50	1.54	1.43
27	c	604	CLA	C1D-ND	3.50	1.42	1.37
27	k	313	CLA	C4B-NB	3.50	1.42	1.37
30	h	309	WVN	C23-C25	3.49	1.53	1.46
27	b	607	CLA	C4B-NB	3.49	1.42	1.37
27	f	601	CLA	C1D-ND	3.49	1.42	1.37
35	d	312	II0	C34-C36	3.49	1.53	1.46
27	i	302	CLA	C4B-NB	3.49	1.42	1.37
27	d	306	CLA	C1D-ND	3.49	1.42	1.37
27	n	606	CLA	C1D-ND	3.49	1.42	1.37
27	j	606	CLA	C1D-ND	3.49	1.42	1.37
35	k	316	II0	C05-C03	3.49	1.65	1.54
35	i	314	II0	C34-C36	3.49	1.53	1.46
35	f	615	II0	C06-C04	3.49	1.65	1.54
35	h	311	II0	C41-C39	3.49	1.54	1.43
35	n	616	II0	C05-C03	3.49	1.65	1.54
27	B	801	CLA	C1D-ND	3.48	1.42	1.37
27	A	856	CLA	CMD-C2D	-3.48	1.43	1.50
35	k	318	II0	C12-C14	-3.48	1.45	1.51
35	f	616	II0	C05-C03	3.48	1.65	1.54
35	j	613	II0	C05-C03	3.48	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	613	CLA	C1D-ND	3.48	1.42	1.37
27	b	604	CLA	C1D-ND	3.48	1.42	1.37
35	k	318	II0	C34-C36	3.47	1.53	1.46
36	g	319	IHT	C40-C37	3.47	1.54	1.43
27	A	811	CLA	C4B-NB	3.47	1.42	1.37
35	n	616	II0	C33-C35	3.47	1.53	1.46
35	d	312	II0	C05-C03	3.47	1.65	1.54
27	g	315	CLA	C1D-ND	3.47	1.42	1.37
27	a	306	CLA	C1D-ND	3.47	1.42	1.37
30	A	846	WVN	C33-C34	3.47	1.53	1.46
35	c	614	II0	C05-C03	3.47	1.65	1.54
35	f	618	II0	C34-C36	3.46	1.53	1.46
35	e	613	II0	C34-C36	3.46	1.53	1.46
36	b	614	IHT	C18-C07	3.46	1.56	1.45
27	k	301	CLA	C1D-ND	3.46	1.42	1.37
38	i	301	LMU	O5'-C1'	3.45	1.50	1.41
27	e	604	CLA	C1D-ND	3.45	1.42	1.37
27	k	309	CLA	C1D-ND	3.45	1.42	1.37
35	l	315	II0	C34-C36	3.45	1.53	1.46
27	a	304	CLA	C1D-ND	3.45	1.42	1.37
35	O	203	II0	C33-C35	3.45	1.53	1.46
27	f	607	CLA	C1D-ND	3.45	1.42	1.37
27	b	603	CLA	C1D-ND	3.45	1.42	1.37
27	B	838	CLA	C1D-ND	3.44	1.42	1.37
27	k	308	CLA	C1D-ND	3.44	1.42	1.37
35	f	615	II0	C05-C03	3.44	1.65	1.54
35	f	614	II0	C33-C35	3.44	1.53	1.46
36	j	616	IHT	C31-C29	3.44	1.53	1.43
36	n	617	IHT	C32-C33	3.43	1.53	1.46
27	L	204	CLA	CMD-C2D	-3.43	1.43	1.50
27	A	852	CLA	C1D-ND	3.43	1.42	1.37
35	n	614	II0	C41-C39	3.43	1.53	1.43
37	n	612	KC2	CHC-C1C	3.43	1.47	1.39
30	L	205	WVN	C30-C28	3.43	1.53	1.43
30	h	309	WVN	C33-C34	3.43	1.53	1.46
35	e	612	II0	C12-C14	-3.43	1.45	1.51
35	j	615	II0	C33-C35	3.42	1.53	1.46
30	A	848	WVN	C02-C11	3.42	1.55	1.50
37	s	204	KC2	CHC-C4B	3.42	1.45	1.38
35	e	616	II0	C05-C03	3.42	1.65	1.54
35	j	615	II0	C05-C03	3.42	1.65	1.54
27	k	313	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	609	CLA	C1D-ND	3.42	1.42	1.37
27	c	607	CLA	C1D-ND	3.42	1.42	1.37
36	f	617	IHT	C32-C33	3.41	1.53	1.46
36	a	317	IHT	C31-C29	3.41	1.53	1.43
27	n	602	CLA	C1D-ND	3.41	1.42	1.37
35	b	615	II0	C05-C03	3.41	1.65	1.54
27	A	839	CLA	C1D-ND	3.41	1.42	1.37
35	m	615	II0	C34-C36	3.40	1.53	1.46
27	f	612	CLA	C4B-NB	3.40	1.42	1.37
35	c	613	II0	C05-C03	3.40	1.65	1.54
27	j	605	CLA	C1D-ND	3.40	1.42	1.37
30	L	205	WVN	C23-C25	3.40	1.53	1.46
27	A	836	CLA	C1D-ND	3.40	1.42	1.37
35	a	318	II0	C33-C35	3.40	1.53	1.46
27	g	307	CLA	C1D-ND	3.40	1.42	1.37
30	A	847	WVN	C39-C36	3.40	1.53	1.43
30	A	846	WVN	C30-C28	3.39	1.53	1.43
27	n	608	CLA	C1D-ND	3.39	1.42	1.37
27	f	608	CLA	C4B-NB	3.39	1.42	1.37
35	c	617	II0	C05-C03	3.39	1.64	1.54
27	n	603	CLA	C1D-ND	3.39	1.42	1.37
30	h	309	WVN	C30-C28	3.39	1.53	1.43
36	b	614	IHT	C14-C02	3.38	1.60	1.53
27	m	604	CLA	CMA-C3A	-3.38	1.46	1.53
27	R	203	CLA	C1D-ND	3.38	1.42	1.37
35	g	320	II0	C05-C03	3.38	1.64	1.54
35	f	615	II0	C27-C25	3.38	1.53	1.50
30	J	101	WVN	C33-C34	3.38	1.53	1.46
27	k	308	CLA	CMC-C2C	-3.38	1.43	1.50
27	i	302	CLA	C1D-ND	3.37	1.42	1.37
37	d	310	KC2	CHB-C4A	3.37	1.46	1.39
37	c	610	KC2	CHB-C4A	3.37	1.46	1.39
27	f	601	CLA	C4B-NB	3.37	1.42	1.37
37	j	610	KC2	CHB-C4A	3.37	1.46	1.39
30	l	316	WVN	C33-C34	3.37	1.53	1.46
27	A	826	CLA	CMC-C2C	-3.37	1.43	1.50
27	f	604	CLA	C1D-ND	3.37	1.42	1.37
27	i	305	CLA	C1D-ND	3.37	1.42	1.37
37	e	609	KC2	CHB-C4A	3.37	1.46	1.39
35	a	316	II0	C05-C03	3.37	1.64	1.54
27	J	105	CLA	CMD-C2D	-3.37	1.43	1.50
27	b	609	CLA	C1D-ND	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	808	CLA	C1D-ND	3.36	1.42	1.37
35	h	311	II0	C05-C03	3.36	1.64	1.54
36	O	204	IHT	C31-C29	3.36	1.53	1.43
36	c	616	IHT	C32-C33	3.36	1.53	1.46
27	c	611	CLA	C1D-ND	3.35	1.42	1.37
27	m	609	CLA	C1D-ND	3.35	1.42	1.37
35	b	613	II0	C30-C26	-3.35	1.30	1.37
27	c	605	CLA	C1D-ND	3.35	1.42	1.37
29	b	617	LHG	O8-C23	3.35	1.43	1.33
35	m	615	II0	C12-C14	-3.35	1.45	1.51
35	g	316	II0	C12-C14	-3.35	1.45	1.51
35	c	615	II0	C34-C36	3.35	1.53	1.46
35	a	315	II0	C34-C36	3.35	1.53	1.46
27	m	604	CLA	C1D-ND	3.35	1.42	1.37
35	e	614	II0	C34-C36	3.35	1.53	1.46
35	b	615	II0	C41-C39	3.35	1.53	1.43
27	L	202	CLA	C1D-ND	3.34	1.42	1.37
30	i	315	WVN	C33-C34	3.34	1.53	1.46
36	R	204	IHT	C32-C33	3.34	1.53	1.46
35	b	613	II0	C05-C03	3.34	1.64	1.54
35	j	613	II0	C27-C25	3.34	1.53	1.50
27	g	305	CLA	C1D-ND	3.34	1.42	1.37
27	j	608	CLA	C1D-ND	3.34	1.42	1.37
35	d	314	II0	C33-C35	3.34	1.53	1.46
35	g	318	II0	C33-C35	3.34	1.53	1.46
37	g	312	KC2	CHB-C4A	3.34	1.46	1.39
27	B	838	CLA	C4B-NB	3.33	1.42	1.37
27	B	840	CLA	C1D-ND	3.33	1.42	1.37
37	g	314	KC2	CHB-C4A	3.33	1.46	1.39
36	k	317	IHT	C31-C29	3.33	1.53	1.43
27	A	804	CLA	CMC-C2C	-3.33	1.43	1.50
37	i	310	KC2	CHB-C4A	3.33	1.46	1.39
36	c	620	IHT	C31-C29	3.33	1.53	1.43
27	m	612	CLA	C1D-ND	3.33	1.42	1.37
27	n	603	CLA	C4B-NB	3.33	1.42	1.37
36	a	317	IHT	C32-C33	3.33	1.53	1.46
27	m	605	CLA	C1D-ND	3.33	1.42	1.37
35	k	318	II0	C33-C35	3.33	1.53	1.46
27	f	610	CLA	C1D-ND	3.33	1.42	1.37
27	n	613	CLA	C1D-ND	3.33	1.42	1.37
27	m	601	CLA	C4B-NB	3.32	1.42	1.37
27	O	206	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	613	CLA	C4B-NB	3.32	1.42	1.37
35	m	614	II0	C41-C39	3.32	1.53	1.43
35	i	318	II0	C33-C35	3.32	1.53	1.46
27	A	819	CLA	C4B-NB	3.32	1.42	1.37
30	J	101	WVN	C30-C28	3.32	1.53	1.43
27	n	601	CLA	C1D-ND	3.31	1.42	1.37
35	c	617	II0	C27-C25	3.31	1.53	1.50
27	b	610	CLA	C4B-NB	3.31	1.42	1.37
27	m	607	CLA	C1D-ND	3.31	1.42	1.37
35	b	613	II0	C41-C39	3.31	1.53	1.43
35	e	613	II0	C05-C03	3.31	1.64	1.54
27	j	607	CLA	C4B-NB	3.31	1.42	1.37
35	b	613	II0	C27-C25	3.31	1.53	1.50
27	f	606	CLA	C1D-ND	3.31	1.42	1.37
27	A	840	CLA	C1D-ND	3.30	1.42	1.37
27	c	606	CLA	C1D-ND	3.30	1.42	1.37
37	k	312	KC2	CHB-C4A	3.30	1.46	1.39
27	B	849	CLA	C1D-ND	3.30	1.42	1.37
30	i	315	WVN	C19-C22	3.30	1.53	1.46
36	c	620	IHT	C41-C38	3.30	1.53	1.43
27	g	308	CLA	C1D-ND	3.30	1.42	1.37
37	f	611	KC2	CHB-C4A	3.30	1.46	1.39
27	d	302	CLA	C1D-ND	3.30	1.42	1.37
35	n	614	II0	C34-C36	3.30	1.53	1.46
36	g	319	IHT	C31-C29	3.30	1.53	1.43
27	l	308	CLA	C1D-ND	3.29	1.42	1.37
30	J	102	WVN	C39-C36	3.29	1.53	1.43
27	s	209	CLA	C1D-ND	3.29	1.42	1.37
27	B	822	CLA	C1D-ND	3.29	1.42	1.37
27	A	805	CLA	C1D-ND	3.29	1.42	1.37
27	B	836	CLA	C1D-ND	3.29	1.42	1.37
35	c	617	II0	C33-C35	3.29	1.53	1.46
27	a	308	CLA	C1D-ND	3.29	1.42	1.37
27	k	302	CLA	C1D-ND	3.28	1.42	1.37
37	d	309	KC2	CHB-C4A	3.28	1.46	1.39
27	B	819	CLA	C1D-ND	3.28	1.42	1.37
27	A	855	CLA	C4B-NB	3.28	1.42	1.37
27	A	838	CLA	CMD-C2D	-3.28	1.44	1.50
27	h	301	CLA	C1D-ND	3.28	1.42	1.37
27	l	306	CLA	C1D-ND	3.28	1.42	1.37
27	A	815	CLA	C1D-ND	3.28	1.42	1.37
35	c	613	II0	C12-C14	-3.28	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	303	CLA	C1D-ND	3.28	1.42	1.37
27	g	322	CLA	C1D-ND	3.28	1.42	1.37
30	B	847	WVN	C23-C25	3.28	1.53	1.46
27	c	609	CLA	C1D-ND	3.28	1.42	1.37
36	O	204	IHT	C28-C26	3.28	1.53	1.50
27	A	852	CLA	C4B-NB	3.27	1.42	1.37
35	n	615	II0	C34-C36	3.27	1.53	1.46
27	s	206	CLA	C4B-NB	3.27	1.42	1.37
36	j	616	IHT	C32-C33	3.27	1.53	1.46
27	A	832	CLA	C1D-ND	3.27	1.42	1.37
27	s	202	CLA	C1D-ND	3.27	1.42	1.37
27	K	101	CLA	C1D-ND	3.27	1.42	1.37
37	f	611	KC2	CHC-C1C	3.27	1.46	1.39
27	l	307	CLA	C1D-ND	3.27	1.42	1.37
27	A	803	CLA	C1D-ND	3.26	1.42	1.37
27	a	308	CLA	C4B-NB	3.26	1.42	1.37
35	g	317	II0	C05-C03	3.26	1.64	1.54
27	n	609	CLA	C1D-ND	3.26	1.42	1.37
30	l	316	WVN	C30-C28	3.26	1.53	1.43
30	A	847	WVN	C19-C22	3.26	1.52	1.46
35	n	615	II0	C05-C03	3.26	1.64	1.54
27	e	608	CLA	C1D-ND	3.26	1.42	1.37
35	e	616	II0	C12-C14	-3.26	1.46	1.51
27	e	610	CLA	C1D-ND	3.26	1.42	1.37
37	i	310	KC2	CHC-C1C	3.26	1.46	1.39
27	n	613	CLA	C4B-NB	3.25	1.42	1.37
37	n	611	KC2	CHB-C4A	3.25	1.46	1.39
30	B	846	WVN	C33-C34	3.25	1.52	1.46
27	B	820	CLA	C1D-ND	3.25	1.42	1.37
27	h	313	CLA	C4B-NB	3.25	1.42	1.37
35	f	614	II0	C12-C14	-3.25	1.46	1.51
30	s	205	WVN	C29-C26	3.25	1.53	1.43
37	m	610	KC2	CHB-C4A	3.25	1.46	1.39
37	g	313	KC2	CHB-C4A	3.25	1.46	1.39
35	c	614	II0	C34-C36	3.25	1.52	1.46
35	a	316	II0	C34-C36	3.25	1.52	1.46
35	J	104	II0	C12-C14	-3.25	1.46	1.51
30	i	315	WVN	C23-C25	3.25	1.52	1.46
35	l	314	II0	C33-C35	3.25	1.52	1.46
35	n	618	II0	C05-C03	3.24	1.64	1.54
27	e	611	CLA	C1D-ND	3.24	1.42	1.37
27	f	606	CLA	C4B-NB	3.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	810	CLA	C1D-ND	3.24	1.42	1.37
35	f	616	II0	C12-C14	-3.24	1.46	1.51
27	d	304	CLA	C1D-ND	3.24	1.42	1.37
27	g	309	CLA	C1D-ND	3.24	1.42	1.37
27	a	312	CLA	C1D-ND	3.23	1.42	1.37
35	j	615	II0	C27-C25	3.23	1.53	1.50
35	d	314	II0	C12-C14	-3.23	1.46	1.51
27	n	607	CLA	C1D-ND	3.23	1.42	1.37
30	R	201	WVN	C02-C11	3.23	1.55	1.50
35	j	614	II0	C34-C36	3.23	1.52	1.46
27	B	831	CLA	C1D-ND	3.23	1.42	1.37
37	k	312	KC2	CHC-C1C	3.23	1.46	1.39
37	j	610	KC2	CHC-C1C	3.23	1.46	1.39
30	l	316	WVN	C40-C37	3.23	1.53	1.43
37	k	310	KC2	CHC-C1C	3.23	1.46	1.39
27	m	606	CLA	C4B-NB	3.23	1.42	1.37
27	d	306	CLA	C4B-NB	3.23	1.42	1.37
30	L	205	WVN	C39-C36	3.23	1.53	1.43
35	J	104	II0	C05-C03	3.22	1.64	1.54
30	L	205	WVN	C31-C32	3.22	1.52	1.46
35	g	316	II0	C05-C03	3.22	1.64	1.54
30	J	102	WVN	C33-C34	3.22	1.52	1.46
35	c	613	II0	C34-C36	3.22	1.52	1.46
30	F	205	WVN	C30-C28	3.22	1.53	1.43
37	k	310	KC2	CHB-C4A	3.22	1.46	1.39
30	A	847	WVN	C29-C26	3.22	1.53	1.43
27	g	310	CLA	C1D-ND	3.21	1.42	1.37
30	F	205	WVN	C40-C37	3.21	1.53	1.43
27	A	807	CLA	C1D-ND	3.21	1.42	1.37
27	O	202	CLA	C1D-ND	3.21	1.42	1.37
27	f	612	CLA	C1D-ND	3.21	1.42	1.37
27	i	304	CLA	C4B-NB	3.21	1.42	1.37
30	s	207	WVN	C40-C37	3.21	1.53	1.43
37	g	314	KC2	CHC-C1C	3.21	1.46	1.39
35	O	203	II0	C34-C36	3.21	1.52	1.46
35	O	203	II0	C12-C14	-3.21	1.46	1.51
35	i	313	II0	C34-C36	3.21	1.52	1.46
27	c	611	CLA	C4B-NB	3.21	1.42	1.37
35	f	618	II0	C33-C35	3.21	1.52	1.46
27	d	305	CLA	C1D-ND	3.21	1.42	1.37
30	A	849	WVN	C33-C34	3.21	1.52	1.46
30	B	846	WVN	C19-C22	3.20	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	846	WVN	C40-C37	3.20	1.53	1.43
27	B	832	CLA	C1D-ND	3.20	1.42	1.37
35	g	318	II0	C12-C14	-3.20	1.46	1.51
27	h	307	CLA	C1D-ND	3.20	1.42	1.37
35	c	614	II0	C12-C14	-3.19	1.46	1.51
27	L	206	CLA	C4B-NB	3.19	1.42	1.37
30	F	205	WVN	C33-C34	3.19	1.52	1.46
30	I	101	WVN	C31-C32	3.19	1.52	1.46
30	I	101	WVN	C29-C26	3.19	1.53	1.43
30	O	201	WVN	C40-C37	3.19	1.53	1.43
30	l	301	WVN	C29-C26	3.19	1.53	1.43
27	A	853	CLA	C1D-ND	3.19	1.42	1.37
30	A	847	WVN	C40-C37	3.19	1.53	1.43
36	O	204	IHT	C32-C33	3.19	1.52	1.46
27	e	606	CLA	C1D-ND	3.19	1.42	1.37
27	n	610	CLA	C1D-ND	3.19	1.42	1.37
27	A	825	CLA	CMD-C2D	-3.19	1.44	1.50
27	n	610	CLA	C4B-NB	3.18	1.42	1.37
27	j	612	CLA	C1D-ND	3.18	1.42	1.37
30	l	301	WVN	C19-C22	3.18	1.52	1.46
37	m	610	KC2	CHC-C1C	3.18	1.46	1.39
30	s	207	WVN	C33-C34	3.18	1.52	1.46
35	J	104	II0	C33-C35	3.18	1.52	1.46
27	b	608	CLA	C1D-ND	3.18	1.42	1.37
27	K	102	CLA	C1D-ND	3.18	1.42	1.37
27	h	302	CLA	CMC-C2C	-3.18	1.44	1.50
27	a	311	CLA	C1D-ND	3.18	1.42	1.37
37	l	311	KC2	CHB-C4A	3.18	1.46	1.39
27	l	307	CLA	C4B-NB	3.18	1.42	1.37
27	B	808	CLA	CAB-C3B	-3.18	1.44	1.50
37	s	201	KC2	C4B-NB	-3.18	1.33	1.37
37	i	317	KC2	C4A-C3A	3.18	1.51	1.44
30	i	315	WVN	C30-C28	3.17	1.53	1.43
27	B	827	CLA	C1D-ND	3.17	1.42	1.37
27	B	834	CLA	C1D-ND	3.17	1.42	1.37
27	k	306	CLA	C4B-NB	3.17	1.42	1.37
27	f	602	CLA	C1D-ND	3.17	1.42	1.37
27	i	305	CLA	C4B-NB	3.17	1.42	1.37
37	c	610	KC2	CHC-C1C	3.17	1.46	1.39
35	i	314	II0	C33-C35	3.17	1.52	1.46
30	L	205	WVN	C29-C26	3.17	1.53	1.43
27	l	309	CLA	C1D-ND	3.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	103	WVN	C40-C37	3.17	1.53	1.43
30	l	316	WVN	C39-C36	3.17	1.53	1.43
27	c	606	CLA	CMB-C2B	-3.17	1.44	1.50
30	l	316	WVN	C29-C26	3.17	1.53	1.43
35	h	312	II0	C41-C39	3.16	1.53	1.43
37	d	309	KC2	CHC-C1C	3.16	1.46	1.39
30	A	846	WVN	C29-C26	3.16	1.53	1.43
27	B	802	CLA	CMC-C2C	-3.16	1.44	1.50
37	n	612	KC2	C1B-NB	-3.16	1.33	1.37
27	B	822	CLA	CMC-C2C	-3.16	1.44	1.50
30	A	847	WVN	C31-C32	3.16	1.52	1.46
27	A	818	CLA	C1D-ND	3.16	1.42	1.37
27	A	835	CLA	C1D-ND	3.16	1.42	1.37
27	F	202	CLA	C4B-NB	3.16	1.42	1.37
37	s	201	KC2	CHC-C1C	3.16	1.46	1.39
30	A	846	WVN	C19-C22	3.16	1.52	1.46
35	l	315	II0	C33-C35	3.16	1.52	1.46
27	l	305	CLA	C4B-NB	3.16	1.42	1.37
27	d	311	CLA	C4B-NB	3.16	1.42	1.37
27	A	823	CLA	C1D-ND	3.16	1.42	1.37
27	b	602	CLA	C1D-ND	3.16	1.42	1.37
27	b	606	CLA	C4B-NB	3.16	1.42	1.37
27	e	607	CLA	C1D-ND	3.16	1.42	1.37
27	h	307	CLA	C4B-NB	3.16	1.42	1.37
27	A	839	CLA	C4B-NB	3.15	1.42	1.37
27	c	608	CLA	C1D-ND	3.15	1.42	1.37
27	k	309	CLA	C4B-NB	3.15	1.42	1.37
27	m	603	CLA	C1D-ND	3.15	1.42	1.37
30	e	615	WVN	C29-C26	3.15	1.53	1.43
30	h	309	WVN	C31-C32	3.15	1.52	1.46
35	e	612	II0	C33-C35	3.15	1.52	1.46
27	s	206	CLA	C1D-ND	3.15	1.42	1.37
30	s	207	WVN	C39-C36	3.15	1.53	1.43
37	g	312	KC2	CHC-C1C	3.15	1.46	1.39
27	g	306	CLA	C1D-ND	3.15	1.42	1.37
27	n	604	CLA	CMD-C2D	-3.15	1.44	1.50
35	n	615	II0	C33-C35	3.15	1.52	1.46
27	A	815	CLA	CMB-C2B	-3.15	1.44	1.50
27	A	823	CLA	C4B-NB	3.15	1.42	1.37
27	a	312	CLA	C4B-NB	3.15	1.42	1.37
30	i	315	WVN	C29-C26	3.15	1.52	1.43
27	F	202	CLA	C1D-ND	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	817	CLA	C1D-ND	3.14	1.42	1.37
27	b	611	CLA	C1D-ND	3.14	1.42	1.37
27	g	304	CLA	C1D-ND	3.14	1.42	1.37
27	A	829	CLA	C1D-ND	3.14	1.42	1.37
30	B	846	WVN	C23-C25	3.14	1.52	1.46
27	n	604	CLA	C4B-NB	3.14	1.42	1.37
36	a	317	IHT	C28-C26	3.14	1.53	1.50
27	A	855	CLA	CMB-C2B	-3.14	1.44	1.50
27	B	806	CLA	C4B-NB	3.14	1.42	1.37
30	B	847	WVN	C30-C28	3.14	1.52	1.43
30	K	103	WVN	C33-C34	3.13	1.52	1.46
36	m	616	IHT	C32-C33	3.13	1.52	1.46
27	l	303	CLA	C1D-ND	3.13	1.42	1.37
36	k	317	IHT	C32-C33	3.13	1.52	1.46
30	A	846	WVN	C40-C37	3.13	1.52	1.43
30	l	316	WVN	C31-C32	3.13	1.52	1.46
30	K	103	WVN	C39-C36	3.13	1.52	1.43
30	i	315	WVN	C39-C36	3.13	1.52	1.43
30	l	316	WVN	C23-C25	3.13	1.52	1.46
27	j	609	CLA	CMD-C2D	-3.13	1.44	1.50
27	l	309	CLA	CMD-C2D	-3.13	1.44	1.50
27	d	301	CLA	C1D-ND	3.13	1.42	1.37
27	g	311	CLA	C4B-NB	3.13	1.42	1.37
30	F	205	WVN	C23-C25	3.12	1.52	1.46
27	i	307	CLA	C1D-ND	3.12	1.42	1.37
30	e	615	WVN	C19-C22	3.12	1.52	1.46
37	s	201	KC2	CHC-C4B	3.12	1.44	1.38
30	s	205	WVN	C19-C22	3.12	1.52	1.46
27	A	837	CLA	C1D-ND	3.12	1.42	1.37
30	B	843	WVN	C30-C28	3.12	1.52	1.43
37	e	609	KC2	CHC-C1C	3.12	1.46	1.39
27	c	605	CLA	C4B-NB	3.12	1.42	1.37
27	b	601	CLA	C1D-ND	3.12	1.42	1.37
27	g	305	CLA	CMB-C2B	-3.12	1.44	1.50
27	B	820	CLA	C4B-NB	3.12	1.42	1.37
35	g	316	II0	C33-C35	3.11	1.52	1.46
27	b	605	CLA	C1D-ND	3.11	1.42	1.37
27	m	604	CLA	C4B-NB	3.11	1.42	1.37
27	l	312	CLA	C4B-NB	3.11	1.41	1.37
30	i	315	WVN	C40-C37	3.11	1.52	1.43
30	h	309	WVN	C29-C26	3.11	1.52	1.43
27	h	303	CLA	C1D-ND	3.11	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	811	CLA	C1D-ND	3.11	1.41	1.37
30	e	615	WVN	C39-C36	3.11	1.52	1.43
27	A	841	CLA	C1D-ND	3.10	1.41	1.37
27	h	305	CLA	C1D-ND	3.10	1.41	1.37
27	f	603	CLA	C1D-ND	3.10	1.41	1.37
30	e	615	WVN	C31-C32	3.10	1.52	1.46
27	A	840	CLA	C4B-NB	3.10	1.41	1.37
27	B	807	CLA	CMB-C2B	-3.10	1.44	1.50
27	B	804	CLA	C1D-ND	3.10	1.41	1.37
27	c	606	CLA	C4B-NB	3.10	1.41	1.37
30	s	207	WVN	C30-C28	3.10	1.52	1.43
27	e	602	CLA	C1D-ND	3.10	1.41	1.37
27	d	304	CLA	C4B-NB	3.10	1.41	1.37
30	L	205	WVN	C40-C37	3.10	1.52	1.43
37	s	204	KC2	CHB-C4A	3.10	1.46	1.39
37	l	311	KC2	CHC-C1C	3.10	1.46	1.39
35	b	613	II0	C34-C36	3.09	1.52	1.46
35	k	316	II0	C12-C14	-3.09	1.46	1.51
27	K	101	CLA	C4B-NB	3.09	1.41	1.37
27	s	203	CLA	CMD-C2D	-3.09	1.44	1.50
27	b	611	CLA	C4B-NB	3.09	1.41	1.37
30	A	849	WVN	C39-C36	3.09	1.52	1.43
27	A	837	CLA	CMC-C2C	-3.09	1.44	1.50
27	k	303	CLA	C1D-ND	3.09	1.41	1.37
35	l	313	II0	C33-C35	3.09	1.52	1.46
27	F	203	CLA	C4B-NB	3.09	1.41	1.37
27	i	304	CLA	C1D-ND	3.09	1.41	1.37
27	h	306	CLA	C1D-ND	3.09	1.41	1.37
27	A	833	CLA	C1D-ND	3.08	1.41	1.37
27	a	310	CLA	C1D-ND	3.08	1.41	1.37
30	h	309	WVN	C39-C36	3.08	1.52	1.43
37	n	611	KC2	CHC-C1C	3.08	1.46	1.39
27	s	209	CLA	C4B-NB	3.08	1.41	1.37
27	A	810	CLA	C4B-NB	3.08	1.41	1.37
30	s	207	WVN	C19-C22	3.08	1.52	1.46
35	h	311	II0	C34-C36	3.08	1.52	1.46
27	c	601	CLA	C4B-NB	3.08	1.41	1.37
27	B	823	CLA	C1D-ND	3.08	1.41	1.37
27	n	601	CLA	C4B-NB	3.08	1.41	1.37
37	d	310	KC2	CHC-C1C	3.08	1.46	1.39
27	B	824	CLA	C1D-ND	3.08	1.41	1.37
27	h	302	CLA	C1D-ND	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	j	616	IHT	C28-C26	3.08	1.52	1.50
27	A	831	CLA	C1D-ND	3.08	1.41	1.37
27	j	611	CLA	C4B-NB	3.08	1.41	1.37
27	A	833	CLA	CMB-C2B	-3.08	1.44	1.50
37	g	313	KC2	CHC-C1C	3.08	1.46	1.39
30	J	102	WVN	C40-C37	3.07	1.52	1.43
30	I	101	WVN	C39-C36	3.07	1.52	1.43
30	A	847	WVN	C33-C34	3.07	1.52	1.46
35	i	313	II0	C33-C35	3.07	1.52	1.46
27	l	312	CLA	C1D-ND	3.07	1.41	1.37
27	g	303	CLA	C1D-ND	3.07	1.41	1.37
37	s	204	KC2	CHC-C1C	3.07	1.46	1.39
27	s	203	CLA	C1D-ND	3.07	1.41	1.37
27	A	818	CLA	CMB-C2B	-3.07	1.44	1.50
27	R	203	CLA	C4B-NB	3.06	1.41	1.37
27	A	829	CLA	CMB-C2B	-3.06	1.44	1.50
35	j	614	II0	C06-C04	3.06	1.64	1.54
30	O	201	WVN	C39-C36	3.06	1.52	1.43
37	k	311	KC2	CHB-C4A	3.06	1.46	1.39
30	A	846	WVN	C31-C32	3.06	1.52	1.46
35	e	616	II0	C33-C35	3.06	1.52	1.46
37	k	311	KC2	C1A-CHA	3.06	1.48	1.40
27	e	601	CLA	C4B-NB	3.06	1.41	1.37
35	J	104	II0	C34-C36	3.06	1.52	1.46
27	A	829	CLA	C4B-NB	3.06	1.41	1.37
30	A	846	WVN	C39-C36	3.06	1.52	1.43
36	m	616	IHT	C28-C26	3.06	1.52	1.50
30	I	101	WVN	C40-C37	3.06	1.52	1.43
27	A	814	CLA	C4B-NB	3.06	1.41	1.37
35	i	314	II0	C12-C14	-3.06	1.46	1.51
27	b	606	CLA	C1D-ND	3.06	1.41	1.37
35	m	614	II0	C34-C36	3.05	1.52	1.46
30	B	848	WVN	C30-C28	3.05	1.52	1.43
35	l	317	II0	C33-C35	3.05	1.52	1.46
27	e	611	CLA	C4B-NB	3.05	1.41	1.37
27	j	604	CLA	C4B-NB	3.05	1.41	1.37
30	l	301	WVN	C40-C37	3.05	1.52	1.43
35	g	320	II0	C33-C35	3.05	1.52	1.46
30	B	846	WVN	C39-C36	3.05	1.52	1.43
27	e	601	CLA	C1D-ND	3.05	1.41	1.37
35	j	615	II0	C12-C14	-3.05	1.46	1.51
30	l	316	WVN	C19-C22	3.04	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	J	102	WVN	C31-C32	3.04	1.52	1.46
35	d	312	II0	C33-C35	3.04	1.52	1.46
27	B	812	CLA	C1D-ND	3.04	1.41	1.37
35	n	618	II0	C33-C35	3.04	1.52	1.46
30	J	102	WVN	C23-C25	3.04	1.52	1.46
27	B	808	CLA	C4B-NB	3.04	1.41	1.37
30	i	315	WVN	C31-C32	3.04	1.52	1.46
30	s	207	WVN	C31-C32	3.04	1.52	1.46
27	A	835	CLA	C4B-NB	3.04	1.41	1.37
27	i	306	CLA	C4B-NB	3.04	1.41	1.37
27	s	208	CLA	C1D-ND	3.03	1.41	1.37
35	k	314	II0	C27-C25	3.03	1.52	1.50
30	J	102	WVN	C19-C22	3.03	1.52	1.46
27	i	303	CLA	C1D-ND	3.03	1.41	1.37
30	J	101	WVN	C39-C36	3.03	1.52	1.43
30	e	615	WVN	C40-C37	3.03	1.52	1.43
35	m	614	II0	C33-C35	3.03	1.52	1.46
30	J	102	WVN	C30-C28	3.03	1.52	1.43
27	d	307	CLA	C4B-NB	3.03	1.41	1.37
30	R	202	WVN	C30-C28	3.03	1.52	1.43
27	l	303	CLA	C4B-NB	3.02	1.41	1.37
35	a	315	II0	C33-C35	3.02	1.52	1.46
35	j	614	II0	C33-C35	3.02	1.52	1.46
30	K	103	WVN	C19-C22	3.02	1.52	1.46
30	L	201	WVN	C31-C32	3.02	1.52	1.46
35	a	316	II0	C33-C35	3.02	1.52	1.46
30	L	201	WVN	C39-C36	3.02	1.52	1.43
27	d	305	CLA	C4B-NB	3.02	1.41	1.37
30	J	101	WVN	C40-C37	3.02	1.52	1.43
27	B	830	CLA	C1D-ND	3.01	1.41	1.37
27	g	302	CLA	C1D-ND	3.01	1.41	1.37
30	B	846	WVN	C29-C26	3.01	1.52	1.43
27	L	202	CLA	C4B-NB	3.01	1.41	1.37
35	d	312	II0	C12-C14	-3.01	1.46	1.51
27	b	610	CLA	C1D-ND	3.01	1.41	1.37
27	e	603	CLA	C4B-NB	3.01	1.41	1.37
30	B	847	WVN	C33-C34	3.01	1.52	1.46
35	d	313	II0	C12-C14	-3.01	1.46	1.51
27	A	817	CLA	C4B-NB	3.01	1.41	1.37
27	h	313	CLA	C1D-ND	3.01	1.41	1.37
27	B	826	CLA	C1D-ND	3.00	1.41	1.37
27	s	202	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	847	WVN	C40-C37	3.00	1.52	1.43
30	l	301	WVN	C31-C32	3.00	1.52	1.46
27	A	824	CLA	C1D-ND	3.00	1.41	1.37
27	B	827	CLA	C4B-NB	3.00	1.41	1.37
27	g	304	CLA	C4B-NB	3.00	1.41	1.37
30	A	849	WVN	C19-C22	3.00	1.52	1.46
27	B	834	CLA	CMD-C2D	-3.00	1.44	1.50
27	A	801	CLA	C4B-NB	3.00	1.41	1.37
27	L	206	CLA	C1D-ND	3.00	1.41	1.37
30	h	309	WVN	C40-C37	3.00	1.52	1.43
35	n	618	II0	C12-C14	-3.00	1.46	1.51
27	e	605	CLA	C1D-ND	2.99	1.41	1.37
30	A	849	WVN	C40-C37	2.99	1.52	1.43
30	B	848	WVN	C40-C37	2.99	1.52	1.43
27	c	603	CLA	C1D-ND	2.99	1.41	1.37
27	B	837	CLA	C1D-ND	2.99	1.41	1.37
30	F	205	WVN	C29-C26	2.99	1.52	1.43
30	B	845	WVN	C30-C28	2.99	1.52	1.43
27	A	822	CLA	C1D-ND	2.99	1.41	1.37
27	B	839	CLA	C4B-NB	2.99	1.41	1.37
35	c	613	II0	C27-C25	2.98	1.52	1.50
30	R	201	WVN	C19-C22	2.98	1.52	1.46
27	A	803	CLA	C4B-NB	2.98	1.41	1.37
27	a	309	CLA	C1D-ND	2.98	1.41	1.37
27	k	308	CLA	C3B-C4B	2.98	1.51	1.42
30	R	202	WVN	C33-C34	2.98	1.52	1.46
30	R	201	WVN	C29-C26	2.98	1.52	1.43
35	j	614	II0	C12-C14	-2.98	1.46	1.51
30	A	849	WVN	C30-C28	2.98	1.52	1.43
27	J	105	CLA	C1D-ND	2.98	1.41	1.37
27	A	822	CLA	CMD-C2D	-2.97	1.44	1.50
27	B	816	CLA	CMB-C2B	-2.97	1.44	1.50
27	m	608	CLA	C4B-NB	2.97	1.41	1.37
27	l	309	CLA	C4B-NB	2.97	1.41	1.37
27	j	611	CLA	C1D-ND	2.97	1.41	1.37
30	B	843	WVN	C40-C37	2.97	1.52	1.43
27	A	815	CLA	MG-NB	-2.97	1.99	2.05
27	n	610	CLA	CMD-C2D	-2.96	1.44	1.50
30	A	848	WVN	C30-C28	2.96	1.52	1.43
27	k	301	CLA	C4B-NB	2.96	1.41	1.37
30	J	101	WVN	C29-C26	2.96	1.52	1.43
27	n	604	CLA	C1D-ND	2.96	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	303	CLA	C4B-NB	2.96	1.41	1.37
27	B	814	CLA	C1D-ND	2.96	1.41	1.37
35	h	312	II0	C34-C36	2.96	1.52	1.46
30	K	103	WVN	C30-C28	2.96	1.52	1.43
27	l	304	CLA	C1D-ND	2.96	1.41	1.37
35	b	615	II0	C34-C36	2.96	1.52	1.46
30	s	205	WVN	C39-C36	2.96	1.52	1.43
27	a	303	CLA	CMD-C2D	-2.96	1.44	1.50
27	j	606	CLA	C4B-NB	2.96	1.41	1.37
30	s	205	WVN	C31-C32	2.96	1.52	1.46
27	f	609	CLA	C4B-NB	2.96	1.41	1.37
27	f	604	CLA	C4B-NB	2.95	1.41	1.37
27	j	605	CLA	C1B-C2B	2.95	1.50	1.43
27	A	811	CLA	C1D-ND	2.95	1.41	1.37
27	c	607	CLA	C4B-NB	2.95	1.41	1.37
30	R	202	WVN	C23-C25	2.95	1.52	1.46
30	A	848	WVN	C40-C37	2.95	1.52	1.43
27	B	816	CLA	C1D-ND	2.95	1.41	1.37
27	g	310	CLA	C4B-NB	2.95	1.41	1.37
27	m	606	CLA	C1D-ND	2.95	1.41	1.37
27	n	608	CLA	C4B-NB	2.95	1.41	1.37
30	B	845	WVN	C33-C34	2.95	1.52	1.46
27	A	855	CLA	C1D-ND	2.94	1.41	1.37
37	n	612	KC2	CHB-C4A	2.94	1.45	1.39
27	i	303	CLA	C4B-NB	2.94	1.41	1.37
35	c	615	II0	C33-C35	2.94	1.52	1.46
27	B	829	CLA	C1D-ND	2.94	1.41	1.37
30	B	847	WVN	C20-C13	2.94	1.55	1.45
30	L	201	WVN	C29-C26	2.94	1.52	1.43
27	B	815	CLA	C1D-ND	2.94	1.41	1.37
27	B	813	CLA	C1D-ND	2.94	1.41	1.37
27	h	313	CLA	CMD-C2D	-2.94	1.44	1.50
30	F	205	WVN	C31-C32	2.94	1.52	1.46
27	l	310	CLA	C4B-NB	2.93	1.41	1.37
30	R	201	WVN	C31-C32	2.93	1.52	1.46
27	B	849	CLA	C4B-NB	2.93	1.41	1.37
27	m	609	CLA	C4B-NB	2.93	1.41	1.37
30	B	843	WVN	C33-C34	2.93	1.52	1.46
30	B	846	WVN	C31-C32	2.93	1.52	1.46
27	A	827	CLA	C1D-ND	2.93	1.41	1.37
35	m	613	II0	C33-C35	2.93	1.52	1.46
27	B	806	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	848	WVN	C39-C36	2.93	1.52	1.43
30	F	204	WVN	C39-C36	2.93	1.52	1.43
27	a	303	CLA	C1D-ND	2.93	1.41	1.37
35	f	615	II0	C33-C35	2.93	1.52	1.46
30	B	845	WVN	C39-C36	2.93	1.52	1.43
27	A	807	CLA	C4B-NB	2.92	1.41	1.37
27	f	603	CLA	C4B-NB	2.92	1.41	1.37
27	i	312	CLA	C4B-NB	2.92	1.41	1.37
27	s	208	CLA	C1B-NB	-2.92	1.34	1.37
27	e	610	CLA	C4B-NB	2.92	1.41	1.37
27	B	811	CLA	C4B-NB	2.92	1.41	1.37
30	O	201	WVN	C29-C26	2.92	1.52	1.43
27	B	801	CLA	C4B-NB	2.92	1.41	1.37
27	g	309	CLA	CMA-C3A	-2.92	1.47	1.53
27	A	812	CLA	C1D-ND	2.92	1.41	1.37
37	k	311	KC2	CHC-C1C	2.92	1.45	1.39
30	I	101	WVN	C19-C22	2.91	1.52	1.46
30	l	301	WVN	C39-C36	2.91	1.52	1.43
27	e	604	CLA	C4B-NB	2.91	1.41	1.37
36	g	319	IHT	C32-C33	2.91	1.52	1.46
35	a	316	II0	C12-C14	-2.90	1.46	1.51
27	A	825	CLA	C4B-NB	2.90	1.41	1.37
30	F	204	WVN	C40-C37	2.90	1.52	1.43
27	A	817	CLA	C1D-ND	2.90	1.41	1.37
30	l	301	WVN	C33-C34	2.90	1.52	1.46
27	A	814	CLA	C1D-ND	2.90	1.41	1.37
27	e	608	CLA	C4B-NB	2.90	1.41	1.37
27	A	831	CLA	C4B-NB	2.90	1.41	1.37
27	i	307	CLA	C3B-C4B	2.90	1.51	1.42
30	B	848	WVN	C23-C25	2.90	1.52	1.46
36	b	614	IHT	C09-C10	-2.90	1.45	1.51
27	A	820	CLA	CMB-C2B	-2.90	1.44	1.50
27	A	809	CLA	CMC-C2C	-2.90	1.44	1.50
27	B	801	CLA	C1B-C2B	2.89	1.49	1.43
27	B	828	CLA	C1D-ND	2.89	1.41	1.37
30	R	201	WVN	C39-C36	2.89	1.52	1.43
27	A	834	CLA	C1D-ND	2.89	1.41	1.37
27	L	204	CLA	C4B-NB	2.89	1.41	1.37
30	e	615	WVN	C30-C28	2.89	1.52	1.43
30	e	615	WVN	C33-C34	2.89	1.52	1.46
30	O	201	WVN	C30-C28	2.89	1.52	1.43
27	B	805	CLA	C1D-ND	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	R	202	WVN	C40-C37	2.88	1.52	1.43
30	F	205	WVN	C19-C22	2.88	1.52	1.46
30	l	301	WVN	C02-C11	2.88	1.54	1.50
35	l	302	II0	C34-C36	2.88	1.52	1.46
35	k	315	II0	C34-C36	2.88	1.52	1.46
30	B	847	WVN	C39-C36	2.88	1.52	1.43
27	A	810	CLA	C1D-ND	2.88	1.41	1.37
27	B	834	CLA	C4B-NB	2.88	1.41	1.37
27	B	805	CLA	C1B-C2B	2.88	1.49	1.43
30	F	204	WVN	C31-C32	2.88	1.52	1.46
27	B	824	CLA	CMD-C2D	-2.87	1.44	1.50
27	c	609	CLA	C4B-NB	2.87	1.41	1.37
27	j	608	CLA	C4B-NB	2.87	1.41	1.37
30	B	843	WVN	C39-C36	2.87	1.52	1.43
27	n	609	CLA	CMA-C3A	-2.87	1.47	1.53
30	F	205	WVN	C39-C36	2.87	1.52	1.43
37	g	313	KC2	C3C-C4C	2.87	1.50	1.44
27	c	602	CLA	C4B-NB	2.87	1.41	1.37
27	f	605	CLA	C1B-C2B	2.87	1.49	1.43
27	i	308	CLA	C1D-ND	2.87	1.41	1.37
27	A	834	CLA	CMD-C2D	-2.87	1.44	1.50
27	k	303	CLA	C4B-NB	2.87	1.41	1.37
27	B	830	CLA	CMD-C2D	-2.87	1.44	1.50
27	h	306	CLA	C4B-NB	2.87	1.41	1.37
30	M	101	WVN	C29-C26	2.87	1.52	1.43
27	A	821	CLA	C4B-NB	2.87	1.41	1.37
27	b	608	CLA	C4B-NB	2.87	1.41	1.37
30	K	103	WVN	C29-C26	2.86	1.52	1.43
27	L	204	CLA	C1D-ND	2.86	1.41	1.37
27	B	809	CLA	C1D-ND	2.86	1.41	1.37
30	B	844	WVN	C30-C28	2.86	1.52	1.43
30	J	101	WVN	C31-C32	2.86	1.52	1.46
27	b	601	CLA	C4B-NB	2.86	1.41	1.37
35	l	302	II0	C33-C35	2.86	1.52	1.46
27	f	605	CLA	C4B-NB	2.86	1.41	1.37
27	O	206	CLA	C4B-NB	2.86	1.41	1.37
30	O	201	WVN	C20-C13	2.86	1.54	1.45
30	s	207	WVN	C29-C26	2.86	1.52	1.43
27	j	612	CLA	C4B-NB	2.86	1.41	1.37
30	R	202	WVN	C29-C26	2.85	1.52	1.43
35	b	612	II0	C33-C35	2.85	1.52	1.46
30	A	849	WVN	C31-C32	2.85	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	j	602	CLA	C1D-ND	2.85	1.41	1.37
30	B	844	WVN	C39-C36	2.85	1.52	1.43
27	A	830	CLA	CMD-C2D	-2.85	1.44	1.50
27	B	814	CLA	C4B-NB	2.85	1.41	1.37
27	B	835	CLA	C1D-ND	2.85	1.41	1.37
30	B	848	WVN	C39-C36	2.85	1.52	1.43
27	g	322	CLA	CMB-C2B	-2.85	1.44	1.50
27	B	814	CLA	CMB-C2B	-2.85	1.44	1.50
35	l	302	II0	C27-C25	2.85	1.52	1.50
30	B	845	WVN	C40-C37	2.85	1.52	1.43
27	j	601	CLA	C1D-ND	2.85	1.41	1.37
30	R	201	WVN	C30-C28	2.85	1.52	1.43
37	s	201	KC2	CHB-C1B	2.84	1.43	1.38
27	g	315	CLA	C4B-NB	2.84	1.41	1.37
30	A	849	WVN	C29-C26	2.84	1.52	1.43
27	c	612	CLA	C4B-NB	2.84	1.41	1.37
27	F	203	CLA	C1D-ND	2.84	1.41	1.37
27	k	302	CLA	C4B-NB	2.84	1.41	1.37
30	M	101	WVN	C31-C32	2.84	1.52	1.46
30	M	101	WVN	C40-C37	2.84	1.52	1.43
27	B	815	CLA	C4B-NB	2.84	1.41	1.37
27	m	611	CLA	C4B-NB	2.84	1.41	1.37
37	d	310	KC2	C1B-NB	-2.84	1.34	1.37
30	K	103	WVN	C31-C32	2.84	1.52	1.46
27	m	611	CLA	C1D-ND	2.84	1.41	1.37
27	j	604	CLA	CMA-C3A	-2.84	1.47	1.53
30	e	615	WVN	C20-C13	2.84	1.54	1.45
30	e	615	WVN	C23-C25	2.83	1.52	1.46
30	M	101	WVN	C30-C28	2.83	1.52	1.43
37	s	204	KC2	CHB-C1B	2.83	1.43	1.38
31	A	851	LMT	O2B-C2B	-2.83	1.35	1.43
27	A	801	CLA	C1B-C2B	2.83	1.49	1.43
27	k	305	CLA	CAA-C2A	-2.83	1.48	1.54
30	l	316	WVN	C02-C11	2.83	1.54	1.50
27	g	322	CLA	C4B-NB	2.83	1.41	1.37
35	f	615	II0	C34-C36	2.83	1.52	1.46
37	g	312	KC2	C1B-NB	-2.83	1.34	1.37
30	B	845	WVN	C23-C25	2.83	1.52	1.46
27	A	802	CLA	C4B-NB	2.83	1.41	1.37
37	n	611	KC2	C1B-NB	-2.83	1.34	1.37
27	m	602	CLA	C1D-ND	2.83	1.41	1.37
37	k	311	KC2	C1B-NB	-2.83	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	314	II0	C33-C35	2.82	1.52	1.46
35	e	614	II0	C33-C35	2.82	1.52	1.46
27	n	603	CLA	C3B-C4B	2.82	1.50	1.42
27	B	809	CLA	C4B-NB	2.82	1.41	1.37
27	g	304	CLA	CMD-C2D	-2.82	1.45	1.50
27	k	307	CLA	C4B-NB	2.82	1.41	1.37
30	O	201	WVN	C33-C34	2.81	1.52	1.46
30	s	205	WVN	C30-C28	2.81	1.51	1.43
35	c	614	II0	C33-C35	2.81	1.52	1.46
27	R	203	CLA	C3B-C4B	2.81	1.50	1.42
27	m	607	CLA	C4B-NB	2.81	1.41	1.37
27	B	833	CLA	CMD-C2D	-2.81	1.45	1.50
37	d	309	KC2	C1B-NB	-2.81	1.34	1.37
27	n	610	CLA	C3B-C4B	2.81	1.50	1.42
27	L	202	CLA	C3B-C4B	2.81	1.50	1.42
27	A	856	CLA	C4B-NB	2.81	1.41	1.37
27	A	806	CLA	C4B-NB	2.81	1.41	1.37
27	B	837	CLA	C4B-NB	2.81	1.41	1.37
27	A	838	CLA	C1D-ND	2.81	1.41	1.37
30	R	201	WVN	C40-C37	2.81	1.51	1.43
27	B	803	CLA	C1D-ND	2.80	1.41	1.37
30	F	204	WVN	C29-C26	2.80	1.51	1.43
35	g	317	II0	C34-C36	2.80	1.51	1.46
27	K	102	CLA	CMC-C2C	-2.80	1.45	1.50
27	B	832	CLA	C4B-NB	2.80	1.41	1.37
30	I	101	WVN	C02-C11	2.80	1.54	1.50
27	B	809	CLA	C3B-C4B	2.80	1.50	1.42
37	j	610	KC2	C1B-NB	-2.80	1.34	1.37
27	c	604	CLA	C4B-NB	2.80	1.41	1.37
37	i	310	KC2	C1B-NB	-2.80	1.34	1.37
30	B	847	WVN	C29-C26	2.80	1.51	1.43
27	s	208	CLA	C4B-NB	2.80	1.41	1.37
27	k	308	CLA	C4B-NB	2.80	1.41	1.37
35	m	615	II0	C33-C35	2.79	1.51	1.46
27	a	313	CLA	CMD-C2D	-2.79	1.45	1.50
27	h	301	CLA	C4B-NB	2.79	1.41	1.37
37	g	314	KC2	C1B-NB	-2.79	1.34	1.37
27	a	307	CLA	C1D-ND	2.79	1.41	1.37
30	s	205	WVN	C02-C11	2.79	1.54	1.50
27	F	201	CLA	C4B-NB	2.79	1.41	1.37
37	k	310	KC2	C1B-NB	-2.79	1.34	1.37
35	c	613	II0	C33-C35	2.79	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	847	WVN	C30-C28	2.79	1.51	1.43
36	O	204	IHT	C18-C07	2.79	1.54	1.45
27	k	307	CLA	C1B-C2B	2.79	1.49	1.43
27	B	817	CLA	C4B-NB	2.79	1.41	1.37
27	c	605	CLA	C1B-C2B	2.79	1.49	1.43
27	g	305	CLA	C4B-NB	2.79	1.41	1.37
30	s	205	WVN	C40-C37	2.79	1.51	1.43
35	c	615	II0	C12-C14	-2.79	1.46	1.51
27	h	303	CLA	C4B-NB	2.78	1.41	1.37
27	B	810	CLA	CMC-C2C	-2.78	1.45	1.50
27	b	609	CLA	C4B-NB	2.78	1.41	1.37
30	M	101	WVN	C39-C36	2.78	1.51	1.43
35	J	104	II0	C27-C25	2.78	1.52	1.50
27	g	310	CLA	C3B-C4B	2.78	1.50	1.42
36	c	620	IHT	C25-C23	2.78	1.56	1.50
27	n	602	CLA	C4B-NB	2.78	1.41	1.37
27	k	303	CLA	CMC-C2C	-2.78	1.45	1.50
27	B	807	CLA	C1D-ND	2.77	1.41	1.37
30	s	205	WVN	C33-C34	2.77	1.51	1.46
27	B	835	CLA	CMB-C2B	-2.77	1.45	1.50
27	A	813	CLA	C4B-NB	2.77	1.41	1.37
36	b	614	IHT	C31-C29	2.77	1.51	1.43
27	f	602	CLA	C4B-NB	2.77	1.41	1.37
27	A	828	CLA	CMD-C2D	-2.77	1.45	1.50
30	B	843	WVN	C29-C26	2.77	1.51	1.43
27	B	818	CLA	C1D-ND	2.77	1.41	1.37
27	B	826	CLA	C4B-NB	2.77	1.41	1.37
27	A	840	CLA	C3B-C4B	2.77	1.50	1.42
30	B	843	WVN	C23-C25	2.77	1.51	1.46
27	B	829	CLA	C4B-NB	2.77	1.41	1.37
37	i	310	KC2	C1A-CHA	2.77	1.47	1.40
27	f	610	CLA	C4B-NB	2.77	1.41	1.37
27	d	308	CLA	C4B-NB	2.76	1.41	1.37
27	B	815	CLA	CMB-C2B	-2.76	1.45	1.50
27	a	313	CLA	C1D-ND	2.76	1.41	1.37
37	l	311	KC2	C1B-NB	-2.76	1.34	1.37
27	A	831	CLA	C1B-C2B	2.76	1.49	1.43
27	g	306	CLA	C1B-C2B	2.76	1.49	1.43
27	g	306	CLA	C4B-NB	2.76	1.41	1.37
30	s	207	WVN	C20-C13	2.76	1.54	1.45
27	g	307	CLA	C4B-NB	2.76	1.41	1.37
27	B	825	CLA	C4B-NB	2.76	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	603	CLA	C4B-NB	2.76	1.41	1.37
27	i	307	CLA	C1B-C2B	2.76	1.49	1.43
27	i	302	CLA	C3B-C4B	2.76	1.50	1.42
30	M	101	WVN	C19-C22	2.76	1.51	1.46
36	c	620	IHT	C32-C33	2.76	1.51	1.46
27	A	828	CLA	C1D-ND	2.76	1.41	1.37
27	J	105	CLA	C4B-NB	2.76	1.41	1.37
27	l	308	CLA	C1B-C2B	2.76	1.49	1.43
27	J	103	CLA	C1D-ND	2.76	1.41	1.37
30	A	847	WVN	C20-C13	2.76	1.54	1.45
30	A	848	WVN	C19-C22	2.75	1.51	1.46
27	A	842	CLA	C1D-ND	2.75	1.41	1.37
37	e	609	KC2	C1B-NB	-2.75	1.34	1.37
35	d	312	II0	C20-C14	2.75	1.55	1.50
30	I	101	WVN	C30-C28	2.75	1.51	1.43
30	J	102	WVN	C20-C13	2.75	1.54	1.45
37	c	610	KC2	C1B-NB	-2.75	1.34	1.37
35	b	613	II0	C33-C35	2.75	1.51	1.46
27	i	308	CLA	C4B-NB	2.75	1.41	1.37
27	n	607	CLA	C4B-NB	2.75	1.41	1.37
27	B	818	CLA	C4B-NB	2.75	1.41	1.37
37	g	313	KC2	C1B-NB	-2.75	1.34	1.37
27	n	613	CLA	C1B-C2B	2.75	1.49	1.43
27	A	856	CLA	C1D-ND	2.75	1.41	1.37
27	B	830	CLA	CMB-C2B	-2.75	1.45	1.50
36	c	616	IHT	C25-C23	2.74	1.56	1.50
36	b	614	IHT	C28-C26	2.74	1.52	1.50
27	A	822	CLA	C4B-NB	2.74	1.41	1.37
37	f	611	KC2	C1B-NB	-2.74	1.34	1.37
30	K	103	WVN	C20-C13	2.74	1.54	1.45
27	i	308	CLA	C3B-C4B	2.74	1.50	1.42
30	K	103	WVN	C23-C25	2.74	1.51	1.46
27	a	313	CLA	C4B-NB	2.74	1.41	1.37
27	B	819	CLA	CMC-C2C	-2.74	1.45	1.50
30	O	201	WVN	C23-C25	2.74	1.51	1.46
27	j	609	CLA	C1D-ND	2.74	1.41	1.37
27	i	311	CLA	C3B-C4B	2.74	1.50	1.42
27	B	819	CLA	C4B-NB	2.74	1.41	1.37
27	F	201	CLA	C1D-ND	2.73	1.41	1.37
37	k	312	KC2	C1B-NB	-2.73	1.34	1.37
30	B	848	WVN	C29-C26	2.73	1.51	1.43
27	h	304	CLA	C1D-ND	2.73	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	g	309	CLA	C4B-NB	2.73	1.41	1.37
27	n	601	CLA	C1B-C2B	2.73	1.49	1.43
35	e	613	II0	C33-C35	2.73	1.51	1.46
27	e	605	CLA	C4B-NB	2.73	1.41	1.37
27	k	305	CLA	CMD-C2D	-2.73	1.45	1.50
30	A	848	WVN	C29-C26	2.73	1.51	1.43
27	B	812	CLA	CMC-C2C	-2.73	1.45	1.50
37	m	610	KC2	C1B-NB	-2.73	1.34	1.37
27	A	841	CLA	C4B-NB	2.72	1.41	1.37
27	h	306	CLA	C3B-C4B	2.72	1.50	1.42
30	A	849	WVN	C23-C25	2.72	1.51	1.46
30	B	846	WVN	C02-C11	2.72	1.54	1.50
27	b	601	CLA	C1B-C2B	2.72	1.49	1.43
27	d	304	CLA	CMB-C2B	-2.72	1.45	1.50
27	l	306	CLA	CMA-C3A	-2.72	1.47	1.53
27	A	808	CLA	C1D-ND	2.72	1.41	1.37
27	B	806	CLA	CMD-C2D	-2.72	1.45	1.50
35	h	310	II0	C33-C35	2.71	1.51	1.46
27	b	611	CLA	C1B-C2B	2.71	1.49	1.43
27	A	811	CLA	C3B-C4B	2.71	1.50	1.42
30	I	101	WVN	C33-C34	2.71	1.51	1.46
27	k	309	CLA	C1B-C2B	2.71	1.49	1.43
27	A	820	CLA	C1D-ND	2.71	1.41	1.37
27	B	835	CLA	C4B-NB	2.71	1.41	1.37
27	n	606	CLA	C4B-NB	2.71	1.41	1.37
27	A	816	CLA	C1D-ND	2.71	1.41	1.37
30	A	848	WVN	C31-C32	2.71	1.51	1.46
27	a	309	CLA	C1B-C2B	2.70	1.49	1.43
27	A	820	CLA	C4B-NB	2.70	1.41	1.37
27	h	301	CLA	CMB-C2B	-2.70	1.45	1.50
27	i	309	CLA	C4B-NB	2.70	1.41	1.37
27	A	804	CLA	C1D-ND	2.70	1.41	1.37
27	A	836	CLA	C4B-NB	2.70	1.41	1.37
27	a	312	CLA	C1B-C2B	2.70	1.49	1.43
30	L	201	WVN	C40-C37	2.70	1.51	1.43
30	A	846	WVN	C23-C25	2.70	1.51	1.46
30	i	315	WVN	C02-C11	2.70	1.54	1.50
27	e	605	CLA	C1B-C2B	2.70	1.49	1.43
36	n	617	IHT	C18-C07	2.70	1.54	1.45
30	F	205	WVN	C02-C11	2.70	1.54	1.50
27	m	601	CLA	C1B-C2B	2.70	1.49	1.43
35	h	311	II0	C30-C26	-2.69	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	m	611	CLA	CMD-C2D	-2.69	1.45	1.50
30	L	205	WVN	C20-C13	2.69	1.54	1.45
27	B	838	CLA	C3B-C4B	2.69	1.50	1.42
37	g	312	KC2	C1A-CHA	2.69	1.47	1.40
35	k	315	II0	C33-C35	2.69	1.51	1.46
27	B	833	CLA	C1D-ND	2.69	1.41	1.37
27	j	611	CLA	C1B-C2B	2.69	1.49	1.43
27	e	606	CLA	C4B-NB	2.69	1.41	1.37
30	J	102	WVN	C29-C26	2.69	1.51	1.43
37	g	314	KC2	C1A-CHA	2.69	1.47	1.40
27	j	603	CLA	C4B-NB	2.69	1.41	1.37
30	L	205	WVN	C19-C22	2.69	1.51	1.46
27	A	823	CLA	C1B-C2B	2.69	1.49	1.43
27	A	807	CLA	C1B-C2B	2.68	1.49	1.43
35	b	612	II0	C34-C36	2.68	1.51	1.46
30	A	848	WVN	C33-C34	2.68	1.51	1.46
27	L	204	CLA	CMB-C2B	-2.68	1.45	1.50
27	A	856	CLA	C1B-C2B	2.68	1.49	1.43
27	c	611	CLA	CMC-C2C	-2.68	1.45	1.50
37	g	313	KC2	C1A-CHA	2.68	1.47	1.40
27	A	812	CLA	CMC-C2C	-2.68	1.45	1.50
30	M	101	WVN	C23-C25	2.68	1.51	1.46
30	B	843	WVN	C31-C32	2.67	1.51	1.46
27	A	821	CLA	C1D-ND	2.67	1.41	1.37
36	n	617	IHT	C25-C23	2.67	1.56	1.50
35	f	616	II0	C33-C35	2.67	1.51	1.46
37	s	204	KC2	C3C-C4C	2.67	1.50	1.44
30	L	201	WVN	C23-C25	2.67	1.51	1.46
27	F	202	CLA	C3B-C4B	2.67	1.50	1.42
27	B	802	CLA	C4B-NB	2.67	1.41	1.37
35	b	615	II0	C33-C35	2.67	1.51	1.46
27	b	603	CLA	C4B-NB	2.67	1.41	1.37
27	A	809	CLA	C4B-NB	2.66	1.41	1.37
30	B	848	WVN	C19-C22	2.66	1.51	1.46
27	m	604	CLA	CMB-C2B	-2.66	1.45	1.50
27	g	311	CLA	C1B-C2B	2.66	1.49	1.43
27	h	308	CLA	C1B-C2B	2.66	1.49	1.43
27	A	842	CLA	C4B-NB	2.66	1.41	1.37
27	B	811	CLA	C1B-C2B	2.66	1.49	1.43
27	g	310	CLA	CMD-C2D	-2.66	1.45	1.50
36	m	616	IHT	C25-C23	2.66	1.56	1.50
27	l	308	CLA	C4B-NB	2.66	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	g	308	CLA	CMD-C2D	-2.66	1.45	1.50
37	c	610	KC2	C1A-CHA	2.66	1.47	1.40
30	J	101	WVN	C19-C22	2.66	1.51	1.46
36	k	317	IHT	C25-C23	2.65	1.56	1.50
27	c	601	CLA	C1B-C2B	2.65	1.49	1.43
27	B	807	CLA	C4B-NB	2.65	1.41	1.37
30	L	201	WVN	C30-C28	2.65	1.51	1.43
30	A	849	WVN	C20-C13	2.65	1.54	1.45
27	c	608	CLA	C4B-NB	2.65	1.41	1.37
27	B	812	CLA	C4B-NB	2.65	1.41	1.37
36	a	317	IHT	C25-C23	2.65	1.56	1.50
30	B	844	WVN	C40-C37	2.65	1.51	1.43
27	j	606	CLA	CAA-C2A	-2.65	1.49	1.54
27	A	819	CLA	C1B-C2B	2.65	1.49	1.43
27	l	304	CLA	C4B-NB	2.65	1.41	1.37
27	e	602	CLA	C4B-NB	2.64	1.41	1.37
27	A	813	CLA	C1B-NB	-2.64	1.34	1.37
30	R	202	WVN	C39-C36	2.64	1.51	1.43
30	l	316	WVN	C20-C13	2.64	1.54	1.45
27	i	303	CLA	CMD-C2D	-2.64	1.45	1.50
27	l	310	CLA	C1B-C2B	2.64	1.49	1.43
27	j	601	CLA	C3B-C4B	2.64	1.50	1.42
37	k	312	KC2	C1A-CHA	2.64	1.47	1.40
27	l	303	CLA	C1B-C2B	2.64	1.49	1.43
27	B	813	CLA	CMC-C2C	-2.64	1.45	1.50
27	c	608	CLA	C1B-C2B	2.64	1.49	1.43
30	B	844	WVN	C23-C25	2.64	1.51	1.46
30	I	101	WVN	C23-C25	2.64	1.51	1.46
27	d	305	CLA	C1B-C2B	2.63	1.49	1.43
36	m	616	IHT	C18-C07	2.63	1.54	1.45
36	g	319	IHT	C25-C23	2.63	1.56	1.50
30	L	201	WVN	C19-C22	2.63	1.51	1.46
36	a	317	IHT	C18-C07	2.63	1.54	1.45
30	R	201	WVN	C33-C34	2.63	1.51	1.46
27	B	828	CLA	MG-NC	2.63	2.12	2.06
27	A	820	CLA	CMD-C2D	-2.63	1.45	1.50
27	J	103	CLA	CMD-C2D	-2.63	1.45	1.50
36	f	617	IHT	C18-C07	2.63	1.54	1.45
30	l	301	WVN	C30-C28	2.63	1.51	1.43
27	B	808	CLA	C4B-C3B	2.63	1.49	1.43
36	f	617	IHT	C25-C23	2.63	1.56	1.50
35	a	315	II0	C30-C26	-2.63	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	812	CLA	C1B-NB	-2.62	1.34	1.37
27	n	604	CLA	CMB-C2B	-2.62	1.45	1.50
30	B	847	WVN	C19-C22	2.62	1.51	1.46
27	h	303	CLA	CMB-C2B	-2.62	1.45	1.50
27	A	804	CLA	C4B-NB	2.62	1.41	1.37
27	n	609	CLA	C3B-C4B	2.62	1.50	1.42
27	n	608	CLA	CMD-C2D	-2.62	1.45	1.50
27	d	301	CLA	C1B-C2B	2.62	1.49	1.43
27	i	309	CLA	C1B-C2B	2.62	1.49	1.43
27	s	202	CLA	CMB-C2B	-2.62	1.45	1.50
27	e	603	CLA	CMD-C2D	-2.62	1.45	1.50
35	j	613	II0	C34-C36	2.62	1.51	1.46
30	R	202	WVN	C31-C32	2.62	1.51	1.46
27	e	603	CLA	C1B-C2B	2.62	1.49	1.43
27	L	204	CLA	C1B-C2B	2.62	1.49	1.43
27	L	203	CLA	C4B-NB	2.62	1.41	1.37
27	f	601	CLA	C1B-C2B	2.62	1.49	1.43
31	a	302	LMT	O1'-C1'	-2.62	1.35	1.40
27	A	817	CLA	CMB-C2B	-2.61	1.45	1.50
27	B	803	CLA	CMD-C2D	-2.61	1.45	1.50
27	c	608	CLA	CMC-C2C	-2.61	1.45	1.50
27	A	804	CLA	CMD-C2D	-2.61	1.45	1.50
27	m	609	CLA	C1B-C2B	2.61	1.49	1.43
36	O	204	IHT	C25-C23	2.61	1.56	1.50
27	k	302	CLA	C3B-C4B	2.61	1.50	1.42
27	B	838	CLA	C1B-C2B	2.61	1.49	1.43
27	c	607	CLA	C1B-C2B	2.61	1.49	1.43
27	A	802	CLA	C1B-NB	-2.61	1.34	1.37
27	h	308	CLA	C4B-NB	2.61	1.41	1.37
27	d	301	CLA	C4B-NB	2.61	1.41	1.37
27	c	604	CLA	C1B-C2B	2.61	1.49	1.43
35	h	312	II0	C33-C35	2.61	1.51	1.46
27	l	307	CLA	C2A-C1A	2.61	1.58	1.52
30	B	845	WVN	C20-C13	2.61	1.54	1.45
27	K	101	CLA	C1B-C2B	2.61	1.49	1.43
35	b	615	II0	C27-C25	2.61	1.52	1.50
27	B	816	CLA	C3B-C4B	2.61	1.50	1.42
27	B	824	CLA	CMB-C2B	-2.61	1.45	1.50
27	j	604	CLA	C1B-C2B	2.60	1.49	1.43
37	s	204	KC2	CBD-CAD	-2.60	1.44	1.56
30	B	847	WVN	C31-C32	2.60	1.51	1.46
27	s	206	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	s	207	WVN	C23-C25	2.60	1.51	1.46
27	a	309	CLA	C4B-NB	2.60	1.41	1.37
27	J	103	CLA	C4B-NB	2.60	1.41	1.37
27	A	825	CLA	C1B-C2B	2.60	1.49	1.43
27	B	830	CLA	C4B-NB	2.60	1.41	1.37
27	a	306	CLA	C4B-NB	2.60	1.41	1.37
27	f	613	CLA	C3B-C4B	2.60	1.50	1.42
27	f	602	CLA	C1B-C2B	2.60	1.49	1.43
27	c	602	CLA	CMD-C2D	-2.59	1.45	1.50
27	l	312	CLA	CMD-C2D	-2.59	1.45	1.50
30	F	204	WVN	C19-C22	2.59	1.51	1.46
27	k	301	CLA	C1B-C2B	2.59	1.49	1.43
27	i	311	CLA	MG-NA	2.59	2.12	2.06
27	s	203	CLA	C1B-C2B	2.59	1.49	1.43
27	A	830	CLA	C4B-NB	2.59	1.41	1.37
27	O	202	CLA	C4B-NB	2.59	1.41	1.37
27	A	838	CLA	CMC-C2C	-2.59	1.45	1.50
27	l	306	CLA	C1B-C2B	2.59	1.49	1.43
27	n	609	CLA	CHC-C1C	2.59	1.43	1.38
27	A	808	CLA	C4B-NB	2.59	1.41	1.37
30	A	846	WVN	C20-C13	2.59	1.53	1.45
27	l	309	CLA	C3B-C4B	2.59	1.50	1.42
30	J	101	WVN	C20-C13	2.59	1.53	1.45
27	b	605	CLA	CMD-C2D	-2.59	1.45	1.50
27	n	610	CLA	C1B-C2B	2.59	1.49	1.43
27	m	612	CLA	C4B-NB	2.59	1.41	1.37
27	g	302	CLA	CMD-C2D	-2.59	1.45	1.50
27	B	816	CLA	C1B-NB	-2.59	1.34	1.37
27	a	305	CLA	C4B-NB	2.59	1.41	1.37
27	A	817	CLA	C3B-C4B	2.58	1.50	1.42
36	j	616	IHT	C25-C23	2.58	1.56	1.50
27	j	609	CLA	C4B-NB	2.58	1.41	1.37
27	f	606	CLA	C1B-C2B	2.58	1.49	1.43
27	J	105	CLA	C1B-C2B	2.58	1.49	1.43
27	h	307	CLA	C1B-C2B	2.58	1.49	1.43
27	A	828	CLA	C4B-NB	2.58	1.41	1.37
27	A	852	CLA	C1B-C2B	2.58	1.49	1.43
27	n	606	CLA	C1B-C2B	2.58	1.49	1.43
37	s	201	KC2	CBD-CAD	-2.58	1.45	1.56
27	A	813	CLA	C1B-C2B	2.58	1.49	1.43
30	B	844	WVN	C33-C34	2.58	1.51	1.46
27	n	602	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	k	305	CLA	C4B-NB	2.58	1.41	1.37
30	F	204	WVN	C30-C28	2.57	1.51	1.43
27	F	201	CLA	C1B-C2B	2.57	1.49	1.43
27	B	839	CLA	O2D-CED	-2.57	1.39	1.45
27	h	304	CLA	C4B-NB	2.57	1.41	1.37
27	h	304	CLA	CMD-C2D	-2.57	1.45	1.50
27	m	605	CLA	CMC-C2C	-2.57	1.45	1.50
27	j	609	CLA	C1B-C2B	2.57	1.49	1.43
27	i	302	CLA	C1B-C2B	2.57	1.49	1.43
37	i	317	KC2	C3B-C4B	2.57	1.50	1.46
27	a	307	CLA	C4B-NB	2.57	1.41	1.37
27	B	829	CLA	CMD-C2D	-2.57	1.45	1.50
27	b	602	CLA	C4B-NB	2.57	1.41	1.37
27	O	202	CLA	C1B-C2B	2.57	1.49	1.43
35	l	314	II0	C18-C04	2.57	1.58	1.53
27	n	609	CLA	C4B-NB	2.57	1.41	1.37
30	i	315	WVN	C20-C13	2.56	1.53	1.45
27	k	304	CLA	C4B-NB	2.56	1.41	1.37
27	k	305	CLA	C1B-C2B	2.56	1.49	1.43
27	A	839	CLA	C1B-C2B	2.56	1.49	1.43
27	l	303	CLA	CMD-C2D	-2.56	1.45	1.50
27	g	308	CLA	C4B-NB	2.56	1.41	1.37
27	B	806	CLA	C3B-C4B	2.56	1.50	1.42
30	h	309	WVN	C20-C13	2.56	1.53	1.45
35	l	314	II0	C16-C03	2.56	1.58	1.53
36	b	614	IHT	C25-C23	2.56	1.56	1.50
36	R	204	IHT	C18-C07	2.56	1.53	1.45
27	B	829	CLA	C1B-C2B	2.55	1.49	1.43
27	A	824	CLA	CMD-C2D	-2.55	1.45	1.50
27	d	307	CLA	C1B-C2B	2.55	1.49	1.43
27	j	607	CLA	C1B-C2B	2.55	1.49	1.43
27	a	304	CLA	CMD-C2D	-2.55	1.45	1.50
30	M	101	WVN	C20-C13	2.55	1.53	1.45
37	d	310	KC2	C4A-C3A	2.55	1.49	1.44
35	g	317	II0	C33-C35	2.55	1.51	1.46
27	K	102	CLA	C1B-C2B	2.55	1.49	1.43
37	e	609	KC2	C3C-C4C	2.55	1.49	1.44
27	f	612	CLA	CMC-C2C	-2.55	1.45	1.50
27	e	606	CLA	C1B-C2B	2.55	1.49	1.43
37	l	311	KC2	C1A-CHA	2.55	1.46	1.40
27	c	601	CLA	CMD-C2D	-2.55	1.45	1.50
36	k	317	IHT	C18-C07	2.55	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	e	609	KC2	C4A-C3A	2.55	1.49	1.44
35	d	314	II0	C16-C03	2.55	1.58	1.53
27	s	209	CLA	C1B-C2B	2.55	1.49	1.43
27	h	305	CLA	C4B-NB	2.55	1.41	1.37
27	f	601	CLA	C3B-C4B	2.54	1.50	1.42
27	f	607	CLA	C3B-C4B	2.54	1.50	1.42
30	O	201	WVN	C19-C22	2.54	1.51	1.46
27	f	608	CLA	C1B-C2B	2.54	1.49	1.43
30	B	845	WVN	C29-C26	2.54	1.51	1.43
27	b	605	CLA	MG-NB	-2.54	2.00	2.05
27	B	804	CLA	C1B-C2B	2.54	1.49	1.43
27	B	822	CLA	C4B-NB	2.54	1.41	1.37
27	f	609	CLA	CMC-C2C	-2.54	1.45	1.50
27	B	849	CLA	C1B-C2B	2.54	1.49	1.43
27	f	609	CLA	C3B-C4B	2.54	1.50	1.42
27	B	813	CLA	C4B-NB	2.54	1.41	1.37
27	d	307	CLA	CMB-C2B	-2.53	1.45	1.50
27	k	308	CLA	CHC-C1C	2.53	1.43	1.38
27	B	825	CLA	CMB-C2B	-2.53	1.45	1.50
27	c	601	CLA	C3B-C4B	2.53	1.50	1.42
27	d	308	CLA	C1B-C2B	2.53	1.49	1.43
27	g	311	CLA	C1D-ND	2.53	1.41	1.37
27	B	837	CLA	CMD-C2D	-2.53	1.45	1.50
35	l	315	II0	C18-C04	2.53	1.58	1.53
37	e	609	KC2	C1A-CHA	2.53	1.46	1.40
37	k	312	KC2	C3C-C4C	2.53	1.49	1.44
27	s	208	CLA	C3B-C4B	2.53	1.50	1.42
30	O	201	WVN	C31-C32	2.53	1.51	1.46
27	l	306	CLA	C4B-NB	2.53	1.41	1.37
27	j	602	CLA	CMC-C2C	-2.53	1.45	1.50
27	m	602	CLA	CMB-C2B	-2.53	1.45	1.50
35	m	615	II0	C27-C25	2.53	1.52	1.50
27	d	306	CLA	C3B-C4B	2.53	1.50	1.42
27	B	802	CLA	C1D-ND	2.53	1.41	1.37
27	B	836	CLA	CMD-C2D	-2.53	1.45	1.50
27	B	802	CLA	C3B-C4B	2.53	1.50	1.42
27	B	823	CLA	CMD-C2D	-2.53	1.45	1.50
27	j	606	CLA	C1B-C2B	2.52	1.49	1.43
27	f	607	CLA	C1B-C2B	2.52	1.49	1.43
27	j	605	CLA	C4B-NB	2.52	1.41	1.37
27	g	309	CLA	C1B-C2B	2.52	1.49	1.43
27	O	202	CLA	CMD-C2D	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	602	CLA	C1D-ND	2.52	1.41	1.37
27	F	201	CLA	CMD-C2D	-2.52	1.45	1.50
31	a	302	LMT	O2'-C2'	-2.52	1.36	1.43
27	m	603	CLA	C4B-NB	2.52	1.41	1.37
27	i	307	CLA	CHC-C1C	2.52	1.43	1.38
27	F	203	CLA	O2A-CGA	2.52	1.40	1.33
27	m	612	CLA	CMD-C2D	-2.52	1.45	1.50
27	A	814	CLA	C1B-C2B	2.52	1.49	1.43
27	B	814	CLA	CMD-C2D	-2.52	1.45	1.50
27	l	305	CLA	C1D-ND	2.52	1.41	1.37
27	A	826	CLA	C3B-C4B	2.52	1.50	1.42
27	A	827	CLA	C3B-C4B	2.51	1.50	1.42
27	d	304	CLA	C1B-C2B	2.51	1.49	1.43
27	i	309	CLA	C1D-ND	2.51	1.41	1.37
27	A	855	CLA	CMD-C2D	-2.51	1.45	1.50
27	L	204	CLA	CMC-C2C	-2.51	1.45	1.50
27	B	812	CLA	C3B-C4B	2.51	1.50	1.42
30	F	204	WVN	C20-C13	2.51	1.53	1.45
27	f	604	CLA	C1B-C2B	2.51	1.49	1.43
27	n	605	CLA	C1B-C2B	2.51	1.49	1.43
27	A	815	CLA	C1B-NB	-2.51	1.34	1.37
37	d	309	KC2	C3C-C4C	2.51	1.49	1.44
27	i	305	CLA	C3B-C4B	2.51	1.50	1.42
27	a	307	CLA	CMD-C2D	-2.51	1.45	1.50
27	h	306	CLA	CHC-C1C	2.51	1.43	1.38
37	j	610	KC2	C1A-CHA	2.51	1.46	1.40
27	A	820	CLA	CMC-C2C	-2.51	1.45	1.50
27	i	304	CLA	C3B-C4B	2.51	1.50	1.42
27	B	810	CLA	C1B-C2B	2.51	1.49	1.43
27	j	604	CLA	C1D-ND	2.51	1.41	1.37
27	B	827	CLA	CHC-C1C	2.51	1.43	1.38
35	a	314	II0	C34-C36	2.50	1.51	1.46
27	i	311	CLA	CMD-C2D	-2.50	1.45	1.50
37	l	311	KC2	C3C-C4C	2.50	1.49	1.44
27	A	818	CLA	C4B-NB	2.50	1.41	1.37
27	a	309	CLA	CMC-C2C	-2.50	1.45	1.50
27	e	602	CLA	CMB-C2B	-2.50	1.45	1.50
27	A	853	CLA	C4B-NB	2.50	1.41	1.37
27	g	302	CLA	C4B-NB	2.50	1.41	1.37
27	a	310	CLA	CMC-C2C	-2.50	1.45	1.50
27	j	612	CLA	CMD-C2D	-2.50	1.45	1.50
37	f	611	KC2	C1A-CHA	2.50	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	816	CLA	C4B-NB	2.50	1.41	1.37
27	L	203	CLA	C1D-ND	2.50	1.41	1.37
27	A	816	CLA	C1B-C2B	2.50	1.49	1.43
27	a	304	CLA	C4B-NB	2.50	1.41	1.37
27	g	309	CLA	CMC-C2C	-2.50	1.45	1.50
27	i	306	CLA	C1B-C2B	2.50	1.49	1.43
27	a	310	CLA	CMD-C2D	-2.50	1.45	1.50
27	B	834	CLA	C3B-C4B	2.50	1.50	1.42
37	m	610	KC2	C3C-C4C	2.50	1.49	1.44
27	a	308	CLA	C1B-C2B	2.49	1.49	1.43
37	g	312	KC2	C3C-C4C	2.49	1.49	1.44
27	s	208	CLA	CMD-C2D	-2.49	1.45	1.50
27	i	303	CLA	C1B-C2B	2.49	1.49	1.43
35	h	311	II0	C33-C35	2.49	1.51	1.46
27	j	601	CLA	CMD-C2D	-2.49	1.45	1.50
27	a	303	CLA	C3B-C4B	2.49	1.50	1.42
27	j	608	CLA	C3B-C4B	2.49	1.50	1.42
37	d	309	KC2	C4A-C3A	2.49	1.49	1.44
27	e	606	CLA	CMC-C2C	-2.49	1.45	1.50
37	g	314	KC2	C3C-C4C	2.49	1.49	1.44
31	b	616	LMT	O3'-C3'	-2.49	1.36	1.43
27	g	310	CLA	CMC-C2C	-2.49	1.45	1.50
27	g	302	CLA	MG-NB	-2.48	2.00	2.05
27	B	840	CLA	C1B-C2B	2.48	1.49	1.43
27	B	816	CLA	CMD-C2D	-2.48	1.45	1.50
27	A	818	CLA	C1B-NB	-2.48	1.34	1.37
37	k	311	KC2	C3C-C4C	2.48	1.49	1.44
35	g	316	II0	C16-C03	2.48	1.58	1.53
30	F	204	WVN	C28-C25	-2.48	1.30	1.35
27	m	604	CLA	C3B-C4B	2.48	1.50	1.42
27	i	306	CLA	C3B-C4B	2.48	1.50	1.42
31	a	302	LMT	O3'-C3'	-2.48	1.36	1.43
27	e	604	CLA	C1B-C2B	2.48	1.48	1.43
27	A	827	CLA	C4B-NB	2.48	1.41	1.37
27	B	839	CLA	C1D-ND	2.48	1.41	1.37
27	c	611	CLA	C3B-C4B	2.48	1.49	1.42
27	B	833	CLA	MG-NB	-2.48	2.00	2.05
27	m	606	CLA	C1B-C2B	2.48	1.48	1.43
27	a	310	CLA	C1B-C2B	2.48	1.48	1.43
30	J	101	WVN	C23-C25	2.48	1.51	1.46
27	A	826	CLA	CMD-C2D	-2.47	1.45	1.50
27	n	603	CLA	C1B-C2B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	317	IHT	C39-C35	2.47	1.55	1.50
27	A	835	CLA	C1B-C2B	2.47	1.48	1.43
37	k	310	KC2	C3C-C4C	2.47	1.49	1.44
27	g	322	CLA	C1B-C2B	2.47	1.48	1.43
27	B	840	CLA	CMD-C2D	-2.47	1.45	1.50
27	c	608	CLA	CMA-C3A	-2.47	1.48	1.53
27	A	834	CLA	C4B-NB	2.47	1.41	1.37
27	B	820	CLA	CMD-C2D	-2.47	1.45	1.50
36	f	617	IHT	C20-C15	2.47	1.54	1.50
36	n	617	IHT	C39-C35	2.47	1.55	1.50
27	B	823	CLA	C4B-NB	2.47	1.41	1.37
27	B	831	CLA	CMC-C2C	-2.47	1.45	1.50
27	A	802	CLA	CMB-C2B	-2.47	1.45	1.50
27	c	602	CLA	CMB-C2B	-2.46	1.45	1.50
37	i	310	KC2	C3C-C4C	2.46	1.49	1.44
27	m	611	CLA	C3B-C4B	2.46	1.49	1.42
27	A	809	CLA	CMD-C2D	-2.46	1.45	1.50
27	k	305	CLA	C1D-ND	2.46	1.41	1.37
27	h	302	CLA	C1B-C2B	2.46	1.48	1.43
27	f	612	CLA	C3B-C4B	2.46	1.49	1.42
27	A	810	CLA	CMD-C2D	-2.46	1.45	1.50
27	B	828	CLA	CMD-C2D	-2.46	1.45	1.50
27	m	603	CLA	C1B-C2B	2.46	1.48	1.43
27	f	609	CLA	C1B-C2B	2.46	1.48	1.43
27	a	303	CLA	CMC-C2C	-2.46	1.45	1.50
27	m	606	CLA	C3B-C4B	2.46	1.49	1.42
27	B	808	CLA	C1B-C2B	2.45	1.48	1.43
27	A	836	CLA	CMD-C2D	-2.45	1.45	1.50
27	g	307	CLA	C1B-C2B	2.45	1.48	1.43
30	B	844	WVN	C26-C22	-2.45	1.30	1.35
27	k	306	CLA	C1B-C2B	2.45	1.48	1.43
30	B	843	WVN	C20-C13	2.45	1.53	1.45
27	b	610	CLA	C1B-C2B	2.45	1.48	1.43
27	k	307	CLA	CMC-C2C	-2.45	1.45	1.50
27	A	817	CLA	CMC-C2C	-2.45	1.45	1.50
27	B	835	CLA	C3B-C4B	2.45	1.49	1.42
27	e	601	CLA	C1B-C2B	2.45	1.48	1.43
36	g	319	IHT	C18-C07	2.45	1.53	1.45
27	k	306	CLA	C3B-C4B	2.45	1.49	1.42
37	k	310	KC2	C1A-CHA	2.45	1.46	1.40
35	i	314	II0	C18-C04	2.45	1.58	1.53
37	n	611	KC2	C3C-C4C	2.45	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	i	317	KC2	C1B-NB	-2.45	1.34	1.37
36	m	616	IHT	C39-C35	2.45	1.55	1.50
27	f	603	CLA	C1B-C2B	2.45	1.48	1.43
37	m	610	KC2	C4A-C3A	2.45	1.49	1.44
27	A	828	CLA	C1B-C2B	2.45	1.48	1.43
27	A	837	CLA	C1B-C2B	2.44	1.48	1.43
27	b	603	CLA	CMD-C2D	-2.44	1.45	1.50
27	A	806	CLA	CMB-C2B	-2.44	1.45	1.50
27	O	206	CLA	C1B-C2B	2.44	1.48	1.43
27	n	603	CLA	CMD-C2D	-2.44	1.45	1.50
37	f	611	KC2	C3C-C4C	2.44	1.49	1.44
27	g	302	CLA	C1B-C2B	2.44	1.48	1.43
35	j	613	II0	C33-C35	2.44	1.51	1.46
27	A	840	CLA	CMB-C2B	-2.44	1.45	1.50
37	d	309	KC2	C1A-CHA	2.44	1.46	1.40
27	A	824	CLA	C1B-C2B	2.44	1.48	1.43
36	b	614	IHT	C39-C35	2.44	1.55	1.50
27	f	603	CLA	CMD-C2D	-2.44	1.45	1.50
35	l	317	II0	C18-C04	2.44	1.58	1.53
27	A	838	CLA	C4B-NB	2.44	1.41	1.37
27	i	308	CLA	CHC-C1C	2.44	1.43	1.38
37	i	317	KC2	C1B-C2B	2.44	1.50	1.45
27	n	602	CLA	CMD-C2D	-2.44	1.45	1.50
27	a	311	CLA	C4B-NB	2.44	1.41	1.37
27	c	609	CLA	C3B-C4B	2.44	1.49	1.42
27	B	839	CLA	C1B-NB	-2.44	1.34	1.37
27	f	602	CLA	CMD-C2D	-2.44	1.45	1.50
37	n	611	KC2	C1A-CHA	2.44	1.46	1.40
27	A	815	CLA	MG-ND	-2.44	2.01	2.05
36	c	620	IHT	C39-C35	2.44	1.55	1.50
37	f	611	KC2	CBD-CAD	-2.44	1.45	1.56
27	B	807	CLA	CMD-C2D	-2.43	1.45	1.50
27	B	825	CLA	C1B-C2B	2.43	1.48	1.43
36	R	204	IHT	C25-C23	2.43	1.55	1.50
27	d	303	CLA	C1B-C2B	2.43	1.48	1.43
27	a	304	CLA	C3B-C4B	2.43	1.49	1.42
35	l	317	II0	C12-C14	-2.43	1.47	1.51
27	k	303	CLA	CMD-C2D	-2.43	1.45	1.50
30	R	202	WVN	C20-C13	2.43	1.53	1.45
27	B	827	CLA	C3B-C4B	2.43	1.49	1.42
27	s	202	CLA	CMD-C2D	-2.43	1.45	1.50
27	A	809	CLA	C1B-C2B	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	n	604	CLA	C1B-C2B	2.43	1.48	1.43
27	B	804	CLA	CMD-C2D	-2.43	1.45	1.50
27	B	808	CLA	CMB-C2B	-2.43	1.45	1.50
27	c	602	CLA	MG-NB	-2.43	2.01	2.05
27	e	610	CLA	C1B-C2B	2.43	1.48	1.43
27	A	805	CLA	CMD-C2D	-2.43	1.45	1.50
27	a	308	CLA	C3B-C4B	2.43	1.49	1.42
27	B	824	CLA	C4B-NB	2.43	1.41	1.37
35	d	314	II0	C18-C04	2.43	1.58	1.53
27	a	312	CLA	CMD-C2D	-2.43	1.45	1.50
36	c	616	IHT	C18-C07	2.43	1.53	1.45
27	K	102	CLA	C4B-NB	2.43	1.41	1.37
27	A	820	CLA	C1B-NB	-2.43	1.34	1.37
27	e	608	CLA	C1B-C2B	2.43	1.48	1.43
30	B	844	WVN	C29-C26	2.43	1.50	1.43
27	n	605	CLA	CHC-C4B	-2.43	1.34	1.39
27	b	604	CLA	C4B-NB	2.43	1.41	1.37
38	i	301	LMU	O5'-C5'	2.42	1.50	1.44
36	c	616	IHT	C39-C35	2.42	1.55	1.50
27	g	304	CLA	C3B-C4B	2.42	1.49	1.42
37	s	201	KC2	C1A-CHA	2.42	1.46	1.40
27	b	603	CLA	C1B-C2B	2.42	1.48	1.43
27	i	305	CLA	C1B-C2B	2.42	1.48	1.43
27	c	606	CLA	CMC-C2C	-2.42	1.45	1.50
27	A	806	CLA	C3B-C4B	2.42	1.49	1.42
27	A	806	CLA	C1B-C2B	2.42	1.48	1.43
27	A	807	CLA	CMB-C2B	-2.42	1.45	1.50
27	F	203	CLA	C1B-C2B	2.42	1.48	1.43
27	A	836	CLA	C1B-C2B	2.42	1.48	1.43
27	b	608	CLA	C3B-C4B	2.42	1.49	1.42
27	L	206	CLA	C1B-C2B	2.41	1.48	1.43
37	s	201	KC2	C3C-C4C	2.41	1.49	1.44
27	A	812	CLA	C4B-NB	2.41	1.41	1.37
27	m	605	CLA	C1B-C2B	2.41	1.48	1.43
30	R	201	WVN	C20-C13	2.41	1.53	1.45
35	g	317	II0	C16-C03	2.41	1.58	1.53
27	c	603	CLA	C1B-C2B	2.41	1.48	1.43
27	g	308	CLA	C1B-C2B	2.41	1.48	1.43
30	M	101	WVN	C33-C34	2.41	1.51	1.46
27	i	312	CLA	C1B-C2B	2.41	1.48	1.43
27	A	840	CLA	CMD-C2D	-2.41	1.45	1.50
27	B	806	CLA	CMB-C2B	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	607	CLA	CMB-C2B	-2.41	1.45	1.50
27	g	315	CLA	CMD-C2D	-2.41	1.45	1.50
27	A	830	CLA	C1D-ND	2.41	1.41	1.37
27	m	607	CLA	CMB-C2B	-2.41	1.45	1.50
27	e	607	CLA	C1B-C2B	2.41	1.48	1.43
27	A	802	CLA	C3B-C4B	2.41	1.49	1.42
27	m	607	CLA	C3B-C4B	2.41	1.49	1.42
27	n	606	CLA	C3B-C4B	2.41	1.49	1.42
27	c	602	CLA	CMC-C2C	-2.41	1.45	1.50
27	A	810	CLA	C3B-C4B	2.41	1.49	1.42
35	a	318	II0	C18-C04	2.40	1.58	1.53
27	b	606	CLA	CMD-C2D	-2.40	1.45	1.50
27	f	604	CLA	C3B-C4B	2.40	1.49	1.42
27	f	613	CLA	C1B-C2B	2.40	1.48	1.43
37	k	312	KC2	C4A-C3A	2.40	1.49	1.44
27	l	307	CLA	C3B-C4B	2.40	1.49	1.42
27	B	807	CLA	C1B-NB	-2.40	1.34	1.37
27	g	315	CLA	C3B-C4B	2.40	1.49	1.42
35	J	104	II0	C16-C03	2.40	1.58	1.53
35	m	615	II0	C16-C03	2.40	1.58	1.53
27	b	608	CLA	C1B-C2B	2.40	1.48	1.43
27	a	306	CLA	C1B-C2B	2.40	1.48	1.43
27	A	803	CLA	C1B-C2B	2.40	1.48	1.43
27	O	206	CLA	CMB-C2B	-2.40	1.45	1.50
30	I	101	WVN	C20-C13	2.40	1.53	1.45
27	B	840	CLA	C4B-NB	2.40	1.41	1.37
36	n	617	IHT	C20-C15	2.40	1.54	1.50
36	f	617	IHT	C39-C35	2.40	1.55	1.50
27	i	307	CLA	CMC-C2C	-2.40	1.45	1.50
36	O	204	IHT	C39-C35	2.39	1.55	1.50
27	A	804	CLA	C1B-C2B	2.39	1.48	1.43
27	B	821	CLA	C3B-C4B	2.39	1.49	1.42
27	n	601	CLA	C3B-C4B	2.39	1.49	1.42
27	b	604	CLA	CMD-C2D	-2.39	1.45	1.50
27	n	604	CLA	C1B-NB	-2.39	1.34	1.37
27	a	309	CLA	C3B-C4B	2.39	1.49	1.42
27	a	307	CLA	MG-NB	-2.39	2.01	2.05
27	a	311	CLA	C1B-C2B	2.39	1.48	1.43
36	c	620	IHT	C18-C07	2.39	1.53	1.45
27	l	306	CLA	CMD-C2D	-2.39	1.45	1.50
36	j	616	IHT	C20-C15	2.39	1.54	1.50
27	c	601	CLA	C1D-ND	2.39	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	612	CLA	MG-NA	2.39	2.11	2.06
27	h	306	CLA	CMD-C2D	-2.39	1.45	1.50
30	A	847	WVN	C23-C25	2.39	1.51	1.46
27	B	830	CLA	C1B-C2B	2.39	1.48	1.43
27	B	808	CLA	CMD-C2D	-2.39	1.45	1.50
27	c	607	CLA	C3B-C4B	2.39	1.49	1.42
27	d	303	CLA	C3B-C4B	2.39	1.49	1.42
27	A	816	CLA	CMD-C2D	-2.38	1.45	1.50
27	k	301	CLA	CMD-C2D	-2.38	1.45	1.50
27	c	611	CLA	C1B-C2B	2.38	1.48	1.43
27	d	304	CLA	CMC-C2C	-2.38	1.45	1.50
27	h	313	CLA	C3B-C4B	2.38	1.49	1.42
36	R	204	IHT	C39-C35	2.38	1.55	1.50
27	B	820	CLA	C1B-C2B	2.38	1.48	1.43
27	j	604	CLA	CMD-C2D	-2.38	1.45	1.50
30	L	201	WVN	C28-C25	-2.38	1.30	1.35
27	h	302	CLA	C4B-NB	2.38	1.41	1.37
27	g	308	CLA	CMB-C2B	-2.38	1.45	1.50
27	B	820	CLA	C3B-C4B	2.38	1.49	1.42
30	F	204	WVN	C23-C25	2.38	1.51	1.46
27	B	822	CLA	CMD-C2D	-2.38	1.45	1.50
27	l	305	CLA	C3B-C4B	2.38	1.49	1.42
27	a	303	CLA	CMB-C2B	-2.38	1.45	1.50
37	c	610	KC2	C3C-C4C	2.38	1.49	1.44
27	b	608	CLA	CMB-C2B	-2.38	1.45	1.50
27	a	312	CLA	C3B-C4B	2.38	1.49	1.42
27	B	821	CLA	C4B-NB	2.38	1.41	1.37
27	B	809	CLA	CMC-C2C	-2.38	1.45	1.50
27	c	606	CLA	CMD-C2D	-2.38	1.45	1.50
35	c	613	II0	C16-C03	2.38	1.58	1.53
27	c	606	CLA	C3B-C4B	2.38	1.49	1.42
36	a	317	IHT	C39-C35	2.38	1.55	1.50
27	R	203	CLA	CHC-C1C	2.38	1.43	1.38
27	L	202	CLA	CMD-C2D	-2.38	1.45	1.50
28	A	843	PQN	O4-C4	-2.38	1.18	1.23
30	B	848	WVN	C31-C32	2.37	1.51	1.46
35	e	613	II0	C16-C03	2.37	1.58	1.53
27	g	322	CLA	CMD-C2D	-2.37	1.45	1.50
30	F	204	WVN	C33-C34	2.37	1.51	1.46
37	n	612	KC2	C4A-C3A	2.37	1.49	1.44
27	b	601	CLA	CMD-C2D	-2.37	1.45	1.50
27	B	832	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	j	616	IHT	C18-C07	2.37	1.53	1.45
35	l	302	II0	C18-C04	2.37	1.58	1.53
37	m	610	KC2	C1A-CHA	2.37	1.46	1.40
27	j	601	CLA	C1B-C2B	2.37	1.48	1.43
27	a	313	CLA	CMC-C2C	-2.37	1.45	1.50
27	f	606	CLA	CMD-C2D	-2.37	1.45	1.50
27	n	606	CLA	CMD-C2D	-2.37	1.45	1.50
27	B	828	CLA	C3B-C4B	2.37	1.49	1.42
27	h	301	CLA	MG-NB	-2.37	2.01	2.05
27	b	609	CLA	CMC-C2C	-2.37	1.45	1.50
27	m	607	CLA	CMC-C2C	-2.37	1.45	1.50
27	k	304	CLA	C1B-C2B	2.37	1.48	1.43
36	b	614	IHT	C20-C15	2.37	1.54	1.50
37	j	610	KC2	C4A-C3A	2.37	1.49	1.44
27	e	606	CLA	O2D-CED	-2.37	1.40	1.45
27	A	824	CLA	C4B-NB	2.37	1.41	1.37
27	b	606	CLA	C1B-C2B	2.37	1.48	1.43
27	b	605	CLA	MG-ND	-2.37	2.01	2.05
37	n	611	KC2	CBD-CAD	-2.37	1.45	1.56
27	A	835	CLA	CMB-C2B	-2.37	1.45	1.50
27	i	309	CLA	MG-ND	-2.36	2.01	2.05
27	m	601	CLA	C3B-C4B	2.36	1.49	1.42
27	b	605	CLA	C4B-NB	2.36	1.41	1.37
37	i	317	KC2	C1A-CHA	2.36	1.46	1.40
27	c	604	CLA	CMB-C2B	-2.36	1.45	1.50
27	d	302	CLA	C4B-NB	2.36	1.41	1.37
27	B	833	CLA	C3B-C4B	2.36	1.49	1.42
27	l	304	CLA	C1B-C2B	2.36	1.48	1.43
30	L	201	WVN	C33-C34	2.36	1.51	1.46
35	f	614	II0	C16-C03	2.36	1.58	1.53
27	A	853	CLA	CMD-C2D	-2.36	1.45	1.50
27	A	822	CLA	C3B-C4B	2.36	1.49	1.42
37	c	610	KC2	C4A-C3A	2.36	1.49	1.44
31	A	851	LMT	O3B-C3B	-2.36	1.37	1.43
27	B	819	CLA	CMD-C2D	-2.36	1.45	1.50
27	O	206	CLA	CMD-C2D	-2.36	1.45	1.50
27	g	305	CLA	C1B-NB	-2.36	1.34	1.37
27	B	804	CLA	C4B-NB	2.36	1.41	1.37
37	n	611	KC2	C4A-C3A	2.36	1.49	1.44
35	l	302	II0	C16-C03	2.36	1.58	1.53
27	i	305	CLA	CMC-C2C	-2.35	1.45	1.50
34	b	619	LMG	O1-C1	2.35	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	605	CLA	CMC-C2C	-2.35	1.45	1.50
36	g	319	IHT	C39-C35	2.35	1.55	1.50
27	a	304	CLA	CHC-C1C	2.35	1.43	1.38
27	a	313	CLA	C1B-C2B	2.35	1.48	1.43
27	m	604	CLA	CMD-C2D	-2.35	1.45	1.50
30	s	205	WVN	C37-C34	-2.35	1.30	1.35
27	e	611	CLA	CHC-C1C	2.35	1.43	1.38
27	m	607	CLA	CMD-C2D	-2.35	1.46	1.50
37	l	311	KC2	CBD-CAD	-2.35	1.46	1.56
27	a	305	CLA	CMD-C2D	-2.35	1.46	1.50
27	A	835	CLA	C3B-C4B	2.35	1.49	1.42
27	b	606	CLA	C3B-C4B	2.35	1.49	1.42
27	B	811	CLA	CMD-C2D	-2.35	1.46	1.50
37	g	313	KC2	CBD-CAD	-2.35	1.46	1.56
27	g	306	CLA	CMC-C2C	-2.35	1.46	1.50
27	n	608	CLA	C1B-C2B	2.35	1.48	1.43
27	A	834	CLA	C1B-NB	-2.35	1.34	1.37
27	j	605	CLA	CMD-C2D	-2.35	1.46	1.50
27	B	817	CLA	C1B-C2B	2.35	1.48	1.43
27	A	809	CLA	C3B-C4B	2.35	1.49	1.42
27	A	826	CLA	C1B-NB	-2.35	1.34	1.37
27	a	305	CLA	C1B-C2B	2.35	1.48	1.43
27	h	305	CLA	CMD-C2D	-2.35	1.46	1.50
27	s	203	CLA	C4B-NB	2.34	1.40	1.37
36	k	317	IHT	C20-C15	2.34	1.54	1.50
27	s	206	CLA	C3B-C4B	2.34	1.49	1.42
37	c	610	KC2	CBD-CAD	-2.34	1.46	1.56
27	B	803	CLA	C4B-NB	2.34	1.40	1.37
37	k	310	KC2	C4A-C3A	2.34	1.49	1.44
27	A	807	CLA	CMD-C2D	-2.34	1.46	1.50
27	A	802	CLA	CMD-C2D	-2.34	1.46	1.50
27	m	608	CLA	C1B-C2B	2.34	1.48	1.43
37	g	312	KC2	CBD-CAD	-2.34	1.46	1.56
27	e	611	CLA	C3B-C4B	2.34	1.49	1.42
27	a	303	CLA	CHC-C1C	2.34	1.43	1.38
27	A	811	CLA	C1B-C2B	2.34	1.48	1.43
27	n	608	CLA	C3B-C4B	2.34	1.49	1.42
27	a	304	CLA	C1B-C2B	2.34	1.48	1.43
27	b	604	CLA	C1B-C2B	2.34	1.48	1.43
27	m	611	CLA	C1B-C2B	2.34	1.48	1.43
27	B	810	CLA	CMD-C2D	-2.34	1.46	1.50
27	A	836	CLA	CMB-C2B	-2.34	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	609	CLA	CMD-C2D	-2.34	1.46	1.50
27	c	611	CLA	CMD-C2D	-2.34	1.46	1.50
27	s	203	CLA	CMB-C2B	-2.34	1.46	1.50
27	j	608	CLA	C1B-C2B	2.34	1.48	1.43
27	i	308	CLA	MG-NB	-2.34	2.01	2.05
27	A	840	CLA	C1B-NB	-2.34	1.34	1.37
27	b	607	CLA	C1D-ND	2.34	1.40	1.37
36	R	204	IHT	C20-C15	2.33	1.54	1.50
37	l	311	KC2	C4A-C3A	2.33	1.49	1.44
27	A	803	CLA	CHC-C1C	2.33	1.43	1.38
27	A	815	CLA	CMD-C2D	-2.33	1.46	1.50
27	m	605	CLA	MG-NB	-2.33	2.01	2.05
35	a	318	II0	C16-C03	2.33	1.58	1.53
27	h	304	CLA	C1B-C2B	2.33	1.48	1.43
27	b	605	CLA	CMB-C2B	-2.33	1.46	1.50
27	c	605	CLA	CMB-C2B	-2.33	1.46	1.50
27	l	304	CLA	CMB-C2B	-2.33	1.46	1.50
36	j	616	IHT	C39-C35	2.33	1.55	1.50
30	A	848	WVN	C20-C13	2.33	1.53	1.45
27	L	203	CLA	CMB-C2B	-2.33	1.46	1.50
27	c	604	CLA	CMD-C2D	-2.33	1.46	1.50
35	i	313	II0	C15-C03	2.33	1.58	1.53
27	A	803	CLA	C3B-C4B	2.33	1.49	1.42
27	B	828	CLA	C1B-C2B	2.33	1.48	1.43
27	l	309	CLA	C1B-C2B	2.33	1.48	1.43
27	B	832	CLA	CHC-C1C	2.33	1.43	1.38
30	B	845	WVN	C02-C11	2.33	1.53	1.50
30	e	615	WVN	C02-C11	2.33	1.53	1.50
27	b	602	CLA	C1B-C2B	2.33	1.48	1.43
27	A	823	CLA	CMB-C2B	-2.32	1.46	1.50
27	g	308	CLA	CHC-C4B	-2.32	1.34	1.39
27	a	308	CLA	CMB-C2B	-2.32	1.46	1.50
27	B	819	CLA	C3B-C4B	2.32	1.49	1.42
37	k	312	KC2	CBD-CAD	-2.32	1.46	1.56
27	d	306	CLA	CMD-C2D	-2.32	1.46	1.50
27	A	839	CLA	C3B-C4B	2.32	1.49	1.42
27	B	807	CLA	MG-NB	-2.32	2.01	2.05
27	F	202	CLA	CMD-C2D	-2.32	1.46	1.50
30	A	846	WVN	C02-C11	2.32	1.53	1.50
27	A	818	CLA	C3C-C2C	2.32	1.41	1.36
27	B	826	CLA	CMB-C2B	-2.32	1.46	1.50
30	F	205	WVN	C36-C32	-2.32	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	m	612	CLA	C3C-C2C	2.32	1.41	1.36
27	a	311	CLA	CMC-C2C	-2.32	1.46	1.50
27	B	822	CLA	CMB-C2B	-2.32	1.46	1.50
27	A	809	CLA	CHC-C1C	2.32	1.43	1.38
27	l	304	CLA	CHC-C1C	2.32	1.43	1.38
37	j	610	KC2	C3C-C4C	2.32	1.49	1.44
30	s	205	WVN	C20-C13	2.32	1.53	1.45
27	c	603	CLA	CHC-C1C	2.32	1.43	1.38
35	c	614	II0	C28-C26	2.32	1.52	1.50
27	f	610	CLA	CMD-C2D	-2.32	1.46	1.50
27	A	824	CLA	C1B-NB	-2.32	1.34	1.37
27	B	820	CLA	CMC-C2C	-2.32	1.46	1.50
37	j	610	KC2	CBD-CAD	-2.32	1.46	1.56
37	n	612	KC2	C1D-C2D	2.32	1.48	1.43
30	R	202	WVN	C19-C22	2.32	1.50	1.46
30	B	844	WVN	C31-C32	2.32	1.50	1.46
27	A	820	CLA	MG-NB	-2.32	2.01	2.05
27	h	308	CLA	CMC-C2C	-2.32	1.46	1.50
27	A	822	CLA	C1B-C2B	2.32	1.48	1.43
27	s	208	CLA	CMB-C2B	-2.31	1.46	1.50
27	m	602	CLA	C4B-NB	2.31	1.40	1.37
37	g	312	KC2	C4A-C3A	2.31	1.49	1.44
27	d	311	CLA	C3B-C4B	2.31	1.49	1.42
27	A	829	CLA	C1B-NB	-2.31	1.34	1.37
27	b	611	CLA	C3B-C4B	2.31	1.49	1.42
27	h	313	CLA	C1B-C2B	2.31	1.48	1.43
27	d	302	CLA	C1B-C2B	2.31	1.48	1.43
27	j	602	CLA	MG-NB	-2.31	2.01	2.05
27	B	818	CLA	CMB-C2B	-2.31	1.46	1.50
27	A	832	CLA	C4B-NB	2.31	1.40	1.37
27	B	818	CLA	C3B-C4B	2.31	1.49	1.42
36	a	317	IHT	C20-C15	2.31	1.54	1.50
35	j	613	II0	C16-C03	2.31	1.58	1.53
37	f	611	KC2	C4A-C3A	2.31	1.49	1.44
28	B	841	PQN	O4-C4	-2.31	1.18	1.23
27	A	819	CLA	CMD-C2D	-2.31	1.46	1.50
27	i	311	CLA	CHC-C1C	2.31	1.43	1.38
27	f	609	CLA	CHC-C1C	2.31	1.43	1.38
37	g	314	KC2	C4A-C3A	2.31	1.49	1.44
27	K	101	CLA	C3B-C4B	2.31	1.49	1.42
27	B	840	CLA	CHC-C1C	2.31	1.43	1.38
27	B	805	CLA	CMD-C2D	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	601	CLA	CMB-C2B	-2.31	1.46	1.50
27	s	209	CLA	CMB-C2B	-2.31	1.46	1.50
27	A	826	CLA	C4B-NB	2.31	1.40	1.37
27	F	203	CLA	C3B-C4B	2.31	1.49	1.42
27	B	836	CLA	C3B-C4B	2.30	1.49	1.42
27	A	808	CLA	CMD-C2D	-2.30	1.46	1.50
27	n	604	CLA	CMC-C2C	-2.30	1.46	1.50
27	A	856	CLA	CMC-C2C	-2.30	1.46	1.50
27	B	826	CLA	CMD-C2D	-2.30	1.46	1.50
27	A	834	CLA	C3B-C4B	2.30	1.49	1.42
27	B	818	CLA	CMC-C2C	-2.30	1.46	1.50
27	h	307	CLA	C3B-C4B	2.30	1.49	1.42
27	i	303	CLA	CMC-C2C	-2.30	1.46	1.50
27	d	301	CLA	CMD-C2D	-2.30	1.46	1.50
27	A	853	CLA	C1B-C2B	2.30	1.48	1.43
27	n	605	CLA	C4B-NB	2.30	1.40	1.37
27	B	835	CLA	CMD-C2D	-2.30	1.46	1.50
27	e	603	CLA	C3B-C4B	2.30	1.49	1.42
27	B	831	CLA	C4B-NB	2.30	1.40	1.37
35	m	613	II0	C16-C03	2.30	1.58	1.53
27	j	607	CLA	C3B-C4B	2.30	1.49	1.42
27	B	803	CLA	CMC-C2C	-2.30	1.46	1.50
31	A	851	LMT	O3'-C3'	-2.30	1.37	1.43
27	d	308	CLA	C3B-C4B	2.30	1.49	1.42
27	A	823	CLA	C3B-C4B	2.30	1.49	1.42
37	k	311	KC2	CBD-CAD	-2.30	1.46	1.56
27	g	311	CLA	C3B-C4B	2.30	1.49	1.42
27	A	817	CLA	CMD-C2D	-2.30	1.46	1.50
35	j	614	II0	C16-C03	2.30	1.58	1.53
27	B	805	CLA	C4B-NB	2.30	1.40	1.37
35	i	313	II0	C16-C03	2.30	1.58	1.53
27	k	303	CLA	C3B-C4B	2.30	1.49	1.42
35	i	314	II0	C27-C25	2.29	1.52	1.50
27	s	202	CLA	C3B-C4B	2.29	1.49	1.42
27	m	612	CLA	C3B-C4B	2.29	1.49	1.42
27	d	306	CLA	CMC-C2C	-2.29	1.46	1.50
27	m	608	CLA	C3B-C4B	2.29	1.49	1.42
27	j	609	CLA	CMB-C2B	-2.29	1.46	1.50
27	l	312	CLA	C3B-C4B	2.29	1.49	1.42
27	a	312	CLA	CHC-C1C	2.29	1.43	1.38
27	B	839	CLA	C3B-C4B	2.29	1.49	1.42
27	m	609	CLA	CMD-C2D	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	s	207	WVN	C02-C11	2.29	1.53	1.50
27	A	840	CLA	CMC-C2C	-2.29	1.46	1.50
27	A	812	CLA	CMD-C2D	-2.29	1.46	1.50
27	A	819	CLA	C3B-C4B	2.29	1.49	1.42
27	B	811	CLA	CMC-C2C	-2.29	1.46	1.50
27	l	312	CLA	CMB-C2B	-2.29	1.46	1.50
35	d	313	II0	C18-C04	2.29	1.58	1.53
27	e	611	CLA	CMD-C2D	-2.29	1.46	1.50
27	A	814	CLA	C3B-C4B	2.29	1.49	1.42
27	B	817	CLA	C3B-C4B	2.29	1.49	1.42
37	d	309	KC2	CBD-CAD	-2.28	1.46	1.56
27	A	802	CLA	CMC-C2C	-2.28	1.46	1.50
27	A	806	CLA	CMD-C2D	-2.28	1.46	1.50
27	s	203	CLA	CMC-C2C	-2.28	1.46	1.50
30	B	843	WVN	C02-C11	2.28	1.53	1.50
27	c	603	CLA	C3B-C4B	2.28	1.49	1.42
27	k	302	CLA	CHC-C1C	2.28	1.43	1.38
27	A	824	CLA	CMB-C2B	-2.28	1.46	1.50
27	a	307	CLA	CMB-C2B	-2.28	1.46	1.50
37	d	310	KC2	CBD-CAD	-2.28	1.46	1.56
35	i	318	II0	C16-C03	2.28	1.58	1.53
27	f	610	CLA	C1B-C2B	2.28	1.48	1.43
35	k	314	II0	C16-C03	2.28	1.58	1.53
35	a	315	II0	C18-C04	2.28	1.58	1.53
27	A	805	CLA	MG-NB	-2.28	2.01	2.05
27	a	307	CLA	C1B-C2B	2.28	1.48	1.43
27	j	603	CLA	C1B-C2B	2.28	1.48	1.43
27	e	608	CLA	C3B-C4B	2.28	1.49	1.42
27	B	836	CLA	C4B-NB	2.28	1.40	1.37
27	f	606	CLA	CMB-C2B	-2.28	1.46	1.50
27	l	307	CLA	C1B-C2B	2.28	1.48	1.43
27	A	834	CLA	CHC-C1C	2.28	1.43	1.38
27	F	202	CLA	C1B-C2B	2.28	1.48	1.43
27	l	305	CLA	C1B-C2B	2.28	1.48	1.43
35	k	316	II0	C18-C04	2.28	1.58	1.53
27	h	301	CLA	CMD-C2D	-2.28	1.46	1.50
27	g	303	CLA	CMD-C2D	-2.28	1.46	1.50
27	g	310	CLA	CHC-C1C	2.28	1.43	1.38
27	A	819	CLA	CMB-C2B	-2.28	1.46	1.50
35	f	616	II0	C18-C04	2.28	1.58	1.53
35	i	313	II0	C18-C04	2.28	1.58	1.53
27	B	831	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	h	303	CLA	CMD-C2D	-2.27	1.46	1.50
27	b	610	CLA	C3B-C4B	2.27	1.49	1.42
27	A	830	CLA	MG-ND	-2.27	2.01	2.05
27	n	613	CLA	CMD-C2D	-2.27	1.46	1.50
27	c	612	CLA	C3B-C4B	2.27	1.49	1.42
27	B	817	CLA	CMD-C2D	-2.27	1.46	1.50
29	b	617	LHG	O8-C6	-2.27	1.40	1.45
27	A	821	CLA	C1B-C2B	2.27	1.48	1.43
27	s	206	CLA	CHC-C1C	2.27	1.43	1.38
27	n	613	CLA	C3B-C4B	2.27	1.49	1.42
27	A	841	CLA	CMD-C2D	-2.27	1.46	1.50
27	b	611	CLA	CMD-C2D	-2.27	1.46	1.50
27	b	609	CLA	MG-NB	-2.27	2.01	2.05
27	c	612	CLA	C1B-C2B	2.27	1.48	1.43
35	d	314	II0	C28-C26	2.27	1.52	1.50
35	k	315	II0	C18-C04	2.27	1.58	1.53
27	A	842	CLA	CMD-C2D	-2.27	1.46	1.50
30	L	201	WVN	C20-C13	2.27	1.52	1.45
37	i	310	KC2	CBD-CAD	-2.27	1.46	1.56
30	K	103	WVN	C02-C11	2.27	1.53	1.50
27	c	602	CLA	CHC-C1C	2.27	1.43	1.38
27	f	608	CLA	C3B-C4B	2.27	1.49	1.42
27	l	305	CLA	CMD-C2D	-2.27	1.46	1.50
27	j	603	CLA	CMD-C2D	-2.27	1.46	1.50
27	h	302	CLA	CMD-C2D	-2.27	1.46	1.50
27	f	606	CLA	C3B-C4B	2.27	1.49	1.42
27	A	816	CLA	CMC-C2C	-2.26	1.46	1.50
27	A	833	CLA	C4B-NB	2.26	1.40	1.37
27	B	826	CLA	C3B-C4B	2.26	1.49	1.42
27	A	814	CLA	CMC-C2C	-2.26	1.46	1.50
27	k	307	CLA	CMD-C2D	-2.26	1.46	1.50
35	m	614	II0	C16-C03	2.26	1.58	1.53
30	B	844	WVN	C36-C32	-2.26	1.30	1.35
27	b	609	CLA	C3B-C4B	2.26	1.49	1.42
27	B	807	CLA	CMC-C2C	-2.26	1.46	1.50
27	B	819	CLA	CMB-C2B	-2.26	1.46	1.50
27	A	812	CLA	C3B-C4B	2.26	1.49	1.42
27	h	301	CLA	C1B-NB	-2.26	1.34	1.37
37	d	310	KC2	C4B-NB	-2.26	1.34	1.37
27	A	855	CLA	CMC-C2C	-2.26	1.46	1.50
27	j	608	CLA	CMC-C2C	-2.26	1.46	1.50
27	m	603	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	k	304	CLA	CHC-C4B	-2.26	1.34	1.39
27	c	608	CLA	C3B-C4B	2.26	1.49	1.42
37	g	314	KC2	CBD-CAD	-2.26	1.46	1.56
35	n	615	II0	C18-C04	2.26	1.58	1.53
27	B	816	CLA	C1B-C2B	2.26	1.48	1.43
27	n	613	CLA	CHC-C1C	2.26	1.43	1.38
27	k	302	CLA	C1B-C2B	2.26	1.48	1.43
27	A	802	CLA	CHC-C1C	2.26	1.43	1.38
27	A	827	CLA	CMD-C2D	-2.26	1.46	1.50
27	m	602	CLA	CMC-C2C	-2.26	1.46	1.50
27	A	841	CLA	CHC-C1C	2.26	1.43	1.38
27	s	202	CLA	CAA-C2A	-2.26	1.50	1.54
35	n	615	II0	C15-C03	2.26	1.58	1.53
30	h	309	WVN	C19-C22	2.26	1.50	1.46
37	e	609	KC2	CBD-CAD	-2.26	1.46	1.56
27	A	811	CLA	CMD-C2D	-2.26	1.46	1.50
27	f	602	CLA	CMC-C2C	-2.26	1.46	1.50
27	d	306	CLA	C1B-C2B	2.26	1.48	1.43
37	m	610	KC2	C1D-C2D	2.26	1.48	1.43
27	b	601	CLA	C3B-C4B	2.26	1.49	1.42
27	A	856	CLA	CAA-C2A	-2.26	1.48	1.53
27	A	827	CLA	CMB-C2B	-2.25	1.46	1.50
27	m	611	CLA	CMC-C2C	-2.25	1.46	1.50
27	A	852	CLA	C3B-C4B	2.25	1.49	1.42
27	A	841	CLA	C3B-C4B	2.25	1.49	1.42
27	B	830	CLA	MG-NB	-2.25	2.01	2.05
27	k	302	CLA	CMD-C2D	-2.25	1.46	1.50
27	s	202	CLA	MG-NB	-2.25	2.01	2.05
36	g	319	IHT	C20-C15	2.25	1.54	1.50
27	A	805	CLA	C1B-NB	-2.25	1.34	1.37
27	B	815	CLA	CMD-C2D	-2.25	1.46	1.50
27	B	831	CLA	CMD-C2D	-2.25	1.46	1.50
27	e	607	CLA	CMD-C2D	-2.25	1.46	1.50
27	A	802	CLA	C1D-ND	2.25	1.40	1.37
27	b	603	CLA	C3B-C4B	2.25	1.49	1.42
27	k	313	CLA	C1B-C2B	2.25	1.48	1.43
27	A	805	CLA	CMB-C2B	-2.25	1.46	1.50
27	B	832	CLA	CMD-C2D	-2.25	1.46	1.50
27	k	303	CLA	C1B-C2B	2.25	1.48	1.43
27	a	313	CLA	C3B-C4B	2.25	1.49	1.42
27	A	817	CLA	MG-NB	-2.25	2.01	2.05
27	A	822	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	831	CLA	CMD-C2D	-2.25	1.46	1.50
27	k	308	CLA	CMD-C2D	-2.25	1.46	1.50
27	i	312	CLA	C3B-C4B	2.25	1.49	1.42
27	i	304	CLA	CHC-C1C	2.25	1.43	1.38
27	d	307	CLA	CMC-C2C	-2.25	1.46	1.50
27	j	609	CLA	MG-NB	-2.25	2.01	2.05
27	g	305	CLA	CHC-C4B	-2.25	1.34	1.39
27	j	611	CLA	C3B-C4B	2.25	1.49	1.42
27	B	831	CLA	MG-NB	-2.25	2.01	2.05
37	i	317	KC2	CBD-CAD	-2.25	1.46	1.56
27	b	609	CLA	CHC-C1C	2.25	1.43	1.38
27	F	201	CLA	CMB-C2B	-2.25	1.46	1.50
27	a	310	CLA	C4B-NB	2.25	1.40	1.37
27	A	838	CLA	CMB-C2B	-2.24	1.46	1.50
37	n	612	KC2	CBD-CAD	-2.24	1.46	1.56
27	L	202	CLA	CMB-C2B	-2.24	1.46	1.50
27	B	825	CLA	C1D-ND	2.24	1.40	1.37
27	f	612	CLA	MG-NC	2.24	2.11	2.06
27	n	610	CLA	MG-ND	-2.24	2.01	2.05
27	j	602	CLA	C1B-C2B	2.24	1.48	1.43
27	g	309	CLA	CHC-C1C	2.24	1.43	1.38
27	b	602	CLA	CMC-C2C	-2.24	1.46	1.50
27	A	830	CLA	MG-NB	-2.24	2.01	2.05
27	A	818	CLA	CMD-C2D	-2.24	1.46	1.50
27	F	202	CLA	CMB-C2B	-2.24	1.46	1.50
35	e	612	II0	C16-C03	2.24	1.58	1.53
27	m	603	CLA	CMD-C2D	-2.24	1.46	1.50
27	B	823	CLA	CHC-C1C	2.24	1.43	1.38
27	A	834	CLA	CMC-C2C	-2.24	1.46	1.50
27	B	804	CLA	CMB-C2B	-2.24	1.46	1.50
27	J	105	CLA	CHC-C1C	2.24	1.43	1.38
27	n	607	CLA	C1B-C2B	2.24	1.48	1.43
30	B	848	WVN	C20-C13	2.24	1.52	1.45
27	K	102	CLA	CMB-C2B	-2.24	1.46	1.50
27	f	612	CLA	C1B-C2B	2.24	1.48	1.43
35	m	613	II0	C18-C04	2.24	1.58	1.53
35	e	612	II0	C15-C03	2.24	1.58	1.53
27	A	832	CLA	CMB-C2B	-2.24	1.46	1.50
30	L	201	WVN	C40-C39	-2.23	1.30	1.36
27	J	103	CLA	CMC-C2C	-2.23	1.46	1.50
27	l	308	CLA	CMD-C2D	-2.23	1.46	1.50
27	n	607	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	203	CLA	CMD-C2D	-2.23	1.46	1.50
27	l	310	CLA	C3B-C4B	2.23	1.49	1.42
27	d	302	CLA	C3B-C4B	2.23	1.49	1.42
27	A	810	CLA	CMB-C2B	-2.23	1.46	1.50
27	h	301	CLA	CMC-C2C	-2.23	1.46	1.50
27	k	313	CLA	C3B-C4B	2.23	1.49	1.42
35	n	616	II0	C16-C03	2.23	1.58	1.53
27	h	308	CLA	C3B-C4B	2.23	1.49	1.42
27	c	611	CLA	CMB-C2B	-2.23	1.46	1.50
27	A	822	CLA	CMC-C2C	-2.23	1.46	1.50
27	A	841	CLA	CMB-C2B	-2.23	1.46	1.50
27	g	311	CLA	MG-ND	-2.23	2.01	2.05
35	J	104	II0	C18-C04	2.23	1.58	1.53
27	g	302	CLA	C3B-C4B	2.23	1.49	1.42
27	b	609	CLA	C1B-C2B	2.23	1.48	1.43
27	A	838	CLA	C1B-NB	-2.23	1.34	1.37
35	a	316	II0	C20-C14	2.23	1.54	1.50
27	B	813	CLA	C3B-C4B	2.23	1.49	1.42
37	d	310	KC2	C1A-CHA	2.23	1.46	1.40
27	B	817	CLA	CMC-C2C	-2.23	1.46	1.50
37	i	310	KC2	C4A-C3A	2.23	1.49	1.44
27	d	301	CLA	CHC-C1C	2.23	1.42	1.38
27	n	606	CLA	CAA-C2A	-2.23	1.50	1.54
37	m	610	KC2	CBD-CAD	-2.23	1.46	1.56
27	f	604	CLA	CMD-C2D	-2.23	1.46	1.50
35	O	203	II0	C16-C03	2.22	1.58	1.53
37	k	310	KC2	CBD-CAD	-2.22	1.46	1.56
27	a	306	CLA	C3B-C4B	2.22	1.49	1.42
27	c	603	CLA	CMC-C2C	-2.22	1.46	1.50
27	k	305	CLA	CMB-C2B	-2.22	1.46	1.50
27	A	853	CLA	CMB-C2B	-2.22	1.46	1.50
35	e	616	II0	C18-C04	2.22	1.58	1.53
27	B	804	CLA	CMC-C2C	-2.22	1.46	1.50
27	s	206	CLA	CMD-C2D	-2.22	1.46	1.50
35	b	612	II0	C16-C03	2.22	1.58	1.53
27	b	607	CLA	C1B-C2B	2.22	1.48	1.43
27	g	305	CLA	CMD-C2D	-2.22	1.46	1.50
27	e	602	CLA	CMD-C2D	-2.22	1.46	1.50
27	A	827	CLA	CMC-C2C	-2.22	1.46	1.50
27	m	605	CLA	CMB-C2B	-2.22	1.46	1.50
27	j	603	CLA	C3B-C4B	2.22	1.49	1.42
27	B	835	CLA	C1B-C2B	2.22	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	839	CLA	CHC-C1C	2.22	1.42	1.38
31	A	851	LMT	O4'-C4B	-2.22	1.37	1.43
27	A	807	CLA	CMC-C2C	-2.22	1.46	1.50
27	B	809	CLA	CMD-C2D	-2.22	1.46	1.50
27	h	307	CLA	CMB-C2B	-2.22	1.46	1.50
27	l	306	CLA	CMC-C2C	-2.22	1.46	1.50
35	i	318	II0	C20-C14	2.22	1.54	1.50
27	a	309	CLA	CHC-C1C	2.22	1.42	1.38
27	B	822	CLA	C3B-C4B	2.22	1.49	1.42
27	A	808	CLA	C1B-C2B	2.22	1.48	1.43
35	f	615	II0	C15-C03	2.22	1.57	1.53
27	c	608	CLA	CMD-C2D	-2.22	1.46	1.50
27	A	855	CLA	C1B-NB	-2.22	1.34	1.37
27	A	821	CLA	CMD-C2D	-2.22	1.46	1.50
27	A	856	CLA	CMB-C2B	-2.22	1.46	1.50
27	A	810	CLA	C1B-C2B	2.22	1.48	1.43
27	m	612	CLA	C1B-C2B	2.22	1.48	1.43
35	k	315	II0	C30-C26	-2.22	1.32	1.37
27	m	602	CLA	C3B-C4B	2.22	1.49	1.42
30	F	205	WVN	C20-C13	2.21	1.52	1.45
27	j	602	CLA	C4B-NB	2.21	1.40	1.37
27	A	806	CLA	CMC-C2C	-2.21	1.46	1.50
27	e	611	CLA	MG-NB	-2.21	2.01	2.05
27	B	803	CLA	CHC-C1C	2.21	1.42	1.38
27	f	603	CLA	C3B-C4B	2.21	1.49	1.42
35	h	312	II0	C16-C03	2.21	1.57	1.53
27	L	202	CLA	C1B-C2B	2.21	1.48	1.43
36	f	617	IHT	C13-C02	2.21	1.57	1.53
27	a	305	CLA	CMB-C2B	-2.21	1.46	1.50
37	k	312	KC2	C1D-C2D	2.21	1.48	1.43
27	B	810	CLA	C4B-NB	2.21	1.40	1.37
27	k	306	CLA	MG-NA	2.21	2.11	2.06
27	c	602	CLA	MG-ND	-2.21	2.01	2.05
27	b	604	CLA	CMC-C2C	-2.21	1.46	1.50
27	j	603	CLA	CMC-C2C	-2.21	1.46	1.50
27	A	818	CLA	C3B-C4B	2.21	1.49	1.42
27	k	305	CLA	CMC-C2C	-2.21	1.46	1.50
27	A	804	CLA	C3B-C4B	2.21	1.49	1.42
27	B	802	CLA	CHC-C1C	2.21	1.42	1.38
27	m	602	CLA	CMD-C2D	-2.21	1.46	1.50
27	n	607	CLA	C1B-NB	-2.21	1.35	1.37
37	s	201	KC2	CHB-C4A	2.21	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	823	CLA	MG-NB	-2.21	2.01	2.05
28	A	843	PQN	O1-C1	-2.21	1.18	1.23
27	A	855	CLA	C3B-C4B	2.21	1.49	1.42
27	A	808	CLA	CMC-C2C	-2.21	1.46	1.50
27	A	842	CLA	CMC-C2C	-2.21	1.46	1.50
27	f	605	CLA	CMD-C2D	-2.21	1.46	1.50
27	h	308	CLA	CMD-C2D	-2.21	1.46	1.50
35	b	613	II0	C15-C03	2.21	1.57	1.53
27	A	811	CLA	CMC-C2C	-2.21	1.46	1.50
27	A	842	CLA	C3B-C4B	2.20	1.49	1.42
27	k	301	CLA	C3B-C4B	2.20	1.49	1.42
27	f	602	CLA	CMB-C2B	-2.20	1.46	1.50
27	f	604	CLA	CMC-C2C	-2.20	1.46	1.50
27	b	607	CLA	C3B-C4B	2.20	1.49	1.42
27	h	308	CLA	CMB-C2B	-2.20	1.46	1.50
27	i	311	CLA	CMC-C2C	-2.20	1.46	1.50
27	L	204	CLA	MG-ND	-2.20	2.01	2.05
27	A	837	CLA	CMD-C2D	-2.20	1.46	1.50
27	B	849	CLA	CMD-C2D	-2.20	1.46	1.50
27	A	831	CLA	CMB-C2B	-2.20	1.46	1.50
27	l	303	CLA	CMB-C2B	-2.20	1.46	1.50
27	c	606	CLA	C1B-NB	-2.20	1.35	1.37
27	A	833	CLA	C1B-C2B	2.20	1.48	1.43
27	n	602	CLA	C3B-C4B	2.20	1.49	1.42
27	B	823	CLA	CMB-C2B	-2.20	1.46	1.50
27	e	601	CLA	CMB-C2B	-2.20	1.46	1.50
27	B	821	CLA	MG-ND	-2.20	2.01	2.05
27	B	816	CLA	MG-NB	-2.20	2.01	2.05
35	k	315	II0	C15-C03	2.20	1.57	1.53
27	A	821	CLA	CMC-C2C	-2.20	1.46	1.50
27	d	308	CLA	CMD-C2D	-2.20	1.46	1.50
27	B	821	CLA	MG-NB	-2.20	2.01	2.05
35	b	615	II0	C30-C26	-2.20	1.32	1.37
27	F	203	CLA	CMD-C2D	-2.20	1.46	1.50
27	k	304	CLA	CMD-C2D	-2.20	1.46	1.50
27	A	814	CLA	CMB-C2B	-2.20	1.46	1.50
35	l	314	II0	C15-C03	2.20	1.57	1.53
27	j	605	CLA	CMB-C2B	-2.19	1.46	1.50
27	e	610	CLA	MG-NB	-2.19	2.01	2.05
27	B	823	CLA	C3B-C4B	2.19	1.49	1.42
27	B	833	CLA	C1B-C2B	2.19	1.48	1.43
27	B	814	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	n	602	CLA	CHC-C1C	2.19	1.42	1.38
37	i	317	KC2	C1D-C2D	2.19	1.48	1.43
35	j	614	II0	C20-C14	2.19	1.54	1.50
27	g	304	CLA	CHC-C1C	2.19	1.42	1.38
27	m	608	CLA	CMC-C2C	-2.19	1.46	1.50
27	A	821	CLA	C3B-C4B	2.19	1.49	1.42
27	n	609	CLA	CMC-C2C	-2.19	1.46	1.50
28	B	841	PQN	O1-C1	-2.19	1.18	1.23
27	m	602	CLA	MG-NB	-2.19	2.01	2.05
35	g	317	II0	C15-C03	2.19	1.57	1.53
30	A	848	WVN	C37-C34	-2.19	1.30	1.35
37	n	612	KC2	C1A-CHA	2.19	1.45	1.40
27	A	835	CLA	CMD-C2D	-2.19	1.46	1.50
27	B	821	CLA	CHC-C1C	2.19	1.42	1.38
27	g	304	CLA	MG-NB	-2.19	2.01	2.05
27	n	606	CLA	CMC-C2C	-2.19	1.46	1.50
27	B	824	CLA	C1B-NB	-2.19	1.35	1.37
27	g	309	CLA	C3B-C4B	2.19	1.49	1.42
37	d	309	KC2	C1D-C2D	2.19	1.48	1.43
27	m	605	CLA	CMD-C2D	-2.19	1.46	1.50
27	J	103	CLA	C3B-C4B	2.19	1.49	1.42
36	m	616	IHT	C20-C15	2.19	1.54	1.50
27	L	206	CLA	C3B-C4B	2.19	1.49	1.42
27	b	606	CLA	CMB-C2B	-2.19	1.46	1.50
27	k	303	CLA	CHC-C4B	-2.19	1.34	1.39
27	j	611	CLA	CMC-C2C	-2.19	1.46	1.50
27	e	604	CLA	CMD-C2D	-2.19	1.46	1.50
27	B	826	CLA	CMC-C2C	-2.19	1.46	1.50
27	n	605	CLA	CMC-C2C	-2.19	1.46	1.50
27	n	608	CLA	CMC-C2C	-2.19	1.46	1.50
27	A	836	CLA	C3B-C4B	2.18	1.49	1.42
27	B	809	CLA	CMB-C2B	-2.18	1.46	1.50
27	B	806	CLA	CMC-C2C	-2.18	1.46	1.50
27	e	601	CLA	MG-NB	-2.18	2.01	2.05
27	L	203	CLA	CMD-C2D	-2.18	1.46	1.50
27	b	611	CLA	CMC-C2C	-2.18	1.46	1.50
27	B	849	CLA	C3B-C4B	2.18	1.49	1.42
27	A	828	CLA	MG-NB	-2.18	2.01	2.05
27	n	610	CLA	MG-NB	-2.18	2.01	2.05
27	B	829	CLA	C3B-C4B	2.18	1.49	1.42
35	a	315	II0	C28-C26	2.18	1.52	1.50
27	B	822	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	202	CLA	MG-NB	-2.18	2.01	2.05
35	l	313	II0	C16-C03	2.18	1.57	1.53
27	a	306	CLA	CMD-C2D	-2.18	1.46	1.50
27	g	304	CLA	C1B-C2B	2.18	1.48	1.43
27	B	833	CLA	CMB-C2B	-2.18	1.46	1.50
27	g	309	CLA	CMD-C2D	-2.18	1.46	1.50
27	B	839	CLA	C1B-C2B	2.18	1.48	1.43
27	i	304	CLA	CMD-C2D	-2.18	1.46	1.50
27	A	805	CLA	C4B-NB	2.18	1.40	1.37
35	j	614	II0	C15-C03	2.18	1.57	1.53
27	A	855	CLA	MG-NB	-2.18	2.01	2.05
27	e	602	CLA	MG-NB	-2.18	2.01	2.05
27	k	305	CLA	MG-NB	-2.18	2.01	2.05
27	j	602	CLA	CMD-C2D	-2.18	1.46	1.50
27	n	609	CLA	C1B-C2B	2.18	1.48	1.43
27	k	305	CLA	CHC-C1C	2.18	1.42	1.38
27	l	303	CLA	C3B-C4B	2.17	1.49	1.42
35	d	313	II0	C20-C14	2.17	1.54	1.50
37	s	204	KC2	C1D-C2D	2.17	1.48	1.43
27	B	820	CLA	CMB-C2B	-2.17	1.46	1.50
27	A	803	CLA	CMC-C2C	-2.17	1.46	1.50
27	B	801	CLA	CMD-C2D	-2.17	1.46	1.50
27	B	808	CLA	CHC-C1C	2.17	1.42	1.38
27	i	309	CLA	MG-NB	-2.17	2.01	2.05
27	A	855	CLA	O2A-CGA	2.17	1.39	1.33
27	A	810	CLA	CMC-C2C	-2.17	1.46	1.50
30	B	843	WVN	C26-C22	-2.17	1.30	1.35
27	A	829	CLA	CMD-C2D	-2.17	1.46	1.50
27	b	603	CLA	CMB-C2B	-2.17	1.46	1.50
27	f	613	CLA	CMD-C2D	-2.17	1.46	1.50
27	B	803	CLA	C1B-NB	-2.17	1.35	1.37
27	e	604	CLA	C3B-C4B	2.17	1.49	1.42
27	e	606	CLA	C3B-C4B	2.17	1.49	1.42
27	f	610	CLA	CMB-C2B	-2.17	1.46	1.50
27	g	311	CLA	CMB-C2B	-2.17	1.46	1.50
27	k	313	CLA	CMD-C2D	-2.17	1.46	1.50
27	h	303	CLA	MG-NB	-2.17	2.01	2.05
27	l	308	CLA	C3B-C4B	2.17	1.49	1.42
27	m	608	CLA	CMD-C2D	-2.17	1.46	1.50
27	g	302	CLA	CMB-C2B	-2.17	1.46	1.50
27	c	609	CLA	C1B-C2B	2.17	1.48	1.43
27	h	304	CLA	C3B-C4B	2.17	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	312	CLA	MG-NA	2.17	2.11	2.06
27	a	312	CLA	MG-NC	2.17	2.11	2.06
27	a	313	CLA	CHC-C1C	2.17	1.42	1.38
35	d	312	II0	C16-C03	2.17	1.57	1.53
35	l	317	II0	C16-C03	2.17	1.57	1.53
27	d	311	CLA	CMC-C2C	-2.17	1.46	1.50
27	d	307	CLA	C3B-C4B	2.17	1.49	1.42
27	f	607	CLA	CMB-C2B	-2.17	1.46	1.50
27	A	824	CLA	MG-NB	-2.17	2.01	2.05
35	i	314	II0	C20-C14	2.17	1.54	1.50
27	s	206	CLA	CMC-C2C	-2.17	1.46	1.50
27	n	602	CLA	CMC-C2C	-2.17	1.46	1.50
27	A	841	CLA	MG-NB	-2.17	2.01	2.05
27	A	827	CLA	CHC-C1C	2.16	1.42	1.38
27	A	804	CLA	C1B-NB	-2.16	1.35	1.37
27	i	308	CLA	C3D-C4D	2.16	1.49	1.44
27	A	825	CLA	MG-NB	-2.16	2.01	2.05
27	A	826	CLA	CMB-C2B	-2.16	1.46	1.50
35	a	315	II0	C16-C03	2.16	1.57	1.53
27	A	842	CLA	MG-NB	-2.16	2.01	2.05
27	m	601	CLA	CMD-C2D	-2.16	1.46	1.50
27	e	605	CLA	CMD-C2D	-2.16	1.46	1.50
27	A	823	CLA	CMC-C2C	-2.16	1.46	1.50
30	B	846	WVN	C20-C13	2.16	1.52	1.45
27	s	208	CLA	CMC-C2C	-2.16	1.46	1.50
27	d	302	CLA	CMD-C2D	-2.16	1.46	1.50
27	e	611	CLA	CMB-C2B	-2.16	1.46	1.50
27	n	601	CLA	CMD-C2D	-2.16	1.46	1.50
27	A	801	CLA	CMB-C2B	-2.16	1.46	1.50
27	a	304	CLA	CMC-C2C	-2.16	1.46	1.50
27	b	605	CLA	CMC-C2C	-2.16	1.46	1.50
27	n	610	CLA	O2D-CGD	2.16	1.38	1.33
27	J	105	CLA	MG-NB	-2.16	2.01	2.05
27	e	607	CLA	CMC-C2C	-2.16	1.46	1.50
27	d	305	CLA	CAC-C3C	-2.16	1.45	1.51
27	A	803	CLA	CMD-C2D	-2.16	1.46	1.50
27	A	803	CLA	CMB-C2B	-2.16	1.46	1.50
27	A	817	CLA	CHC-C1C	2.16	1.42	1.38
30	B	845	WVN	C19-C22	2.16	1.50	1.46
27	B	826	CLA	CHC-C1C	2.16	1.42	1.38
27	B	811	CLA	C1B-NB	-2.16	1.35	1.37
27	A	805	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	610	CLA	CMD-C2D	-2.15	1.46	1.50
27	A	822	CLA	CHC-C1C	2.15	1.42	1.38
27	a	311	CLA	CMB-C2B	-2.15	1.46	1.50
27	e	608	CLA	CMD-C2D	-2.15	1.46	1.50
30	L	201	WVN	C37-C34	-2.15	1.30	1.35
27	A	830	CLA	CMB-C2B	-2.15	1.46	1.50
27	B	839	CLA	CMB-C2B	-2.15	1.46	1.50
27	F	201	CLA	MG-NB	-2.15	2.01	2.05
27	A	825	CLA	CHC-C1C	2.15	1.42	1.38
27	B	803	CLA	C3B-C4B	2.15	1.49	1.42
27	n	605	CLA	CMD-C2D	-2.15	1.46	1.50
27	B	833	CLA	C4B-NB	2.15	1.40	1.37
35	m	614	II0	C20-C14	2.15	1.54	1.50
27	b	602	CLA	CHC-C1C	2.15	1.42	1.38
27	L	206	CLA	CMD-C2D	-2.15	1.46	1.50
27	A	814	CLA	CMD-C2D	-2.15	1.46	1.50
27	A	816	CLA	CMB-C2B	-2.15	1.46	1.50
36	O	204	IHT	C13-C02	2.15	1.57	1.53
27	f	605	CLA	CMB-C2B	-2.15	1.46	1.50
27	h	304	CLA	MG-NB	-2.15	2.01	2.05
27	g	322	CLA	C3B-C4B	2.15	1.49	1.42
27	j	601	CLA	CMB-C2B	-2.15	1.46	1.50
27	A	856	CLA	CAC-C3C	-2.15	1.45	1.51
30	A	849	WVN	C02-C11	2.15	1.53	1.50
27	m	611	CLA	MG-ND	-2.15	2.01	2.05
27	m	606	CLA	CMD-C2D	-2.15	1.46	1.50
27	B	837	CLA	C1B-C2B	2.15	1.48	1.43
37	e	609	KC2	C1D-C2D	2.15	1.48	1.43
27	L	203	CLA	C1B-NB	-2.15	1.35	1.37
27	l	307	CLA	CMD-C2D	-2.15	1.46	1.50
27	n	603	CLA	CMC-C2C	-2.15	1.46	1.50
35	n	615	II0	C30-C26	-2.15	1.32	1.37
27	B	819	CLA	CHC-C1C	2.15	1.42	1.38
27	a	310	CLA	CMB-C2B	-2.15	1.46	1.50
27	m	604	CLA	C1B-C2B	2.14	1.48	1.43
27	L	203	CLA	C3B-C4B	2.14	1.49	1.42
27	A	815	CLA	CHC-C4B	-2.14	1.34	1.39
35	l	315	II0	C16-C03	2.14	1.57	1.53
27	B	839	CLA	CMD-C2D	-2.14	1.46	1.50
27	i	303	CLA	C3B-C4B	2.14	1.49	1.42
27	e	602	CLA	CMC-C2C	-2.14	1.46	1.50
27	e	610	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	617	II0	C18-C04	2.14	1.57	1.53
27	j	602	CLA	CMB-C2B	-2.14	1.46	1.50
27	f	610	CLA	C3B-C4B	2.14	1.49	1.42
27	e	602	CLA	CHC-C1C	2.14	1.42	1.38
27	B	815	CLA	C1B-C2B	2.14	1.48	1.43
27	c	607	CLA	CMB-C2B	-2.14	1.46	1.50
27	m	606	CLA	CMB-C2B	-2.14	1.46	1.50
27	l	310	CLA	CMD-C2D	-2.14	1.46	1.50
27	n	609	CLA	CMD-C2D	-2.14	1.46	1.50
35	f	614	II0	C18-C04	2.14	1.57	1.53
27	l	309	CLA	CHC-C1C	2.14	1.42	1.38
35	i	318	II0	C15-C03	2.14	1.57	1.53
27	A	838	CLA	C1B-C2B	2.14	1.48	1.43
27	k	306	CLA	CMD-C2D	-2.14	1.46	1.50
27	e	610	CLA	C3B-C4B	2.14	1.49	1.42
27	f	613	CLA	CMB-C2B	-2.14	1.46	1.50
29	b	617	LHG	O7-C5	-2.14	1.41	1.46
27	h	304	CLA	MG-ND	-2.14	2.01	2.05
27	A	801	CLA	CMD-C2D	-2.14	1.46	1.50
27	B	828	CLA	CMB-C2B	-2.14	1.46	1.50
27	i	305	CLA	CHC-C1C	2.14	1.42	1.38
27	j	607	CLA	CHC-C1C	2.14	1.42	1.38
27	A	820	CLA	C3B-C4B	2.14	1.49	1.42
27	k	302	CLA	CMC-C2C	-2.14	1.46	1.50
27	a	307	CLA	C3B-C4B	2.14	1.49	1.42
27	B	840	CLA	C3B-C4B	2.13	1.49	1.42
30	R	201	WVN	C37-C34	-2.13	1.30	1.35
35	g	320	II0	C20-C14	2.13	1.54	1.50
27	B	813	CLA	C1B-C2B	2.13	1.48	1.43
27	A	821	CLA	CMB-C2B	-2.13	1.46	1.50
27	c	607	CLA	CMD-C2D	-2.13	1.46	1.50
27	a	307	CLA	CMC-C2C	-2.13	1.46	1.50
27	A	813	CLA	CMD-C2D	-2.13	1.46	1.50
27	e	604	CLA	CMC-C2C	-2.13	1.46	1.50
27	B	839	CLA	CHC-C1C	2.13	1.42	1.38
27	J	105	CLA	C3B-C4B	2.13	1.49	1.42
27	A	825	CLA	C3B-C4B	2.13	1.49	1.42
27	B	806	CLA	C1B-NB	-2.13	1.35	1.37
27	c	602	CLA	C3B-C4B	2.13	1.49	1.42
27	k	307	CLA	CMB-C2B	-2.13	1.46	1.50
35	g	317	II0	C18-C04	2.13	1.57	1.53
27	j	612	CLA	C1B-C2B	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	203	CLA	C1B-C2B	2.13	1.48	1.43
27	A	825	CLA	MG-ND	-2.13	2.01	2.05
27	B	818	CLA	MG-NB	-2.13	2.01	2.05
27	j	609	CLA	C3B-C4B	2.13	1.48	1.42
27	B	819	CLA	C1B-C2B	2.13	1.48	1.43
27	m	607	CLA	CHC-C1C	2.13	1.42	1.38
35	n	614	II0	C20-C14	2.13	1.54	1.50
35	m	615	II0	C15-C03	2.13	1.57	1.53
27	d	306	CLA	CMB-C2B	-2.13	1.46	1.50
27	A	841	CLA	C1B-C2B	2.13	1.48	1.43
27	B	834	CLA	C1B-C2B	2.13	1.48	1.43
27	R	203	CLA	C1B-C2B	2.13	1.48	1.43
36	k	317	IHT	C13-C02	2.13	1.57	1.53
27	A	828	CLA	CMB-C2B	-2.13	1.46	1.50
27	B	838	CLA	CMC-C2C	-2.13	1.46	1.50
36	c	620	IHT	C20-C15	2.13	1.54	1.50
27	J	105	CLA	CMB-C2B	-2.13	1.46	1.50
27	e	607	CLA	C3B-C4B	2.12	1.48	1.42
27	e	608	CLA	MG-NB	-2.12	2.01	2.05
27	h	308	CLA	C3D-C4D	2.12	1.49	1.44
35	h	311	II0	C28-C26	2.12	1.52	1.50
27	A	856	CLA	C3B-C4B	2.12	1.48	1.42
27	J	103	CLA	CHC-C1C	2.12	1.42	1.38
27	b	606	CLA	CMC-C2C	-2.12	1.46	1.50
30	R	202	WVN	C36-C32	-2.12	1.30	1.35
27	K	102	CLA	CMD-C2D	-2.12	1.46	1.50
27	c	604	CLA	CMC-C2C	-2.12	1.46	1.50
27	B	831	CLA	C1B-NB	-2.12	1.35	1.37
27	B	812	CLA	CHC-C1C	2.12	1.42	1.38
27	A	807	CLA	C3B-C4B	2.12	1.48	1.42
27	d	303	CLA	CMB-C2B	-2.12	1.46	1.50
27	K	102	CLA	MG-NB	-2.12	2.01	2.05
27	A	826	CLA	CHC-C1C	2.12	1.42	1.38
27	i	307	CLA	CMD-C2D	-2.12	1.46	1.50
27	i	312	CLA	CMD-C2D	-2.12	1.46	1.50
27	O	202	CLA	CMC-C2C	-2.12	1.46	1.50
27	K	101	CLA	CMC-C2C	-2.12	1.46	1.50
27	d	307	CLA	CMD-C2D	-2.12	1.46	1.50
35	e	613	II0	C20-C14	2.12	1.54	1.50
27	l	312	CLA	C1B-C2B	2.12	1.48	1.43
27	j	608	CLA	CMD-C2D	-2.12	1.46	1.50
27	K	101	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	847	WVN	C02-C11	2.12	1.53	1.50
27	B	837	CLA	MG-NB	-2.12	2.01	2.05
27	j	604	CLA	C3B-C4B	2.12	1.48	1.42
27	m	603	CLA	CMC-C2C	-2.12	1.46	1.50
27	B	830	CLA	CMC-C2C	-2.12	1.46	1.50
27	k	301	CLA	CMB-C2B	-2.12	1.46	1.50
27	e	611	CLA	C1B-C2B	2.12	1.48	1.43
27	j	602	CLA	CAC-C3C	-2.12	1.45	1.51
27	B	811	CLA	C3B-C4B	2.12	1.48	1.42
27	i	309	CLA	CMB-C2B	-2.12	1.46	1.50
27	n	601	CLA	CMB-C2B	-2.12	1.46	1.50
27	k	309	CLA	MG-ND	-2.12	2.01	2.05
30	B	844	WVN	C19-C22	2.12	1.50	1.46
27	B	810	CLA	CMB-C2B	-2.11	1.46	1.50
30	M	101	WVN	C28-C25	-2.11	1.30	1.35
37	s	201	KC2	C1D-C2D	2.11	1.48	1.43
27	B	830	CLA	MG-ND	-2.11	2.01	2.05
27	i	304	CLA	C1B-C2B	2.11	1.48	1.43
27	B	801	CLA	C3B-C4B	2.11	1.48	1.42
27	d	301	CLA	CMC-C2C	-2.11	1.46	1.50
27	e	606	CLA	C3D-C4D	2.11	1.48	1.44
27	h	301	CLA	C3B-C4B	2.11	1.48	1.42
27	A	852	CLA	CMB-C2B	-2.11	1.46	1.50
27	b	604	CLA	C3B-C4B	2.11	1.48	1.42
37	g	314	KC2	C1D-C2D	2.11	1.48	1.43
27	A	832	CLA	CMD-C2D	-2.11	1.46	1.50
27	A	828	CLA	CMC-C2C	-2.11	1.46	1.50
27	B	813	CLA	CMD-C2D	-2.11	1.46	1.50
27	c	603	CLA	CMD-C2D	-2.11	1.46	1.50
27	B	830	CLA	C1B-NB	-2.11	1.35	1.37
27	A	833	CLA	CMC-C2C	-2.11	1.46	1.50
27	A	836	CLA	CMC-C2C	-2.11	1.46	1.50
27	F	201	CLA	CMC-C2C	-2.11	1.46	1.50
27	B	840	CLA	MG-NB	-2.11	2.01	2.05
35	i	314	II0	C28-C26	-2.11	1.49	1.50
27	h	302	CLA	CMB-C2B	-2.11	1.46	1.50
27	k	304	CLA	C3B-C4B	2.11	1.48	1.42
27	A	825	CLA	CMB-C2B	-2.11	1.46	1.50
35	c	613	II0	C18-C04	2.11	1.57	1.53
27	e	601	CLA	C3B-C4B	2.11	1.48	1.42
27	k	304	CLA	C3D-C4D	2.11	1.48	1.44
27	B	823	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	j	615	II0	C18-C04	2.11	1.57	1.53
27	c	604	CLA	C1B-NB	-2.10	1.35	1.37
27	n	604	CLA	C3B-C4B	2.10	1.48	1.42
27	a	309	CLA	CMD-C2D	-2.10	1.46	1.50
27	A	830	CLA	C3B-C4B	2.10	1.48	1.42
27	B	812	CLA	CMD-C2D	-2.10	1.46	1.50
27	h	305	CLA	CMB-C2B	-2.10	1.46	1.50
27	O	206	CLA	C3B-C4B	2.10	1.48	1.42
27	f	612	CLA	CMD-C2D	-2.10	1.46	1.50
27	a	307	CLA	MG-ND	-2.10	2.01	2.05
27	a	306	CLA	CHC-C1C	2.10	1.42	1.38
27	g	305	CLA	C1B-C2B	2.10	1.48	1.43
27	m	612	CLA	CMB-C2B	-2.10	1.46	1.50
27	n	607	CLA	CHC-C4B	-2.10	1.34	1.39
27	B	804	CLA	MG-NB	-2.10	2.01	2.05
27	A	804	CLA	CMB-C2B	-2.10	1.46	1.50
27	A	830	CLA	CMC-C2C	-2.10	1.46	1.50
27	F	203	CLA	CMB-C2B	-2.10	1.46	1.50
27	b	609	CLA	CMD-C2D	-2.10	1.46	1.50
27	B	803	CLA	C1B-C2B	2.10	1.48	1.43
27	l	303	CLA	CAC-C3C	-2.10	1.45	1.51
27	b	602	CLA	C3B-C4B	2.10	1.48	1.42
27	A	832	CLA	C1B-C2B	2.10	1.48	1.43
30	B	844	WVN	C28-C25	-2.10	1.30	1.35
27	A	829	CLA	CMC-C2C	-2.10	1.46	1.50
27	e	608	CLA	CMB-C2B	-2.10	1.46	1.50
27	f	608	CLA	CMD-C2D	-2.10	1.46	1.50
35	g	320	II0	C18-C04	2.10	1.57	1.53
27	B	834	CLA	CMC-C2C	-2.10	1.46	1.50
27	f	606	CLA	MG-NC	2.10	2.11	2.06
27	f	608	CLA	CHC-C1C	2.10	1.42	1.38
27	b	603	CLA	CMC-C2C	-2.10	1.46	1.50
27	h	306	CLA	CMC-C2C	-2.10	1.46	1.50
27	k	305	CLA	C3B-C4B	2.10	1.48	1.42
27	j	603	CLA	MG-NB	-2.10	2.01	2.05
27	f	603	CLA	MG-NB	-2.10	2.01	2.05
27	k	313	CLA	MG-NA	2.10	2.11	2.06
35	g	320	II0	C16-C03	2.10	1.57	1.53
27	l	306	CLA	C3B-C4B	2.10	1.48	1.42
27	c	611	CLA	CHC-C1C	2.10	1.42	1.38
27	B	811	CLA	CMB-C2B	-2.10	1.46	1.50
27	e	607	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	837	CLA	CMB-C2B	-2.09	1.46	1.50
35	c	613	II0	C20-C14	2.09	1.54	1.50
27	B	832	CLA	CMB-C2B	-2.09	1.46	1.50
37	i	310	KC2	C1D-C2D	2.09	1.48	1.43
27	h	304	CLA	CMB-C2B	-2.09	1.46	1.50
35	g	316	II0	C15-C03	2.09	1.57	1.53
27	b	606	CLA	CHC-C1C	2.09	1.42	1.38
35	e	616	II0	C16-C03	2.09	1.57	1.53
27	d	304	CLA	C3B-C4B	2.09	1.48	1.42
27	B	831	CLA	CMB-C2B	-2.09	1.46	1.50
27	e	606	CLA	CMD-C2D	-2.09	1.46	1.50
27	B	821	CLA	C1D-ND	2.09	1.40	1.37
35	a	314	II0	C16-C03	2.09	1.57	1.53
30	I	101	WVN	C28-C25	-2.09	1.31	1.35
27	A	812	CLA	MG-NB	-2.09	2.01	2.05
27	a	305	CLA	MG-NB	-2.09	2.01	2.05
27	A	812	CLA	C1B-C2B	2.09	1.48	1.43
35	d	312	II0	C15-C03	2.09	1.57	1.53
27	f	601	CLA	CMD-C2D	-2.09	1.46	1.50
37	c	610	KC2	C1D-C2D	2.09	1.48	1.43
30	s	207	WVN	C26-C22	-2.09	1.31	1.35
27	e	605	CLA	CMB-C2B	-2.09	1.46	1.50
27	A	819	CLA	CAC-C3C	-2.09	1.45	1.51
27	B	812	CLA	CMB-C2B	-2.09	1.46	1.50
27	l	305	CLA	CMB-C2B	-2.09	1.46	1.50
27	A	852	CLA	CHC-C1C	2.09	1.42	1.38
36	j	616	IHT	C13-C02	2.09	1.57	1.53
35	g	317	II0	C30-C26	-2.09	1.32	1.37
27	B	820	CLA	CHC-C1C	2.09	1.42	1.38
35	a	314	II0	C18-C04	2.09	1.57	1.53
27	A	809	CLA	CMB-C2B	-2.09	1.46	1.50
27	s	209	CLA	CMD-C2D	-2.09	1.46	1.50
27	l	308	CLA	CHC-C1C	2.09	1.42	1.38
30	F	204	WVN	C14-C15	2.09	1.54	1.51
27	A	805	CLA	MG-ND	-2.09	2.01	2.05
35	f	618	II0	C16-C03	2.09	1.57	1.53
35	k	315	II0	C16-C03	2.08	1.57	1.53
36	c	616	IHT	C20-C15	2.08	1.54	1.50
27	J	103	CLA	C1B-C2B	2.08	1.48	1.43
27	d	311	CLA	C1B-C2B	2.08	1.48	1.43
31	b	616	LMT	O5'-C5'	-2.08	1.39	1.44
30	J	101	WVN	C26-C22	-2.08	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	i	313	II0	C30-C26	-2.08	1.32	1.37
27	A	837	CLA	C4B-NB	2.08	1.40	1.37
35	a	315	II0	C15-C03	2.08	1.57	1.53
27	B	814	CLA	C1B-C2B	2.08	1.48	1.43
27	e	610	CLA	CMD-C2D	-2.08	1.46	1.50
27	a	311	CLA	C3B-C4B	2.08	1.48	1.42
30	B	844	WVN	C37-C34	-2.08	1.31	1.35
27	A	839	CLA	CMD-C2D	-2.08	1.46	1.50
27	A	842	CLA	C1B-NB	-2.08	1.35	1.37
35	f	615	II0	C30-C26	-2.08	1.32	1.37
27	L	206	CLA	CMC-C2C	-2.08	1.46	1.50
27	l	304	CLA	CMD-C2D	-2.08	1.46	1.50
27	A	852	CLA	CMD-C2D	-2.08	1.46	1.50
27	B	832	CLA	CMC-C2C	-2.08	1.46	1.50
27	n	610	CLA	CMB-C2B	-2.08	1.46	1.50
35	b	613	II0	C20-C14	2.08	1.54	1.50
27	L	204	CLA	CHC-C1C	2.08	1.42	1.38
27	b	608	CLA	CMD-C2D	-2.08	1.46	1.50
27	d	305	CLA	CMD-C2D	-2.08	1.46	1.50
27	B	813	CLA	MG-NB	-2.08	2.01	2.05
27	c	609	CLA	CHC-C1C	2.08	1.42	1.38
27	a	306	CLA	CMC-C2C	-2.08	1.46	1.50
27	a	303	CLA	MG-NB	-2.08	2.01	2.05
27	c	605	CLA	C3B-C4B	2.08	1.48	1.42
27	A	811	CLA	CMB-C2B	-2.08	1.46	1.50
27	L	204	CLA	MG-NB	-2.08	2.01	2.05
27	e	601	CLA	CMD-C2D	-2.08	1.46	1.50
27	g	307	CLA	CMD-C2D	-2.08	1.46	1.50
27	B	805	CLA	C3B-C4B	2.08	1.48	1.42
35	f	615	II0	C18-C04	2.08	1.57	1.53
27	j	606	CLA	MG-NB	-2.08	2.01	2.05
30	R	202	WVN	C37-C34	-2.08	1.31	1.35
27	h	305	CLA	C3B-C4B	2.07	1.48	1.42
35	m	614	II0	C18-C04	2.07	1.57	1.53
27	l	307	CLA	CMB-C2B	-2.07	1.46	1.50
27	f	609	CLA	CMD-C2D	-2.07	1.46	1.50
27	B	825	CLA	CMC-C2C	-2.07	1.46	1.50
27	h	304	CLA	C3D-C4D	2.07	1.48	1.44
30	s	205	WVN	C14-C15	2.07	1.54	1.51
27	l	304	CLA	CMC-C2C	-2.07	1.46	1.50
27	f	607	CLA	CMD-C2D	-2.07	1.46	1.50
27	B	802	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	b	613	II0	C16-C03	2.07	1.57	1.53
27	B	827	CLA	CMD-C2D	-2.07	1.46	1.50
27	A	824	CLA	CMC-C2C	-2.07	1.46	1.50
27	c	609	CLA	CMB-C2B	-2.07	1.46	1.50
27	a	308	CLA	CMD-C2D	-2.07	1.46	1.50
27	g	304	CLA	C1B-NB	-2.07	1.35	1.37
27	B	805	CLA	CMC-C2C	-2.07	1.46	1.50
27	h	313	CLA	CHC-C1C	2.07	1.42	1.38
27	B	818	CLA	MG-ND	-2.07	2.01	2.05
30	A	849	WVN	C26-C22	-2.07	1.31	1.35
35	d	312	II0	C28-C26	-2.07	1.49	1.50
30	l	301	WVN	C20-C13	2.07	1.52	1.45
27	A	839	CLA	CMC-C2C	-2.07	1.46	1.50
27	n	607	CLA	CMB-C2B	-2.07	1.46	1.50
29	A	845	LHG	O7-C5	-2.07	1.41	1.46
27	B	827	CLA	CMB-C2B	-2.07	1.46	1.50
27	g	307	CLA	CMB-C2B	-2.07	1.46	1.50
27	B	815	CLA	C3B-C4B	2.07	1.48	1.42
27	k	309	CLA	C3B-C4B	2.07	1.48	1.42
36	O	204	IHT	C20-C15	2.07	1.54	1.50
34	J	106	LMG	O7-C8	-2.07	1.41	1.46
27	f	605	CLA	C3D-C4D	2.07	1.48	1.44
27	B	849	CLA	CMB-C2B	-2.07	1.46	1.50
27	e	606	CLA	CMB-C2B	-2.07	1.46	1.50
27	f	601	CLA	CMB-C2B	-2.07	1.46	1.50
30	R	202	WVN	C40-C39	-2.07	1.30	1.36
27	l	305	CLA	CHC-C1C	2.07	1.42	1.38
27	i	306	CLA	CHC-C1C	2.07	1.42	1.38
27	m	612	CLA	C1B-NB	-2.07	1.35	1.37
36	a	317	IHT	C13-C02	2.07	1.57	1.53
27	B	817	CLA	MG-NB	-2.07	2.01	2.05
27	g	303	CLA	MG-NB	-2.06	2.01	2.05
27	A	841	CLA	CMC-C2C	-2.06	1.46	1.50
27	B	823	CLA	CMC-C2C	-2.06	1.46	1.50
27	B	824	CLA	CMC-C2C	-2.06	1.46	1.50
27	k	301	CLA	CHC-C1C	2.06	1.42	1.38
30	F	205	WVN	C27-C25	2.06	1.55	1.50
27	g	304	CLA	MG-ND	-2.06	2.01	2.05
27	h	302	CLA	C3B-C4B	2.06	1.48	1.42
27	A	801	CLA	C3B-C4B	2.06	1.48	1.42
37	k	311	KC2	C4B-NB	-2.06	1.35	1.37
35	n	618	II0	C16-C03	2.06	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	602	CLA	CMD-C2D	-2.06	1.46	1.50
27	l	307	CLA	C3D-C4D	2.06	1.48	1.44
27	B	819	CLA	MG-NB	-2.06	2.01	2.05
27	l	312	CLA	MG-NB	-2.06	2.01	2.05
27	j	606	CLA	CMC-C2C	-2.06	1.46	1.50
35	a	316	II0	C18-C04	2.06	1.57	1.53
27	d	304	CLA	CMD-C2D	-2.06	1.46	1.50
35	c	615	II0	C18-C04	2.06	1.57	1.53
27	A	823	CLA	CMD-C2D	-2.06	1.46	1.50
27	n	605	CLA	CMB-C2B	-2.06	1.46	1.50
27	j	604	CLA	CHC-C4B	-2.06	1.34	1.39
27	B	835	CLA	MG-NB	-2.06	2.01	2.05
27	B	834	CLA	MG-ND	-2.06	2.01	2.05
27	m	601	CLA	CMB-C2B	-2.06	1.46	1.50
27	j	605	CLA	CMC-C2C	-2.06	1.46	1.50
30	B	847	WVN	C26-C22	-2.06	1.31	1.35
37	s	204	KC2	C1A-CHA	2.06	1.45	1.40
27	b	611	CLA	CMB-C2B	-2.06	1.46	1.50
27	i	311	CLA	C1B-C2B	2.06	1.48	1.43
27	n	607	CLA	CMC-C2C	-2.06	1.46	1.50
35	h	311	II0	C20-C14	2.06	1.54	1.50
27	B	849	CLA	CHC-C4B	-2.06	1.34	1.39
27	O	206	CLA	MG-NB	-2.06	2.01	2.05
27	m	603	CLA	CMB-C2B	-2.06	1.46	1.50
27	e	610	CLA	O2D-CED	-2.06	1.40	1.45
27	B	832	CLA	C1B-C2B	2.06	1.48	1.43
27	e	611	CLA	CMC-C2C	-2.06	1.46	1.50
27	l	309	CLA	CMC-C2C	-2.06	1.46	1.50
31	A	851	LMT	O1'-C1'	-2.06	1.36	1.40
27	B	804	CLA	C1B-NB	-2.06	1.35	1.37
27	a	309	CLA	C1B-NB	-2.06	1.35	1.37
27	B	812	CLA	C1B-C2B	2.06	1.48	1.43
27	c	601	CLA	MG-ND	-2.05	2.01	2.05
27	A	842	CLA	C1B-C2B	2.05	1.47	1.43
27	d	302	CLA	CMC-C2C	-2.05	1.46	1.50
27	b	604	CLA	CHC-C1C	2.05	1.42	1.38
27	n	607	CLA	C3B-C4B	2.05	1.48	1.42
37	d	310	KC2	C1D-C2D	2.05	1.47	1.43
35	e	612	II0	C18-C04	2.05	1.57	1.53
27	L	203	CLA	CMC-C2C	-2.05	1.46	1.50
27	d	305	CLA	CMB-C2B	-2.05	1.46	1.50
27	m	602	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	828	CLA	C3B-C4B	2.05	1.48	1.42
27	l	310	CLA	CMB-C2B	-2.05	1.46	1.50
27	f	607	CLA	CMC-C2C	-2.05	1.46	1.50
27	h	303	CLA	C1B-C2B	2.05	1.47	1.43
27	h	301	CLA	MG-ND	-2.05	2.01	2.05
35	f	615	II0	C20-C14	2.05	1.54	1.50
27	a	305	CLA	CMC-C2C	-2.05	1.46	1.50
35	n	618	II0	C20-C14	2.05	1.54	1.50
35	a	314	II0	C28-C26	-2.05	1.49	1.50
27	n	608	CLA	CMB-C2B	-2.05	1.46	1.50
36	n	617	IHT	C13-C02	2.05	1.57	1.53
27	A	802	CLA	MG-NB	-2.05	2.01	2.05
27	a	305	CLA	C1B-NB	-2.05	1.35	1.37
27	A	833	CLA	MG-NB	-2.05	2.01	2.05
27	B	814	CLA	CHC-C1C	2.05	1.42	1.38
27	h	313	CLA	CMC-C2C	-2.05	1.46	1.50
27	l	306	CLA	CHC-C1C	2.05	1.42	1.38
37	g	313	KC2	C4A-C3A	2.05	1.48	1.44
27	B	834	CLA	CMB-C2B	-2.05	1.46	1.50
30	L	201	WVN	C26-C22	-2.05	1.31	1.35
27	A	821	CLA	C1B-NB	-2.05	1.35	1.37
27	B	810	CLA	C3B-C4B	2.05	1.48	1.42
27	A	805	CLA	C1B-C2B	2.05	1.47	1.43
27	B	825	CLA	MG-ND	-2.05	2.01	2.05
27	B	832	CLA	C1B-NB	-2.05	1.35	1.37
27	h	305	CLA	CMC-C2C	-2.05	1.46	1.50
27	e	607	CLA	C4B-NB	2.05	1.40	1.37
27	h	303	CLA	C3B-C4B	2.05	1.48	1.42
35	e	613	II0	C30-C26	-2.05	1.32	1.37
27	h	303	CLA	C1B-NB	-2.04	1.35	1.37
27	a	305	CLA	C3B-C4B	2.04	1.48	1.42
27	A	856	CLA	MG-ND	-2.04	2.01	2.05
31	b	616	LMT	O2'-C2'	-2.04	1.37	1.43
27	A	835	CLA	CMC-C2C	-2.04	1.46	1.50
27	c	609	CLA	CMC-C2C	-2.04	1.46	1.50
27	h	307	CLA	CMC-C2C	-2.04	1.46	1.50
27	n	604	CLA	MG-ND	-2.04	2.01	2.05
27	A	856	CLA	MG-NB	-2.04	2.01	2.05
27	m	605	CLA	C4B-NB	2.04	1.40	1.37
27	L	202	CLA	MG-NB	-2.04	2.01	2.05
27	f	610	CLA	CMC-C2C	-2.04	1.46	1.50
27	i	302	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	g	304	CLA	CMC-C2C	-2.04	1.46	1.50
27	A	820	CLA	MG-ND	-2.04	2.01	2.05
27	g	311	CLA	CAC-C3C	-2.04	1.45	1.51
27	g	315	CLA	CMC-C2C	-2.04	1.46	1.50
27	L	204	CLA	C3B-C4B	2.04	1.48	1.42
27	k	307	CLA	C3B-C4B	2.04	1.48	1.42
27	h	305	CLA	CHC-C1C	2.04	1.42	1.38
27	i	303	CLA	CHC-C1C	2.04	1.42	1.38
35	n	614	II0	C16-C03	2.04	1.57	1.53
27	A	831	CLA	CMC-C2C	-2.04	1.46	1.50
27	A	831	CLA	CAA-C2A	-2.04	1.50	1.54
37	k	311	KC2	C1D-C2D	2.04	1.47	1.43
27	B	809	CLA	C1B-NB	-2.04	1.35	1.37
27	k	305	CLA	MG-ND	-2.04	2.01	2.05
27	c	612	CLA	CMD-C2D	-2.04	1.46	1.50
27	b	610	CLA	CMB-C2B	-2.04	1.46	1.50
27	j	607	CLA	CMD-C2D	-2.04	1.46	1.50
30	F	205	WVN	C21-C15	2.04	1.54	1.50
30	B	844	WVN	C40-C39	-2.04	1.30	1.36
27	A	825	CLA	C1B-NB	-2.04	1.35	1.37
27	A	830	CLA	C1B-NB	-2.04	1.35	1.37
35	c	617	II0	C16-C03	2.04	1.57	1.53
27	j	612	CLA	MG-NB	-2.04	2.01	2.05
35	m	615	II0	C18-C04	2.04	1.57	1.53
27	B	810	CLA	MG-NB	-2.04	2.01	2.05
30	B	848	WVN	C36-C32	-2.04	1.31	1.35
27	A	821	CLA	MG-NB	-2.03	2.01	2.05
27	e	605	CLA	MG-ND	-2.03	2.01	2.05
27	A	817	CLA	MG-ND	-2.03	2.01	2.05
27	B	840	CLA	CMC-C2C	-2.03	1.46	1.50
27	a	311	CLA	CMD-C2D	-2.03	1.46	1.50
30	M	101	WVN	C37-C34	-2.03	1.31	1.35
27	g	306	CLA	CMB-C2B	-2.03	1.46	1.50
27	B	818	CLA	C1B-C2B	2.03	1.47	1.43
27	b	604	CLA	O2D-CED	-2.03	1.40	1.45
27	A	853	CLA	CMC-C2C	-2.03	1.46	1.50
35	J	104	II0	C20-C14	2.03	1.54	1.50
36	R	204	IHT	C13-C02	2.03	1.57	1.53
27	b	603	CLA	MG-NB	-2.03	2.01	2.05
27	h	306	CLA	MG-NB	-2.03	2.01	2.05
35	n	615	II0	C16-C03	2.03	1.57	1.53
30	L	205	WVN	C02-C11	2.03	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	i	311	CLA	MG-NC	2.03	2.11	2.06
27	j	612	CLA	C3B-C4B	2.03	1.48	1.42
27	e	602	CLA	MG-ND	-2.03	2.01	2.05
35	l	315	II0	C20-C14	2.03	1.54	1.50
27	i	305	CLA	CMD-C2D	-2.03	1.46	1.50
27	d	303	CLA	CMD-C2D	-2.03	1.46	1.50
27	l	309	CLA	MG-NB	-2.03	2.01	2.05
30	B	845	WVN	C26-C22	-2.03	1.31	1.35
27	g	310	CLA	C1B-C2B	2.03	1.47	1.43
27	f	608	CLA	CMB-C2B	-2.03	1.46	1.50
27	A	842	CLA	CMB-C2B	-2.03	1.46	1.50
27	i	304	CLA	CMB-C2B	-2.03	1.46	1.50
27	B	801	CLA	CMB-C2B	-2.03	1.46	1.50
27	a	303	CLA	C1B-C2B	2.03	1.47	1.43
27	B	821	CLA	CMB-C2B	-2.03	1.46	1.50
27	m	606	CLA	CMC-C2C	-2.03	1.46	1.50
30	L	201	WVN	C36-C32	-2.03	1.31	1.35
27	l	310	CLA	CHC-C1C	2.03	1.42	1.38
27	m	611	CLA	MG-NB	-2.03	2.01	2.05
35	n	616	II0	C15-C03	2.03	1.57	1.53
27	f	601	CLA	CHC-C1C	2.03	1.42	1.38
27	m	609	CLA	C3B-C4B	2.03	1.48	1.42
27	b	609	CLA	CMB-C2B	-2.03	1.46	1.50
27	d	311	CLA	CMD-C2D	-2.03	1.46	1.50
30	s	205	WVN	C28-C25	-2.02	1.31	1.35
27	l	307	CLA	C3C-C2C	2.02	1.41	1.36
27	B	822	CLA	MG-ND	-2.02	2.01	2.05
27	f	609	CLA	CMB-C2B	-2.02	1.46	1.50
27	B	824	CLA	MG-NB	-2.02	2.01	2.05
27	m	611	CLA	CMB-C2B	-2.02	1.46	1.50
27	e	605	CLA	CMC-C2C	-2.02	1.46	1.50
27	n	608	CLA	CHC-C1C	2.02	1.42	1.38
27	A	829	CLA	C3B-C4B	2.02	1.48	1.42
27	j	609	CLA	MG-ND	-2.02	2.01	2.05
27	A	840	CLA	O2D-CED	-2.02	1.40	1.45
37	g	312	KC2	C1D-C2D	2.02	1.47	1.43
35	e	613	II0	C15-C03	2.02	1.57	1.53
27	m	605	CLA	MG-ND	-2.02	2.01	2.05
27	L	206	CLA	CHC-C1C	2.02	1.42	1.38
30	B	848	WVN	C40-C39	-2.02	1.30	1.36
27	f	604	CLA	C1A-CHA	-2.02	1.34	1.43
27	A	855	CLA	C1B-C2B	2.02	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	h	305	CLA	C1B-C2B	2.02	1.47	1.43
27	a	309	CLA	CMB-C2B	-2.02	1.46	1.50
27	A	828	CLA	CHC-C1C	2.02	1.42	1.38
27	b	605	CLA	C1B-C2B	2.02	1.47	1.43
27	k	304	CLA	CMC-C2C	-2.02	1.46	1.50
37	s	204	KC2	O2A-CGA	-2.02	1.25	1.30
30	J	102	WVN	C26-C22	-2.02	1.31	1.35
27	g	308	CLA	CMC-C2C	-2.02	1.46	1.50
27	c	603	CLA	MG-NB	-2.02	2.01	2.05
27	l	304	CLA	C3B-C4B	2.02	1.48	1.42
27	g	307	CLA	C3B-C4B	2.02	1.48	1.42
35	j	613	II0	C18-C04	2.02	1.57	1.53
27	A	812	CLA	CMB-C2B	-2.02	1.46	1.50
35	e	612	II0	C29-C25	-2.02	1.32	1.37
27	s	202	CLA	C1D-C2D	2.02	1.49	1.45
35	l	317	II0	C15-C03	2.02	1.57	1.53
27	O	202	CLA	CHC-C1C	2.02	1.42	1.38
27	B	829	CLA	CMC-C2C	-2.02	1.46	1.50
27	l	309	CLA	CMB-C2B	-2.02	1.46	1.50
37	l	311	KC2	C1D-C2D	2.02	1.47	1.43
35	b	612	II0	C18-C04	2.02	1.57	1.53
27	j	611	CLA	CMD-C2D	-2.02	1.46	1.50
37	g	313	KC2	C1D-C2D	2.02	1.47	1.43
27	a	312	CLA	CMB-C2B	-2.02	1.46	1.50
27	g	305	CLA	CMC-C2C	-2.02	1.46	1.50
27	g	303	CLA	C1B-NB	-2.02	1.35	1.37
37	s	204	KC2	C4B-NB	-2.02	1.35	1.37
27	m	611	CLA	CHC-C1C	2.02	1.42	1.38
27	B	839	CLA	CMC-C2C	-2.01	1.46	1.50
27	F	203	CLA	CMC-C2C	-2.01	1.46	1.50
30	B	847	WVN	C37-C34	-2.01	1.31	1.35
27	B	838	CLA	CMB-C2B	-2.01	1.46	1.50
27	j	603	CLA	CMB-C2B	-2.01	1.46	1.50
27	B	827	CLA	C1B-C2B	2.01	1.47	1.43
27	j	609	CLA	CHC-C4B	-2.01	1.34	1.39
27	K	101	CLA	CMB-C2B	-2.01	1.46	1.50
27	L	202	CLA	C1B-NB	-2.01	1.35	1.37
27	A	830	CLA	C1B-C2B	2.01	1.47	1.43
27	l	305	CLA	CMC-C2C	-2.01	1.46	1.50
27	B	829	CLA	CMB-C2B	-2.01	1.46	1.50
27	n	604	CLA	MG-NB	-2.01	2.01	2.05
27	e	601	CLA	C3D-C4D	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	601	CLA	CAC-C3C	-2.01	1.45	1.51
27	d	301	CLA	C3B-C4B	2.01	1.48	1.42
27	b	603	CLA	CHC-C1C	2.01	1.42	1.38
27	i	303	CLA	CMB-C2B	-2.01	1.46	1.50
27	d	301	CLA	CMB-C2B	-2.01	1.46	1.50
27	g	303	CLA	CMC-C2C	-2.01	1.46	1.50
27	e	603	CLA	CHC-C1C	2.01	1.42	1.38
27	s	209	CLA	C3B-C4B	2.01	1.48	1.42
27	n	601	CLA	CMC-C2C	-2.01	1.46	1.50
27	l	305	CLA	MG-NB	-2.01	2.01	2.05
27	A	804	CLA	CHC-C1C	2.01	1.42	1.38
27	n	603	CLA	CMB-C2B	-2.01	1.46	1.50
27	B	801	CLA	CHC-C1C	2.01	1.42	1.38
27	K	101	CLA	CHC-C1C	2.01	1.42	1.38
35	l	314	II0	C20-C14	2.01	1.54	1.50
35	g	316	II0	C18-C04	2.01	1.57	1.53
27	A	840	CLA	C1B-C2B	2.01	1.47	1.43
30	A	848	WVN	C36-C32	-2.01	1.31	1.35
27	B	828	CLA	C1B-NB	-2.01	1.35	1.37
27	O	202	CLA	CMB-C2B	-2.01	1.46	1.50
27	A	817	CLA	C1B-NB	-2.01	1.35	1.37
27	R	203	CLA	CMC-C2C	-2.01	1.46	1.50
27	B	809	CLA	MG-ND	-2.01	2.01	2.05
27	B	802	CLA	CMD-C2D	-2.00	1.46	1.50
27	B	814	CLA	MG-NB	-2.00	2.01	2.05
27	A	837	CLA	C3B-C4B	2.00	1.48	1.42
27	A	828	CLA	C1B-NB	-2.00	1.35	1.37
27	h	304	CLA	C1B-NB	-2.00	1.35	1.37
27	A	813	CLA	CMB-C2B	-2.00	1.46	1.50
35	e	614	II0	C20-C14	2.00	1.54	1.50
27	b	605	CLA	CHC-C1C	2.00	1.42	1.38
37	i	317	KC2	C1C-C2C	2.00	1.48	1.44
30	l	301	WVN	C28-C25	-2.00	1.31	1.35
27	g	303	CLA	C1B-C2B	2.00	1.47	1.43
27	i	306	CLA	CMD-C2D	-2.00	1.46	1.50
27	m	606	CLA	MG-NB	-2.00	2.01	2.05
27	B	837	CLA	CMC-C2C	-2.00	1.46	1.50
27	B	838	CLA	CMD-C2D	-2.00	1.46	1.50
27	e	604	CLA	CMB-C2B	-2.00	1.46	1.50
27	i	309	CLA	C3B-C4B	2.00	1.48	1.42
27	s	208	CLA	CHC-C4B	-2.00	1.34	1.39
35	c	614	II0	C16-C03	2.00	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	303	CLA	C1B-NB	-2.00	1.35	1.37
27	B	825	CLA	C3B-C4B	2.00	1.48	1.42
30	A	848	WVN	C23-C25	2.00	1.50	1.46
27	O	202	CLA	C3B-C4B	2.00	1.48	1.42
27	m	607	CLA	MG-NB	-2.00	2.01	2.05

All (4638) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	813	CLA	C4A-NA-C1A	13.35	112.77	106.68
37	n	612	KC2	C1A-NA-C4A	-12.43	101.01	106.68
37	l	311	KC2	C1A-NA-C4A	-12.02	101.20	106.68
37	n	611	KC2	C1A-NA-C4A	-11.76	101.31	106.68
37	m	610	KC2	C1A-NA-C4A	-11.65	101.36	106.68
37	k	310	KC2	C1A-NA-C4A	-11.65	101.36	106.68
37	d	309	KC2	C1A-NA-C4A	-11.41	101.47	106.68
27	B	833	CLA	C4A-NA-C1A	11.27	111.82	106.68
37	f	611	KC2	C1A-NA-C4A	-11.01	101.66	106.68
37	g	313	KC2	C1A-NA-C4A	-10.98	101.67	106.68
37	e	609	KC2	C1A-NA-C4A	-10.97	101.68	106.68
37	j	610	KC2	C1A-NA-C4A	-10.93	101.69	106.68
37	g	314	KC2	C1A-NA-C4A	-10.78	101.76	106.68
37	k	312	KC2	C1A-NA-C4A	-10.70	101.80	106.68
37	s	204	KC2	C1A-NA-C4A	-10.62	101.83	106.68
37	g	312	KC2	C1A-NA-C4A	-10.44	101.91	106.68
37	i	310	KC2	C1A-NA-C4A	-10.02	102.11	106.68
37	c	610	KC2	C1A-NA-C4A	-10.02	102.11	106.68
27	A	856	CLA	C4A-NA-C1A	9.88	111.19	106.68
37	k	311	KC2	C1A-NA-C4A	-9.87	102.18	106.68
37	n	612	KC2	CHD-C4C-NC	9.81	139.08	124.31
37	d	310	KC2	C1A-NA-C4A	-9.50	102.35	106.68
37	i	317	KC2	CHD-C4C-NC	9.33	138.37	124.31
27	j	606	CLA	C4A-NA-C1A	9.24	110.89	106.68
35	a	318	II0	C42-C40-C36	-9.23	114.34	127.28
30	F	205	WVN	C20-C23-C25	-9.20	112.62	126.23
37	d	310	KC2	CHD-C4C-NC	9.15	138.09	124.31
30	s	207	WVN	C04-C09-C05	-9.11	116.13	124.83
37	s	201	KC2	C1A-NA-C4A	-9.04	102.56	106.68
37	c	610	KC2	CHD-C4C-NC	9.03	137.91	124.31
37	j	610	KC2	CHD-C4C-NC	8.98	137.83	124.31
37	s	201	KC2	CHD-C4C-NC	8.93	137.77	124.31
37	g	312	KC2	CHD-C4C-NC	8.87	137.68	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	i	310	KC2	CHD-C4C-NC	8.87	137.68	124.31
37	f	611	KC2	CHD-C4C-NC	8.84	137.62	124.31
30	F	205	WVN	C30-C28-C25	-8.82	114.91	127.28
37	e	609	KC2	CHD-C4C-NC	8.80	137.56	124.31
37	n	611	KC2	CHD-C4C-NC	8.79	137.54	124.31
37	d	309	KC2	CHD-C4C-NC	8.78	137.53	124.31
37	m	610	KC2	CHD-C4C-NC	8.77	137.52	124.31
37	k	312	KC2	CHD-C4C-NC	8.77	137.51	124.31
27	g	302	CLA	C4A-NA-C1A	8.63	110.62	106.68
37	g	314	KC2	CHD-C4C-NC	8.62	137.29	124.31
37	l	311	KC2	CHD-C4C-NC	8.59	137.25	124.31
37	k	310	KC2	CHD-C4C-NC	8.58	137.23	124.31
27	e	601	CLA	C4A-NA-C1A	8.54	110.58	106.68
27	A	804	CLA	C4A-NA-C1A	8.52	110.57	106.68
37	k	311	KC2	CHD-C4C-NC	8.27	136.76	124.31
27	g	309	CLA	C4A-NA-C1A	8.27	110.45	106.68
37	s	204	KC2	CHD-C4C-NC	8.23	136.71	124.31
27	B	805	CLA	C4A-NA-C1A	8.20	110.42	106.68
37	g	313	KC2	CHD-C4C-NC	8.16	136.60	124.31
30	R	202	WVN	C29-C26-C22	-8.15	115.85	127.28
30	B	846	WVN	C20-C23-C25	-8.14	114.19	126.23
27	h	308	CLA	C4A-NA-C1A	8.11	110.38	106.68
35	j	613	II0	C41-C39-C35	-7.97	116.09	127.28
37	s	201	KC2	CHB-C4A-C3A	-7.89	112.57	125.03
27	J	105	CLA	C4A-NA-C1A	7.88	110.28	106.68
27	e	604	CLA	C4A-NA-C1A	7.87	110.27	106.68
27	a	312	CLA	C4A-NA-C1A	7.85	110.26	106.68
35	k	315	II0	C41-C39-C35	-7.83	116.30	127.28
35	d	314	II0	C41-C39-C35	-7.78	116.36	127.28
30	R	201	WVN	C02-C11-C19	-7.75	112.53	124.58
37	s	204	KC2	C1A-C2A-C3A	-7.75	100.16	107.28
27	A	836	CLA	C4A-NA-C1A	7.67	110.18	106.68
35	n	614	II0	C42-C40-C36	-7.64	116.56	127.28
30	B	848	WVN	C02-C11-C19	-7.57	112.80	124.58
36	c	616	IHT	C18-C22-C23	-7.44	115.23	126.23
27	A	807	CLA	C4A-NA-C1A	7.43	110.07	106.68
30	B	844	WVN	C02-C11-C19	-7.35	113.14	124.58
27	c	604	CLA	C4A-NA-C1A	7.33	110.02	106.68
27	B	830	CLA	C4A-NA-C1A	7.27	110.00	106.68
35	c	615	II0	C42-C40-C36	-7.27	117.08	127.28
37	k	311	KC2	CHB-C4A-C3A	-7.27	113.55	125.03
35	l	314	II0	C41-C39-C35	-7.25	117.11	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	848	WVN	C30-C28-C25	-7.25	117.11	127.28
35	b	615	II0	C42-C40-C36	-7.23	117.14	127.28
30	B	845	WVN	C02-C11-C19	-7.23	113.33	124.58
30	F	205	WVN	C40-C39-C36	-7.22	108.74	123.52
35	l	302	II0	C41-C39-C35	-7.20	117.18	127.28
27	B	802	CLA	CAC-C3C-C4C	7.18	134.13	124.79
27	b	609	CLA	C4A-NA-C1A	7.17	109.95	106.68
36	R	204	IHT	C30-C27-C23	-7.17	117.22	127.28
37	e	609	KC2	CHC-C4B-C3B	-7.17	113.11	125.21
37	k	311	KC2	CHC-C4B-C3B	-7.15	113.16	125.21
37	g	313	KC2	CHB-C4A-C3A	-7.10	113.82	125.03
37	l	311	KC2	CHC-C4B-C3B	-7.09	113.25	125.21
27	F	203	CLA	C4A-NA-C1A	7.09	109.91	106.68
27	j	605	CLA	C4A-NA-C1A	7.07	109.90	106.68
37	g	312	KC2	CHC-C4B-C3B	-7.06	113.31	125.21
27	a	309	CLA	C4A-NA-C1A	7.04	109.89	106.68
37	g	313	KC2	CHC-C4B-C3B	-7.02	113.37	125.21
27	n	606	CLA	C4A-NA-C1A	7.01	109.88	106.68
37	d	309	KC2	CHC-C4B-C3B	-7.00	113.41	125.21
27	A	819	CLA	C4A-NA-C1A	6.99	109.87	106.68
36	b	614	IHT	C02-C07-C10	-6.99	113.09	122.64
36	n	617	IHT	C30-C27-C23	-6.97	117.50	127.28
37	k	312	KC2	CHC-C4B-C3B	-6.96	113.47	125.21
37	i	317	KC2	C1A-NA-C4A	-6.96	103.50	106.68
37	m	610	KC2	CHC-C4B-C3B	-6.93	113.53	125.21
27	f	605	CLA	C4A-NA-C1A	6.93	109.84	106.68
30	R	201	WVN	C30-C28-C25	-6.89	117.62	127.28
37	j	610	KC2	CHC-C4B-C3B	-6.88	113.61	125.21
30	F	205	WVN	C40-C37-C34	-6.88	117.63	127.28
30	B	844	WVN	C20-C23-C25	-6.87	116.07	126.23
37	c	610	KC2	CHC-C4B-C3B	-6.87	113.63	125.21
37	s	201	KC2	CHB-C1B-NB	6.87	134.47	124.80
27	A	821	CLA	C4A-NA-C1A	6.86	109.81	106.68
37	g	314	KC2	CHC-C4B-C3B	-6.85	113.66	125.21
30	B	843	WVN	C24-C22-C19	6.84	128.54	118.09
37	g	313	KC2	C2C-C1C-NC	6.83	118.90	110.45
35	c	615	II0	C41-C39-C35	-6.82	117.71	127.28
27	A	826	CLA	C4A-NA-C1A	6.81	109.78	106.68
37	f	611	KC2	CHC-C4B-C3B	-6.80	113.74	125.21
27	B	838	CLA	C4A-NA-C1A	6.79	109.78	106.68
27	c	603	CLA	C4A-NA-C1A	6.79	109.78	106.68
35	a	318	II0	C30-C32-C34	-6.78	103.55	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	l	306	CLA	C4A-NA-C1A	6.76	109.76	106.68
37	k	311	KC2	C2C-C1C-NC	6.76	118.82	110.45
37	l	311	KC2	CHB-C4A-C3A	-6.75	114.36	125.03
37	n	611	KC2	CHC-C4B-C3B	-6.75	113.82	125.21
27	A	831	CLA	C4A-NA-C1A	6.75	109.76	106.68
37	i	317	KC2	OBD-CAD-C3D	-6.74	112.65	128.42
37	s	204	KC2	CHC-C4B-C3B	-6.73	113.86	125.21
27	B	816	CLA	CMB-C2B-C1B	-6.73	115.18	125.42
30	A	846	WVN	C21-C15-C13	-6.72	117.15	124.48
37	i	310	KC2	CHC-C4B-C3B	-6.72	113.88	125.21
27	B	811	CLA	C4A-NA-C1A	6.70	109.74	106.68
37	n	611	KC2	CMD-C2D-C1D	-6.70	115.22	125.42
37	k	310	KC2	CHC-C4B-C3B	-6.68	113.94	125.21
27	A	824	CLA	C4A-NA-C1A	6.68	109.73	106.68
27	e	608	CLA	C4A-NA-C1A	6.68	109.73	106.68
37	s	201	KC2	CHB-C1B-C2B	-6.68	111.60	125.49
27	A	809	CLA	C4A-NA-C1A	6.67	109.72	106.68
35	g	317	II0	C42-C40-C36	-6.66	117.94	127.28
27	a	311	CLA	C4A-NA-C1A	6.65	109.71	106.68
30	L	201	WVN	C20-C23-C25	-6.65	116.40	126.23
35	j	615	II0	C42-C40-C36	-6.64	117.97	127.28
35	c	613	II0	C41-C39-C35	-6.64	117.97	127.28
37	n	612	KC2	CHB-C4A-C3A	-6.63	114.56	125.03
27	K	101	CLA	C4A-NA-C1A	6.63	109.70	106.68
37	k	311	KC2	CHC-C4B-NB	6.63	134.13	124.80
37	l	311	KC2	C2C-C1C-NC	6.60	118.62	110.45
27	f	613	CLA	C4A-NA-C1A	6.60	109.69	106.68
37	l	311	KC2	CHC-C4B-NB	6.59	134.08	124.80
27	A	840	CLA	C4A-NA-C1A	6.59	109.68	106.68
36	O	204	IHT	C40-C37-C33	-6.58	118.05	127.28
30	h	309	WVN	C02-C11-C19	-6.58	114.34	124.58
37	e	609	KC2	CHC-C4B-NB	6.57	134.04	124.80
37	i	310	KC2	OBD-CAD-C3D	-6.56	113.08	128.42
37	n	611	KC2	CHB-C4A-C3A	-6.55	114.69	125.03
37	d	310	KC2	CHC-C4B-C3B	-6.55	114.17	125.21
37	g	312	KC2	CHB-C4A-C3A	-6.54	114.69	125.03
37	e	609	KC2	C2C-C1C-NC	6.54	118.55	110.45
27	f	606	CLA	C4A-NA-C1A	6.53	109.66	106.68
37	i	310	KC2	CHB-C4A-C3A	-6.53	114.72	125.03
37	g	312	KC2	CHC-C4B-NB	6.51	133.96	124.80
30	A	846	WVN	C30-C28-C25	-6.50	118.16	127.28
37	e	609	KC2	OBD-CAD-C3D	-6.49	113.24	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	d	310	KC2	C2C-C1C-NC	6.48	118.47	110.45
37	k	310	KC2	CHC-C4B-NB	6.48	133.93	124.80
37	d	309	KC2	CHC-C4B-NB	6.48	133.92	124.80
37	g	314	KC2	C2C-C1C-NC	6.47	118.46	110.45
37	s	204	KC2	C2C-C1C-NC	6.47	118.45	110.45
27	A	856	CLA	CAA-C2A-C3A	-6.47	101.40	116.23
37	k	312	KC2	CHC-C4B-NB	6.47	133.90	124.80
37	g	314	KC2	CHB-C4A-C3A	-6.46	114.82	125.03
27	g	308	CLA	C4A-NA-C1A	6.46	109.63	106.68
37	g	314	KC2	CHC-C4B-NB	6.46	133.89	124.80
35	g	317	II0	C41-C39-C35	-6.44	118.25	127.28
37	j	610	KC2	CHC-C4B-NB	6.44	133.86	124.80
37	d	309	KC2	C2C-C1C-NC	6.43	118.42	110.45
37	k	312	KC2	CHB-C4A-C3A	-6.43	114.87	125.03
37	m	610	KC2	CHB-C4A-C3A	-6.43	114.88	125.03
37	f	611	KC2	CHC-C4B-NB	6.42	133.85	124.80
37	g	312	KC2	C2C-C1C-NC	6.42	118.39	110.45
37	n	611	KC2	CHC-C4B-NB	6.41	133.82	124.80
37	k	310	KC2	CHB-C4A-C3A	-6.41	114.92	125.03
37	c	610	KC2	CHC-C4B-NB	6.40	133.82	124.80
30	L	201	WVN	C04-C09-C05	-6.40	118.72	124.83
37	f	611	KC2	C1A-C2A-C3A	-6.39	101.41	107.28
30	B	847	WVN	C02-C11-C19	-6.37	114.67	124.58
37	n	611	KC2	C2C-C1C-NC	6.37	118.33	110.45
27	B	817	CLA	C4A-NA-C1A	6.36	109.58	106.68
27	L	202	CLA	C4A-NA-C1A	6.35	109.58	106.68
37	j	610	KC2	CHB-C4A-C3A	-6.35	115.00	125.03
37	k	310	KC2	C2C-C1C-NC	6.35	118.31	110.45
37	f	611	KC2	CHB-C4A-C3A	-6.35	115.00	125.03
27	m	603	CLA	C4A-NA-C1A	6.35	109.58	106.68
37	i	310	KC2	CHC-C4B-NB	6.35	133.74	124.80
37	m	610	KC2	C2C-C1C-NC	6.35	118.31	110.45
29	n	619	LHG	O7-C7-C8	6.34	125.21	111.48
37	g	313	KC2	CHC-C4B-NB	6.34	133.73	124.80
27	O	206	CLA	C4A-NA-C1A	6.33	109.57	106.68
37	d	309	KC2	CHB-C4A-C3A	-6.33	115.03	125.03
30	i	315	WVN	C02-C11-C19	-6.33	114.73	124.58
27	m	609	CLA	C4A-NA-C1A	6.33	109.57	106.68
37	k	312	KC2	C2C-C1C-NC	6.32	118.28	110.45
27	e	605	CLA	C4A-NA-C1A	6.32	109.56	106.68
37	m	610	KC2	CHC-C4B-NB	6.32	133.69	124.80
37	n	611	KC2	C4C-C3C-C2C	-6.31	101.48	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	n	612	KC2	C1A-C2A-C3A	-6.31	101.48	107.28
37	g	314	KC2	OBD-CAD-C3D	-6.31	113.67	128.42
27	A	815	CLA	C4A-NA-C1A	6.31	109.56	106.68
30	B	843	WVN	C04-C09-C05	-6.30	118.81	124.83
37	j	610	KC2	C4C-C3C-C2C	-6.30	101.49	107.28
27	l	303	CLA	C4A-NA-C1A	6.30	109.55	106.68
36	a	317	IHT	C30-C27-C23	-6.29	118.45	127.28
37	g	313	KC2	C4C-C3C-C2C	-6.29	101.50	107.28
36	j	616	IHT	C18-C22-C23	-6.29	116.93	126.23
37	d	310	KC2	C1A-C2A-C3A	-6.29	101.50	107.28
30	A	847	WVN	C39-C36-C32	-6.28	118.47	127.28
30	i	315	WVN	C21-C15-C13	-6.28	117.63	124.48
37	i	310	KC2	C2C-C1C-NC	6.27	118.21	110.45
37	c	610	KC2	CHB-C4A-C3A	-6.27	115.13	125.03
37	j	610	KC2	C2C-C1C-NC	6.27	118.21	110.45
37	j	610	KC2	OBD-CAD-C3D	-6.27	113.77	128.42
27	B	829	CLA	C4A-NA-C1A	6.26	109.54	106.68
30	R	202	WVN	C02-C11-C19	-6.26	114.84	124.58
37	n	611	KC2	OBD-CAD-C3D	-6.25	113.82	128.42
27	A	832	CLA	C4A-NA-C1A	6.24	109.53	106.68
37	e	609	KC2	CHB-C4A-C3A	-6.24	115.18	125.03
37	f	611	KC2	C2C-C1C-NC	6.23	118.16	110.45
37	l	311	KC2	C4C-C3C-C2C	-6.22	101.56	107.28
30	B	845	WVN	C35-C32-C31	6.21	127.58	118.09
30	B	848	WVN	C38-C34-C33	6.21	127.58	118.09
35	l	302	II0	C41-C42-C40	-6.21	110.81	123.52
27	a	306	CLA	C4A-NA-C1A	6.21	109.51	106.68
27	l	307	CLA	C4A-NA-C1A	6.21	109.51	106.68
27	b	607	CLA	CAC-C3C-C4C	-6.20	116.72	124.79
37	f	611	KC2	C4C-C3C-C2C	-6.19	101.59	107.28
27	k	305	CLA	C4A-NA-C1A	6.18	109.50	106.68
37	d	310	KC2	CHC-C4B-NB	6.18	133.50	124.80
35	c	614	II0	C41-C39-C35	-6.18	118.62	127.28
37	g	314	KC2	C4C-C3C-C2C	-6.17	101.61	107.28
30	h	309	WVN	C29-C26-C22	-6.16	118.64	127.28
36	f	617	IHT	C19-C10-C07	-6.16	117.76	124.48
37	n	611	KC2	C1A-C2A-C3A	-6.16	101.62	107.28
27	O	202	CLA	C4A-NA-C1A	6.15	109.49	106.68
27	m	606	CLA	C4A-NA-C1A	6.15	109.49	106.68
27	B	812	CLA	C4A-NA-C1A	6.15	109.48	106.68
30	A	847	WVN	C30-C28-C25	-6.15	118.66	127.28
37	k	310	KC2	C1A-C2A-C3A	-6.13	101.64	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	605	CLA	C4A-NA-C1A	6.13	109.48	106.68
37	c	610	KC2	C2C-C1C-NC	6.13	118.04	110.45
35	l	314	II0	C42-C40-C36	-6.13	118.68	127.28
27	k	304	CLA	C4A-NA-C1A	6.12	109.47	106.68
37	k	310	KC2	C4C-C3C-C2C	-6.12	101.66	107.28
37	g	313	KC2	OBD-CAD-C3D	-6.10	114.15	128.42
36	R	204	IHT	C40-C37-C33	-6.10	118.72	127.28
30	B	846	WVN	C40-C37-C34	-6.09	118.74	127.28
37	i	317	KC2	C1A-C2A-C3A	-6.09	101.68	107.28
27	h	303	CLA	C4A-NA-C1A	6.08	109.45	106.68
27	B	803	CLA	C4A-NA-C1A	6.08	109.45	106.68
27	B	832	CLA	C4A-NA-C1A	6.08	109.45	106.68
35	l	315	II0	C42-C40-C36	-6.08	118.75	127.28
37	e	609	KC2	C1A-C2A-C3A	-6.08	101.69	107.28
36	k	317	IHT	C18-C22-C23	-6.07	117.25	126.23
27	b	601	CLA	C4A-NA-C1A	6.07	109.45	106.68
36	g	319	IHT	C41-C38-C35	-6.07	118.77	127.28
27	d	305	CLA	C4A-NA-C1A	6.06	109.44	106.68
27	B	820	CLA	C4A-NA-C1A	6.05	109.44	106.68
37	k	311	KC2	OBD-CAD-C3D	-6.04	114.29	128.42
37	s	201	KC2	C2C-C1C-NC	6.04	117.93	110.45
30	l	316	WVN	C08-C01-C07	-6.04	99.08	107.87
27	e	602	CLA	C4A-NA-C1A	6.03	109.43	106.68
37	k	311	KC2	C4C-C3C-C2C	-6.03	101.74	107.28
27	A	811	CLA	C4A-NA-C1A	6.02	109.42	106.68
37	n	612	KC2	CHB-C1B-NB	6.01	133.27	124.80
27	m	605	CLA	C4A-NA-C1A	6.01	109.42	106.68
27	A	828	CLA	C4A-NA-C1A	6.01	109.42	106.68
36	c	616	IHT	C40-C37-C33	-6.00	118.87	127.28
36	g	319	IHT	C19-C10-C07	-5.99	117.94	124.48
37	c	610	KC2	C1A-C2A-C3A	-5.99	101.78	107.28
30	F	204	WVN	C20-C23-C25	-5.99	117.38	126.23
27	A	803	CLA	C4A-NA-C1A	5.98	109.41	106.68
27	A	808	CLA	C4A-NA-C1A	5.97	109.40	106.68
37	k	312	KC2	C4C-C3C-C2C	-5.97	101.79	107.28
30	L	201	WVN	C08-C01-C02	-5.97	100.51	109.55
27	b	603	CLA	C4A-NA-C1A	5.96	109.40	106.68
35	j	614	II0	C41-C39-C35	-5.96	118.93	127.28
37	l	311	KC2	C1A-C2A-C3A	-5.95	101.81	107.28
35	f	618	II0	C41-C39-C35	-5.95	118.93	127.28
27	g	307	CLA	C4A-NA-C1A	5.95	109.39	106.68
27	B	835	CLA	C4A-NA-C1A	5.95	109.39	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	m	610	KC2	C1A-C2A-C3A	-5.95	101.81	107.28
37	j	610	KC2	C1A-C2A-C3A	-5.94	101.82	107.28
37	g	313	KC2	C1A-C2A-C3A	-5.94	101.82	107.28
30	A	846	WVN	C04-C09-C05	-5.93	119.17	124.83
35	c	617	II0	C42-C40-C36	-5.93	118.97	127.28
35	h	312	II0	C42-C40-C36	-5.92	118.97	127.28
27	m	604	CLA	C4A-NA-C1A	5.92	109.38	106.68
27	c	602	CLA	CAC-C3C-C4C	5.92	132.49	124.79
37	e	609	KC2	C4C-C3C-C2C	-5.90	101.85	107.28
37	d	309	KC2	C1A-C2A-C3A	-5.90	101.85	107.28
27	h	304	CLA	C4A-NA-C1A	5.89	109.37	106.68
30	J	101	WVN	C02-C11-C19	-5.89	115.41	124.58
27	B	802	CLA	C4A-NA-C1A	5.89	109.37	106.68
35	h	312	II0	C41-C39-C35	-5.89	119.02	127.28
37	s	201	KC2	C4C-C3C-C2C	-5.89	101.87	107.28
37	n	612	KC2	C2C-C1C-NC	5.89	117.73	110.45
36	O	204	IHT	C41-C38-C35	-5.88	119.03	127.28
36	c	616	IHT	C02-C07-C10	-5.88	114.60	122.64
37	n	612	KC2	CHC-C4B-C3B	-5.88	115.29	125.21
37	s	204	KC2	CMD-C2D-C1D	-5.87	116.48	125.42
37	i	317	KC2	C4C-C3C-C2C	-5.86	101.89	107.28
30	A	848	WVN	C20-C23-C25	-5.86	117.57	126.23
37	c	610	KC2	OBD-CAD-C3D	-5.85	114.73	128.42
27	e	606	CLA	C4A-NA-C1A	5.85	109.35	106.68
37	i	310	KC2	C4C-C3C-C2C	-5.85	101.91	107.28
37	d	309	KC2	OBD-CAD-C3D	-5.84	114.77	128.42
35	j	613	II0	C42-C40-C36	-5.83	119.10	127.28
37	s	204	KC2	C4C-C3C-C2C	-5.83	101.92	107.28
27	A	805	CLA	C4A-NA-C1A	5.82	109.34	106.68
30	L	201	WVN	C39-C36-C32	-5.81	119.13	127.28
37	m	610	KC2	C4C-C3C-C2C	-5.81	101.94	107.28
35	l	317	II0	C42-C40-C36	-5.80	119.14	127.28
27	j	611	CLA	C4A-NA-C1A	5.80	109.32	106.68
37	f	611	KC2	OBD-CAD-C3D	-5.80	114.87	128.42
37	k	312	KC2	C1A-C2A-C3A	-5.80	101.95	107.28
27	B	818	CLA	C4A-NA-C1A	5.79	109.32	106.68
37	d	309	KC2	C4C-C3C-C2C	-5.77	101.97	107.28
35	n	618	II0	C41-C39-C35	-5.77	119.19	127.28
37	d	310	KC2	OBD-CAD-C3D	-5.77	114.93	128.42
27	A	812	CLA	C4A-NA-C1A	5.76	109.31	106.68
35	e	614	II0	C41-C39-C35	-5.76	119.20	127.28
37	k	310	KC2	OBD-CAD-C3D	-5.76	114.96	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	848	WVN	C20-C23-C25	-5.75	117.73	126.23
35	i	318	II0	C41-C39-C35	-5.75	119.22	127.28
27	B	840	CLA	C4A-NA-C1A	5.75	109.30	106.68
37	k	312	KC2	OBD-CAD-C3D	-5.74	114.99	128.42
30	l	316	WVN	C29-C26-C22	-5.74	119.23	127.28
27	n	602	CLA	C4A-NA-C1A	5.73	109.30	106.68
27	n	603	CLA	C4A-NA-C1A	5.73	109.29	106.68
35	g	320	II0	C41-C39-C35	-5.73	119.25	127.28
30	L	201	WVN	C40-C37-C34	-5.73	119.25	127.28
27	d	307	CLA	C4A-NA-C1A	5.72	109.29	106.68
27	A	830	CLA	C4A-NA-C1A	5.72	109.29	106.68
37	s	201	KC2	CHC-C4B-C3B	-5.71	115.58	125.21
30	B	846	WVN	C02-C11-C19	-5.70	115.70	124.58
35	e	613	II0	C41-C39-C35	-5.70	119.28	127.28
27	F	201	CLA	C4A-NA-C1A	5.70	109.28	106.68
27	d	304	CLA	C4A-NA-C1A	5.69	109.28	106.68
37	g	312	KC2	OBD-CAD-C3D	-5.69	115.11	128.42
37	n	612	KC2	CHB-C1B-C2B	-5.69	113.66	125.49
30	A	848	WVN	C08-C01-C02	5.68	118.15	109.55
35	g	318	II0	C41-C39-C35	-5.67	119.32	127.28
35	k	318	II0	C42-C40-C36	-5.67	119.32	127.28
37	i	317	KC2	CHD-C1D-ND	-5.67	115.54	124.05
37	m	610	KC2	OBD-CAD-C3D	-5.66	115.17	128.42
37	c	610	KC2	C4C-C3C-C2C	-5.66	102.07	107.28
27	B	837	CLA	C4A-NA-C1A	5.66	109.26	106.68
37	n	612	KC2	OBD-CAD-C3D	-5.66	115.19	128.42
37	d	310	KC2	C4C-C3C-C2C	-5.65	102.08	107.28
35	h	311	II0	C42-C40-C36	-5.65	119.35	127.28
37	g	312	KC2	C4C-C3C-C2C	-5.65	102.09	107.28
34	L	208	LMG	O7-C10-C11	5.65	123.70	111.48
27	f	601	CLA	C4A-NA-C1A	5.64	109.25	106.68
27	e	611	CLA	C4A-NA-C1A	5.64	109.25	106.68
37	i	317	KC2	CHC-C1C-NC	-5.64	115.49	124.23
36	k	317	IHT	C40-C37-C33	-5.64	119.37	127.28
27	A	838	CLA	C4A-NA-C1A	5.63	109.25	106.68
27	A	815	CLA	CMB-C2B-C1B	-5.63	116.84	125.42
30	F	204	WVN	C39-C40-C37	-5.63	112.00	123.52
37	s	204	KC2	CHB-C4A-C3A	-5.63	116.15	125.03
37	k	310	KC2	CMD-C2D-C1D	-5.62	116.86	125.42
36	a	317	IHT	C41-C38-C35	-5.62	119.40	127.28
35	h	310	II0	C42-C40-C36	-5.62	119.40	127.28
27	B	810	CLA	C4A-NA-C1A	5.61	109.24	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	618	LHG	O7-C7-C8	5.61	123.61	111.48
35	i	313	II0	C41-C39-C35	-5.61	119.42	127.28
35	m	614	II0	C42-C41-C39	-5.59	112.09	123.52
37	g	314	KC2	C1A-C2A-C3A	-5.58	102.15	107.28
29	e	617	LHG	O7-C7-C8	5.58	123.56	111.48
29	g	301	LHG	O7-C7-C8	5.58	123.55	111.48
35	n	615	II0	C41-C39-C35	-5.57	119.46	127.28
27	B	827	CLA	C4A-NA-C1A	5.57	109.22	106.68
30	l	301	WVN	C30-C28-C25	-5.56	119.48	127.28
27	k	307	CLA	C4A-NA-C1A	5.56	109.22	106.68
30	F	204	WVN	C06-C13-C15	-5.56	115.04	122.64
30	O	201	WVN	C02-C11-C19	-5.56	115.93	124.58
35	h	312	II0	C18-C04-C17	-5.56	92.73	108.63
30	J	102	WVN	C39-C36-C32	-5.55	119.49	127.28
30	L	205	WVN	C29-C26-C22	-5.55	119.50	127.28
27	n	609	CLA	C4A-NA-C1A	5.55	109.21	106.68
35	b	612	II0	C42-C40-C36	-5.54	119.50	127.28
36	c	616	IHT	C09-C10-C07	-5.54	115.22	122.70
30	h	309	WVN	C21-C15-C13	-5.54	118.44	124.48
35	d	314	II0	C41-C42-C40	-5.54	112.18	123.52
27	a	307	CLA	C4A-NA-C1A	5.54	109.21	106.68
27	g	311	CLA	C4A-NA-C1A	5.54	109.21	106.68
30	l	316	WVN	C02-C11-C19	-5.53	115.97	124.58
35	f	615	II0	C41-C39-C35	-5.53	119.52	127.28
30	e	615	WVN	C30-C28-C25	-5.52	119.53	127.28
37	f	611	KC2	CMD-C2D-C1D	-5.52	117.01	125.42
35	f	616	II0	C42-C40-C36	-5.52	119.54	127.28
27	A	842	CLA	C4A-NA-C1A	5.52	109.20	106.68
27	K	102	CLA	C4A-NA-C1A	5.51	109.19	106.68
35	O	203	II0	C42-C40-C36	-5.51	119.55	127.28
27	a	310	CLA	C4A-NA-C1A	5.50	109.19	106.68
27	g	305	CLA	C4A-NA-C1A	5.50	109.19	106.68
37	l	311	KC2	CMD-C2D-C1D	-5.49	117.05	125.42
37	s	201	KC2	OBD-CAD-C3D	-5.49	115.58	128.42
37	g	312	KC2	C1A-C2A-C3A	-5.49	102.23	107.28
27	A	833	CLA	C4A-NA-C1A	5.48	109.18	106.68
36	b	614	IHT	C19-C10-C07	-5.48	118.50	124.48
27	i	302	CLA	C4A-NA-C1A	5.48	109.18	106.68
27	l	310	CLA	C4A-NA-C1A	5.47	109.18	106.68
35	f	614	II0	C20-C14-C10	-5.46	113.95	124.16
36	j	616	IHT	C02-C07-C10	-5.46	115.18	122.64
27	s	203	CLA	C4A-NA-C1A	5.46	109.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	610	KC2	CMD-C2D-C1D	-5.45	117.12	125.42
36	c	616	IHT	C30-C27-C23	-5.44	119.65	127.28
35	c	614	II0	C42-C40-C36	-5.44	119.65	127.28
37	s	204	KC2	CHC-C4B-NB	5.42	132.43	124.80
35	g	320	II0	C42-C40-C36	-5.42	119.68	127.28
36	n	617	IHT	C09-C10-C07	-5.42	115.38	122.70
30	h	309	WVN	C04-C09-C05	-5.41	119.66	124.83
27	A	855	CLA	C4A-NA-C1A	5.41	109.15	106.68
35	j	613	II0	C41-C42-C40	-5.41	112.45	123.52
37	s	204	KC2	C4B-C3B-C2B	-5.41	102.12	106.81
37	g	312	KC2	CMD-C2D-C1D	-5.41	117.18	125.42
37	j	610	KC2	CHD-C4C-C3C	-5.41	107.72	125.91
37	n	612	KC2	CHC-C4B-NB	5.40	132.40	124.80
36	O	204	IHT	C02-C07-C10	-5.40	115.26	122.64
37	n	611	KC2	CHC-C1C-NC	-5.38	115.89	124.23
27	g	322	CLA	C4A-NA-C1A	5.38	109.13	106.68
30	A	849	WVN	C30-C28-C25	-5.38	119.74	127.28
27	g	306	CLA	C4A-NA-C1A	5.37	109.13	106.68
27	B	816	CLA	C4A-NA-C1A	5.37	109.13	106.68
37	d	310	KC2	CHB-C4A-C3A	-5.37	116.55	125.03
35	c	617	II0	C20-C14-C10	-5.36	114.13	124.16
37	s	201	KC2	C1B-CHB-C4A	-5.36	114.63	126.02
27	B	823	CLA	C4A-NA-C1A	5.35	109.12	106.68
35	J	104	II0	C42-C40-C36	-5.35	119.77	127.28
35	e	614	II0	C42-C40-C36	-5.35	119.78	127.28
27	j	602	CLA	C4A-NA-C1A	5.34	109.12	106.68
27	A	802	CLA	CMB-C2B-C1B	-5.34	117.28	125.42
37	d	310	KC2	CHD-C4C-C3C	-5.34	107.93	125.91
37	i	310	KC2	C1A-C2A-C3A	-5.34	102.37	107.28
30	l	301	WVN	C04-C09-C05	-5.34	119.73	124.83
30	B	844	WVN	C30-C28-C25	-5.33	119.80	127.28
37	n	612	KC2	CHD-C4C-C3C	-5.33	107.97	125.91
35	b	613	II0	C42-C40-C36	-5.33	119.80	127.28
37	n	611	KC2	CHD-C4C-C3C	-5.33	107.98	125.91
27	A	835	CLA	C4A-NA-C1A	5.33	109.11	106.68
27	A	823	CLA	C4A-NA-C1A	5.32	109.11	106.68
37	i	317	KC2	C1D-ND-C4D	5.32	110.05	106.31
30	B	848	WVN	C04-C09-C05	-5.32	119.75	124.83
37	s	201	KC2	C3A-C4A-NA	5.32	117.03	110.45
37	i	317	KC2	CHD-C4C-C3C	-5.31	108.03	125.91
35	a	315	II0	C41-C39-C35	-5.30	119.84	127.28
36	n	617	IHT	C40-C37-C33	-5.30	119.85	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	809	CLA	C4A-NA-C1A	5.29	109.09	106.68
37	k	311	KC2	C1B-CHB-C4A	-5.29	114.77	126.02
27	j	609	CLA	O2D-CGD-CBD	5.29	120.48	111.23
27	B	839	CLA	C4A-NA-C1A	5.29	109.09	106.68
36	f	617	IHT	C09-C10-C07	-5.28	115.56	122.70
30	M	101	WVN	C20-C23-C25	-5.28	118.42	126.23
36	m	616	IHT	C40-C37-C33	-5.28	119.87	127.28
35	f	615	II0	C42-C40-C36	-5.27	119.89	127.28
37	g	313	KC2	CMD-C2D-C1D	-5.27	117.39	125.42
30	I	101	WVN	C29-C26-C22	-5.27	119.89	127.28
37	f	611	KC2	CHD-C4C-C3C	-5.26	108.19	125.91
36	n	617	IHT	C41-C38-C35	-5.26	119.90	127.28
35	J	104	II0	C32-C34-C36	-5.26	111.95	126.36
27	A	822	CLA	C4A-NA-C1A	5.26	109.08	106.68
35	n	616	II0	C41-C39-C35	-5.25	119.91	127.28
30	s	207	WVN	C30-C28-C25	-5.25	119.91	127.28
37	c	610	KC2	CMD-C2D-C1D	-5.25	117.43	125.42
27	g	322	CLA	CAC-C3C-C4C	5.25	131.62	124.79
30	J	101	WVN	C30-C28-C25	-5.24	119.92	127.28
27	j	609	CLA	C4A-NA-C1A	5.24	109.07	106.68
36	c	616	IHT	C41-C38-C35	-5.24	119.93	127.28
27	B	835	CLA	CAC-C3C-C4C	5.24	131.60	124.79
35	f	614	II0	C41-C39-C35	-5.24	119.94	127.28
27	A	853	CLA	C4A-NA-C1A	5.23	109.07	106.68
35	d	312	II0	C19-C13-C11	5.23	124.03	114.42
37	d	310	KC2	CHC-C1C-NC	-5.23	116.13	124.23
30	l	301	WVN	C40-C37-C34	-5.23	119.95	127.28
37	n	611	KC2	CHB-C1B-NB	5.22	132.16	124.80
30	s	205	WVN	C02-C11-C19	-5.22	116.46	124.58
30	B	846	WVN	C21-C15-C13	-5.22	118.79	124.48
27	c	608	CLA	C4A-NA-C1A	5.22	109.06	106.68
37	l	311	KC2	OBD-CAD-C3D	-5.21	116.23	128.42
37	d	310	KC2	CMD-C2D-C1D	-5.20	117.50	125.42
37	l	311	KC2	CHD-C4C-C3C	-5.20	108.41	125.91
27	l	308	CLA	C4A-NA-C1A	5.20	109.05	106.68
37	g	314	KC2	CHD-C4C-C3C	-5.20	108.42	125.91
27	b	604	CLA	C4A-NA-C1A	5.19	109.05	106.68
37	i	317	KC2	CMD-C2D-C1D	-5.19	117.52	125.42
37	i	310	KC2	CHD-C4C-C3C	-5.19	108.45	125.91
29	j	617	LHG	O7-C7-C8	5.19	122.70	111.48
35	b	612	II0	C41-C39-C35	-5.19	120.00	127.28
37	k	310	KC2	CHB-C1B-NB	5.18	132.10	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	k	312	KC2	CHB-C1B-NB	5.18	132.09	124.80
37	e	609	KC2	CHD-C4C-C3C	-5.18	108.49	125.91
37	c	610	KC2	CHD-C4C-C3C	-5.17	108.51	125.91
37	s	204	KC2	C1D-ND-C4D	5.16	109.94	106.31
27	n	605	CLA	CAC-C3C-C4C	5.16	131.50	124.79
30	F	205	WVN	C30-C33-C34	-5.15	112.23	126.36
27	A	820	CLA	C4A-NA-C1A	5.15	109.03	106.68
37	m	610	KC2	CHB-C1B-NB	5.15	132.06	124.80
27	A	806	CLA	C4A-NA-C1A	5.15	109.03	106.68
27	B	815	CLA	C4A-NA-C1A	5.15	109.03	106.68
37	k	310	KC2	CHC-C1C-NC	-5.14	116.26	124.23
37	g	312	KC2	CHD-C4C-C3C	-5.14	108.60	125.91
36	g	319	IHT	C18-C22-C23	-5.14	118.63	126.23
35	f	615	II0	C19-C13-C11	5.13	123.86	114.42
37	c	610	KC2	CHB-C1B-NB	5.13	132.03	124.80
37	k	310	KC2	CHD-C4C-C3C	-5.13	108.65	125.91
27	b	607	CLA	C4A-NA-C1A	5.12	109.02	106.68
37	k	312	KC2	CHD-C4C-C3C	-5.12	108.68	125.91
30	B	848	WVN	C30-C28-C25	-5.12	120.10	127.28
30	F	204	WVN	C02-C11-C19	-5.11	116.62	124.58
27	c	601	CLA	C4A-NA-C1A	5.11	109.01	106.68
37	c	610	KC2	CHC-C1C-NC	-5.11	116.31	124.23
37	f	611	KC2	CHC-C1C-NC	-5.11	116.31	124.23
27	B	801	CLA	C4A-NA-C1A	5.11	109.01	106.68
37	f	611	KC2	CHB-C1B-NB	5.11	131.99	124.80
36	n	617	IHT	C02-C07-C10	-5.10	115.66	122.64
27	d	303	CLA	C4A-NA-C1A	5.10	109.01	106.68
37	m	610	KC2	CHD-C4C-C3C	-5.10	108.75	125.91
30	A	847	WVN	C11-C19-C22	-5.10	115.36	126.32
30	F	204	WVN	C26-C29-C31	-5.08	108.47	123.20
37	d	309	KC2	CHD-C4C-C3C	-5.08	108.81	125.91
30	R	202	WVN	C39-C36-C32	-5.08	120.15	127.28
37	g	314	KC2	CHB-C1B-NB	5.08	131.95	124.80
30	i	315	WVN	C29-C26-C22	-5.08	120.16	127.28
27	k	309	CLA	O2D-CGD-O1D	-5.07	113.98	123.85
37	j	610	KC2	CHC-C1C-NC	-5.07	116.37	124.23
37	d	309	KC2	CHB-C1B-NB	5.07	131.94	124.80
36	j	616	IHT	C09-C10-C07	-5.07	115.85	122.70
27	b	608	CLA	C4A-NA-C1A	5.07	108.99	106.68
27	n	604	CLA	C4A-NA-C1A	5.06	108.99	106.68
30	B	843	WVN	C02-C11-C19	5.06	132.45	124.58
37	l	311	KC2	CHC-C1C-NC	-5.05	116.40	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	n	612	KC2	CMD-C2D-C1D	-5.05	117.72	125.42
37	i	310	KC2	CHB-C1B-NB	5.05	131.91	124.80
37	k	311	KC2	C3A-C4A-NA	5.05	116.70	110.45
36	k	317	IHT	C41-C38-C35	-5.05	120.20	127.28
37	m	610	KC2	CHC-C1C-NC	-5.04	116.41	124.23
37	e	609	KC2	CHB-C1B-NB	5.04	131.90	124.80
37	k	311	KC2	CHD-C4C-C3C	-5.04	108.96	125.91
35	f	616	II0	C41-C39-C35	-5.03	120.22	127.28
37	g	312	KC2	CHB-C1B-NB	5.03	131.89	124.80
35	i	318	II0	C31-C33-C35	-5.03	112.56	126.36
27	A	814	CLA	C4A-NA-C1A	5.03	108.97	106.68
35	e	612	II0	C42-C40-C36	-5.03	120.22	127.28
30	A	847	WVN	C04-C09-C05	-5.03	120.03	124.83
29	c	621	LHG	O7-C7-C8	5.03	122.36	111.48
37	e	609	KC2	CHC-C1C-NC	-5.02	116.44	124.23
30	B	843	WVN	C11-C19-C22	5.02	137.13	126.32
27	n	610	CLA	C4A-NA-C1A	5.02	108.97	106.68
37	s	204	KC2	O2D-CGD-CBD	5.02	120.01	111.23
35	l	313	II0	C42-C40-C36	-5.02	120.24	127.28
27	l	305	CLA	C4A-NA-C1A	5.01	108.97	106.68
36	f	617	IHT	C18-C22-C23	-5.01	118.82	126.23
37	i	317	KC2	C4B-C3B-C2B	-5.01	102.47	106.81
37	j	610	KC2	CHB-C1B-NB	5.00	131.83	124.80
37	g	313	KC2	C4B-CHC-C1C	-4.99	115.41	126.02
37	n	612	KC2	C4B-CHC-C1C	-4.99	115.41	126.02
27	b	611	CLA	C4A-NA-C1A	4.99	108.95	106.68
30	B	847	WVN	C30-C28-C25	-4.98	120.29	127.28
30	M	101	WVN	C07-C01-C02	4.98	117.09	109.55
35	m	615	II0	C41-C39-C35	-4.98	120.30	127.28
27	b	602	CLA	C4A-NA-C1A	4.97	108.95	106.68
27	m	602	CLA	C4A-NA-C1A	4.97	108.95	106.68
27	a	308	CLA	C4A-NA-C1A	4.97	108.95	106.68
27	l	304	CLA	O2D-CGD-O1D	-4.97	114.17	123.85
37	g	313	KC2	CHC-C1C-NC	-4.97	116.53	124.23
37	s	201	KC2	CHD-C4C-C3C	-4.96	109.22	125.91
37	g	314	KC2	CMD-C2D-C1D	-4.95	117.88	125.42
27	l	304	CLA	C4A-NA-C1A	4.95	108.94	106.68
37	c	610	KC2	C4B-CHC-C1C	-4.95	115.50	126.02
37	s	204	KC2	OBD-CAD-C3D	-4.95	116.85	128.42
37	d	309	KC2	CHC-C1C-NC	-4.95	116.56	124.23
37	g	312	KC2	CHC-C1C-NC	-4.95	116.56	124.23
30	s	205	WVN	C20-C23-C25	-4.95	118.92	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	n	611	KC2	C4B-CHC-C1C	-4.95	115.51	126.02
37	g	313	KC2	CHD-C4C-C3C	-4.94	109.30	125.91
30	L	201	WVN	C07-C01-C02	4.94	117.02	109.55
35	k	318	II0	C19-C13-C11	4.93	123.49	114.42
27	b	610	CLA	O2D-CGD-O1D	-4.93	114.25	123.85
30	A	846	WVN	C39-C36-C32	-4.92	120.37	127.28
37	k	312	KC2	CHC-C1C-NC	-4.92	116.60	124.23
37	i	310	KC2	CHC-C1C-NC	-4.92	116.60	124.23
37	g	314	KC2	CHC-C1C-NC	-4.92	116.60	124.23
37	s	201	KC2	CHD-C1D-ND	-4.92	116.66	124.05
37	n	612	KC2	C4C-C3C-C2C	-4.92	102.75	107.28
35	h	311	II0	C20-C14-C12	4.92	123.47	114.42
30	A	849	WVN	C39-C36-C32	-4.92	120.38	127.28
35	g	316	II0	C42-C40-C36	-4.92	120.38	127.28
37	k	311	KC2	C4B-CHC-C1C	-4.91	115.58	126.02
37	l	311	KC2	C3A-C4A-NA	4.91	116.53	110.45
37	l	311	KC2	CHB-C1B-NB	4.91	131.71	124.80
27	B	802	CLA	CMB-C2B-C1B	-4.91	117.95	125.42
35	c	614	II0	C20-C14-C12	4.90	123.44	114.42
35	e	614	II0	C16-C03-C09	-4.90	101.73	110.52
27	l	307	CLA	C2A-C1A-CHA	4.90	132.37	123.87
30	A	847	WVN	C19-C22-C26	4.90	126.72	119.01
37	s	201	KC2	CHC-C4B-NB	4.90	131.70	124.80
30	M	101	WVN	C40-C37-C34	-4.90	120.41	127.28
37	i	310	KC2	CMD-C2D-C1D	-4.89	117.97	125.42
29	a	319	LHG	O7-C7-C8	4.89	122.07	111.48
30	s	205	WVN	C39-C36-C32	-4.89	120.42	127.28
37	g	313	KC2	CHB-C1B-NB	4.89	131.68	124.80
27	A	841	CLA	C4A-NA-C1A	4.89	108.91	106.68
37	n	612	KC2	C3A-C4A-NA	4.88	116.49	110.45
30	R	202	WVN	C40-C37-C34	-4.88	120.43	127.28
37	g	312	KC2	C4B-CHC-C1C	-4.88	115.65	126.02
27	f	604	CLA	C4A-NA-C1A	4.87	108.90	106.68
27	l	304	CLA	O2D-CGD-CBD	4.87	119.75	111.23
35	c	617	II0	C19-C13-C09	-4.87	115.06	124.16
33	B	842	DGD	O2G-C1B-C2B	4.87	122.02	111.48
27	s	209	CLA	C4A-NA-C1A	4.87	108.90	106.68
36	b	614	IHT	C41-C38-C35	-4.86	120.46	127.28
37	k	311	KC2	CHC-C1C-NC	-4.86	116.69	124.23
37	d	309	KC2	CMD-C2D-C1D	-4.86	118.03	125.42
35	d	312	II0	C41-C39-C35	-4.85	120.47	127.28
27	s	208	CLA	C4A-NA-C1A	4.85	108.89	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	n	614	II0	C42-C41-C39	-4.85	113.60	123.52
30	h	309	WVN	C30-C28-C25	-4.85	120.48	127.28
27	B	826	CLA	C4A-NA-C1A	4.85	108.89	106.68
35	g	316	II0	C19-C13-C09	-4.84	115.11	124.16
36	m	616	IHT	C30-C27-C23	-4.84	120.50	127.28
27	A	837	CLA	C4A-NA-C1A	4.84	108.89	106.68
37	l	311	KC2	C4B-CHC-C1C	-4.83	115.75	126.02
30	l	316	WVN	C06-C13-C15	-4.83	116.04	122.64
37	e	609	KC2	C4B-CHC-C1C	-4.83	115.76	126.02
37	m	610	KC2	CMD-C2D-C1D	-4.83	118.07	125.42
27	R	203	CLA	CAA-C2A-C3A	-4.83	99.96	113.00
27	B	836	CLA	C4A-NA-C1A	4.82	108.88	106.68
37	m	610	KC2	C4B-CHC-C1C	-4.81	115.79	126.02
27	A	829	CLA	CMB-C2B-C1B	-4.81	118.09	125.42
35	a	316	II0	C42-C40-C36	-4.81	120.53	127.28
37	k	312	KC2	CMD-C2D-C1D	-4.81	118.10	125.42
37	j	610	KC2	C4B-CHC-C1C	-4.81	115.80	126.02
27	b	606	CLA	C4A-NA-C1A	4.81	108.87	106.68
37	g	314	KC2	C4B-CHC-C1C	-4.81	115.80	126.02
27	j	603	CLA	C4A-NA-C1A	4.80	108.87	106.68
30	i	315	WVN	C30-C28-C25	-4.80	120.54	127.28
27	n	605	CLA	C4A-NA-C1A	4.80	108.87	106.68
30	K	103	WVN	C30-C28-C25	-4.80	120.54	127.28
36	R	204	IHT	C02-C07-C10	-4.80	116.08	122.64
35	h	312	II0	C41-C42-C40	-4.80	113.70	123.52
27	a	305	CLA	C4A-NA-C1A	4.79	108.86	106.68
37	i	317	KC2	CHC-C4B-C3B	-4.79	117.13	125.21
27	A	820	CLA	CMB-C2B-C1B	-4.79	118.12	125.42
35	a	318	II0	C28-C26-C30	-4.78	114.89	124.18
27	B	822	CLA	C4A-NA-C1A	4.78	108.86	106.68
35	l	315	II0	C19-C13-C11	4.78	123.20	114.42
35	h	310	II0	C41-C39-C35	-4.78	120.58	127.28
29	i	316	LHG	O7-C7-C8	4.77	121.81	111.48
37	k	312	KC2	C4B-CHC-C1C	-4.77	115.89	126.02
35	l	315	II0	C19-C13-C09	-4.76	115.26	124.16
37	i	317	KC2	C4B-CHC-C1C	-4.76	115.91	126.02
37	d	309	KC2	C4B-CHC-C1C	-4.76	115.91	126.02
27	f	602	CLA	C4A-NA-C1A	4.75	108.85	106.68
30	A	847	WVN	C26-C29-C31	-4.75	109.43	123.20
35	a	314	II0	C41-C39-C35	-4.75	120.61	127.28
37	s	204	KC2	CHD-C1D-ND	-4.75	116.93	124.05
37	f	611	KC2	C4B-CHC-C1C	-4.75	115.93	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	i	310	KC2	C1D-ND-C4D	4.74	109.64	106.31
37	g	313	KC2	C3A-C4A-NA	4.74	116.31	110.45
35	f	618	II0	C41-C42-C40	-4.73	113.83	123.52
37	l	311	KC2	C1B-CHB-C4A	-4.73	115.96	126.02
37	n	612	KC2	CHD-C1D-ND	-4.73	116.95	124.05
37	c	610	KC2	C1D-ND-C4D	4.73	109.63	106.31
37	d	310	KC2	CHD-C1D-ND	-4.73	116.95	124.05
30	M	101	WVN	C01-C02-C11	-4.73	107.39	112.83
37	d	310	KC2	CHB-C1B-NB	4.72	131.45	124.80
36	c	620	IHT	C41-C38-C35	-4.72	120.66	127.28
27	c	606	CLA	O2D-CGD-O1D	-4.72	114.66	123.85
36	j	616	IHT	C41-C38-C35	-4.71	120.67	127.28
37	i	310	KC2	C4B-CHC-C1C	-4.71	116.00	126.02
27	J	103	CLA	C4A-NA-C1A	4.71	108.83	106.68
35	a	318	II0	C34-C36-C40	4.71	126.42	119.01
36	f	617	IHT	C41-C38-C35	-4.71	120.68	127.28
35	j	614	II0	C42-C40-C36	-4.70	120.68	127.28
27	e	604	CLA	O2D-CGD-O1D	-4.70	114.70	123.85
36	f	617	IHT	C40-C37-C33	-4.70	120.69	127.28
30	J	101	WVN	C23-C25-C28	4.69	126.39	119.01
30	s	205	WVN	C04-C09-C05	-4.69	120.35	124.83
37	m	610	KC2	CHB-C1B-C2B	-4.69	115.73	125.49
37	s	204	KC2	CHB-C1B-C2B	-4.69	115.74	125.49
37	k	310	KC2	C4B-CHC-C1C	-4.67	116.08	126.02
36	R	204	IHT	C18-C22-C23	-4.67	119.32	126.23
27	n	601	CLA	C4A-NA-C1A	4.67	108.81	106.68
37	k	311	KC2	C1D-ND-C4D	4.67	109.59	106.31
37	s	204	KC2	C4B-CHC-C1C	-4.66	116.11	126.02
30	A	847	WVN	C24-C22-C26	-4.66	115.26	122.82
27	e	607	CLA	C4A-NA-C1A	4.66	108.81	106.68
27	b	602	CLA	O2D-CGD-CBD	4.66	119.38	111.23
37	k	310	KC2	C3A-C4A-NA	4.66	116.21	110.45
37	n	612	KC2	CHC-C1C-NC	-4.66	117.01	124.23
27	c	611	CLA	C4A-NA-C1A	4.66	108.80	106.68
27	d	306	CLA	C4A-NA-C1A	4.66	108.80	106.68
29	i	316	LHG	C5-O7-C7	-4.65	106.66	117.80
35	a	314	II0	C42-C40-C36	-4.65	120.76	127.28
35	b	615	II0	C20-C14-C10	-4.65	115.47	124.16
27	B	807	CLA	C4A-NA-C1A	4.64	108.80	106.68
30	A	846	WVN	C02-C11-C19	-4.64	117.35	124.58
37	s	204	KC2	CHD-C4C-C3C	-4.64	110.29	125.91
30	B	844	WVN	C26-C29-C31	-4.64	109.77	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	k	312	KC2	CHB-C1B-C2B	-4.64	115.85	125.49
30	l	301	WVN	C02-C11-C19	-4.64	117.37	124.58
37	n	611	KC2	CHB-C1B-C2B	-4.63	115.85	125.49
27	g	305	CLA	CMB-C2B-C1B	-4.63	118.37	125.42
27	a	307	CLA	CAC-C3C-C4C	4.63	130.81	124.79
37	e	609	KC2	CMD-C2D-C1D	-4.62	118.38	125.42
37	k	310	KC2	C1B-CHB-C4A	-4.62	116.20	126.02
30	l	316	WVN	C21-C15-C13	-4.62	119.44	124.48
37	i	317	KC2	CHC-C4B-NB	4.62	131.30	124.80
30	M	101	WVN	C39-C36-C32	-4.61	120.81	127.28
35	h	312	II0	C20-C14-C10	-4.61	115.55	124.16
35	f	618	II0	C06-C04-C10	4.60	118.56	109.49
27	A	834	CLA	C4A-NA-C1A	4.60	108.78	106.68
37	k	310	KC2	CHB-C1B-C2B	-4.60	115.91	125.49
35	g	316	II0	C20-C14-C10	-4.60	115.56	124.16
30	e	615	WVN	C11-C19-C22	-4.60	116.43	126.32
37	k	312	KC2	C1D-ND-C4D	4.60	109.54	106.31
30	B	846	WVN	C30-C28-C25	4.59	133.72	127.28
37	g	314	KC2	CHB-C1B-C2B	-4.59	115.93	125.49
35	g	316	II0	C31-C33-C35	-4.59	113.77	126.36
35	k	316	II0	C05-C03-C09	4.59	118.54	109.49
35	m	614	II0	C19-C13-C11	4.59	122.86	114.42
27	B	814	CLA	C4A-NA-C1A	4.59	108.77	106.68
30	h	309	WVN	C30-C33-C34	-4.59	113.79	126.36
30	s	207	WVN	C39-C36-C32	-4.58	120.85	127.28
35	k	316	II0	C16-C03-C09	-4.58	102.32	110.52
35	e	612	II0	C19-C13-C09	-4.57	115.61	124.16
37	k	311	KC2	CHD-C1D-ND	-4.57	117.19	124.05
27	B	828	CLA	O2D-CGD-CBD	4.57	119.22	111.23
27	B	813	CLA	C4A-NA-C1A	4.57	108.76	106.68
27	j	601	CLA	C4A-NA-C1A	4.57	108.76	106.68
37	f	611	KC2	CHB-C1B-C2B	-4.56	116.00	125.49
37	g	312	KC2	CHB-C1B-C2B	-4.56	116.00	125.49
37	n	611	KC2	C3A-C4A-NA	4.56	116.10	110.45
30	e	615	WVN	C40-C37-C34	-4.56	120.88	127.28
37	g	314	KC2	C3A-C4A-NA	4.56	116.09	110.45
35	j	615	II0	C19-C13-C11	4.56	122.80	114.42
27	B	808	CLA	C4A-NA-C1A	4.55	108.76	106.68
37	i	310	KC2	CHB-C1B-C2B	-4.55	116.01	125.49
30	M	101	WVN	C29-C26-C22	-4.55	120.90	127.28
27	h	302	CLA	C4A-NA-C1A	4.55	108.75	106.68
37	d	309	KC2	C3A-C4A-NA	4.55	116.08	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	610	KC2	CHB-C1B-C2B	-4.55	116.03	125.49
37	g	313	KC2	CHB-C1B-C2B	-4.55	116.03	125.49
30	B	844	WVN	C40-C37-C34	-4.54	120.90	127.28
37	s	204	KC2	CHB-C1B-NB	4.54	131.20	124.80
27	f	603	CLA	C4A-NA-C1A	4.54	108.75	106.68
37	s	201	KC2	C1D-ND-C4D	4.54	109.50	106.31
37	d	309	KC2	CHB-C1B-C2B	-4.54	116.04	125.49
27	K	101	CLA	C1-C2-C3	-4.54	118.75	126.20
35	n	614	II0	C37-C35-C39	-4.54	115.46	122.82
27	B	804	CLA	C4A-NA-C1A	4.54	108.75	106.68
27	F	202	CLA	C4A-NA-C1A	4.54	108.75	106.68
30	K	103	WVN	C02-C11-C19	-4.54	117.52	124.58
37	d	309	KC2	CHD-C1D-ND	-4.53	117.25	124.05
37	g	314	KC2	C1B-CHB-C4A	-4.53	116.38	126.02
27	B	828	CLA	C4A-NA-C1A	4.53	108.75	106.68
30	J	102	WVN	C16-C05-C09	-4.53	107.14	122.37
37	m	610	KC2	C3A-C4A-NA	4.53	116.06	110.45
35	i	313	II0	C42-C40-C36	-4.53	120.93	127.28
35	e	613	II0	C42-C40-C36	-4.52	120.93	127.28
37	k	311	KC2	C1A-C2A-C3A	-4.52	103.12	107.28
34	c	619	LMG	O7-C10-C11	4.52	121.25	111.48
27	b	610	CLA	C4A-NA-C1A	4.52	108.74	106.68
36	c	616	IHT	C03-C05-C08	-4.52	103.69	113.59
37	j	610	KC2	CHB-C1B-C2B	-4.52	116.09	125.49
35	a	318	II0	C32-C34-C36	4.51	138.74	126.36
27	k	301	CLA	C4A-NA-C1A	4.51	108.74	106.68
37	l	311	KC2	CHB-C1B-C2B	-4.51	116.11	125.49
29	d	315	LHG	O7-C7-C8	4.50	121.22	111.48
36	c	620	IHT	C18-C22-C23	-4.50	119.58	126.23
37	k	312	KC2	CHD-C1D-ND	-4.50	117.30	124.05
30	B	845	WVN	C04-C09-C05	-4.50	120.54	124.83
30	B	844	WVN	C04-C09-C05	-4.50	120.54	124.83
29	g	321	LHG	O7-C7-C8	4.50	121.21	111.48
30	R	202	WVN	C20-C23-C25	-4.49	119.59	126.23
27	A	818	CLA	CMB-C2B-C1B	-4.49	118.58	125.42
36	j	616	IHT	C30-C27-C23	-4.49	120.98	127.28
35	b	613	II0	C42-C41-C39	-4.49	114.34	123.52
35	n	616	II0	C42-C40-C36	-4.49	120.99	127.28
27	s	203	CLA	O2D-CGD-O1D	-4.48	115.12	123.85
37	s	201	KC2	C4B-C3B-C2B	-4.48	102.93	106.81
27	s	206	CLA	C4A-NA-C1A	4.48	108.72	106.68
27	B	831	CLA	C4A-NA-C1A	4.48	108.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	f	608	CLA	C4A-NA-C1A	4.48	108.72	106.68
27	j	604	CLA	C4A-NA-C1A	4.47	108.72	106.68
30	e	615	WVN	C04-C09-C05	-4.47	120.56	124.83
35	d	312	II0	C42-C40-C36	-4.47	121.01	127.28
27	A	852	CLA	C4A-NA-C1A	4.47	108.72	106.68
27	L	206	CLA	C4A-NA-C1A	4.47	108.72	106.68
37	k	312	KC2	C3A-C4A-NA	4.47	115.98	110.45
27	A	839	CLA	C4A-NA-C1A	4.47	108.72	106.68
30	I	101	WVN	C06-C13-C15	-4.47	116.53	122.64
27	h	301	CLA	C4A-NA-C1A	4.46	108.72	106.68
30	l	301	WVN	C23-C20-C13	-4.46	115.08	127.00
37	d	310	KC2	C1B-CHB-C4A	-4.46	116.53	126.02
30	L	201	WVN	C29-C26-C22	-4.46	121.02	127.28
29	l	318	LHG	O7-C7-C8	4.46	121.13	111.48
27	B	849	CLA	C4A-NA-C1A	4.46	108.71	106.68
30	F	204	WVN	C28-C30-C33	-4.46	110.29	123.20
35	a	315	II0	C19-C13-C11	4.45	122.61	114.42
36	j	616	IHT	C40-C37-C33	-4.45	121.03	127.28
35	i	314	II0	C05-C03-C09	4.45	118.26	109.49
37	s	201	KC2	C4B-CHC-C1C	-4.45	116.56	126.02
37	j	610	KC2	C1B-CHB-C4A	-4.45	116.56	126.02
27	A	801	CLA	C4A-NA-C1A	4.45	108.71	106.68
27	m	601	CLA	C4A-NA-C1A	4.45	108.71	106.68
30	s	205	WVN	C21-C15-C13	-4.44	119.64	124.48
37	d	309	KC2	C1B-CHB-C4A	-4.44	116.58	126.02
37	m	610	KC2	CHD-C1D-ND	-4.44	117.39	124.05
37	s	201	KC2	CHC-C1C-NC	-4.44	117.35	124.23
37	i	310	KC2	CHD-C1D-ND	-4.44	117.39	124.05
37	n	612	KC2	C1D-ND-C4D	4.44	109.42	106.31
27	a	303	CLA	C4A-NA-C1A	4.44	108.70	106.68
37	i	310	KC2	C3A-C4A-NA	4.44	115.94	110.45
37	s	201	KC2	O2D-CGD-CBD	4.44	118.98	111.23
35	b	612	II0	C19-C13-C11	4.43	122.58	114.42
30	J	102	WVN	C40-C37-C34	-4.43	121.06	127.28
30	A	847	WVN	C29-C26-C22	4.43	133.49	127.28
37	n	611	KC2	C1B-CHB-C4A	-4.43	116.61	126.02
37	m	610	KC2	C1B-CHB-C4A	-4.43	116.61	126.02
27	d	311	CLA	C4A-NA-C1A	4.43	108.70	106.68
37	g	314	KC2	C1D-ND-C4D	4.42	109.42	106.31
37	g	312	KC2	C3A-C4A-NA	4.42	115.92	110.45
37	e	609	KC2	CHB-C1B-C2B	-4.42	116.29	125.49
27	A	827	CLA	C4A-NA-C1A	4.42	108.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	R	203	CLA	CMB-C2B-C1B	-4.41	118.70	125.42
27	i	311	CLA	CMB-C2B-C1B	-4.41	118.70	125.42
27	B	824	CLA	CMB-C2B-C1B	-4.41	118.71	125.42
37	e	609	KC2	CHD-C1D-ND	-4.41	117.44	124.05
30	l	301	WVN	C39-C36-C32	-4.41	121.10	127.28
37	g	313	KC2	C1B-CHB-C4A	-4.39	116.68	126.02
37	j	610	KC2	C3A-C4A-NA	4.39	115.89	110.45
37	c	610	KC2	CHD-C1D-ND	-4.39	117.46	124.05
37	d	310	KC2	C4B-CHC-C1C	-4.39	116.69	126.02
27	h	313	CLA	C4A-NA-C1A	4.39	108.68	106.68
37	e	609	KC2	C3A-C4A-NA	4.38	115.88	110.45
30	K	103	WVN	C14-C15-C13	-4.38	116.78	122.70
37	k	311	KC2	CHB-C1B-NB	4.38	130.97	124.80
37	f	611	KC2	C3A-C4A-NA	4.38	115.87	110.45
30	B	847	WVN	C39-C36-C32	-4.37	121.14	127.28
30	M	101	WVN	C30-C28-C25	-4.37	121.14	127.28
30	l	316	WVN	C39-C36-C32	-4.37	121.15	127.28
37	e	609	KC2	C1B-CHB-C4A	-4.37	116.74	126.02
29	A	844	LHG	O7-C7-C8	4.37	120.92	111.48
35	b	613	II0	C20-C14-C12	4.36	122.44	114.42
37	g	312	KC2	C1D-ND-C4D	4.36	109.37	106.31
30	R	202	WVN	C06-C13-C15	-4.36	116.68	122.64
27	a	303	CLA	CMB-C2B-C1B	-4.36	118.79	125.42
37	k	312	KC2	C1B-CHB-C4A	-4.36	116.76	126.02
37	g	312	KC2	C1B-CHB-C4A	-4.35	116.76	126.02
27	i	311	CLA	CED-O2D-CGD	4.35	125.79	115.92
27	L	204	CLA	C4A-NA-C1A	4.35	108.66	106.68
30	s	205	WVN	C06-C13-C15	-4.35	116.69	122.64
37	g	312	KC2	CHD-C1D-ND	-4.35	117.53	124.05
27	A	817	CLA	C4A-NA-C1A	4.35	108.66	106.68
37	k	311	KC2	CMD-C2D-C1D	-4.35	118.80	125.42
37	f	611	KC2	C1B-CHB-C4A	-4.34	116.79	126.02
27	B	816	CLA	C4B-C3B-C2B	-4.34	101.90	107.30
27	m	607	CLA	C4A-NA-C1A	4.34	108.66	106.68
30	F	204	WVN	C21-C15-C13	-4.34	119.75	124.48
30	J	102	WVN	C04-C09-C05	-4.34	120.69	124.83
27	A	855	CLA	O2D-CGD-CBD	4.34	118.82	111.23
37	g	314	KC2	CHD-C1D-ND	-4.33	117.55	124.05
35	k	315	II0	C20-C14-C12	4.33	122.39	114.42
37	k	310	KC2	C1D-ND-C4D	4.33	109.35	106.31
36	b	614	IHT	C34-C35-C38	4.33	125.82	119.01
27	A	826	CLA	CMB-C2B-C1B	-4.33	118.83	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	e	609	KC2	C1D-ND-C4D	4.33	109.35	106.31
27	j	607	CLA	C4A-NA-C1A	4.32	108.65	106.68
37	i	310	KC2	C1B-CHB-C4A	-4.32	116.83	126.02
27	B	836	CLA	CMB-C2B-C1B	-4.31	118.85	125.42
27	B	822	CLA	CMB-C2B-C1B	-4.31	118.86	125.42
30	B	845	WVN	C19-C22-C26	-4.31	112.23	119.01
27	A	842	CLA	CMB-C2B-C1B	-4.30	118.86	125.42
37	n	612	KC2	C1B-CHB-C4A	-4.30	116.88	126.02
30	e	615	WVN	C07-C01-C02	4.30	116.05	109.55
37	e	609	KC2	C4B-C3B-C2B	-4.29	103.09	106.81
30	B	845	WVN	C30-C33-C34	-4.29	114.59	126.36
27	c	606	CLA	C4A-NA-C1A	4.29	108.64	106.68
27	B	825	CLA	C4A-NA-C1A	4.29	108.64	106.68
30	l	316	WVN	C07-C01-C02	4.29	116.04	109.55
37	f	611	KC2	CHD-C1D-ND	-4.28	117.62	124.05
35	j	614	II0	O02-C08-C06	-4.28	100.99	109.75
30	B	845	WVN	C40-C37-C34	-4.28	121.27	127.28
34	F	206	LMG	O7-C10-C11	4.28	120.74	111.48
27	d	301	CLA	C4A-NA-C1A	4.28	108.63	106.68
27	i	304	CLA	C4A-NA-C1A	4.28	108.63	106.68
30	s	207	WVN	C02-C11-C19	-4.28	117.93	124.58
27	B	831	CLA	CMB-C2B-C1B	-4.27	118.91	125.42
35	l	302	II0	C42-C40-C36	-4.27	121.28	127.28
30	B	848	WVN	C39-C36-C32	-4.27	121.29	127.28
27	L	203	CLA	C4A-NA-C1A	4.27	108.63	106.68
27	A	855	CLA	C4-C3-C2	-4.27	112.67	123.63
37	n	611	KC2	CMD-C2D-C3D	4.27	139.12	125.67
35	n	615	II0	C42-C40-C36	-4.26	121.30	127.28
35	f	615	II0	C20-C14-C10	-4.26	116.19	124.16
37	d	310	KC2	C1D-ND-C4D	4.26	109.30	106.31
35	k	314	II0	C42-C40-C36	-4.26	121.30	127.28
37	j	610	KC2	CHD-C1D-ND	-4.26	117.66	124.05
37	k	311	KC2	CHB-C1B-C2B	-4.26	116.63	125.49
37	g	313	KC2	C1D-ND-C4D	4.26	109.30	106.31
36	c	620	IHT	C41-C40-C37	-4.25	114.81	123.52
37	k	310	KC2	CHD-C1D-ND	-4.25	117.67	124.05
35	b	615	II0	C06-C04-C10	4.25	117.86	109.49
37	f	611	KC2	C1D-ND-C4D	4.25	109.29	106.31
37	n	612	KC2	C4B-C3B-C2B	-4.25	103.13	106.81
35	a	314	II0	C41-C42-C40	-4.24	114.83	123.52
30	e	615	WVN	C39-C36-C32	-4.24	121.33	127.28
27	c	612	CLA	CMB-C2B-C1B	-4.24	118.96	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	k	316	II0	C41-C39-C35	-4.24	121.33	127.28
37	l	311	KC2	CHD-C1D-ND	-4.24	117.69	124.05
37	i	317	KC2	C2C-C1C-NC	4.24	115.69	110.45
37	s	204	KC2	CHC-C1C-NC	-4.23	117.67	124.23
27	n	605	CLA	CBC-CAC-C3C	4.23	123.89	112.42
27	A	834	CLA	CMB-C2B-C1B	-4.23	118.98	125.42
27	h	307	CLA	C4A-NA-C1A	4.23	108.61	106.68
30	B	845	WVN	C40-C39-C36	-4.23	114.86	123.52
35	a	318	II0	C31-C33-C35	-4.23	114.77	126.36
27	k	303	CLA	CMB-C2B-C1B	-4.23	118.98	125.42
35	O	203	II0	C41-C39-C35	-4.22	121.36	127.28
35	O	203	II0	C20-C14-C10	-4.22	116.27	124.16
36	c	620	IHT	C40-C37-C33	-4.22	121.36	127.28
27	g	304	CLA	CMB-C2B-C1B	-4.22	118.99	125.42
30	s	205	WVN	C39-C40-C37	-4.22	114.88	123.52
37	m	610	KC2	C1D-ND-C4D	4.22	109.27	106.31
37	i	317	KC2	CHB-C1B-NB	4.21	130.73	124.80
35	j	613	II0	C21-C23-C25	-4.21	161.92	176.23
27	b	607	CLA	CAC-C3C-C2C	4.21	135.29	127.56
27	c	605	CLA	C4A-NA-C1A	4.21	108.60	106.68
27	j	602	CLA	CMB-C2B-C1B	-4.20	119.02	125.42
37	c	610	KC2	C1B-CHB-C4A	-4.20	117.09	126.02
28	B	841	PQN	C11-C12-C13	-4.20	119.60	126.83
30	A	846	WVN	C20-C23-C25	-4.20	120.03	126.23
37	l	311	KC2	O2D-CGD-CBD	4.19	118.56	111.23
36	a	317	IHT	C41-C40-C37	-4.19	114.94	123.52
35	c	613	II0	C42-C40-C36	-4.19	121.40	127.28
35	e	612	II0	C41-C39-C35	-4.19	121.41	127.28
27	B	806	CLA	C4A-NA-C1A	4.19	108.59	106.68
27	e	610	CLA	C4A-NA-C1A	4.19	108.59	106.68
27	i	306	CLA	C4A-NA-C1A	4.19	108.59	106.68
27	A	805	CLA	CAA-C2A-C3A	-4.19	101.69	113.00
35	f	616	II0	C20-C14-C10	-4.19	116.33	124.16
35	g	317	II0	C19-C13-C11	4.18	122.11	114.42
37	c	610	KC2	O2D-CGD-CBD	4.18	118.54	111.23
27	i	307	CLA	CMB-C2B-C1B	-4.18	119.05	125.42
37	d	309	KC2	C1D-ND-C4D	4.18	109.25	106.31
30	A	848	WVN	C39-C36-C32	-4.18	121.42	127.28
27	n	607	CLA	CMB-C2B-C1B	-4.17	119.06	125.42
34	b	619	LMG	O7-C10-C11	4.17	120.51	111.48
27	B	821	CLA	CMB-C2B-C1B	-4.17	119.07	125.42
30	L	205	WVN	C40-C37-C34	-4.17	121.43	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	g	310	CLA	CMB-C2B-C1B	-4.17	119.07	125.42
27	A	818	CLA	C1-C2-C3	-4.17	119.37	126.20
30	J	101	WVN	C40-C37-C34	-4.17	121.43	127.28
30	s	207	WVN	C40-C37-C34	-4.17	121.43	127.28
35	h	311	II0	C42-C41-C39	-4.17	114.99	123.52
27	m	604	CLA	CMB-C2B-C1B	-4.16	119.08	125.42
27	d	301	CLA	C1-C2-C3	-4.16	120.03	126.76
27	h	305	CLA	C4A-NA-C1A	4.16	108.58	106.68
27	f	609	CLA	C4A-NA-C1A	4.16	108.58	106.68
35	d	314	II0	C42-C40-C36	-4.15	121.45	127.28
27	f	607	CLA	C4-C3-C5	4.15	122.43	115.23
27	A	812	CLA	CMB-C2B-C1B	-4.15	119.10	125.42
36	O	204	IHT	C30-C27-C23	-4.15	121.46	127.28
35	j	614	II0	C20-C14-C10	-4.14	116.41	124.16
27	j	609	CLA	O2D-CGD-O1D	-4.14	115.79	123.85
30	A	848	WVN	C29-C26-C22	-4.14	121.47	127.28
37	g	312	KC2	C4B-C3B-C2B	-4.14	103.23	106.81
35	h	310	II0	C42-C41-C39	-4.14	115.06	123.52
31	A	851	LMT	C3'-C4'-C5'	-4.14	101.76	110.93
37	g	313	KC2	C4B-C3B-C2B	-4.13	103.23	106.81
35	a	316	II0	C42-C41-C39	-4.13	115.07	123.52
35	e	616	II0	C19-C13-C11	4.13	122.02	114.42
36	m	616	IHT	C18-C22-C23	-4.13	120.12	126.23
35	i	314	II0	C19-C13-C11	4.13	122.01	114.42
37	s	201	KC2	C2A-C3A-C4A	-4.13	103.31	106.41
35	g	316	II0	C19-C13-C11	4.13	122.01	114.42
30	L	205	WVN	C14-C15-C13	-4.13	117.13	122.70
30	O	201	WVN	C20-C23-C25	-4.12	120.13	126.23
35	k	315	II0	C19-C13-C11	4.12	122.00	114.42
35	b	615	II0	C41-C39-C35	-4.12	121.50	127.28
37	c	610	KC2	C3A-C4A-NA	4.12	115.55	110.45
27	B	803	CLA	CHB-C4A-NA	4.12	130.34	124.40
30	h	309	WVN	C20-C23-C25	-4.12	120.14	126.23
36	g	319	IHT	C40-C37-C33	-4.11	121.51	127.28
27	h	301	CLA	CMB-C2B-C1B	-4.11	119.16	125.42
30	J	101	WVN	C27-C25-C23	-4.11	111.81	118.09
30	s	205	WVN	C30-C28-C25	-4.11	121.52	127.28
37	m	610	KC2	C4B-C3B-C2B	-4.11	103.25	106.81
27	c	608	CLA	CED-O2D-CGD	4.11	125.23	115.92
27	k	309	CLA	C4A-NA-C1A	4.10	108.55	106.68
37	k	312	KC2	C4B-C3B-C2B	-4.10	103.26	106.81
35	O	203	II0	C19-C13-C11	4.09	121.95	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	R	202	WVN	C18-C06-C13	4.09	116.66	110.24
35	l	314	II0	C19-C13-C11	4.09	121.95	114.42
37	d	309	KC2	C4B-C3B-C2B	-4.09	103.27	106.81
35	g	318	II0	C42-C40-C36	-4.09	121.54	127.28
29	b	618	LHG	O7-C7-C8	4.09	120.32	111.48
27	i	308	CLA	C4A-NA-C1A	4.08	108.54	106.68
30	i	315	WVN	C39-C36-C32	-4.08	121.56	127.28
36	c	616	IHT	C19-C10-C07	-4.08	120.03	124.48
30	F	204	WVN	C29-C26-C22	-4.08	121.56	127.28
27	g	304	CLA	C4A-NA-C1A	4.07	108.53	106.68
30	A	849	WVN	C30-C33-C34	-4.06	115.23	126.36
27	B	813	CLA	CMB-C2B-C1B	-4.06	119.24	125.42
37	c	610	KC2	C4B-C3B-C2B	-4.06	103.30	106.81
27	h	304	CLA	CMB-C2B-C1B	-4.05	119.25	125.42
36	g	319	IHT	C41-C40-C37	-4.05	115.23	123.52
27	d	308	CLA	C4A-NA-C1A	4.05	108.53	106.68
27	k	309	CLA	C2D-C1D-ND	-4.05	106.12	110.13
30	O	201	WVN	C40-C37-C34	-4.05	121.60	127.28
35	m	615	II0	C42-C40-C36	-4.05	121.61	127.28
27	B	807	CLA	CMB-C2B-C1B	-4.04	119.26	125.42
35	c	613	II0	C19-C13-C11	4.04	121.85	114.42
30	A	847	WVN	C01-C02-C11	-4.04	108.18	112.83
27	s	202	CLA	CAA-CBA-CGA	-4.03	101.76	113.21
27	g	311	CLA	O2D-CGD-O1D	-4.03	116.00	123.85
27	B	817	CLA	CAA-CBA-CGA	-4.03	101.76	113.21
27	a	304	CLA	C4A-NA-C1A	4.03	108.52	106.68
35	f	618	II0	C20-C14-C12	4.03	121.83	114.42
35	a	316	II0	C20-C14-C10	-4.03	116.63	124.16
35	b	615	II0	C30-C32-C34	-4.02	111.54	123.20
30	i	315	WVN	C40-C37-C34	-4.02	121.64	127.28
27	c	602	CLA	C4A-NA-C1A	4.02	108.51	106.68
37	n	611	KC2	C1D-ND-C4D	4.02	109.13	106.31
36	f	617	IHT	C02-C07-C10	-4.02	117.15	122.64
35	g	318	II0	C20-C14-C12	4.02	121.81	114.42
27	A	838	CLA	CMB-C2B-C1B	-4.02	119.30	125.42
35	b	612	II0	C20-C14-C12	4.02	121.81	114.42
30	A	849	WVN	C29-C26-C22	-4.02	121.65	127.28
28	A	843	PQN	C11-C12-C13	-4.02	119.91	126.83
30	L	201	WVN	C30-C28-C25	-4.01	121.65	127.28
37	d	310	KC2	CHB-C1B-C2B	-4.01	117.14	125.49
36	j	616	IHT	C19-C10-C09	4.01	122.14	113.60
27	A	856	CLA	CMA-C3A-C2A	-4.01	107.04	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	311	CLA	O2A-CGA-O1A	-4.01	113.60	123.63
30	l	316	WVN	C30-C28-C25	-4.00	121.66	127.28
27	A	837	CLA	CAC-C3C-C4C	4.00	129.99	124.79
35	c	617	II0	C32-C34-C36	-3.99	115.41	126.36
27	g	309	CLA	CHB-C4A-NA	3.99	130.16	124.40
35	h	310	II0	C19-C13-C11	3.99	121.76	114.42
27	A	829	CLA	C4A-NA-C1A	3.99	108.50	106.68
36	R	204	IHT	C41-C38-C35	-3.99	121.69	127.28
36	g	319	IHT	C30-C27-C23	-3.98	121.69	127.28
30	K	103	WVN	C06-C13-C15	-3.98	117.20	122.64
37	j	610	KC2	C4B-C3B-C2B	-3.98	103.36	106.81
37	s	201	KC2	CHB-C4A-NA	3.98	130.40	124.23
27	A	818	CLA	CMC-C2C-C1C	-3.98	118.82	125.03
35	a	314	II0	C19-C13-C11	3.97	121.72	114.42
35	n	615	II0	C20-C14-C12	3.97	121.72	114.42
37	l	311	KC2	C4B-C3B-C2B	-3.96	103.38	106.81
37	g	312	KC2	O2D-CGD-CBD	3.96	118.16	111.23
37	l	311	KC2	C1D-ND-C4D	3.96	109.09	106.31
35	e	612	II0	C19-C13-C11	3.96	121.70	114.42
35	l	313	II0	C19-C13-C09	-3.96	116.76	124.16
27	A	805	CLA	CMB-C2B-C1B	-3.95	119.40	125.42
36	g	319	IHT	C09-C10-C07	-3.95	117.36	122.70
36	c	616	IHT	C31-C34-C35	-3.95	115.53	126.36
30	A	847	WVN	C21-C15-C13	-3.95	120.17	124.48
34	c	619	LMG	C7-O1-C1	-3.95	105.33	113.80
27	B	838	CLA	CAA-C2A-C3A	-3.95	102.33	113.00
30	L	205	WVN	C39-C36-C32	-3.95	121.74	127.28
34	L	208	LMG	C3-C4-C5	3.95	117.39	110.23
35	b	612	II0	C20-C14-C10	-3.95	116.78	124.16
27	b	605	CLA	C3B-C4B-NB	-3.94	107.01	110.53
30	L	205	WVN	C02-C11-C19	-3.94	118.45	124.58
36	f	617	IHT	C30-C27-C23	-3.94	121.75	127.28
36	b	614	IHT	C04-C02-C07	3.94	116.16	110.44
30	R	202	WVN	C29-C31-C32	-3.94	115.56	126.36
36	O	204	IHT	C09-C10-C07	-3.94	117.39	122.70
37	k	310	KC2	O2D-CGD-CBD	3.93	118.11	111.23
30	A	848	WVN	C06-C13-C20	3.93	126.32	115.65
27	i	303	CLA	C4A-NA-C1A	3.93	108.47	106.68
37	g	313	KC2	CHD-C1D-ND	-3.93	118.15	124.05
30	e	615	WVN	C18-C06-C13	3.93	116.40	110.24
29	A	845	LHG	O8-C23-C24	3.93	123.07	111.15
35	J	104	II0	C41-C39-C35	-3.92	121.78	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	f	611	KC2	C4B-C3B-C2B	-3.92	103.41	106.81
27	e	608	CLA	O2D-CGD-O1D	-3.92	116.21	123.85
35	j	613	II0	C20-C14-C12	3.92	121.63	114.42
29	g	321	LHG	C6-C5-C4	-3.92	102.65	111.78
27	g	309	CLA	O2D-CGD-CBD	3.92	118.08	111.23
35	h	311	II0	C41-C39-C35	-3.91	121.79	127.28
37	i	310	KC2	C4B-C3B-C2B	-3.91	103.42	106.81
29	L	207	LHG	O7-C7-C8	3.91	119.94	111.48
27	f	607	CLA	CAA-CBA-CGA	-3.90	102.13	113.21
27	B	802	CLA	CMB-C2B-C3B	3.90	135.72	126.55
30	L	205	WVN	C06-C13-C15	-3.90	117.31	122.64
38	i	301	LMU	O1B-C4'-C3'	3.90	117.14	107.23
37	g	314	KC2	C4B-C3B-C2B	-3.90	103.44	106.81
27	a	304	CLA	CMB-C2B-C1B	-3.89	119.49	125.42
37	n	611	KC2	C4B-C3B-C2B	-3.89	103.44	106.81
37	d	310	KC2	C3A-C4A-NA	3.89	115.26	110.45
35	l	302	II0	C37-C35-C33	3.88	124.02	118.09
37	d	310	KC2	C4B-C3B-C2B	-3.88	103.45	106.81
27	J	103	CLA	CMB-C2B-C1B	-3.88	119.51	125.42
30	M	101	WVN	C14-C15-C13	-3.88	117.46	122.70
27	A	810	CLA	C4A-NA-C1A	3.87	108.45	106.68
27	B	824	CLA	C4A-NA-C1A	3.87	108.45	106.68
27	i	309	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
30	K	103	WVN	C04-C09-C05	-3.87	121.13	124.83
27	f	612	CLA	CAC-C3C-C4C	3.87	129.83	124.79
27	F	203	CLA	C1-O2A-CGA	3.87	126.02	116.65
37	s	204	KC2	C2A-C1A-NA	3.87	115.54	109.34
27	A	822	CLA	C3B-C4B-NB	-3.87	107.08	110.53
27	A	832	CLA	O2D-CGD-CBD	3.87	117.99	111.23
37	s	204	KC2	C1B-CHB-C4A	-3.87	117.80	126.02
27	e	603	CLA	C4A-NA-C1A	3.87	108.44	106.68
35	m	613	II0	C41-C39-C35	-3.87	121.86	127.28
35	m	614	II0	C42-C40-C36	-3.86	121.86	127.28
27	B	836	CLA	C1-C2-C3	-3.86	119.87	126.20
29	A	845	LHG	O7-C7-C8	3.86	119.83	111.48
27	J	105	CLA	CHB-C4A-NA	3.86	129.97	124.40
35	l	315	II0	C42-C41-C39	-3.86	115.62	123.52
27	A	841	CLA	CMB-C2B-C1B	-3.86	119.55	125.42
35	k	318	II0	C20-C14-C10	-3.86	116.95	124.16
30	O	201	WVN	C07-C01-C02	3.86	115.39	109.55
30	I	101	WVN	C07-C01-C02	3.85	115.38	109.55
27	c	608	CLA	O2D-CGD-CBD	3.85	117.97	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	i	316	LHG	O8-C23-C24	3.85	123.58	111.83
27	s	208	CLA	CHB-C4A-NA	3.85	129.96	124.40
30	B	843	WVN	C19-C22-C26	-3.85	112.95	119.01
37	s	201	KC2	CBC-CAC-C3C	-3.85	108.30	127.53
27	l	309	CLA	C1-C2-C3	-3.84	119.90	126.20
27	A	816	CLA	C4A-NA-C1A	3.84	108.43	106.68
27	a	312	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
35	e	614	II0	C20-C14-C10	-3.84	116.98	124.16
27	m	604	CLA	CHB-C4A-NA	3.84	129.94	124.40
35	n	614	II0	C37-C35-C33	3.84	123.95	118.09
35	f	618	II0	C31-C33-C35	-3.84	115.85	126.36
35	b	613	II0	C19-C13-C09	-3.83	116.99	124.16
30	B	847	WVN	C26-C29-C31	-3.83	112.10	123.20
35	m	614	II0	C32-C34-C36	-3.83	115.86	126.36
35	g	318	II0	C30-C32-C34	-3.83	112.10	123.20
30	B	843	WVN	C07-C01-C02	3.83	115.35	109.55
36	n	617	IHT	C19-C10-C07	-3.83	120.31	124.48
36	m	616	IHT	C41-C38-C35	-3.83	121.91	127.28
36	n	617	IHT	C30-C32-C33	-3.83	115.87	126.36
30	I	101	WVN	C39-C40-C37	-3.83	115.69	123.52
37	s	201	KC2	C2B-C1B-NB	3.82	113.91	110.13
27	c	608	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
27	A	817	CLA	C3B-C4B-NB	-3.82	107.12	110.53
27	B	812	CLA	CMB-C2B-C1B	-3.82	119.60	125.42
30	J	101	WVN	C04-C09-C05	-3.82	121.19	124.83
35	c	614	II0	C41-C42-C40	-3.81	115.72	123.52
27	B	817	CLA	CMB-C2B-C1B	-3.81	119.61	125.42
36	R	204	IHT	C09-C10-C07	-3.81	117.55	122.70
35	e	614	II0	C19-C13-C11	3.81	121.43	114.42
27	m	612	CLA	CMC-C2C-C1C	-3.81	119.08	125.03
30	A	846	WVN	C40-C37-C34	-3.80	121.94	127.28
30	J	101	WVN	C39-C36-C32	-3.80	121.94	127.28
36	k	317	IHT	C30-C27-C23	-3.80	121.94	127.28
36	a	317	IHT	C02-C07-C10	-3.80	117.44	122.64
27	f	604	CLA	CHB-C4A-NA	3.80	129.89	124.40
27	A	802	CLA	CMB-C2B-C3B	3.80	135.48	126.55
27	f	607	CLA	C4A-NA-C1A	3.80	108.41	106.68
30	B	845	WVN	C30-C28-C25	-3.80	121.95	127.28
30	A	846	WVN	C23-C25-C28	3.80	124.98	119.01
27	A	825	CLA	C4A-NA-C1A	3.80	108.41	106.68
27	l	306	CLA	CHB-C4A-NA	3.79	129.88	124.40
35	i	318	II0	C20-C14-C12	3.79	121.39	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	k	317	IHT	C09-C10-C07	-3.79	117.58	122.70
27	A	804	CLA	CHB-C4A-NA	3.79	129.86	124.40
37	f	611	KC2	CMD-C2D-C3D	3.78	137.61	125.67
35	g	318	II0	C19-C13-C09	-3.78	117.09	124.16
30	B	843	WVN	C40-C37-C34	-3.78	121.97	127.28
35	j	614	II0	C41-C42-C40	-3.78	115.78	123.52
37	j	610	KC2	C1D-ND-C4D	3.78	108.97	106.31
27	j	608	CLA	CMB-C2B-C1B	-3.78	119.67	125.42
35	h	310	II0	C31-C33-C35	-3.78	116.01	126.36
27	m	611	CLA	CAA-C2A-C3A	-3.77	102.80	113.00
35	m	613	II0	C19-C13-C11	3.77	121.36	114.42
30	B	848	WVN	C40-C37-C34	-3.77	121.99	127.28
30	h	309	WVN	C39-C36-C32	-3.77	121.99	127.28
27	A	836	CLA	CAA-CBA-CGA	-3.77	102.50	113.21
35	j	613	II0	C31-C33-C35	-3.77	116.03	126.36
35	k	318	II0	C20-C14-C12	3.77	121.35	114.42
30	e	615	WVN	C29-C26-C22	-3.77	122.00	127.28
27	B	802	CLA	CAC-C3C-C2C	-3.76	120.64	127.56
27	s	208	CLA	O2D-CGD-O1D	-3.76	116.52	123.85
35	n	614	II0	C05-C03-C09	3.76	116.90	109.49
27	d	311	CLA	CMB-C2B-C1B	-3.76	119.69	125.42
34	F	206	LMG	C8-O7-C10	-3.76	108.80	117.80
36	b	614	IHT	C39-C35-C38	-3.76	116.73	122.82
27	k	309	CLA	CAC-C3C-C4C	3.76	129.68	124.79
27	b	608	CLA	O2D-CGD-O1D	-3.75	116.54	123.85
36	c	620	IHT	C19-C10-C07	-3.75	120.39	124.48
37	n	611	KC2	CHD-C1D-ND	-3.75	118.43	124.05
36	m	616	IHT	C09-C10-C07	-3.75	117.64	122.70
35	k	314	II0	C33-C35-C39	3.74	124.89	119.01
30	B	847	WVN	C07-C01-C02	3.74	115.21	109.55
27	e	605	CLA	O2D-CGD-CBD	3.74	117.77	111.23
37	n	612	KC2	C2A-C1A-NA	3.74	115.33	109.34
27	J	105	CLA	C2A-C1A-CHA	3.74	130.35	123.87
35	c	614	II0	C18-C04-C10	-3.73	103.83	110.52
37	j	610	KC2	CMD-C2D-C3D	3.73	137.45	125.67
30	B	846	WVN	C04-C09-C05	-3.73	121.27	124.83
27	f	604	CLA	CMB-C2B-C1B	-3.73	119.74	125.42
27	i	308	CLA	CMB-C2B-C1B	-3.73	119.74	125.42
35	m	613	II0	C42-C40-C36	-3.73	122.05	127.28
27	c	612	CLA	C4A-NA-C1A	3.73	108.38	106.68
37	f	611	KC2	O2D-CGD-CBD	3.72	117.74	111.23
27	B	823	CLA	CMB-C2B-C1B	-3.72	119.75	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	s	204	KC2	CMD-C2D-C3D	3.72	137.41	125.67
27	A	815	CLA	CMB-C2B-C3B	3.72	135.30	126.55
30	B	847	WVN	C40-C37-C34	-3.72	122.06	127.28
37	l	311	KC2	CMD-C2D-C3D	3.72	137.40	125.67
35	a	318	II0	C32-C30-C26	3.72	137.02	126.61
30	R	201	WVN	C39-C36-C32	-3.71	122.07	127.28
35	g	320	II0	C06-C04-C10	3.71	116.80	109.49
27	A	821	CLA	CMB-C2B-C1B	-3.71	119.77	125.42
37	i	317	KC2	C1B-CHB-C4A	-3.71	118.14	126.02
35	i	313	II0	C19-C13-C09	-3.71	117.23	124.16
30	B	848	WVN	C21-C15-C13	-3.71	120.44	124.48
35	m	615	II0	C20-C14-C10	-3.70	117.23	124.16
27	f	602	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
30	R	202	WVN	C03-C04-C09	-3.70	105.85	112.07
27	d	302	CLA	C4A-NA-C1A	3.70	108.37	106.68
27	g	303	CLA	C4A-NA-C1A	3.70	108.37	106.68
37	s	201	KC2	C3B-C2B-C1B	-3.70	103.55	107.05
37	k	311	KC2	C4B-C3B-C2B	-3.69	103.61	106.81
37	g	312	KC2	CMD-C2D-C3D	3.69	137.32	125.67
27	m	611	CLA	C4A-NA-C1A	3.69	108.36	106.68
30	A	848	WVN	C17-C06-C13	3.69	116.03	110.24
30	A	849	WVN	C26-C29-C31	-3.69	112.51	123.20
27	A	832	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
30	i	315	WVN	C04-C09-C05	-3.69	121.31	124.83
30	A	848	WVN	C14-C15-C13	-3.68	117.73	122.70
27	j	611	CLA	C1-C2-C3	-3.68	120.17	126.20
35	m	613	II0	C20-C14-C10	-3.68	117.28	124.16
27	l	309	CLA	CMB-C2B-C1B	-3.68	119.82	125.42
35	O	203	II0	C17-C04-C10	-3.68	103.93	110.52
27	c	602	CLA	CMC-C2C-C1C	3.68	130.78	125.03
27	A	837	CLA	CAA-CBA-CGA	-3.68	102.77	113.21
30	i	315	WVN	C40-C39-C36	-3.68	116.00	123.52
27	A	856	CLA	CHB-C4A-NA	3.67	129.70	124.40
27	k	306	CLA	C1-C2-C3	-3.67	120.18	126.20
27	b	609	CLA	CMB-C2B-C1B	-3.67	119.83	125.42
37	k	311	KC2	O2D-CGD-O1D	-3.67	116.70	123.85
35	k	314	II0	C37-C35-C33	-3.67	112.48	118.09
30	M	101	WVN	C11-C19-C22	-3.67	118.44	126.32
27	A	834	CLA	CMB-C2B-C3B	3.66	135.16	126.55
27	A	829	CLA	O2D-CGD-CBD	3.66	117.63	111.23
37	d	309	KC2	O2D-CGD-CBD	3.66	117.62	111.23
35	e	613	II0	C41-C42-C40	-3.66	116.03	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	k	310	KC2	C4B-C3B-C2B	-3.66	103.64	106.81
30	s	205	WVN	C40-C37-C34	-3.66	122.15	127.28
36	c	620	IHT	C20-C15-C11	-3.66	117.32	124.16
35	d	314	II0	C19-C13-C11	3.65	121.14	114.42
37	k	310	KC2	CMD-C2D-C3D	3.65	137.18	125.67
30	A	848	WVN	C39-C40-C37	-3.65	116.05	123.52
29	A	844	LHG	O8-C23-C24	3.65	122.96	111.83
27	n	609	CLA	CHB-C4A-NA	3.65	129.67	124.40
30	s	207	WVN	C30-C33-C34	-3.65	116.36	126.36
35	l	302	II0	C21-C23-C25	-3.65	163.84	176.23
27	B	810	CLA	C7-C6-C5	-3.65	103.54	113.26
35	h	312	II0	C17-C04-C10	3.64	117.05	110.52
30	B	843	WVN	C39-C40-C37	-3.64	116.07	123.52
27	A	829	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
35	n	618	II0	C19-C13-C11	3.64	121.12	114.42
35	h	310	II0	C30-C32-C34	-3.64	117.97	125.28
27	B	836	CLA	CMB-C2B-C3B	3.63	135.10	126.55
37	g	313	KC2	CHB-C4A-NA	3.63	129.87	124.23
35	j	615	II0	C20-C14-C10	-3.63	117.37	124.16
36	m	616	IHT	C02-C07-C10	-3.63	117.67	122.64
27	c	609	CLA	C4A-NA-C1A	3.63	108.33	106.68
27	a	310	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
38	i	301	LMU	C3'-C4'-C5'	-3.63	102.89	110.93
27	i	309	CLA	C4A-NA-C1A	3.63	108.33	106.68
27	B	838	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
27	d	307	CLA	CAA-C2A-C3A	-3.62	107.93	116.23
37	i	317	KC2	CMD-C2D-C3D	3.62	137.09	125.67
36	c	620	IHT	C19-C10-C09	3.62	121.31	113.60
27	i	304	CLA	CMB-C2B-C1B	-3.62	119.91	125.42
29	m	617	LHG	O7-C7-C8	3.62	119.31	111.48
37	g	313	KC2	CMD-C2D-C3D	3.62	137.08	125.67
35	k	316	II0	C20-C14-C10	-3.62	117.39	124.16
35	O	203	II0	C31-C33-C35	-3.62	116.44	126.36
36	a	317	IHT	C09-C10-C07	-3.62	117.82	122.70
27	k	309	CLA	O2D-CGD-CBD	3.61	117.55	111.23
27	B	835	CLA	CBC-CAC-C3C	3.61	122.21	112.42
30	I	101	WVN	C02-C11-C19	-3.61	118.96	124.58
35	b	615	II0	C20-C14-C12	3.61	121.06	114.42
27	e	604	CLA	CHB-C4A-NA	3.61	129.61	124.40
27	A	826	CLA	CMC-C2C-C1C	-3.61	119.40	125.03
37	n	611	KC2	O2D-CGD-CBD	3.60	117.52	111.23
30	A	849	WVN	C40-C37-C34	-3.60	122.23	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	L	208	LMG	C8-O7-C10	-3.60	109.19	117.80
30	B	845	WVN	C29-C26-C22	-3.59	122.24	127.28
35	a	316	II0	C19-C13-C11	3.59	121.02	114.42
30	B	845	WVN	C29-C31-C32	3.59	136.20	126.36
37	c	610	KC2	CMD-C2D-C3D	3.59	136.98	125.67
35	J	104	II0	C31-C33-C35	-3.58	116.54	126.36
27	k	302	CLA	CAA-C2A-C3A	-3.58	103.32	113.00
27	g	303	CLA	CMB-C2B-C3B	3.58	134.97	126.55
27	s	206	CLA	O2D-CGD-CBD	3.58	117.48	111.23
27	j	602	CLA	CMB-C2B-C3B	3.58	134.96	126.55
37	k	310	KC2	C2A-C1A-NA	3.57	115.07	109.34
27	A	802	CLA	C4A-NA-C1A	3.57	108.31	106.68
27	k	309	CLA	CED-O2D-CGD	3.57	124.02	115.92
35	i	314	II0	C41-C39-C35	-3.57	122.27	127.28
29	a	301	LHG	O7-C7-C8	3.57	119.21	111.48
27	B	810	CLA	CBC-CAC-C3C	3.57	122.10	112.42
29	a	301	LHG	O8-C23-C24	3.57	122.71	111.83
37	m	610	KC2	C2A-C1A-NA	3.56	115.05	109.34
36	a	317	IHT	C40-C37-C33	-3.56	122.28	127.28
27	k	302	CLA	CMB-C2B-C1B	-3.56	119.99	125.42
30	F	205	WVN	C07-C01-C02	3.56	114.94	109.55
29	k	319	LHG	O7-C7-C8	3.56	119.18	111.48
35	l	313	II0	C42-C41-C39	-3.56	116.23	123.52
35	n	615	II0	C41-C42-C40	-3.56	116.25	123.52
30	B	844	WVN	C39-C36-C32	-3.55	122.29	127.28
37	i	317	KC2	CBC-CAC-C3C	-3.55	109.77	127.53
27	j	603	CLA	CMB-C2B-C1B	-3.55	120.01	125.42
37	k	311	KC2	CHB-C4A-NA	3.55	129.74	124.23
27	c	602	CLA	CMB-C2B-C1B	-3.55	120.02	125.42
27	A	855	CLA	O2A-CGA-CBA	3.54	122.64	111.83
35	J	104	II0	C19-C13-C11	3.54	120.93	114.42
27	B	827	CLA	CMB-C2B-C1B	-3.54	120.03	125.42
27	c	602	CLA	O2D-CGD-O1D	-3.54	116.97	123.85
27	B	831	CLA	CMB-C2B-C3B	3.53	134.86	126.55
27	g	309	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
30	R	202	WVN	C04-C09-C05	-3.53	121.46	124.83
35	a	314	II0	C32-C30-C26	-3.53	116.74	126.61
27	g	310	CLA	CMB-C2B-C3B	3.53	134.85	126.55
30	h	309	WVN	C06-C13-C15	-3.53	117.82	122.64
35	k	314	II0	C19-C13-C11	3.53	120.91	114.42
37	d	309	KC2	C2A-C1A-NA	3.52	114.99	109.34
27	R	203	CLA	C4A-NA-C1A	3.52	108.29	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	604	CLA	CMB-C2B-C1B	-3.52	120.06	125.42
27	B	835	CLA	C4-C3-C5	3.52	121.34	115.23
30	A	849	WVN	C07-C01-C02	3.52	114.88	109.55
36	c	620	IHT	C27-C30-C32	-3.52	113.00	123.20
27	s	208	CLA	CMA-C3A-C4A	-3.52	102.31	111.77
37	d	310	KC2	C2A-C1A-NA	3.52	114.98	109.34
27	A	842	CLA	CMB-C2B-C3B	3.52	134.83	126.55
30	I	101	WVN	C23-C20-C13	-3.52	117.60	127.00
27	h	308	CLA	C2A-C1A-CHA	3.52	129.97	123.87
27	c	606	CLA	CAA-C2A-C3A	-3.52	103.49	113.00
27	a	311	CLA	CMB-C2B-C1B	-3.52	120.06	125.42
27	e	611	CLA	C7-C6-C5	-3.52	103.89	113.26
27	h	304	CLA	C2A-C1A-CHA	3.51	129.97	123.87
27	i	309	CLA	CAC-C3C-C4C	3.51	129.36	124.79
37	l	311	KC2	C2A-C1A-NA	3.51	114.97	109.34
27	g	310	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
27	g	303	CLA	CMB-C2B-C1B	-3.51	120.07	125.42
27	A	832	CLA	CMC-C2C-C1C	-3.51	119.55	125.03
27	B	834	CLA	C4A-NA-C1A	3.51	108.28	106.68
27	A	824	CLA	C2A-C1A-CHA	3.51	129.96	123.87
35	l	302	II0	C20-C14-C10	-3.51	117.60	124.16
27	L	206	CLA	CMB-C2B-C1B	-3.51	120.08	125.42
27	B	835	CLA	CAC-C3C-C2C	-3.51	121.11	127.56
29	A	850	LHG	O7-C7-C8	3.51	119.07	111.48
36	O	204	IHT	C18-C22-C23	-3.51	121.05	126.23
27	b	604	CLA	CMB-C2B-C1B	-3.51	120.08	125.42
30	F	205	WVN	C39-C40-C37	3.51	130.69	123.52
37	e	609	KC2	C2A-C1A-NA	3.50	114.96	109.34
37	n	612	KC2	CBC-CAC-C3C	-3.50	110.02	127.53
27	B	822	CLA	O2D-CGD-CBD	3.50	117.36	111.23
30	F	205	WVN	C29-C26-C22	-3.50	122.37	127.28
37	n	611	KC2	C2A-C1A-NA	3.50	114.95	109.34
35	f	614	II0	C19-C13-C11	3.49	120.85	114.42
27	e	602	CLA	CMB-C2B-C1B	-3.49	120.10	125.42
27	J	105	CLA	C3B-C4B-NB	-3.49	107.41	110.53
27	k	307	CLA	CBA-CAA-C2A	3.49	124.18	113.79
35	b	615	II0	C16-C03-C15	-3.49	98.64	108.63
35	g	318	II0	C19-C13-C11	3.49	120.84	114.42
27	n	613	CLA	C4A-NA-C1A	3.49	108.27	106.68
27	B	825	CLA	CMB-C2B-C1B	-3.49	120.11	125.42
30	L	201	WVN	C26-C29-C31	-3.49	113.09	123.20
27	F	201	CLA	O2D-CGD-CBD	3.49	117.33	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	103	WVN	C26-C29-C31	-3.49	113.09	123.20
30	B	848	WVN	C38-C34-C37	-3.49	117.17	122.82
27	f	610	CLA	C4A-NA-C1A	3.49	108.27	106.68
27	A	803	CLA	CAA-CBA-CGA	-3.49	103.31	113.21
27	i	311	CLA	CMB-C2B-C3B	3.49	134.75	126.55
37	i	310	KC2	CMD-C2D-C3D	3.48	136.66	125.67
35	e	612	II0	C32-C34-C36	-3.48	116.81	126.36
27	k	304	CLA	CMC-C2C-C1C	-3.48	119.59	125.03
35	c	615	II0	C19-C13-C09	-3.48	117.65	124.16
27	A	830	CLA	CMB-C2B-C1B	-3.48	120.12	125.42
27	l	307	CLA	O2A-CGA-O1A	-3.48	114.93	123.63
37	k	311	KC2	CBC-CAC-C3C	-3.48	110.16	127.53
35	a	318	II0	C38-C36-C40	-3.47	117.19	122.82
27	B	835	CLA	CAA-CBA-CGA	-3.47	103.35	113.21
27	d	304	CLA	O2D-CGD-CBD	3.47	117.30	111.23
37	k	310	KC2	O2D-CGD-O1D	-3.47	117.09	123.85
29	L	207	LHG	C5-O7-C7	-3.47	109.49	117.80
37	f	611	KC2	C2A-C1A-NA	3.47	114.90	109.34
35	k	316	II0	C27-C25-C29	-3.47	117.45	124.18
37	d	310	KC2	CMD-C2D-C3D	3.47	136.60	125.67
35	k	318	II0	C31-C33-C35	-3.46	116.86	126.36
27	j	604	CLA	CHB-C4A-NA	3.46	129.40	124.40
27	c	603	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
30	B	844	WVN	C21-C15-C13	-3.46	120.71	124.48
35	c	613	II0	C20-C14-C10	-3.46	117.69	124.16
35	j	613	II0	C30-C32-C34	-3.46	113.17	123.20
37	g	314	KC2	CMD-C2D-C3D	3.46	136.58	125.67
37	c	610	KC2	CBC-CAC-C3C	-3.46	110.24	127.53
35	g	317	II0	C29-C31-C33	-3.46	113.18	123.20
35	e	616	II0	C41-C42-C40	-3.46	116.45	123.52
37	n	612	KC2	O2D-CGD-CBD	3.46	117.27	111.23
27	a	306	CLA	CMB-C2B-C1B	-3.45	120.16	125.42
27	e	603	CLA	CMB-C2B-C1B	-3.45	120.17	125.42
35	c	617	II0	C42-C41-C39	-3.45	116.46	123.52
35	m	614	II0	C31-C29-C25	-3.45	116.97	126.61
27	i	303	CLA	O2D-CGD-CBD	3.45	117.26	111.23
36	m	616	IHT	C19-C10-C09	3.45	120.94	113.60
27	R	203	CLA	CMB-C2B-C3B	3.44	134.65	126.55
35	n	618	II0	C31-C33-C35	-3.44	116.92	126.36
35	l	317	II0	C33-C35-C39	-3.44	113.59	119.01
37	g	312	KC2	CBC-CAC-C3C	-3.44	110.33	127.53
30	M	101	WVN	C06-C13-C15	-3.44	117.94	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	i	305	CLA	CMB-C2B-C1B	-3.44	120.18	125.42
37	k	311	KC2	C3B-C2B-C1B	-3.44	103.79	107.05
30	A	848	WVN	C30-C33-C34	-3.43	116.95	126.36
35	j	614	II0	C32-C34-C36	-3.43	116.95	126.36
27	s	206	CLA	CMB-C2B-C1B	-3.43	120.19	125.42
27	j	606	CLA	CHB-C4A-NA	3.43	129.35	124.40
27	k	308	CLA	CMB-C2B-C1B	-3.43	120.19	125.42
36	a	317	IHT	C29-C31-C34	-3.43	113.26	123.20
27	c	612	CLA	CMB-C2B-C3B	3.43	134.62	126.55
37	k	312	KC2	CMD-C2D-C3D	3.43	136.48	125.67
27	a	307	CLA	O2D-CGD-CBD	3.43	117.22	111.23
35	f	618	II0	C11-C13-C09	-3.43	113.37	120.50
27	g	308	CLA	CHB-C4A-NA	3.43	129.34	124.40
27	A	827	CLA	CMB-C2B-C1B	-3.43	120.20	125.42
35	a	314	II0	C19-C13-C09	-3.43	117.75	124.16
27	h	302	CLA	CMB-C2B-C1B	-3.42	120.20	125.42
30	s	207	WVN	C29-C26-C22	-3.42	122.47	127.28
30	J	102	WVN	C20-C23-C25	-3.42	121.17	126.23
30	B	846	WVN	C27-C25-C23	-3.42	112.86	118.09
27	J	103	CLA	CMB-C2B-C3B	3.42	134.60	126.55
27	B	836	CLA	CHB-C4A-NA	3.42	129.34	124.40
27	B	839	CLA	CMB-C2B-C1B	-3.42	120.21	125.42
36	b	614	IHT	C31-C29-C26	-3.42	117.05	126.61
37	n	612	KC2	CMD-C2D-C3D	3.42	136.44	125.67
30	I	101	WVN	C40-C37-C34	-3.41	122.49	127.28
30	L	205	WVN	C30-C28-C25	-3.41	122.49	127.28
27	n	609	CLA	CMB-C2B-C1B	-3.41	120.22	125.42
27	a	303	CLA	C1-C2-C3	-3.41	120.61	126.20
35	k	315	II0	C03-C05-C07	3.41	121.07	113.59
37	d	309	KC2	CMD-C2D-C3D	3.41	136.42	125.67
27	h	306	CLA	CMB-C2B-C1B	-3.41	120.23	125.42
27	A	840	CLA	C12-C11-C10	3.41	128.55	113.28
27	j	604	CLA	CMA-C3A-C4A	-3.41	102.62	111.77
27	A	826	CLA	CMB-C2B-C3B	3.41	134.56	126.55
30	O	201	WVN	C39-C40-C37	-3.40	116.55	123.52
35	k	314	II0	C19-C13-C09	-3.40	117.80	124.16
37	k	311	KC2	C1D-CHD-C4C	-3.40	118.25	126.25
27	l	306	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
35	f	615	II0	C38-C36-C34	3.40	123.28	118.09
30	A	848	WVN	C21-C15-C14	3.40	120.84	113.60
27	A	825	CLA	CMB-C2B-C1B	-3.40	120.24	125.42
27	A	816	CLA	O2D-CGD-O1D	-3.40	117.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	614	IHT	C29-C31-C34	-3.40	113.35	123.20
35	b	612	II0	C42-C41-C39	-3.40	116.56	123.52
35	a	314	II0	C20-C14-C12	3.40	120.67	114.42
35	a	318	II0	C20-C14-C12	3.40	120.67	114.42
27	A	816	CLA	CBA-CAA-C2A	3.40	123.90	113.79
35	l	317	II0	C20-C14-C10	-3.40	117.81	124.16
30	B	848	WVN	C30-C33-C34	3.39	135.67	126.36
30	J	101	WVN	C26-C29-C31	-3.39	113.36	123.20
35	g	318	II0	C16-C03-C09	-3.39	104.44	110.52
35	b	615	II0	C17-C04-C10	-3.39	104.44	110.52
37	i	310	KC2	CBC-CAC-C3C	-3.39	110.57	127.53
27	k	305	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
35	a	315	II0	C42-C40-C36	-3.39	122.52	127.28
35	k	315	II0	C05-C03-C09	3.39	116.17	109.49
35	i	314	II0	C42-C40-C36	-3.39	122.52	127.28
27	B	803	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
27	k	304	CLA	CHB-C4A-NA	3.39	129.29	124.40
27	c	603	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
27	B	802	CLA	CBC-CAC-C3C	3.39	121.60	112.42
27	B	801	CLA	C1-C2-C3	-3.39	120.65	126.20
27	d	308	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
35	c	613	II0	C19-C13-C09	-3.39	117.83	124.16
38	i	301	LMU	O1'-C1'-C2'	3.38	113.41	108.27
35	n	615	II0	C17-C04-C10	-3.38	104.46	110.52
35	J	104	II0	C20-C14-C10	-3.38	117.84	124.16
27	h	308	CLA	CHB-C4A-NA	3.38	129.28	124.40
27	n	605	CLA	CHB-C4A-NA	3.38	129.28	124.40
35	d	314	II0	C20-C14-C10	-3.38	117.85	124.16
27	m	608	CLA	CMB-C2B-C1B	-3.38	120.28	125.42
35	m	614	II0	C20-C14-C12	3.38	120.63	114.42
27	A	813	CLA	CAA-CBA-CGA	-3.37	103.49	112.49
35	c	615	II0	C05-C03-C09	3.37	116.14	109.49
35	j	614	II0	C19-C13-C09	-3.37	117.85	124.16
37	g	314	KC2	O2D-CGD-CBD	3.37	117.13	111.23
27	A	832	CLA	CAA-CBA-CGA	-3.37	103.63	113.21
37	e	609	KC2	CMD-C2D-C3D	3.37	136.31	125.67
34	F	206	LMG	C7-O1-C1	-3.37	106.57	113.80
27	k	308	CLA	CED-O2D-CGD	3.37	123.56	115.92
35	i	314	II0	C20-C14-C10	-3.37	117.86	124.16
27	A	836	CLA	CMB-C2B-C1B	-3.37	120.29	125.42
27	n	602	CLA	CMB-C2B-C1B	-3.37	120.30	125.42
27	K	101	CLA	O2D-CGD-O1D	-3.37	117.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	820	CLA	C7-C6-C5	-3.36	104.29	113.26
27	B	819	CLA	C4A-NA-C1A	3.36	108.21	106.68
35	l	314	II0	C31-C33-C35	-3.36	117.14	126.36
35	b	612	II0	C29-C31-C33	-3.36	113.45	123.20
27	B	813	CLA	CMB-C2B-C3B	3.36	134.46	126.55
27	B	822	CLA	CMB-C2B-C3B	3.36	134.46	126.55
35	J	104	II0	C42-C41-C39	-3.36	116.64	123.52
27	c	602	CLA	CAC-C3C-C2C	-3.36	121.38	127.56
27	k	303	CLA	CMB-C2B-C3B	3.36	134.46	126.55
37	m	610	KC2	CMD-C2D-C3D	3.36	136.27	125.67
27	a	304	CLA	CMB-C2B-C3B	3.36	134.45	126.55
35	a	315	II0	C31-C33-C35	-3.36	117.16	126.36
27	j	605	CLA	C2A-C1A-CHA	3.36	129.69	123.87
37	d	310	KC2	C1D-CHD-C4C	-3.36	118.36	126.25
35	d	312	II0	C20-C14-C12	3.35	120.58	114.42
35	J	104	II0	C19-C13-C09	-3.35	117.89	124.16
35	a	314	II0	C30-C32-C34	-3.35	113.49	123.20
27	g	308	CLA	CMB-C2B-C1B	-3.35	120.32	125.42
27	g	304	CLA	CMB-C2B-C3B	3.35	134.43	126.55
27	B	803	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
27	i	308	CLA	C3B-C4B-NB	-3.35	107.54	110.53
30	R	202	WVN	C21-C15-C13	-3.35	120.83	124.48
27	d	311	CLA	O2D-CGD-O1D	-3.35	117.34	123.85
27	n	608	CLA	C4A-NA-C1A	3.34	108.20	106.68
29	m	617	LHG	C5-O7-C7	-3.34	109.80	117.80
27	a	309	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
27	B	821	CLA	CMB-C2B-C3B	3.34	134.40	126.55
27	j	604	CLA	CAA-CBA-CGA	-3.34	103.74	113.21
30	J	102	WVN	C08-C01-C03	-3.34	102.07	109.01
36	a	317	IHT	C18-C22-C23	-3.34	121.30	126.23
37	k	311	KC2	CMD-C2D-C3D	3.33	136.19	125.67
35	i	314	II0	C37-C35-C33	-3.33	113.00	118.09
27	l	312	CLA	C4A-NA-C1A	3.33	108.20	106.68
27	B	809	CLA	CHB-C4A-NA	3.33	129.21	124.40
30	R	201	WVN	C30-C33-C34	-3.33	117.22	126.36
27	m	605	CLA	C3B-C4B-NB	-3.33	107.56	110.53
27	k	302	CLA	C4A-NA-C1A	3.33	108.20	106.68
27	h	306	CLA	C3B-C4B-NB	-3.33	107.56	110.53
27	A	834	CLA	C1-C2-C3	-3.33	120.75	126.20
27	n	603	CLA	CAA-C2A-C3A	-3.33	104.01	113.00
27	B	837	CLA	O2A-CGA-O1A	-3.33	115.31	123.63
36	k	317	IHT	C19-C10-C07	-3.32	120.86	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	805	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
30	O	201	WVN	C21-C15-C13	-3.32	120.86	124.48
37	d	309	KC2	CBC-CAC-C3C	-3.32	110.92	127.53
37	g	312	KC2	CHB-C4A-NA	3.32	129.38	124.23
30	B	843	WVN	C39-C36-C32	-3.32	122.62	127.28
34	c	619	LMG	O6-C1-O1	3.32	117.89	110.04
27	F	203	CLA	CHB-C4A-NA	3.32	129.19	124.40
27	B	820	CLA	CHB-C4A-NA	3.32	129.19	124.40
27	m	609	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
27	k	303	CLA	CHB-C4A-NA	3.32	129.19	124.40
30	O	201	WVN	C06-C13-C20	3.32	124.64	115.65
35	l	314	II0	C32-C34-C36	-3.32	117.27	126.36
34	c	619	LMG	C1-O6-C5	3.31	120.19	113.72
27	A	808	CLA	CMB-C2B-C1B	-3.31	120.37	125.42
27	s	203	CLA	O2A-CGA-CBA	3.31	121.94	111.83
27	g	302	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
30	A	849	WVN	C08-C01-C07	-3.31	103.05	107.87
27	h	313	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
27	B	802	CLA	C3B-C4B-NB	-3.31	107.57	110.53
27	m	612	CLA	CMC-C2C-C3C	3.31	135.10	126.15
37	s	204	KC2	C3A-C4A-NA	3.31	114.55	110.45
27	k	305	CLA	O2D-CGD-CBD	3.31	117.01	111.23
27	i	306	CLA	CMB-C2B-C1B	-3.31	120.39	125.42
35	e	616	II0	C20-C14-C12	3.30	120.50	114.42
27	f	602	CLA	CAA-CBA-CGA	-3.30	103.83	113.21
27	i	308	CLA	CMB-C2B-C3B	3.30	134.32	126.55
30	A	849	WVN	C02-C11-C19	-3.30	119.44	124.58
37	j	610	KC2	C2A-C1A-NA	3.30	114.63	109.34
35	l	313	II0	C41-C39-C35	-3.30	122.65	127.28
35	g	320	II0	C20-C14-C10	-3.30	118.00	124.16
27	n	606	CLA	CBA-CAA-C2A	-3.30	103.99	113.79
27	A	812	CLA	C4-C3-C5	3.30	120.95	115.23
30	B	845	WVN	C24-C22-C19	3.30	123.12	118.09
37	i	310	KC2	CHB-C4A-NA	3.29	129.34	124.23
27	A	812	CLA	CMB-C2B-C3B	3.29	134.29	126.55
37	k	312	KC2	CBC-CAC-C3C	-3.29	111.08	127.53
35	c	617	II0	C31-C29-C25	-3.29	117.40	126.61
27	A	817	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
35	m	615	II0	C19-C13-C11	3.29	120.47	114.42
35	k	314	II0	C31-C33-C35	-3.29	117.35	126.36
27	A	824	CLA	O2D-CGD-CBD	3.29	116.98	111.23
35	h	311	II0	C30-C32-C34	-3.29	113.68	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	602	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
36	m	616	IHT	C30-C32-C33	-3.29	117.35	126.36
27	j	606	CLA	CBA-CAA-C2A	-3.29	104.02	113.79
27	h	304	CLA	CMB-C2B-C3B	3.29	134.28	126.55
35	d	313	II0	C06-C04-C10	3.29	115.96	109.49
27	A	838	CLA	CMB-C2B-C3B	3.29	134.28	126.55
30	F	205	WVN	C35-C32-C31	3.28	123.11	118.09
30	I	101	WVN	C04-C09-C05	-3.28	121.69	124.83
29	A	850	LHG	C5-O7-C7	-3.28	109.94	117.80
37	m	610	KC2	CBC-CAC-C3C	-3.28	111.12	127.53
27	l	307	CLA	CHB-C4A-NA	3.28	129.14	124.40
37	c	610	KC2	CHB-C4A-NA	3.28	129.32	124.23
27	A	815	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
30	A	848	WVN	C20-C13-C15	-3.28	114.00	121.56
36	k	317	IHT	C31-C34-C35	-3.28	117.38	126.36
37	s	204	KC2	CHB-C4A-NA	3.27	129.31	124.23
36	c	620	IHT	C09-C10-C07	-3.27	118.28	122.70
27	e	602	CLA	CHB-C4A-NA	3.27	129.12	124.40
30	I	101	WVN	C28-C30-C33	-3.27	113.72	123.20
35	b	612	II0	C32-C30-C26	-3.27	117.46	126.61
27	A	856	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
35	j	613	II0	C32-C30-C26	-3.27	117.47	126.61
27	n	605	CLA	CAC-C3C-C2C	-3.27	121.55	127.56
35	g	316	II0	C31-C29-C25	-3.27	117.47	126.61
27	j	604	CLA	CMA-C3A-C2A	-3.26	101.36	113.98
35	b	612	II0	C32-C34-C36	-3.26	117.41	126.36
30	F	204	WVN	C21-C15-C14	3.26	120.54	113.60
35	a	316	II0	C22-C24-C26	-3.26	165.16	176.23
27	B	832	CLA	CMB-C2B-C1B	-3.26	120.46	125.42
29	e	617	LHG	C6-C5-C4	-3.25	104.20	111.78
27	i	312	CLA	CHB-C4A-NA	3.25	129.10	124.40
37	k	312	KC2	O2D-CGD-O1D	-3.25	117.52	123.85
30	l	301	WVN	C26-C29-C31	-3.25	113.77	123.20
37	i	317	KC2	O2D-CGD-CBD	3.25	116.92	111.23
35	l	314	II0	C20-C14-C10	-3.25	118.08	124.16
35	l	315	II0	C20-C14-C10	-3.25	118.08	124.16
27	m	604	CLA	CMA-C3A-C4A	-3.25	103.04	111.77
30	l	316	WVN	C14-C15-C13	-3.25	118.31	122.70
37	i	317	KC2	C2A-C1A-NA	3.25	114.55	109.34
27	s	202	CLA	C3B-C4B-NB	-3.25	107.63	110.53
35	l	317	II0	C31-C29-C25	-3.25	117.53	126.61
35	f	616	II0	C12-C14-C10	-3.25	113.74	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	607	CLA	CMB-C2B-C3B	3.25	134.18	126.55
27	n	609	CLA	CMB-C2B-C3B	3.25	134.18	126.55
34	J	106	LMG	O7-C10-C11	3.25	118.50	111.48
27	k	306	CLA	CAC-C3C-C4C	3.24	129.01	124.79
36	m	616	IHT	C22-C18-C07	-3.24	118.33	127.00
35	h	312	II0	C19-C13-C11	3.24	120.39	114.42
27	n	602	CLA	CGD-CBD-CAD	-3.24	100.34	110.85
35	m	614	II0	C38-C36-C34	3.24	123.04	118.09
30	h	309	WVN	C40-C37-C34	-3.24	122.73	127.28
27	h	306	CLA	C4A-NA-C1A	3.24	108.16	106.68
27	B	849	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
36	c	620	IHT	C31-C34-C35	-3.24	117.48	126.36
27	f	612	CLA	CMB-C2B-C1B	-3.24	120.49	125.42
37	k	312	KC2	C2A-C1A-NA	3.24	114.53	109.34
35	n	618	II0	C20-C14-C10	-3.23	118.12	124.16
27	b	602	CLA	CHB-C4A-NA	3.23	129.06	124.40
27	B	826	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
35	h	312	II0	C31-C29-C25	-3.23	117.58	126.61
35	j	613	II0	C27-C25-C29	-3.23	117.91	124.18
27	k	308	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
27	B	812	CLA	C1-C2-C3	-3.23	120.91	126.20
35	c	614	II0	C06-C04-C10	3.23	115.84	109.49
30	F	204	WVN	C18-C06-C17	-3.22	99.40	108.63
27	h	301	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
36	c	620	IHT	C30-C27-C23	-3.22	122.76	127.28
27	b	601	CLA	O2D-CGD-CBD	3.22	116.86	111.23
27	h	313	CLA	CMB-C2B-C1B	-3.22	120.51	125.42
27	i	308	CLA	CMD-C2D-C3D	3.22	135.07	127.69
27	i	312	CLA	CAA-C2A-C3A	-3.22	104.30	113.00
30	B	847	WVN	C30-C33-C34	-3.22	117.54	126.36
27	n	608	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
27	B	805	CLA	CHB-C4A-NA	3.22	129.04	124.40
30	A	846	WVN	C39-C40-C37	-3.22	116.94	123.52
30	l	301	WVN	C30-C33-C34	-3.22	117.54	126.36
37	c	610	KC2	C2A-C1A-NA	3.22	114.50	109.34
27	k	313	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
35	n	616	II0	C19-C13-C11	3.22	120.33	114.42
35	d	313	II0	C41-C39-C35	-3.21	122.77	127.28
27	A	816	CLA	C4-C3-C2	-3.21	115.37	123.63
27	A	825	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
27	B	815	CLA	CMB-C2B-C1B	-3.21	120.53	125.42
35	g	318	II0	C15-C03-C09	-3.21	104.76	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	n	611	KC2	CHB-C4A-NA	3.21	129.21	124.23
27	B	840	CLA	C7-C6-C5	-3.21	104.70	113.26
35	d	313	II0	C42-C40-C36	-3.21	122.78	127.28
30	R	202	WVN	C17-C06-C13	-3.21	105.21	110.24
27	a	303	CLA	CMB-C2B-C3B	3.21	134.10	126.55
27	i	308	CLA	CAA-CBA-CGA	3.21	122.32	113.21
27	m	608	CLA	C4A-NA-C1A	3.21	108.14	106.68
27	A	822	CLA	O2A-CGA-O1A	-3.21	115.60	123.63
27	B	803	CLA	CMB-C2B-C3B	3.21	134.10	126.55
27	A	830	CLA	CHB-C4A-NA	3.21	129.03	124.40
27	B	826	CLA	C3B-C4B-NB	-3.21	107.67	110.53
27	g	302	CLA	C2A-C1A-CHA	3.21	129.43	123.87
35	j	615	II0	C19-C13-C09	-3.20	118.17	124.16
27	B	849	CLA	CHB-C4A-NA	3.20	129.02	124.40
30	B	845	WVN	C39-C36-C32	-3.20	122.79	127.28
30	e	615	WVN	C03-C04-C09	-3.20	106.69	112.07
27	j	604	CLA	C1-C2-C3	-3.20	120.95	126.20
35	l	314	II0	C06-C04-C10	3.20	115.80	109.49
27	A	819	CLA	CAC-C3C-C4C	-3.20	120.62	124.79
35	m	614	II0	C34-C36-C40	-3.20	113.97	119.01
30	h	309	WVN	C07-C01-C02	3.20	114.39	109.55
35	k	316	II0	C42-C40-C36	-3.20	122.79	127.28
37	e	609	KC2	O2D-CGD-CBD	3.20	116.82	111.23
27	A	828	CLA	C1-C2-C3	-3.20	120.95	126.20
27	B	806	CLA	CBA-CAA-C2A	3.20	123.31	113.79
27	m	612	CLA	CBC-CAC-C3C	3.20	121.09	112.42
27	A	804	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
27	g	306	CLA	CAC-C3C-C4C	3.20	128.95	124.79
27	h	306	CLA	CMB-C2B-C3B	3.20	134.07	126.55
27	g	307	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
27	B	831	CLA	CAA-C2A-C3A	-3.20	104.36	113.00
31	b	616	LMT	C4'-C3'-C2'	3.20	116.44	110.83
27	e	608	CLA	CAA-C2A-C3A	-3.19	104.37	113.00
27	n	605	CLA	C2A-C1A-CHA	3.19	129.41	123.87
27	i	303	CLA	C1-C2-C3	-3.19	121.61	126.76
27	j	605	CLA	CAA-C2A-C1A	3.19	122.42	111.97
36	k	317	IHT	C12-C15-C11	-3.19	113.87	120.50
27	m	604	CLA	CMA-C3A-C2A	-3.18	101.67	113.98
30	e	615	WVN	C07-C01-C03	-3.18	102.39	109.01
30	l	316	WVN	C04-C09-C05	-3.18	121.79	124.83
37	g	313	KC2	O2D-CGD-CBD	3.18	116.79	111.23
27	i	312	CLA	CMB-C2B-C1B	-3.18	120.57	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	s	207	WVN	C21-C15-C13	-3.18	121.01	124.48
30	s	207	WVN	C02-C05-C09	-3.18	117.55	121.47
27	A	820	CLA	CMB-C2B-C3B	3.18	134.03	126.55
35	c	614	II0	C19-C13-C11	3.18	120.27	114.42
30	l	301	WVN	C14-C15-C13	-3.18	118.41	122.70
30	F	205	WVN	C28-C30-C33	3.18	132.41	123.20
27	F	202	CLA	C3B-C4B-NB	-3.18	107.69	110.53
27	a	307	CLA	CAC-C3C-C2C	-3.18	121.72	127.56
27	l	304	CLA	CHB-C4A-NA	3.18	128.98	124.40
36	c	620	IHT	C40-C41-C38	-3.18	117.02	123.52
30	A	847	WVN	C31-C32-C36	3.18	124.00	119.01
35	e	616	II0	C42-C40-C36	-3.18	122.82	127.28
27	B	813	CLA	O2D-CGD-CBD	3.17	116.78	111.23
30	L	205	WVN	C04-C09-C05	-3.17	121.80	124.83
35	i	314	II0	C12-C14-C10	-3.17	113.89	120.50
27	A	814	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
27	b	606	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
27	A	818	CLA	CMC-C2C-C3C	3.17	134.73	126.15
27	n	606	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
37	k	312	KC2	CHB-C4A-NA	3.17	129.15	124.23
37	g	313	KC2	C3B-C2B-C1B	-3.17	104.05	107.05
30	A	848	WVN	C21-C15-C13	-3.17	121.03	124.48
30	B	845	WVN	C10-C06-C13	3.17	115.04	110.44
27	c	602	CLA	O2D-CGD-CBD	3.16	116.76	111.23
30	R	202	WVN	C11-C19-C22	-3.16	119.52	126.32
27	g	302	CLA	O2D-CGD-CBD	3.16	116.76	111.23
35	c	617	II0	C41-C39-C35	-3.16	122.84	127.28
30	F	205	WVN	C20-C13-C15	-3.16	114.27	121.56
37	n	612	KC2	C3B-C2B-C1B	-3.16	104.05	107.05
34	c	619	LMG	C9-C8-C7	-3.16	104.41	111.78
35	f	616	II0	C20-C14-C12	3.16	120.24	114.42
27	b	610	CLA	O1D-CGD-CBD	3.16	130.75	124.52
37	f	611	KC2	CHB-C4A-NA	3.16	129.13	124.23
37	g	313	KC2	C2A-C1A-NA	3.16	114.41	109.34
27	B	822	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
27	j	608	CLA	CMB-C2B-C3B	3.16	133.99	126.55
30	s	205	WVN	C03-C04-C09	-3.16	106.76	112.07
30	B	848	WVN	C26-C29-C31	-3.16	114.04	123.20
27	m	609	CLA	CHB-C4A-NA	3.16	128.96	124.40
35	n	615	II0	C20-C14-C10	-3.16	118.25	124.16
35	e	614	II0	C05-C03-C09	3.16	115.72	109.49
27	i	307	CLA	CMB-C2B-C3B	3.16	133.98	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	R	204	IHT	C19-C10-C09	3.16	120.33	113.60
37	g	314	KC2	C3B-C2B-C1B	-3.16	104.06	107.05
35	e	616	II0	C32-C34-C36	-3.16	117.71	126.36
35	n	614	II0	C06-C04-C10	3.16	115.71	109.49
27	B	816	CLA	CMB-C2B-C3B	3.15	133.97	126.55
35	f	614	II0	C32-C34-C36	-3.15	117.72	126.36
27	k	304	CLA	CMC-C2C-C3C	3.15	134.68	126.15
37	l	311	KC2	C3B-C2B-C1B	-3.15	104.06	107.05
35	f	615	II0	C12-C14-C10	-3.15	113.94	120.50
30	F	204	WVN	C39-C36-C32	-3.15	122.86	127.28
37	j	610	KC2	CHB-C4A-NA	3.15	129.12	124.23
37	e	609	KC2	CBC-CAC-C3C	-3.15	111.79	127.53
35	d	313	II0	C20-C14-C10	-3.15	118.27	124.16
36	O	204	IHT	C29-C31-C34	-3.15	114.08	123.20
35	c	615	II0	C20-C14-C12	3.15	120.21	114.42
27	A	830	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
35	h	311	II0	C11-C13-C09	-3.15	113.95	120.50
30	l	316	WVN	C10-C12-C14	-3.15	104.36	111.28
27	c	608	CLA	CHB-C4A-NA	3.15	128.94	124.40
37	l	311	KC2	CHB-C4A-NA	3.15	129.11	124.23
35	m	613	II0	C15-C03-C09	-3.14	104.88	110.52
27	s	208	CLA	CMB-C2B-C1B	-3.14	120.63	125.42
27	n	603	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
27	A	803	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
27	A	803	CLA	O2D-CGD-CBD	3.14	116.72	111.23
35	l	313	II0	C15-C03-C09	-3.14	104.89	110.52
36	R	204	IHT	C19-C10-C07	-3.14	121.06	124.48
27	B	804	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
35	l	302	II0	C31-C33-C35	-3.14	117.75	126.36
27	i	307	CLA	C4A-NA-C1A	3.14	108.11	106.68
34	L	208	LMG	C1-C2-C3	3.14	116.61	110.01
27	K	101	CLA	CHB-C4A-NA	3.14	128.93	124.40
37	k	310	KC2	C3B-C2B-C1B	-3.13	104.08	107.05
27	k	302	CLA	CMB-C2B-C3B	3.13	133.92	126.55
37	d	310	KC2	O2D-CGD-O1D	-3.13	117.75	123.85
35	g	320	II0	C32-C34-C36	-3.13	117.77	126.36
27	A	826	CLA	CHB-C4A-NA	3.13	128.92	124.40
35	d	313	II0	C05-C03-C09	3.13	115.66	109.49
27	A	816	CLA	CMB-C2B-C1B	-3.13	120.65	125.42
27	e	605	CLA	CHB-C4A-NA	3.13	128.92	124.40
27	b	606	CLA	C3B-C4B-NB	-3.13	107.73	110.53
27	c	606	CLA	O2D-CGD-CBD	3.13	116.70	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	602	CLA	CHB-C4A-NA	3.13	128.92	124.40
27	e	607	CLA	CMC-C2C-C1C	3.13	129.93	125.03
27	B	819	CLA	C3B-C4B-NB	-3.13	107.74	110.53
37	g	314	KC2	CHB-C4A-NA	3.13	129.08	124.23
27	A	838	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
27	e	601	CLA	C2A-C1A-CHA	3.13	129.30	123.87
27	d	302	CLA	CMB-C2B-C1B	-3.13	120.66	125.42
27	m	602	CLA	C3B-C4B-NB	-3.13	107.74	110.53
27	b	601	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
27	g	311	CLA	CHB-C4A-NA	3.12	128.91	124.40
27	l	308	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
27	d	301	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
37	d	310	KC2	O2D-CGD-CBD	3.12	116.69	111.23
35	a	316	II0	C05-C03-C09	3.12	115.64	109.49
35	c	613	II0	C32-C34-C36	-3.12	117.81	126.36
36	c	616	IHT	C30-C32-C33	-3.12	117.81	126.36
27	A	807	CLA	CHB-C4A-NA	3.12	128.90	124.40
35	m	615	II0	C31-C33-C35	-3.12	117.82	126.36
27	B	812	CLA	CMB-C2B-C3B	3.11	133.88	126.55
27	B	801	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
37	m	610	KC2	CHB-C4A-NA	3.11	129.06	124.23
35	e	612	II0	C20-C14-C12	3.11	120.15	114.42
30	l	301	WVN	C39-C40-C37	-3.11	117.15	123.52
27	k	304	CLA	C2A-C1A-CHA	3.11	129.27	123.87
37	m	610	KC2	C3B-C2B-C1B	-3.11	104.10	107.05
27	b	611	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
35	n	614	II0	C19-C13-C09	-3.11	118.35	124.16
30	B	845	WVN	C31-C32-C36	-3.11	114.12	119.01
27	l	312	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
27	B	816	CLA	C3B-C2B-C1B	3.11	110.83	107.17
30	l	316	WVN	C20-C23-C25	-3.11	121.64	126.23
27	h	301	CLA	O2D-CGD-CBD	3.11	116.66	111.23
36	c	620	IHT	C36-C33-C32	3.11	122.83	118.09
27	h	313	CLA	O2D-CGD-CBD	3.10	116.66	111.23
37	g	314	KC2	C2A-C1A-NA	3.10	114.32	109.34
30	B	843	WVN	C26-C29-C31	-3.10	114.21	123.20
27	c	608	CLA	CAA-CBA-CGA	-3.10	104.40	113.21
27	A	828	CLA	CMB-C2B-C1B	-3.10	120.69	125.42
27	j	605	CLA	CHB-C4A-NA	3.10	128.88	124.40
27	A	818	CLA	C4A-NA-C1A	3.10	108.09	106.68
37	e	609	KC2	O2D-CGD-O1D	-3.10	117.81	123.85
30	B	843	WVN	C30-C28-C25	-3.10	122.93	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	833	CLA	CHB-C4A-NA	3.10	128.87	124.40
37	j	610	KC2	O2D-CGD-O1D	-3.10	117.81	123.85
27	d	304	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
35	a	318	II0	C05-C03-C09	3.10	115.59	109.49
27	i	312	CLA	C4A-NA-C1A	3.10	108.09	106.68
30	A	849	WVN	C04-C09-C05	-3.10	121.87	124.83
27	i	309	CLA	C2D-C1D-ND	-3.09	107.06	110.13
27	s	202	CLA	C1-C2-C3	-3.09	121.13	126.20
27	B	833	CLA	C3B-C4B-NB	-3.09	107.77	110.53
31	a	320	LMT	C1'-O5'-C5'	3.09	119.76	113.72
35	b	613	II0	C29-C31-C33	-3.09	114.24	123.20
35	c	615	II0	C19-C13-C11	3.09	120.11	114.42
30	A	847	WVN	C17-C06-C13	3.09	115.09	110.24
29	b	617	LHG	O7-C7-O9	-3.09	116.48	123.70
27	A	825	CLA	O2D-CGD-CBD	3.09	116.63	111.23
35	f	614	II0	C31-C33-C35	-3.09	117.89	126.36
29	a	319	LHG	O8-C23-C24	3.09	121.25	111.83
36	b	614	IHT	C31-C34-C35	-3.09	117.90	126.36
27	s	202	CLA	CAA-C2A-C3A	-3.09	104.66	113.00
27	B	810	CLA	CHB-C4A-NA	3.09	128.85	124.40
27	B	824	CLA	CMB-C2B-C3B	3.09	133.81	126.55
35	k	314	II0	C38-C36-C40	-3.09	117.82	122.82
29	g	321	LHG	O8-C23-C24	3.09	121.25	111.83
37	n	611	KC2	C3B-C2B-C1B	-3.08	104.13	107.05
27	l	309	CLA	C4A-NA-C1A	3.08	108.09	106.68
35	i	318	II0	C19-C13-C09	-3.08	118.39	124.16
35	g	317	II0	C32-C34-C36	-3.08	117.91	126.36
27	B	815	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
27	c	602	CLA	CHB-C4A-NA	3.08	128.85	124.40
34	b	619	LMG	C4-C3-C2	3.08	116.24	110.83
27	A	813	CLA	C2C-C1C-NC	3.08	113.22	109.98
27	A	827	CLA	CMB-C2B-C3B	3.08	133.79	126.55
27	A	855	CLA	O2A-CGA-O1A	-3.08	115.92	123.63
27	k	308	CLA	C3B-C4B-NB	-3.08	107.78	110.53
27	a	306	CLA	CBA-CAA-C2A	3.08	122.95	113.79
37	k	312	KC2	C3B-C2B-C1B	-3.08	104.13	107.05
27	g	304	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
27	A	840	CLA	CHB-C4A-NA	3.08	128.84	124.40
27	m	611	CLA	C4-C3-C5	3.08	119.75	116.13
27	A	823	CLA	O2A-CGA-O1A	-3.08	115.93	123.63
27	k	304	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
30	R	202	WVN	C02-C05-C09	-3.08	117.68	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	317	IHT	C19-C10-C09	3.08	120.15	113.60
29	J	107	LHG	O7-C7-C8	3.07	118.13	111.48
27	A	805	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
27	g	322	CLA	CAC-C3C-C2C	-3.07	121.91	127.56
35	g	317	II0	C41-C42-C40	-3.07	117.23	123.52
30	s	205	WVN	C01-C02-C11	3.07	116.36	112.83
27	A	805	CLA	CMB-C2B-C3B	3.07	133.78	126.55
27	j	603	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
35	k	318	II0	C16-C03-C09	-3.07	105.01	110.52
27	d	311	CLA	CMB-C2B-C3B	3.07	133.78	126.55
27	A	803	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
27	a	306	CLA	CMB-C2B-C3B	3.07	133.77	126.55
27	n	602	CLA	CMB-C2B-C3B	3.07	133.77	126.55
27	B	830	CLA	CHB-C4A-NA	3.07	128.83	124.40
27	c	601	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
27	m	603	CLA	CHB-C4A-NA	3.07	128.83	124.40
27	k	309	CLA	C4D-C3D-CAD	3.07	111.44	108.11
35	j	613	II0	C32-C34-C36	-3.07	117.96	126.36
35	f	615	II0	C34-C36-C40	-3.06	114.19	119.01
27	f	604	CLA	CMB-C2B-C3B	3.06	133.76	126.55
27	h	301	CLA	C3B-C4B-NB	-3.06	107.80	110.53
37	m	610	KC2	O2D-CGD-CBD	3.06	116.58	111.23
27	m	605	CLA	CHC-C4B-NB	3.06	128.64	124.05
35	c	613	II0	C29-C31-C33	-3.06	114.33	123.20
27	g	303	CLA	CHB-C4A-NA	3.06	128.82	124.40
27	K	102	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
27	f	606	CLA	CHB-C4A-NA	3.06	128.82	124.40
35	j	613	II0	C19-C13-C09	-3.06	118.44	124.16
37	j	610	KC2	C3B-C2B-C1B	-3.06	104.15	107.05
27	s	206	CLA	CGD-CBD-CAD	-3.06	100.95	110.85
35	d	314	II0	C32-C30-C26	-3.06	118.06	126.61
27	c	606	CLA	CMB-C2B-C1B	-3.06	120.77	125.42
30	J	102	WVN	C29-C31-C32	-3.06	117.98	126.36
37	f	611	KC2	C3B-C2B-C1B	-3.06	104.15	107.05
27	B	804	CLA	CMB-C2B-C1B	-3.06	120.77	125.42
27	B	837	CLA	C3B-C4B-NB	-3.05	107.80	110.53
30	R	201	WVN	C21-C15-C13	3.05	127.82	124.48
27	c	604	CLA	CMB-C2B-C1B	-3.05	120.77	125.42
27	k	307	CLA	O2A-CGA-O1A	-3.05	115.99	123.63
27	f	606	CLA	C4-C3-C5	3.05	119.72	116.13
27	d	303	CLA	CHB-C4A-NA	3.05	128.80	124.40
27	b	603	CLA	CMB-C2B-C1B	-3.05	120.77	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	l	302	II0	C32-C30-C26	-3.05	118.08	126.61
27	j	606	CLA	C3A-C2A-C1A	3.05	105.91	101.34
27	l	307	CLA	CMC-C2C-C1C	-3.05	120.27	125.03
27	l	307	CLA	CBA-CAA-C2A	3.05	122.87	113.79
30	s	205	WVN	C02-C05-C09	-3.05	117.72	121.47
30	s	205	WVN	C23-C20-C13	-3.05	118.85	127.00
35	l	313	II0	C31-C33-C35	-3.05	118.00	126.36
35	l	315	II0	C31-C29-C25	-3.05	118.09	126.61
30	l	316	WVN	C40-C37-C34	-3.05	123.00	127.28
27	a	305	CLA	CAA-C2A-C3A	-3.05	104.76	113.00
34	c	619	LMG	C4-C3-C2	3.05	116.18	110.83
35	m	615	II0	C31-C29-C25	-3.05	118.09	126.61
31	A	851	LMT	C3B-C4B-C5B	-3.04	104.71	110.23
37	e	609	KC2	CHB-C4A-NA	3.04	128.95	124.23
37	n	612	KC2	CHB-C4A-NA	3.04	128.95	124.23
35	c	613	II0	C38-C36-C34	3.04	122.73	118.09
27	s	203	CLA	CBA-CAA-C2A	-3.04	104.75	113.79
36	m	616	IHT	C04-C02-C07	3.04	114.86	110.44
27	b	605	CLA	CHB-C4A-NA	3.04	128.79	124.40
35	l	313	II0	C38-C36-C34	3.04	122.73	118.09
35	f	614	II0	C41-C42-C40	-3.04	117.30	123.52
27	j	605	CLA	CHC-C4B-NB	3.04	128.61	124.05
35	k	318	II0	C18-C04-C10	-3.04	105.08	110.52
35	l	317	II0	O02-C08-C06	-3.04	103.54	109.75
30	J	102	WVN	C31-C32-C36	3.04	123.78	119.01
35	c	614	II0	C20-C14-C10	-3.04	118.48	124.16
30	R	201	WVN	C40-C37-C34	-3.04	123.02	127.28
27	c	602	CLA	CAA-CBA-CGA	-3.04	104.59	113.21
37	f	611	KC2	CBC-CAC-C3C	-3.03	112.37	127.53
27	k	302	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
30	A	847	WVN	C30-C33-C34	-3.03	118.05	126.36
36	f	617	IHT	C20-C15-C12	3.03	120.00	114.42
27	e	603	CLA	CMB-C2B-C3B	3.03	133.68	126.55
27	m	603	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
36	a	317	IHT	C19-C10-C07	-3.03	121.18	124.48
35	i	313	II0	C42-C41-C39	-3.03	117.32	123.52
30	K	103	WVN	C30-C33-C34	-3.03	118.06	126.36
35	f	615	II0	C19-C13-C09	-3.03	118.50	124.16
35	d	313	II0	C19-C13-C11	3.03	119.99	114.42
35	l	315	II0	C06-C04-C10	3.03	115.45	109.49
27	g	302	CLA	C3B-C4B-NB	-3.03	107.83	110.53
27	b	607	CLA	CMC-C2C-C3C	3.03	134.34	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	j	603	CLA	CMB-C2B-C3B	3.03	133.67	126.55
35	a	315	II0	C05-C03-C09	3.03	115.45	109.49
27	l	307	CLA	O2D-CGD-CBD	3.02	116.52	111.23
27	k	303	CLA	O2A-CGA-O1A	-3.02	116.07	123.63
37	g	312	KC2	C3B-C2B-C1B	-3.02	104.19	107.05
27	A	809	CLA	CHB-C4A-NA	3.02	128.76	124.40
30	B	846	WVN	C40-C39-C36	-3.02	117.34	123.52
37	d	309	KC2	C3B-C2B-C1B	-3.02	104.19	107.05
35	n	616	II0	C42-C41-C39	-3.02	117.34	123.52
27	k	309	CLA	CHB-C4A-NA	3.02	128.75	124.40
35	b	615	II0	C19-C13-C09	-3.01	118.52	124.16
27	m	603	CLA	CAA-C2A-C3A	-3.01	104.85	113.00
35	d	314	II0	C32-C34-C36	-3.01	118.10	126.36
27	B	823	CLA	CMB-C2B-C3B	3.01	133.64	126.55
27	A	837	CLA	CHB-C4A-NA	3.01	128.75	124.40
27	d	305	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
35	n	614	II0	C32-C34-C36	-3.01	118.11	126.36
27	A	837	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
35	e	613	II0	C19-C13-C11	3.01	119.96	114.42
30	B	844	WVN	C40-C39-C36	-3.01	117.36	123.52
35	f	614	II0	C05-C03-C09	3.01	115.42	109.49
27	n	605	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
30	i	315	WVN	C20-C23-C25	-3.01	121.78	126.23
27	B	832	CLA	CHB-C4A-NA	3.01	128.74	124.40
35	a	315	II0	C32-C34-C36	-3.01	118.11	126.36
36	c	620	IHT	C22-C18-C07	-3.01	118.96	127.00
37	g	314	KC2	O2D-CGD-O1D	-3.01	117.99	123.85
30	R	201	WVN	C07-C01-C02	3.01	114.10	109.55
37	i	317	KC2	C1D-CHD-C4C	-3.01	119.18	126.25
27	f	601	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
27	j	604	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
27	b	604	CLA	CMB-C2B-C3B	3.01	133.62	126.55
27	g	302	CLA	CHB-C4A-NA	3.01	128.74	124.40
37	d	309	KC2	CHB-C4A-NA	3.00	128.89	124.23
30	B	848	WVN	C29-C26-C22	-3.00	123.06	127.28
27	d	305	CLA	CHB-C4A-NA	3.00	128.74	124.40
27	B	827	CLA	CMB-C2B-C3B	3.00	133.61	126.55
35	f	615	II0	C41-C42-C40	-3.00	117.38	123.52
35	k	314	II0	C30-C32-C34	-3.00	114.50	123.20
35	k	318	II0	C06-C04-C10	3.00	115.40	109.49
30	J	101	WVN	C21-C15-C13	-3.00	121.21	124.48
27	j	603	CLA	CHB-C4A-NA	3.00	128.73	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	315	II0	C11-C13-C09	-3.00	114.26	120.50
35	m	615	II0	C42-C41-C39	-3.00	117.38	123.52
37	c	610	KC2	C3B-C2B-C1B	-3.00	104.21	107.05
27	A	832	CLA	CMC-C2C-C3C	3.00	134.26	126.15
27	e	611	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
34	L	208	LMG	O7-C10-O9	-3.00	116.70	123.70
36	n	617	IHT	C18-C22-C23	-3.00	121.80	126.23
35	h	310	II0	C31-C29-C25	-3.00	118.23	126.61
37	g	312	KC2	C2A-C1A-NA	3.00	114.14	109.34
27	A	842	CLA	CAA-CBA-CGA	-3.00	104.70	113.21
27	B	804	CLA	O1D-CGD-CBD	3.00	130.43	124.52
27	l	309	CLA	CMB-C2B-C3B	3.00	133.60	126.55
29	a	319	LHG	O7-C7-O9	-2.99	116.71	123.70
27	A	842	CLA	O2A-CGA-O1A	-2.99	116.14	123.63
37	k	310	KC2	CHB-C4A-NA	2.99	128.87	124.23
27	g	308	CLA	CAA-CBA-CGA	-2.99	104.71	113.21
27	f	606	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	A	824	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
27	A	816	CLA	C4-C3-C5	2.99	120.42	115.23
35	i	313	II0	C20-C14-C10	-2.99	118.57	124.16
27	h	303	CLA	CHB-C4A-NA	2.99	128.72	124.40
35	i	314	II0	C29-C31-C33	-2.99	114.53	123.20
27	d	311	CLA	CHB-C4A-NA	2.99	128.71	124.40
27	f	603	CLA	CMB-C2B-C1B	-2.99	120.87	125.42
37	i	310	KC2	C3B-C2B-C1B	-2.99	104.22	107.05
30	O	201	WVN	C20-C13-C15	-2.99	114.68	121.56
27	a	308	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
27	d	306	CLA	CHB-C4A-NA	2.98	128.70	124.40
27	J	105	CLA	CAA-C2A-C3A	-2.98	104.94	113.00
27	s	203	CLA	O2D-CGD-CBD	2.98	116.44	111.23
30	h	309	WVN	C03-C04-C09	-2.98	107.07	112.07
35	n	615	II0	C32-C34-C36	-2.98	118.19	126.36
27	k	303	CLA	C4A-NA-C1A	2.98	108.04	106.68
27	j	607	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	m	612	CLA	CAC-C3C-C2C	2.98	133.03	127.56
27	A	839	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
27	B	833	CLA	C2A-C1A-CHA	2.97	129.03	123.87
30	J	101	WVN	C17-C06-C13	2.97	114.91	110.24
27	h	313	CLA	CHB-C4A-NA	2.97	128.69	124.40
27	l	307	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
29	j	617	LHG	O8-C23-C24	2.97	120.90	111.83
27	B	810	CLA	CAA-C2A-C3A	-2.97	104.97	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	308	CLA	CMB-C2B-C3B	2.97	133.54	126.55
27	B	819	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
27	g	310	CLA	C4A-NA-C1A	2.97	108.03	106.68
35	k	315	II0	C29-C31-C33	-2.97	114.59	123.20
27	m	609	CLA	CAA-CBA-CGA	-2.97	104.77	113.21
35	f	616	II0	C31-C33-C35	-2.97	118.22	126.36
29	b	617	LHG	O7-C7-C8	2.97	117.91	111.48
27	m	607	CLA	CHB-C4A-NA	2.97	128.69	124.40
27	d	311	CLA	C2A-C1A-CHA	2.97	129.02	123.87
35	d	312	II0	C38-C36-C34	2.97	122.63	118.09
27	m	612	CLA	C4A-NA-C1A	2.97	108.03	106.68
36	a	317	IHT	C22-C18-C07	-2.97	119.07	127.00
35	j	615	II0	C30-C32-C34	-2.97	114.60	123.20
30	M	101	WVN	C39-C40-C37	-2.97	117.44	123.52
27	A	830	CLA	O2D-CGD-CBD	2.97	116.42	111.23
27	i	303	CLA	CMD-C2D-C1D	2.97	129.96	124.73
27	i	308	CLA	O2D-CGD-CBD	2.97	116.42	111.23
30	B	848	WVN	C12-C14-C15	-2.97	108.77	114.06
37	d	310	KC2	C3B-C2B-C1B	-2.97	104.24	107.05
37	i	317	KC2	CHB-C1B-C2B	-2.96	119.32	125.49
30	I	101	WVN	C30-C28-C25	-2.96	123.12	127.28
27	b	602	CLA	CAA-CBA-CGA	-2.96	104.80	113.21
27	s	206	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
27	m	607	CLA	CMB-C2B-C1B	-2.96	120.91	125.42
37	s	204	KC2	C2B-C1B-NB	2.96	113.06	110.13
27	A	814	CLA	CMB-C2B-C1B	-2.96	120.91	125.42
36	k	317	IHT	C41-C40-C37	-2.96	117.46	123.52
27	F	201	CLA	CMB-C2B-C1B	-2.96	120.91	125.42
27	A	818	CLA	CMB-C2B-C3B	2.96	133.51	126.55
30	h	309	WVN	C24-C22-C19	-2.96	113.57	118.09
27	B	820	CLA	C6-C5-C3	-2.96	106.27	113.47
34	L	208	LMG	C1-O6-C5	-2.95	107.95	113.72
36	g	319	IHT	C27-C30-C32	-2.95	114.64	123.20
35	f	618	II0	C05-C03-C09	2.95	115.31	109.49
30	R	201	WVN	C16-C05-C09	-2.95	112.44	122.37
35	f	616	II0	C31-C29-C25	-2.95	118.35	126.61
27	A	802	CLA	C1-C2-C3	-2.95	121.36	126.20
27	A	832	CLA	C6-C7-C8	-2.95	106.16	115.97
27	B	814	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
35	c	614	II0	C05-C03-C09	2.95	115.30	109.49
27	d	301	CLA	CAA-CBA-CGA	-2.95	104.84	113.21
27	A	811	CLA	O2D-CGD-O1D	-2.95	118.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	817	CLA	CMB-C2B-C3B	2.95	133.48	126.55
27	L	202	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
35	h	311	II0	C38-C36-C34	2.95	122.59	118.09
27	A	824	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
28	A	843	PQN	C14-C13-C15	2.94	120.34	115.23
27	j	609	CLA	CMC-C2C-C3C	2.94	134.11	126.15
27	k	306	CLA	O2A-CGA-O1A	-2.94	116.27	123.63
30	F	204	WVN	C01-C02-C11	-2.94	109.44	112.83
27	A	808	CLA	CMB-C2B-C3B	2.94	133.47	126.55
27	L	203	CLA	O2D-CGD-CBD	2.94	116.37	111.23
27	g	322	CLA	O2D-CGD-CBD	2.94	116.37	111.23
27	m	602	CLA	CAC-C3C-C4C	2.94	128.62	124.79
27	A	805	CLA	C7-C6-C5	-2.94	105.43	113.26
35	b	615	II0	C42-C41-C39	-2.94	117.50	123.52
27	s	208	CLA	O2A-CGA-O1A	-2.94	116.28	123.63
29	c	618	LHG	O8-C23-C24	2.94	120.79	111.83
35	i	314	II0	C19-C13-C09	-2.94	118.67	124.16
35	g	317	II0	C20-C14-C10	-2.94	118.67	124.16
35	f	615	II0	C32-C34-C36	-2.94	118.31	126.36
35	g	320	II0	C19-C13-C11	2.94	119.82	114.42
35	d	312	II0	O02-C08-C06	-2.94	103.74	109.75
37	n	612	KC2	C2B-C1B-NB	2.94	113.03	110.13
35	c	617	II0	C17-C04-C10	-2.93	105.26	110.52
30	A	846	WVN	C30-C33-C34	-2.93	118.32	126.36
37	i	317	KC2	O2D-CGD-O1D	-2.93	118.14	123.85
30	A	848	WVN	C40-C37-C34	-2.93	123.17	127.28
27	b	608	CLA	CHB-C4A-NA	2.93	128.63	124.40
27	k	308	CLA	C1-C2-C3	-2.93	121.39	126.20
27	A	855	CLA	C4-C3-C5	2.93	120.32	115.23
30	A	847	WVN	C20-C23-C25	-2.93	121.90	126.23
37	l	311	KC2	CBC-CAC-C3C	-2.93	112.88	127.53
29	e	617	LHG	O8-C23-C24	2.93	120.77	111.83
30	A	847	WVN	C18-C06-C17	-2.93	100.24	108.63
27	h	303	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
27	B	820	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
27	A	818	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
35	m	613	II0	C19-C13-C09	-2.93	118.68	124.16
27	f	612	CLA	CMB-C2B-C3B	2.93	133.44	126.55
27	B	822	CLA	CHB-C4A-NA	2.93	128.62	124.40
35	n	616	II0	C20-C14-C10	-2.93	118.69	124.16
27	A	834	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
27	g	315	CLA	CMB-C2B-C1B	-2.92	120.97	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	j	602	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
27	A	811	CLA	CHB-C4A-NA	2.92	128.62	124.40
37	i	317	KC2	CHD-C1D-C2D	2.92	135.91	127.43
27	A	841	CLA	CMB-C2B-C3B	2.92	133.42	126.55
27	f	609	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
27	L	206	CLA	CMB-C2B-C3B	2.92	133.42	126.55
27	a	311	CLA	CHB-C4A-NA	2.92	128.62	124.40
37	l	311	KC2	C1D-CHD-C4C	-2.92	119.38	126.25
27	B	823	CLA	O2D-CGD-CBD	2.92	116.34	111.23
27	A	829	CLA	CMB-C2B-C3B	2.92	133.42	126.55
35	f	615	II0	C05-C03-C09	2.92	115.24	109.49
35	m	615	II0	C20-C14-C12	2.92	119.79	114.42
27	b	609	CLA	CMB-C2B-C3B	2.92	133.42	126.55
27	j	604	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
27	h	302	CLA	CMB-C2B-C3B	2.92	133.41	126.55
35	m	614	II0	C19-C13-C09	-2.92	118.70	124.16
27	k	308	CLA	O2D-CGD-CBD	2.92	116.33	111.23
27	A	836	CLA	C11-C12-C13	-2.92	106.27	115.97
27	a	311	CLA	CMB-C2B-C3B	2.92	133.41	126.55
29	b	618	LHG	C5-O7-C7	-2.92	110.81	117.80
35	i	313	II0	C32-C34-C36	-2.92	118.37	126.36
27	g	308	CLA	CMC-C2C-C1C	-2.92	120.48	125.03
27	A	808	CLA	CAA-CBA-CGA	-2.92	104.93	113.21
27	B	805	CLA	O2D-CGD-CBD	2.91	116.33	111.23
27	m	604	CLA	CMB-C2B-C3B	2.91	133.40	126.55
27	b	608	CLA	C1-C2-C3	-2.91	121.42	126.20
35	l	314	II0	C19-C13-C09	-2.91	118.71	124.16
36	c	616	IHT	C19-C10-C09	2.91	119.81	113.60
30	J	102	WVN	C10-C06-C13	2.91	114.67	110.44
35	m	614	II0	C06-C04-C10	2.91	115.23	109.49
27	A	816	CLA	CMB-C2B-C3B	2.91	133.40	126.55
27	A	855	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
27	c	611	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
30	R	201	WVN	C03-C04-C09	-2.91	107.19	112.07
36	j	616	IHT	C19-C10-C07	-2.91	121.31	124.48
35	n	614	II0	C41-C39-C35	-2.91	123.20	127.28
27	b	604	CLA	O1D-CGD-CBD	2.91	130.25	124.52
27	e	608	CLA	CHB-C4A-NA	2.91	128.60	124.40
35	l	313	II0	C32-C34-C36	-2.91	118.39	126.36
27	B	818	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
27	i	302	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
27	i	305	CLA	CMB-C2B-C3B	2.91	133.38	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	l	317	II0	C37-C35-C33	2.91	122.53	118.09
35	b	612	II0	C05-C03-C09	2.90	115.21	109.49
27	b	607	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
35	l	302	II0	C20-C14-C12	2.90	119.76	114.42
27	n	613	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
35	c	614	II0	C32-C34-C36	-2.90	118.41	126.36
27	B	821	CLA	C4A-NA-C1A	2.90	108.00	106.68
30	J	101	WVN	C39-C40-C37	-2.90	117.58	123.52
27	A	855	CLA	C1-O2A-CGA	2.90	123.67	116.65
35	k	316	II0	C31-C29-C25	-2.90	118.50	126.61
27	l	310	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
27	i	304	CLA	CHB-C4A-NA	2.90	128.58	124.40
27	a	308	CLA	CAA-C2A-C3A	-2.90	105.17	113.00
27	l	306	CLA	C1-C2-C3	-2.90	121.45	126.20
27	c	604	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
27	i	303	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
27	l	307	CLA	CMC-C2C-C3C	2.90	133.98	126.15
35	f	616	II0	C27-C25-C29	-2.90	118.56	124.18
27	a	307	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
27	A	836	CLA	CHB-C4A-NA	2.90	128.58	124.40
35	g	316	II0	C41-C42-C40	-2.90	117.59	123.52
27	A	830	CLA	CMB-C2B-C3B	2.90	133.36	126.55
35	g	318	II0	C05-C03-C09	2.90	115.19	109.49
27	s	202	CLA	C4A-NA-C1A	2.90	108.00	106.68
35	i	314	II0	C31-C33-C35	-2.89	118.43	126.36
27	e	602	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
27	A	818	CLA	CHB-C1B-NB	2.89	128.39	124.05
27	l	312	CLA	C1-C2-C3	-2.89	121.45	126.20
27	B	820	CLA	CMB-C2B-C1B	-2.89	121.01	125.42
36	g	319	IHT	C02-C07-C10	-2.89	118.68	122.64
31	A	851	LMT	O5B-C5B-C4B	2.89	114.91	109.70
27	A	815	CLA	CHC-C4B-NB	2.89	128.39	124.05
27	j	608	CLA	C4A-NA-C1A	2.89	108.00	106.68
27	B	809	CLA	CMB-C2B-C1B	-2.89	121.01	125.42
37	j	610	KC2	CBC-CAC-C3C	-2.89	113.07	127.53
27	s	206	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
30	L	201	WVN	C39-C40-C37	-2.89	117.60	123.52
27	i	306	CLA	CMB-C2B-C3B	2.89	133.35	126.55
27	A	802	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
27	A	802	CLA	C3B-C4B-NB	-2.89	107.95	110.53
35	a	316	II0	C19-C13-C09	-2.89	118.76	124.16
35	a	316	II0	C41-C39-C35	-2.89	123.23	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	844	WVN	C06-C13-C20	2.89	123.48	115.65
30	B	843	WVN	C28-C30-C33	-2.89	114.84	123.20
34	O	205	LMG	C8-O7-C10	-2.89	110.89	117.80
27	A	813	CLA	CHB-C4A-NA	2.88	128.56	124.40
36	O	204	IHT	C05-C03-C11	2.88	115.17	109.49
27	l	305	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
29	b	617	LHG	C5-O7-C7	-2.88	110.90	117.80
27	A	820	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	F	203	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	B	823	CLA	C1-C2-C3	-2.88	121.47	126.20
36	j	616	IHT	C20-C15-C12	2.88	119.72	114.42
27	j	611	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	A	835	CLA	CHB-C4A-NA	2.88	128.56	124.40
27	f	610	CLA	CBC-CAC-C3C	-2.88	104.61	112.42
34	F	206	LMG	O1-C1-C2	2.88	112.65	108.27
27	m	601	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
27	B	813	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
27	k	305	CLA	CBA-CAA-C2A	-2.88	105.23	113.79
27	n	607	CLA	CHB-C4A-NA	2.88	128.55	124.40
27	A	838	CLA	O2D-CGD-CBD	2.88	116.26	111.23
37	d	310	KC2	CBC-CAC-C3C	-2.88	113.16	127.53
35	b	615	II0	C31-C29-C25	-2.88	118.57	126.61
35	k	315	II0	C32-C30-C26	-2.88	118.57	126.61
30	L	205	WVN	C40-C39-C36	-2.88	117.64	123.52
27	l	304	CLA	C3B-C4B-NB	-2.88	107.96	110.53
27	n	603	CLA	CHB-C4A-NA	2.87	128.55	124.40
27	k	309	CLA	C4D-CHA-C1A	-2.87	117.82	121.24
27	B	817	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
27	f	603	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
27	A	817	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
30	L	201	WVN	C02-C11-C19	-2.87	120.11	124.58
27	c	603	CLA	CMB-C2B-C3B	2.87	133.30	126.55
27	B	806	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
27	B	833	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
27	A	852	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	K	103	WVN	C21-C15-C13	-2.87	121.35	124.48
29	f	619	LHG	O7-C7-C8	2.87	117.69	111.48
27	B	808	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
27	g	315	CLA	CHB-C1B-NB	2.87	128.35	124.05
30	L	201	WVN	C28-C30-C33	-2.87	114.89	123.20
30	e	615	WVN	C21-C15-C13	-2.86	121.36	124.48
27	A	841	CLA	C4-C3-C5	2.86	120.20	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	O	201	WVN	C28-C30-C33	-2.86	114.90	123.20
27	B	832	CLA	C16-C15-C13	-2.86	106.45	115.97
27	g	303	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
27	e	611	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
27	d	304	CLA	CHB-C4A-NA	2.86	128.53	124.40
29	m	617	LHG	O8-C23-C24	2.86	120.55	111.83
27	B	825	CLA	CAA-CBA-CGA	-2.86	105.09	113.21
27	A	821	CLA	CMB-C2B-C3B	2.86	133.27	126.55
27	n	605	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
35	h	310	II0	C19-C13-C09	-2.85	118.83	124.16
27	a	303	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	m	608	CLA	CMB-C2B-C3B	2.85	133.26	126.55
27	A	856	CLA	C2A-C1A-CHA	2.85	128.80	123.86
27	B	840	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
27	B	823	CLA	C3B-C4B-NB	-2.85	107.99	110.53
27	d	306	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	m	602	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	A	816	CLA	CAA-C2A-C3A	-2.85	105.30	113.00
27	a	304	CLA	CHB-C4A-NA	2.85	128.51	124.40
30	O	201	WVN	C12-C14-C15	-2.85	108.98	114.06
36	n	617	IHT	C22-C18-C07	-2.85	119.39	127.00
37	g	314	KC2	C1D-CHD-C4C	-2.85	119.55	126.25
27	h	308	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
27	O	206	CLA	CHB-C4A-NA	2.85	128.51	124.40
30	s	207	WVN	C24-C22-C19	2.85	122.44	118.09
27	h	304	CLA	CHB-C4A-NA	2.85	128.51	124.40
35	g	317	II0	C19-C13-C09	-2.84	118.84	124.16
27	A	812	CLA	CHB-C4A-NA	2.84	128.50	124.40
34	O	205	LMG	O8-C28-C29	2.84	120.50	111.83
37	k	310	KC2	CBC-CAC-C3C	-2.84	113.32	127.53
27	b	609	CLA	C3B-C4B-NB	-2.84	107.99	110.53
27	f	608	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
27	B	834	CLA	CHB-C4A-NA	2.84	128.50	124.40
34	L	208	LMG	C4-C3-C2	2.84	115.82	110.83
27	B	829	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
30	B	843	WVN	C23-C20-C13	-2.84	119.42	127.00
27	A	842	CLA	CAA-C2A-C3A	-2.84	105.34	113.00
35	e	613	II0	C20-C14-C10	-2.84	118.86	124.16
27	m	605	CLA	CAA-C2A-C1A	2.84	118.42	112.14
27	a	305	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
27	g	305	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
30	A	849	WVN	C40-C39-C36	-2.83	117.72	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	601	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
27	l	306	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
35	n	618	II0	C18-C04-C17	-2.83	100.53	108.63
30	K	103	WVN	C39-C36-C32	-2.83	123.31	127.28
27	l	312	CLA	C3B-C4B-NB	-2.83	108.00	110.53
27	A	836	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
35	f	614	II0	C16-C03-C09	-2.83	105.45	110.52
27	d	302	CLA	CMB-C2B-C3B	2.83	133.21	126.55
35	g	317	II0	C31-C29-C25	-2.83	118.70	126.61
36	O	204	IHT	C19-C10-C07	-2.83	121.40	124.48
30	B	846	WVN	C14-C15-C13	-2.83	118.88	122.70
27	f	605	CLA	C2A-C1A-CHA	2.83	128.78	123.87
36	m	616	IHT	C19-C10-C07	-2.83	121.40	124.48
30	B	847	WVN	C19-C22-C26	-2.83	114.56	119.01
27	d	307	CLA	CHB-C4A-NA	2.83	128.48	124.40
27	B	827	CLA	C3B-C4B-NB	-2.83	108.01	110.53
27	m	607	CLA	C3B-C4B-NB	-2.83	108.01	110.53
31	A	851	LMT	O1B-C4'-C3'	2.82	114.41	107.23
35	e	616	II0	C42-C41-C39	2.82	129.30	123.52
27	m	612	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
27	c	603	CLA	CHB-C4A-NA	2.82	128.47	124.40
27	B	822	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
27	B	839	CLA	CHB-C4A-NA	2.82	128.47	124.40
35	f	614	II0	C42-C40-C36	-2.82	123.32	127.28
37	i	310	KC2	C2A-C1A-NA	2.82	113.86	109.34
35	k	315	II0	C31-C29-C25	-2.82	118.72	126.61
37	j	610	KC2	C1D-CHD-C4C	-2.82	119.61	126.25
27	B	839	CLA	CBC-CAC-C3C	2.82	120.06	112.42
37	n	611	KC2	CBC-CAC-C3C	-2.82	113.44	127.53
30	M	101	WVN	C04-C09-C05	-2.82	122.14	124.83
27	f	613	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
27	m	603	CLA	C16-C15-C13	-2.82	106.60	115.97
27	B	812	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
27	K	102	CLA	CHB-C4A-NA	2.82	128.47	124.40
28	B	841	PQN	C14-C13-C15	2.82	120.12	115.23
27	l	309	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
27	k	301	CLA	C1-C2-C3	-2.81	122.21	126.76
27	b	601	CLA	CBC-CAC-C3C	-2.81	104.79	112.42
30	A	848	WVN	C27-C25-C23	-2.81	113.79	118.09
27	B	830	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
27	A	811	CLA	O2A-CGA-O1A	-2.81	116.59	123.63
37	m	610	KC2	O2D-CGD-O1D	-2.81	118.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	302	CLA	CHB-C4A-NA	2.81	128.46	124.40
27	B	828	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
35	h	312	II0	C32-C34-C36	-2.81	118.66	126.36
27	i	303	CLA	CAA-CBA-CGA	-2.81	105.23	113.21
27	d	305	CLA	CED-O2D-CGD	2.81	122.29	115.92
27	e	610	CLA	C3B-C4B-NB	-2.81	108.02	110.53
36	R	204	IHT	C30-C32-C33	-2.81	118.67	126.36
30	J	101	WVN	C29-C26-C22	-2.81	123.34	127.28
30	K	103	WVN	C40-C37-C34	-2.81	123.34	127.28
35	b	613	II0	C12-C14-C10	-2.81	114.66	120.50
27	g	305	CLA	CMB-C2B-C3B	2.81	133.15	126.55
29	A	845	LHG	O8-C23-O10	-2.81	116.61	123.63
27	B	832	CLA	CMB-C2B-C3B	2.81	133.15	126.55
29	a	301	LHG	O8-C23-O10	-2.81	116.61	123.63
27	A	819	CLA	CHB-C4A-NA	2.81	128.45	124.40
27	A	835	CLA	CAC-C3C-C4C	2.81	128.44	124.79
27	b	606	CLA	O2A-CGA-O1A	-2.81	116.61	123.63
27	A	833	CLA	CHB-C4A-NA	2.80	128.45	124.40
35	c	617	II0	C31-C33-C35	-2.80	118.67	126.36
36	k	317	IHT	C19-C10-C09	2.80	119.57	113.60
27	A	853	CLA	C1-C2-C3	-2.80	121.60	126.20
27	L	202	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
30	J	101	WVN	C03-C04-C09	-2.80	107.36	112.07
27	A	813	CLA	C2A-C1A-CHA	2.80	128.73	123.87
27	m	606	CLA	C3B-C4B-NB	-2.80	108.03	110.53
27	d	307	CLA	CAC-C3C-C4C	2.80	128.44	124.79
27	a	313	CLA	C3B-C4B-NB	-2.80	108.03	110.53
36	j	616	IHT	C40-C41-C38	-2.80	117.79	123.52
27	f	612	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	l	308	CLA	C6-C7-C8	-2.80	106.66	115.97
27	A	815	CLA	CHB-C1B-NB	2.80	128.25	124.05
27	e	608	CLA	O2D-CGD-CBD	2.80	116.12	111.23
27	h	304	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
30	l	301	WVN	C21-C15-C14	2.80	119.56	113.60
36	j	616	IHT	C22-C18-C07	-2.80	119.53	127.00
30	B	848	WVN	C28-C30-C33	2.80	131.30	123.20
37	e	609	KC2	C3B-C2B-C1B	-2.80	104.40	107.05
27	e	602	CLA	CMB-C2B-C3B	2.80	133.12	126.55
27	i	305	CLA	CHB-C4A-NA	2.80	128.43	124.40
30	B	845	WVN	C35-C32-C36	-2.79	118.29	122.82
35	c	614	II0	C31-C33-C35	-2.79	118.70	126.36
27	h	305	CLA	CHB-C4A-NA	2.79	128.43	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	604	CLA	CBA-CAA-C2A	2.79	122.11	113.79
27	l	303	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
37	f	611	KC2	O2D-CGD-O1D	-2.79	118.41	123.85
27	g	305	CLA	CHB-C4A-NA	2.79	128.43	124.40
30	B	846	WVN	C26-C29-C31	-2.79	115.11	123.20
35	k	318	II0	C41-C39-C35	-2.79	123.36	127.28
27	c	601	CLA	CMD-C2D-C3D	2.79	134.09	127.69
27	n	604	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
35	c	615	II0	C42-C41-C39	-2.79	117.81	123.52
27	a	304	CLA	CAA-CBA-CGA	-2.79	105.28	113.21
27	d	301	CLA	CMB-C2B-C3B	2.79	133.12	126.55
27	l	309	CLA	CHB-C4A-NA	2.79	128.43	124.40
30	L	201	WVN	C11-C19-C22	-2.79	120.32	126.32
35	n	618	II0	C41-C42-C40	-2.79	117.81	123.52
27	L	204	CLA	CMA-C3A-C2A	-2.79	103.19	113.98
27	B	809	CLA	CAC-C3C-C4C	2.79	128.42	124.79
27	B	828	CLA	CAA-CBA-CGA	-2.79	105.28	113.21
27	b	607	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
27	B	807	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	s	205	WVN	C38-C34-C33	2.79	122.35	118.09
27	L	206	CLA	CHB-C4A-NA	2.79	128.42	124.40
27	j	612	CLA	C4A-NA-C1A	2.79	107.95	106.68
37	s	204	KC2	O2D-CGD-O1D	-2.79	118.42	123.85
27	e	605	CLA	CMD-C2D-C1D	-2.79	119.82	124.73
27	A	826	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
35	k	316	II0	C29-C31-C33	-2.79	115.13	123.20
27	B	812	CLA	CHB-C4A-NA	2.79	128.42	124.40
35	g	318	II0	C20-C14-C10	-2.79	118.95	124.16
35	c	613	II0	C05-C03-C09	2.79	114.98	109.49
27	c	603	CLA	C1-O2A-CGA	2.78	123.39	116.65
30	s	207	WVN	C26-C29-C31	-2.78	115.13	123.20
37	i	310	KC2	O2D-CGD-O1D	-2.78	118.43	123.85
36	c	616	IHT	C28-C26-C29	-2.78	118.78	124.18
35	n	616	II0	C32-C34-C36	-2.78	118.73	126.36
30	B	846	WVN	C16-C05-C09	-2.78	113.02	122.37
27	c	612	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
37	s	204	KC2	C3B-C2B-C1B	-2.78	104.41	107.05
30	l	301	WVN	C20-C23-C25	-2.78	122.12	126.23
27	l	305	CLA	C3B-C4B-NB	-2.78	108.05	110.53
27	i	308	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
35	f	616	II0	C32-C34-C36	-2.78	118.74	126.36
37	g	314	KC2	CBC-CAC-C3C	-2.78	113.64	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	m	614	II0	C41-C42-C40	-2.78	117.83	123.52
27	A	819	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
27	e	607	CLA	CHB-C4A-NA	2.78	128.41	124.40
35	l	314	II0	C12-C14-C10	-2.78	114.72	120.50
27	i	312	CLA	CMB-C2B-C3B	2.78	133.08	126.55
27	b	605	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
27	c	609	CLA	CMB-C2B-C1B	-2.77	121.19	125.42
27	c	608	CLA	CMB-C2B-C1B	-2.77	121.19	125.42
27	f	605	CLA	CHB-C4A-NA	2.77	128.40	124.40
27	b	602	CLA	C1-C2-C3	-2.77	121.65	126.20
35	k	315	II0	C30-C32-C34	-2.77	115.17	123.20
35	a	315	II0	C41-C42-C40	-2.77	117.84	123.52
27	m	611	CLA	CMC-C2C-C1C	-2.77	120.70	125.03
27	f	605	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
27	n	609	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
37	k	310	KC2	C1D-CHD-C4C	-2.77	119.73	126.25
37	s	204	KC2	CAB-C3B-C2B	2.77	137.44	128.43
27	A	819	CLA	CMC-C2C-C3C	2.77	133.64	126.15
27	s	209	CLA	CHB-C4A-NA	2.77	128.40	124.40
35	f	616	II0	C29-C31-C33	-2.77	115.18	123.20
35	f	614	II0	C33-C35-C39	2.77	123.36	119.01
27	a	304	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
27	e	611	CLA	C12-C11-C10	2.77	125.68	113.28
27	A	812	CLA	C4-C3-C2	-2.77	116.52	123.63
27	i	303	CLA	CHB-C4A-NA	2.77	128.39	124.40
27	e	606	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
27	i	304	CLA	CMB-C2B-C3B	2.77	133.06	126.55
30	J	102	WVN	C03-C04-C09	-2.77	107.43	112.07
30	A	846	WVN	C27-C25-C23	-2.77	113.86	118.09
30	s	207	WVN	C07-C01-C02	2.76	113.73	109.55
27	A	807	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
27	l	305	CLA	CHB-C4A-NA	2.76	128.39	124.40
27	A	835	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
27	c	602	CLA	CMB-C2B-C3B	2.76	133.05	126.55
27	b	606	CLA	C4-C3-C5	2.76	120.02	115.23
27	c	607	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
35	d	312	II0	C31-C29-C25	-2.76	118.88	126.61
27	A	832	CLA	CHB-C4A-NA	2.76	128.38	124.40
37	i	317	KC2	CHB-C4A-C3A	-2.76	120.67	125.03
27	c	609	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
35	l	317	II0	C19-C13-C09	-2.76	119.00	124.16
27	A	835	CLA	C1-C2-C3	-2.76	121.67	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	848	WVN	C40-C39-C36	-2.76	117.87	123.52
27	B	803	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
27	e	603	CLA	CHB-C4A-NA	2.76	128.38	124.40
27	L	206	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
37	n	612	KC2	C1D-CHD-C4C	-2.76	119.76	126.25
36	k	317	IHT	C02-C07-C10	-2.76	118.87	122.64
35	h	311	II0	C31-C33-C35	-2.76	118.81	126.36
35	j	613	II0	C05-C03-C09	2.76	114.92	109.49
30	A	847	WVN	C29-C31-C32	2.76	133.92	126.36
27	d	308	CLA	CAA-C2A-C3A	-2.76	109.91	116.23
27	A	803	CLA	CHB-C4A-NA	2.76	128.38	124.40
30	l	301	WVN	C21-C15-C13	-2.75	121.48	124.48
35	l	315	II0	C12-C14-C10	-2.75	114.77	120.50
35	b	615	II0	C12-C14-C10	-2.75	114.77	120.50
36	b	614	IHT	C19-C10-C09	2.75	119.46	113.60
27	l	306	CLA	CAA-CBA-CGA	-2.75	105.39	113.21
29	g	301	LHG	O9-C7-C8	-2.75	113.02	123.78
27	h	307	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
30	B	847	WVN	C40-C39-C36	-2.75	117.89	123.52
27	J	103	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	k	305	CLA	C3B-C4B-NB	-2.75	108.08	110.53
27	c	611	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
35	a	316	II0	C20-C14-C12	2.75	119.47	114.42
27	m	602	CLA	CBC-CAC-C3C	2.75	119.87	112.42
35	i	314	II0	C33-C35-C39	2.75	123.33	119.01
27	A	832	CLA	C7-C6-C5	-2.75	105.94	113.26
27	L	204	CLA	CAA-CBA-CGA	-2.75	105.41	113.21
27	e	604	CLA	CGD-CBD-CAD	-2.75	101.95	110.85
30	A	848	WVN	C16-C05-C09	-2.75	113.14	122.37
35	a	315	II0	C38-C36-C34	2.75	122.28	118.09
27	e	601	CLA	CHB-C4A-NA	2.75	128.36	124.40
27	B	825	CLA	CMB-C2B-C3B	2.74	133.01	126.55
37	s	201	KC2	CHD-C1D-C2D	2.74	135.39	127.43
27	J	103	CLA	CHB-C4A-NA	2.74	128.36	124.40
27	d	302	CLA	CHB-C4A-NA	2.74	128.36	124.40
27	A	813	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
27	B	806	CLA	C3B-C4B-NB	-2.74	108.08	110.53
27	h	303	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
30	B	846	WVN	C30-C33-C34	-2.74	118.84	126.36
29	k	319	LHG	O8-C23-O10	-2.74	116.77	123.63
27	e	605	CLA	CMD-C2D-C3D	2.74	133.98	127.69
27	h	308	CLA	CAA-C2A-C1A	2.74	120.96	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	610	CLA	C3B-C4B-NB	-2.74	108.08	110.53
27	B	823	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
27	j	608	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
30	J	102	WVN	C01-C02-C11	-2.74	109.68	112.83
27	m	602	CLA	CHB-C4A-NA	2.74	128.35	124.40
36	m	616	IHT	C31-C34-C35	-2.74	118.86	126.36
27	A	805	CLA	O2D-CGD-CBD	2.74	116.01	111.23
27	B	806	CLA	O2D-CGD-CBD	2.74	116.01	111.23
27	A	808	CLA	C1-C2-C3	-2.74	121.72	126.20
27	B	821	CLA	C3B-C4B-NB	-2.73	108.09	110.53
30	R	201	WVN	C23-C20-C13	-2.73	119.69	127.00
27	d	306	CLA	C3B-C4B-NB	-2.73	108.09	110.53
27	j	601	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
27	A	818	CLA	CHB-C4A-NA	2.73	128.34	124.40
35	h	311	II0	C06-C04-C10	2.73	114.86	109.49
27	k	301	CLA	CHB-C4A-NA	2.73	128.34	124.40
35	h	311	II0	C19-C13-C11	2.73	119.44	114.42
27	l	312	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
27	g	306	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
27	m	606	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
30	i	315	WVN	C06-C13-C20	2.73	123.05	115.65
35	c	615	II0	C15-C03-C09	-2.73	105.64	110.52
38	i	301	LMU	O1B-C1B-C2B	2.73	114.79	108.09
27	A	831	CLA	C7-C6-C5	-2.72	106.00	113.26
30	B	847	WVN	C08-C01-C02	-2.72	105.42	109.55
27	m	609	CLA	CMC-C2C-C1C	-2.72	120.78	125.03
27	a	306	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
27	L	204	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
35	j	613	II0	C06-C04-C10	2.72	114.85	109.49
27	g	315	CLA	CHB-C4A-NA	2.72	128.33	124.40
27	d	301	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
27	n	605	CLA	CHA-C1A-NA	-2.72	120.23	126.39
36	f	617	IHT	C22-C18-C07	-2.72	119.73	127.00
27	L	203	CLA	C3B-C4B-NB	-2.72	108.10	110.53
36	g	319	IHT	C20-C15-C12	2.72	119.42	114.42
27	h	301	CLA	CMB-C2B-C3B	2.72	132.95	126.55
37	k	311	KC2	CAA-CBA-CGA	-2.72	113.22	127.05
35	f	615	II0	C29-C31-C33	-2.72	115.32	123.20
35	a	318	II0	C04-C06-C08	2.72	119.56	113.59
27	B	826	CLA	CHB-C4A-NA	2.72	128.32	124.40
27	m	611	CLA	C3B-C4B-NB	-2.72	108.10	110.53
35	n	618	II0	C03-C05-C07	-2.72	107.63	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	e	614	II0	C06-C04-C10	2.72	114.84	109.49
36	n	617	IHT	C31-C34-C35	-2.72	118.92	126.36
27	a	303	CLA	CAA-CBA-CGA	-2.72	105.50	113.21
27	A	805	CLA	CHB-C4A-NA	2.72	128.32	124.40
27	i	302	CLA	CHB-C4A-NA	2.71	128.32	124.40
27	J	105	CLA	CMA-C3A-C4A	2.71	119.07	111.77
27	m	605	CLA	CBC-CAC-C3C	2.71	119.78	112.42
36	n	617	IHT	C19-C10-C09	2.71	119.38	113.60
35	d	314	II0	C19-C13-C09	-2.71	119.09	124.16
35	d	313	II0	C31-C33-C35	-2.71	118.93	126.36
27	A	838	CLA	CHB-C4A-NA	2.71	128.31	124.40
27	m	609	CLA	O2D-CGD-CBD	2.71	115.97	111.23
36	n	617	IHT	C31-C29-C26	-2.71	119.03	126.61
34	L	208	LMG	O6-C5-C6	2.71	113.15	106.44
27	B	802	CLA	C1C-C2C-C3C	2.71	109.83	106.98
30	A	848	WVN	C26-C29-C31	-2.71	115.35	123.20
27	a	310	CLA	CHB-C4A-NA	2.71	128.31	124.40
27	B	832	CLA	C4-C3-C5	2.71	119.93	115.23
27	s	209	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
27	b	607	CLA	C1-C2-C3	-2.71	121.76	126.20
27	g	315	CLA	CHB-C1B-C2B	-2.71	119.57	127.43
27	g	306	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
37	c	610	KC2	CAB-C3B-C2B	2.71	137.23	128.43
37	i	310	KC2	O2D-CGD-CBD	2.71	115.96	111.23
27	s	203	CLA	CHB-C4A-NA	2.71	128.31	124.40
35	k	314	II0	C20-C14-C12	2.71	119.40	114.42
30	R	201	WVN	C39-C40-C37	-2.71	117.98	123.52
35	c	615	II0	C20-C14-C10	-2.70	119.10	124.16
27	A	801	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
35	l	315	II0	C27-C25-C29	-2.70	118.93	124.18
27	a	307	CLA	CHB-C4A-NA	2.70	128.30	124.40
35	e	612	II0	C42-C41-C39	-2.70	117.99	123.52
30	l	316	WVN	C12-C14-C15	-2.70	109.23	114.06
27	B	837	CLA	CHB-C4A-NA	2.70	128.30	124.40
27	n	602	CLA	O2D-CGD-CBD	2.70	115.95	111.23
35	e	616	II0	C27-C25-C29	-2.70	118.93	124.18
35	c	614	II0	C29-C31-C33	-2.70	115.37	123.20
37	d	309	KC2	O2D-CGD-O1D	-2.70	118.59	123.85
27	a	309	CLA	CMB-C2B-C3B	2.70	132.90	126.55
37	n	611	KC2	C1D-CHD-C4C	-2.70	119.89	126.25
36	j	616	IHT	C30-C32-C33	-2.70	118.96	126.36
35	g	318	II0	C38-C36-C34	2.70	122.21	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	613	II0	C41-C42-C40	-2.70	117.99	123.52
27	B	829	CLA	CHB-C4A-NA	2.70	128.30	124.40
27	n	608	CLA	CHB-C4A-NA	2.70	128.30	124.40
37	k	312	KC2	CAB-C3B-C2B	2.70	137.21	128.43
35	e	613	II0	C31-C33-C35	-2.70	118.96	126.36
36	g	319	IHT	C22-C18-C07	-2.70	119.79	127.00
30	B	847	WVN	C18-C06-C13	2.70	114.47	110.24
27	d	308	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
35	k	315	II0	C41-C42-C40	-2.70	118.00	123.52
35	a	316	II0	C31-C33-C35	-2.70	118.97	126.36
27	c	603	CLA	O2D-CGD-CBD	2.70	115.95	111.23
37	e	609	KC2	CAB-C3B-C2B	2.70	137.20	128.43
27	k	304	CLA	CMB-C2B-C3B	2.70	132.89	126.55
37	s	201	KC2	CMD-C2D-C1D	-2.70	121.31	125.42
35	d	313	II0	C16-C03-C09	-2.70	105.69	110.52
37	s	204	KC2	CBC-CAC-C3C	-2.70	114.06	127.53
27	A	834	CLA	CHB-C4A-NA	2.69	128.29	124.40
36	n	617	IHT	C20-C15-C12	2.69	119.38	114.42
35	k	315	II0	C42-C41-C39	-2.69	118.01	123.52
27	b	608	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
30	K	103	WVN	C39-C40-C37	-2.69	118.01	123.52
35	j	615	II0	C05-C03-C09	2.69	114.79	109.49
27	d	307	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
27	B	840	CLA	CMB-C2B-C3B	2.69	132.88	126.55
27	B	802	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
27	m	611	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
27	k	309	CLA	CHA-C4D-ND	2.69	138.09	132.55
27	j	609	CLA	CBC-CAC-C3C	2.69	119.70	112.42
27	i	303	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
27	B	818	CLA	C3B-C4B-NB	-2.69	108.13	110.53
27	j	604	CLA	C6-C5-C3	-2.68	106.93	113.47
35	a	316	II0	C32-C34-C36	-2.68	119.00	126.36
30	B	848	WVN	C02-C05-C09	-2.68	118.17	121.47
36	R	204	IHT	C29-C31-C34	-2.68	115.42	123.20
27	c	608	CLA	CMB-C2B-C3B	2.68	132.86	126.55
27	a	310	CLA	C3B-C4B-NB	-2.68	108.14	110.53
35	n	615	II0	C19-C13-C09	-2.68	119.14	124.16
27	A	831	CLA	CHB-C4A-NA	2.68	128.27	124.40
27	d	308	CLA	CHB-C4A-NA	2.68	128.27	124.40
30	B	843	WVN	C24-C22-C26	-2.68	118.47	122.82
27	A	853	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
35	j	613	II0	C20-C14-C10	-2.68	119.15	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	s	206	CLA	CMB-C2B-C3B	2.68	132.85	126.55
35	a	318	II0	C06-C04-C10	2.68	114.77	109.49
27	A	827	CLA	CHB-C4A-NA	2.68	128.26	124.40
27	m	612	CLA	CAC-C3C-C4C	-2.68	121.31	124.79
30	B	843	WVN	C02-C05-C09	-2.68	118.17	121.47
35	l	302	II0	C19-C13-C09	-2.68	119.16	124.16
35	m	613	II0	C31-C33-C35	-2.68	119.03	126.36
27	A	836	CLA	CMB-C2B-C3B	2.67	132.84	126.55
27	m	603	CLA	C3A-C2A-C1A	2.67	105.34	101.34
27	A	813	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
29	b	617	LHG	O3-P-O5	-2.67	98.34	108.94
27	b	611	CLA	CHB-C4A-NA	2.67	128.26	124.40
27	l	306	CLA	CMB-C2B-C3B	2.67	132.83	126.55
35	e	613	II0	C38-C36-C34	2.67	122.17	118.09
27	g	315	CLA	CMB-C2B-C3B	2.67	132.83	126.55
27	l	307	CLA	CHA-C1A-NA	-2.67	120.34	126.39
27	B	823	CLA	CAA-C2A-C1A	2.67	120.73	111.97
27	k	307	CLA	CHB-C4A-NA	2.67	128.25	124.40
27	e	611	CLA	C11-C10-C8	-2.67	107.09	115.97
27	A	817	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
27	K	101	CLA	CAA-CBA-CGA	-2.67	105.63	113.21
35	g	316	II0	C38-C36-C34	2.67	122.16	118.09
27	c	601	CLA	CHB-C4A-NA	2.67	128.25	124.40
27	c	606	CLA	CHB-C4A-NA	2.67	128.25	124.40
27	B	832	CLA	C3B-C4B-NB	-2.67	108.15	110.53
37	m	610	KC2	CAB-C3B-C2B	2.67	137.10	128.43
37	g	313	KC2	CAB-C3B-C2B	2.67	137.10	128.43
27	e	611	CLA	C6-C5-C3	-2.67	106.98	113.47
35	n	615	II0	C31-C33-C35	-2.66	119.06	126.36
27	L	202	CLA	CHB-C4A-NA	2.66	128.24	124.40
35	a	318	II0	C41-C42-C40	-2.66	118.07	123.52
29	g	301	LHG	O8-C23-C24	2.66	119.95	111.83
27	i	305	CLA	C4A-NA-C1A	2.66	107.89	106.68
27	A	825	CLA	CMB-C2B-C3B	2.66	132.81	126.55
27	A	804	CLA	CMB-C2B-C3B	2.66	132.81	126.55
30	i	315	WVN	C06-C13-C15	-2.66	119.00	122.64
35	j	614	II0	C12-C14-C10	-2.66	114.96	120.50
30	B	846	WVN	C24-C22-C19	2.66	122.15	118.09
27	m	604	CLA	C2A-C3A-C4A	2.66	106.16	101.87
27	h	306	CLA	CHB-C1B-NB	2.66	128.03	124.05
27	k	301	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
27	h	313	CLA	CMB-C2B-C3B	2.66	132.80	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	603	CLA	CHB-C4A-NA	2.65	128.23	124.40
27	j	609	CLA	CMC-C2C-C1C	-2.65	120.89	125.03
27	B	832	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
27	s	208	CLA	CHB-C1B-C2B	-2.65	119.73	127.43
27	B	811	CLA	CHB-C4A-NA	2.65	128.23	124.40
35	n	615	II0	C32-C30-C26	-2.65	119.20	126.61
30	B	844	WVN	C30-C33-C34	-2.65	119.10	126.36
27	i	311	CLA	C1D-ND-C4D	-2.65	104.45	106.31
30	F	205	WVN	C26-C29-C31	-2.65	115.52	123.20
27	i	308	CLA	CMD-C2D-C1D	-2.65	120.06	124.73
30	e	615	WVN	C30-C33-C34	-2.65	119.10	126.36
27	h	306	CLA	CHB-C4A-NA	2.65	128.22	124.40
35	d	314	II0	C31-C29-C25	-2.65	119.21	126.61
35	a	314	II0	C34-C36-C40	-2.65	114.85	119.01
36	f	617	IHT	C30-C32-C33	-2.65	119.11	126.36
27	f	607	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
35	b	615	II0	C29-C31-C33	-2.64	115.54	123.20
27	B	818	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
27	A	820	CLA	CHB-C4A-NA	2.64	128.22	124.40
29	c	618	LHG	O7-C7-O9	-2.64	117.52	123.70
27	g	310	CLA	C1-C2-C3	-2.64	121.87	126.20
36	k	317	IHT	C27-C30-C32	-2.64	115.55	123.20
27	B	805	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
27	n	602	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
27	A	802	CLA	CAA-C2A-C1A	-2.64	103.32	111.97
27	c	611	CLA	CHB-C4A-NA	2.64	128.21	124.40
27	l	303	CLA	CHB-C4A-NA	2.64	128.21	124.40
27	k	305	CLA	CHB-C4A-NA	2.64	128.21	124.40
35	h	311	II0	C29-C31-C33	-2.64	115.55	123.20
27	k	308	CLA	C4A-NA-C1A	2.64	107.88	106.68
30	I	101	WVN	C39-C36-C32	-2.64	123.58	127.28
27	k	306	CLA	CAA-C2A-C1A	2.64	120.62	111.97
35	h	310	II0	C15-C03-C09	-2.64	105.79	110.52
30	F	204	WVN	C14-C15-C13	-2.64	119.14	122.70
27	i	306	CLA	CHB-C4A-NA	2.64	128.21	124.40
37	f	611	KC2	C1D-CHD-C4C	-2.64	120.05	126.25
35	l	314	II0	C17-C04-C10	-2.64	105.80	110.52
35	d	312	II0	C41-C42-C40	-2.64	118.13	123.52
37	k	311	KC2	CMB-C2B-C1B	2.63	129.37	124.73
35	a	316	II0	C30-C32-C34	-2.63	115.57	123.20
36	O	204	IHT	C40-C41-C38	-2.63	118.13	123.52
27	h	301	CLA	CGD-CBD-CAD	-2.63	102.32	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	s	201	KC2	C1D-CHD-C4C	-2.63	120.05	126.25
27	n	606	CLA	CHB-C4A-NA	2.63	128.20	124.40
27	B	821	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
27	g	308	CLA	CMC-C2C-C3C	2.63	133.27	126.15
27	h	303	CLA	C1-O2A-CGA	2.63	123.02	116.65
27	c	606	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
27	h	306	CLA	CHB-C1B-C2B	-2.63	119.79	127.43
27	j	609	CLA	C3A-C2A-C1A	2.63	105.28	101.34
27	B	835	CLA	CHB-C4A-NA	2.63	128.20	124.40
27	A	802	CLA	C11-C12-C13	-2.63	107.22	115.97
35	j	614	II0	C29-C31-C33	-2.63	115.58	123.20
27	A	821	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
27	g	310	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
29	g	321	LHG	O8-C6-C5	2.63	115.98	108.40
30	J	102	WVN	C30-C28-C25	-2.63	123.59	127.28
27	A	823	CLA	CHB-C4A-NA	2.63	128.19	124.40
27	a	309	CLA	CHB-C4A-NA	2.63	128.19	124.40
27	f	613	CLA	CHB-C4A-NA	2.63	128.19	124.40
27	d	302	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
27	b	602	CLA	CMB-C2B-C1B	-2.63	121.42	125.42
27	h	305	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
35	h	311	II0	C41-C42-C40	-2.63	118.14	123.52
27	O	202	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
27	n	607	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
27	c	601	CLA	CMD-C2D-C1D	-2.63	120.10	124.73
27	A	803	CLA	CMB-C2B-C3B	2.62	132.72	126.55
27	j	602	CLA	CHB-C4A-NA	2.62	128.19	124.40
27	h	303	CLA	C1-C2-C3	-2.62	122.52	126.76
27	B	832	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
35	m	613	II0	C29-C31-C33	-2.62	115.60	123.20
27	j	606	CLA	CAA-C2A-C1A	-2.62	103.38	111.97
35	a	314	II0	C05-C03-C09	2.62	114.66	109.49
27	f	603	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
37	s	201	KC2	C1A-C2A-C3A	-2.62	104.87	107.28
27	R	203	CLA	C1-C2-C3	-2.62	121.90	126.20
35	i	318	II0	O02-C08-C06	2.62	115.11	109.75
36	O	204	IHT	C19-C10-C09	2.62	119.18	113.60
30	J	102	WVN	C12-C14-C15	2.62	118.73	114.06
27	B	807	CLA	C4-C3-C5	2.62	119.78	115.23
27	s	202	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
27	g	308	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
27	k	308	CLA	C6-C7-C8	-2.62	107.26	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	845	LHG	C6-C5-C4	-2.62	105.68	111.78
35	f	618	II0	C42-C40-C36	-2.62	123.61	127.28
36	R	204	IHT	C22-C18-C07	-2.62	120.01	127.00
27	n	609	CLA	CMA-C3A-C2A	-2.62	103.87	113.98
36	b	614	IHT	C13-C02-C07	-2.62	106.14	110.24
27	A	802	CLA	CHB-C1B-NB	2.62	127.97	124.05
27	g	308	CLA	CMB-C2B-C3B	2.61	132.70	126.55
27	m	602	CLA	C1-C2-C3	-2.61	121.91	126.20
35	c	617	II0	C19-C13-C11	2.61	119.23	114.42
29	n	619	LHG	O7-C7-O9	-2.61	117.60	123.70
27	i	306	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
27	m	603	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
27	k	304	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
27	A	838	CLA	C1-C2-C3	-2.61	121.92	126.20
27	g	307	CLA	CHB-C4A-NA	2.61	128.17	124.40
30	L	201	WVN	C10-C06-C13	2.61	114.23	110.44
27	A	804	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
37	d	309	KC2	C1D-CHD-C4C	-2.61	120.11	126.25
27	h	302	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
27	A	817	CLA	CHB-C1B-NB	2.61	127.96	124.05
27	B	838	CLA	CHB-C4A-NA	2.61	128.17	124.40
27	B	831	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	m	606	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	d	306	CLA	O2D-CGD-CBD	2.61	115.79	111.23
27	a	313	CLA	C4A-NA-C1A	2.61	107.87	106.68
27	A	842	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	j	612	CLA	CHB-C1B-NB	2.61	127.96	124.05
27	A	801	CLA	C1-C2-C3	-2.61	121.93	126.20
27	k	305	CLA	C1-C2-C3	-2.61	121.93	126.20
27	m	608	CLA	C1D-ND-C4D	-2.61	104.48	106.31
27	J	103	CLA	C3B-C4B-NB	-2.61	108.20	110.53
35	n	618	II0	C38-C36-C34	2.61	122.07	118.09
27	f	607	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	A	820	CLA	CBC-CAC-C3C	2.61	119.48	112.42
29	g	321	LHG	C5-O7-C7	-2.61	111.56	117.80
27	c	605	CLA	CAA-CBA-CGA	-2.61	105.81	113.21
27	f	602	CLA	O1D-CGD-CBD	2.60	129.66	124.52
27	n	605	CLA	C2C-C1C-NC	2.60	112.72	109.98
27	a	306	CLA	CHB-C4A-NA	2.60	128.16	124.40
27	e	606	CLA	CHB-C4A-NA	2.60	128.16	124.40
27	f	609	CLA	CMB-C2B-C3B	2.60	132.67	126.55
27	i	312	CLA	O2D-CGD-O1D	-2.60	118.78	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	i	313	II0	C30-C32-C34	-2.60	115.66	123.20
37	e	609	KC2	C1D-CHD-C4C	-2.60	120.13	126.25
36	b	614	IHT	C20-C15-C11	-2.60	119.29	124.16
34	O	205	LMG	O7-C10-C11	2.60	120.49	110.93
34	s	210	LMG	O8-C28-C29	2.60	119.77	111.83
27	B	839	CLA	CAC-C3C-C4C	2.60	128.18	124.79
30	F	205	WVN	C04-C09-C05	-2.60	122.35	124.83
35	g	318	II0	C06-C04-C10	2.60	114.61	109.49
27	m	609	CLA	CMC-C2C-C3C	2.60	133.18	126.15
30	i	315	WVN	C29-C31-C32	-2.60	119.23	126.36
27	l	308	CLA	CHB-C4A-NA	2.60	128.15	124.40
27	g	310	CLA	CHB-C1B-NB	2.60	127.95	124.05
35	h	311	II0	C12-C14-C10	-2.60	115.09	120.50
35	j	615	II0	C41-C39-C35	-2.60	123.63	127.28
37	n	611	KC2	CAB-C3B-C2B	2.60	136.88	128.43
37	n	611	KC2	O2D-CGD-O1D	-2.60	118.79	123.85
35	f	615	II0	C30-C32-C34	-2.60	115.67	123.20
30	s	205	WVN	C28-C30-C33	-2.60	115.67	123.20
27	O	206	CLA	C2A-C1A-CHA	2.60	128.38	123.87
37	d	309	KC2	CAB-C3B-C2B	2.60	136.87	128.43
30	A	848	WVN	C06-C13-C15	-2.60	119.09	122.64
30	B	848	WVN	C23-C20-C13	-2.60	120.06	127.00
35	n	618	II0	C19-C13-C09	-2.60	119.31	124.16
27	L	203	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
27	f	602	CLA	CHB-C4A-NA	2.59	128.14	124.40
27	O	206	CLA	C4-C3-C5	2.59	119.73	115.23
27	m	604	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
30	R	202	WVN	C14-C15-C13	-2.59	119.20	122.70
27	A	807	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
35	m	613	II0	C05-C03-C09	2.59	114.60	109.49
27	a	310	CLA	O2D-CGD-CBD	2.59	115.76	111.23
27	B	814	CLA	CHB-C4A-NA	2.59	128.14	124.40
27	b	606	CLA	CHB-C4A-NA	2.59	128.14	124.40
35	h	311	II0	C05-C03-C09	2.59	114.60	109.49
27	A	841	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
27	l	308	CLA	CMB-C2B-C3B	2.59	132.64	126.55
36	m	616	IHT	C02-C07-C18	2.59	122.67	115.65
36	O	204	IHT	C31-C29-C26	-2.59	119.37	126.61
27	A	828	CLA	CMB-C2B-C3B	2.59	132.64	126.55
30	L	205	WVN	C31-C32-C36	2.59	123.08	119.01
30	h	309	WVN	C14-C15-C13	-2.59	119.21	122.70
27	L	204	CLA	CBA-CAA-C2A	2.59	121.50	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	615	II0	C37-C35-C33	2.59	122.04	118.09
27	c	612	CLA	CHB-C4A-NA	2.59	128.13	124.40
27	B	810	CLA	C1-C2-C3	-2.59	121.96	126.20
27	i	303	CLA	C1D-ND-C4D	-2.59	104.50	106.31
27	A	808	CLA	CHB-C4A-NA	2.59	128.13	124.40
35	b	612	II0	C30-C32-C34	-2.59	115.71	123.20
27	n	608	CLA	O2D-CGD-CBD	2.58	115.75	111.23
37	s	204	KC2	CHD-C1D-C2D	2.58	134.93	127.43
27	n	613	CLA	O1D-CGD-CBD	2.58	129.61	124.52
27	A	809	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
27	a	308	CLA	CAA-C2A-C1A	-2.58	103.51	111.97
27	B	824	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
27	A	811	CLA	C3B-C4B-NB	-2.58	108.22	110.53
35	g	316	II0	C21-C23-C25	-2.58	167.46	176.23
30	J	102	WVN	C28-C30-C33	-2.58	115.72	123.20
27	i	309	CLA	CHB-C4A-NA	2.58	128.12	124.40
27	B	839	CLA	CMB-C2B-C3B	2.58	132.62	126.55
27	A	840	CLA	C5-C3-C2	-2.58	115.37	121.17
27	A	833	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
34	s	210	LMG	O7-C10-C11	2.58	117.06	111.48
35	m	614	II0	C12-C14-C10	-2.58	115.13	120.50
35	c	613	II0	C31-C33-C35	-2.58	119.30	126.36
37	g	314	KC2	CAB-C3B-C2B	2.58	136.81	128.43
30	B	846	WVN	C28-C30-C33	2.58	130.67	123.20
27	B	806	CLA	CHB-C4A-NA	2.58	128.12	124.40
37	j	610	KC2	CAB-C3B-C2B	2.58	136.81	128.43
27	g	310	CLA	CHB-C1B-C2B	-2.58	119.95	127.43
27	b	610	CLA	C4-C3-C5	2.58	119.70	115.23
30	B	846	WVN	C20-C13-C15	-2.57	115.63	121.56
33	B	842	DGD	O1G-C1A-C2A	2.57	119.68	111.83
30	R	202	WVN	C08-C01-C02	-2.57	105.65	109.55
27	A	842	CLA	C3A-C2A-C1A	2.57	105.19	101.34
27	k	309	CLA	C3A-C2A-C1A	2.57	105.19	101.34
27	A	834	CLA	CAA-CBA-CGA	-2.57	105.91	113.21
27	h	307	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
27	e	611	CLA	C3B-C4B-NB	-2.57	108.24	110.53
27	j	604	CLA	CMB-C2B-C3B	2.57	132.59	126.55
30	h	309	WVN	C29-C31-C32	-2.57	119.32	126.36
35	n	614	II0	C16-C03-C09	-2.57	105.92	110.52
37	i	310	KC2	C1D-CHD-C4C	-2.57	120.21	126.25
27	g	308	CLA	CHC-C1C-NC	2.57	128.18	124.31
27	c	605	CLA	O2D-CGD-O1D	-2.57	118.85	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	e	606	CLA	O1D-CGD-CBD	2.57	129.58	124.52
27	d	311	CLA	O2D-CGD-CBD	2.57	115.72	111.23
27	A	819	CLA	C2A-C1A-CHA	2.57	128.32	123.87
27	i	307	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
30	e	615	WVN	C16-C05-C09	-2.56	113.75	122.37
35	c	614	II0	C16-C03-C09	-2.56	105.92	110.52
27	A	812	CLA	C7-C6-C5	2.56	120.09	113.26
35	n	618	II0	C28-C26-C30	-2.56	119.20	124.18
37	f	611	KC2	CAA-CBA-CGA	-2.56	114.02	127.05
27	B	809	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
27	e	611	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
27	a	311	CLA	C3A-C2A-C1A	2.56	105.17	101.34
27	i	305	CLA	C1-C2-C3	-2.56	122.00	126.20
37	l	311	KC2	CAB-C3B-C2B	2.56	136.76	128.43
27	l	304	CLA	CAA-CBA-CGA	-2.56	105.94	113.21
27	g	322	CLA	CHB-C4A-NA	2.56	128.09	124.40
27	b	603	CLA	C4-C3-C5	2.56	119.67	115.23
36	k	317	IHT	C31-C29-C26	-2.56	119.45	126.61
29	g	321	LHG	O8-C23-O10	-2.56	117.23	123.63
27	A	839	CLA	C1-C2-C3	-2.56	122.01	126.20
35	e	614	II0	C41-C42-C40	-2.56	118.29	123.52
27	g	304	CLA	O2D-CGD-CBD	2.56	115.70	111.23
27	A	813	CLA	CHC-C4B-NB	2.56	127.89	124.05
27	B	805	CLA	CMB-C2B-C3B	2.56	132.56	126.55
34	F	206	LMG	O8-C28-C29	2.56	119.63	111.83
27	A	810	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
27	g	310	CLA	O2D-CGD-CBD	2.56	115.70	111.23
30	s	205	WVN	C12-C14-C15	-2.56	109.50	114.06
30	R	202	WVN	C30-C28-C25	-2.55	123.69	127.28
35	n	614	II0	C41-C42-C40	-2.55	118.29	123.52
35	a	318	II0	C19-C13-C11	2.55	119.12	114.42
27	f	613	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
27	i	311	CLA	C4-C3-C5	-2.55	113.12	116.13
27	k	301	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
27	B	837	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	m	611	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	A	837	CLA	C16-C15-C13	-2.55	107.48	115.97
30	F	204	WVN	C16-C05-C09	-2.55	113.79	122.37
37	d	310	KC2	CHB-C4A-NA	2.55	128.19	124.23
27	g	311	CLA	O1D-CGD-CBD	2.55	129.55	124.52
27	l	306	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
27	A	824	CLA	CHA-C1A-NA	-2.55	120.61	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	f	611	KC2	CAB-C3B-C2B	2.55	136.72	128.43
27	d	311	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
27	k	306	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
27	l	312	CLA	C4-C3-C5	2.55	119.65	115.23
27	e	604	CLA	O2D-CGD-CBD	2.55	115.69	111.23
30	e	615	WVN	C39-C40-C37	-2.55	118.30	123.52
35	g	320	II0	C29-C31-C33	-2.55	115.82	123.20
30	R	201	WVN	C17-C06-C13	2.55	114.24	110.24
30	i	315	WVN	C30-C33-C34	-2.55	119.38	126.36
29	c	621	LHG	O8-C23-C24	2.55	119.60	111.83
35	O	203	II0	C06-C04-C10	2.55	114.51	109.49
27	B	821	CLA	C2D-C1D-ND	-2.55	107.61	110.13
27	O	206	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
27	A	820	CLA	CHB-C1B-NB	2.54	127.86	124.05
27	l	304	CLA	O2A-CGA-CBA	2.54	119.59	111.83
35	f	616	II0	C05-C03-C09	2.54	114.50	109.49
27	L	206	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
27	A	806	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
27	j	609	CLA	C2C-C1C-NC	2.54	112.65	109.98
31	a	320	LMT	O5'-C5'-C6'	2.54	112.73	106.44
30	R	202	WVN	C20-C13-C15	-2.54	115.70	121.56
27	k	309	CLA	CAC-C3C-C2C	-2.54	122.89	127.56
30	M	101	WVN	C30-C33-C34	-2.54	119.40	126.36
35	e	612	II0	C06-C04-C10	2.54	114.49	109.49
35	n	616	II0	C31-C29-C25	-2.54	119.51	126.61
27	A	803	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
35	k	315	II0	C19-C13-C09	-2.54	119.41	124.16
27	B	814	CLA	O2D-CGD-CBD	2.54	115.67	111.23
35	a	314	II0	C31-C33-C35	-2.54	119.40	126.36
27	A	811	CLA	C1-C2-C3	-2.54	122.04	126.20
34	c	619	LMG	O8-C28-C29	2.54	119.57	111.83
27	A	826	CLA	CAA-CBA-CGA	-2.54	106.00	113.21
27	n	602	CLA	CMA-C3A-C4A	-2.54	104.95	111.77
27	c	604	CLA	CHB-C4A-NA	2.54	128.06	124.40
27	c	609	CLA	CHB-C4A-NA	2.54	128.06	124.40
27	g	322	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
27	a	308	CLA	CHB-C4A-NA	2.54	128.06	124.40
27	a	312	CLA	CHB-C4A-NA	2.54	128.06	124.40
36	g	319	IHT	C31-C34-C35	-2.53	119.42	126.36
35	f	618	II0	C19-C13-C09	-2.53	119.42	124.16
27	b	602	CLA	CMB-C2B-C3B	2.53	132.51	126.55
35	n	616	II0	C06-C04-C10	2.53	114.48	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	819	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
35	c	613	II0	C15-C03-C09	-2.53	105.98	110.52
27	A	835	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
27	c	608	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
27	b	603	CLA	CMB-C2B-C3B	2.53	132.50	126.55
30	s	207	WVN	C23-C20-C13	-2.53	120.23	127.00
27	h	303	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
31	A	851	LMT	C1B-O5B-C5B	2.53	118.66	113.72
27	L	203	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
27	A	806	CLA	CAA-CBA-CGA	-2.53	106.03	113.21
27	h	301	CLA	CHB-C1B-NB	2.53	127.84	124.05
27	n	601	CLA	CHB-C4A-NA	2.53	128.05	124.40
27	B	834	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
27	A	823	CLA	C3B-C4B-NB	-2.53	108.28	110.53
27	c	602	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
34	L	208	LMG	O8-C28-C29	2.53	119.54	111.83
27	h	302	CLA	C1-O2A-CGA	2.52	122.76	116.65
27	s	208	CLA	CMB-C2B-C3B	2.52	132.49	126.55
27	k	304	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
27	a	308	CLA	CAC-C3C-C4C	2.52	128.07	124.79
30	J	101	WVN	C23-C20-C13	-2.52	120.26	127.00
27	L	202	CLA	C3B-C4B-NB	-2.52	108.28	110.53
27	a	309	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
27	B	804	CLA	CMB-C2B-C3B	2.52	132.48	126.55
27	A	835	CLA	O2D-CGD-CBD	2.52	115.64	111.23
27	B	810	CLA	O2D-CGD-CBD	2.52	115.64	111.23
27	A	810	CLA	C3B-C4B-NB	-2.52	108.28	110.53
27	n	602	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
37	g	312	KC2	CAB-C3B-C2B	2.52	136.63	128.43
27	h	308	CLA	CMA-C3A-C4A	2.52	118.55	111.77
35	a	315	II0	C34-C36-C40	-2.52	115.04	119.01
35	c	617	II0	C27-C25-C29	-2.52	119.29	124.18
27	g	306	CLA	CHB-C4A-NA	2.52	128.04	124.40
35	l	302	II0	C06-C04-C10	2.52	114.45	109.49
27	B	829	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
27	m	606	CLA	CBA-CAA-C2A	-2.52	106.30	113.79
29	a	319	LHG	C25-C24-C23	-2.52	104.46	113.69
27	k	308	CLA	C4D-CHA-C1A	2.52	124.25	121.24
27	f	606	CLA	O1D-CGD-CBD	2.52	129.49	124.52
35	e	616	II0	C20-C14-C10	-2.52	119.45	124.16
27	c	601	CLA	O2D-CGD-CBD	2.52	115.63	111.23
27	e	608	CLA	C3B-C4B-NB	-2.52	108.28	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	842	DGD	O6E-C5E-C6E	2.52	112.68	106.44
27	h	305	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
29	A	850	LHG	O8-C23-C24	2.52	119.51	111.83
27	k	307	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
36	j	616	IHT	C31-C34-C35	-2.52	119.46	126.36
27	L	203	CLA	CHD-C1D-ND	-2.52	121.26	124.80
37	g	312	KC2	C1D-CHD-C4C	-2.52	120.33	126.25
27	c	609	CLA	CMB-C2B-C3B	2.52	132.47	126.55
27	k	308	CLA	CHB-C1B-NB	2.52	127.82	124.05
27	h	308	CLA	CAA-C2A-C3A	-2.51	106.20	113.00
27	a	308	CLA	C6-C7-C8	-2.51	107.61	115.97
27	l	304	CLA	C1-C2-C3	-2.51	122.08	126.20
27	d	308	CLA	CMB-C2B-C3B	2.51	132.46	126.55
27	b	601	CLA	CHB-C4A-NA	2.51	128.03	124.40
27	j	604	CLA	C11-C12-C13	-2.51	107.62	115.97
27	g	315	CLA	CAA-CBA-CGA	-2.51	106.08	113.21
29	i	316	LHG	O8-C23-O10	-2.51	117.35	123.63
27	i	303	CLA	CMB-C2B-C3B	2.51	132.46	126.55
27	A	803	CLA	C3B-C4B-NB	-2.51	108.29	110.53
27	f	604	CLA	C2A-C3A-C4A	2.51	105.92	101.87
27	m	609	CLA	C2A-C1A-CHA	2.51	128.22	123.87
27	b	609	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
27	f	610	CLA	CHB-C4A-NA	2.51	128.02	124.40
35	k	316	II0	C20-C14-C12	2.51	119.03	114.42
35	e	614	II0	C29-C31-C33	-2.51	115.94	123.20
35	n	615	II0	C06-C04-C10	2.51	114.43	109.49
27	n	605	CLA	CHC-C1C-NC	2.51	128.09	124.31
30	s	205	WVN	C21-C15-C14	2.51	118.94	113.60
35	j	615	II0	C41-C42-C40	-2.51	118.39	123.52
27	i	309	CLA	O1D-CGD-CBD	2.51	129.46	124.52
27	B	820	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
35	f	614	II0	C20-C14-C12	2.50	119.03	114.42
27	e	602	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
27	A	808	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
27	A	827	CLA	C3B-C4B-NB	-2.50	108.30	110.53
27	i	304	CLA	C3B-C4B-NB	-2.50	108.30	110.53
27	g	309	CLA	C3B-C4B-NB	-2.50	108.30	110.53
27	b	603	CLA	C1-C2-C3	-2.50	122.10	126.20
27	R	203	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
27	A	853	CLA	CAA-CBA-CGA	-2.50	106.11	113.21
27	A	824	CLA	CBA-CAA-C2A	2.50	121.24	113.79
27	B	836	CLA	O2A-CGA-O1A	-2.50	117.37	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	615	II0	C41-C42-C40	-2.50	118.40	123.52
27	A	855	CLA	C5-C3-C2	2.50	126.78	121.17
27	e	604	CLA	O1D-CGD-CBD	2.50	129.45	124.52
37	j	610	KC2	O2D-CGD-CBD	2.50	115.60	111.23
27	l	305	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
35	i	314	II0	C32-C30-C26	-2.50	119.62	126.61
27	O	206	CLA	CAA-C2A-C3A	-2.50	106.24	113.00
36	k	317	IHT	C20-C15-C12	2.50	119.02	114.42
35	g	317	II0	C30-C32-C34	-2.50	115.96	123.20
35	j	613	II0	C18-C04-C17	-2.50	101.48	108.63
35	b	613	II0	C31-C33-C35	-2.50	119.51	126.36
35	e	613	II0	C20-C14-C12	2.50	119.02	114.42
27	B	831	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
27	s	202	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
27	m	611	CLA	CHB-C4A-NA	2.50	128.00	124.40
34	O	205	LMG	O6-C5-C6	2.50	112.63	106.44
27	B	813	CLA	CHB-C4A-NA	2.50	128.00	124.40
27	m	607	CLA	CMB-C2B-C3B	2.50	132.42	126.55
27	B	807	CLA	CHB-C1B-NB	2.50	127.79	124.05
27	B	810	CLA	CAC-C3C-C4C	2.49	128.04	124.79
37	k	312	KC2	C1D-CHD-C4C	-2.49	120.38	126.25
27	h	304	CLA	CHA-C1A-NA	-2.49	120.74	126.39
37	l	311	KC2	CAA-CBA-CGA	-2.49	114.36	127.05
30	l	301	WVN	C06-C13-C15	-2.49	119.23	122.64
27	A	841	CLA	C3B-C4B-NB	-2.49	108.30	110.53
27	a	307	CLA	C3B-C4B-NB	-2.49	108.30	110.53
27	B	826	CLA	O2D-CGD-CBD	2.49	115.59	111.23
27	A	825	CLA	CAC-C3C-C4C	2.49	128.03	124.79
27	f	609	CLA	C7-C6-C5	2.49	119.91	113.26
30	K	103	WVN	C24-C22-C19	2.49	121.89	118.09
27	h	305	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
37	g	313	KC2	C1D-CHD-C4C	-2.49	120.39	126.25
35	g	320	II0	C05-C03-C09	2.49	114.40	109.49
27	B	840	CLA	CHB-C4A-NA	2.49	127.99	124.40
29	a	301	LHG	C5-O7-C7	-2.49	111.84	117.80
34	J	106	LMG	O8-C28-C29	2.49	119.42	111.83
27	n	607	CLA	CMC-C2C-C1C	-2.49	121.14	125.03
27	A	824	CLA	CHB-C4A-NA	2.49	127.99	124.40
30	B	848	WVN	C03-C04-C09	-2.49	107.89	112.07
35	f	615	II0	C16-C03-C09	-2.49	106.06	110.52
27	a	313	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
27	A	818	CLA	CBC-CAC-C3C	2.49	119.16	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	e	614	II0	C32-C34-C36	-2.49	119.55	126.36
27	h	301	CLA	C7-C6-C5	-2.49	106.64	113.26
35	g	320	II0	C15-C03-C09	-2.48	106.07	110.52
27	c	607	CLA	CMB-C2B-C3B	2.48	132.39	126.55
37	c	610	KC2	O2D-CGD-O1D	-2.48	119.02	123.85
27	B	823	CLA	C2A-C1A-CHA	2.48	128.18	123.87
35	g	320	II0	C20-C14-C12	2.48	118.98	114.42
27	d	307	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
27	f	612	CLA	CMC-C2C-C1C	-2.48	121.16	125.03
27	A	840	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
27	B	827	CLA	CHB-C4A-NA	2.48	127.98	124.40
27	j	603	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
27	A	853	CLA	CHB-C4A-NA	2.48	127.98	124.40
27	m	606	CLA	CAC-C3C-C4C	2.48	128.01	124.79
35	d	313	II0	C27-C25-C29	-2.48	119.37	124.18
35	k	318	II0	C31-C29-C25	-2.48	119.68	126.61
27	J	105	CLA	CHA-C1A-NA	-2.48	120.78	126.39
35	k	318	II0	C37-C35-C33	2.48	121.87	118.09
27	n	605	CLA	CMB-C2B-C3B	2.48	132.38	126.55
35	m	614	II0	C31-C33-C35	-2.48	119.57	126.36
27	A	817	CLA	CHB-C4A-NA	2.48	127.97	124.40
27	L	203	CLA	CHB-C4A-NA	2.48	127.97	124.40
35	f	615	II0	C31-C29-C25	-2.48	119.68	126.61
30	B	844	WVN	C11-C19-C22	-2.48	121.00	126.32
27	m	612	CLA	CHB-C4A-NA	2.48	127.97	124.40
27	e	602	CLA	C3B-C4B-NB	-2.48	108.32	110.53
37	m	610	KC2	C1D-CHD-C4C	-2.47	120.43	126.25
27	a	312	CLA	C3B-C4B-NB	-2.47	108.32	110.53
27	j	606	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
27	c	605	CLA	CAC-C3C-C4C	2.47	128.01	124.79
27	i	309	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
35	l	313	II0	C20-C14-C10	-2.47	119.54	124.16
27	B	815	CLA	O2D-CGD-CBD	2.47	115.55	111.23
27	B	810	CLA	C2A-C1A-CHA	2.47	128.16	123.87
27	f	603	CLA	CMB-C2B-C3B	2.47	132.36	126.55
34	c	619	LMG	O1-C1-C2	2.47	112.02	108.27
35	k	318	II0	C12-C14-C10	-2.47	115.36	120.50
27	A	814	CLA	CHB-C4A-NA	2.47	127.96	124.40
27	F	201	CLA	CMB-C2B-C3B	2.47	132.36	126.55
35	j	614	II0	C05-C03-C09	2.47	114.35	109.49
27	B	849	CLA	O2D-CGD-CBD	2.47	115.54	111.23
37	g	313	KC2	CAC-C3C-C4C	2.47	135.29	124.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	810	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
35	l	313	II0	C05-C03-C09	2.47	114.35	109.49
27	B	811	CLA	CBA-CAA-C2A	2.47	121.13	113.79
35	g	316	II0	C12-C14-C10	-2.47	115.37	120.50
27	A	837	CLA	CMB-C2B-C3B	2.47	132.35	126.55
27	k	306	CLA	C2C-C1C-NC	2.47	112.57	109.98
36	a	317	IHT	C30-C32-C33	-2.47	119.60	126.36
27	s	206	CLA	C11-C12-C13	-2.46	107.77	115.97
27	h	304	CLA	CBA-CAA-C2A	2.46	121.13	113.79
27	j	611	CLA	CHB-C4A-NA	2.46	127.96	124.40
27	g	303	CLA	C3B-C4B-NB	-2.46	108.33	110.53
27	d	301	CLA	CHB-C4A-NA	2.46	127.95	124.40
37	i	317	KC2	CMB-C2B-C1B	2.46	129.06	124.73
27	n	610	CLA	C4D-CHA-C1A	2.46	124.18	121.24
27	a	312	CLA	O2D-CGD-CBD	2.46	115.53	111.23
27	d	305	CLA	O2D-CGD-CBD	2.46	115.53	111.23
35	i	313	II0	C05-C03-C09	2.46	114.33	109.49
30	R	201	WVN	C18-C06-C13	2.46	114.10	110.24
27	f	612	CLA	C4-C3-C5	2.46	119.02	116.13
27	B	803	CLA	O2D-CGD-CBD	2.46	115.53	111.23
27	n	605	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
35	g	320	II0	C12-C14-C10	-2.46	115.39	120.50
27	f	612	CLA	CHB-C1B-C2B	-2.46	120.30	127.43
30	B	844	WVN	C19-C22-C26	-2.46	115.15	119.01
27	c	603	CLA	CAC-C3C-C4C	2.46	127.98	124.79
27	A	840	CLA	C1-O2A-CGA	-2.45	110.71	116.65
27	F	202	CLA	C1-C2-C3	-2.45	122.17	126.20
30	B	844	WVN	C23-C20-C13	-2.45	120.44	127.00
27	A	834	CLA	C3B-C4B-NB	-2.45	108.34	110.53
27	d	305	CLA	CAC-C3C-C4C	-2.45	121.60	124.79
27	m	604	CLA	CHD-C1D-ND	-2.45	121.35	124.80
27	A	823	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
27	A	856	CLA	C3A-C2A-C1A	2.45	105.80	101.64
37	s	204	KC2	CAA-CBA-CGA	-2.45	114.58	127.05
30	K	103	WVN	C20-C23-C25	-2.45	122.61	126.23
27	j	604	CLA	C7-C6-C5	-2.45	106.73	113.26
30	l	301	WVN	C29-C26-C22	-2.45	123.84	127.28
27	B	806	CLA	CHB-C1B-NB	2.45	127.72	124.05
35	h	312	II0	C31-C33-C35	-2.45	119.65	126.36
30	B	846	WVN	C27-C25-C28	2.45	126.78	122.82
35	O	203	II0	C37-C35-C33	2.45	121.83	118.09
27	A	802	CLA	CHB-C4A-NA	2.45	127.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	K	101	CLA	O2D-CGD-CBD	2.45	115.51	111.23
27	i	311	CLA	CMC-C2C-C3C	2.45	132.77	126.15
30	B	843	WVN	C20-C23-C25	-2.45	122.61	126.23
30	h	309	WVN	C40-C39-C36	-2.45	118.51	123.52
27	a	313	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
27	i	306	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
37	s	201	KC2	CBA-CAA-C2A	-2.45	115.63	125.45
37	i	317	KC2	C3A-C4A-NA	2.45	113.48	110.45
27	A	821	CLA	CAA-CBA-CGA	-2.45	106.26	113.21
27	K	102	CLA	CAC-C3C-C4C	2.45	127.97	124.79
27	h	303	CLA	O2D-CGD-CBD	2.45	115.51	111.23
27	e	607	CLA	C11-C12-C13	-2.45	107.83	115.97
27	B	839	CLA	CHD-C1D-ND	-2.45	121.36	124.80
30	R	202	WVN	C39-C40-C37	-2.45	118.52	123.52
27	l	310	CLA	CHB-C4A-NA	2.44	127.93	124.40
27	B	815	CLA	CMB-C2B-C3B	2.44	132.30	126.55
37	d	309	KC2	CAA-CBA-CGA	-2.44	114.62	127.05
27	f	612	CLA	CBC-CAC-C3C	2.44	119.05	112.42
27	k	304	CLA	CMD-C2D-C1D	2.44	129.03	124.73
27	g	322	CLA	O2A-C1-C2	2.44	117.51	108.11
27	g	309	CLA	C2A-C1A-CHA	2.44	128.10	123.87
27	B	827	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
27	k	304	CLA	C1D-ND-C4D	-2.44	104.60	106.31
27	B	811	CLA	CAA-CBA-CGA	-2.44	106.28	113.21
35	d	314	II0	C38-C36-C40	-2.44	118.86	122.82
27	c	606	CLA	C2A-C1A-CHA	2.44	128.10	123.87
27	g	311	CLA	CMD-C2D-C1D	-2.44	120.43	124.73
27	n	607	CLA	CMC-C2C-C3C	2.44	132.75	126.15
36	c	616	IHT	C20-C15-C11	-2.44	119.60	124.16
27	h	305	CLA	CMB-C2B-C3B	2.44	132.29	126.55
27	B	835	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
35	J	104	II0	C38-C36-C34	2.44	121.81	118.09
27	B	818	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	b	609	CLA	CHB-C4A-NA	2.44	127.92	124.40
29	g	301	LHG	C5-O7-C7	2.44	123.63	117.80
27	s	202	CLA	CHD-C1D-ND	-2.44	121.37	124.80
35	O	203	II0	C30-C32-C34	-2.44	116.14	123.20
35	f	618	II0	C32-C30-C26	-2.44	119.80	126.61
27	b	607	CLA	CHD-C1D-ND	-2.43	121.38	124.80
27	B	838	CLA	C1-C2-C3	-2.43	122.21	126.20
27	s	202	CLA	CMD-C2D-C1D	2.43	129.01	124.73
27	n	608	CLA	CMA-C3A-C4A	-2.43	105.23	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	l	311	KC2	O2D-CGD-O1D	-2.43	119.11	123.85
30	M	101	WVN	C16-C05-C09	-2.43	114.19	122.37
35	e	616	II0	C06-C04-C10	2.43	114.28	109.49
27	g	304	CLA	CAA-C2A-C3A	-2.43	106.43	113.00
27	a	308	CLA	O2D-CGD-CBD	2.43	115.48	111.23
27	k	308	CLA	CAC-C3C-C4C	2.43	127.95	124.79
30	h	309	WVN	C28-C30-C33	2.43	130.25	123.20
34	c	619	LMG	O6-C5-C4	2.43	114.08	109.70
27	k	302	CLA	CAC-C3C-C4C	2.43	127.95	124.79
35	d	312	II0	C42-C41-C39	-2.43	118.55	123.52
27	J	105	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
30	I	101	WVN	C27-C25-C23	2.43	121.80	118.09
27	l	306	CLA	C11-C12-C13	-2.43	107.89	115.97
35	m	613	II0	C32-C34-C36	-2.43	119.70	126.36
35	m	613	II0	C41-C42-C40	-2.43	118.55	123.52
27	k	308	CLA	CHB-C1B-C2B	-2.43	120.37	127.43
27	A	842	CLA	C2A-C1A-CHA	2.43	128.08	123.87
27	B	820	CLA	C2A-C1A-CHA	2.43	128.08	123.87
30	A	848	WVN	C11-C19-C22	-2.43	121.10	126.32
27	e	604	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
27	j	604	CLA	CHD-C1D-ND	-2.43	121.39	124.80
35	b	613	II0	C04-C06-C08	-2.43	108.27	113.59
35	c	614	II0	C19-C13-C09	-2.43	119.62	124.16
27	A	821	CLA	CHB-C4A-NA	2.43	127.90	124.40
35	i	313	II0	C31-C33-C35	-2.43	119.71	126.36
29	k	319	LHG	O8-C23-C24	2.43	119.23	111.83
27	e	605	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
35	l	317	II0	C20-C14-C12	2.42	118.88	114.42
34	b	619	LMG	O8-C28-C29	2.42	119.23	111.83
35	b	615	II0	C18-C04-C17	-2.42	101.69	108.63
27	A	842	CLA	C3B-C4B-NB	-2.42	108.37	110.53
37	n	612	KC2	CHD-C1D-C2D	2.42	134.46	127.43
27	g	315	CLA	C1-C2-C3	-2.42	122.23	126.20
35	a	314	II0	C20-C14-C10	-2.42	119.63	124.16
35	b	612	II0	C41-C42-C40	-2.42	118.56	123.52
27	B	801	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	j	607	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	g	315	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
27	B	802	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	m	605	CLA	CAC-C3C-C4C	2.42	127.94	124.79
27	f	601	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	B	815	CLA	CHB-C4A-NA	2.42	127.89	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	O	204	IHT	C41-C40-C37	-2.42	118.57	123.52
27	A	813	CLA	CMB-C2B-C3B	2.42	132.23	126.55
37	d	310	KC2	CMB-C2B-C1B	2.42	128.98	124.73
27	A	812	CLA	CAC-C3C-C4C	2.42	127.93	124.79
30	B	848	WVN	C06-C13-C15	-2.42	119.33	122.64
37	k	310	KC2	CAA-CBA-CGA	-2.42	114.77	127.05
35	m	615	II0	C19-C13-C09	-2.42	119.64	124.16
27	l	309	CLA	C2D-C1D-ND	-2.41	107.74	110.13
30	B	844	WVN	C03-C04-C09	-2.41	108.02	112.07
27	f	606	CLA	C1-C2-C3	-2.41	122.24	126.20
27	n	610	CLA	CHA-C1A-NA	-2.41	120.92	126.39
27	A	810	CLA	CHB-C4A-NA	2.41	127.88	124.40
35	e	614	II0	C31-C33-C35	-2.41	119.75	126.36
27	a	306	CLA	O1D-CGD-CBD	2.41	129.28	124.52
27	l	304	CLA	C4-C3-C5	2.41	119.42	115.23
37	s	201	KC2	O2D-CGD-O1D	-2.41	119.15	123.85
30	L	205	WVN	C08-C01-C02	2.41	113.20	109.55
27	e	608	CLA	C2A-C1A-CHA	2.41	128.05	123.87
29	n	619	LHG	O8-C23-C24	2.41	119.19	111.83
27	A	817	CLA	C6-C7-C8	-2.41	107.95	115.97
27	a	306	CLA	C11-C10-C8	-2.41	107.95	115.97
27	c	605	CLA	CHB-C4A-NA	2.41	127.88	124.40
30	R	201	WVN	C20-C23-C25	-2.41	122.67	126.23
27	i	307	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
27	O	202	CLA	CHB-C4A-NA	2.41	127.88	124.40
27	A	822	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
27	e	606	CLA	CMB-C2B-C3B	2.41	132.22	126.55
27	e	607	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
35	O	203	II0	C42-C41-C39	-2.41	118.59	123.52
27	g	310	CLA	CHB-C4A-NA	2.41	127.87	124.40
36	g	319	IHT	C29-C31-C34	-2.41	116.22	123.20
27	m	608	CLA	CHB-C4A-NA	2.41	127.87	124.40
27	B	822	CLA	CGD-CBD-CAD	2.41	118.64	110.85
35	l	302	II0	C30-C32-C34	-2.41	116.23	123.20
36	g	319	IHT	C20-C15-C11	-2.41	119.66	124.16
27	K	102	CLA	C2A-C1A-CHA	2.41	128.04	123.87
27	g	308	CLA	CHC-C1C-C2C	-2.41	120.11	126.95
27	k	309	CLA	C3D-C2D-C1D	2.40	109.11	105.83
35	l	317	II0	C31-C33-C35	-2.40	119.77	126.36
27	l	305	CLA	C4-C3-C5	2.40	118.96	116.13
27	B	818	CLA	O2D-CGD-CBD	2.40	115.43	111.23
30	J	101	WVN	C30-C33-C34	-2.40	119.77	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	j	614	II0	C32-C30-C26	-2.40	119.89	126.61
27	A	814	CLA	CMB-C2B-C3B	2.40	132.20	126.55
27	d	305	CLA	C1C-C2C-C3C	-2.40	104.45	106.98
35	h	311	II0	O01-C07-C05	-2.40	104.83	109.75
27	j	605	CLA	CHA-C1A-NA	-2.40	120.95	126.39
30	B	843	WVN	C29-C26-C22	-2.40	123.91	127.28
27	B	836	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
27	i	308	CLA	C4D-C3D-CAD	-2.40	105.50	108.11
27	d	305	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
27	B	822	CLA	CAC-C3C-C4C	2.40	127.91	124.79
27	B	811	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
27	B	829	CLA	O2D-CGD-CBD	2.40	115.43	111.23
37	d	310	KC2	CHD-C1D-C2D	2.40	134.39	127.43
27	b	606	CLA	C1-C2-C3	-2.40	122.27	126.20
27	b	609	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
35	c	614	II0	C32-C30-C26	-2.40	119.90	126.61
27	h	301	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
37	k	311	KC2	CAB-C3B-C2B	2.40	136.23	128.43
27	A	808	CLA	CAA-C2A-C1A	2.40	119.83	111.97
27	A	806	CLA	C11-C10-C8	-2.40	108.00	115.97
37	i	317	KC2	CHC-C1C-C2C	2.40	128.81	125.03
27	A	831	CLA	C2A-C1A-CHA	2.40	128.03	123.87
27	n	607	CLA	C4A-NA-C1A	2.40	107.77	106.68
30	B	847	WVN	C06-C13-C15	-2.40	119.36	122.64
27	a	303	CLA	CHB-C4A-NA	2.40	127.86	124.40
30	B	848	WVN	C33-C34-C37	-2.40	115.24	119.01
27	j	604	CLA	C2A-C3A-C4A	2.40	105.74	101.87
27	A	824	CLA	CMB-C2B-C3B	2.39	132.18	126.55
27	A	816	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
37	d	310	KC2	CAB-C3B-C2B	2.39	136.21	128.43
27	n	609	CLA	CAA-CBA-CGA	-2.39	106.41	113.21
27	f	609	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
27	s	206	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	B	837	CLA	CAC-C3C-C4C	2.39	127.90	124.79
27	A	836	CLA	C2A-C1A-CHA	2.39	128.01	123.87
27	O	206	CLA	C3B-C4B-NB	-2.39	108.40	110.53
27	e	610	CLA	CAA-CBA-CGA	-2.39	106.42	113.21
27	B	820	CLA	CMB-C2B-C3B	2.39	132.17	126.55
29	A	844	LHG	O8-C23-O10	-2.39	117.65	123.63
27	A	808	CLA	C2A-C1A-CHA	2.39	128.01	123.87
27	j	608	CLA	CAC-C3C-C4C	2.39	127.90	124.79
27	A	822	CLA	CHB-C4A-NA	2.39	127.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	j	612	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
35	a	315	II0	C19-C13-C09	-2.39	119.70	124.16
30	O	201	WVN	C18-C06-C13	2.39	113.98	110.24
27	j	602	CLA	CBC-CAC-C3C	-2.39	105.95	112.42
35	h	312	II0	C29-C31-C33	-2.39	116.29	123.20
35	a	314	II0	C12-C14-C10	-2.38	115.54	120.50
27	g	322	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
27	B	824	CLA	CHB-C4A-NA	2.38	127.84	124.40
35	b	613	II0	C30-C32-C34	-2.38	116.30	123.20
35	k	316	II0	C30-C32-C34	-2.38	116.30	123.20
27	k	306	CLA	CHB-C1B-NB	2.38	127.62	124.05
27	f	608	CLA	CHB-C4A-NA	2.38	127.84	124.40
35	l	317	II0	C32-C34-C36	-2.38	119.84	126.36
27	s	202	CLA	O2D-CGD-CBD	2.38	115.39	111.23
27	d	301	CLA	O2A-CGA-CBA	2.38	119.09	111.83
27	B	828	CLA	C2A-C1A-CHA	2.38	128.00	123.87
27	K	101	CLA	C2A-C1A-CHA	2.38	128.00	123.87
35	c	615	II0	C32-C30-C26	-2.38	119.96	126.61
35	h	310	II0	C34-C36-C40	2.38	122.75	119.01
35	j	613	II0	C33-C35-C39	2.38	122.75	119.01
27	B	806	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
27	i	302	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
27	c	606	CLA	CHB-C1B-NB	2.38	127.61	124.05
27	O	202	CLA	CBC-CAC-C3C	2.38	118.86	112.42
35	g	318	II0	C41-C42-C40	-2.38	118.66	123.52
35	k	318	II0	C32-C34-C36	-2.37	119.85	126.36
27	j	611	CLA	CMB-C2B-C1B	-2.37	121.80	125.42
27	k	304	CLA	O2A-CGA-O1A	-2.37	117.23	123.33
27	B	802	CLA	O1D-CGD-CBD	2.37	129.20	124.52
35	h	312	II0	C30-C32-C34	-2.37	116.32	123.20
27	m	611	CLA	CMB-C2B-C3B	2.37	132.13	126.55
27	n	606	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
27	j	604	CLA	CMC-C2C-C1C	-2.37	121.33	125.03
30	s	205	WVN	C24-C22-C19	2.37	121.71	118.09
36	f	617	IHT	C19-C10-C09	2.37	118.65	113.60
27	b	603	CLA	C2A-C1A-CHA	2.37	127.98	123.87
27	i	308	CLA	C4D-CHA-C1A	2.37	124.07	121.24
35	m	613	II0	C30-C32-C34	-2.37	116.34	123.20
27	a	311	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
27	k	313	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
30	M	101	WVN	C08-C01-C07	-2.37	104.42	107.87
36	R	204	IHT	C40-C41-C38	-2.37	118.67	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	313	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
36	b	614	IHT	C20-C15-C12	2.37	118.78	114.42
36	a	317	IHT	C20-C15-C11	-2.37	119.73	124.16
27	f	612	CLA	CAA-C2A-C1A	2.37	119.73	111.97
35	k	315	II0	C32-C34-C36	-2.37	119.87	126.36
37	i	310	KC2	CMB-C2B-C1B	2.37	128.89	124.73
27	j	605	CLA	O2A-CGA-O1A	-2.37	117.25	123.33
36	c	620	IHT	C39-C35-C34	2.37	121.70	118.09
30	M	101	WVN	C35-C32-C31	2.36	121.70	118.09
27	f	603	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	B	825	CLA	C2D-C1D-ND	-2.36	107.79	110.13
27	n	604	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
27	m	607	CLA	C1-C2-C3	-2.36	122.32	126.20
35	l	317	II0	C19-C13-C11	2.36	118.77	114.42
27	B	816	CLA	C1-C2-C3	-2.36	122.33	126.20
30	A	848	WVN	C23-C25-C28	2.36	122.73	119.01
35	d	313	II0	C19-C13-C09	-2.36	119.74	124.16
30	F	205	WVN	C02-C11-C19	-2.36	120.90	124.58
27	k	313	CLA	CHC-C4B-NB	2.36	127.59	124.05
27	A	827	CLA	CHB-C1B-C2B	-2.36	120.57	127.43
27	d	307	CLA	CMA-C3A-C2A	-2.36	110.82	116.23
30	B	843	WVN	C21-C15-C13	-2.36	121.91	124.48
27	A	827	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
27	b	609	CLA	C1-C2-C3	-2.36	122.33	126.20
27	n	604	CLA	CMB-C2B-C3B	2.36	132.09	126.55
27	h	306	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
27	A	811	CLA	C4-C3-C5	2.36	119.32	115.23
27	h	307	CLA	CHB-C4A-NA	2.36	127.80	124.40
35	l	315	II0	C41-C39-C35	-2.36	123.97	127.28
27	A	831	CLA	C1-C2-C3	-2.35	122.34	126.20
27	j	602	CLA	C3B-C4B-NB	-2.35	108.43	110.53
27	j	612	CLA	C3B-C4B-NB	-2.35	108.43	110.53
27	k	308	CLA	CHB-C4A-NA	2.35	127.80	124.40
27	j	612	CLA	CHC-C4B-NB	2.35	127.58	124.05
35	h	311	II0	C22-C24-C26	-2.35	168.23	176.23
38	i	301	LMU	C2'-C3'-C4'	2.35	115.02	109.68
27	f	603	CLA	CAC-C3C-C4C	2.35	127.85	124.79
27	b	610	CLA	CHB-C4A-NA	2.35	127.80	124.40
35	a	314	II0	C29-C31-C33	-2.35	116.39	123.20
35	c	615	II0	C27-C25-C29	-2.35	119.61	124.18
27	B	807	CLA	CMB-C2B-C3B	2.35	132.08	126.55
30	l	316	WVN	C23-C20-C13	-2.35	120.72	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	819	CLA	CAA-CBA-CGA	-2.35	106.22	112.49
27	B	824	CLA	CHB-C1B-NB	2.35	127.58	124.05
27	A	826	CLA	O2D-CGD-CBD	2.35	115.34	111.23
27	n	606	CLA	O2D-CGD-CBD	2.35	115.34	111.23
27	A	826	CLA	CAC-C3C-C2C	2.35	131.88	127.56
27	A	855	CLA	CHB-C4A-NA	2.35	127.79	124.40
30	B	848	WVN	C21-C15-C14	2.35	118.61	113.60
36	c	620	IHT	C32-C33-C37	-2.35	115.31	119.01
30	B	845	WVN	C23-C20-C13	-2.35	120.72	127.00
30	L	205	WVN	C20-C23-C25	-2.35	122.76	126.23
35	a	315	II0	C16-C03-C09	-2.35	106.31	110.52
30	L	201	WVN	C02-C05-C09	-2.35	118.58	121.47
30	A	847	WVN	C06-C13-C15	-2.35	119.43	122.64
27	B	809	CLA	C3B-C4B-NB	-2.35	108.43	110.53
27	J	105	CLA	CBA-CAA-C2A	-2.35	106.81	113.79
35	j	614	II0	C22-C24-C26	-2.35	168.25	176.23
29	l	318	LHG	C5-O7-C7	-2.35	112.18	117.80
27	A	802	CLA	CAA-CBA-CGA	-2.35	106.54	113.21
27	f	602	CLA	CMA-C3A-C2A	-2.35	104.91	113.98
27	i	306	CLA	CAA-C2A-C1A	-2.35	104.29	111.97
27	g	304	CLA	CHB-C4A-NA	2.35	127.78	124.40
27	A	812	CLA	C2A-C1A-CHA	2.35	127.94	123.87
27	b	604	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	B	815	CLA	C1-O2A-CGA	2.34	122.33	116.65
27	s	202	CLA	CHB-C1B-NB	2.34	127.56	124.05
27	m	611	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
27	A	809	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
27	A	840	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
35	c	613	II0	C42-C41-C39	-2.34	118.73	123.52
27	n	604	CLA	CGD-CBD-CAD	-2.34	103.26	110.85
27	m	603	CLA	CMB-C2B-C3B	2.34	132.06	126.55
35	g	320	II0	C31-C33-C35	-2.34	119.94	126.36
27	A	832	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
27	B	818	CLA	CHB-C1B-NB	2.34	127.56	124.05
36	O	204	IHT	C03-C05-C08	2.34	118.73	113.59
37	n	612	KC2	O2D-CGD-O1D	-2.34	119.29	123.85
27	B	839	CLA	CHA-C1A-NA	-2.34	121.09	126.39
30	i	315	WVN	C14-C15-C13	-2.34	119.54	122.70
27	B	809	CLA	CHB-C1B-NB	2.34	127.56	124.05
27	m	606	CLA	C3A-C2A-C1A	2.34	104.84	101.34
27	d	303	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
27	A	836	CLA	O2D-CGD-CBD	2.34	115.32	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	s	201	KC2	C2D-C1D-ND	-2.34	107.90	110.33
27	i	308	CLA	CHB-C1B-NB	2.34	127.56	124.05
27	j	604	CLA	CMC-C2C-C3C	2.34	132.47	126.15
27	s	208	CLA	CHB-C1B-NB	2.34	127.55	124.05
27	A	816	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	m	601	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	k	308	CLA	CHA-C1A-NA	-2.34	121.10	126.39
27	A	809	CLA	C3B-C4B-NB	-2.34	108.44	110.53
27	B	849	CLA	CMC-C2C-C3C	2.33	132.46	126.15
36	O	204	IHT	O01-C08-C05	-2.33	104.97	109.75
35	h	311	II0	C31-C29-C25	-2.33	120.08	126.61
35	j	614	II0	C15-C03-C09	-2.33	106.34	110.52
34	J	106	LMG	O8-C28-O10	-2.33	117.79	123.63
29	f	619	LHG	C5-O7-C7	-2.33	112.21	117.80
37	k	310	KC2	CAB-C3B-C2B	2.33	136.01	128.43
30	B	844	WVN	C07-C01-C02	2.33	113.08	109.55
30	M	101	WVN	C26-C29-C31	-2.33	116.45	123.20
27	A	828	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
27	B	826	CLA	CHD-C1D-ND	-2.33	121.52	124.80
27	J	105	CLA	C1-C2-C3	-2.33	122.38	126.20
27	B	831	CLA	CHB-C4A-NA	2.33	127.76	124.40
27	B	803	CLA	C11-C12-C13	-2.33	108.22	115.97
27	A	812	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
27	B	829	CLA	CMB-C2B-C3B	2.33	132.03	126.55
37	g	313	KC2	CBC-CAC-C3C	-2.33	115.90	127.53
27	s	202	CLA	CHD-C1D-C2D	2.33	130.32	125.49
27	a	305	CLA	C3B-C4B-NB	-2.33	108.45	110.53
27	h	304	CLA	CAA-CBA-CGA	-2.33	106.61	113.21
28	B	841	PQN	C2M-C2-C3	-2.33	120.63	124.45
27	l	312	CLA	CHD-C1D-ND	-2.33	121.53	124.80
35	c	615	II0	C30-C32-C34	-2.33	116.46	123.20
27	g	304	CLA	C3B-C4B-NB	-2.32	108.45	110.53
27	g	302	CLA	C3A-C2A-C1A	2.32	104.82	101.34
27	e	610	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
38	i	301	LMU	O5'-C5'-C4'	2.32	114.53	109.72
27	j	609	CLA	CHB-C4A-NA	2.32	127.75	124.40
27	n	613	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
27	B	829	CLA	C11-C10-C8	-2.32	108.25	115.97
30	A	849	WVN	C06-C13-C15	-2.32	119.46	122.64
27	e	601	CLA	CHA-C1A-NA	-2.32	121.13	126.39
27	k	305	CLA	C3A-C2A-C1A	2.32	104.82	101.34
27	f	601	CLA	C3B-C4B-NB	-2.32	108.46	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	607	CLA	C1-C2-C3	-2.32	122.39	126.20
27	B	829	CLA	CMA-C3A-C2A	-2.32	105.01	113.98
35	f	616	II0	C19-C13-C11	2.32	118.69	114.42
27	i	308	CLA	CMA-C3A-C4A	2.32	118.01	111.77
27	c	611	CLA	O2A-CGA-O1A	-2.32	117.37	123.33
35	l	315	II0	C30-C32-C34	-2.32	116.48	123.20
29	k	319	LHG	O4-P-O5	2.32	123.22	112.44
27	B	835	CLA	C5-C3-C2	-2.32	115.97	121.17
27	j	608	CLA	CHB-C4A-NA	2.32	127.74	124.40
27	a	313	CLA	O1D-CGD-CBD	2.32	129.09	124.52
27	B	822	CLA	C1-C2-C3	-2.32	122.40	126.20
27	B	829	CLA	C3B-C4B-NB	-2.32	108.46	110.53
30	L	201	WVN	C30-C33-C34	-2.32	120.01	126.36
36	k	317	IHT	C22-C18-C07	-2.32	120.81	127.00
27	m	612	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
29	e	617	LHG	O7-C7-O9	-2.32	118.29	123.70
30	R	201	WVN	C21-C15-C14	-2.32	108.66	113.60
27	R	203	CLA	C2A-C1A-CHA	2.32	127.89	123.87
27	g	315	CLA	C3B-C4B-NB	-2.32	108.46	110.53
37	g	312	KC2	O2D-CGD-O1D	-2.32	119.34	123.85
27	B	827	CLA	CHD-C1D-ND	-2.32	121.54	124.80
27	f	605	CLA	CHA-C1A-NA	-2.32	121.15	126.39
31	A	851	LMT	O1B-C1B-C2B	2.31	113.78	108.09
27	g	304	CLA	C2A-C1A-CHA	2.31	127.88	123.87
35	a	315	II0	C20-C14-C10	-2.31	119.83	124.16
30	h	309	WVN	C11-C19-C22	-2.31	121.35	126.32
37	k	312	KC2	O2D-CGD-CBD	2.31	115.27	111.23
35	d	313	II0	C32-C30-C26	-2.31	120.14	126.61
27	k	309	CLA	CAA-CBA-CGA	-2.31	106.64	113.21
27	B	834	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	i	305	CLA	CHB-C1B-C2B	-2.31	120.72	127.43
27	B	839	CLA	C2A-C1A-CHA	2.31	127.88	123.87
27	k	313	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	B	801	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
27	A	809	CLA	CMB-C2B-C3B	2.31	131.98	126.55
27	A	827	CLA	CHB-C1B-NB	2.31	127.51	124.05
27	k	304	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
27	A	801	CLA	CHB-C4A-NA	2.31	127.73	124.40
30	e	615	WVN	C23-C20-C13	-2.31	120.83	127.00
35	k	318	II0	C32-C30-C26	-2.31	120.16	126.61
27	k	301	CLA	CMB-C2B-C3B	2.31	131.98	126.55
27	c	607	CLA	O1D-CGD-CBD	2.31	129.07	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	e	604	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
27	m	605	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
27	A	837	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
27	e	603	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
27	b	607	CLA	CHD-C4C-NC	2.31	127.81	124.23
27	e	605	CLA	CBA-CAA-C2A	-2.31	106.93	113.79
30	R	202	WVN	C40-C39-C36	-2.31	118.80	123.52
35	k	318	II0	C30-C32-C34	-2.31	116.52	123.20
27	B	811	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
37	s	204	KC2	CAA-C2A-C1A	2.31	134.74	124.64
27	A	834	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
35	m	613	II0	C38-C36-C34	2.30	121.61	118.09
35	h	311	II0	C19-C13-C09	-2.30	119.85	124.16
27	b	602	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
27	A	830	CLA	C3B-C4B-NB	-2.30	108.47	110.53
27	c	607	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
35	a	314	II0	C42-C41-C39	-2.30	118.81	123.52
37	e	609	KC2	CAA-CBA-CGA	-2.30	115.34	127.05
27	B	810	CLA	C14-C13-C12	-2.30	103.07	111.27
27	A	825	CLA	CMD-C2D-C1D	-2.30	120.68	124.73
35	b	612	II0	C06-C04-C10	2.30	114.02	109.49
27	B	840	CLA	CHA-C1A-NA	-2.30	121.18	126.39
35	k	314	II0	C38-C36-C34	2.30	121.60	118.09
27	m	611	CLA	CMC-C2C-C3C	2.30	132.37	126.15
35	d	312	II0	C11-C13-C09	-2.30	115.71	120.50
36	g	319	IHT	C19-C10-C09	2.30	118.50	113.60
27	B	828	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
35	l	313	II0	C20-C14-C12	2.30	118.65	114.42
27	A	839	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
35	k	316	II0	C18-C04-C10	-2.30	106.40	110.52
27	f	610	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
27	s	208	CLA	C2B-C1B-NB	2.30	112.71	110.33
27	A	828	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
35	c	613	II0	C17-C04-C10	-2.30	106.40	110.52
37	k	311	KC2	C2B-C1B-NB	2.30	112.40	110.13
27	B	828	CLA	CHB-C4A-NA	2.30	127.71	124.40
27	B	839	CLA	C1-O2A-CGA	2.30	122.21	116.65
27	n	606	CLA	C1-C2-C3	-2.30	122.44	126.20
27	e	602	CLA	C1-C2-C3	-2.30	123.05	126.76
27	A	826	CLA	C2A-C1A-CHA	2.30	127.85	123.87
27	B	829	CLA	C11-C12-C13	-2.29	108.34	115.97
27	c	608	CLA	C1-C2-C3	-2.29	122.44	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	m	603	CLA	CAA-C2A-C1A	-2.29	104.45	111.97
30	B	845	WVN	C12-C14-C15	-2.29	109.97	114.06
27	b	606	CLA	C11-C12-C13	-2.29	108.34	115.97
27	L	204	CLA	CAC-C3C-C4C	2.29	127.77	124.79
30	s	205	WVN	C30-C33-C34	-2.29	120.08	126.36
34	s	210	LMG	C7-O1-C1	-2.29	108.88	113.80
27	f	608	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
27	n	608	CLA	C3B-C4B-NB	-2.29	108.48	110.53
30	J	101	WVN	C02-C05-C09	-2.29	118.65	121.47
36	n	617	IHT	C41-C40-C37	-2.29	118.83	123.52
27	A	834	CLA	C3A-C2A-C1A	2.29	104.77	101.34
37	c	610	KC2	C1D-CHD-C4C	-2.29	120.86	126.25
35	c	615	II0	C38-C36-C34	2.29	121.59	118.09
37	i	317	KC2	CMA-C3A-C4A	2.29	128.61	125.03
30	F	204	WVN	C12-C14-C15	-2.29	109.97	114.06
27	f	613	CLA	C7-C6-C5	-2.29	107.16	113.26
27	e	604	CLA	CMB-C2B-C3B	2.29	131.93	126.55
29	i	316	LHG	O7-C7-O9	-2.29	118.36	123.70
35	b	613	II0	C06-C04-C10	2.29	114.00	109.49
35	f	614	II0	C06-C04-C10	2.29	114.00	109.49
27	A	841	CLA	CHB-C4A-NA	2.29	127.70	124.40
27	c	611	CLA	CMB-C2B-C3B	2.29	131.93	126.55
30	F	205	WVN	C31-C32-C36	-2.29	115.41	119.01
27	k	306	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
35	k	318	II0	C42-C41-C39	-2.29	118.84	123.52
27	F	202	CLA	CHA-C1A-NA	-2.29	121.22	126.39
27	m	609	CLA	C3B-C4B-NB	-2.29	108.49	110.53
27	j	605	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
27	k	313	CLA	CHB-C1B-NB	2.28	127.48	124.05
35	f	615	II0	C42-C41-C39	-2.28	118.84	123.52
30	R	201	WVN	C26-C29-C31	-2.28	116.58	123.20
27	s	208	CLA	CHC-C1C-NC	2.28	127.75	124.31
35	m	615	II0	C29-C31-C33	-2.28	116.59	123.20
27	d	302	CLA	C3B-C4B-NB	-2.28	108.49	110.53
27	g	310	CLA	C3B-C4B-NB	-2.28	108.49	110.53
27	A	842	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
27	B	811	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
27	d	303	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
27	m	603	CLA	CAC-C3C-C4C	2.28	127.76	124.79
27	l	312	CLA	CHB-C1B-NB	2.28	127.47	124.05
30	B	848	WVN	C19-C22-C26	-2.28	115.42	119.01
27	c	609	CLA	C3B-C4B-NB	-2.28	108.50	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	852	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
36	c	620	IHT	C04-C02-C07	2.28	113.75	110.44
30	M	101	WVN	C28-C30-C33	-2.28	116.60	123.20
30	B	846	WVN	C03-C04-C09	-2.28	108.24	112.07
27	m	607	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
27	B	818	CLA	C2D-C1D-ND	-2.28	107.87	110.13
27	k	308	CLA	C2A-C1A-CHA	2.28	127.82	123.87
27	b	602	CLA	O2A-CGA-CBA	2.28	118.78	111.83
27	h	302	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
35	h	312	II0	C06-C04-C10	2.28	113.98	109.49
27	a	308	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
37	s	204	KC2	C1D-CHD-C4C	-2.28	120.89	126.25
27	a	307	CLA	CHD-C4C-C3C	2.28	128.09	124.77
35	c	617	II0	C15-C03-C09	-2.28	106.44	110.52
27	B	812	CLA	C3B-C4B-NB	-2.28	108.50	110.53
27	c	609	CLA	O2D-CGD-CBD	2.28	115.21	111.23
35	n	616	II0	C32-C30-C26	-2.28	120.25	126.61
36	k	317	IHT	C25-C23-C22	2.28	121.56	118.09
27	k	305	CLA	CMD-C2D-C1D	-2.28	120.72	124.73
30	J	101	WVN	C07-C01-C02	2.27	112.99	109.55
27	m	605	CLA	CMA-C3A-C4A	2.27	117.89	111.77
35	e	612	II0	C38-C36-C34	2.27	121.56	118.09
35	J	104	II0	O01-C07-C11	-2.27	104.59	109.71
35	b	612	II0	C31-C33-C35	-2.27	120.13	126.36
27	A	809	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
36	a	317	IHT	C20-C15-C12	2.27	118.60	114.42
27	A	827	CLA	C1-C2-C3	-2.27	122.48	126.20
37	k	311	KC2	C2A-C1A-NA	2.27	112.98	109.34
27	l	303	CLA	CAA-CBA-CGA	-2.27	106.76	113.21
27	A	816	CLA	C1-C2-C3	2.27	129.92	126.20
29	j	617	LHG	O7-C7-O9	-2.27	118.40	123.70
35	c	615	II0	C37-C35-C33	2.27	121.55	118.09
27	A	816	CLA	O2D-CGD-CBD	2.27	115.19	111.23
30	A	846	WVN	C29-C26-C22	-2.27	124.10	127.28
27	g	309	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
27	B	810	CLA	C3A-C2A-C1A	2.27	104.73	101.34
27	f	609	CLA	CHB-C4A-NA	2.27	127.67	124.40
37	k	311	KC2	O1D-CGD-CBD	-2.26	120.05	124.52
27	j	607	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
36	b	614	IHT	C18-C22-C23	2.26	129.58	126.23
27	m	607	CLA	CHA-C1A-NA	-2.26	121.27	126.39
27	A	802	CLA	O2A-CGA-CBA	2.26	118.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	615	II0	C31-C33-C35	-2.26	120.16	126.36
30	B	844	WVN	C39-C40-C37	-2.26	118.89	123.52
27	B	825	CLA	CHB-C4A-NA	2.26	127.66	124.40
27	n	613	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
27	A	804	CLA	CBA-CAA-C2A	2.26	120.52	113.79
30	i	315	WVN	C31-C32-C36	2.26	122.56	119.01
27	A	806	CLA	O2D-CGD-CBD	2.26	115.18	111.23
30	B	844	WVN	C21-C15-C14	2.26	118.41	113.60
29	J	107	LHG	C5-O7-C7	-2.26	112.39	117.80
27	A	839	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
27	A	818	CLA	O2D-CGD-CBD	2.26	115.18	111.23
30	K	103	WVN	C07-C01-C02	2.26	112.97	109.55
27	g	310	CLA	CBA-CAA-C2A	2.26	120.51	113.79
35	g	316	II0	C06-C04-C10	2.26	113.94	109.49
27	l	306	CLA	C12-C11-C10	-2.26	103.17	113.28
27	B	816	CLA	CHB-C1B-NB	2.26	127.43	124.05
30	M	101	WVN	C40-C39-C36	-2.26	118.90	123.52
35	n	616	II0	C05-C03-C09	2.26	113.93	109.49
27	g	303	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
27	k	309	CLA	CMD-C2D-C3D	-2.26	122.52	127.69
27	n	607	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
30	A	846	WVN	C38-C34-C37	-2.25	119.16	122.82
27	d	307	CLA	C2A-C3A-C4A	2.25	104.23	101.59
27	h	305	CLA	C3B-C4B-NB	-2.25	108.52	110.53
27	A	816	CLA	CAA-C2A-C1A	2.25	119.36	111.97
27	A	855	CLA	C2A-C1A-CHA	2.25	127.78	123.87
27	c	612	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
27	n	609	CLA	C1-C2-C3	-2.25	122.51	126.20
27	b	611	CLA	CAC-C3C-C4C	2.25	127.72	124.79
27	R	203	CLA	CHB-C4A-NA	2.25	127.65	124.40
36	c	620	IHT	C18-C07-C10	-2.25	116.37	121.56
35	a	315	II0	C42-C41-C39	-2.25	118.91	123.52
29	i	316	LHG	O4-P-O5	2.25	122.91	112.44
27	f	602	CLA	C3B-C4B-NB	-2.25	108.52	110.53
27	g	309	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
27	B	819	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
27	b	607	CLA	CMC-C2C-C1C	-2.25	121.52	125.03
27	f	607	CLA	C4-C3-C2	-2.25	117.85	123.63
27	B	836	CLA	CHB-C1B-C2B	-2.25	120.90	127.43
27	B	834	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
37	s	201	KC2	CAB-C3B-C2B	2.25	135.74	128.43
37	m	610	KC2	CAA-CBA-CGA	-2.25	115.62	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	e	614	II0	C38-C36-C34	2.25	121.52	118.09
27	d	304	CLA	CAA-C2A-C1A	-2.25	104.62	111.97
27	B	839	CLA	O1D-CGD-CBD	2.25	128.95	124.52
27	A	855	CLA	CMD-C2D-C3D	2.24	132.84	127.69
27	A	855	CLA	CMD-C2D-C1D	-2.24	120.78	124.73
27	k	302	CLA	C3A-C2A-C1A	2.24	104.70	101.34
27	s	203	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
27	A	833	CLA	CHC-C4B-NB	2.24	127.42	124.05
27	l	306	CLA	O1D-CGD-CBD	2.24	128.94	124.52
27	j	606	CLA	CBB-CAB-C3B	2.24	138.73	127.53
27	k	303	CLA	C1-C2-C3	-2.24	122.52	126.20
27	f	602	CLA	C4-C3-C5	2.24	119.12	115.23
27	k	313	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
27	m	604	CLA	C11-C12-C13	-2.24	108.51	115.97
27	b	606	CLA	C4-C3-C2	-2.24	117.87	123.63
35	g	318	II0	C18-C04-C17	-2.24	102.22	108.63
27	e	611	CLA	CBA-CAA-C2A	-2.24	107.13	113.79
27	j	609	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
27	k	304	CLA	C2C-C1C-NC	2.24	112.33	109.98
27	B	837	CLA	C1-O2A-CGA	2.24	122.07	116.65
34	c	619	LMG	O7-C8-C9	2.24	116.38	108.34
37	c	610	KC2	CAB-C3B-C4B	-2.24	119.47	124.82
36	R	204	IHT	C20-C15-C11	-2.24	119.97	124.16
29	n	619	LHG	C6-C5-C4	-2.24	106.57	111.78
27	i	308	CLA	CHB-C1B-C2B	-2.24	120.93	127.43
27	A	855	CLA	CAA-C2A-C1A	2.24	119.31	111.97
30	J	102	WVN	C26-C29-C31	-2.24	116.72	123.20
27	i	308	CLA	C2A-C1A-CHA	2.24	127.75	123.87
27	B	822	CLA	C7-C6-C5	-2.24	107.30	113.26
27	l	307	CLA	C2B-C1B-NB	2.24	112.64	110.33
30	O	201	WVN	C23-C25-C28	-2.24	115.49	119.01
35	f	618	II0	C20-C14-C10	-2.24	119.98	124.16
27	A	829	CLA	C4B-C3B-C2B	-2.23	104.52	107.30
27	A	833	CLA	CHD-C1D-ND	-2.23	121.66	124.80
27	e	607	CLA	CAA-CBA-CGA	-2.23	106.86	113.21
35	g	317	II0	C32-C30-C26	-2.23	120.37	126.61
35	k	315	II0	C31-C33-C35	-2.23	120.24	126.36
37	k	312	KC2	CAA-CBA-CGA	-2.23	115.70	127.05
27	m	602	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
35	a	314	II0	C16-C03-C09	-2.23	106.52	110.52
27	A	841	CLA	CHB-C1B-NB	2.23	127.40	124.05
27	f	606	CLA	CBA-CAA-C2A	-2.23	107.15	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	819	CLA	CHA-C1A-NA	-2.23	121.34	126.39
27	n	610	CLA	CHB-C4A-NA	2.23	127.62	124.40
36	O	204	IHT	C20-C15-C12	2.23	118.52	114.42
27	h	306	CLA	C16-C15-C13	-2.23	108.55	115.97
35	f	618	II0	C28-C26-C30	-2.23	119.85	124.18
35	i	314	II0	C30-C32-C34	-2.23	116.74	123.20
27	A	806	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
27	i	309	CLA	CMB-C2B-C3B	2.23	131.80	126.55
27	k	304	CLA	O1A-CGA-CBA	2.23	130.16	123.09
27	l	312	CLA	C7-C6-C5	-2.23	107.32	113.26
27	A	818	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
37	k	312	KC2	CHD-C1D-C2D	2.23	133.90	127.43
27	B	801	CLA	C3B-C4B-NB	-2.23	108.54	110.53
27	b	602	CLA	C3B-C4B-NB	-2.23	108.54	110.53
35	f	615	II0	C20-C14-C12	2.23	118.52	114.42
27	e	607	CLA	C4-C3-C5	2.23	119.09	115.23
27	l	309	CLA	O1D-CGD-CBD	2.23	128.91	124.52
27	e	601	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
27	K	101	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
28	A	843	PQN	C2M-C2-C3	-2.23	120.79	124.45
27	L	202	CLA	CAA-CBA-CGA	-2.23	106.89	113.21
27	j	601	CLA	C3B-C4B-NB	-2.22	108.54	110.53
27	R	203	CLA	C3B-C4B-NB	-2.22	108.55	110.53
35	e	616	II0	C31-C33-C35	-2.22	120.27	126.36
27	i	311	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
30	F	204	WVN	C40-C39-C36	2.22	128.07	123.52
27	i	309	CLA	CAC-C3C-C2C	-2.22	123.48	127.56
27	O	206	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
27	c	601	CLA	C1-C2-C3	-2.22	122.56	126.20
27	m	604	CLA	C1-C2-C3	-2.22	122.56	126.20
30	h	309	WVN	C08-C01-C02	-2.22	106.18	109.55
30	B	844	WVN	C20-C13-C15	-2.22	116.44	121.56
27	A	817	CLA	CMB-C2B-C3B	2.22	131.77	126.55
36	b	614	IHT	C36-C33-C37	-2.22	119.22	122.82
27	j	601	CLA	O2D-CGD-CBD	2.22	115.11	111.23
35	i	313	II0	C41-C42-C40	-2.22	118.98	123.52
35	d	313	II0	C28-C26-C30	-2.22	119.87	124.18
27	e	603	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
27	a	303	CLA	C2D-C1D-ND	-2.22	107.93	110.13
27	A	829	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
27	n	603	CLA	C3A-C2A-C1A	2.22	104.66	101.34
27	g	304	CLA	CHB-C1B-NB	2.22	127.38	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	811	CLA	CMB-C2B-C3B	2.22	131.77	126.55
35	i	318	II0	C41-C42-C40	-2.22	118.98	123.52
35	d	312	II0	C31-C33-C35	-2.22	120.28	126.36
37	i	317	KC2	CAA-CBA-CGA	-2.22	115.77	127.05
27	s	208	CLA	C2A-C1A-CHA	2.22	127.72	123.87
35	k	318	II0	C05-C03-C09	2.22	113.86	109.49
27	a	303	CLA	C3B-C4B-NB	-2.22	108.55	110.53
36	f	617	IHT	C02-C07-C18	2.22	121.66	115.65
27	l	307	CLA	CAA-C2A-C1A	2.22	119.24	111.97
30	B	844	WVN	C35-C32-C31	2.22	121.47	118.09
30	h	309	WVN	C06-C13-C20	2.22	121.66	115.65
37	k	312	KC2	CAB-C3B-C4B	-2.22	119.53	124.82
27	B	827	CLA	CHB-C1B-NB	2.22	127.37	124.05
27	h	308	CLA	CBA-CAA-C2A	2.21	120.38	113.79
27	l	309	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
27	B	830	CLA	C2A-C1A-CHA	2.21	127.71	123.87
27	a	303	CLA	O2D-CGD-CBD	2.21	115.10	111.23
30	I	101	WVN	C23-C25-C28	-2.21	115.53	119.01
30	L	201	WVN	C40-C39-C36	-2.21	118.99	123.52
27	B	834	CLA	CHA-C1A-NA	-2.21	121.38	126.39
29	A	845	LHG	C9-C8-C7	-2.21	105.59	113.69
35	d	312	II0	C27-C25-C29	-2.21	119.89	124.18
37	k	311	KC2	O2D-CGD-CBD	2.21	115.10	111.23
27	A	815	CLA	CHB-C4A-NA	2.21	127.59	124.40
30	L	205	WVN	C01-C02-C11	-2.21	110.28	112.83
36	m	616	IHT	C20-C15-C11	-2.21	120.03	124.16
28	B	841	PQN	C11-C3-C2	-2.21	121.10	124.89
27	j	603	CLA	C2A-C1A-CHA	2.21	127.70	123.87
27	j	602	CLA	CMC-C2C-C1C	2.21	128.49	125.03
27	i	312	CLA	C2A-C1A-CHA	2.21	127.70	123.87
27	F	201	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
27	L	204	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
27	h	301	CLA	CHB-C4A-NA	2.21	127.59	124.40
27	A	822	CLA	O2D-CGD-CBD	2.21	115.09	111.23
27	s	206	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
27	f	613	CLA	C2A-C1A-CHA	2.21	127.70	123.87
27	L	204	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
27	s	208	CLA	O1D-CGD-CBD	2.21	128.87	124.52
37	d	309	KC2	CHD-C1D-C2D	2.21	133.83	127.43
27	c	607	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
27	B	825	CLA	C1-C2-C3	-2.21	122.58	126.20
27	B	849	CLA	C1-C2-C3	-2.21	122.58	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	831	CLA	CHB-C1B-NB	2.21	127.36	124.05
30	s	207	WVN	C08-C01-C07	-2.21	104.66	107.87
27	A	824	CLA	CAC-C3C-C4C	2.21	127.66	124.79
27	k	302	CLA	CHB-C1B-C2B	-2.21	121.02	127.43
27	e	604	CLA	C1-C2-C3	-2.21	122.58	126.20
27	a	311	CLA	C2A-C1A-CHA	2.21	127.69	123.87
37	m	610	KC2	CHD-C1D-C2D	2.20	133.82	127.43
35	j	614	II0	C31-C33-C35	-2.20	120.32	126.36
27	B	816	CLA	C2C-C1C-NC	2.20	112.30	109.98
36	g	319	IHT	C36-C33-C32	2.20	121.45	118.09
27	a	303	CLA	CHA-C1A-NA	-2.20	121.40	126.39
27	f	602	CLA	CMC-C2C-C1C	2.20	128.48	125.03
35	d	312	II0	C06-C04-C10	2.20	113.83	109.49
27	f	613	CLA	C3A-C2A-C1A	2.20	104.64	101.34
27	A	829	CLA	CHB-C4A-NA	2.20	127.58	124.40
27	e	610	CLA	CHA-C1A-NA	-2.20	121.41	126.39
27	A	827	CLA	CBA-CAA-C2A	2.20	120.34	113.79
27	A	828	CLA	CHB-C4A-NA	2.20	127.57	124.40
27	c	607	CLA	C2A-C1A-CHA	2.20	127.68	123.87
27	a	307	CLA	C2A-C1A-CHA	2.20	127.68	123.87
27	h	302	CLA	CHB-C4A-NA	2.20	127.57	124.40
27	B	825	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
27	e	606	CLA	C2A-C1A-CHA	2.20	127.68	123.87
30	F	204	WVN	C07-C01-C02	2.20	112.87	109.55
27	d	311	CLA	CHB-C1B-C2B	-2.20	121.05	127.43
27	A	855	CLA	CHB-C1B-NB	2.20	127.34	124.05
27	e	602	CLA	CHB-C1B-NB	2.20	127.34	124.05
27	B	832	CLA	CBA-CAA-C2A	2.20	120.33	113.79
27	b	611	CLA	C3B-C4B-NB	-2.20	108.57	110.53
27	B	804	CLA	CHB-C4A-NA	2.20	127.57	124.40
31	b	616	LMT	C1-O1'-C1'	2.20	117.43	113.68
27	m	602	CLA	CMB-C2B-C3B	2.20	131.71	126.55
37	g	312	KC2	CAA-CBA-CGA	-2.19	115.89	127.05
27	h	304	CLA	CMD-C2D-C3D	2.19	132.72	127.69
27	a	305	CLA	C4-C3-C5	2.19	118.71	116.13
27	K	102	CLA	CHA-C1A-NA	-2.19	121.42	126.39
27	h	304	CLA	O2D-CGD-CBD	2.19	115.07	111.23
27	B	833	CLA	O2D-CGD-CBD	2.19	115.06	111.23
36	b	614	IHT	C06-C09-C10	2.19	117.97	114.06
37	i	310	KC2	CHD-C1D-C2D	2.19	133.79	127.43
27	a	303	CLA	CHB-C1B-NB	2.19	127.34	124.05
27	c	602	CLA	C3B-C4B-NB	-2.19	108.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	s	209	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
27	A	837	CLA	C1-C2-C3	-2.19	122.61	126.20
27	A	840	CLA	C2A-C1A-CHA	2.19	127.67	123.87
29	l	318	LHG	O7-C7-O9	-2.19	118.58	123.70
27	A	802	CLA	CHB-C1B-C2B	-2.19	121.07	127.43
27	b	607	CLA	CHB-C4A-NA	2.19	127.56	124.40
27	j	608	CLA	CHB-C1B-NB	2.19	127.33	124.05
30	A	848	WVN	C07-C01-C02	-2.19	106.23	109.55
29	c	621	LHG	C5-O7-C7	-2.19	112.56	117.80
27	n	604	CLA	C1-C2-C3	-2.19	122.61	126.20
27	B	837	CLA	O2A-CGA-CBA	2.19	118.51	111.83
27	B	823	CLA	O2A-C1-C2	-2.19	99.68	108.11
27	j	604	CLA	C16-C15-C13	-2.19	108.69	115.97
27	A	813	CLA	C3A-C2A-C1A	2.19	104.62	101.34
27	c	611	CLA	CHB-C1B-NB	2.19	127.33	124.05
38	i	301	LMU	C4B-C3B-C2B	2.19	114.67	110.83
35	e	612	II0	C20-C14-C10	-2.19	120.07	124.16
27	d	304	CLA	C3B-C4B-NB	-2.19	108.58	110.53
27	B	804	CLA	CHA-C1A-NA	-2.19	121.44	126.39
30	I	101	WVN	C11-C19-C22	-2.19	121.62	126.32
37	k	311	KC2	C4D-CHA-C1A	-2.19	115.79	122.45
35	l	313	II0	C31-C29-C25	-2.19	120.50	126.61
27	g	311	CLA	C2C-C1C-NC	2.19	112.28	109.98
27	f	604	CLA	CBA-CAA-C2A	2.19	120.30	113.79
27	m	608	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
29	b	618	LHG	O8-C23-C24	2.19	118.50	111.83
37	g	313	KC2	C2B-C1B-NB	2.18	112.29	110.13
27	e	610	CLA	CMB-C2B-C3B	2.18	131.69	126.55
35	c	615	II0	C12-C14-C10	-2.18	115.95	120.50
27	B	818	CLA	CMB-C2B-C3B	2.18	131.69	126.55
27	A	826	CLA	C3A-C2A-C1A	2.18	104.61	101.34
27	f	607	CLA	CAC-C3C-C4C	2.18	127.63	124.79
27	b	609	CLA	C2A-C1A-CHA	2.18	127.66	123.87
35	c	617	II0	C06-C04-C10	2.18	113.79	109.49
35	a	314	II0	C32-C34-C36	-2.18	120.38	126.36
35	d	312	II0	C19-C13-C09	-2.18	120.08	124.16
27	n	603	CLA	C3B-C4B-NB	-2.18	108.58	110.53
27	B	829	CLA	C16-C15-C13	-2.18	108.71	115.97
35	e	614	II0	C19-C13-C09	-2.18	120.08	124.16
37	c	610	KC2	CHD-C1D-C2D	2.18	133.76	127.43
30	B	846	WVN	C39-C36-C32	-2.18	124.22	127.28
35	a	314	II0	C38-C36-C34	2.18	121.42	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	g	302	CLA	CHA-C1A-NA	-2.18	121.45	126.39
35	g	318	II0	C31-C33-C35	-2.18	120.38	126.36
27	A	806	CLA	CHB-C4A-NA	2.18	127.55	124.40
36	n	617	IHT	C25-C23-C27	-2.18	119.28	122.82
27	g	304	CLA	CHA-C1A-NA	-2.18	121.45	126.39
27	A	812	CLA	C1-C2-C3	-2.18	122.62	126.20
27	B	810	CLA	C11-C12-C13	-2.18	108.72	115.97
27	f	609	CLA	C3B-C4B-NB	-2.18	108.58	110.53
35	l	302	II0	C38-C36-C34	2.18	121.42	118.09
27	i	312	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
27	B	831	CLA	C1-C2-C3	-2.18	122.63	126.20
35	b	612	II0	C18-C04-C10	-2.18	106.61	110.52
27	m	605	CLA	CHA-C1A-NA	-2.18	121.46	126.39
27	l	309	CLA	C3B-C4B-NB	-2.18	108.58	110.53
30	A	847	WVN	C06-C13-C20	2.18	121.56	115.65
27	j	609	CLA	C11-C12-C13	-2.18	108.72	115.97
27	m	605	CLA	CHB-C4A-NA	2.18	127.54	124.40
27	s	208	CLA	CMC-C2C-C3C	2.18	132.04	126.15
27	B	822	CLA	CHA-C4D-ND	2.18	137.04	132.55
27	k	304	CLA	CHD-C1D-ND	-2.18	121.74	124.80
27	g	306	CLA	CHA-C1A-NA	-2.18	121.46	126.39
27	B	822	CLA	CHA-C1A-NA	-2.18	121.46	126.39
35	i	314	II0	C41-C42-C40	-2.18	119.07	123.52
27	c	611	CLA	CBC-CAC-C3C	2.18	118.32	112.42
37	k	311	KC2	CHD-C1D-C2D	2.18	133.74	127.43
27	g	305	CLA	C1-C2-C3	-2.17	122.63	126.20
30	B	846	WVN	C02-C05-C09	-2.17	118.79	121.47
27	A	856	CLA	C2D-C1D-ND	-2.17	107.97	110.13
27	g	308	CLA	C1-O2A-CGA	-2.17	111.39	116.65
35	i	313	II0	C31-C29-C25	-2.17	120.53	126.61
37	k	310	KC2	O1D-CGD-CBD	-2.17	120.23	124.52
37	i	310	KC2	CAB-C3B-C2B	2.17	135.50	128.43
27	c	602	CLA	CHB-C1B-NB	2.17	127.31	124.05
30	l	316	WVN	C19-C22-C26	2.17	122.43	119.01
27	g	305	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
27	b	606	CLA	O1D-CGD-CBD	2.17	128.80	124.52
35	k	316	II0	C12-C14-C10	-2.17	115.98	120.50
27	j	612	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
35	l	302	II0	C33-C35-C39	-2.17	115.59	119.01
27	B	807	CLA	O2D-CGD-CBD	2.17	115.03	111.23
27	B	809	CLA	CMC-C2C-C1C	-2.17	121.64	125.03
36	c	620	IHT	C02-C07-C18	2.17	121.54	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	602	CLA	C3B-C4B-NB	-2.17	108.59	110.53
37	d	310	KC2	CAA-CBA-CGA	-2.17	116.02	127.05
27	A	801	CLA	CBA-CAA-C2A	-2.17	107.34	113.79
27	A	824	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
27	a	304	CLA	O2D-CGD-CBD	2.17	115.02	111.23
27	f	602	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
27	A	817	CLA	C16-C15-C13	-2.17	108.76	115.97
27	A	829	CLA	CHB-C1B-NB	2.17	127.30	124.05
35	l	314	II0	C31-C29-C25	-2.17	120.55	126.61
27	B	835	CLA	CHB-C1B-NB	2.17	127.30	124.05
27	c	612	CLA	CHD-C1D-ND	-2.17	121.75	124.80
27	j	606	CLA	C2A-C1A-CHA	2.17	127.63	123.87
27	l	305	CLA	O2D-CGD-CBD	2.17	115.02	111.23
37	m	610	KC2	CAB-C3B-C4B	-2.17	119.65	124.82
27	g	315	CLA	C4A-NA-C1A	2.17	107.67	106.68
27	h	302	CLA	CAC-C3C-C4C	2.17	127.61	124.79
27	F	203	CLA	C3B-C4B-NB	-2.16	108.60	110.53
35	f	618	II0	C38-C36-C34	2.16	121.39	118.09
27	O	206	CLA	CHA-C1A-NA	-2.16	121.49	126.39
27	B	809	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
35	n	615	II0	C05-C03-C09	2.16	113.75	109.49
37	s	201	KC2	CAC-C3C-C4C	2.16	133.95	124.39
27	B	836	CLA	C11-C10-C8	-2.16	108.78	115.97
27	e	611	CLA	C3A-C2A-C1A	2.16	104.58	101.34
27	O	202	CLA	C3B-C4B-NB	-2.16	108.60	110.53
27	f	612	CLA	CHB-C4A-NA	2.16	127.52	124.40
35	c	615	II0	C38-C36-C40	-2.16	119.31	122.82
27	i	311	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
35	l	314	II0	O02-C08-C06	-2.16	105.33	109.75
27	B	822	CLA	C2A-C1A-CHA	2.16	127.62	123.87
27	R	203	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
35	d	313	II0	C31-C29-C25	-2.16	120.57	126.61
30	L	205	WVN	C29-C31-C32	-2.16	120.44	126.36
27	e	605	CLA	CGD-CBD-CAD	-2.16	103.86	110.85
27	l	305	CLA	CMB-C2B-C3B	2.16	131.63	126.55
35	k	318	II0	C41-C42-C40	-2.16	119.10	123.52
29	f	619	LHG	O8-C23-C24	2.16	118.42	111.83
27	a	310	CLA	CMC-C2C-C1C	-2.16	121.66	125.03
30	F	205	WVN	C21-C15-C13	-2.16	122.13	124.48
27	B	822	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
27	a	313	CLA	CHB-C4A-NA	2.16	127.51	124.40
37	n	611	KC2	CAC-C3C-C4C	2.16	133.92	124.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	808	CLA	CMB-C2B-C3B	2.16	129.26	123.53
27	B	820	CLA	C16-C15-C13	-2.16	108.80	115.97
27	A	821	CLA	O2D-CGD-CBD	2.16	115.00	111.23
37	g	313	KC2	CAB-C3B-C4B	-2.16	119.67	124.82
27	B	814	CLA	CHB-C1B-NB	2.16	127.28	124.05
27	A	855	CLA	C3B-C4B-NB	-2.16	108.61	110.53
31	A	851	LMT	O5'-C1'-O1'	-2.16	104.95	110.04
35	d	314	II0	C16-C03-C15	-2.16	102.46	108.63
27	A	841	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
27	B	824	CLA	CAA-CBA-CGA	-2.15	107.09	113.21
27	c	604	CLA	CMB-C2B-C3B	2.15	131.62	126.55
37	n	611	KC2	CAB-C3B-C4B	-2.15	119.68	124.82
27	l	306	CLA	C16-C15-C13	-2.15	108.81	115.97
27	d	308	CLA	CMC-C2C-C3C	2.15	131.97	126.15
35	c	617	II0	C05-C03-C09	2.15	113.73	109.49
27	i	303	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
27	g	322	CLA	CBC-CAC-C3C	2.15	118.25	112.42
27	m	609	CLA	CGD-CBD-CAD	2.15	117.81	110.85
27	m	605	CLA	C2A-C1A-CHA	2.15	127.60	123.87
27	n	610	CLA	C2A-C1A-CHA	2.15	127.60	123.87
30	i	315	WVN	C08-C01-C07	-2.15	104.74	107.87
27	B	809	CLA	CMB-C2B-C3B	2.15	131.61	126.55
27	A	826	CLA	CMC-C2C-C3C	2.15	131.97	126.15
27	k	303	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
27	m	611	CLA	C2A-C1A-CHA	2.15	127.60	123.87
27	A	832	CLA	CMB-C2B-C3B	2.15	131.61	126.55
27	f	610	CLA	C4-C3-C5	2.15	118.96	115.23
27	g	307	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	n	606	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	n	607	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
27	B	809	CLA	O2D-CGD-CBD	2.15	114.99	111.23
27	l	308	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
27	A	807	CLA	CMB-C2B-C3B	2.15	131.60	126.55
36	m	616	IHT	C40-C41-C38	-2.15	119.12	123.52
27	B	836	CLA	C2A-C1A-CHA	2.15	127.59	123.87
30	R	201	WVN	C07-C01-C03	-2.15	104.54	109.01
27	k	306	CLA	CAC-C3C-C2C	-2.15	123.61	127.56
27	j	606	CLA	C1-O2A-CGA	2.15	121.85	116.65
27	A	816	CLA	C6-C7-C8	-2.15	108.83	115.97
27	B	828	CLA	C2C-C1C-NC	2.15	112.24	109.98
27	A	812	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
37	g	312	KC2	CMB-C2B-C1B	2.15	128.51	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	m	607	CLA	CHB-C1B-NB	2.15	127.27	124.05
30	K	103	WVN	C19-C22-C26	-2.15	115.63	119.01
35	j	615	II0	C16-C03-C09	-2.15	106.67	110.52
27	A	802	CLA	CHD-C1D-ND	-2.15	121.78	124.80
27	f	612	CLA	C2B-C1B-NB	2.15	112.55	110.33
27	n	609	CLA	CGD-CBD-CAD	2.15	117.79	110.85
27	m	607	CLA	C2A-C1A-CHA	2.15	127.59	123.87
27	d	308	CLA	O1D-CGD-CBD	2.15	128.75	124.52
27	A	828	CLA	CHA-C1A-NA	-2.14	121.53	126.39
34	b	619	LMG	C9-C8-C7	-2.14	106.78	111.78
27	f	608	CLA	CMB-C2B-C3B	2.14	131.59	126.55
35	O	203	II0	C32-C34-C36	-2.14	120.48	126.36
27	f	612	CLA	CHA-C1A-NA	-2.14	121.53	126.39
27	c	607	CLA	CHA-C1A-NA	-2.14	121.54	126.39
27	A	839	CLA	CMB-C2B-C3B	2.14	131.59	126.55
27	j	609	CLA	C1C-C2C-C3C	-2.14	104.73	106.98
30	A	848	WVN	C12-C10-C06	-2.14	106.85	114.43
35	n	614	II0	C11-C13-C09	-2.14	116.04	120.50
27	m	604	CLA	CBC-CAC-C3C	2.14	118.22	112.42
27	g	306	CLA	C2A-C1A-CHA	2.14	127.58	123.87
27	n	613	CLA	CHB-C4A-NA	2.14	127.49	124.40
27	j	603	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
27	d	305	CLA	CHD-C4C-NC	2.14	127.55	124.23
27	b	608	CLA	CMB-C2B-C3B	2.14	131.58	126.55
37	e	609	KC2	CAB-C3B-C4B	-2.14	119.71	124.82
27	A	855	CLA	C1-C2-C3	-2.14	122.69	126.20
27	k	308	CLA	C4D-C3D-CAD	-2.14	105.78	108.11
27	A	801	CLA	C3B-C4B-NB	-2.14	108.62	110.53
35	l	313	II0	C06-C04-C10	2.14	113.70	109.49
27	F	201	CLA	C11-C12-C13	-2.14	108.85	115.97
27	B	817	CLA	O2D-CGD-CBD	2.14	114.97	111.23
27	b	605	CLA	CMB-C2B-C3B	2.14	131.58	126.55
27	a	303	CLA	C2A-C1A-CHA	2.14	127.58	123.87
27	m	602	CLA	CMC-C2C-C1C	2.14	128.38	125.03
27	l	307	CLA	C3A-C2A-C1A	2.14	104.54	101.34
27	k	303	CLA	C2B-C1B-NB	2.14	112.54	110.33
27	l	312	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
27	A	832	CLA	C11-C10-C8	-2.14	108.86	115.97
27	j	608	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
27	B	831	CLA	C7-C6-C5	-2.14	107.57	113.26
37	e	609	KC2	CHD-C1D-C2D	2.14	133.63	127.43
27	i	304	CLA	O2D-CGD-O1D	-2.14	119.69	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	843	PQN	C11-C3-C2	-2.14	121.23	124.89
35	l	302	II0	C32-C34-C36	-2.14	120.50	126.36
35	f	616	II0	C32-C30-C26	-2.14	120.64	126.61
37	l	311	KC2	CMB-C2B-C1B	2.14	128.49	124.73
36	f	617	IHT	C40-C41-C38	-2.14	119.15	123.52
27	s	208	CLA	CMC-C2C-C1C	-2.14	121.70	125.03
27	b	608	CLA	C11-C12-C13	-2.14	108.87	115.97
37	s	201	KC2	CMD-C2D-C3D	2.14	132.40	125.67
29	k	319	LHG	C5-O7-C7	-2.14	112.69	117.80
27	K	102	CLA	O1D-CGD-CBD	2.13	128.73	124.52
29	J	107	LHG	O8-C23-C24	2.13	118.34	111.83
27	J	105	CLA	CHA-C4D-ND	2.13	136.95	132.55
27	g	307	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
35	d	314	II0	C27-C25-C29	-2.13	120.04	124.18
27	b	607	CLA	C3B-C4B-NB	-2.13	108.63	110.53
27	A	832	CLA	CBC-CAC-C3C	2.13	118.20	112.42
35	j	613	II0	C37-C35-C33	-2.13	114.83	118.09
27	A	813	CLA	C1D-ND-C4D	-2.13	104.82	106.31
27	n	609	CLA	C3B-C4B-NB	-2.13	108.63	110.53
27	h	306	CLA	CHA-C1A-NA	-2.13	121.57	126.39
35	f	618	II0	C16-C03-C15	-2.13	102.53	108.63
27	B	829	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
36	j	616	IHT	C31-C29-C26	-2.13	120.65	126.61
27	A	839	CLA	CHB-C4A-NA	2.13	127.47	124.40
27	c	606	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
30	A	849	WVN	C20-C23-C25	-2.13	123.08	126.23
27	B	834	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
35	e	614	II0	C42-C41-C39	-2.13	119.16	123.52
27	f	613	CLA	O2A-CGA-CBA	2.13	118.33	111.83
35	j	613	II0	C18-C04-C10	-2.13	106.70	110.52
35	g	316	II0	C07-C11-C13	-2.13	106.88	112.18
27	A	820	CLA	C3B-C4B-NB	-2.13	108.63	110.53
27	f	613	CLA	CGD-CBD-CAD	2.13	117.73	110.85
27	n	603	CLA	O1D-CGD-CBD	2.13	128.72	124.52
27	k	303	CLA	CHA-C1A-NA	-2.13	121.57	126.39
27	l	312	CLA	CHB-C4A-NA	2.13	127.47	124.40
27	n	609	CLA	O2D-CGD-CBD	2.13	114.95	111.23
27	c	611	CLA	C3B-C4B-NB	-2.13	108.63	110.53
27	b	607	CLA	CMD-C2D-C3D	2.13	132.57	127.69
27	j	612	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
35	e	613	II0	C31-C29-C25	-2.13	120.67	126.61
27	b	603	CLA	CHA-C1A-NA	-2.13	121.58	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	821	CLA	O1D-CGD-CBD	2.13	128.71	124.52
36	f	617	IHT	C31-C34-C35	-2.13	120.53	126.36
27	B	834	CLA	C4-C3-C5	2.13	118.92	115.23
27	B	837	CLA	CHB-C1B-NB	2.13	127.24	124.05
29	g	321	LHG	C25-C24-C23	-2.13	105.91	113.69
30	h	309	WVN	C19-C22-C26	2.13	122.35	119.01
27	B	812	CLA	C2A-C1A-CHA	2.13	127.56	123.87
27	i	307	CLA	CHD-C4C-NC	2.12	127.53	124.23
27	a	312	CLA	C1-C2-C3	-2.12	122.72	126.20
27	e	603	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
27	s	209	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
27	m	603	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
36	c	620	IHT	C25-C23-C22	2.12	121.33	118.09
27	j	602	CLA	CMA-C3A-C2A	-2.12	105.77	113.98
29	j	617	LHG	C6-C5-C4	-2.12	106.83	111.78
37	n	612	KC2	CAB-C3B-C2B	2.12	135.33	128.43
27	b	608	CLA	O1D-CGD-CBD	2.12	128.71	124.52
27	j	607	CLA	CMB-C2B-C3B	2.12	131.54	126.55
37	g	314	KC2	CAB-C3B-C4B	-2.12	119.75	124.82
27	f	609	CLA	C4-C3-C5	2.12	118.91	115.23
36	R	204	IHT	C03-C05-C08	-2.12	108.94	113.59
35	n	618	II0	C32-C30-C26	-2.12	120.68	126.61
27	A	801	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
27	B	849	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
27	A	804	CLA	C1-O2A-CGA	2.12	121.78	116.65
27	J	105	CLA	CAA-C2A-C1A	2.12	118.92	111.97
27	d	304	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
29	a	319	LHG	C6-C5-C4	-2.12	106.84	111.78
27	A	813	CLA	O2D-CGD-CBD	2.12	114.94	111.23
37	k	310	KC2	CHD-C1D-C2D	2.12	133.58	127.43
27	A	853	CLA	CAC-C3C-C4C	2.12	127.55	124.79
27	B	831	CLA	C3A-C2A-C1A	2.12	104.51	101.34
35	l	302	II0	C17-C04-C10	-2.12	106.72	110.52
37	g	314	KC2	CHD-C1D-C2D	2.12	133.58	127.43
27	i	309	CLA	C3D-C2D-C1D	2.12	108.72	105.83
35	j	613	II0	C12-C14-C10	-2.12	116.09	120.50
27	A	823	CLA	C1-C2-C3	2.12	129.66	126.20
27	m	608	CLA	C1-O2A-CGA	2.12	121.77	116.65
27	A	825	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	i	304	CLA	CHB-C1B-NB	2.12	127.22	124.05
27	B	819	CLA	CAC-C3C-C4C	2.12	127.54	124.79
27	i	309	CLA	CBA-CAA-C2A	2.12	120.09	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	h	312	II0	C38-C36-C34	2.12	121.32	118.09
35	f	618	II0	C19-C13-C11	2.11	118.31	114.42
27	f	607	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
35	n	616	II0	C19-C13-C09	-2.11	120.21	124.16
27	m	611	CLA	CHA-C1A-NA	-2.11	121.61	126.39
27	e	607	CLA	C3B-C4B-NB	-2.11	108.64	110.53
27	A	808	CLA	O1D-CGD-CBD	2.11	128.69	124.52
27	f	601	CLA	O2D-CGD-CBD	2.11	114.92	111.23
27	g	304	CLA	CHA-C4D-ND	2.11	136.91	132.55
27	m	605	CLA	O1D-CGD-CBD	2.11	128.68	124.52
35	b	613	II0	C18-C04-C10	-2.11	106.74	110.52
27	n	601	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
27	B	840	CLA	C2A-C1A-CHA	2.11	127.53	123.87
27	f	607	CLA	C9-C8-C10	-2.11	103.75	111.27
27	b	608	CLA	CHD-C1D-ND	-2.11	121.83	124.80
27	j	601	CLA	CHB-C4A-NA	2.11	127.44	124.40
27	A	826	CLA	C12-C11-C10	-2.11	103.82	113.28
37	s	204	KC2	C2D-C1D-ND	-2.11	108.14	110.33
27	B	806	CLA	C1-C2-C3	-2.11	122.74	126.20
35	g	320	II0	C11-C13-C09	-2.11	116.11	120.50
27	A	827	CLA	C2A-C1A-CHA	2.11	127.53	123.87
27	A	804	CLA	C6-C7-C8	-2.11	108.96	115.97
27	j	603	CLA	CHB-C1B-NB	2.11	127.21	124.05
35	a	315	II0	C31-C29-C25	-2.11	120.72	126.61
27	B	814	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
27	a	306	CLA	C7-C6-C5	-2.11	107.65	113.26
27	n	609	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
27	A	835	CLA	C6-C7-C8	-2.11	108.97	115.97
27	B	825	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
37	m	610	KC2	C2B-C1B-NB	2.11	112.21	110.13
35	n	618	II0	C32-C34-C36	-2.11	120.59	126.36
27	a	309	CLA	CMA-C3A-C2A	-2.10	105.85	113.98
27	A	806	CLA	C6-C7-C8	-2.10	108.97	115.97
27	m	612	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
27	B	840	CLA	C11-C12-C13	-2.10	108.97	115.97
35	g	316	II0	C16-C03-C09	-2.10	106.75	110.52
35	j	613	II0	C31-C29-C25	-2.10	120.73	126.61
35	a	318	II0	C22-C24-C26	-2.10	169.09	176.23
27	c	609	CLA	CHB-C1B-NB	2.10	127.20	124.05
27	B	833	CLA	C3A-C2A-C1A	2.10	104.49	101.34
27	j	603	CLA	C3A-C2A-C1A	2.10	104.49	101.34
27	a	307	CLA	CGD-CBD-CAD	2.10	117.65	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	k	317	IHT	C40-C41-C38	-2.10	119.22	123.52
35	l	315	II0	C31-C33-C35	-2.10	120.60	126.36
27	g	309	CLA	C2A-C3A-C4A	2.10	105.26	101.87
27	A	827	CLA	CAC-C3C-C4C	2.10	127.52	124.79
37	g	314	KC2	CAA-CBA-CGA	-2.10	116.37	127.05
30	R	201	WVN	C38-C34-C33	2.10	121.30	118.09
27	c	601	CLA	C3B-C4B-NB	-2.10	108.66	110.53
27	e	604	CLA	CAA-C2A-C3A	-2.10	107.32	113.00
27	m	609	CLA	CHA-C1A-NA	-2.10	121.64	126.39
35	e	616	II0	C11-C13-C09	-2.10	116.13	120.50
27	B	809	CLA	C2A-C1A-CHA	2.10	127.51	123.87
35	k	318	II0	C11-C13-C09	-2.10	116.13	120.50
27	c	605	CLA	O2D-CGD-CBD	2.10	114.90	111.23
27	A	834	CLA	CBA-CAA-C2A	-2.10	107.55	113.79
27	B	801	CLA	CBA-CAA-C2A	-2.10	107.55	113.79
27	n	603	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
27	n	607	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
27	B	838	CLA	O2D-CGD-CBD	2.10	114.89	111.23
35	e	613	II0	C42-C41-C39	-2.10	119.23	123.52
27	a	311	CLA	C6-C7-C8	-2.10	109.00	115.97
27	k	313	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
27	B	834	CLA	CMB-C2B-C3B	2.09	131.48	126.55
27	l	310	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	f	603	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
27	j	611	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	f	612	CLA	CMC-C2C-C3C	2.09	131.81	126.15
27	A	839	CLA	C3B-C4B-NB	-2.09	108.66	110.53
29	d	315	LHG	O4-P-O5	2.09	122.18	112.44
27	B	849	CLA	CHD-C1D-ND	-2.09	121.86	124.80
27	n	601	CLA	C3B-C4B-NB	-2.09	108.66	110.53
36	c	616	IHT	C16-C03-C11	-2.09	106.77	110.52
37	j	610	KC2	CAB-C3B-C4B	-2.09	119.83	124.82
30	h	309	WVN	C21-C15-C14	2.09	118.05	113.60
30	J	102	WVN	C02-C11-C19	-2.09	121.33	124.58
27	a	311	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
27	A	808	CLA	CHA-C1A-NA	-2.09	121.66	126.39
27	A	821	CLA	CHD-C1D-ND	-2.09	121.86	124.80
35	m	614	II0	C05-C03-C09	2.09	113.61	109.49
27	h	305	CLA	C4-C3-C5	2.09	118.59	116.13
27	f	604	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
27	l	304	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
27	i	303	CLA	O2A-CGA-O1A	-2.09	118.40	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	204	WVN	C18-C06-C13	2.09	113.52	110.24
27	B	831	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
35	n	618	II0	C15-C03-C09	-2.09	106.78	110.52
35	n	618	II0	C08-C12-C14	2.09	117.38	112.18
29	l	318	LHG	C6-C5-C4	-2.09	106.92	111.78
27	s	202	CLA	C2A-C1A-CHA	2.09	127.49	123.87
27	B	836	CLA	O2D-CGD-CBD	2.09	114.88	111.23
27	e	603	CLA	O2D-CGD-CBD	2.09	114.88	111.23
27	A	815	CLA	O1D-CGD-CBD	2.09	128.63	124.52
27	k	313	CLA	CBC-CAC-C3C	2.09	118.08	112.42
30	B	844	WVN	C02-C05-C09	-2.09	118.90	121.47
27	A	852	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
27	F	202	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
30	B	843	WVN	C06-C13-C15	-2.09	119.78	122.64
27	d	311	CLA	CHD-C1D-ND	-2.09	121.87	124.80
27	l	309	CLA	CHA-C4D-ND	2.09	136.85	132.55
35	c	614	II0	C31-C29-C25	-2.09	120.78	126.61
27	a	305	CLA	CHB-C4A-NA	2.08	127.41	124.40
27	c	606	CLA	O1D-CGD-CBD	2.08	128.63	124.52
30	B	843	WVN	C29-C31-C32	-2.08	120.65	126.36
27	a	309	CLA	C1-C2-C3	-2.08	122.78	126.20
27	A	804	CLA	C2A-C1A-CHA	2.08	127.48	123.87
30	B	848	WVN	C39-C40-C37	-2.08	119.26	123.52
27	A	833	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
27	B	815	CLA	CHC-C4B-NB	2.08	127.17	124.05
27	B	821	CLA	CHB-C1B-NB	2.08	127.17	124.05
30	J	101	WVN	C24-C22-C19	2.08	121.27	118.09
27	A	855	CLA	C3B-C2B-C1B	2.08	109.62	107.17
27	k	306	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
27	B	827	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
27	B	813	CLA	C2A-C1A-CHA	2.08	127.48	123.87
35	a	316	II0	C15-C03-C09	-2.08	106.79	110.52
35	e	612	II0	C17-C04-C10	-2.08	106.79	110.52
36	R	204	IHT	C20-C15-C12	2.08	118.25	114.42
29	j	617	LHG	C5-O7-C7	-2.08	112.81	117.80
35	n	618	II0	C20-C14-C12	2.08	118.25	114.42
37	g	313	KC2	CAA-CBA-CGA	-2.08	116.47	127.05
27	c	609	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
27	d	308	CLA	CMC-C2C-C1C	-2.08	121.78	125.03
30	l	316	WVN	C18-C06-C13	2.08	113.50	110.24
27	h	303	CLA	CMB-C2B-C3B	2.08	131.44	126.55
27	B	802	CLA	CHB-C1B-NB	2.08	127.17	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	834	CLA	C2D-C1D-ND	-2.08	108.07	110.13
27	B	810	CLA	CHA-C1A-NA	-2.08	121.69	126.39
27	k	306	CLA	CHA-C1A-NA	-2.08	121.69	126.39
27	A	805	CLA	C3A-C2A-C1A	2.08	104.45	101.34
37	d	309	KC2	CAB-C3B-C4B	-2.08	119.86	124.82
27	b	605	CLA	C2A-C1A-CHA	2.08	127.47	123.87
27	i	308	CLA	CHA-C1A-NA	-2.08	121.69	126.39
30	B	847	WVN	C24-C22-C19	2.08	121.26	118.09
35	k	315	II0	C11-C13-C09	-2.08	116.18	120.50
27	m	612	CLA	CMB-C2B-C3B	2.08	131.43	126.55
35	k	314	II0	C05-C03-C09	2.08	113.58	109.49
37	l	311	KC2	C2B-C1B-NB	2.07	112.18	110.13
37	f	611	KC2	CAB-C3B-C4B	-2.07	119.87	124.82
27	K	102	CLA	CHC-C1C-NC	2.07	127.44	124.31
27	b	610	CLA	O2D-CGD-CBD	2.07	114.86	111.23
37	l	311	KC2	CAB-C3B-C4B	-2.07	119.87	124.82
29	j	617	LHG	C25-C24-C23	-2.07	106.09	113.69
30	B	845	WVN	C02-C05-C09	-2.07	118.92	121.47
27	k	302	CLA	O2D-CGD-CBD	2.07	114.85	111.23
27	j	606	CLA	O2D-CGD-CBD	2.07	114.85	111.23
27	a	305	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
27	B	817	CLA	CHD-C1D-ND	-2.07	121.89	124.80
27	m	612	CLA	C3B-C4B-NB	-2.07	108.68	110.53
30	R	201	WVN	C10-C06-C13	-2.07	107.43	110.44
27	f	603	CLA	O2D-CGD-CBD	2.07	114.85	111.23
27	n	613	CLA	CHC-C4B-NB	2.07	127.16	124.05
37	e	609	KC2	CMB-C2B-C1B	2.07	128.38	124.73
30	s	207	WVN	C06-C13-C15	-2.07	119.81	122.64
27	J	105	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
27	K	101	CLA	CAA-C2A-C1A	2.07	118.76	111.97
27	B	831	CLA	O2D-CGD-CBD	2.07	114.85	111.23
37	g	312	KC2	CHD-C1D-C2D	2.07	133.44	127.43
35	k	314	II0	C41-C39-C35	-2.07	124.38	127.28
27	j	608	CLA	CHD-C1D-ND	-2.07	121.89	124.80
27	F	202	CLA	CHB-C4A-NA	2.07	127.39	124.40
27	e	610	CLA	C4D-CHA-C1A	2.07	123.71	121.24
27	h	301	CLA	C1-O2A-CGA	2.07	121.66	116.65
27	B	838	CLA	C3B-C4B-NB	-2.07	108.68	110.53
27	f	604	CLA	CHD-C1D-ND	-2.07	121.89	124.80
27	j	608	CLA	CHA-C1A-NA	-2.07	121.71	126.39
27	j	611	CLA	CMB-C2B-C3B	2.07	131.41	126.55
27	e	608	CLA	C3A-C2A-C1A	2.07	104.44	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	610	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
27	s	208	CLA	CHA-C1A-NA	-2.07	121.71	126.39
27	a	310	CLA	CHC-C4B-NB	2.07	127.15	124.05
27	j	612	CLA	CMB-C2B-C3B	2.07	131.41	126.55
36	O	204	IHT	C27-C30-C32	-2.07	117.22	123.20
35	d	313	II0	C20-C14-C12	2.07	118.22	114.42
27	e	606	CLA	CHC-C4B-NB	2.07	127.15	124.05
35	d	314	II0	C29-C31-C33	-2.06	117.22	123.20
27	B	840	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
27	g	304	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
27	B	849	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
27	A	856	CLA	CAA-C2A-C1A	2.06	116.91	111.81
27	l	312	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
27	g	304	CLA	C3A-C2A-C1A	2.06	104.43	101.34
27	d	302	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	n	605	CLA	CHD-C4C-C3C	2.06	127.78	124.77
30	B	844	WVN	C14-C15-C13	-2.06	119.92	122.70
29	g	301	LHG	O7-C5-C4	2.06	115.74	108.34
27	B	809	CLA	CHC-C1C-NC	2.06	127.42	124.31
27	n	613	CLA	CMB-C2B-C3B	2.06	131.40	126.55
27	g	310	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
27	f	613	CLA	O2D-CGD-CBD	2.06	114.84	111.23
27	A	826	CLA	C3B-C4B-NB	-2.06	108.69	110.53
27	k	302	CLA	C3B-C4B-NB	-2.06	108.69	110.53
27	n	607	CLA	C2C-C1C-NC	2.06	112.15	109.98
29	a	301	LHG	O4-P-O5	2.06	122.04	112.44
27	L	202	CLA	CMB-C2B-C3B	2.06	131.40	126.55
27	i	311	CLA	CMC-C2C-C1C	-2.06	121.81	125.03
27	B	837	CLA	C2A-C1A-CHA	2.06	127.44	123.87
27	g	303	CLA	O2D-CGD-CBD	2.06	114.83	111.23
27	A	836	CLA	C7-C6-C5	-2.06	107.77	113.26
27	A	831	CLA	C3B-C4B-NB	-2.06	108.69	110.53
27	A	801	CLA	O1D-CGD-CBD	2.06	128.58	124.52
27	k	309	CLA	CMD-C2D-C1D	2.06	128.36	124.73
27	f	605	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
27	g	305	CLA	CBA-CAA-C2A	2.06	119.92	113.79
27	n	610	CLA	C3B-C4B-NB	-2.06	108.69	110.53
35	k	315	II0	C42-C40-C36	-2.06	124.39	127.28
27	B	839	CLA	C4D-CHA-C1A	2.06	123.70	121.24
30	K	103	WVN	C23-C20-C13	-2.06	121.50	127.00
35	b	612	II0	C22-C24-C26	-2.06	169.23	176.23
36	g	319	IHT	C12-C15-C11	-2.06	116.22	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	R	203	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
27	B	804	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
30	s	205	WVN	C14-C15-C13	-2.06	119.92	122.70
36	R	204	IHT	C25-C23-C27	-2.06	119.48	122.82
27	B	824	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
27	B	803	CLA	C2A-C3A-C4A	2.06	105.19	101.87
27	A	834	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
27	B	828	CLA	CHA-C1A-NA	-2.06	121.73	126.39
27	s	208	CLA	CHD-C1D-ND	-2.06	121.91	124.80
27	B	830	CLA	CGD-CBD-CAD	-2.06	104.19	110.85
27	b	603	CLA	O2D-CGD-O1D	-2.06	119.85	123.85
35	c	617	II0	C38-C36-C34	2.06	121.23	118.09
27	A	820	CLA	CAC-C3C-C4C	2.06	127.46	124.79
27	B	811	CLA	CAA-C2A-C1A	2.06	118.71	111.97
27	j	608	CLA	C4D-C3D-CAD	-2.06	105.87	108.11
27	B	807	CLA	C11-C12-C13	-2.05	109.14	115.97
35	g	317	II0	C31-C33-C35	-2.05	120.73	126.36
27	A	830	CLA	C1-C2-C3	-2.05	123.44	126.76
27	A	837	CLA	C11-C12-C13	-2.05	109.14	115.97
27	A	811	CLA	CHA-C1A-NA	-2.05	121.74	126.39
27	k	302	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
35	n	614	II0	C18-C04-C10	-2.05	106.84	110.52
27	A	817	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
27	f	602	CLA	O2A-CGA-CBA	2.05	118.09	111.83
36	O	204	IHT	C20-C15-C11	-2.05	120.32	124.16
29	m	617	LHG	O8-C23-O10	-2.05	118.49	123.63
29	g	321	LHG	O4-P-O5	2.05	121.99	112.44
27	c	611	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
30	R	202	WVN	C30-C33-C34	-2.05	120.74	126.36
35	a	315	II0	C06-C04-C10	2.05	113.53	109.49
27	j	603	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
30	l	316	WVN	C06-C13-C20	2.05	121.21	115.65
27	B	828	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
27	a	307	CLA	C3C-C4C-NC	-2.05	107.80	110.43
35	n	616	II0	C31-C33-C35	-2.05	120.74	126.36
27	A	806	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
27	A	829	CLA	CHA-C4D-ND	2.05	136.78	132.55
27	B	820	CLA	C3B-C4B-NB	-2.05	108.70	110.53
27	k	313	CLA	CMB-C2B-C3B	2.05	131.37	126.55
27	i	311	CLA	CHB-C4A-NA	2.05	127.36	124.40
30	R	202	WVN	C21-C15-C14	2.05	117.96	113.60
27	l	304	CLA	C11-C12-C13	-2.05	109.16	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	f	612	CLA	CHB-C1B-NB	2.05	127.12	124.05
27	c	609	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
27	n	610	CLA	CBC-CAC-C3C	2.05	117.97	112.42
36	m	616	IHT	C20-C15-C12	2.05	118.18	114.42
35	i	318	II0	C24-C22-C10	-2.05	170.71	175.48
31	a	320	LMT	C1-O1'-C1'	-2.05	110.19	113.68
27	A	812	CLA	C3A-C2A-C1A	2.05	104.40	101.34
35	e	613	II0	C29-C31-C33	-2.05	117.27	123.20
35	c	615	II0	C41-C42-C40	-2.04	119.33	123.52
35	l	315	II0	C20-C14-C12	2.04	118.18	114.42
27	a	313	CLA	CHB-C1B-NB	2.04	127.12	124.05
36	j	616	IHT	C06-C09-C10	-2.04	110.41	114.06
35	k	318	II0	C19-C13-C09	-2.04	120.34	124.16
37	n	611	KC2	CAA-CBA-CGA	-2.04	116.66	127.05
27	i	308	CLA	CHB-C4A-NA	2.04	127.35	124.40
30	O	201	WVN	C16-C05-C09	-2.04	115.50	122.37
27	B	839	CLA	C1-C2-C3	2.04	129.54	126.20
27	e	611	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
35	f	616	II0	C41-C42-C40	-2.04	119.34	123.52
27	O	202	CLA	C11-C12-C13	-2.04	109.18	115.97
27	g	307	CLA	O2D-CGD-CBD	2.04	114.80	111.23
35	i	318	II0	O02-C08-C12	-2.04	105.11	109.71
27	l	312	CLA	O1D-CGD-CBD	2.04	128.54	124.52
27	d	301	CLA	C3B-C4B-NB	-2.04	108.71	110.53
27	A	836	CLA	C3A-C2A-C1A	2.04	104.40	101.34
37	d	309	KC2	CMB-C2B-C1B	2.04	128.32	124.73
27	k	303	CLA	CHC-C1C-NC	2.04	127.38	124.31
27	B	809	CLA	CHA-C1A-NA	-2.04	121.77	126.39
27	j	608	CLA	C3B-C4B-NB	-2.04	108.71	110.53
27	A	810	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
35	f	614	II0	C17-C04-C10	-2.04	106.86	110.52
35	f	614	II0	C18-C04-C10	-2.04	106.86	110.52
27	m	612	CLA	CHB-C1B-NB	2.04	127.11	124.05
27	d	311	CLA	CHB-C1B-NB	2.04	127.11	124.05
27	n	609	CLA	CHD-C1D-ND	-2.04	121.93	124.80
27	g	315	CLA	CHD-C1D-ND	-2.04	121.93	124.80
37	n	612	KC2	CAA-C2A-C1A	2.04	133.57	124.64
27	A	853	CLA	C3B-C4B-NB	-2.04	108.71	110.53
27	B	835	CLA	C3B-C4B-NB	-2.04	108.71	110.53
27	i	311	CLA	C2C-C1C-NC	2.04	112.12	109.98
31	a	320	LMT	O5'-C1'-C2'	2.04	114.56	110.37
37	n	611	KC2	C4D-CHA-C1A	-2.04	116.25	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	k	310	KC2	CMB-C2B-C1B	2.04	128.31	124.73
27	B	829	CLA	C1-O2A-CGA	2.04	121.58	116.65
35	a	314	II0	C17-C04-C10	-2.04	106.87	110.52
35	a	315	II0	C04-C06-C08	-2.04	109.13	113.59
35	e	613	II0	C30-C32-C34	-2.03	117.30	123.20
30	J	102	WVN	C17-C06-C13	2.03	113.43	110.24
37	i	310	KC2	CAA-CBA-CGA	-2.03	116.70	127.05
27	A	805	CLA	C3B-C4B-NB	-2.03	108.71	110.53
35	n	615	II0	C04-C06-C08	2.03	118.06	113.59
27	b	607	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
27	g	309	CLA	CBC-CAC-C3C	2.03	117.93	112.42
35	j	615	II0	C28-C26-C30	-2.03	120.23	124.18
27	f	601	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
30	K	103	WVN	C16-C05-C09	-2.03	115.54	122.37
27	i	304	CLA	C1-C2-C3	-2.03	122.87	126.20
35	l	317	II0	C06-C04-C10	2.03	113.49	109.49
27	B	840	CLA	CAC-C3C-C4C	2.03	127.43	124.79
27	A	828	CLA	C2A-C1A-CHA	2.03	127.39	123.87
27	e	607	CLA	OBD-CAD-C3D	2.03	133.17	128.42
36	j	616	IHT	C41-C40-C37	-2.03	119.36	123.52
27	c	601	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	m	605	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
27	h	306	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	n	603	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
27	A	826	CLA	C9-C8-C10	-2.03	104.03	111.27
27	a	308	CLA	C3B-C4B-NB	-2.03	108.72	110.53
30	F	205	WVN	C33-C34-C37	2.03	122.20	119.01
27	g	305	CLA	CMC-C2C-C3C	2.03	131.64	126.15
27	j	611	CLA	O1D-CGD-CBD	2.03	128.52	124.52
27	i	304	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
27	f	602	CLA	CHC-C4B-NB	2.03	127.09	124.05
27	b	611	CLA	O1D-CGD-CBD	2.03	128.52	124.52
35	g	317	II0	C38-C36-C34	2.03	121.19	118.09
36	k	317	IHT	C36-C33-C32	2.03	121.19	118.09
35	a	318	II0	C19-C13-C09	-2.03	120.37	124.16
27	i	311	CLA	C1-O2A-CGA	2.03	121.56	116.65
35	l	315	II0	C17-C04-C10	-2.03	106.88	110.52
36	n	617	IHT	C40-C41-C38	-2.03	119.37	123.52
35	n	614	II0	C20-C14-C10	-2.03	120.37	124.16
27	F	203	CLA	C2A-C1A-CHA	2.03	127.39	123.87
27	f	610	CLA	CHA-C1A-NA	-2.03	121.80	126.39
27	b	601	CLA	CMB-C2B-C1B	-2.03	122.33	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	l	308	CLA	CMA-C3A-C2A	-2.03	106.14	113.98
27	k	309	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
35	J	104	II0	C41-C42-C40	-2.03	119.37	123.52
36	O	204	IHT	C30-C32-C33	-2.03	120.80	126.36
37	j	610	KC2	CMB-C2B-C1B	2.03	128.30	124.73
27	A	814	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
27	A	830	CLA	CHB-C1B-NB	2.03	127.09	124.05
37	k	312	KC2	CAC-C3C-C4C	2.03	133.34	124.39
30	B	845	WVN	C21-C15-C13	-2.03	122.27	124.48
37	k	311	KC2	CAC-C3C-C4C	2.03	133.34	124.39
27	B	813	CLA	CHB-C1B-C2B	-2.03	121.55	127.43
27	a	304	CLA	C3B-C4B-NB	-2.03	108.72	110.53
27	a	312	CLA	CAA-C2A-C3A	-2.03	107.53	113.00
27	h	308	CLA	CHA-C1A-NA	-2.03	121.81	126.39
27	B	837	CLA	C3A-C2A-C1A	2.02	104.37	101.34
27	f	610	CLA	C2A-C1A-CHA	2.02	127.38	123.87
27	B	813	CLA	CHB-C1B-NB	2.02	127.09	124.05
27	m	604	CLA	CAC-C3C-C2C	2.02	131.28	127.56
27	K	101	CLA	C3B-C4B-NB	-2.02	108.72	110.53
27	m	601	CLA	C3B-C4B-NB	-2.02	108.72	110.53
27	a	312	CLA	C2D-C1D-ND	-2.02	108.12	110.13
27	b	606	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
27	i	312	CLA	C1-C2-C3	-2.02	122.88	126.20
27	m	604	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
27	i	305	CLA	C16-C17-C18	-2.02	106.91	115.94
35	h	312	II0	C19-C13-C09	-2.02	120.38	124.16
27	A	823	CLA	CHD-C1D-ND	-2.02	121.96	124.80
27	A	808	CLA	C3B-C4B-NB	-2.02	108.72	110.53
34	b	619	LMG	C1-C2-C3	2.02	114.26	110.01
27	h	301	CLA	O2A-C1-C2	2.02	115.88	108.11
35	n	616	II0	C12-C14-C10	-2.02	116.29	120.50
27	B	812	CLA	O2D-CGD-CBD	2.02	114.76	111.23
29	g	301	LHG	O8-C23-O10	-2.02	118.58	123.63
35	l	314	II0	C16-C03-C09	-2.02	106.90	110.52
27	d	302	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
27	j	602	CLA	CHC-C4B-NB	2.02	127.08	124.05
27	B	831	CLA	C2A-C1A-CHA	2.02	127.37	123.87
27	d	302	CLA	CHA-C1A-NA	-2.02	121.82	126.39
27	j	604	CLA	O1D-CGD-CBD	2.02	128.50	124.52
36	O	204	IHT	C22-C18-C07	-2.02	121.61	127.00
27	L	204	CLA	O2D-CGD-CBD	2.02	114.75	111.23
27	A	823	CLA	C4-C3-C2	-2.02	118.45	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	822	CLA	C16-C15-C13	-2.02	109.27	115.97
27	B	808	CLA	CMA-C3A-C2A	-2.02	106.19	113.98
34	c	619	LMG	O6-C1-C2	-2.02	106.23	110.37
27	F	202	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
27	A	835	CLA	CGD-CBD-CAD	2.01	117.37	110.85
27	c	605	CLA	C4-C3-C5	2.01	118.50	116.13
27	n	607	CLA	CGD-CBD-CAD	-2.01	104.33	110.85
27	B	839	CLA	C11-C10-C8	-2.01	109.27	115.97
27	b	608	CLA	O2D-CGD-CBD	2.01	114.75	111.23
35	f	614	II0	C19-C13-C09	-2.01	120.39	124.16
27	B	817	CLA	C1D-ND-C4D	-2.01	104.90	106.31
30	l	316	WVN	C16-C05-C09	-2.01	115.60	122.37
27	f	607	CLA	CHA-C1A-NA	-2.01	121.83	126.39
27	m	612	CLA	O2D-CGD-CBD	2.01	114.75	111.23
27	A	820	CLA	O2D-CGD-CBD	2.01	114.75	111.23
27	A	827	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
27	A	814	CLA	CHD-C1D-ND	-2.01	121.97	124.80
27	B	815	CLA	C3B-C4B-NB	-2.01	108.73	110.53
30	F	204	WVN	C35-C32-C31	2.01	121.16	118.09
34	c	619	LMG	O6-C5-C6	2.01	111.42	106.44
37	g	312	KC2	C2B-C1B-NB	2.01	112.12	110.13
37	g	314	KC2	C2B-C1B-NB	2.01	112.12	110.13
27	b	605	CLA	CHA-C1A-NA	-2.01	121.84	126.39
27	g	305	CLA	CBC-CAC-C3C	2.01	117.87	112.42
35	f	618	II0	C37-C35-C39	-2.01	119.56	122.82
27	A	828	CLA	C3B-C4B-NB	-2.01	108.74	110.53
27	A	836	CLA	C1-C2-C3	-2.01	122.91	126.20
27	g	307	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
27	n	603	CLA	C2A-C1A-CHA	2.01	127.35	123.87
35	j	615	II0	C29-C31-C33	-2.01	117.38	123.20
30	F	205	WVN	C11-C19-C22	-2.01	122.00	126.32
27	B	819	CLA	O1D-CGD-CBD	2.01	128.48	124.52
27	b	601	CLA	C3B-C4B-NB	-2.01	108.74	110.53
27	h	301	CLA	CHA-C4D-ND	2.01	136.69	132.55
27	c	606	CLA	CHA-C1A-NA	-2.01	121.85	126.39
27	s	208	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
35	e	613	II0	C05-C03-C09	2.01	113.44	109.49
37	f	611	KC2	CAC-C3C-C4C	2.01	133.26	124.39
27	d	306	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
27	l	306	CLA	C11-C10-C8	-2.01	109.30	115.97
37	s	204	KC2	C2A-C3A-C4A	2.01	107.92	106.41
27	A	819	CLA	CHC-C1C-C2C	-2.01	121.25	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	204	WVN	C07-C01-C03	2.01	113.18	109.01
35	h	310	II0	C05-C03-C09	2.01	113.44	109.49
27	a	310	CLA	CMC-C2C-C3C	2.01	131.57	126.15
27	A	830	CLA	CHA-C1A-NA	-2.00	121.85	126.39
27	B	823	CLA	CHA-C1A-NA	-2.00	121.85	126.39
30	B	843	WVN	C08-C01-C02	-2.00	106.51	109.55
27	f	610	CLA	CHB-C1B-NB	2.00	127.06	124.05
30	B	844	WVN	C01-C02-C11	-2.00	110.52	112.83
27	a	307	CLA	CHA-C1A-NA	-2.00	121.85	126.39
27	g	310	CLA	CHA-C1A-NA	-2.00	121.85	126.39
27	m	608	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
35	h	312	II0	C05-C03-C09	2.00	113.44	109.49
35	f	615	II0	C31-C33-C35	-2.00	120.87	126.36
27	j	609	CLA	CGD-CBD-CAD	2.00	117.33	110.85
30	B	844	WVN	C06-C13-C15	-2.00	119.90	122.64
27	n	608	CLA	CHA-C4D-ND	2.00	136.68	132.55
27	c	612	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
35	f	618	II0	C30-C32-C34	-2.00	117.40	123.20
30	O	201	WVN	C19-C22-C26	-2.00	115.86	119.01
27	e	605	CLA	CHC-C4B-NB	2.00	127.05	124.05
37	i	317	KC2	CMC-C2C-C1C	2.00	128.16	125.03
27	A	853	CLA	CBA-CAA-C2A	2.00	119.75	113.79
27	k	309	CLA	O1D-CGD-CBD	2.00	128.46	124.52
35	j	614	II0	C20-C14-C12	2.00	118.10	114.42
27	n	604	CLA	C2A-C1A-CHA	2.00	127.34	123.87
27	f	612	CLA	CAA-CBA-CGA	-2.00	107.53	113.21
31	b	616	LMT	C4-C3-C2	-2.00	104.26	114.37

All (218) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	801	CLA	ND
27	A	802	CLA	ND
27	A	803	CLA	ND
27	A	804	CLA	ND
27	A	805	CLA	ND
27	A	807	CLA	ND
27	A	808	CLA	ND
27	A	809	CLA	ND
27	A	810	CLA	ND
27	A	812	CLA	ND
27	A	813	CLA	ND

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Mol	Chain	Res	Type	Atom
27	A	814	CLA	ND
27	A	815	CLA	ND
27	A	816	CLA	ND
27	A	817	CLA	ND
27	A	818	CLA	ND
27	A	819	CLA	ND
27	A	820	CLA	ND
27	A	822	CLA	ND
27	A	823	CLA	ND
27	A	824	CLA	ND
27	A	826	CLA	ND
27	A	827	CLA	ND
27	A	828	CLA	ND
27	A	829	CLA	ND
27	A	831	CLA	ND
27	A	832	CLA	ND
27	A	833	CLA	ND
27	A	834	CLA	ND
27	A	835	CLA	ND
27	A	837	CLA	ND
27	A	838	CLA	ND
27	A	839	CLA	ND
27	A	841	CLA	ND
27	A	842	CLA	ND
27	A	852	CLA	ND
27	A	853	CLA	ND
27	A	855	CLA	ND
27	A	856	CLA	ND
27	B	801	CLA	ND
27	B	802	CLA	ND
27	B	803	CLA	ND
27	B	804	CLA	ND
27	B	805	CLA	ND
27	B	806	CLA	ND
27	B	807	CLA	ND
27	B	808	CLA	ND
27	B	809	CLA	ND
27	B	810	CLA	ND
27	B	811	CLA	ND
27	B	812	CLA	ND
27	B	813	CLA	ND
27	B	814	CLA	ND

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Mol	Chain	Res	Type	Atom
27	B	816	CLA	ND
27	B	818	CLA	ND
27	B	819	CLA	ND
27	B	820	CLA	ND
27	B	821	CLA	ND
27	B	822	CLA	ND
27	B	823	CLA	ND
27	B	824	CLA	ND
27	B	825	CLA	ND
27	B	826	CLA	ND
27	B	827	CLA	ND
27	B	828	CLA	ND
27	B	829	CLA	ND
27	B	830	CLA	ND
27	B	831	CLA	ND
27	B	832	CLA	ND
27	B	833	CLA	ND
27	B	834	CLA	ND
27	B	835	CLA	ND
27	B	836	CLA	ND
27	B	837	CLA	ND
27	B	838	CLA	ND
27	B	839	CLA	ND
27	B	840	CLA	ND
27	F	201	CLA	ND
27	F	202	CLA	ND
27	F	203	CLA	ND
27	J	103	CLA	ND
27	J	105	CLA	ND
27	L	202	CLA	ND
27	L	204	CLA	ND
27	L	206	CLA	ND
27	O	202	CLA	ND
27	O	206	CLA	ND
27	K	101	CLA	ND
27	K	102	CLA	ND
27	s	202	CLA	ND
27	s	206	CLA	ND
27	s	209	CLA	ND
27	c	601	CLA	ND
27	c	602	CLA	ND
27	c	603	CLA	ND

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Mol	Chain	Res	Type	Atom
27	c	605	CLA	ND
27	c	607	CLA	ND
27	c	608	CLA	ND
27	c	609	CLA	ND
27	c	612	CLA	ND
27	a	303	CLA	ND
27	a	304	CLA	ND
27	a	305	CLA	ND
27	a	306	CLA	ND
27	a	308	CLA	ND
27	a	309	CLA	ND
27	a	310	CLA	ND
27	a	311	CLA	ND
27	a	313	CLA	ND
27	b	601	CLA	ND
27	b	602	CLA	ND
27	b	603	CLA	ND
27	b	605	CLA	ND
27	b	606	CLA	ND
27	b	607	CLA	ND
27	b	608	CLA	ND
27	b	610	CLA	ND
27	b	611	CLA	ND
27	h	301	CLA	ND
27	h	302	CLA	ND
27	h	303	CLA	ND
27	h	304	CLA	ND
27	h	305	CLA	ND
27	h	306	CLA	ND
27	h	307	CLA	ND
27	h	308	CLA	ND
27	h	313	CLA	ND
27	m	601	CLA	ND
27	m	602	CLA	ND
27	m	603	CLA	ND
27	m	605	CLA	ND
27	m	606	CLA	ND
27	m	607	CLA	ND
27	m	608	CLA	ND
27	m	609	CLA	ND
27	m	611	CLA	ND
27	m	612	CLA	ND

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Mol	Chain	Res	Type	Atom
27	e	601	CLA	ND
27	e	602	CLA	ND
27	e	603	CLA	ND
27	e	606	CLA	ND
27	e	607	CLA	ND
27	e	608	CLA	ND
27	e	610	CLA	ND
27	l	303	CLA	ND
27	l	304	CLA	ND
27	l	305	CLA	ND
27	l	307	CLA	ND
27	l	308	CLA	ND
27	l	309	CLA	ND
27	l	310	CLA	ND
27	l	312	CLA	ND
27	k	301	CLA	ND
27	k	302	CLA	ND
27	k	303	CLA	ND
27	k	304	CLA	ND
27	k	305	CLA	ND
27	k	306	CLA	ND
27	k	307	CLA	ND
27	k	308	CLA	ND
27	k	309	CLA	ND
27	k	313	CLA	ND
27	f	601	CLA	ND
27	f	602	CLA	ND
27	f	603	CLA	ND
27	f	604	CLA	ND
27	f	607	CLA	ND
27	f	608	CLA	ND
27	f	609	CLA	ND
27	f	610	CLA	ND
27	f	612	CLA	ND
27	i	302	CLA	ND
27	i	303	CLA	ND
27	i	304	CLA	ND
27	i	305	CLA	ND
27	i	306	CLA	ND
27	i	307	CLA	ND
27	i	308	CLA	ND
27	i	309	CLA	ND

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Mol	Chain	Res	Type	Atom
27	i	311	CLA	ND
27	i	312	CLA	ND
27	j	601	CLA	ND
27	j	602	CLA	ND
27	j	603	CLA	ND
27	j	604	CLA	ND
27	j	607	CLA	ND
27	j	608	CLA	ND
27	j	609	CLA	ND
27	j	611	CLA	ND
27	j	612	CLA	ND
27	d	301	CLA	ND
27	d	302	CLA	ND
27	d	303	CLA	ND
27	d	305	CLA	ND
27	d	306	CLA	ND
27	d	308	CLA	ND
27	g	302	CLA	ND
27	g	303	CLA	ND
27	g	304	CLA	ND
27	g	305	CLA	ND
27	g	306	CLA	ND
27	g	308	CLA	ND
27	g	309	CLA	ND
27	g	310	CLA	ND
27	g	311	CLA	ND
27	g	322	CLA	ND
27	R	203	CLA	ND
27	n	601	CLA	ND
27	n	602	CLA	ND
27	n	603	CLA	ND
27	n	604	CLA	ND
27	n	605	CLA	ND
27	n	606	CLA	ND
27	n	607	CLA	ND
27	n	608	CLA	ND
27	n	609	CLA	ND
27	n	610	CLA	ND
27	n	613	CLA	ND

All (3615) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	801	CLA	CBD-CGD-O2D-CED
27	A	802	CLA	C1A-C2A-CAA-CBA
27	A	802	CLA	CBA-CGA-O2A-C1
27	A	802	CLA	O1A-CGA-O2A-C1
27	A	803	CLA	C1A-C2A-CAA-CBA
27	A	803	CLA	C3A-C2A-CAA-CBA
27	A	804	CLA	C3A-C2A-CAA-CBA
27	A	805	CLA	C1A-C2A-CAA-CBA
27	A	807	CLA	CHA-CBD-CGD-O1D
27	A	807	CLA	CHA-CBD-CGD-O2D
27	A	810	CLA	C1A-C2A-CAA-CBA
27	A	810	CLA	C11-C10-C8-C7
27	A	811	CLA	CBA-CGA-O2A-C1
27	A	813	CLA	C1A-C2A-CAA-CBA
27	A	814	CLA	C3A-C2A-CAA-CBA
27	A	815	CLA	CBD-CGD-O2D-CED
27	A	816	CLA	C1A-C2A-CAA-CBA
27	A	816	CLA	CHA-CBD-CGD-O1D
27	A	816	CLA	CHA-CBD-CGD-O2D
27	A	817	CLA	C1A-C2A-CAA-CBA
27	A	817	CLA	C3A-C2A-CAA-CBA
27	A	818	CLA	C1A-C2A-CAA-CBA
27	A	818	CLA	C3A-C2A-CAA-CBA
27	A	822	CLA	C4B-C3B-CAB-CBB
27	A	827	CLA	C11-C12-C13-C14
27	A	829	CLA	CHA-CBD-CGD-O1D
27	A	829	CLA	CHA-CBD-CGD-O2D
27	A	830	CLA	C1A-C2A-CAA-CBA
27	A	831	CLA	C2B-C3B-CAB-CBB
27	A	831	CLA	C4B-C3B-CAB-CBB
27	A	832	CLA	CHA-CBD-CGD-O1D
27	A	832	CLA	CHA-CBD-CGD-O2D
27	A	837	CLA	C3A-C2A-CAA-CBA
27	A	838	CLA	C1A-C2A-CAA-CBA
27	A	839	CLA	C11-C10-C8-C9
27	A	840	CLA	C11-C10-C8-C9
27	A	855	CLA	CBA-CGA-O2A-C1
27	A	855	CLA	O1A-CGA-O2A-C1
27	A	856	CLA	C2B-C3B-CAB-CBB
27	A	856	CLA	C4B-C3B-CAB-CBB
27	A	856	CLA	CBD-CGD-O2D-CED
27	B	801	CLA	CBD-CGD-O2D-CED
27	B	802	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	803	CLA	C3A-C2A-CAA-CBA
27	B	804	CLA	CBD-CGD-O2D-CED
27	B	806	CLA	CHA-CBD-CGD-O1D
27	B	806	CLA	CHA-CBD-CGD-O2D
27	B	806	CLA	C14-C13-C15-C16
27	B	810	CLA	C14-C13-C15-C16
27	B	813	CLA	C1A-C2A-CAA-CBA
27	B	815	CLA	C3A-C2A-CAA-CBA
27	B	819	CLA	C2B-C3B-CAB-CBB
27	B	819	CLA	C4B-C3B-CAB-CBB
27	B	820	CLA	C6-C7-C8-C9
27	B	824	CLA	C1A-C2A-CAA-CBA
27	B	826	CLA	C3A-C2A-CAA-CBA
27	B	830	CLA	C1A-C2A-CAA-CBA
27	B	830	CLA	C2B-C3B-CAB-CBB
27	B	830	CLA	C4B-C3B-CAB-CBB
27	B	831	CLA	C1A-C2A-CAA-CBA
27	B	831	CLA	C3A-C2A-CAA-CBA
27	B	836	CLA	C11-C12-C13-C14
27	B	838	CLA	C1A-C2A-CAA-CBA
27	B	849	CLA	CHA-CBD-CGD-O1D
27	B	849	CLA	CHA-CBD-CGD-O2D
27	F	202	CLA	C11-C12-C13-C14
27	F	203	CLA	C1A-C2A-CAA-CBA
27	F	203	CLA	C3A-C2A-CAA-CBA
27	J	103	CLA	C1A-C2A-CAA-CBA
27	J	105	CLA	CBA-CGA-O2A-C1
27	J	105	CLA	O1A-CGA-O2A-C1
27	J	105	CLA	C2B-C3B-CAB-CBB
27	J	105	CLA	C4B-C3B-CAB-CBB
27	J	105	CLA	C2-C3-C5-C6
27	L	202	CLA	C1A-C2A-CAA-CBA
27	L	202	CLA	C3A-C2A-CAA-CBA
27	L	203	CLA	C11-C12-C13-C14
27	L	204	CLA	C1A-C2A-CAA-CBA
27	L	204	CLA	C3A-C2A-CAA-CBA
27	L	206	CLA	C2-C3-C5-C6
27	L	206	CLA	C4-C3-C5-C6
27	O	202	CLA	C1A-C2A-CAA-CBA
27	O	202	CLA	CBD-CGD-O2D-CED
27	O	202	CLA	C11-C10-C8-C9
27	O	206	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	O	206	CLA	C4B-C3B-CAB-CBB
27	K	101	CLA	C2B-C3B-CAB-CBB
27	K	101	CLA	C4B-C3B-CAB-CBB
27	K	101	CLA	C2-C3-C5-C6
27	K	101	CLA	C4-C3-C5-C6
27	K	102	CLA	CBD-CGD-O2D-CED
27	s	202	CLA	C4B-C3B-CAB-CBB
27	s	203	CLA	C1A-C2A-CAA-CBA
27	s	206	CLA	C1A-C2A-CAA-CBA
27	s	208	CLA	C1A-C2A-CAA-CBA
27	s	208	CLA	C3A-C2A-CAA-CBA
27	s	209	CLA	C2B-C3B-CAB-CBB
27	s	209	CLA	C4B-C3B-CAB-CBB
27	c	601	CLA	C1A-C2A-CAA-CBA
27	c	601	CLA	CHA-CBD-CGD-O1D
27	c	601	CLA	CHA-CBD-CGD-O2D
27	c	602	CLA	C3A-C2A-CAA-CBA
27	c	602	CLA	CHA-CBD-CGD-O1D
27	c	602	CLA	CHA-CBD-CGD-O2D
27	c	605	CLA	C4B-C3B-CAB-CBB
27	c	605	CLA	C2-C3-C5-C6
27	c	605	CLA	C4-C3-C5-C6
27	c	606	CLA	C1A-C2A-CAA-CBA
27	c	606	CLA	CBD-CGD-O2D-CED
27	c	608	CLA	C3A-C2A-CAA-CBA
27	c	608	CLA	CBD-CGD-O2D-CED
27	c	608	CLA	O1D-CGD-O2D-CED
27	c	611	CLA	CBD-CGD-O2D-CED
27	c	612	CLA	CBD-CGD-O2D-CED
27	a	303	CLA	C1A-C2A-CAA-CBA
27	a	303	CLA	C3A-C2A-CAA-CBA
27	a	304	CLA	C1A-C2A-CAA-CBA
27	a	304	CLA	C3A-C2A-CAA-CBA
27	a	305	CLA	C2-C3-C5-C6
27	a	305	CLA	C4-C3-C5-C6
27	a	307	CLA	C2B-C3B-CAB-CBB
27	a	307	CLA	C4B-C3B-CAB-CBB
27	a	308	CLA	CHA-CBD-CGD-O1D
27	a	308	CLA	CHA-CBD-CGD-O2D
27	a	308	CLA	C11-C10-C8-C9
27	a	308	CLA	C14-C13-C15-C16
27	a	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	a	310	CLA	C4B-C3B-CAB-CBB
27	a	311	CLA	CHA-CBD-CGD-O1D
27	a	311	CLA	CHA-CBD-CGD-O2D
27	a	312	CLA	CBA-CGA-O2A-C1
27	a	312	CLA	C4B-C3B-CAB-CBB
27	a	313	CLA	C2B-C3B-CAB-CBB
27	a	313	CLA	C4B-C3B-CAB-CBB
27	b	602	CLA	C3A-C2A-CAA-CBA
27	b	602	CLA	CHA-CBD-CGD-O1D
27	b	602	CLA	CHA-CBD-CGD-O2D
27	b	603	CLA	C4-C3-C5-C6
27	b	603	CLA	C12-C13-C15-C16
27	b	605	CLA	C2B-C3B-CAB-CBB
27	b	605	CLA	C4B-C3B-CAB-CBB
27	b	605	CLA	C6-C7-C8-C9
27	b	606	CLA	C2B-C3B-CAB-CBB
27	b	606	CLA	C4B-C3B-CAB-CBB
27	b	606	CLA	CBD-CGD-O2D-CED
27	b	607	CLA	C2B-C3B-CAB-CBB
27	b	607	CLA	C4B-C3B-CAB-CBB
27	b	608	CLA	CBD-CGD-O2D-CED
27	b	610	CLA	C2B-C3B-CAB-CBB
27	b	610	CLA	C4B-C3B-CAB-CBB
27	b	610	CLA	CBD-CGD-O2D-CED
27	b	611	CLA	CBD-CGD-O2D-CED
27	h	302	CLA	C1A-C2A-CAA-CBA
27	h	303	CLA	C2B-C3B-CAB-CBB
27	h	303	CLA	C4B-C3B-CAB-CBB
27	h	304	CLA	C3A-C2A-CAA-CBA
27	h	304	CLA	CHA-CBD-CGD-O1D
27	h	304	CLA	CHA-CBD-CGD-O2D
27	h	305	CLA	C1A-C2A-CAA-CBA
27	h	305	CLA	C2-C3-C5-C6
27	h	305	CLA	C4-C3-C5-C6
27	h	307	CLA	C4B-C3B-CAB-CBB
27	h	308	CLA	C2B-C3B-CAB-CBB
27	h	308	CLA	C4B-C3B-CAB-CBB
27	h	308	CLA	C2-C3-C5-C6
27	m	602	CLA	C1A-C2A-CAA-CBA
27	m	602	CLA	C3A-C2A-CAA-CBA
27	m	602	CLA	CHA-CBD-CGD-O1D
27	m	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	m	604	CLA	CAD-CBD-CGD-O1D
27	m	604	CLA	CAD-CBD-CGD-O2D
27	m	605	CLA	C1A-C2A-CAA-CBA
27	m	605	CLA	C3A-C2A-CAA-CBA
27	m	607	CLA	C1A-C2A-CAA-CBA
27	m	607	CLA	C3A-C2A-CAA-CBA
27	m	608	CLA	C3A-C2A-CAA-CBA
27	m	609	CLA	C1A-C2A-CAA-CBA
27	m	609	CLA	C2B-C3B-CAB-CBB
27	m	609	CLA	C4B-C3B-CAB-CBB
27	m	611	CLA	CAD-CBD-CGD-O1D
27	m	611	CLA	CAD-CBD-CGD-O2D
27	m	611	CLA	C2-C3-C5-C6
27	m	611	CLA	C4-C3-C5-C6
27	m	612	CLA	C1A-C2A-CAA-CBA
27	m	612	CLA	C3A-C2A-CAA-CBA
27	e	601	CLA	C1A-C2A-CAA-CBA
27	e	601	CLA	C3A-C2A-CAA-CBA
27	e	601	CLA	C2B-C3B-CAB-CBB
27	e	601	CLA	C4B-C3B-CAB-CBB
27	e	602	CLA	C1A-C2A-CAA-CBA
27	e	602	CLA	C3A-C2A-CAA-CBA
27	e	602	CLA	CHA-CBD-CGD-O1D
27	e	602	CLA	CHA-CBD-CGD-O2D
27	e	604	CLA	CBD-CGD-O2D-CED
27	e	605	CLA	C2B-C3B-CAB-CBB
27	e	605	CLA	C4B-C3B-CAB-CBB
27	e	606	CLA	CHA-CBD-CGD-O1D
27	e	606	CLA	CHA-CBD-CGD-O2D
27	e	607	CLA	C1A-C2A-CAA-CBA
27	e	608	CLA	C1A-C2A-CAA-CBA
27	e	608	CLA	C2B-C3B-CAB-CBB
27	e	608	CLA	C4B-C3B-CAB-CBB
27	e	611	CLA	O1A-CGA-O2A-C1
27	e	611	CLA	C2B-C3B-CAB-CBB
27	e	611	CLA	C4B-C3B-CAB-CBB
27	l	303	CLA	C2B-C3B-CAB-CBB
27	l	303	CLA	C4B-C3B-CAB-CBB
27	l	304	CLA	C3A-C2A-CAA-CBA
27	l	304	CLA	C4B-C3B-CAB-CBB
27	l	304	CLA	CHA-CBD-CGD-O1D
27	l	304	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	l	305	CLA	C2-C3-C5-C6
27	l	305	CLA	C4-C3-C5-C6
27	l	306	CLA	CBD-CGD-O2D-CED
27	l	307	CLA	C2B-C3B-CAB-CBB
27	l	307	CLA	C4B-C3B-CAB-CBB
27	l	308	CLA	C1A-C2A-CAA-CBA
27	l	308	CLA	C3A-C2A-CAA-CBA
27	l	309	CLA	C3A-C2A-CAA-CBA
27	l	310	CLA	CBD-CGD-O2D-CED
27	k	301	CLA	C1A-C2A-CAA-CBA
27	k	301	CLA	C3A-C2A-CAA-CBA
27	k	305	CLA	C1A-C2A-CAA-CBA
27	k	305	CLA	C2B-C3B-CAB-CBB
27	k	305	CLA	C4B-C3B-CAB-CBB
27	k	306	CLA	C1A-C2A-CAA-CBA
27	k	306	CLA	CBA-CGA-O2A-C1
27	k	306	CLA	O1A-CGA-O2A-C1
27	k	306	CLA	CBD-CGD-O2D-CED
27	k	306	CLA	C2-C3-C5-C6
27	k	307	CLA	C1A-C2A-CAA-CBA
27	k	307	CLA	C3A-C2A-CAA-CBA
27	k	307	CLA	C2B-C3B-CAB-CBB
27	k	307	CLA	C4B-C3B-CAB-CBB
27	k	308	CLA	CBD-CGD-O2D-CED
27	k	309	CLA	C1A-C2A-CAA-CBA
27	k	309	CLA	C3A-C2A-CAA-CBA
27	k	309	CLA	C2B-C3B-CAB-CBB
27	k	309	CLA	C4B-C3B-CAB-CBB
27	k	309	CLA	CBD-CGD-O2D-CED
27	k	313	CLA	C1A-C2A-CAA-CBA
27	k	313	CLA	C2B-C3B-CAB-CBB
27	k	313	CLA	C4B-C3B-CAB-CBB
27	k	313	CLA	CBD-CGD-O2D-CED
27	k	313	CLA	O1D-CGD-O2D-CED
27	f	602	CLA	C1A-C2A-CAA-CBA
27	f	602	CLA	C3A-C2A-CAA-CBA
27	f	602	CLA	C2B-C3B-CAB-CBB
27	f	602	CLA	C4B-C3B-CAB-CBB
27	f	605	CLA	CBD-CGD-O2D-CED
27	f	606	CLA	C2-C3-C5-C6
27	f	607	CLA	C1A-C2A-CAA-CBA
27	f	607	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	f	610	CLA	C1A-C2A-CAA-CBA
27	f	610	CLA	C3A-C2A-CAA-CBA
27	f	610	CLA	C2B-C3B-CAB-CBB
27	f	610	CLA	C4B-C3B-CAB-CBB
27	f	612	CLA	CBD-CGD-O2D-CED
27	f	612	CLA	C2-C3-C5-C6
27	f	613	CLA	C1A-C2A-CAA-CBA
27	f	613	CLA	C11-C12-C13-C14
27	i	302	CLA	C1A-C2A-CAA-CBA
27	i	302	CLA	C3A-C2A-CAA-CBA
27	i	303	CLA	C3A-C2A-CAA-CBA
27	i	303	CLA	CHA-CBD-CGD-O1D
27	i	303	CLA	CHA-CBD-CGD-O2D
27	i	305	CLA	C6-C7-C8-C9
27	i	309	CLA	C1A-C2A-CAA-CBA
27	i	309	CLA	CBD-CGD-O2D-CED
27	i	311	CLA	C3A-C2A-CAA-CBA
27	i	312	CLA	C1A-C2A-CAA-CBA
27	j	601	CLA	CHA-CBD-CGD-O1D
27	j	601	CLA	CHA-CBD-CGD-O2D
27	j	602	CLA	CHA-CBD-CGD-O1D
27	j	602	CLA	CHA-CBD-CGD-O2D
27	j	604	CLA	C1A-C2A-CAA-CBA
27	j	606	CLA	CHA-CBD-CGD-O1D
27	j	606	CLA	CHA-CBD-CGD-O2D
27	j	609	CLA	C1A-C2A-CAA-CBA
27	j	609	CLA	C3A-C2A-CAA-CBA
27	j	609	CLA	C6-C7-C8-C9
27	j	611	CLA	CBD-CGD-O2D-CED
27	j	611	CLA	C2-C3-C5-C6
27	j	612	CLA	C14-C13-C15-C16
27	d	301	CLA	C1A-C2A-CAA-CBA
27	d	301	CLA	C3A-C2A-CAA-CBA
27	d	302	CLA	CHA-CBD-CGD-O2D
27	d	304	CLA	C2B-C3B-CAB-CBB
27	d	304	CLA	C4B-C3B-CAB-CBB
27	d	304	CLA	CHA-CBD-CGD-O1D
27	d	304	CLA	CHA-CBD-CGD-O2D
27	d	305	CLA	C1A-C2A-CAA-CBA
27	d	305	CLA	C3A-C2A-CAA-CBA
27	d	305	CLA	CBD-CGD-O2D-CED
27	d	306	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	d	308	CLA	CBD-CGD-O2D-CED
27	g	303	CLA	C3A-C2A-CAA-CBA
27	g	303	CLA	CHA-CBD-CGD-O1D
27	g	303	CLA	CHA-CBD-CGD-O2D
27	g	306	CLA	C1A-C2A-CAA-CBA
27	g	310	CLA	CBA-CGA-O2A-C1
27	g	310	CLA	O1A-CGA-O2A-C1
27	g	315	CLA	C2B-C3B-CAB-CBB
27	g	315	CLA	C4B-C3B-CAB-CBB
27	g	322	CLA	CHA-CBD-CGD-O1D
27	g	322	CLA	CHA-CBD-CGD-O2D
27	n	601	CLA	C1A-C2A-CAA-CBA
27	n	601	CLA	C2B-C3B-CAB-CBB
27	n	601	CLA	C4B-C3B-CAB-CBB
27	n	603	CLA	C1A-C2A-CAA-CBA
27	n	603	CLA	C3A-C2A-CAA-CBA
27	n	604	CLA	C1A-C2A-CAA-CBA
27	n	604	CLA	C3A-C2A-CAA-CBA
27	n	605	CLA	C3A-C2A-CAA-CBA
27	n	606	CLA	C1A-C2A-CAA-CBA
27	n	606	CLA	C3A-C2A-CAA-CBA
27	n	606	CLA	CBA-CGA-O2A-C1
27	n	606	CLA	O1A-CGA-O2A-C1
27	n	607	CLA	CHA-CBD-CGD-O1D
27	n	607	CLA	CHA-CBD-CGD-O2D
27	n	608	CLA	C3A-C2A-CAA-CBA
27	n	608	CLA	C4B-C3B-CAB-CBB
27	n	610	CLA	C1A-C2A-CAA-CBA
27	n	610	CLA	C3A-C2A-CAA-CBA
27	n	613	CLA	C1A-C2A-CAA-CBA
27	n	613	CLA	CBD-CGD-O2D-CED
29	A	844	LHG	C4-O6-P-O3
29	A	844	LHG	C4-O6-P-O5
29	A	845	LHG	O1-C1-C2-C3
29	A	845	LHG	C3-O3-P-O5
29	A	850	LHG	C3-O3-P-O5
29	A	850	LHG	C3-O3-P-O6
29	A	850	LHG	C4-O6-P-O3
29	A	850	LHG	C8-C7-O7-C5
29	J	107	LHG	C1-C2-C3-O3
29	J	107	LHG	C3-O3-P-O4
29	J	107	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
29	L	207	LHG	C3-O3-P-O5
29	L	207	LHG	C3-O3-P-O6
29	L	207	LHG	C4-O6-P-O3
29	L	207	LHG	C4-O6-P-O5
29	c	618	LHG	C4-O6-P-O3
29	c	618	LHG	C4-O6-P-O4
29	c	618	LHG	O9-C7-O7-C5
29	c	618	LHG	C8-C7-O7-C5
29	c	621	LHG	O1-C1-C2-C3
29	c	621	LHG	C3-O3-P-O4
29	c	621	LHG	C4-O6-P-O3
29	c	621	LHG	C4-O6-P-O4
29	a	301	LHG	C3-O3-P-O6
29	a	301	LHG	O9-C7-O7-C5
29	a	319	LHG	O7-C5-C6-O8
29	b	617	LHG	C3-O3-P-O4
29	b	617	LHG	C3-O3-P-O6
29	b	617	LHG	O9-C7-O7-C5
29	b	617	LHG	C8-C7-O7-C5
29	m	617	LHG	C4-O6-P-O4
29	e	617	LHG	C4-O6-P-O3
29	e	617	LHG	O9-C7-O7-C5
29	l	318	LHG	C3-O3-P-O6
29	k	319	LHG	C4-O6-P-O3
29	k	319	LHG	C4-O6-P-O4
29	k	319	LHG	C8-C7-O7-C5
29	f	619	LHG	C3-O3-P-O5
29	f	619	LHG	C3-O3-P-O6
29	f	619	LHG	C4-O6-P-O5
29	f	619	LHG	O9-C7-O7-C5
29	i	316	LHG	C3-O3-P-O6
29	i	316	LHG	O9-C7-O7-C5
29	i	316	LHG	C8-C7-O7-C5
29	i	316	LHG	O10-C23-O8-C6
29	i	316	LHG	C24-C23-O8-C6
29	j	617	LHG	C4-O6-P-O3
29	j	617	LHG	C4-O6-P-O4
29	d	315	LHG	C1-C2-C3-O3
29	d	315	LHG	C3-O3-P-O4
29	d	315	LHG	C3-O3-P-O6
29	d	315	LHG	C4-O6-P-O3
29	d	315	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
29	d	315	LHG	C8-C7-O7-C5
29	g	301	LHG	C3-O3-P-O4
29	g	301	LHG	C3-O3-P-O5
29	g	301	LHG	C3-O3-P-O6
29	g	301	LHG	C4-O6-P-O5
29	g	321	LHG	C3-O3-P-O4
29	g	321	LHG	C3-O3-P-O6
29	g	321	LHG	C4-O6-P-O3
29	g	321	LHG	C4-O6-P-O4
29	g	321	LHG	O9-C7-O7-C5
29	g	321	LHG	C8-C7-O7-C5
29	n	619	LHG	C3-O3-P-O6
29	n	619	LHG	C4-O6-P-O3
29	n	619	LHG	C4-O6-P-O4
29	n	619	LHG	C4-O6-P-O5
30	A	847	WVN	C06-C13-C20-C23
30	A	847	WVN	C15-C13-C20-C23
30	A	847	WVN	C20-C23-C25-C27
30	A	847	WVN	C20-C23-C25-C28
30	A	847	WVN	C29-C31-C32-C35
30	A	847	WVN	C29-C31-C32-C36
30	A	847	WVN	C30-C33-C34-C37
30	A	847	WVN	C30-C33-C34-C38
30	A	848	WVN	C05-C02-C11-C19
30	A	848	WVN	C06-C13-C20-C23
30	A	848	WVN	C15-C13-C20-C23
30	A	848	WVN	C30-C33-C34-C37
30	A	849	WVN	C11-C19-C22-C24
30	A	849	WVN	C11-C19-C22-C26
30	A	849	WVN	C29-C31-C32-C35
30	A	849	WVN	C29-C31-C32-C36
30	A	849	WVN	C30-C33-C34-C38
30	B	843	WVN	C29-C31-C32-C35
30	B	843	WVN	C29-C31-C32-C36
30	B	843	WVN	C30-C33-C34-C37
30	B	845	WVN	C25-C28-C30-C33
30	B	845	WVN	C30-C33-C34-C37
30	B	845	WVN	C30-C33-C34-C38
30	B	846	WVN	C15-C13-C20-C23
30	B	846	WVN	C20-C23-C25-C27
30	B	846	WVN	C20-C23-C25-C28
30	B	847	WVN	C11-C19-C22-C24

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Mol	Chain	Res	Type	Atoms
30	B	847	WVN	C11-C19-C22-C26
30	B	847	WVN	C20-C23-C25-C27
30	B	847	WVN	C20-C23-C25-C28
30	B	847	WVN	C30-C33-C34-C37
30	B	847	WVN	C30-C33-C34-C38
30	B	848	WVN	C29-C31-C32-C36
30	F	204	WVN	C11-C19-C22-C24
30	F	204	WVN	C11-C19-C22-C26
30	F	204	WVN	C22-C26-C29-C31
30	F	204	WVN	C29-C31-C32-C36
30	F	205	WVN	C05-C02-C11-C19
30	F	205	WVN	C15-C13-C20-C23
30	I	101	WVN	C01-C02-C11-C19
30	I	101	WVN	C05-C02-C11-C19
30	I	101	WVN	C11-C19-C22-C24
30	I	101	WVN	C11-C19-C22-C26
30	J	101	WVN	C15-C13-C20-C23
30	J	101	WVN	C29-C31-C32-C36
30	J	102	WVN	C11-C19-C22-C24
30	J	102	WVN	C11-C19-C22-C26
30	J	102	WVN	C20-C23-C25-C27
30	J	102	WVN	C20-C23-C25-C28
30	J	102	WVN	C30-C33-C34-C37
30	J	102	WVN	C30-C33-C34-C38
30	L	201	WVN	C05-C02-C11-C19
30	L	201	WVN	C11-C19-C22-C26
30	L	205	WVN	C06-C13-C20-C23
30	L	205	WVN	C11-C19-C22-C24
30	L	205	WVN	C11-C19-C22-C26
30	M	101	WVN	C05-C02-C11-C19
30	M	101	WVN	C20-C23-C25-C27
30	M	101	WVN	C20-C23-C25-C28
30	M	101	WVN	C30-C33-C34-C37
30	M	101	WVN	C30-C33-C34-C38
30	O	201	WVN	C06-C13-C20-C23
30	O	201	WVN	C15-C13-C20-C23
30	O	201	WVN	C20-C23-C25-C27
30	O	201	WVN	C20-C23-C25-C28
30	h	309	WVN	C20-C23-C25-C27
30	h	309	WVN	C20-C23-C25-C28
30	h	309	WVN	C30-C33-C34-C37
30	h	309	WVN	C30-C33-C34-C38

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Mol	Chain	Res	Type	Atoms
30	e	615	WVN	C01-C02-C11-C19
30	e	615	WVN	C05-C02-C11-C19
30	e	615	WVN	C15-C13-C20-C23
30	e	615	WVN	C30-C33-C34-C37
30	l	316	WVN	C15-C13-C20-C23
30	l	316	WVN	C29-C31-C32-C35
30	l	316	WVN	C29-C31-C32-C36
30	i	315	WVN	C29-C31-C32-C36
30	R	202	WVN	C15-C13-C20-C23
30	R	202	WVN	C29-C31-C32-C35
30	R	202	WVN	C29-C31-C32-C36
31	A	851	LMT	O5B-C1B-O1B-C4'
31	A	851	LMT	C2'-C1'-O1'-C1
31	A	851	LMT	O5'-C1'-O1'-C1
31	a	302	LMT	C2'-C1'-O1'-C1
31	a	302	LMT	O5'-C1'-O1'-C1
31	a	320	LMT	C2-C1-O1'-C1'
31	b	616	LMT	O5'-C1'-O1'-C1
34	L	208	LMG	O6-C1-O1-C7
34	s	210	LMG	O7-C8-C9-O8
34	b	619	LMG	O9-C10-O7-C8
34	b	619	LMG	C11-C10-O7-C8
35	J	104	II0	C25-C29-C31-C33
35	J	104	II0	C32-C34-C36-C38
35	J	104	II0	C32-C34-C36-C40
35	c	617	II0	C32-C34-C36-C40
35	a	318	II0	C25-C29-C31-C33
35	a	318	II0	C31-C33-C35-C37
35	a	318	II0	C31-C33-C35-C39
35	a	318	II0	C35-C39-C41-C42
35	b	613	II0	C31-C33-C35-C39
35	h	311	II0	C26-C30-C32-C34
35	h	311	II0	C32-C34-C36-C40
35	h	312	II0	C25-C29-C31-C33
35	m	613	II0	C32-C34-C36-C38
35	m	613	II0	C32-C34-C36-C40
35	e	612	II0	C26-C30-C32-C34
35	e	612	II0	C32-C34-C36-C38
35	e	612	II0	C32-C34-C36-C40
35	e	614	II0	C32-C34-C36-C38
35	e	614	II0	C32-C34-C36-C40
35	l	302	II0	C31-C33-C35-C37

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Mol	Chain	Res	Type	Atoms
35	l	302	II0	C31-C33-C35-C39
35	l	302	II0	C32-C34-C36-C38
35	l	302	II0	C32-C34-C36-C40
35	l	313	II0	C32-C34-C36-C38
35	l	313	II0	C32-C34-C36-C40
35	l	314	II0	C31-C33-C35-C39
35	l	315	II0	C32-C34-C36-C38
35	l	315	II0	C32-C34-C36-C40
35	l	317	II0	C32-C34-C36-C38
35	l	317	II0	C32-C34-C36-C40
35	k	315	II0	C25-C29-C31-C33
35	k	315	II0	C31-C33-C35-C39
35	k	315	II0	C32-C34-C36-C38
35	k	315	II0	C32-C34-C36-C40
35	k	316	II0	C25-C29-C31-C33
35	k	318	II0	C31-C33-C35-C37
35	k	318	II0	C31-C33-C35-C39
35	f	615	II0	C32-C34-C36-C40
35	f	616	II0	C31-C33-C35-C37
35	f	616	II0	C31-C33-C35-C39
35	f	618	II0	C25-C29-C31-C33
35	f	618	II0	C32-C34-C36-C40
35	i	313	II0	C32-C34-C36-C38
35	i	313	II0	C32-C34-C36-C40
35	i	314	II0	C32-C34-C36-C40
35	i	318	II0	C31-C33-C35-C37
35	i	318	II0	C31-C33-C35-C39
35	j	615	II0	C31-C33-C35-C37
35	j	615	II0	C31-C33-C35-C39
35	j	615	II0	C32-C34-C36-C38
35	j	615	II0	C32-C34-C36-C40
35	d	313	II0	C26-C30-C32-C34
35	d	313	II0	C31-C33-C35-C39
35	d	313	II0	C32-C34-C36-C38
35	d	313	II0	C32-C34-C36-C40
35	g	317	II0	C32-C34-C36-C40
35	g	320	II0	C32-C34-C36-C38
35	g	320	II0	C32-C34-C36-C40
35	n	615	II0	C31-C33-C35-C39
35	n	618	II0	C31-C33-C35-C37
35	n	618	II0	C31-C33-C35-C39
36	O	204	IHT	C18-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
36	O	204	IHT	C30-C32-C33-C36
36	O	204	IHT	C30-C32-C33-C37
36	c	616	IHT	C30-C32-C33-C37
36	c	620	IHT	C31-C34-C35-C38
36	c	620	IHT	C31-C34-C35-C39
36	b	614	IHT	C10-C07-C18-C22
36	m	616	IHT	C31-C34-C35-C38
36	f	617	IHT	C23-C27-C30-C32
36	f	617	IHT	C30-C32-C33-C36
36	f	617	IHT	C30-C32-C33-C37
36	j	616	IHT	C30-C32-C33-C36
36	j	616	IHT	C30-C32-C33-C37
37	s	201	KC2	C3A-C2A-CAA-CBA
37	s	201	KC2	C2C-C3C-CAC-CBC
37	s	201	KC2	C4C-C3C-CAC-CBC
37	s	201	KC2	C2A-CAA-CBA-CGA
37	s	204	KC2	C3A-C2A-CAA-CBA
37	c	610	KC2	C3A-C2A-CAA-CBA
37	c	610	KC2	C2C-C3C-CAC-CBC
37	c	610	KC2	C4C-C3C-CAC-CBC
37	c	610	KC2	CHA-CBD-CGD-O1D
37	c	610	KC2	CHA-CBD-CGD-O2D
37	m	610	KC2	C2C-C3C-CAC-CBC
37	m	610	KC2	C4C-C3C-CAC-CBC
37	e	609	KC2	C2C-C3C-CAC-CBC
37	e	609	KC2	CBD-CGD-O2D-CED
37	l	311	KC2	C2C-C3C-CAC-CBC
37	k	310	KC2	C2C-C3C-CAC-CBC
37	k	310	KC2	C4C-C3C-CAC-CBC
37	k	310	KC2	CHA-CBD-CGD-O2D
37	k	311	KC2	C2B-C3B-CAB-CBB
37	k	311	KC2	C4B-C3B-CAB-CBB
37	k	311	KC2	C2C-C3C-CAC-CBC
37	k	311	KC2	C4C-C3C-CAC-CBC
37	k	311	KC2	CBD-CGD-O2D-CED
37	k	312	KC2	C2C-C3C-CAC-CBC
37	k	312	KC2	C4C-C3C-CAC-CBC
37	k	312	KC2	C2A-CAA-CBA-CGA
37	k	312	KC2	CAD-CBD-CGD-O1D
37	k	312	KC2	CAD-CBD-CGD-O2D
37	f	611	KC2	C2C-C3C-CAC-CBC
37	f	611	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
37	i	310	KC2	C1A-C2A-CAA-CBA
37	i	310	KC2	C2B-C3B-CAB-CBB
37	i	310	KC2	C2C-C3C-CAC-CBC
37	i	310	KC2	C4C-C3C-CAC-CBC
37	i	310	KC2	CAA-CBA-CGA-O2A
37	i	317	KC2	C2B-C3B-CAB-CBB
37	i	317	KC2	C2C-C3C-CAC-CBC
37	i	317	KC2	C4C-C3C-CAC-CBC
37	i	317	KC2	CHA-CBD-CGD-O2D
37	j	610	KC2	C3A-C2A-CAA-CBA
37	d	309	KC2	C2C-C3C-CAC-CBC
37	d	309	KC2	CHA-CBD-CGD-O2D
37	d	310	KC2	C2C-C3C-CAC-CBC
37	d	310	KC2	C4C-C3C-CAC-CBC
37	g	312	KC2	C3A-C2A-CAA-CBA
37	g	312	KC2	C2C-C3C-CAC-CBC
37	g	312	KC2	C4C-C3C-CAC-CBC
37	g	313	KC2	C2C-C3C-CAC-CBC
37	g	314	KC2	C3A-C2A-CAA-CBA
37	g	314	KC2	C2C-C3C-CAC-CBC
37	n	611	KC2	C1A-C2A-CAA-CBA
37	n	611	KC2	C3A-C2A-CAA-CBA
37	n	611	KC2	C2C-C3C-CAC-CBC
37	n	612	KC2	C3A-C2A-CAA-CBA
37	n	612	KC2	C2C-C3C-CAC-CBC
37	n	612	KC2	C4C-C3C-CAC-CBC
37	n	612	KC2	C2A-CAA-CBA-CGA
37	n	612	KC2	CHA-CBD-CGD-O1D
37	n	612	KC2	CHA-CBD-CGD-O2D
38	i	301	LMU	C2'-C1'-O1'-C1
27	A	801	CLA	O1D-CGD-O2D-CED
27	A	815	CLA	O1D-CGD-O2D-CED
27	B	801	CLA	O1D-CGD-O2D-CED
27	c	603	CLA	O1D-CGD-O2D-CED
27	m	612	CLA	O1D-CGD-O2D-CED
27	k	306	CLA	O1D-CGD-O2D-CED
37	e	609	KC2	O1D-CGD-O2D-CED
37	k	311	KC2	O1D-CGD-O2D-CED
27	K	102	CLA	O1D-CGD-O2D-CED
27	f	613	CLA	O1D-CGD-O2D-CED
27	i	309	CLA	O1D-CGD-O2D-CED
27	i	312	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	d	305	CLA	O1D-CGD-O2D-CED
37	k	310	KC2	O1D-CGD-O2D-CED
27	A	813	CLA	CBD-CGD-O2D-CED
27	A	816	CLA	CBD-CGD-O2D-CED
27	A	839	CLA	CBD-CGD-O2D-CED
27	F	203	CLA	CBD-CGD-O2D-CED
27	J	103	CLA	CBD-CGD-O2D-CED
27	s	203	CLA	CBD-CGD-O2D-CED
27	c	602	CLA	CBD-CGD-O2D-CED
27	c	603	CLA	CBD-CGD-O2D-CED
27	c	604	CLA	CBD-CGD-O2D-CED
27	b	601	CLA	CBD-CGD-O2D-CED
27	h	302	CLA	CBD-CGD-O2D-CED
27	m	612	CLA	CBD-CGD-O2D-CED
27	e	607	CLA	CBD-CGD-O2D-CED
27	k	305	CLA	CBD-CGD-O2D-CED
27	k	307	CLA	CBD-CGD-O2D-CED
27	f	606	CLA	CBD-CGD-O2D-CED
27	f	613	CLA	CBD-CGD-O2D-CED
27	i	303	CLA	CBD-CGD-O2D-CED
27	i	308	CLA	CBD-CGD-O2D-CED
27	i	311	CLA	CBD-CGD-O2D-CED
27	i	312	CLA	CBD-CGD-O2D-CED
27	j	604	CLA	CBD-CGD-O2D-CED
27	j	606	CLA	CBD-CGD-O2D-CED
27	j	608	CLA	CBD-CGD-O2D-CED
27	j	609	CLA	CBD-CGD-O2D-CED
27	j	612	CLA	CBD-CGD-O2D-CED
27	d	302	CLA	CBD-CGD-O2D-CED
27	d	311	CLA	CBD-CGD-O2D-CED
27	g	302	CLA	CBD-CGD-O2D-CED
27	g	305	CLA	CBD-CGD-O2D-CED
27	g	310	CLA	CBD-CGD-O2D-CED
27	n	603	CLA	CBD-CGD-O2D-CED
37	k	310	KC2	CBD-CGD-O2D-CED
27	A	811	CLA	O1A-CGA-O2A-C1
27	A	842	CLA	O1A-CGA-O2A-C1
27	B	849	CLA	O1A-CGA-O2A-C1
27	F	202	CLA	O1A-CGA-O2A-C1
27	O	206	CLA	O1A-CGA-O2A-C1
27	c	601	CLA	O1A-CGA-O2A-C1
27	a	311	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	a	312	CLA	O1A-CGA-O2A-C1
27	h	302	CLA	O1A-CGA-O2A-C1
27	e	606	CLA	O1A-CGA-O2A-C1
27	l	307	CLA	O1A-CGA-O2A-C1
27	l	308	CLA	O1A-CGA-O2A-C1
27	i	306	CLA	O1A-CGA-O2A-C1
29	A	850	LHG	O10-C23-O8-C6
29	e	617	LHG	O10-C23-O8-C6
27	d	306	CLA	O1A-CGA-O2A-C1
27	m	612	CLA	C4C-C3C-CAC-CBC
27	B	802	CLA	C2C-C3C-CAC-CBC
27	A	856	CLA	O1D-CGD-O2D-CED
27	f	610	CLA	C5-C6-C7-C8
38	i	301	LMU	O5B-C1B-O1B-C4'
27	s	203	CLA	O1D-CGD-O2D-CED
27	h	302	CLA	O1D-CGD-O2D-CED
27	k	308	CLA	O1D-CGD-O2D-CED
27	A	842	CLA	CBA-CGA-O2A-C1
27	a	311	CLA	CBA-CGA-O2A-C1
27	h	302	CLA	CBA-CGA-O2A-C1
27	e	606	CLA	CBA-CGA-O2A-C1
27	l	307	CLA	CBA-CGA-O2A-C1
27	i	306	CLA	CBA-CGA-O2A-C1
29	A	850	LHG	C24-C23-O8-C6
29	e	617	LHG	C24-C23-O8-C6
27	b	609	CLA	CBD-CGD-O2D-CED
27	A	803	CLA	O1A-CGA-O2A-C1
27	A	821	CLA	O1A-CGA-O2A-C1
27	B	809	CLA	O1A-CGA-O2A-C1
27	B	811	CLA	O1A-CGA-O2A-C1
27	B	829	CLA	O1A-CGA-O2A-C1
27	h	303	CLA	O1A-CGA-O2A-C1
27	h	305	CLA	O1A-CGA-O2A-C1
27	j	611	CLA	O1A-CGA-O2A-C1
29	c	618	LHG	O10-C23-O8-C6
34	b	619	LMG	O10-C28-O8-C9
27	e	604	CLA	C10-C11-C12-C13
27	B	804	CLA	O1D-CGD-O2D-CED
27	O	202	CLA	O1D-CGD-O2D-CED
27	c	611	CLA	O1D-CGD-O2D-CED
27	c	612	CLA	O1D-CGD-O2D-CED
27	b	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	b	610	CLA	O1D-CGD-O2D-CED
27	k	305	CLA	O1D-CGD-O2D-CED
27	j	608	CLA	O1D-CGD-O2D-CED
27	c	606	CLA	O1D-CGD-O2D-CED
27	b	608	CLA	O1D-CGD-O2D-CED
27	l	306	CLA	O1D-CGD-O2D-CED
27	k	309	CLA	O1D-CGD-O2D-CED
27	f	605	CLA	O1D-CGD-O2D-CED
27	f	612	CLA	O1D-CGD-O2D-CED
27	j	611	CLA	O1D-CGD-O2D-CED
27	d	308	CLA	O1D-CGD-O2D-CED
27	n	613	CLA	O1D-CGD-O2D-CED
27	A	835	CLA	O1A-CGA-O2A-C1
27	b	606	CLA	O1A-CGA-O2A-C1
27	m	612	CLA	C2C-C3C-CAC-CBC
29	d	315	LHG	O9-C7-O7-C5
27	l	310	CLA	O1D-CGD-O2D-CED
27	c	607	CLA	CBA-CGA-O2A-C1
27	c	607	CLA	O1A-CGA-O2A-C1
27	A	802	CLA	C3-C5-C6-C7
27	A	820	CLA	C3-C5-C6-C7
27	A	841	CLA	C3-C5-C6-C7
27	B	806	CLA	C3-C5-C6-C7
27	B	821	CLA	C3-C5-C6-C7
27	B	829	CLA	C3-C5-C6-C7
27	B	835	CLA	C3-C5-C6-C7
27	b	607	CLA	C3-C5-C6-C7
27	e	605	CLA	C3-C5-C6-C7
27	l	304	CLA	C3-C5-C6-C7
27	k	307	CLA	C3-C5-C6-C7
27	f	610	CLA	C3-C5-C6-C7
28	A	843	PQN	C13-C15-C16-C17
28	B	841	PQN	C13-C15-C16-C17
27	B	802	CLA	O1D-CGD-O2D-CED
27	g	305	CLA	O1D-CGD-O2D-CED
27	A	803	CLA	CBA-CGA-O2A-C1
27	A	821	CLA	CBA-CGA-O2A-C1
27	B	849	CLA	CBA-CGA-O2A-C1
27	F	202	CLA	CBA-CGA-O2A-C1
27	O	206	CLA	CBA-CGA-O2A-C1
27	b	601	CLA	CBA-CGA-O2A-C1
27	h	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	h	305	CLA	CBA-CGA-O2A-C1
27	e	611	CLA	CBA-CGA-O2A-C1
27	l	308	CLA	CBA-CGA-O2A-C1
27	f	610	CLA	CBA-CGA-O2A-C1
27	j	606	CLA	CBA-CGA-O2A-C1
27	j	611	CLA	CBA-CGA-O2A-C1
27	g	308	CLA	CBA-CGA-O2A-C1
31	b	616	LMT	O5'-C5'-C6'-O6'
38	i	301	LMU	O5'-C5'-C6'-O6'
27	A	814	CLA	CBD-CGD-O2D-CED
27	A	840	CLA	CBD-CGD-O2D-CED
27	B	818	CLA	CBD-CGD-O2D-CED
27	B	838	CLA	CBD-CGD-O2D-CED
27	L	202	CLA	CBD-CGD-O2D-CED
27	s	206	CLA	CBD-CGD-O2D-CED
27	a	306	CLA	CBD-CGD-O2D-CED
27	m	605	CLA	CBD-CGD-O2D-CED
27	e	602	CLA	CBD-CGD-O2D-CED
27	l	304	CLA	CBD-CGD-O2D-CED
27	l	312	CLA	CBD-CGD-O2D-CED
27	i	307	CLA	CBD-CGD-O2D-CED
27	j	605	CLA	CBD-CGD-O2D-CED
27	g	307	CLA	CBD-CGD-O2D-CED
27	g	311	CLA	CBD-CGD-O2D-CED
27	g	315	CLA	CBD-CGD-O2D-CED
27	n	601	CLA	CBD-CGD-O2D-CED
37	k	312	KC2	CBD-CGD-O2D-CED
29	a	301	LHG	C8-C7-O7-C5
29	e	617	LHG	C8-C7-O7-C5
29	f	619	LHG	C8-C7-O7-C5
27	e	604	CLA	O1D-CGD-O2D-CED
27	A	814	CLA	O1A-CGA-O2A-C1
27	b	611	CLA	O1D-CGD-O2D-CED
27	A	811	CLA	C4-C3-C5-C6
27	A	829	CLA	C4-C3-C5-C6
27	A	835	CLA	C4-C3-C5-C6
27	A	838	CLA	C4-C3-C5-C6
27	A	841	CLA	C4-C3-C5-C6
27	B	820	CLA	C4-C3-C5-C6
27	b	608	CLA	C4-C3-C5-C6
27	l	312	CLA	C4-C3-C5-C6
27	n	609	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	829	CLA	C2-C3-C5-C6
27	A	838	CLA	C2-C3-C5-C6
27	A	841	CLA	C2-C3-C5-C6
27	b	603	CLA	C2-C3-C5-C6
27	b	608	CLA	C2-C3-C5-C6
27	n	609	CLA	C2-C3-C5-C6
27	j	607	CLA	CBD-CGD-O2D-CED
27	B	807	CLA	C2A-CAA-CBA-CGA
27	a	312	CLA	C2A-CAA-CBA-CGA
27	A	823	CLA	O1A-CGA-O2A-C1
27	g	308	CLA	O1A-CGA-O2A-C1
27	O	202	CLA	C3-C5-C6-C7
27	g	322	CLA	C3-C5-C6-C7
27	B	835	CLA	C2C-C3C-CAC-CBC
27	A	823	CLA	CBA-CGA-O2A-C1
27	A	830	CLA	CBA-CGA-O2A-C1
27	A	835	CLA	CBA-CGA-O2A-C1
27	B	801	CLA	CBA-CGA-O2A-C1
27	B	809	CLA	CBA-CGA-O2A-C1
27	B	811	CLA	CBA-CGA-O2A-C1
27	B	813	CLA	CBA-CGA-O2A-C1
27	B	829	CLA	CBA-CGA-O2A-C1
27	B	836	CLA	CBA-CGA-O2A-C1
27	c	601	CLA	CBA-CGA-O2A-C1
27	c	606	CLA	CBA-CGA-O2A-C1
27	c	608	CLA	CBA-CGA-O2A-C1
27	b	606	CLA	CBA-CGA-O2A-C1
27	f	602	CLA	CBA-CGA-O2A-C1
27	f	607	CLA	CBA-CGA-O2A-C1
27	i	307	CLA	CBA-CGA-O2A-C1
27	g	322	CLA	CBA-CGA-O2A-C1
27	n	609	CLA	CBA-CGA-O2A-C1
29	c	618	LHG	C24-C23-O8-C6
34	b	619	LMG	C29-C28-O8-C9
30	I	101	WVN	C22-C26-C29-C31
35	J	104	II0	C26-C30-C32-C34
35	O	203	II0	C25-C29-C31-C33
35	c	615	II0	C36-C40-C42-C41
35	c	617	II0	C26-C30-C32-C34
35	h	311	II0	C36-C40-C42-C41
35	m	613	II0	C26-C30-C32-C34
35	e	614	II0	C26-C30-C32-C34

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Mol	Chain	Res	Type	Atoms
35	e	616	II0	C36-C40-C42-C41
35	f	614	II0	C26-C30-C32-C34
35	j	615	II0	C25-C29-C31-C33
35	j	615	II0	C36-C40-C42-C41
36	b	614	IHT	C26-C29-C31-C34
27	A	841	CLA	O1A-CGA-O2A-C1
27	B	827	CLA	O1A-CGA-O2A-C1
27	B	836	CLA	O1A-CGA-O2A-C1
27	c	605	CLA	O1A-CGA-O2A-C1
27	c	608	CLA	O1A-CGA-O2A-C1
27	b	601	CLA	O1A-CGA-O2A-C1
27	f	602	CLA	O1A-CGA-O2A-C1
27	f	610	CLA	O1A-CGA-O2A-C1
29	A	850	LHG	O9-C7-O7-C5
29	k	319	LHG	O9-C7-O7-C5
27	k	307	CLA	O1D-CGD-O2D-CED
27	J	103	CLA	O1D-CGD-O2D-CED
37	e	609	KC2	CAA-CBA-CGA-O2A
37	i	310	KC2	CAA-CBA-CGA-O1A
27	A	829	CLA	C3-C5-C6-C7
27	B	812	CLA	C3-C5-C6-C7
27	e	611	CLA	C3-C5-C6-C7
27	c	607	CLA	CBD-CGD-O2D-CED
27	a	313	CLA	CBD-CGD-O2D-CED
27	h	301	CLA	CBD-CGD-O2D-CED
27	h	306	CLA	CBD-CGD-O2D-CED
29	J	107	LHG	O2-C2-C3-O3
29	d	315	LHG	O2-C2-C3-O3
27	A	816	CLA	O1D-CGD-O2D-CED
27	i	303	CLA	O1D-CGD-O2D-CED
27	i	308	CLA	O1D-CGD-O2D-CED
27	i	311	CLA	O1D-CGD-O2D-CED
27	d	311	CLA	O1D-CGD-O2D-CED
27	A	818	CLA	CBA-CGA-O2A-C1
27	A	841	CLA	CBA-CGA-O2A-C1
27	b	611	CLA	CBA-CGA-O2A-C1
27	k	305	CLA	CBA-CGA-O2A-C1
27	f	613	CLA	CBA-CGA-O2A-C1
27	d	311	CLA	CBA-CGA-O2A-C1
27	n	605	CLA	CBA-CGA-O2A-C1
29	g	301	LHG	C24-C23-O8-C6
27	j	606	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	g	322	CLA	O1A-CGA-O2A-C1
27	A	839	CLA	O1D-CGD-O2D-CED
31	b	616	LMT	C4'-C5'-C6'-O6'
38	i	301	LMU	C4'-C5'-C6'-O6'
27	s	209	CLA	CBD-CGD-O2D-CED
27	k	301	CLA	CBD-CGD-O2D-CED
29	e	617	LHG	C26-C27-C28-C29
27	b	607	CLA	C2C-C3C-CAC-CBC
27	F	203	CLA	O1D-CGD-O2D-CED
27	c	604	CLA	O1D-CGD-O2D-CED
27	e	607	CLA	O1D-CGD-O2D-CED
27	f	606	CLA	O1D-CGD-O2D-CED
27	B	810	CLA	C3-C5-C6-C7
27	a	308	CLA	C3-C5-C6-C7
27	l	310	CLA	C3-C5-C6-C7
27	a	309	CLA	CBD-CGD-O2D-CED
27	m	603	CLA	CBD-CGD-O2D-CED
27	f	601	CLA	CBD-CGD-O2D-CED
27	f	602	CLA	CBD-CGD-O2D-CED
27	j	604	CLA	O1D-CGD-O2D-CED
27	j	612	CLA	O1D-CGD-O2D-CED
27	g	310	CLA	O1D-CGD-O2D-CED
27	A	814	CLA	CBA-CGA-O2A-C1
27	B	827	CLA	CBA-CGA-O2A-C1
27	c	605	CLA	CBA-CGA-O2A-C1
27	B	835	CLA	C4-C3-C5-C6
27	O	206	CLA	C4-C3-C5-C6
27	c	606	CLA	C4-C3-C5-C6
27	b	610	CLA	C4-C3-C5-C6
27	f	602	CLA	C4-C3-C5-C6
27	f	607	CLA	C4-C3-C5-C6
27	f	610	CLA	C4-C3-C5-C6
27	A	811	CLA	C2-C3-C5-C6
27	A	816	CLA	C2-C3-C5-C6
27	A	855	CLA	C2-C3-C5-C6
27	B	820	CLA	C2-C3-C5-C6
27	B	835	CLA	C2-C3-C5-C6
27	O	206	CLA	C2-C3-C5-C6
27	b	610	CLA	C2-C3-C5-C6
27	l	312	CLA	C2-C3-C5-C6
27	f	607	CLA	C2-C3-C5-C6
27	f	610	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	818	CLA	O1A-CGA-O2A-C1
27	B	801	CLA	O1A-CGA-O2A-C1
27	B	813	CLA	O1A-CGA-O2A-C1
27	c	606	CLA	O1A-CGA-O2A-C1
27	b	611	CLA	O1A-CGA-O2A-C1
27	f	607	CLA	O1A-CGA-O2A-C1
27	f	613	CLA	O1A-CGA-O2A-C1
27	i	307	CLA	O1A-CGA-O2A-C1
27	d	311	CLA	O1A-CGA-O2A-C1
29	g	301	LHG	O10-C23-O8-C6
34	b	619	LMG	O6-C5-C6-O5
27	c	602	CLA	O1D-CGD-O2D-CED
27	d	307	CLA	CBD-CGD-O2D-CED
37	j	610	KC2	CBD-CGD-O2D-CED
27	A	821	CLA	C2A-CAA-CBA-CGA
27	A	842	CLA	C2A-CAA-CBA-CGA
27	b	609	CLA	O1D-CGD-O2D-CED
27	d	302	CLA	O1D-CGD-O2D-CED
27	B	803	CLA	O1A-CGA-O2A-C1
27	k	305	CLA	O1A-CGA-O2A-C1
34	s	210	LMG	O6-C1-O1-C7
34	c	619	LMG	O6-C1-O1-C7
31	A	851	LMT	C4'-C5'-C6'-O6'
27	A	813	CLA	O1D-CGD-O2D-CED
27	b	601	CLA	O1D-CGD-O2D-CED
27	j	606	CLA	O1D-CGD-O2D-CED
27	A	801	CLA	CBA-CGA-O2A-C1
27	B	815	CLA	CBA-CGA-O2A-C1
27	n	607	CLA	CBA-CGA-O2A-C1
29	f	619	LHG	C28-C29-C30-C31
27	A	805	CLA	CBD-CGD-O2D-CED
27	A	817	CLA	CBD-CGD-O2D-CED
27	A	818	CLA	CBD-CGD-O2D-CED
27	A	832	CLA	CBD-CGD-O2D-CED
27	A	837	CLA	CBD-CGD-O2D-CED
27	B	807	CLA	CBD-CGD-O2D-CED
27	c	601	CLA	CBD-CGD-O2D-CED
27	a	307	CLA	CBD-CGD-O2D-CED
27	h	313	CLA	CBD-CGD-O2D-CED
27	k	303	CLA	CBD-CGD-O2D-CED
27	g	322	CLA	CBD-CGD-O2D-CED
27	n	605	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	i	310	KC2	CBD-CGD-O2D-CED
37	i	317	KC2	CBD-CGD-O2D-CED
27	A	818	CLA	C4C-C3C-CAC-CBC
27	n	605	CLA	O1A-CGA-O2A-C1
31	a	320	LMT	C11-C10-C9-C8
27	n	603	CLA	O1D-CGD-O2D-CED
31	a	320	LMT	C4B-C5B-C6B-O6B
29	l	318	LHG	C24-C25-C26-C27
27	B	829	CLA	CBD-CGD-O2D-CED
27	B	849	CLA	CBD-CGD-O2D-CED
34	J	106	LMG	C28-C29-C30-C31
30	e	615	WVN	C25-C28-C30-C33
30	l	316	WVN	C22-C26-C29-C31
30	R	202	WVN	C22-C26-C29-C31
35	h	311	II0	C35-C39-C41-C42
35	e	613	II0	C25-C29-C31-C33
35	l	302	II0	C25-C29-C31-C33
35	l	313	II0	C26-C30-C32-C34
35	k	318	II0	C25-C29-C31-C33
35	f	616	II0	C25-C29-C31-C33
35	i	313	II0	C26-C30-C32-C34
35	j	613	II0	C26-C30-C32-C34
35	d	312	II0	C25-C29-C31-C33
35	g	316	II0	C26-C30-C32-C34
35	g	320	II0	C26-C30-C32-C34
35	n	615	II0	C25-C29-C31-C33
36	c	616	IHT	C26-C29-C31-C34
36	c	620	IHT	C26-C29-C31-C34
27	A	830	CLA	O1A-CGA-O2A-C1
27	B	815	CLA	O1A-CGA-O2A-C1
27	B	837	CLA	O1A-CGA-O2A-C1
27	n	609	CLA	O1A-CGA-O2A-C1
29	b	618	LHG	C1-C2-C3-O3
27	A	822	CLA	CBA-CGA-O2A-C1
27	A	837	CLA	CBA-CGA-O2A-C1
27	B	803	CLA	CBA-CGA-O2A-C1
27	B	807	CLA	CBA-CGA-O2A-C1
27	B	825	CLA	CBA-CGA-O2A-C1
27	B	826	CLA	CBA-CGA-O2A-C1
27	B	837	CLA	CBA-CGA-O2A-C1
27	F	203	CLA	CBA-CGA-O2A-C1
27	L	203	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	s	208	CLA	CBA-CGA-O2A-C1
27	a	310	CLA	CBA-CGA-O2A-C1
27	m	602	CLA	CBA-CGA-O2A-C1
27	e	607	CLA	CBA-CGA-O2A-C1
27	k	309	CLA	CBA-CGA-O2A-C1
27	f	603	CLA	CBA-CGA-O2A-C1
27	i	303	CLA	CBA-CGA-O2A-C1
27	j	609	CLA	CBA-CGA-O2A-C1
27	g	306	CLA	CBA-CGA-O2A-C1
29	k	319	LHG	C24-C23-O8-C6
29	g	321	LHG	C24-C23-O8-C6
34	c	619	LMG	C29-C28-O8-C9
29	b	617	LHG	C26-C27-C28-C29
29	f	619	LHG	C33-C34-C35-C36
27	e	611	CLA	CBD-CGD-O2D-CED
27	A	814	CLA	O1D-CGD-O2D-CED
27	l	304	CLA	O1D-CGD-O2D-CED
27	j	609	CLA	O1D-CGD-O2D-CED
37	s	201	KC2	CAA-CBA-CGA-O2A
37	f	611	KC2	CAA-CBA-CGA-O2A
27	A	816	CLA	C4-C3-C5-C6
27	A	855	CLA	C4-C3-C5-C6
27	b	606	CLA	C4-C3-C5-C6
27	A	835	CLA	C2-C3-C5-C6
27	c	606	CLA	C2-C3-C5-C6
27	b	606	CLA	C2-C3-C5-C6
27	f	602	CLA	C2-C3-C5-C6
27	b	604	CLA	C3-C5-C6-C7
27	A	802	CLA	C11-C10-C8-C9
27	A	806	CLA	C11-C12-C13-C14
27	A	809	CLA	C6-C7-C8-C9
27	A	812	CLA	C11-C12-C13-C14
27	A	817	CLA	C11-C10-C8-C9
27	A	839	CLA	C11-C12-C13-C14
27	A	840	CLA	C14-C13-C15-C16
27	A	841	CLA	C14-C13-C15-C16
27	A	842	CLA	C14-C13-C15-C16
27	A	853	CLA	C14-C13-C15-C16
27	B	801	CLA	C11-C12-C13-C14
27	B	804	CLA	C11-C10-C8-C9
27	B	805	CLA	C6-C7-C8-C9
27	B	812	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	B	820	CLA	C11-C12-C13-C14
27	B	821	CLA	C11-C10-C8-C9
27	B	834	CLA	C11-C12-C13-C14
27	B	835	CLA	C6-C7-C8-C9
27	B	838	CLA	C11-C12-C13-C14
27	B	838	CLA	C14-C13-C15-C16
27	F	202	CLA	C11-C10-C8-C9
27	L	203	CLA	C6-C7-C8-C9
27	c	608	CLA	C11-C10-C8-C9
27	c	608	CLA	C14-C13-C15-C16
27	a	309	CLA	C6-C7-C8-C9
27	a	312	CLA	C11-C12-C13-C14
27	a	312	CLA	C14-C13-C15-C16
27	b	605	CLA	C14-C13-C15-C16
27	b	607	CLA	C14-C13-C15-C16
27	b	611	CLA	C11-C12-C13-C14
27	h	306	CLA	C11-C10-C8-C9
27	e	605	CLA	C11-C10-C8-C9
27	e	606	CLA	C6-C7-C8-C9
27	e	606	CLA	C11-C10-C8-C9
27	e	607	CLA	C11-C10-C8-C9
27	e	607	CLA	C14-C13-C15-C16
27	e	610	CLA	C11-C12-C13-C14
27	k	307	CLA	C11-C10-C8-C9
27	f	607	CLA	C6-C7-C8-C9
27	f	607	CLA	C11-C12-C13-C14
27	f	609	CLA	C11-C10-C8-C9
27	i	305	CLA	C11-C12-C13-C14
27	j	604	CLA	C11-C10-C8-C9
27	g	308	CLA	C11-C12-C13-C14
27	g	308	CLA	C14-C13-C15-C16
27	g	309	CLA	C11-C10-C8-C9
27	n	604	CLA	C6-C7-C8-C9
27	n	607	CLA	C14-C13-C15-C16
27	n	609	CLA	C14-C13-C15-C16
27	n	610	CLA	C14-C13-C15-C16
28	A	843	PQN	C16-C17-C18-C19
28	B	841	PQN	C16-C17-C18-C19
27	m	605	CLA	O1D-CGD-O2D-CED
27	l	312	CLA	O1D-CGD-O2D-CED
31	b	616	LMT	C2'-C1'-O1'-C1
34	L	208	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	s	210	LMG	C2-C1-O1-C7
34	c	619	LMG	C2-C1-O1-C7
29	a	319	LHG	O2-C2-C3-O3
29	b	618	LHG	O2-C2-C3-O3
27	j	605	CLA	O1D-CGD-O2D-CED
27	h	306	CLA	CBA-CGA-O2A-C1
27	A	840	CLA	O1D-CGD-O2D-CED
27	g	302	CLA	O1D-CGD-O2D-CED
30	A	848	WVN	C30-C33-C34-C38
30	B	843	WVN	C30-C33-C34-C38
30	B	845	WVN	C20-C23-C25-C27
30	B	847	WVN	C29-C31-C32-C35
30	B	848	WVN	C11-C19-C22-C24
30	B	848	WVN	C20-C23-C25-C27
30	B	848	WVN	C29-C31-C32-C35
30	F	204	WVN	C29-C31-C32-C35
30	F	204	WVN	C30-C33-C34-C38
30	F	205	WVN	C11-C19-C22-C24
30	F	205	WVN	C29-C31-C32-C35
30	J	101	WVN	C29-C31-C32-C35
30	L	201	WVN	C11-C19-C22-C24
30	L	205	WVN	C20-C23-C25-C27
30	e	615	WVN	C20-C23-C25-C27
30	e	615	WVN	C30-C33-C34-C38
30	l	316	WVN	C11-C19-C22-C24
30	i	315	WVN	C29-C31-C32-C35
30	R	201	WVN	C11-C19-C22-C24
35	J	104	II0	C31-C33-C35-C37
35	c	613	II0	C32-C34-C36-C38
35	c	617	II0	C32-C34-C36-C38
35	a	314	II0	C32-C34-C36-C38
35	a	315	II0	C32-C34-C36-C38
35	b	613	II0	C31-C33-C35-C37
35	h	311	II0	C32-C34-C36-C38
35	m	614	II0	C31-C33-C35-C37
35	m	614	II0	C32-C34-C36-C38
35	l	314	II0	C31-C33-C35-C37
35	k	315	II0	C31-C33-C35-C37
35	k	318	II0	C32-C34-C36-C38
35	f	614	II0	C32-C34-C36-C38
35	f	615	II0	C32-C34-C36-C38
35	f	618	II0	C32-C34-C36-C38

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Mol	Chain	Res	Type	Atoms
35	i	314	II0	C32-C34-C36-C38
35	j	613	II0	C32-C34-C36-C38
35	d	312	II0	C32-C34-C36-C38
35	d	313	II0	C31-C33-C35-C37
35	g	316	II0	C32-C34-C36-C38
35	g	317	II0	C32-C34-C36-C38
35	n	615	II0	C31-C33-C35-C37
36	c	616	IHT	C30-C32-C33-C36
36	c	620	IHT	C30-C32-C33-C36
36	a	317	IHT	C18-C22-C23-C25
36	b	614	IHT	C31-C34-C35-C39
36	m	616	IHT	C18-C22-C23-C25
36	m	616	IHT	C31-C34-C35-C39
36	f	617	IHT	C18-C22-C23-C25
36	j	616	IHT	C18-C22-C23-C25
36	R	204	IHT	C18-C22-C23-C25
36	n	617	IHT	C30-C32-C33-C36
30	A	849	WVN	C30-C33-C34-C37
30	B	845	WVN	C20-C23-C25-C28
30	B	847	WVN	C29-C31-C32-C36
30	F	205	WVN	C29-C31-C32-C36
30	L	205	WVN	C20-C23-C25-C28
30	h	309	WVN	C11-C19-C22-C26
30	e	615	WVN	C20-C23-C25-C28
30	l	316	WVN	C11-C19-C22-C26
30	R	201	WVN	C11-C19-C22-C26
35	J	104	II0	C31-C33-C35-C39
35	O	203	II0	C31-C33-C35-C39
35	c	613	II0	C32-C34-C36-C40
35	a	315	II0	C32-C34-C36-C40
35	m	614	II0	C32-C34-C36-C40
35	m	615	II0	C32-C34-C36-C40
35	f	614	II0	C32-C34-C36-C40
35	j	613	II0	C32-C34-C36-C40
35	d	312	II0	C32-C34-C36-C40
35	g	316	II0	C32-C34-C36-C40
36	O	204	IHT	C18-C22-C23-C27
36	O	204	IHT	C31-C34-C35-C38
36	c	620	IHT	C18-C22-C23-C27
36	a	317	IHT	C18-C22-C23-C27
36	b	614	IHT	C31-C34-C35-C38
36	m	616	IHT	C18-C22-C23-C27

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Mol	Chain	Res	Type	Atoms
36	f	617	IHT	C18-C22-C23-C27
36	j	616	IHT	C18-C22-C23-C27
36	R	204	IHT	C18-C22-C23-C27
36	n	617	IHT	C30-C32-C33-C37
27	a	303	CLA	C3-C5-C6-C7
27	l	308	CLA	C2A-CAA-CBA-CGA
27	k	304	CLA	C2A-CAA-CBA-CGA
29	J	107	LHG	C23-C24-C25-C26
27	A	822	CLA	O1A-CGA-O2A-C1
27	B	807	CLA	O1A-CGA-O2A-C1
27	B	825	CLA	O1A-CGA-O2A-C1
27	B	826	CLA	O1A-CGA-O2A-C1
27	a	310	CLA	O1A-CGA-O2A-C1
27	m	602	CLA	O1A-CGA-O2A-C1
29	k	319	LHG	O10-C23-O8-C6
34	c	619	LMG	O10-C28-O8-C9
27	b	603	CLA	C15-C16-C17-C18
37	k	311	KC2	CAA-CBA-CGA-O2A
27	F	201	CLA	CBA-CGA-O2A-C1
27	h	306	CLA	C8-C10-C11-C12
27	h	301	CLA	C2-C1-O2A-CGA
27	B	818	CLA	O1D-CGD-O2D-CED
27	B	838	CLA	O1D-CGD-O2D-CED
27	L	202	CLA	O1D-CGD-O2D-CED
27	a	306	CLA	O1D-CGD-O2D-CED
27	e	602	CLA	O1D-CGD-O2D-CED
31	A	851	LMT	O5'-C5'-C6'-O6'
27	A	818	CLA	C2C-C3C-CAC-CBC
27	A	832	CLA	C15-C16-C17-C18
27	B	837	CLA	C5-C6-C7-C8
27	b	602	CLA	C5-C6-C7-C8
27	b	605	CLA	C8-C10-C11-C12
27	f	602	CLA	C8-C10-C11-C12
27	s	203	CLA	C3-C5-C6-C7
27	e	604	CLA	C3-C5-C6-C7
27	s	208	CLA	O1A-CGA-O2A-C1
27	B	812	CLA	CBD-CGD-O2D-CED
27	b	602	CLA	CBD-CGD-O2D-CED
27	b	604	CLA	CBD-CGD-O2D-CED
27	l	307	CLA	CBD-CGD-O2D-CED
27	A	812	CLA	C6-C7-C8-C10
27	A	818	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	A	826	CLA	C12-C13-C15-C16
27	A	831	CLA	C11-C12-C13-C15
27	A	836	CLA	C6-C7-C8-C10
27	A	840	CLA	C11-C12-C13-C15
27	A	841	CLA	C11-C12-C13-C15
27	B	804	CLA	C11-C12-C13-C15
27	B	810	CLA	C11-C10-C8-C7
27	B	829	CLA	C6-C7-C8-C10
27	F	202	CLA	C6-C7-C8-C10
27	L	203	CLA	C12-C13-C15-C16
27	a	308	CLA	C11-C12-C13-C15
27	a	312	CLA	C6-C7-C8-C10
27	b	608	CLA	C11-C10-C8-C7
27	b	610	CLA	C11-C10-C8-C7
27	b	611	CLA	C6-C7-C8-C10
27	h	301	CLA	C11-C12-C13-C15
27	h	306	CLA	C6-C7-C8-C10
27	h	307	CLA	C6-C7-C8-C10
27	h	313	CLA	C12-C13-C15-C16
27	e	606	CLA	C11-C12-C13-C15
27	e	611	CLA	C12-C13-C15-C16
27	l	304	CLA	C6-C7-C8-C10
27	k	303	CLA	C11-C12-C13-C15
27	k	307	CLA	C12-C13-C15-C16
27	i	305	CLA	C12-C13-C15-C16
27	n	607	CLA	C6-C7-C8-C10
27	n	607	CLA	C11-C12-C13-C15
28	A	843	PQN	C22-C23-C25-C26
28	B	841	PQN	C22-C23-C25-C26
27	A	832	CLA	CBA-CGA-O2A-C1
27	f	612	CLA	CBA-CGA-O2A-C1
29	f	619	LHG	C12-C13-C14-C15
37	s	201	KC2	CAA-CBA-CGA-O1A
27	A	812	CLA	C4-C3-C5-C6
29	l	318	LHG	C23-C24-C25-C26
34	F	206	LMG	C10-C11-C12-C13
30	F	204	WVN	C32-C36-C39-C40
30	F	205	WVN	C22-C26-C29-C31
30	s	207	WVN	C25-C28-C30-C33
30	h	309	WVN	C25-C28-C30-C33
30	h	309	WVN	C34-C37-C40-C39
35	c	615	II0	C25-C29-C31-C33

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Mol	Chain	Res	Type	Atoms
35	a	315	II0	C26-C30-C32-C34
35	a	318	II0	C36-C40-C42-C41
35	m	614	II0	C26-C30-C32-C34
35	m	615	II0	C26-C30-C32-C34
35	k	315	II0	C36-C40-C42-C41
35	i	318	II0	C25-C29-C31-C33
35	g	317	II0	C25-C29-C31-C33
35	g	318	II0	C25-C29-C31-C33
36	O	204	IHT	C26-C29-C31-C34
36	k	317	IHT	C33-C37-C40-C41
27	c	607	CLA	O1D-CGD-O2D-CED
27	g	311	CLA	O1D-CGD-O2D-CED
34	L	208	LMG	C38-C39-C40-C41
27	l	307	CLA	C3-C5-C6-C7
27	F	202	CLA	C5-C6-C7-C8
27	b	611	CLA	C5-C6-C7-C8
27	l	304	CLA	C15-C16-C17-C18
27	f	607	CLA	C15-C16-C17-C18
29	i	316	LHG	C7-C8-C9-C10
27	L	203	CLA	O1A-CGA-O2A-C1
27	k	309	CLA	O1A-CGA-O2A-C1
27	m	611	CLA	CBD-CGD-O2D-CED
27	n	601	CLA	O1D-CGD-O2D-CED
27	A	802	CLA	C5-C6-C7-C8
27	b	603	CLA	C5-C6-C7-C8
27	l	306	CLA	C10-C11-C12-C13
27	l	307	CLA	C13-C15-C16-C17
27	A	819	CLA	C2A-CAA-CBA-CGA
27	A	822	CLA	C2A-CAA-CBA-CGA
27	B	811	CLA	C2A-CAA-CBA-CGA
27	B	834	CLA	C2A-CAA-CBA-CGA
27	B	839	CLA	C2A-CAA-CBA-CGA
27	L	204	CLA	C2A-CAA-CBA-CGA
27	s	202	CLA	C2A-CAA-CBA-CGA
27	s	206	CLA	C2A-CAA-CBA-CGA
27	c	602	CLA	C2A-CAA-CBA-CGA
27	c	608	CLA	C2A-CAA-CBA-CGA
27	c	611	CLA	C2A-CAA-CBA-CGA
27	h	302	CLA	C2A-CAA-CBA-CGA
27	f	612	CLA	C2A-CAA-CBA-CGA
27	i	303	CLA	C2A-CAA-CBA-CGA
27	i	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	g	315	CLA	C2A-CAA-CBA-CGA
27	g	322	CLA	C2A-CAA-CBA-CGA
37	k	312	KC2	CAA-CBA-CGA-O2A
27	A	826	CLA	C5-C6-C7-C8
27	B	812	CLA	C8-C10-C11-C12
27	b	610	CLA	C5-C6-C7-C8
27	b	611	CLA	C8-C10-C11-C12
27	m	603	CLA	C15-C16-C17-C18
27	m	606	CLA	C5-C6-C7-C8
27	e	604	CLA	C5-C6-C7-C8
27	e	606	CLA	C15-C16-C17-C18
27	e	607	CLA	C5-C6-C7-C8
27	f	613	CLA	C10-C11-C12-C13
31	a	302	LMT	O5'-C5'-C6'-O6'
31	a	302	LMT	C4'-C5'-C6'-O6'
29	a	301	LHG	C7-C8-C9-C10
27	s	206	CLA	O1D-CGD-O2D-CED
27	F	203	CLA	O1A-CGA-O2A-C1
27	n	607	CLA	O1A-CGA-O2A-C1
38	i	301	LMU	O5'-C1'-O1'-C1
31	a	320	LMT	O5B-C5B-C6B-O6B
27	A	842	CLA	C15-C16-C17-C18
27	B	835	CLA	C10-C11-C12-C13
27	B	835	CLA	C13-C15-C16-C17
27	B	838	CLA	C10-C11-C12-C13
27	b	606	CLA	C10-C11-C12-C13
27	h	306	CLA	C15-C16-C17-C18
27	l	304	CLA	C10-C11-C12-C13
27	f	602	CLA	C13-C15-C16-C17
27	g	309	CLA	C5-C6-C7-C8
34	c	619	LMG	C37-C38-C39-C40
29	m	617	LHG	O2-C2-C3-O3
29	e	617	LHG	O2-C2-C3-O3
29	f	619	LHG	O2-C2-C3-O3
27	B	821	CLA	CBA-CGA-O2A-C1
27	A	827	CLA	CBD-CGD-O2D-CED
27	B	816	CLA	CBD-CGD-O2D-CED
27	A	801	CLA	O1A-CGA-O2A-C1
27	A	837	CLA	O1A-CGA-O2A-C1
27	e	607	CLA	O1A-CGA-O2A-C1
27	f	603	CLA	O1A-CGA-O2A-C1
27	i	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	g	321	LHG	O10-C23-O8-C6
27	B	815	CLA	C8-C10-C11-C12
27	B	818	CLA	C5-C6-C7-C8
27	B	840	CLA	C13-C15-C16-C17
27	c	604	CLA	C13-C15-C16-C17
27	a	308	CLA	C15-C16-C17-C18
27	b	603	CLA	C8-C10-C11-C12
27	b	607	CLA	C13-C15-C16-C17
31	a	320	LMT	O1'-C1-C2-C3
27	B	802	CLA	C4C-C3C-CAC-CBC
31	b	616	LMT	C7-C8-C9-C10
27	h	306	CLA	O1D-CGD-O2D-CED
27	i	307	CLA	O1D-CGD-O2D-CED
27	j	607	CLA	O1D-CGD-O2D-CED
27	g	307	CLA	O1D-CGD-O2D-CED
27	g	315	CLA	O1D-CGD-O2D-CED
27	A	802	CLA	C8-C10-C11-C12
27	A	807	CLA	C8-C10-C11-C12
27	O	202	CLA	C5-C6-C7-C8
27	a	312	CLA	C8-C10-C11-C12
27	e	604	CLA	C13-C15-C16-C17
28	B	841	PQN	C18-C20-C21-C22
29	e	617	LHG	C7-C8-C9-C10
29	f	619	LHG	C23-C24-C25-C26
27	B	832	CLA	C13-C15-C16-C17
27	f	613	CLA	C15-C16-C17-C18
27	g	305	CLA	C13-C15-C16-C17
27	g	322	CLA	C5-C6-C7-C8
27	A	805	CLA	CBA-CGA-O2A-C1
27	c	602	CLA	CBA-CGA-O2A-C1
27	A	808	CLA	CBD-CGD-O2D-CED
27	A	822	CLA	CBD-CGD-O2D-CED
29	n	619	LHG	C8-C7-O7-C5
37	c	610	KC2	C2A-CAA-CBA-CGA
37	e	609	KC2	C2A-CAA-CBA-CGA
27	f	602	CLA	O1D-CGD-O2D-CED
27	l	306	CLA	C8-C10-C11-C12
27	k	308	CLA	C3-C5-C6-C7
27	k	304	CLA	C2C-C3C-CAC-CBC
27	B	830	CLA	CBD-CGD-O2D-CED
30	B	843	WVN	C32-C36-C39-C40
30	K	103	WVN	C32-C36-C39-C40

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Mol	Chain	Res	Type	Atoms
35	c	613	II0	C26-C30-C32-C34
35	h	310	II0	C36-C40-C42-C41
35	l	314	II0	C25-C29-C31-C33
35	k	315	II0	C26-C30-C32-C34
35	d	314	II0	C26-C30-C32-C34
35	n	618	II0	C25-C29-C31-C33
36	c	620	IHT	C23-C27-C30-C32
36	c	620	IHT	C35-C38-C41-C40
36	n	617	IHT	C23-C27-C30-C32
27	m	604	CLA	C15-C16-C17-C18
27	e	610	CLA	C5-C6-C7-C8
27	g	306	CLA	O1A-CGA-O2A-C1
29	e	617	LHG	C23-C24-C25-C26
33	B	842	DGD	C1B-C2B-C3B-C4B
29	n	619	LHG	O9-C7-O7-C5
29	m	617	LHG	C1-C2-C3-O3
29	e	617	LHG	C1-C2-C3-O3
29	f	619	LHG	C1-C2-C3-O3
27	A	811	CLA	C2A-CAA-CBA-CGA
27	F	203	CLA	C2A-CAA-CBA-CGA
27	h	303	CLA	C2A-CAA-CBA-CGA
27	e	601	CLA	C2A-CAA-CBA-CGA
27	j	606	CLA	C2A-CAA-CBA-CGA
27	A	826	CLA	CBA-CGA-O2A-C1
27	A	840	CLA	CBA-CGA-O2A-C1
27	B	820	CLA	CBA-CGA-O2A-C1
27	B	824	CLA	CBA-CGA-O2A-C1
27	L	206	CLA	CBA-CGA-O2A-C1
27	l	306	CLA	CBA-CGA-O2A-C1
29	n	619	LHG	C24-C23-O8-C6
34	O	205	LMG	C29-C28-O8-C9
27	A	829	CLA	C8-C10-C11-C12
27	B	820	CLA	C5-C6-C7-C8
27	O	206	CLA	C10-C11-C12-C13
27	b	607	CLA	C15-C16-C17-C18
27	b	608	CLA	C13-C15-C16-C17
27	e	611	CLA	C5-C6-C7-C8
27	k	307	CLA	C8-C10-C11-C12
27	f	602	CLA	C10-C11-C12-C13
27	f	604	CLA	C8-C10-C11-C12
27	j	609	CLA	C10-C11-C12-C13
27	n	607	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	A	843	PQN	C18-C20-C21-C22
29	g	321	LHG	C25-C26-C27-C28
27	a	313	CLA	O1D-CGD-O2D-CED
27	A	838	CLA	CBD-CGD-O2D-CED
27	f	613	CLA	C3-C5-C6-C7
27	F	202	CLA	C15-C16-C17-C18
27	e	606	CLA	C13-C15-C16-C17
27	f	613	CLA	C8-C10-C11-C12
27	g	309	CLA	C10-C11-C12-C13
29	d	315	LHG	C24-C25-C26-C27
27	k	301	CLA	O1D-CGD-O2D-CED
31	a	320	LMT	O5'-C5'-C6'-O6'
27	A	835	CLA	C15-C16-C17-C18
27	B	805	CLA	C5-C6-C7-C8
27	c	612	CLA	C8-C10-C11-C12
27	b	610	CLA	C10-C11-C12-C13
27	f	610	CLA	C15-C16-C17-C18
27	d	303	CLA	C5-C6-C7-C8
27	s	209	CLA	O1D-CGD-O2D-CED
27	l	304	CLA	C4-C3-C5-C6
27	A	842	CLA	C8-C10-C11-C12
27	O	206	CLA	C5-C6-C7-C8
27	h	306	CLA	C10-C11-C12-C13
27	A	805	CLA	C3-C5-C6-C7
27	A	840	CLA	C3-C5-C6-C7
34	c	619	LMG	C11-C10-O7-C8
27	e	605	CLA	C11-C12-C13-C14
29	b	618	LHG	O9-C7-O7-C5
27	A	829	CLA	C15-C16-C17-C18
27	d	303	CLA	C15-C16-C17-C18
34	b	619	LMG	C4-C5-C6-O5
27	b	607	CLA	C4C-C3C-CAC-CBC
27	h	306	CLA	O1A-CGA-O2A-C1
27	j	604	CLA	C3-C5-C6-C7
37	k	311	KC2	CAA-CBA-CGA-O1A
30	A	846	WVN	C11-C19-C22-C24
30	B	843	WVN	C20-C23-C25-C27
30	B	846	WVN	C30-C33-C34-C38
30	F	205	WVN	C30-C33-C34-C38
30	I	101	WVN	C29-C31-C32-C35
30	L	201	WVN	C20-C23-C25-C27
30	L	201	WVN	C29-C31-C32-C35

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Mol	Chain	Res	Type	Atoms
30	h	309	WVN	C11-C19-C22-C24
30	e	615	WVN	C11-C19-C22-C24
30	i	315	WVN	C20-C23-C25-C27
30	R	201	WVN	C30-C33-C34-C38
35	O	203	II0	C31-C33-C35-C37
35	a	318	II0	C32-C34-C36-C38
35	h	310	II0	C32-C34-C36-C38
35	h	312	II0	C31-C33-C35-C37
35	m	615	II0	C32-C34-C36-C38
35	i	318	II0	C32-C34-C36-C38
35	d	314	II0	C31-C33-C35-C37
36	O	204	IHT	C31-C34-C35-C39
36	c	616	IHT	C31-C34-C35-C39
36	c	620	IHT	C18-C22-C23-C25
36	k	317	IHT	C18-C22-C23-C25
36	g	319	IHT	C18-C22-C23-C25
36	n	617	IHT	C18-C22-C23-C25
30	A	846	WVN	C20-C23-C25-C28
30	B	843	WVN	C20-C23-C25-C28
30	F	205	WVN	C11-C19-C22-C26
30	I	101	WVN	C29-C31-C32-C36
30	J	101	WVN	C11-C19-C22-C26
30	L	201	WVN	C20-C23-C25-C28
30	i	315	WVN	C20-C23-C25-C28
35	h	310	II0	C32-C34-C36-C40
35	h	312	II0	C31-C33-C35-C39
35	k	318	II0	C32-C34-C36-C40
35	i	318	II0	C32-C34-C36-C40
36	c	616	IHT	C31-C34-C35-C38
36	c	620	IHT	C30-C32-C33-C37
36	k	317	IHT	C18-C22-C23-C27
36	n	617	IHT	C18-C22-C23-C27
27	A	808	CLA	C2A-CAA-CBA-CGA
27	A	817	CLA	C2A-CAA-CBA-CGA
27	A	828	CLA	C2A-CAA-CBA-CGA
27	B	813	CLA	C2A-CAA-CBA-CGA
27	B	814	CLA	C2A-CAA-CBA-CGA
27	B	826	CLA	C2A-CAA-CBA-CGA
27	a	303	CLA	C2A-CAA-CBA-CGA
27	b	602	CLA	C2A-CAA-CBA-CGA
27	b	611	CLA	C2A-CAA-CBA-CGA
27	h	307	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	m	604	CLA	C2A-CAA-CBA-CGA
27	m	611	CLA	C2A-CAA-CBA-CGA
27	f	607	CLA	C2A-CAA-CBA-CGA
27	j	604	CLA	C2A-CAA-CBA-CGA
27	n	601	CLA	C2A-CAA-CBA-CGA
29	J	107	LHG	O1-C1-C2-C3
29	b	617	LHG	O1-C1-C2-C3
29	m	617	LHG	O1-C1-C2-C3
29	e	617	LHG	O1-C1-C2-C3
29	l	318	LHG	O1-C1-C2-C3
29	f	619	LHG	O1-C1-C2-C3
29	g	301	LHG	O1-C1-C2-C3
27	f	601	CLA	O1D-CGD-O2D-CED
30	B	843	WVN	C34-C37-C40-C39
36	a	317	IHT	C23-C27-C30-C32
27	a	306	CLA	C16-C17-C18-C19
27	d	303	CLA	C16-C17-C18-C19
28	B	841	PQN	C26-C27-C28-C29
27	m	603	CLA	O1D-CGD-O2D-CED
27	d	307	CLA	O1D-CGD-O2D-CED
27	A	826	CLA	O1A-CGA-O2A-C1
27	A	832	CLA	O1A-CGA-O2A-C1
27	f	612	CLA	O1A-CGA-O2A-C1
27	j	609	CLA	O1A-CGA-O2A-C1
34	O	205	LMG	O10-C28-O8-C9
27	b	611	CLA	C3-C5-C6-C7
34	c	619	LMG	O9-C10-O7-C8
27	a	309	CLA	O1D-CGD-O2D-CED
29	b	618	LHG	C8-C7-O7-C5
34	L	208	LMG	C11-C10-O7-C8
27	A	841	CLA	C10-C11-C12-C13
27	B	823	CLA	C13-C15-C16-C17
27	B	835	CLA	C5-C6-C7-C8
27	e	605	CLA	C5-C6-C7-C8
27	F	201	CLA	O1A-CGA-O2A-C1
27	A	828	CLA	CBA-CGA-O2A-C1
27	A	852	CLA	CBA-CGA-O2A-C1
27	B	838	CLA	CBA-CGA-O2A-C1
27	O	202	CLA	CBA-CGA-O2A-C1
27	k	313	CLA	CBA-CGA-O2A-C1
27	b	605	CLA	CBD-CGD-O2D-CED
29	l	318	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	j	609	CLA	C4C-C3C-CAC-CBC
27	B	829	CLA	C2-C1-O2A-CGA
27	e	607	CLA	C2-C1-O2A-CGA
27	B	832	CLA	C16-C17-C18-C19
27	B	832	CLA	C16-C17-C18-C20
27	s	203	CLA	C16-C17-C18-C19
27	s	203	CLA	C16-C17-C18-C20
27	b	611	CLA	C16-C17-C18-C19
27	h	306	CLA	C16-C17-C18-C20
27	n	610	CLA	C16-C17-C18-C19
28	B	841	PQN	C26-C27-C28-C30
27	B	821	CLA	O1A-CGA-O2A-C1
27	a	311	CLA	C15-C16-C17-C18
27	b	608	CLA	C15-C16-C17-C18
27	A	817	CLA	O1D-CGD-O2D-CED
27	A	832	CLA	C4C-C3C-CAC-CBC
29	e	617	LHG	C28-C29-C30-C31
29	b	617	LHG	C11-C10-C9-C8
29	m	617	LHG	C29-C30-C31-C32
27	g	322	CLA	C2C-C3C-CAC-CBC
27	B	812	CLA	C5-C6-C7-C8
27	e	611	CLA	C13-C15-C16-C17
29	a	301	LHG	C9-C10-C11-C12
34	L	208	LMG	C18-C19-C20-C21
27	A	805	CLA	O1A-CGA-O2A-C1
29	A	844	LHG	C11-C12-C13-C14
34	b	619	LMG	C21-C22-C23-C24
29	A	845	LHG	O1-C1-C2-O2
29	c	621	LHG	O1-C1-C2-O2
29	l	318	LHG	O1-C1-C2-O2
31	A	851	LMT	C2-C1-O1'-C1'
35	J	104	II0	C10-C22-C24-C26
35	c	613	II0	C09-C21-C23-C25
35	c	617	II0	C10-C22-C24-C26
35	b	613	II0	C09-C21-C23-C25
35	e	613	II0	C10-C22-C24-C26
38	i	301	LMU	C2-C1-O1'-C1'
29	f	619	LHG	C26-C27-C28-C29
31	A	851	LMT	C7-C8-C9-C10
27	h	301	CLA	O1D-CGD-O2D-CED
27	m	603	CLA	C5-C6-C7-C8
27	g	322	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	A	810	CLA	C4B-C3B-CAB-CBB
27	A	823	CLA	C4B-C3B-CAB-CBB
27	B	826	CLA	C4B-C3B-CAB-CBB
27	B	828	CLA	C4B-C3B-CAB-CBB
27	B	837	CLA	C4B-C3B-CAB-CBB
27	B	849	CLA	C4B-C3B-CAB-CBB
27	K	102	CLA	C4B-C3B-CAB-CBB
27	a	305	CLA	C4B-C3B-CAB-CBB
27	b	601	CLA	C4B-C3B-CAB-CBB
27	m	605	CLA	C4B-C3B-CAB-CBB
27	m	612	CLA	C4B-C3B-CAB-CBB
27	e	607	CLA	C4B-C3B-CAB-CBB
27	j	609	CLA	C4B-C3B-CAB-CBB
27	j	612	CLA	C4B-C3B-CAB-CBB
27	g	302	CLA	C4B-C3B-CAB-CBB
27	g	306	CLA	C4B-C3B-CAB-CBB
27	g	307	CLA	C4B-C3B-CAB-CBB
27	g	309	CLA	C4B-C3B-CAB-CBB
29	A	850	LHG	C11-C10-C9-C8
27	B	822	CLA	C16-C17-C18-C19
27	d	303	CLA	C16-C17-C18-C20
27	n	610	CLA	C16-C17-C18-C20
27	n	605	CLA	O1D-CGD-O2D-CED
27	d	305	CLA	C2A-CAA-CBA-CGA
29	e	617	LHG	C9-C10-C11-C12
27	B	805	CLA	C15-C16-C17-C18
27	m	607	CLA	C13-C15-C16-C17
27	e	606	CLA	C5-C6-C7-C8
29	c	621	LHG	C8-C7-O7-C5
29	m	617	LHG	C8-C7-O7-C5
27	A	832	CLA	O1D-CGD-O2D-CED
27	A	852	CLA	C11-C10-C8-C7
27	F	201	CLA	C6-C7-C8-C10
27	c	608	CLA	C11-C10-C8-C7
27	f	609	CLA	C11-C10-C8-C7
29	b	617	LHG	C23-C24-C25-C26
27	B	839	CLA	C2C-C3C-CAC-CBC
27	a	306	CLA	C15-C16-C17-C18
31	A	851	LMT	C1-C2-C3-C4
29	e	617	LHG	C30-C31-C32-C33
29	f	619	LHG	C10-C11-C12-C13
34	J	106	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	B	820	CLA	O1A-CGA-O2A-C1
27	B	801	CLA	C3-C5-C6-C7
27	A	802	CLA	C3A-C2A-CAA-CBA
27	A	810	CLA	C3A-C2A-CAA-CBA
27	A	812	CLA	C3A-C2A-CAA-CBA
27	A	813	CLA	C3A-C2A-CAA-CBA
27	A	816	CLA	C3A-C2A-CAA-CBA
27	A	830	CLA	C3A-C2A-CAA-CBA
27	A	831	CLA	C3A-C2A-CAA-CBA
27	A	834	CLA	C3A-C2A-CAA-CBA
27	A	838	CLA	C3A-C2A-CAA-CBA
27	A	842	CLA	C3A-C2A-CAA-CBA
27	B	813	CLA	C3A-C2A-CAA-CBA
27	B	824	CLA	C3A-C2A-CAA-CBA
27	B	830	CLA	C3A-C2A-CAA-CBA
27	J	105	CLA	C3A-C2A-CAA-CBA
27	O	202	CLA	C3A-C2A-CAA-CBA
27	s	202	CLA	C3A-C2A-CAA-CBA
27	s	203	CLA	C3A-C2A-CAA-CBA
27	c	601	CLA	C3A-C2A-CAA-CBA
27	a	307	CLA	C3A-C2A-CAA-CBA
27	a	308	CLA	C3A-C2A-CAA-CBA
27	h	305	CLA	C3A-C2A-CAA-CBA
27	h	307	CLA	C3A-C2A-CAA-CBA
27	e	607	CLA	C3A-C2A-CAA-CBA
27	e	608	CLA	C3A-C2A-CAA-CBA
27	k	305	CLA	C3A-C2A-CAA-CBA
27	k	306	CLA	C3A-C2A-CAA-CBA
27	f	605	CLA	C3A-C2A-CAA-CBA
27	i	309	CLA	C3A-C2A-CAA-CBA
27	j	604	CLA	C3A-C2A-CAA-CBA
27	j	606	CLA	C3A-C2A-CAA-CBA
27	g	306	CLA	C3A-C2A-CAA-CBA
27	g	315	CLA	C3A-C2A-CAA-CBA
27	n	601	CLA	C3A-C2A-CAA-CBA
27	A	818	CLA	O1D-CGD-O2D-CED
27	c	601	CLA	O1D-CGD-O2D-CED
27	A	812	CLA	C2-C3-C5-C6
34	b	619	LMG	C12-C13-C14-C15
27	A	809	CLA	C5-C6-C7-C8
27	A	841	CLA	C5-C6-C7-C8
27	a	308	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	m	606	CLA	C13-C15-C16-C17
27	k	308	CLA	C8-C10-C11-C12
27	g	322	CLA	C10-C11-C12-C13
27	B	849	CLA	O1D-CGD-O2D-CED
30	B	847	WVN	C32-C36-C39-C40
35	a	316	II0	C25-C29-C31-C33
35	h	312	II0	C26-C30-C32-C34
35	d	312	II0	C36-C40-C42-C41
35	d	314	II0	C36-C40-C42-C41
35	n	616	II0	C36-C40-C42-C41
36	j	616	IHT	C23-C27-C30-C32
27	A	841	CLA	C16-C17-C18-C20
27	B	836	CLA	C16-C17-C18-C20
27	b	611	CLA	C16-C17-C18-C20
27	B	824	CLA	O1A-CGA-O2A-C1
27	L	206	CLA	O1A-CGA-O2A-C1
27	O	202	CLA	O1A-CGA-O2A-C1
27	c	602	CLA	O1A-CGA-O2A-C1
27	k	313	CLA	O1A-CGA-O2A-C1
27	g	322	CLA	O1D-CGD-O2D-CED
27	b	607	CLA	C5-C6-C7-C8
27	a	311	CLA	CBD-CGD-O2D-CED
27	e	608	CLA	CBD-CGD-O2D-CED
37	d	310	KC2	CBD-CGD-O2D-CED
34	L	208	LMG	O9-C10-O7-C8
27	a	310	CLA	O2A-C1-C2-C3
27	B	804	CLA	CBA-CGA-O2A-C1
27	n	608	CLA	CBA-CGA-O2A-C1
29	b	618	LHG	C4-C5-C6-O8
29	e	617	LHG	C11-C12-C13-C14
27	a	312	CLA	C5-C6-C7-C8
29	J	107	LHG	C12-C13-C14-C15
27	B	838	CLA	O1A-CGA-O2A-C1
37	g	312	KC2	CAA-CBA-CGA-O2A
31	b	616	LMT	C4-C5-C6-C7
27	B	807	CLA	O1D-CGD-O2D-CED
27	k	303	CLA	O1D-CGD-O2D-CED
27	A	818	CLA	C13-C15-C16-C17
38	i	301	LMU	C1-C2-C3-C4
27	A	837	CLA	O1D-CGD-O2D-CED
27	B	829	CLA	O1D-CGD-O2D-CED
29	f	619	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	A	835	CLA	C16-C17-C18-C19
29	c	621	LHG	C7-C8-C9-C10
34	b	619	LMG	C28-C29-C30-C31
27	A	828	CLA	O1A-CGA-O2A-C1
27	A	852	CLA	O1A-CGA-O2A-C1
27	B	804	CLA	O1A-CGA-O2A-C1
27	A	810	CLA	C2B-C3B-CAB-CBB
27	A	822	CLA	C2B-C3B-CAB-CBB
27	A	823	CLA	C2B-C3B-CAB-CBB
27	s	202	CLA	C2B-C3B-CAB-CBB
27	c	605	CLA	C2B-C3B-CAB-CBB
27	a	312	CLA	C2B-C3B-CAB-CBB
27	b	601	CLA	C2B-C3B-CAB-CBB
27	h	307	CLA	C2B-C3B-CAB-CBB
27	m	612	CLA	C2B-C3B-CAB-CBB
27	l	304	CLA	C2B-C3B-CAB-CBB
27	j	609	CLA	C2B-C3B-CAB-CBB
27	g	302	CLA	C2B-C3B-CAB-CBB
27	n	608	CLA	C2B-C3B-CAB-CBB
30	A	846	WVN	C06-C13-C20-C23
30	A	849	WVN	C15-C13-C20-C23
30	B	846	WVN	C06-C13-C20-C23
30	B	847	WVN	C15-C13-C20-C23
30	J	101	WVN	C06-C13-C20-C23
30	L	201	WVN	C15-C13-C20-C23
30	L	205	WVN	C15-C13-C20-C23
30	M	101	WVN	C06-C13-C20-C23
30	M	101	WVN	C15-C13-C20-C23
30	K	103	WVN	C06-C13-C20-C23
30	s	205	WVN	C15-C13-C20-C23
30	s	207	WVN	C06-C13-C20-C23
30	s	207	WVN	C15-C13-C20-C23
30	e	615	WVN	C06-C13-C20-C23
36	c	616	IHT	C02-C07-C18-C22
36	c	620	IHT	C10-C07-C18-C22
27	A	809	CLA	CBA-CGA-O2A-C1
27	e	602	CLA	CBA-CGA-O2A-C1
27	h	307	CLA	C5-C6-C7-C8
29	l	318	LHG	C10-C11-C12-C13
27	L	203	CLA	C3-C5-C6-C7
34	L	208	LMG	C19-C20-C21-C22
27	B	824	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	L	202	CLA	C2A-CAA-CBA-CGA
27	m	609	CLA	C2A-CAA-CBA-CGA
27	k	309	CLA	C2A-CAA-CBA-CGA
27	k	313	CLA	C2A-CAA-CBA-CGA
27	f	610	CLA	C2A-CAA-CBA-CGA
27	n	608	CLA	C2A-CAA-CBA-CGA
29	g	301	LHG	C7-C8-C9-C10
29	L	207	LHG	C14-C15-C16-C17
27	e	602	CLA	O1A-CGA-O2A-C1
29	n	619	LHG	O10-C23-O8-C6
29	m	617	LHG	O9-C7-O7-C5
27	d	303	CLA	C4-C3-C5-C6
29	f	619	LHG	C17-C18-C19-C20
34	L	208	LMG	C32-C33-C34-C35
34	b	619	LMG	C33-C34-C35-C36
27	A	829	CLA	C5-C6-C7-C8
29	f	619	LHG	C19-C20-C21-C22
29	c	621	LHG	C28-C29-C30-C31
27	m	611	CLA	CBA-CGA-O2A-C1
27	i	302	CLA	CBA-CGA-O2A-C1
27	B	807	CLA	C3-C5-C6-C7
27	A	808	CLA	C6-C7-C8-C9
27	f	607	CLA	C14-C13-C15-C16
27	n	604	CLA	C11-C10-C8-C9
34	b	619	LMG	C22-C23-C24-C25
27	b	604	CLA	C5-C6-C7-C8
31	a	320	LMT	C1-C2-C3-C4
34	F	206	LMG	C11-C12-C13-C14
38	i	301	LMU	C4-C5-C6-C7
27	l	307	CLA	C5-C6-C7-C8
30	A	849	WVN	C34-C37-C40-C39
30	B	847	WVN	C22-C26-C29-C31
30	I	101	WVN	C32-C36-C39-C40
30	I	101	WVN	C34-C37-C40-C39
30	l	301	WVN	C22-C26-C29-C31
35	e	616	II0	C35-C39-C41-C42
35	l	317	II0	C35-C39-C41-C42
35	f	618	II0	C35-C39-C41-C42
35	i	314	II0	C25-C29-C31-C33
36	k	317	IHT	C35-C38-C41-C40
36	j	616	IHT	C33-C37-C40-C41
34	F	206	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
29	L	207	LHG	C8-C7-O7-C5
29	a	319	LHG	C23-C24-C25-C26
29	c	621	LHG	C31-C32-C33-C34
27	f	607	CLA	C10-C11-C12-C13
27	l	307	CLA	C2C-C3C-CAC-CBC
29	f	619	LHG	C35-C36-C37-C38
30	A	846	WVN	C20-C23-C25-C27
30	A	848	WVN	C20-C23-C25-C27
30	J	101	WVN	C11-C19-C22-C24
30	J	101	WVN	C20-C23-C25-C27
30	s	207	WVN	C20-C23-C25-C27
30	i	315	WVN	C11-C19-C22-C24
34	s	210	LMG	C17-C18-C19-C20
30	A	848	WVN	C20-C23-C25-C28
30	B	848	WVN	C20-C23-C25-C28
30	J	101	WVN	C20-C23-C25-C28
30	s	207	WVN	C20-C23-C25-C28
30	i	315	WVN	C11-C19-C22-C26
35	a	318	II0	C32-C34-C36-C40
35	f	618	II0	C31-C33-C35-C39
35	d	314	II0	C31-C33-C35-C39
27	c	612	CLA	C2A-CAA-CBA-CGA
27	e	607	CLA	C2A-CAA-CBA-CGA
27	f	613	CLA	C2A-CAA-CBA-CGA
37	d	309	KC2	CAA-CBA-CGA-O2A
27	b	606	CLA	C14-C13-C15-C16
27	B	805	CLA	C16-C17-C18-C19
27	B	805	CLA	C16-C17-C18-C20
27	B	809	CLA	C6-C7-C8-C9
27	B	809	CLA	C6-C7-C8-C10
27	B	835	CLA	C16-C17-C18-C20
27	B	836	CLA	C16-C17-C18-C19
27	e	606	CLA	C16-C17-C18-C19
27	n	604	CLA	C11-C12-C13-C15
27	b	611	CLA	C4-C3-C5-C6
27	b	611	CLA	C2-C3-C5-C6
37	s	204	KC2	C2C-C3C-CAC-CBC
31	b	616	LMT	C3-C4-C5-C6
27	e	611	CLA	O1D-CGD-O2D-CED
27	B	835	CLA	C8-C10-C11-C12
27	s	203	CLA	C5-C6-C7-C8
27	b	605	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	e	617	LHG	C27-C28-C29-C30
34	L	208	LMG	C34-C35-C36-C37
27	A	840	CLA	O1A-CGA-O2A-C1
27	m	611	CLA	O1A-CGA-O2A-C1
27	l	306	CLA	O1A-CGA-O2A-C1
27	n	608	CLA	O1A-CGA-O2A-C1
27	F	201	CLA	C10-C11-C12-C13
27	c	608	CLA	C13-C15-C16-C17
29	A	850	LHG	C9-C10-C11-C12
34	O	205	LMG	O6-C5-C6-O5
27	B	835	CLA	C15-C16-C17-C18
27	b	605	CLA	C10-C11-C12-C13
37	e	609	KC2	C4C-C3C-CAC-CBC
37	l	311	KC2	C4C-C3C-CAC-CBC
37	i	310	KC2	C4B-C3B-CAB-CBB
37	i	317	KC2	C4B-C3B-CAB-CBB
37	d	309	KC2	C4C-C3C-CAC-CBC
37	d	310	KC2	C2A-CAA-CBA-CGA
37	g	314	KC2	C4C-C3C-CAC-CBC
37	n	611	KC2	C4C-C3C-CAC-CBC
27	h	313	CLA	O1D-CGD-O2D-CED
31	A	851	LMT	C3-C4-C5-C6
29	l	318	LHG	C7-C8-C9-C10
27	m	609	CLA	C5-C6-C7-C8
27	f	610	CLA	C8-C10-C11-C12
27	b	604	CLA	O1D-CGD-O2D-CED
29	c	621	LHG	O7-C5-C6-O8
29	m	617	LHG	O7-C5-C6-O8
34	F	206	LMG	O7-C8-C9-O8
27	A	805	CLA	O1D-CGD-O2D-CED
29	f	619	LHG	C31-C32-C33-C34
27	a	308	CLA	C8-C10-C11-C12
27	a	312	CLA	C15-C16-C17-C18
29	b	617	LHG	C32-C33-C34-C35
34	c	619	LMG	C35-C36-C37-C38
27	B	838	CLA	C16-C17-C18-C20
27	d	303	CLA	C8-C10-C11-C12
29	k	319	LHG	C25-C26-C27-C28
27	d	303	CLA	C2-C3-C5-C6
29	L	207	LHG	O9-C7-O7-C5
29	c	621	LHG	O9-C7-O7-C5
27	A	815	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	A	838	CLA	C2A-CAA-CBA-CGA
27	B	836	CLA	C2A-CAA-CBA-CGA
27	e	602	CLA	C2A-CAA-CBA-CGA
27	i	305	CLA	C2A-CAA-CBA-CGA
27	e	608	CLA	O1D-CGD-O2D-CED
29	J	107	LHG	C24-C23-O8-C6
29	i	316	LHG	C27-C28-C29-C30
31	a	320	LMT	C6-C7-C8-C9
29	c	618	LHG	C5-C6-O8-C23
27	B	803	CLA	C10-C11-C12-C13
27	j	609	CLA	C5-C6-C7-C8
29	g	301	LHG	C8-C7-O7-C5
29	c	621	LHG	C26-C27-C28-C29
27	A	812	CLA	C16-C17-C18-C20
27	a	306	CLA	C16-C17-C18-C20
27	n	604	CLA	C11-C12-C13-C14
27	i	302	CLA	O1A-CGA-O2A-C1
37	s	204	KC2	CAA-CBA-CGA-O1A
27	A	804	CLA	C1A-C2A-CAA-CBA
27	A	808	CLA	C1A-C2A-CAA-CBA
27	A	809	CLA	C1A-C2A-CAA-CBA
27	A	814	CLA	C1A-C2A-CAA-CBA
27	A	822	CLA	C1A-C2A-CAA-CBA
27	A	831	CLA	C1A-C2A-CAA-CBA
27	A	833	CLA	C1A-C2A-CAA-CBA
27	A	834	CLA	C1A-C2A-CAA-CBA
27	A	837	CLA	C1A-C2A-CAA-CBA
27	A	841	CLA	C1A-C2A-CAA-CBA
27	A	842	CLA	C1A-C2A-CAA-CBA
27	A	855	CLA	C1A-C2A-CAA-CBA
27	B	803	CLA	C1A-C2A-CAA-CBA
27	B	811	CLA	C1A-C2A-CAA-CBA
27	B	815	CLA	C1A-C2A-CAA-CBA
27	B	826	CLA	C1A-C2A-CAA-CBA
27	B	840	CLA	C1A-C2A-CAA-CBA
27	F	201	CLA	C1A-C2A-CAA-CBA
27	J	105	CLA	C1A-C2A-CAA-CBA
27	L	203	CLA	C1A-C2A-CAA-CBA
27	L	206	CLA	C1A-C2A-CAA-CBA
27	s	202	CLA	C1A-C2A-CAA-CBA
27	c	602	CLA	C1A-C2A-CAA-CBA
27	c	608	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	a	307	CLA	C1A-C2A-CAA-CBA
27	a	308	CLA	C1A-C2A-CAA-CBA
27	a	310	CLA	C1A-C2A-CAA-CBA
27	a	312	CLA	C1A-C2A-CAA-CBA
27	b	602	CLA	C1A-C2A-CAA-CBA
27	b	610	CLA	C1A-C2A-CAA-CBA
27	h	304	CLA	C1A-C2A-CAA-CBA
27	h	307	CLA	C1A-C2A-CAA-CBA
27	h	308	CLA	C1A-C2A-CAA-CBA
27	m	608	CLA	C1A-C2A-CAA-CBA
27	e	610	CLA	C1A-C2A-CAA-CBA
27	l	304	CLA	C1A-C2A-CAA-CBA
27	l	309	CLA	C1A-C2A-CAA-CBA
27	l	312	CLA	C1A-C2A-CAA-CBA
27	f	605	CLA	C1A-C2A-CAA-CBA
27	i	303	CLA	C1A-C2A-CAA-CBA
27	i	311	CLA	C1A-C2A-CAA-CBA
27	j	601	CLA	C1A-C2A-CAA-CBA
27	j	602	CLA	C1A-C2A-CAA-CBA
27	j	606	CLA	C1A-C2A-CAA-CBA
27	g	303	CLA	C1A-C2A-CAA-CBA
27	g	315	CLA	C1A-C2A-CAA-CBA
27	n	605	CLA	C1A-C2A-CAA-CBA
27	n	608	CLA	C1A-C2A-CAA-CBA
27	n	609	CLA	C13-C15-C16-C17
27	A	812	CLA	O1A-CGA-O2A-C1
29	J	107	LHG	C29-C30-C31-C32
29	g	301	LHG	O6-C4-C5-C6
27	c	612	CLA	C3-C5-C6-C7
27	A	806	CLA	C6-C7-C8-C10
27	A	810	CLA	C11-C12-C13-C15
27	A	812	CLA	C11-C12-C13-C15
27	A	817	CLA	C11-C10-C8-C7
27	A	825	CLA	C11-C12-C13-C15
27	A	826	CLA	C6-C7-C8-C10
27	A	831	CLA	C12-C13-C15-C16
27	A	841	CLA	C12-C13-C15-C16
27	A	855	CLA	C6-C7-C8-C10
27	B	801	CLA	C11-C12-C13-C15
27	B	804	CLA	C12-C13-C15-C16
27	B	805	CLA	C11-C10-C8-C7
27	B	806	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	B	812	CLA	C6-C7-C8-C10
27	B	816	CLA	C11-C12-C13-C15
27	B	816	CLA	C12-C13-C15-C16
27	F	201	CLA	C12-C13-C15-C16
27	F	202	CLA	C11-C12-C13-C15
27	F	202	CLA	C12-C13-C15-C16
27	c	612	CLA	C11-C12-C13-C15
27	a	308	CLA	C12-C13-C15-C16
27	a	309	CLA	C6-C7-C8-C10
27	a	309	CLA	C11-C12-C13-C15
27	a	309	CLA	C12-C13-C15-C16
27	b	607	CLA	C12-C13-C15-C16
27	b	608	CLA	C12-C13-C15-C16
27	b	610	CLA	C11-C12-C13-C15
27	e	606	CLA	C11-C10-C8-C7
27	e	607	CLA	C11-C10-C8-C7
27	e	607	CLA	C11-C12-C13-C15
27	l	306	CLA	C12-C13-C15-C16
27	k	308	CLA	C12-C13-C15-C16
27	f	610	CLA	C6-C7-C8-C10
27	f	613	CLA	C6-C7-C8-C10
27	i	305	CLA	C6-C7-C8-C10
27	i	307	CLA	C6-C7-C8-C10
27	d	303	CLA	C6-C7-C8-C10
27	g	305	CLA	C11-C12-C13-C15
27	g	309	CLA	C11-C10-C8-C7
27	n	607	CLA	C12-C13-C15-C16
27	n	610	CLA	C11-C12-C13-C15
28	A	843	PQN	C21-C22-C23-C25
34	c	619	LMG	C38-C39-C40-C41
27	A	839	CLA	C16-C17-C18-C20
27	A	841	CLA	C16-C17-C18-C19
27	B	829	CLA	C16-C17-C18-C19
27	f	604	CLA	C16-C17-C18-C19
27	d	303	CLA	C10-C11-C12-C13
34	J	106	LMG	C20-C21-C22-C23
27	J	103	CLA	C3A-C2A-CAA-CBA
27	A	806	CLA	C8-C10-C11-C12
27	A	841	CLA	C8-C10-C11-C12
27	B	834	CLA	C10-C11-C12-C13
27	b	603	CLA	C10-C11-C12-C13
27	e	606	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	850	LHG	C16-C17-C18-C19
27	b	611	CLA	C10-C11-C12-C13
27	l	312	CLA	C8-C10-C11-C12
27	l	309	CLA	C2A-CAA-CBA-CGA
27	n	609	CLA	C2A-CAA-CBA-CGA
27	A	824	CLA	C11-C10-C8-C9
27	A	825	CLA	C6-C7-C8-C9
27	A	825	CLA	C11-C10-C8-C9
27	A	831	CLA	C14-C13-C15-C16
27	A	855	CLA	C6-C7-C8-C9
27	B	802	CLA	C6-C7-C8-C9
27	B	812	CLA	C6-C7-C8-C9
27	B	816	CLA	C11-C12-C13-C14
27	B	816	CLA	C14-C13-C15-C16
27	F	201	CLA	C14-C13-C15-C16
27	L	203	CLA	C14-C13-C15-C16
27	s	202	CLA	C6-C7-C8-C9
27	c	612	CLA	C11-C12-C13-C14
27	a	312	CLA	C6-C7-C8-C9
27	b	604	CLA	C11-C12-C13-C14
27	h	306	CLA	C11-C12-C13-C14
27	h	307	CLA	C6-C7-C8-C9
27	m	603	CLA	C11-C10-C8-C9
27	e	606	CLA	C11-C12-C13-C14
27	e	607	CLA	C11-C12-C13-C14
27	k	303	CLA	C11-C12-C13-C14
27	f	610	CLA	C6-C7-C8-C9
27	f	613	CLA	C6-C7-C8-C9
27	i	305	CLA	C14-C13-C15-C16
27	g	305	CLA	C11-C10-C8-C9
28	B	841	PQN	C24-C23-C25-C26
27	K	101	CLA	CBA-CGA-O2A-C1
27	h	301	CLA	CBA-CGA-O2A-C1
29	c	621	LHG	C24-C23-O8-C6
29	c	621	LHG	C23-C24-C25-C26
29	f	619	LHG	C7-C8-C9-C10
29	g	321	LHG	C4-C5-C6-O8
34	s	210	LMG	C7-C8-C9-O8
29	g	301	LHG	C24-C25-C26-C27
27	k	308	CLA	CBA-CGA-O2A-C1
27	L	203	CLA	C16-C17-C18-C20
27	f	604	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	B	821	CLA	C5-C6-C7-C8
27	m	604	CLA	C10-C11-C12-C13
27	B	812	CLA	O1D-CGD-O2D-CED
27	a	307	CLA	O1D-CGD-O2D-CED
29	J	107	LHG	C9-C10-C11-C12
37	g	312	KC2	CAA-CBA-CGA-O1A
27	A	809	CLA	O1A-CGA-O2A-C1
27	B	818	CLA	C4-C3-C5-C6
27	F	201	CLA	C4-C3-C5-C6
27	e	606	CLA	C4-C3-C5-C6
27	b	605	CLA	C2-C3-C5-C6
27	A	806	CLA	C15-C16-C17-C18
27	A	818	CLA	C8-C10-C11-C12
30	A	849	WVN	C20-C23-C25-C27
30	R	202	WVN	C11-C19-C22-C24
35	j	613	II0	C31-C33-C35-C37
30	A	849	WVN	C20-C23-C25-C28
30	B	846	WVN	C30-C33-C34-C37
30	R	201	WVN	C20-C23-C25-C28
27	i	307	CLA	C5-C6-C7-C8
27	j	609	CLA	C8-C10-C11-C12
27	B	809	CLA	C2A-CAA-CBA-CGA
27	l	306	CLA	C2A-CAA-CBA-CGA
27	B	817	CLA	CBA-CGA-O2A-C1
31	b	616	LMT	C2-C3-C4-C5
27	k	308	CLA	O1A-CGA-O2A-C1
27	A	838	CLA	O1D-CGD-O2D-CED
27	A	806	CLA	CBA-CGA-O2A-C1
27	A	812	CLA	CBA-CGA-O2A-C1
27	a	313	CLA	CBA-CGA-O2A-C1
27	k	302	CLA	CBA-CGA-O2A-C1
27	n	603	CLA	CBA-CGA-O2A-C1
27	g	322	CLA	O2A-C1-C2-C3
29	J	107	LHG	C33-C34-C35-C36
29	b	617	LHG	C13-C14-C15-C16
35	c	614	II0	C25-C29-C31-C33
35	a	315	II0	C25-C29-C31-C33
35	b	612	II0	C26-C30-C32-C34
35	m	614	II0	C25-C29-C31-C33
35	e	612	II0	C25-C29-C31-C33
35	l	317	II0	C36-C40-C42-C41
27	A	808	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	m	611	CLA	O1D-CGD-O2D-CED
29	A	850	LHG	C10-C11-C12-C13
29	J	107	LHG	O6-C4-C5-O7
27	d	305	CLA	CBA-CGA-O2A-C1
29	f	619	LHG	C24-C23-O8-C6
31	A	851	LMT	C4B-C5B-C6B-O6B
34	L	208	LMG	C36-C37-C38-C39
27	b	605	CLA	C4-C3-C5-C6
27	A	828	CLA	C2-C3-C5-C6
27	B	818	CLA	C2-C3-C5-C6
27	l	306	CLA	C2-C3-C5-C6
29	m	617	LHG	C26-C27-C28-C29
29	l	318	LHG	C9-C10-C11-C12
34	b	619	LMG	C14-C15-C16-C17
29	e	617	LHG	C31-C32-C33-C34
29	k	319	LHG	O7-C5-C6-O8
27	A	817	CLA	CBA-CGA-O2A-C1
29	g	301	LHG	C30-C31-C32-C33
27	B	837	CLA	CAA-CBA-CGA-O2A
27	i	302	CLA	CAA-CBA-CGA-O2A
34	J	106	LMG	C18-C19-C20-C21
27	B	802	CLA	C2A-CAA-CBA-CGA
29	a	319	LHG	C19-C20-C21-C22
27	h	301	CLA	O1A-CGA-O2A-C1
27	b	602	CLA	CBA-CGA-O2A-C1
27	m	609	CLA	CBD-CGD-O2D-CED
29	J	107	LHG	C15-C16-C17-C18
29	f	619	LHG	C27-C28-C29-C30
34	F	206	LMG	C15-C16-C17-C18
27	A	842	CLA	C10-C11-C12-C13
27	A	835	CLA	C13-C15-C16-C17
27	B	834	CLA	C8-C10-C11-C12
27	b	606	CLA	C5-C6-C7-C8
27	b	602	CLA	O1D-CGD-O2D-CED
30	B	846	WVN	C25-C28-C30-C33
27	b	608	CLA	C16-C17-C18-C19
27	m	604	CLA	C16-C17-C18-C20
27	n	613	CLA	CAA-CBA-CGA-O2A
27	F	201	CLA	C2-C3-C5-C6
27	f	609	CLA	CBA-CGA-O2A-C1
27	c	612	CLA	C10-C11-C12-C13
27	k	304	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	J	107	LHG	C25-C26-C27-C28
31	a	320	LMT	C4-C5-C6-C7
34	c	619	LMG	C29-C30-C31-C32
35	O	203	II0	C10-C22-C24-C26
35	a	314	II0	C09-C21-C23-C25
35	a	314	II0	C10-C22-C24-C26
35	b	613	II0	C10-C22-C24-C26
35	h	311	II0	C09-C21-C23-C25
35	m	613	II0	C10-C22-C24-C26
35	m	614	II0	C10-C22-C24-C26
35	l	315	II0	C09-C21-C23-C25
35	i	313	II0	C10-C22-C24-C26
36	O	204	IHT	C11-C21-C24-C26
36	k	317	IHT	C11-C21-C24-C26
27	A	802	CLA	C11-C12-C13-C14
27	A	806	CLA	C6-C7-C8-C9
27	A	810	CLA	C11-C12-C13-C14
27	A	816	CLA	C14-C13-C15-C16
27	A	824	CLA	C11-C12-C13-C14
27	A	829	CLA	C11-C10-C8-C9
27	A	841	CLA	C11-C12-C13-C14
27	B	801	CLA	C6-C7-C8-C9
27	B	803	CLA	C14-C13-C15-C16
27	B	804	CLA	C14-C13-C15-C16
27	B	807	CLA	C11-C12-C13-C14
27	B	811	CLA	C6-C7-C8-C9
27	B	832	CLA	C11-C12-C13-C14
27	B	832	CLA	C14-C13-C15-C16
27	B	835	CLA	C14-C13-C15-C16
27	s	202	CLA	C11-C12-C13-C14
27	s	203	CLA	C6-C7-C8-C9
27	s	203	CLA	C14-C13-C15-C16
27	s	206	CLA	C14-C13-C15-C16
27	a	306	CLA	C6-C7-C8-C9
27	a	309	CLA	C11-C12-C13-C14
27	a	309	CLA	C14-C13-C15-C16
27	b	610	CLA	C11-C12-C13-C14
27	h	306	CLA	C6-C7-C8-C9
27	m	607	CLA	C14-C13-C15-C16
27	e	611	CLA	C14-C13-C15-C16
27	l	306	CLA	C14-C13-C15-C16
27	f	602	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	f	613	CLA	C14-C13-C15-C16
27	i	305	CLA	C11-C10-C8-C9
27	i	307	CLA	C6-C7-C8-C9
27	j	612	CLA	C6-C7-C8-C9
27	d	303	CLA	C11-C12-C13-C14
27	n	607	CLA	C6-C7-C8-C9
27	n	610	CLA	C11-C12-C13-C14
28	B	841	PQN	C21-C22-C23-C24
27	n	604	CLA	O1A-CGA-O2A-C1
27	A	832	CLA	C4B-C3B-CAB-CBB
27	A	853	CLA	C4B-C3B-CAB-CBB
27	B	801	CLA	C4B-C3B-CAB-CBB
27	B	814	CLA	C4B-C3B-CAB-CBB
27	h	301	CLA	C4B-C3B-CAB-CBB
27	m	606	CLA	C4B-C3B-CAB-CBB
27	e	610	CLA	C4B-C3B-CAB-CBB
27	l	305	CLA	C4B-C3B-CAB-CBB
27	l	312	CLA	C4B-C3B-CAB-CBB
27	f	605	CLA	C4B-C3B-CAB-CBB
27	d	303	CLA	C4B-C3B-CAB-CBB
34	F	206	LMG	C19-C20-C21-C22
34	L	208	LMG	C22-C23-C24-C25
27	B	803	CLA	CAA-CBA-CGA-O2A
27	R	203	CLA	CAA-CBA-CGA-O2A
27	m	604	CLA	C2C-C3C-CAC-CBC
27	A	839	CLA	C2A-CAA-CBA-CGA
27	f	602	CLA	C2A-CAA-CBA-CGA
27	B	837	CLA	C8-C10-C11-C12
29	m	617	LHG	C27-C28-C29-C30
29	g	301	LHG	C25-C26-C27-C28
34	s	210	LMG	C18-C19-C20-C21
29	J	107	LHG	O6-C4-C5-C6
29	e	617	LHG	O6-C4-C5-C6
29	n	619	LHG	O6-C4-C5-C6
27	B	816	CLA	O1D-CGD-O2D-CED
27	A	801	CLA	CAA-CBA-CGA-O2A
31	a	320	LMT	C4'-C5'-C6'-O6'
27	A	802	CLA	C11-C12-C13-C15
27	A	812	CLA	C12-C13-C15-C16
27	A	816	CLA	C11-C10-C8-C7
27	A	824	CLA	C11-C10-C8-C7
27	A	825	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	A	829	CLA	C11-C10-C8-C7
27	A	835	CLA	C6-C7-C8-C10
27	A	840	CLA	C6-C7-C8-C10
27	A	840	CLA	C11-C10-C8-C7
27	A	853	CLA	C12-C13-C15-C16
27	B	801	CLA	C6-C7-C8-C10
27	B	802	CLA	C6-C7-C8-C10
27	B	810	CLA	C12-C13-C15-C16
27	B	811	CLA	C6-C7-C8-C10
27	B	815	CLA	C11-C10-C8-C7
27	B	820	CLA	C6-C7-C8-C10
27	B	820	CLA	C11-C12-C13-C15
27	B	832	CLA	C12-C13-C15-C16
27	B	835	CLA	C12-C13-C15-C16
27	O	202	CLA	C11-C10-C8-C7
27	O	206	CLA	C11-C12-C13-C15
27	s	202	CLA	C6-C7-C8-C10
27	s	202	CLA	C11-C12-C13-C15
27	s	203	CLA	C6-C7-C8-C10
27	s	203	CLA	C12-C13-C15-C16
27	a	306	CLA	C6-C7-C8-C10
27	b	604	CLA	C11-C12-C13-C15
27	b	605	CLA	C6-C7-C8-C10
27	b	607	CLA	C11-C12-C13-C15
27	h	306	CLA	C11-C12-C13-C15
27	m	603	CLA	C11-C10-C8-C7
27	m	606	CLA	C11-C12-C13-C15
27	e	604	CLA	C11-C12-C13-C15
27	e	606	CLA	C6-C7-C8-C10
27	l	306	CLA	C11-C10-C8-C7
27	l	310	CLA	C11-C12-C13-C15
27	f	608	CLA	C11-C12-C13-C15
27	f	613	CLA	C11-C12-C13-C15
27	j	609	CLA	C6-C7-C8-C10
27	j	612	CLA	C6-C7-C8-C10
27	j	612	CLA	C12-C13-C15-C16
27	d	303	CLA	C11-C10-C8-C7
27	d	303	CLA	C11-C12-C13-C15
27	g	305	CLA	C11-C10-C8-C7
27	n	604	CLA	C6-C7-C8-C10
27	n	610	CLA	C6-C7-C8-C10
27	n	610	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	B	841	PQN	C21-C22-C23-C25
27	K	101	CLA	O1A-CGA-O2A-C1
29	c	621	LHG	O10-C23-O8-C6
29	L	207	LHG	C35-C36-C37-C38
27	B	835	CLA	CBD-CGD-O2D-CED
27	A	842	CLA	C13-C15-C16-C17
27	A	839	CLA	C16-C17-C18-C19
27	b	608	CLA	C16-C17-C18-C20
34	J	106	LMG	C41-C42-C43-C44
29	J	107	LHG	O10-C23-O8-C6
27	A	809	CLA	C3A-C2A-CAA-CBA
27	B	817	CLA	C3A-C2A-CAA-CBA
27	m	609	CLA	C3A-C2A-CAA-CBA
27	f	613	CLA	C3A-C2A-CAA-CBA
27	B	821	CLA	C8-C10-C11-C12
27	A	822	CLA	O1D-CGD-O2D-CED
29	a	319	LHG	C31-C32-C33-C34
27	m	608	CLA	CBA-CGA-O2A-C1
27	j	612	CLA	CBA-CGA-O2A-C1
27	g	307	CLA	CBA-CGA-O2A-C1
30	A	849	WVN	C32-C36-C39-C40
30	B	847	WVN	C34-C37-C40-C39
30	O	201	WVN	C32-C36-C39-C40
30	O	201	WVN	C34-C37-C40-C39
35	a	314	II0	C26-C30-C32-C34
35	b	613	II0	C25-C29-C31-C33
35	e	613	II0	C26-C30-C32-C34
35	l	315	II0	C26-C30-C32-C34
35	f	615	II0	C25-C29-C31-C33
35	j	614	II0	C35-C39-C41-C42
35	j	615	II0	C35-C39-C41-C42
35	n	614	II0	C36-C40-C42-C41
30	s	205	WVN	C20-C23-C25-C27
30	l	301	WVN	C20-C23-C25-C27
30	R	201	WVN	C20-C23-C25-C27
35	e	613	II0	C31-C33-C35-C37
35	f	618	II0	C31-C33-C35-C37
27	f	606	CLA	C4-C3-C5-C6
27	f	612	CLA	C4-C3-C5-C6
27	j	611	CLA	C4-C3-C5-C6
27	d	305	CLA	O1A-CGA-O2A-C1
27	n	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	c	621	LHG	C10-C11-C12-C13
27	F	201	CLA	CBD-CGD-O2D-CED
27	g	304	CLA	CBD-CGD-O2D-CED
29	g	301	LHG	O9-C7-O7-C5
29	b	617	LHG	C24-C25-C26-C27
27	L	202	CLA	O2A-C1-C2-C3
27	l	307	CLA	C2A-CAA-CBA-CGA
27	m	606	CLA	CBA-CGA-O2A-C1
27	n	613	CLA	CBA-CGA-O2A-C1
29	c	618	LHG	C4-C5-C6-O8
29	a	319	LHG	C4-C5-C6-O8
29	m	617	LHG	C4-C5-C6-O8
29	e	617	LHG	C4-C5-C6-O8
29	f	619	LHG	C4-C5-C6-O8
34	F	206	LMG	C7-C8-C9-O8
34	O	205	LMG	C7-C8-C9-O8
29	J	107	LHG	C16-C17-C18-C19
27	A	812	CLA	C16-C17-C18-C19
27	B	838	CLA	C16-C17-C18-C19
27	f	607	CLA	C16-C17-C18-C20
29	n	619	LHG	C12-C13-C14-C15
27	B	812	CLA	C11-C12-C13-C14
27	B	801	CLA	C5-C6-C7-C8
27	A	828	CLA	C4-C3-C5-C6
27	B	801	CLA	C4-C3-C5-C6
27	l	306	CLA	C4-C3-C5-C6
27	B	839	CLA	O1A-CGA-O2A-C1
27	B	830	CLA	O1D-CGD-O2D-CED
27	A	832	CLA	C2C-C3C-CAC-CBC
27	B	810	CLA	C16-C17-C18-C19
27	B	810	CLA	C16-C17-C18-C20
27	B	829	CLA	C16-C17-C18-C20
29	b	618	LHG	O6-C4-C5-O7
29	e	617	LHG	O6-C4-C5-O7
29	d	315	LHG	C27-C28-C29-C30
34	b	619	LMG	C36-C37-C38-C39
27	B	837	CLA	C2B-C3B-CAB-CBB
27	m	606	CLA	C2B-C3B-CAB-CBB
30	B	843	WVN	C15-C13-C20-C23
30	F	205	WVN	C06-C13-C20-C23
30	l	316	WVN	C06-C13-C20-C23
30	i	315	WVN	C06-C13-C20-C23

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Mol	Chain	Res	Type	Atoms
30	R	202	WVN	C06-C13-C20-C23
36	a	317	IHT	C02-C07-C18-C22
36	b	614	IHT	C02-C07-C18-C22
36	n	617	IHT	C02-C07-C18-C22
27	A	829	CLA	C10-C11-C12-C13
34	c	619	LMG	C31-C32-C33-C34
37	e	609	KC2	CAA-CBA-CGA-O1A
27	A	826	CLA	C3-C5-C6-C7
27	A	853	CLA	C8-C10-C11-C12
27	O	206	CLA	C15-C16-C17-C18
27	b	610	CLA	C15-C16-C17-C18
27	k	307	CLA	C13-C15-C16-C17
27	e	605	CLA	O1D-CGD-O2D-CED
29	c	621	LHG	C9-C10-C11-C12
29	a	301	LHG	C27-C28-C29-C30
27	B	822	CLA	C16-C17-C18-C20
27	h	306	CLA	C16-C17-C18-C19
27	m	606	CLA	C16-C17-C18-C19
27	a	308	CLA	CAA-CBA-CGA-O2A
27	A	807	CLA	C2A-CAA-CBA-CGA
27	R	203	CLA	C2A-CAA-CBA-CGA
27	n	610	CLA	C2A-CAA-CBA-CGA
29	L	207	LHG	O7-C5-C6-O8
29	f	619	LHG	O7-C5-C6-O8
29	g	321	LHG	O7-C5-C6-O8
31	a	320	LMT	C2-C3-C4-C5
29	a	319	LHG	C15-C16-C17-C18
27	g	311	CLA	C6-C7-C8-C9
27	i	307	CLA	C4-C3-C5-C6
34	J	106	LMG	C42-C43-C44-C45
27	A	806	CLA	C16-C17-C18-C20
29	L	207	LHG	C32-C33-C34-C35
27	B	820	CLA	C8-C10-C11-C12
27	a	308	CLA	C10-C11-C12-C13
34	c	619	LMG	C39-C40-C41-C42
27	h	307	CLA	C3-C5-C6-C7
27	A	817	CLA	C11-C12-C13-C14
27	A	818	CLA	C11-C12-C13-C14
27	A	835	CLA	C6-C7-C8-C9
27	B	805	CLA	C11-C10-C8-C9
27	B	835	CLA	C11-C12-C13-C14
27	B	838	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	F	202	CLA	C14-C13-C15-C16
27	b	603	CLA	C11-C12-C13-C14
27	b	610	CLA	C11-C10-C8-C9
27	b	611	CLA	C14-C13-C15-C16
27	m	606	CLA	C11-C12-C13-C14
27	e	604	CLA	C6-C7-C8-C9
27	e	607	CLA	C6-C7-C8-C9
27	e	605	CLA	CBD-CGD-O2D-CED
37	c	610	KC2	CAA-CBA-CGA-O2A
27	A	817	CLA	O1A-CGA-O2A-C1
27	A	835	CLA	C16-C17-C18-C20
27	A	827	CLA	O1D-CGD-O2D-CED
27	A	806	CLA	O1A-CGA-O2A-C1
29	b	617	LHG	C28-C29-C30-C31
27	K	102	CLA	C1A-C2A-CAA-CBA
27	i	302	CLA	C2A-CAA-CBA-CGA
27	g	305	CLA	C2C-C3C-CAC-CBC
27	A	829	CLA	CBA-CGA-O2A-C1
27	B	819	CLA	CBA-CGA-O2A-C1
27	b	609	CLA	CBA-CGA-O2A-C1
29	f	619	LHG	C14-C15-C16-C17
27	j	609	CLA	CAA-CBA-CGA-O2A
27	g	306	CLA	CAA-CBA-CGA-O2A
27	g	307	CLA	CAA-CBA-CGA-O2A
27	B	801	CLA	C2-C3-C5-C6
27	a	313	CLA	O1A-CGA-O2A-C1
27	k	302	CLA	O1A-CGA-O2A-C1
27	A	826	CLA	O1D-CGD-O2D-CED
29	a	319	LHG	C14-C15-C16-C17
29	a	319	LHG	C1-C2-C3-O3
27	B	801	CLA	CAA-CBA-CGA-O2A
27	B	839	CLA	CBA-CGA-O2A-C1
27	s	209	CLA	CBA-CGA-O2A-C1
27	e	605	CLA	CBA-CGA-O2A-C1
27	m	604	CLA	C16-C17-C18-C19
27	e	606	CLA	C16-C17-C18-C20
29	J	107	LHG	C14-C15-C16-C17
27	e	604	CLA	C8-C10-C11-C12
30	K	103	WVN	C20-C23-C25-C27
30	R	202	WVN	C30-C33-C34-C38
35	k	314	II0	C32-C34-C36-C38
36	c	616	IHT	C18-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
29	f	619	LHG	C32-C33-C34-C35
29	n	619	LHG	C27-C28-C29-C30
27	A	816	CLA	C12-C13-C15-C16
27	A	817	CLA	C11-C12-C13-C15
27	A	827	CLA	C11-C12-C13-C15
27	A	837	CLA	C12-C13-C15-C16
27	A	840	CLA	C12-C13-C15-C16
27	A	853	CLA	C11-C12-C13-C15
27	B	803	CLA	C11-C12-C13-C15
27	B	823	CLA	C6-C7-C8-C10
27	B	835	CLA	C11-C12-C13-C15
27	L	203	CLA	C11-C12-C13-C15
27	c	608	CLA	C12-C13-C15-C16
27	c	612	CLA	C11-C10-C8-C7
27	a	308	CLA	C11-C10-C8-C7
27	a	312	CLA	C12-C13-C15-C16
27	b	603	CLA	C11-C12-C13-C15
27	b	604	CLA	C6-C7-C8-C10
27	m	602	CLA	C6-C7-C8-C10
27	m	607	CLA	C12-C13-C15-C16
27	e	604	CLA	C6-C7-C8-C10
27	e	605	CLA	C11-C10-C8-C7
27	j	604	CLA	C11-C10-C8-C7
27	j	609	CLA	C11-C10-C8-C7
27	g	308	CLA	C11-C10-C8-C7
27	n	607	CLA	C11-C10-C8-C7
27	n	609	CLA	C12-C13-C15-C16
27	A	826	CLA	CBD-CGD-O2D-CED
27	m	607	CLA	C15-C16-C17-C18
30	A	846	WVN	C11-C19-C22-C26
30	B	848	WVN	C11-C19-C22-C26
30	O	201	WVN	C29-C31-C32-C36
30	K	103	WVN	C20-C23-C25-C28
30	e	615	WVN	C11-C19-C22-C26
30	l	301	WVN	C20-C23-C25-C28
30	R	201	WVN	C30-C33-C34-C37
30	R	202	WVN	C11-C19-C22-C26
35	a	314	II0	C32-C34-C36-C40
35	j	613	II0	C31-C33-C35-C39
35	n	618	II0	C32-C34-C36-C40
36	c	616	IHT	C18-C22-C23-C27
36	g	319	IHT	C18-C22-C23-C27

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Mol	Chain	Res	Type	Atoms
27	d	303	CLA	CBA-CGA-O2A-C1
34	L	208	LMG	C41-C42-C43-C44
27	m	606	CLA	O1A-CGA-O2A-C1
27	m	608	CLA	O1A-CGA-O2A-C1
27	e	605	CLA	O1A-CGA-O2A-C1
27	f	609	CLA	O1A-CGA-O2A-C1
27	k	308	CLA	C15-C16-C17-C18
27	e	610	CLA	C2A-CAA-CBA-CGA
27	a	311	CLA	C16-C17-C18-C20
29	l	318	LHG	C8-C7-O7-C5
27	B	806	CLA	C4-C3-C5-C6
27	g	307	CLA	O1A-CGA-O2A-C1
29	f	619	LHG	O10-C23-O8-C6
37	k	310	KC2	C2B-C3B-CAB-CBB
37	j	610	KC2	C2C-C3C-CAC-CBC
27	B	804	CLA	C15-C16-C17-C18
34	b	619	LMG	C13-C14-C15-C16
27	h	301	CLA	O2A-C1-C2-C3
29	e	617	LHG	C6-C5-O7-C7
27	j	609	CLA	C2C-C3C-CAC-CBC
27	B	828	CLA	O1A-CGA-O2A-C1
27	j	612	CLA	O1A-CGA-O2A-C1
29	a	301	LHG	C14-C15-C16-C17
35	g	318	II0	C26-C30-C32-C34
27	A	807	CLA	C16-C17-C18-C20
27	n	613	CLA	O1A-CGA-O2A-C1
29	b	617	LHG	O2-C2-C3-O3
29	J	107	LHG	C11-C10-C9-C8
27	B	838	CLA	C13-C15-C16-C17
29	L	207	LHG	O6-C4-C5-O7
29	n	619	LHG	O6-C4-C5-O7
27	A	821	CLA	O2A-C1-C2-C3
27	a	311	CLA	O1D-CGD-O2D-CED
29	L	207	LHG	C4-C5-C6-O8
29	k	319	LHG	C7-C8-C9-C10
27	c	604	CLA	C5-C6-C7-C8
37	s	204	KC2	C4C-C3C-CAC-CBC
37	i	317	KC2	C2A-CAA-CBA-CGA
37	g	313	KC2	C4C-C3C-CAC-CBC
27	B	801	CLA	C16-C17-C18-C20
27	B	818	CLA	C6-C7-C8-C9
27	a	312	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	l	304	CLA	C16-C17-C18-C20
28	A	843	PQN	C26-C27-C28-C29
27	b	603	CLA	C3-C5-C6-C7
29	J	107	LHG	C34-C35-C36-C37
27	A	818	CLA	C4-C3-C5-C6
27	B	810	CLA	C4-C3-C5-C6
27	e	607	CLA	C2-C3-C5-C6
27	A	855	CLA	C3-C5-C6-C7
29	c	618	LHG	O7-C5-C6-O8
29	b	618	LHG	O7-C5-C6-O8
29	g	301	LHG	O7-C5-C6-O8
27	g	322	CLA	C15-C16-C17-C18
27	A	831	CLA	C11-C12-C13-C14
27	A	836	CLA	C6-C7-C8-C9
27	e	604	CLA	C11-C12-C13-C14
27	f	610	CLA	C11-C10-C8-C9
27	j	612	CLA	C11-C12-C13-C14
27	d	303	CLA	C11-C10-C8-C9
28	A	843	PQN	C21-C22-C23-C24
27	A	855	CLA	C16-C17-C18-C20
27	A	829	CLA	O1A-CGA-O2A-C1
27	g	311	CLA	O1A-CGA-O2A-C1
30	B	843	WVN	C02-C11-C19-C22
29	L	207	LHG	C7-C8-C9-C10
29	c	621	LHG	C30-C31-C32-C33
34	L	208	LMG	C17-C18-C19-C20
27	e	610	CLA	C10-C11-C12-C13
27	B	819	CLA	O1A-CGA-O2A-C1
27	h	303	CLA	C2-C1-O2A-CGA
27	k	313	CLA	C2-C1-O2A-CGA
30	A	846	WVN	C32-C36-C39-C40
27	B	807	CLA	C16-C17-C18-C19
27	B	835	CLA	C16-C17-C18-C19
27	A	839	CLA	C4-C3-C5-C6
27	b	607	CLA	C4-C3-C5-C6
27	e	607	CLA	C4-C3-C5-C6
27	f	609	CLA	C4-C3-C5-C6
27	B	806	CLA	C2-C3-C5-C6
27	b	605	CLA	O1D-CGD-O2D-CED
29	d	315	LHG	C28-C29-C30-C31
27	l	312	CLA	CBA-CGA-O2A-C1
29	a	301	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
27	m	609	CLA	C4C-C3C-CAC-CBC
27	A	807	CLA	C16-C17-C18-C19
27	b	609	CLA	O1A-CGA-O2A-C1
34	F	206	LMG	C32-C33-C34-C35
27	l	310	CLA	C14-C13-C15-C16
27	l	307	CLA	O1D-CGD-O2D-CED
27	g	304	CLA	O1D-CGD-O2D-CED
27	g	305	CLA	C4C-C3C-CAC-CBC
27	B	807	CLA	C16-C17-C18-C20
27	g	322	CLA	C16-C17-C18-C20
27	l	307	CLA	C4C-C3C-CAC-CBC
35	b	615	II0	C09-C21-C23-C25
35	f	614	II0	C09-C21-C23-C25
36	n	617	IHT	C11-C21-C24-C26
27	s	209	CLA	O1A-CGA-O2A-C1
27	n	610	CLA	O1A-CGA-O2A-C1
27	A	812	CLA	CBD-CGD-O2D-CED
31	a	320	LMT	C3-C4-C5-C6
35	h	311	II0	C31-C33-C35-C37
27	A	812	CLA	C1A-C2A-CAA-CBA
27	A	817	CLA	C4B-C3B-CAB-CBB
27	B	812	CLA	C1A-C2A-CAA-CBA
27	B	827	CLA	C1A-C2A-CAA-CBA
27	B	833	CLA	C4B-C3B-CAB-CBB
27	B	834	CLA	C4B-C3B-CAB-CBB
27	F	203	CLA	C4B-C3B-CAB-CBB
27	c	601	CLA	C4B-C3B-CAB-CBB
27	b	611	CLA	C4B-C3B-CAB-CBB
27	k	306	CLA	C4B-C3B-CAB-CBB
27	k	308	CLA	C1A-C2A-CAA-CBA
27	j	611	CLA	C1A-C2A-CAA-CBA
27	d	306	CLA	C1A-C2A-CAA-CBA
27	d	306	CLA	C4B-C3B-CAB-CBB
27	g	311	CLA	C4B-C3B-CAB-CBB
27	n	606	CLA	C4B-C3B-CAB-CBB
27	h	303	CLA	O1D-CGD-O2D-CED
27	B	828	CLA	CBA-CGA-O2A-C1
27	n	604	CLA	CBA-CGA-O2A-C1
29	b	617	LHG	C9-C10-C11-C12
27	B	810	CLA	C2-C3-C5-C6
27	l	304	CLA	C2-C3-C5-C6
29	L	207	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	a	311	CLA	C2A-CAA-CBA-CGA
29	L	207	LHG	O6-C4-C5-C6
29	f	619	LHG	O6-C4-C5-C6
27	n	604	CLA	CBD-CGD-O2D-CED
31	a	320	LMT	C5-C6-C7-C8
27	d	304	CLA	C2-C3-C5-C6
27	d	311	CLA	C2-C3-C5-C6
27	R	203	CLA	C2-C3-C5-C6
27	n	603	CLA	C2-C3-C5-C6
34	F	206	LMG	C23-C24-C25-C26
27	A	828	CLA	C12-C13-C15-C16
27	A	839	CLA	C11-C12-C13-C15
27	B	811	CLA	C11-C10-C8-C7
27	B	831	CLA	C11-C10-C8-C7
27	B	834	CLA	C11-C10-C8-C7
27	B	834	CLA	C11-C12-C13-C15
27	B	835	CLA	C6-C7-C8-C10
27	B	836	CLA	C11-C10-C8-C7
27	B	838	CLA	C11-C12-C13-C15
27	B	838	CLA	C12-C13-C15-C16
27	F	202	CLA	C11-C10-C8-C7
27	s	206	CLA	C11-C12-C13-C15
27	b	605	CLA	C12-C13-C15-C16
27	b	610	CLA	C6-C7-C8-C10
27	m	604	CLA	C6-C7-C8-C10
27	l	310	CLA	C6-C7-C8-C10
27	l	312	CLA	C6-C7-C8-C10
27	k	303	CLA	C12-C13-C15-C16
27	k	307	CLA	C11-C10-C8-C7
27	f	607	CLA	C6-C7-C8-C10
27	f	607	CLA	C11-C12-C13-C15
27	f	613	CLA	C12-C13-C15-C16
27	g	308	CLA	C11-C12-C13-C15
27	b	603	CLA	C16-C17-C18-C20
27	B	835	CLA	O1D-CGD-O2D-CED
27	l	312	CLA	O1A-CGA-O2A-C1
27	s	203	CLA	C15-C16-C17-C18
27	n	602	CLA	O1A-CGA-O2A-C1
27	a	312	CLA	C10-C11-C12-C13
29	k	319	LHG	C9-C10-C11-C12
27	A	805	CLA	C3A-C2A-CAA-CBA
27	B	810	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	B	811	CLA	C3A-C2A-CAA-CBA
27	c	606	CLA	C3A-C2A-CAA-CBA
27	b	607	CLA	C2-C3-C5-C6
29	f	619	LHG	O6-C4-C5-O7
29	g	301	LHG	O6-C4-C5-O7
27	l	303	CLA	CBD-CGD-O2D-CED
27	k	305	CLA	C2A-CAA-CBA-CGA
27	j	601	CLA	C2A-CAA-CBA-CGA
27	A	816	CLA	C11-C10-C8-C9
27	A	837	CLA	C14-C13-C15-C16
27	A	840	CLA	C11-C12-C13-C14
27	B	815	CLA	C11-C10-C8-C9
27	B	823	CLA	C6-C7-C8-C9
27	O	206	CLA	C11-C12-C13-C14
27	c	612	CLA	C11-C10-C8-C9
27	b	603	CLA	C14-C13-C15-C16
27	b	604	CLA	C6-C7-C8-C9
27	b	610	CLA	C14-C13-C15-C16
27	m	602	CLA	C6-C7-C8-C9
27	l	307	CLA	C6-C7-C8-C9
27	k	307	CLA	C14-C13-C15-C16
27	f	608	CLA	C11-C12-C13-C14
27	j	609	CLA	C11-C10-C8-C9
27	g	308	CLA	C11-C10-C8-C9
27	n	610	CLA	C6-C7-C8-C9
30	A	849	WVN	C25-C28-C30-C33
30	B	845	WVN	C34-C37-C40-C39
30	i	315	WVN	C34-C37-C40-C39
35	m	614	II0	C35-C39-C41-C42
35	l	315	II0	C25-C29-C31-C33
35	k	315	II0	C35-C39-C41-C42
35	f	615	II0	C26-C30-C32-C34
35	j	614	II0	C36-C40-C42-C41
35	n	616	II0	C35-C39-C41-C42
36	f	617	IHT	C33-C37-C40-C41
27	m	609	CLA	C6-C7-C8-C10
27	A	821	CLA	C1-C2-C3-C4
27	B	827	CLA	C1-C2-C3-C4
30	s	207	WVN	C01-C02-C11-C19
37	s	201	KC2	C1A-C2A-CAA-CBA
37	s	204	KC2	C1A-C2A-CAA-CBA
37	f	611	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	i	310	KC2	C3A-C2A-CAA-CBA
37	g	313	KC2	C3A-C2A-CAA-CBA
37	g	314	KC2	C1A-C2A-CAA-CBA
27	g	308	CLA	O1D-CGD-O2D-CED
27	d	303	CLA	O1A-CGA-O2A-C1
29	e	617	LHG	O7-C5-C6-O8
29	a	319	LHG	C10-C11-C12-C13
27	B	819	CLA	CBD-CGD-O2D-CED
27	b	607	CLA	CBD-CGD-O2D-CED
29	c	621	LHG	C4-C5-C6-O8
29	k	319	LHG	C4-C5-C6-O8
27	A	802	CLA	C4-C3-C5-C6
27	A	842	CLA	C4-C3-C5-C6
27	A	804	CLA	CAD-CBD-CGD-O2D
27	A	813	CLA	CAD-CBD-CGD-O2D
27	A	814	CLA	CAD-CBD-CGD-O2D
27	A	855	CLA	CAD-CBD-CGD-O2D
27	O	202	CLA	CAD-CBD-CGD-O2D
27	a	306	CLA	CAD-CBD-CGD-O2D
27	a	313	CLA	CAD-CBD-CGD-O2D
27	b	604	CLA	CAD-CBD-CGD-O2D
27	b	611	CLA	CAD-CBD-CGD-O2D
27	h	308	CLA	CAD-CBD-CGD-O2D
27	h	313	CLA	CAD-CBD-CGD-O2D
27	l	306	CLA	CAD-CBD-CGD-O2D
27	k	303	CLA	CAD-CBD-CGD-O2D
27	f	604	CLA	CAD-CBD-CGD-O2D
27	j	604	CLA	CAD-CBD-CGD-O2D
27	d	303	CLA	CAD-CBD-CGD-O2D
27	d	305	CLA	CAD-CBD-CGD-O2D
27	g	305	CLA	CAD-CBD-CGD-O2D
27	g	309	CLA	CAD-CBD-CGD-O2D
27	a	306	CLA	C13-C15-C16-C17
27	g	305	CLA	C15-C16-C17-C18
34	L	208	LMG	C29-C28-O8-C9
27	A	840	CLA	C5-C6-C7-C8
27	O	206	CLA	C13-C15-C16-C17
27	A	806	CLA	C16-C17-C18-C19
27	B	811	CLA	C11-C12-C13-C14
27	L	203	CLA	C16-C17-C18-C19
27	b	604	CLA	C16-C17-C18-C19
27	f	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
34	J	106	LMG	C37-C38-C39-C40
27	e	604	CLA	C2A-CAA-CBA-CGA
27	b	602	CLA	O1A-CGA-O2A-C1
34	s	210	LMG	C22-C23-C24-C25
27	A	804	CLA	CAD-CBD-CGD-O1D
27	A	813	CLA	CAD-CBD-CGD-O1D
27	A	814	CLA	CAD-CBD-CGD-O1D
27	A	835	CLA	CAD-CBD-CGD-O1D
27	A	855	CLA	CAD-CBD-CGD-O1D
27	B	820	CLA	CHA-CBD-CGD-O1D
27	B	820	CLA	CHA-CBD-CGD-O2D
27	B	836	CLA	CHA-CBD-CGD-O1D
27	B	836	CLA	CHA-CBD-CGD-O2D
27	O	202	CLA	CAD-CBD-CGD-O1D
27	s	203	CLA	CHA-CBD-CGD-O1D
27	s	203	CLA	CHA-CBD-CGD-O2D
27	c	604	CLA	CHA-CBD-CGD-O1D
27	c	604	CLA	CHA-CBD-CGD-O2D
27	a	304	CLA	CHA-CBD-CGD-O1D
27	a	304	CLA	CHA-CBD-CGD-O2D
27	a	305	CLA	CHA-CBD-CGD-O1D
27	a	305	CLA	CHA-CBD-CGD-O2D
27	a	306	CLA	CAD-CBD-CGD-O1D
27	a	313	CLA	CAD-CBD-CGD-O1D
27	b	601	CLA	CHA-CBD-CGD-O1D
27	b	601	CLA	CHA-CBD-CGD-O2D
27	b	604	CLA	CAD-CBD-CGD-O1D
27	b	611	CLA	CAD-CBD-CGD-O1D
27	h	308	CLA	CAD-CBD-CGD-O1D
27	h	313	CLA	CAD-CBD-CGD-O1D
27	l	306	CLA	CAD-CBD-CGD-O1D
27	k	303	CLA	CAD-CBD-CGD-O1D
27	f	601	CLA	CHA-CBD-CGD-O1D
27	f	601	CLA	CHA-CBD-CGD-O2D
27	f	603	CLA	CHA-CBD-CGD-O1D
27	f	603	CLA	CHA-CBD-CGD-O2D
27	f	604	CLA	CAD-CBD-CGD-O1D
27	i	304	CLA	CHA-CBD-CGD-O1D
27	i	304	CLA	CHA-CBD-CGD-O2D
27	i	305	CLA	CAD-CBD-CGD-O1D
27	i	308	CLA	CHA-CBD-CGD-O1D
27	i	308	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	j	604	CLA	CAD-CBD-CGD-O1D
27	d	301	CLA	CHA-CBD-CGD-O1D
27	d	301	CLA	CHA-CBD-CGD-O2D
27	d	302	CLA	CHA-CBD-CGD-O1D
27	d	303	CLA	CAD-CBD-CGD-O1D
27	d	305	CLA	CAD-CBD-CGD-O1D
27	g	305	CLA	CAD-CBD-CGD-O1D
27	g	309	CLA	CAD-CBD-CGD-O1D
29	A	850	LHG	C3-O3-P-O4
29	A	850	LHG	C4-O6-P-O5
29	c	618	LHG	C4-O6-P-O5
29	c	621	LHG	C4-O6-P-O5
29	a	301	LHG	C3-O3-P-O5
29	a	319	LHG	C3-O3-P-O5
29	b	617	LHG	C4-O6-P-O5
29	b	618	LHG	C3-O3-P-O5
29	b	618	LHG	C4-O6-P-O3
29	e	617	LHG	C4-O6-P-O5
29	l	318	LHG	C3-O3-P-O5
29	i	316	LHG	C3-O3-P-O5
29	i	316	LHG	C4-O6-P-O3
29	j	617	LHG	C4-O6-P-O5
29	d	315	LHG	C3-O3-P-O5
29	d	315	LHG	C4-O6-P-O4
29	g	321	LHG	C3-O3-P-O5
29	n	619	LHG	C3-O3-P-O5
30	A	848	WVN	C25-C28-C30-C33
30	F	204	WVN	C34-C37-C40-C39
30	F	205	WVN	C25-C28-C30-C33
30	F	205	WVN	C34-C37-C40-C39
30	i	315	WVN	C32-C36-C39-C40
30	R	202	WVN	C25-C28-C30-C33
35	b	613	II0	C35-C39-C41-C42
35	h	312	II0	C35-C39-C41-C42
35	k	314	II0	C35-C39-C41-C42
37	s	204	KC2	CHA-CBD-CGD-O2D
37	l	311	KC2	CHA-CBD-CGD-O1D
37	l	311	KC2	CHA-CBD-CGD-O2D
37	i	317	KC2	CHA-CBD-CGD-O1D
37	g	312	KC2	CHA-CBD-CGD-O1D
37	g	312	KC2	CHA-CBD-CGD-O2D
27	n	610	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	l	318	LHG	C26-C27-C28-C29
29	b	618	LHG	C9-C10-C11-C12
27	B	826	CLA	C2B-C3B-CAB-CBB
27	B	828	CLA	C2B-C3B-CAB-CBB
27	B	849	CLA	C2B-C3B-CAB-CBB
27	K	102	CLA	C2B-C3B-CAB-CBB
27	h	301	CLA	C2B-C3B-CAB-CBB
27	e	607	CLA	C2B-C3B-CAB-CBB
27	l	312	CLA	C2B-C3B-CAB-CBB
27	j	612	CLA	C2B-C3B-CAB-CBB
27	g	306	CLA	C2B-C3B-CAB-CBB
27	g	307	CLA	C2B-C3B-CAB-CBB
27	g	309	CLA	C2B-C3B-CAB-CBB
27	g	311	CLA	C2B-C3B-CAB-CBB
27	n	606	CLA	C2B-C3B-CAB-CBB
27	B	840	CLA	CAA-CBA-CGA-O2A
37	k	310	KC2	C2A-CAA-CBA-CGA
34	c	619	LMG	C34-C35-C36-C37
29	A	850	LHG	C5-C4-O6-P
29	L	207	LHG	C2-C3-O3-P
29	e	617	LHG	C2-C3-O3-P
29	n	619	LHG	C5-C4-O6-P
30	O	201	WVN	C29-C31-C32-C35
36	g	319	IHT	C30-C32-C33-C36
27	s	202	CLA	C3-C5-C6-C7
27	e	606	CLA	C8-C10-C11-C12
27	A	803	CLA	C6-C7-C8-C10
27	B	811	CLA	C11-C12-C13-C15
27	b	604	CLA	C16-C17-C18-C20
27	f	607	CLA	C16-C17-C18-C19
37	f	611	KC2	CAA-CBA-CGA-O1A
29	A	844	LHG	C10-C11-C12-C13
29	e	617	LHG	C10-C11-C12-C13
34	J	106	LMG	C31-C32-C33-C34
29	J	107	LHG	O1-C1-C2-O2
27	n	609	CLA	C3-C5-C6-C7
29	b	617	LHG	C30-C31-C32-C33
29	g	321	LHG	C4-C5-O7-C7
30	B	845	WVN	C26-C29-C31-C32
30	B	848	WVN	C28-C30-C33-C34
27	B	814	CLA	CAA-CBA-CGA-O2A
27	s	203	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	h	313	CLA	C5-C6-C7-C8
27	m	604	CLA	C8-C10-C11-C12
29	b	617	LHG	C29-C30-C31-C32
27	A	801	CLA	C16-C17-C18-C20
27	B	823	CLA	C16-C17-C18-C20
27	b	610	CLA	C16-C17-C18-C19
27	e	605	CLA	C16-C17-C18-C19
31	A	851	LMT	C6-C7-C8-C9
29	b	618	LHG	O6-C4-C5-C6
27	B	817	CLA	O1A-CGA-O2A-C1
27	A	812	CLA	C6-C7-C8-C9
27	A	853	CLA	C11-C12-C13-C14
27	B	829	CLA	C6-C7-C8-C9
27	B	834	CLA	C11-C10-C8-C9
27	m	604	CLA	C6-C7-C8-C9
27	l	304	CLA	C6-C7-C8-C9
27	l	306	CLA	C11-C10-C8-C9
27	l	310	CLA	C11-C12-C13-C14
27	g	308	CLA	C6-C7-C8-C9
27	g	309	CLA	C6-C7-C8-C9
27	n	607	CLA	C11-C10-C8-C9
28	A	843	PQN	C24-C23-C25-C26
27	A	818	CLA	C11-C12-C13-C15
27	B	805	CLA	C6-C7-C8-C10
27	B	807	CLA	C11-C12-C13-C15
27	B	836	CLA	C11-C12-C13-C15
27	b	610	CLA	C12-C13-C15-C16
27	h	306	CLA	C11-C10-C8-C7
27	m	603	CLA	C12-C13-C15-C16
27	e	610	CLA	C11-C12-C13-C15
27	f	607	CLA	C12-C13-C15-C16
27	f	608	CLA	C12-C13-C15-C16
27	g	322	CLA	C6-C7-C8-C10
28	B	841	PQN	C16-C17-C18-C20
27	B	823	CLA	CBD-CGD-O2D-CED
27	A	855	CLA	C2A-CAA-CBA-CGA
27	m	609	CLA	C6-C7-C8-C9
28	A	843	PQN	C26-C27-C28-C30
27	n	610	CLA	CBA-CGA-O2A-C1
27	h	301	CLA	CAA-CBA-CGA-O2A
37	m	610	KC2	CAA-CBA-CGA-O2A
27	B	823	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	817	CLA	CAA-CBA-CGA-O2A
27	A	817	CLA	C16-C17-C18-C19
27	e	605	CLA	C16-C17-C18-C20
27	A	824	CLA	C8-C10-C11-C12
29	l	318	LHG	O9-C7-O7-C5
34	J	106	LMG	O1-C7-C8-O7
34	O	205	LMG	O7-C8-C9-O8
33	B	842	DGD	C8B-C9B-CAB-CBB
29	f	619	LHG	C34-C35-C36-C37
35	n	616	II0	C26-C30-C32-C34
36	g	319	IHT	C23-C27-C30-C32
29	a	301	LHG	O10-C23-O8-C6
27	A	804	CLA	CAA-CBA-CGA-O2A
27	B	839	CLA	C3-C5-C6-C7
27	a	312	CLA	C4C-C3C-CAC-CBC
27	F	203	CLA	C2-C1-O2A-CGA
27	s	206	CLA	C4-C3-C5-C6
29	J	107	LHG	C27-C28-C29-C30
27	d	304	CLA	CAA-CBA-CGA-O2A
27	A	816	CLA	C8-C10-C11-C12
35	b	613	II0	C32-C34-C36-C38
27	e	610	CLA	C16-C17-C18-C19
37	m	610	KC2	CBD-CGD-O2D-CED
27	g	311	CLA	CBA-CGA-O2A-C1
27	f	613	CLA	CAA-CBA-CGA-O2A
33	B	842	DGD	C5D-C6D-O5D-C1E
27	s	206	CLA	C5-C6-C7-C8
27	b	604	CLA	C8-C10-C11-C12
27	d	303	CLA	C13-C15-C16-C17
27	k	308	CLA	C2A-CAA-CBA-CGA
27	g	305	CLA	C2A-CAA-CBA-CGA
30	L	201	WVN	C22-C26-C29-C31
35	a	316	II0	C36-C40-C42-C41
35	b	613	II0	C26-C30-C32-C34
35	d	313	II0	C25-C29-C31-C33
27	A	840	CLA	C16-C17-C18-C20
27	k	303	CLA	C16-C17-C18-C20
27	g	308	CLA	C4-C3-C5-C6
27	B	823	CLA	C2-C3-C5-C6
27	a	308	CLA	O1D-CGD-O2D-CED
29	g	301	LHG	C31-C32-C33-C34
27	i	302	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
35	e	614	II0	C10-C22-C24-C26
35	k	318	II0	C10-C22-C24-C26
27	B	818	CLA	C6-C7-C8-C10
27	m	606	CLA	CAA-CBA-CGA-O2A
29	c	618	LHG	C25-C26-C27-C28
29	k	319	LHG	C31-C32-C33-C34
27	A	812	CLA	C14-C13-C15-C16
27	A	828	CLA	C14-C13-C15-C16
27	B	811	CLA	C11-C10-C8-C9
27	B	823	CLA	C14-C13-C15-C16
27	b	607	CLA	C11-C12-C13-C14
27	l	310	CLA	C6-C7-C8-C9
27	B	834	CLA	CBA-CGA-O2A-C1
27	O	206	CLA	O1D-CGD-O2D-CED
27	c	609	CLA	C4B-C3B-CAB-CBB
27	e	602	CLA	C4B-C3B-CAB-CBB
27	e	604	CLA	C4B-C3B-CAB-CBB
27	g	322	CLA	C4B-C3B-CAB-CBB
27	A	820	CLA	C2C-C3C-CAC-CBC
33	B	842	DGD	O1A-C1A-O1G-C1G
27	j	612	CLA	C5-C6-C7-C8
27	s	202	CLA	C16-C17-C18-C20
27	a	311	CLA	C16-C17-C18-C19
27	h	301	CLA	C16-C17-C18-C20
33	B	842	DGD	C2A-C1A-O1G-C1G
27	s	202	CLA	C8-C10-C11-C12
27	b	604	CLA	C10-C11-C12-C13
27	A	842	CLA	C2-C3-C5-C6
35	g	318	II0	C36-C40-C42-C41
37	k	310	KC2	C4B-C3B-CAB-CBB
27	A	811	CLA	O1D-CGD-O2D-CED
27	A	807	CLA	C12-C13-C15-C16
27	A	855	CLA	C11-C10-C8-C7
27	B	816	CLA	C6-C7-C8-C10
27	e	604	CLA	C11-C10-C8-C7
27	e	605	CLA	C12-C13-C15-C16
27	e	607	CLA	C12-C13-C15-C16
27	f	608	CLA	C6-C7-C8-C10
27	A	811	CLA	CBD-CGD-O2D-CED
29	L	207	LHG	O2-C2-C3-O3
34	c	619	LMG	C14-C15-C16-C17
34	J	106	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
27	A	801	CLA	C16-C17-C18-C19
27	A	803	CLA	C6-C7-C8-C9
27	F	201	CLA	C16-C17-C18-C19
27	B	804	CLA	C10-C11-C12-C13
27	m	604	CLA	C4C-C3C-CAC-CBC
27	A	808	CLA	C3A-C2A-CAA-CBA
27	B	824	CLA	C4-C3-C5-C6
27	B	838	CLA	C3A-C2A-CAA-CBA
27	s	206	CLA	C3A-C2A-CAA-CBA
27	c	611	CLA	C3A-C2A-CAA-CBA
27	a	313	CLA	C3A-C2A-CAA-CBA
27	e	604	CLA	C3A-C2A-CAA-CBA
27	e	611	CLA	C4-C3-C5-C6
27	n	613	CLA	C3A-C2A-CAA-CBA
27	e	611	CLA	C2-C3-C5-C6
27	k	306	CLA	C2A-CAA-CBA-CGA
29	L	207	LHG	C33-C34-C35-C36
30	A	847	WVN	C24-C22-C26-C29
35	l	314	II0	C38-C36-C40-C42
27	f	604	CLA	C2C-C3C-CAC-CBC
29	m	617	LHG	C10-C11-C12-C13
29	f	619	LHG	C11-C12-C13-C14
30	A	847	WVN	C25-C28-C30-C33
30	A	849	WVN	C22-C26-C29-C31
30	K	103	WVN	C22-C26-C29-C31
35	l	302	II0	C35-C39-C41-C42
36	O	204	IHT	C33-C37-C40-C41
30	B	845	WVN	C29-C31-C32-C35
35	n	618	II0	C32-C34-C36-C38
27	c	602	CLA	C2C-C3C-CAC-CBC
27	k	305	CLA	C4-C3-C5-C6
27	d	304	CLA	C4-C3-C5-C6
27	d	311	CLA	C4-C3-C5-C6
27	n	603	CLA	C4-C3-C5-C6
27	B	836	CLA	C15-C16-C17-C18
34	L	208	LMG	C39-C40-C41-C42
27	B	819	CLA	O1D-CGD-O2D-CED
27	a	308	CLA	C13-C15-C16-C17
30	L	201	WVN	C29-C31-C32-C36
35	m	614	II0	C31-C33-C35-C39
35	e	613	II0	C31-C33-C35-C39
27	m	606	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	i	312	CLA	C2A-CAA-CBA-CGA
29	A	850	LHG	C24-C25-C26-C27
27	B	805	CLA	C3-C5-C6-C7
29	g	301	LHG	C11-C10-C9-C8
27	j	605	CLA	CAA-CBA-CGA-O2A
27	A	808	CLA	C11-C12-C13-C14
27	A	818	CLA	C14-C13-C15-C16
27	A	820	CLA	C11-C10-C8-C9
27	A	825	CLA	C14-C13-C15-C16
27	A	827	CLA	C14-C13-C15-C16
27	B	803	CLA	C6-C7-C8-C9
27	B	820	CLA	C14-C13-C15-C16
27	O	206	CLA	C11-C10-C8-C9
27	c	612	CLA	C14-C13-C15-C16
27	a	306	CLA	C14-C13-C15-C16
27	a	308	CLA	C11-C12-C13-C14
27	b	604	CLA	C11-C10-C8-C9
27	b	606	CLA	C6-C7-C8-C9
27	h	307	CLA	C11-C10-C8-C9
27	e	610	CLA	C6-C7-C8-C9
27	l	304	CLA	C11-C10-C8-C9
27	k	307	CLA	C11-C12-C13-C14
27	i	307	CLA	C11-C10-C8-C9
29	L	207	LHG	O1-C1-C2-C3
29	n	619	LHG	O1-C1-C2-C3
27	g	306	CLA	CAA-CBA-CGA-O1A
27	A	824	CLA	C13-C15-C16-C17
34	F	206	LMG	C14-C15-C16-C17
29	g	301	LHG	C6-C5-O7-C7
27	B	834	CLA	CBD-CGD-O2D-CED
27	B	834	CLA	O1D-CGD-O2D-CED
35	f	618	II0	C36-C40-C42-C41
27	A	827	CLA	C4-C3-C5-C6
27	a	309	CLA	C16-C17-C18-C20
27	k	303	CLA	C16-C17-C18-C19
27	B	828	CLA	CBD-CGD-O2D-CED
27	f	609	CLA	C2-C3-C5-C6
29	m	617	LHG	O1-C1-C2-O2
27	A	852	CLA	C2A-CAA-CBA-CGA
27	R	203	CLA	CAA-CBA-CGA-O1A
27	B	810	CLA	C1A-C2A-CAA-CBA
27	B	817	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	B	823	CLA	C1A-C2A-CAA-CBA
27	c	605	CLA	C1A-C2A-CAA-CBA
27	c	609	CLA	C1A-C2A-CAA-CBA
27	a	313	CLA	C1A-C2A-CAA-CBA
27	b	606	CLA	C1A-C2A-CAA-CBA
27	h	301	CLA	C1A-C2A-CAA-CBA
27	m	611	CLA	C1A-C2A-CAA-CBA
27	f	604	CLA	C1A-C2A-CAA-CBA
27	j	605	CLA	C1A-C2A-CAA-CBA
30	A	847	WVN	C19-C22-C26-C29
35	l	314	II0	C34-C36-C40-C42
29	a	319	LHG	C33-C34-C35-C36
34	s	210	LMG	C15-C16-C17-C18
27	A	817	CLA	C2B-C3B-CAB-CBB
27	A	832	CLA	C2B-C3B-CAB-CBB
27	A	833	CLA	C2B-C3B-CAB-CBB
27	A	853	CLA	C2B-C3B-CAB-CBB
27	B	801	CLA	C2B-C3B-CAB-CBB
27	B	814	CLA	C2B-C3B-CAB-CBB
27	B	833	CLA	C2B-C3B-CAB-CBB
27	B	834	CLA	C2B-C3B-CAB-CBB
27	F	203	CLA	C2B-C3B-CAB-CBB
27	L	203	CLA	C2B-C3B-CAB-CBB
27	s	203	CLA	C2B-C3B-CAB-CBB
27	c	609	CLA	C2B-C3B-CAB-CBB
27	a	305	CLA	C2B-C3B-CAB-CBB
27	b	611	CLA	C2B-C3B-CAB-CBB
27	m	611	CLA	C2B-C3B-CAB-CBB
27	e	602	CLA	C2B-C3B-CAB-CBB
27	e	610	CLA	C2B-C3B-CAB-CBB
27	l	305	CLA	C2B-C3B-CAB-CBB
27	k	306	CLA	C2B-C3B-CAB-CBB
27	f	605	CLA	C2B-C3B-CAB-CBB
27	d	303	CLA	C2B-C3B-CAB-CBB
27	d	306	CLA	C2B-C3B-CAB-CBB
27	n	603	CLA	C2B-C3B-CAB-CBB
30	A	846	WVN	C15-C13-C20-C23
30	B	845	WVN	C06-C13-C20-C23
30	B	845	WVN	C15-C13-C20-C23
30	J	102	WVN	C15-C13-C20-C23
36	O	204	IHT	C02-C07-C18-C22
36	k	317	IHT	C02-C07-C18-C22

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Mol	Chain	Res	Type	Atoms
36	f	617	IHT	C02-C07-C18-C22
27	b	607	CLA	O1D-CGD-O2D-CED
27	h	303	CLA	CBD-CGD-O2D-CED
27	f	612	CLA	C4C-C3C-CAC-CBC
29	J	107	LHG	C32-C33-C34-C35
27	A	824	CLA	C12-C13-C15-C16
27	A	829	CLA	C6-C7-C8-C10
27	B	814	CLA	C6-C7-C8-C10
27	B	823	CLA	C12-C13-C15-C16
27	L	203	CLA	C6-C7-C8-C10
27	s	202	CLA	C11-C10-C8-C7
27	a	306	CLA	C11-C10-C8-C7
27	a	312	CLA	C11-C12-C13-C15
27	l	308	CLA	C6-C7-C8-C10
27	l	310	CLA	C11-C10-C8-C7
27	i	305	CLA	C11-C10-C8-C7
28	A	843	PQN	C16-C17-C18-C20
27	j	612	CLA	C16-C17-C18-C19
27	a	304	CLA	C2A-CAA-CBA-CGA
27	a	313	CLA	C2A-CAA-CBA-CGA
27	h	306	CLA	C2A-CAA-CBA-CGA
31	A	851	LMT	C2-C3-C4-C5
27	A	825	CLA	CBA-CGA-O2A-C1
27	i	312	CLA	CAA-CBA-CGA-O2A
29	a	319	LHG	C24-C25-C26-C27
27	B	823	CLA	C15-C16-C17-C18
27	m	603	CLA	C13-C15-C16-C17
27	l	310	CLA	C5-C6-C7-C8
27	F	201	CLA	O1D-CGD-O2D-CED
27	l	303	CLA	O1D-CGD-O2D-CED
27	A	809	CLA	C11-C10-C8-C7
27	b	606	CLA	C12-C13-C15-C16
30	s	205	WVN	C30-C33-C34-C38
27	F	202	CLA	C4-C3-C5-C6
27	O	202	CLA	C4-C3-C5-C6
27	e	605	CLA	C4-C3-C5-C6
27	l	312	CLA	C5-C6-C7-C8
27	A	818	CLA	C2-C3-C5-C6
27	A	827	CLA	C2-C3-C5-C6
27	c	608	CLA	C15-C16-C17-C18
30	R	202	WVN	C30-C33-C34-C37
35	h	311	II0	C31-C33-C35-C39

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Mol	Chain	Res	Type	Atoms
36	g	319	IHT	C30-C32-C33-C37
27	F	201	CLA	C16-C17-C18-C20
29	J	107	LHG	C17-C18-C19-C20
27	B	816	CLA	CBA-CGA-O2A-C1
34	O	205	LMG	C28-C29-C30-C31
29	J	107	LHG	C30-C31-C32-C33
27	j	605	CLA	CAA-CBA-CGA-O1A
27	B	801	CLA	C11-C10-C8-C9
27	b	611	CLA	C6-C7-C8-C9
27	l	310	CLA	C11-C10-C8-C9
34	c	619	LMG	C12-C13-C14-C15
27	l	308	CLA	C5-C6-C7-C8
27	a	312	CLA	C16-C17-C18-C20
27	f	607	CLA	C5-C6-C7-C8
34	L	208	LMG	O10-C28-O8-C9
27	k	313	CLA	C2C-C3C-CAC-CBC
27	B	838	CLA	C4-C3-C5-C6
27	j	607	CLA	CAA-CBA-CGA-O2A
29	a	301	LHG	C5-C4-O6-P
29	f	619	LHG	C2-C3-O3-P
27	i	307	CLA	C2-C3-C5-C6
34	c	619	LMG	C32-C33-C34-C35
27	O	206	CLA	CBD-CGD-O2D-CED
27	m	607	CLA	C16-C17-C18-C20
27	B	835	CLA	C4C-C3C-CAC-CBC
27	A	835	CLA	C2A-CAA-CBA-CGA
27	c	604	CLA	C2A-CAA-CBA-CGA
27	l	304	CLA	C2A-CAA-CBA-CGA
27	j	612	CLA	C2A-CAA-CBA-CGA
29	i	316	LHG	C26-C27-C28-C29
31	a	302	LMT	C4-C5-C6-C7
27	f	613	CLA	C13-C15-C16-C17
29	l	318	LHG	C25-C26-C27-C28
27	A	819	CLA	CAA-CBA-CGA-O2A
27	B	832	CLA	C5-C6-C7-C8
27	A	801	CLA	CAA-CBA-CGA-O1A
29	a	319	LHG	C29-C30-C31-C32
31	b	616	LMT	O1'-C1-C2-C3
29	g	301	LHG	O1-C1-C2-O2
35	a	318	II0	C09-C21-C23-C25
35	f	614	II0	C10-C22-C24-C26
35	f	615	II0	C10-C22-C24-C26

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Mol	Chain	Res	Type	Atoms
35	j	615	II0	C09-C21-C23-C25
35	j	615	II0	C10-C22-C24-C26
35	d	312	II0	C10-C22-C24-C26
35	d	314	II0	C10-C22-C24-C26
35	g	316	II0	C09-C21-C23-C25
29	c	621	LHG	O6-C4-C5-O7
27	n	602	CLA	CBA-CGA-O2A-C1
29	b	617	LHG	C27-C28-C29-C30
27	n	613	CLA	CAA-CBA-CGA-O1A
27	A	855	CLA	C16-C17-C18-C19
27	s	202	CLA	C16-C17-C18-C19
27	e	610	CLA	C16-C17-C18-C20
27	F	201	CLA	C15-C16-C17-C18
29	m	617	LHG	C25-C26-C27-C28
27	A	801	CLA	C4B-C3B-CAB-CBB
27	A	830	CLA	C4B-C3B-CAB-CBB
27	A	833	CLA	C4B-C3B-CAB-CBB
27	B	818	CLA	C4B-C3B-CAB-CBB
27	L	203	CLA	C4B-C3B-CAB-CBB
27	m	602	CLA	C4B-C3B-CAB-CBB
27	m	611	CLA	C4B-C3B-CAB-CBB
27	A	812	CLA	O1D-CGD-O2D-CED
27	g	308	CLA	C8-C10-C11-C12
27	B	806	CLA	C16-C17-C18-C19
27	e	610	CLA	C6-C7-C8-C10
27	j	612	CLA	C11-C12-C13-C15
29	b	618	LHG	C25-C26-C27-C28
30	l	316	WVN	C32-C36-C39-C40
30	l	316	WVN	C34-C37-C40-C39
27	k	305	CLA	CAA-CBA-CGA-O2A
27	B	806	CLA	C16-C17-C18-C20
27	j	612	CLA	C3-C5-C6-C7
27	g	308	CLA	CBD-CGD-O2D-CED
29	L	207	LHG	C12-C13-C14-C15
27	A	810	CLA	C11-C10-C8-C9
27	A	836	CLA	C11-C12-C13-C14
27	A	852	CLA	C14-C13-C15-C16
27	A	853	CLA	C11-C10-C8-C9
27	B	804	CLA	C11-C12-C13-C14
27	B	810	CLA	C11-C10-C8-C9
27	B	831	CLA	C11-C10-C8-C9
27	a	309	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	b	610	CLA	C6-C7-C8-C9
27	e	610	CLA	C11-C10-C8-C9
27	l	312	CLA	C6-C7-C8-C9
27	k	308	CLA	C11-C12-C13-C14
27	f	608	CLA	C11-C10-C8-C9
27	n	607	CLA	C11-C12-C13-C14
34	b	619	LMG	C16-C17-C18-C19
34	J	106	LMG	C8-C7-O1-C1
27	c	606	CLA	C2A-CAA-CBA-CGA
27	k	303	CLA	C2A-CAA-CBA-CGA
27	A	805	CLA	C2-C1-O2A-CGA
27	A	832	CLA	C2-C1-O2A-CGA
27	A	833	CLA	C2-C1-O2A-CGA
27	B	803	CLA	C2-C1-O2A-CGA
27	J	105	CLA	C2-C1-O2A-CGA
27	a	303	CLA	C2-C1-O2A-CGA
27	j	603	CLA	C2-C1-O2A-CGA
27	l	304	CLA	C16-C17-C18-C19
34	c	619	LMG	C24-C25-C26-C27
27	e	606	CLA	O1D-CGD-O2D-CED
27	B	807	CLA	C3A-C2A-CAA-CBA
27	F	201	CLA	C3A-C2A-CAA-CBA
27	c	605	CLA	C3A-C2A-CAA-CBA
27	h	301	CLA	C3A-C2A-CAA-CBA
27	h	302	CLA	C3A-C2A-CAA-CBA
27	A	819	CLA	CAA-CBA-CGA-O1A
27	A	839	CLA	C2-C3-C5-C6
37	g	312	KC2	C2B-C3B-CAB-CBB
31	a	302	LMT	C1-C2-C3-C4
34	L	208	LMG	C11-C12-C13-C14
29	a	301	LHG	O1-C1-C2-C3
27	B	837	CLA	CAA-CBA-CGA-O1A
27	B	823	CLA	O1D-CGD-O2D-CED
27	j	606	CLA	CAA-CBA-CGA-O2A
29	b	617	LHG	C18-C19-C20-C21
27	j	607	CLA	CAA-CBA-CGA-O1A
27	e	605	CLA	C15-C16-C17-C18
31	A	851	LMT	C5'-C4'-O1B-C1B
27	B	840	CLA	C16-C17-C18-C20
27	A	812	CLA	C8-C10-C11-C12
27	B	805	CLA	C2A-CAA-CBA-CGA
29	n	619	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	B	824	CLA	C2-C3-C5-C6
27	B	808	CLA	CBA-CGA-O2A-C1
27	L	204	CLA	CBA-CGA-O2A-C1
27	f	604	CLA	C4C-C3C-CAC-CBC
27	a	308	CLA	CBD-CGD-O2D-CED
27	e	604	CLA	CBA-CGA-O2A-C1
34	b	619	LMG	C7-C8-C9-O8
37	j	610	KC2	C4C-C3C-CAC-CBC
37	d	310	KC2	C4B-C3B-CAB-CBB
37	g	312	KC2	C4B-C3B-CAB-CBB
27	A	812	CLA	C3-C5-C6-C7
37	m	610	KC2	CAA-CBA-CGA-O1A
29	f	619	LHG	O7-C7-C8-C9
35	e	616	II0	C25-C29-C31-C33
27	l	303	CLA	C2-C1-O2A-CGA
27	A	828	CLA	CAA-CBA-CGA-O2A
27	B	839	CLA	CAA-CBA-CGA-O2A
28	A	843	PQN	C15-C16-C17-C18
34	c	619	LMG	C4-C5-C6-O5
27	A	839	CLA	C13-C15-C16-C17
27	l	310	CLA	C8-C10-C11-C12
27	A	840	CLA	C6-C7-C8-C9
27	B	803	CLA	C11-C12-C13-C14
27	B	821	CLA	C14-C13-C15-C16
27	k	303	CLA	C14-C13-C15-C16
27	B	801	CLA	C16-C17-C18-C19
27	B	823	CLA	C16-C17-C18-C19
27	A	812	CLA	CAA-CBA-CGA-O2A
27	B	801	CLA	CAA-CBA-CGA-O1A
27	a	308	CLA	CAA-CBA-CGA-O1A
34	J	106	LMG	C34-C35-C36-C37
27	b	603	CLA	O1D-CGD-O2D-CED
34	s	210	LMG	C32-C33-C34-C35
27	s	203	CLA	CAA-CBA-CGA-O2A
27	l	308	CLA	CAA-CBA-CGA-O2A
27	l	307	CLA	C16-C17-C18-C19
27	c	609	CLA	CAA-CBA-CGA-O2A
27	b	607	CLA	C2A-CAA-CBA-CGA
27	A	802	CLA	C11-C10-C8-C7
27	A	808	CLA	C6-C7-C8-C10
27	A	816	CLA	C11-C12-C13-C15
27	A	839	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	A	842	CLA	C11-C10-C8-C7
27	A	853	CLA	C11-C10-C8-C7
27	B	801	CLA	C11-C10-C8-C7
27	B	804	CLA	C11-C10-C8-C7
27	B	812	CLA	C11-C10-C8-C7
27	B	821	CLA	C11-C10-C8-C7
27	c	604	CLA	C11-C10-C8-C7
27	c	608	CLA	C6-C7-C8-C10
27	a	311	CLA	C6-C7-C8-C10
27	k	307	CLA	C11-C12-C13-C15
27	f	609	CLA	C6-C7-C8-C10
27	g	309	CLA	C6-C7-C8-C10
27	A	852	CLA	C2B-C3B-CAB-CBB
27	B	818	CLA	C2B-C3B-CAB-CBB
27	c	607	CLA	C2B-C3B-CAB-CBB
27	m	602	CLA	C2B-C3B-CAB-CBB
27	m	605	CLA	C2B-C3B-CAB-CBB
27	e	604	CLA	C2B-C3B-CAB-CBB
27	j	611	CLA	C2B-C3B-CAB-CBB
27	g	322	CLA	C2B-C3B-CAB-CBB
30	J	102	WVN	C06-C13-C20-C23
36	c	620	IHT	C02-C07-C18-C22
36	k	317	IHT	C10-C07-C18-C22
34	L	208	LMG	C37-C38-C39-C40
29	A	845	LHG	O7-C7-C8-C9
27	b	601	CLA	C2-C1-O2A-CGA
27	b	609	CLA	C2-C1-O2A-CGA
27	h	307	CLA	C2-C1-O2A-CGA
27	l	309	CLA	C2-C1-O2A-CGA
27	k	305	CLA	C2-C1-O2A-CGA
34	F	206	LMG	C24-C25-C26-C27
27	g	308	CLA	CAA-CBA-CGA-O2A
27	F	203	CLA	C4-C3-C5-C6
34	c	619	LMG	C17-C18-C19-C20
27	e	604	CLA	C2-C3-C5-C6
27	n	601	CLA	CAA-CBA-CGA-O1A
27	f	604	CLA	C2A-CAA-CBA-CGA
27	g	310	CLA	C2A-CAA-CBA-CGA
27	k	304	CLA	CBD-CGD-O2D-CED
27	B	804	CLA	CAA-CBA-CGA-O2A
27	K	101	CLA	CAA-CBA-CGA-O2A
27	n	610	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	A	825	CLA	C8-C10-C11-C12
27	A	842	CLA	C5-C6-C7-C8
27	j	604	CLA	CAA-CBA-CGA-O2A
29	J	107	LHG	O7-C7-C8-C9
27	A	809	CLA	C11-C10-C8-C9
27	l	310	CLA	C12-C13-C15-C16
27	e	604	CLA	C4-C3-C5-C6
27	B	826	CLA	CAA-CBA-CGA-O2A
27	j	603	CLA	CAA-CBA-CGA-O2A
27	F	202	CLA	C2-C3-C5-C6
27	s	206	CLA	C2-C3-C5-C6
27	j	604	CLA	O1A-CGA-O2A-C1
34	L	208	LMG	C23-C24-C25-C26
27	B	835	CLA	CAA-CBA-CGA-O2A
35	c	617	II0	C09-C21-C23-C25
35	b	615	II0	C10-C22-C24-C26
27	B	834	CLA	O1A-CGA-O2A-C1
29	b	617	LHG	C10-C11-C12-C13
27	A	805	CLA	C11-C10-C8-C9
27	A	837	CLA	C6-C7-C8-C9
27	B	836	CLA	C11-C10-C8-C9
27	l	308	CLA	C6-C7-C8-C9
27	d	303	CLA	C6-C7-C8-C9
27	A	824	CLA	CAA-CBA-CGA-O2A
27	B	838	CLA	CAA-CBA-CGA-O2A
27	L	202	CLA	CAA-CBA-CGA-O2A
27	m	604	CLA	CAA-CBA-CGA-O2A
27	h	308	CLA	O1A-CGA-O2A-C1
29	c	621	LHG	O2-C2-C3-O3
27	A	835	CLA	C4B-C3B-CAB-CBB
27	B	818	CLA	C1A-C2A-CAA-CBA
27	B	822	CLA	C1A-C2A-CAA-CBA
27	B	839	CLA	C1A-C2A-CAA-CBA
27	s	208	CLA	C4B-C3B-CAB-CBB
27	c	611	CLA	C1A-C2A-CAA-CBA
27	m	601	CLA	C4B-C3B-CAB-CBB
27	i	304	CLA	C4B-C3B-CAB-CBB
27	n	605	CLA	C4B-C3B-CAB-CBB
27	c	609	CLA	CAA-CBA-CGA-O1A
27	a	303	CLA	C4-C3-C5-C6
27	h	307	CLA	C4-C3-C5-C6
27	O	206	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	h	303	CLA	CAA-CBA-CGA-O2A
27	l	309	CLA	CAA-CBA-CGA-O2A
27	k	309	CLA	CAA-CBA-CGA-O2A
27	i	311	CLA	CAA-CBA-CGA-O2A
29	b	618	LHG	O7-C7-C8-C9
29	J	107	LHG	O7-C5-C6-O8
30	F	205	WVN	C30-C33-C34-C37
30	s	205	WVN	C30-C33-C34-C37
35	e	616	II0	C32-C34-C36-C40
35	k	314	II0	C32-C34-C36-C40
30	O	201	WVN	C22-C26-C29-C31
35	e	614	II0	C25-C29-C31-C33
36	n	617	IHT	C33-C37-C40-C41
37	d	309	KC2	CBD-CGD-O2D-CED
29	f	619	LHG	C25-C26-C27-C28
27	A	836	CLA	CAA-CBA-CGA-O2A
27	B	849	CLA	CAA-CBA-CGA-O2A
27	c	606	CLA	CAA-CBA-CGA-O2A
27	h	308	CLA	CAA-CBA-CGA-O2A
27	m	607	CLA	CAA-CBA-CGA-O2A
29	j	617	LHG	O8-C23-C24-C25
27	j	604	CLA	C4C-C3C-CAC-CBC
27	m	609	CLA	C2C-C3C-CAC-CBC
27	g	308	CLA	C16-C17-C18-C20
27	e	603	CLA	CAA-CBA-CGA-O2A
27	e	607	CLA	CAA-CBA-CGA-O2A
27	B	803	CLA	CAA-CBA-CGA-O1A
29	b	618	LHG	C11-C12-C13-C14
27	c	601	CLA	C2-C3-C5-C6
27	b	601	CLA	C2-C3-C5-C6
27	f	603	CLA	C2-C3-C5-C6
27	n	613	CLA	C2-C3-C5-C6
27	h	306	CLA	C4-C3-C5-C6
27	h	313	CLA	C4-C3-C5-C6
28	A	843	PQN	C14-C13-C15-C16
27	B	810	CLA	C2C-C3C-CAC-CBC
27	A	816	CLA	C2-C1-O2A-CGA
27	l	307	CLA	C2-C1-O2A-CGA
27	B	815	CLA	C6-C7-C8-C10
27	O	202	CLA	C12-C13-C15-C16
27	e	610	CLA	C11-C10-C8-C7
27	l	304	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	f	604	CLA	C12-C13-C15-C16
27	i	307	CLA	C11-C12-C13-C15
27	j	604	CLA	C12-C13-C15-C16
27	d	303	CLA	C12-C13-C15-C16
27	c	612	CLA	CBA-CGA-O2A-C1
27	A	842	CLA	C16-C17-C18-C19
27	m	607	CLA	C16-C17-C18-C19
29	d	315	LHG	C7-C8-C9-C10
27	l	312	CLA	C15-C16-C17-C18
37	l	311	KC2	CAA-CBA-CGA-O1A
27	B	816	CLA	O1A-CGA-O2A-C1
27	c	608	CLA	CAA-CBA-CGA-O2A
29	d	315	LHG	C25-C26-C27-C28
27	h	306	CLA	C13-C15-C16-C17
29	m	617	LHG	C9-C10-C11-C12
27	A	810	CLA	CBA-CGA-O2A-C1
27	B	832	CLA	CBA-CGA-O2A-C1
27	j	602	CLA	C2A-CAA-CBA-CGA
27	A	836	CLA	C8-C10-C11-C12
27	e	606	CLA	C10-C11-C12-C13
27	c	612	CLA	CAA-CBA-CGA-O2A
27	B	804	CLA	CAA-CBA-CGA-O1A
34	c	619	LMG	C13-C14-C15-C16
27	h	306	CLA	C5-C6-C7-C8
27	j	604	CLA	C2C-C3C-CAC-CBC
27	B	822	CLA	C3A-C2A-CAA-CBA
27	b	610	CLA	C3A-C2A-CAA-CBA
27	d	311	CLA	C3A-C2A-CAA-CBA
27	R	203	CLA	C3A-C2A-CAA-CBA
27	g	307	CLA	CAA-CBA-CGA-O1A
27	b	611	CLA	C15-C16-C17-C18
27	A	837	CLA	C16-C17-C18-C20
27	A	852	CLA	CAA-CBA-CGA-O2A
27	g	315	CLA	CAA-CBA-CGA-O2A
34	J	106	LMG	O8-C28-C29-C30
27	A	802	CLA	C2-C3-C5-C6
27	a	303	CLA	C2-C3-C5-C6
27	A	855	CLA	C10-C11-C12-C13
27	l	308	CLA	CAA-CBA-CGA-O1A
27	g	308	CLA	CAA-CBA-CGA-O1A
29	J	107	LHG	O9-C7-C8-C9
27	A	804	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	f	601	CLA	CBA-CGA-O2A-C1
27	b	603	CLA	C13-C15-C16-C17
27	n	609	CLA	CBD-CGD-O2D-CED
29	i	316	LHG	O8-C23-C24-C25
29	c	621	LHG	C11-C10-C9-C8
27	A	812	CLA	CAA-CBA-CGA-O1A
27	A	816	CLA	C11-C12-C13-C14
27	c	604	CLA	C11-C10-C8-C9
27	a	306	CLA	C11-C10-C8-C9
27	a	311	CLA	C6-C7-C8-C9
27	m	603	CLA	C14-C13-C15-C16
27	m	606	CLA	C6-C7-C8-C9
27	l	304	CLA	C11-C12-C13-C14
27	k	308	CLA	C14-C13-C15-C16
27	d	303	CLA	C14-C13-C15-C16
27	g	305	CLA	C11-C12-C13-C14
27	c	608	CLA	CAA-CBA-CGA-O1A
27	j	603	CLA	CAA-CBA-CGA-O1A
34	c	619	LMG	C40-C41-C42-C43
27	A	809	CLA	C3-C5-C6-C7
27	F	201	CLA	C8-C10-C11-C12
27	g	311	CLA	C4-C3-C5-C6
27	B	839	CLA	CAA-CBA-CGA-O1A
27	K	101	CLA	CAA-CBA-CGA-O1A
27	h	303	CLA	CAA-CBA-CGA-O1A
27	h	307	CLA	CAA-CBA-CGA-O2A
27	F	203	CLA	C2-C3-C5-C6
27	h	307	CLA	C2-C3-C5-C6
27	k	307	CLA	C2-C3-C5-C6
27	J	105	CLA	C4-C3-C5-C6
27	h	308	CLA	C4-C3-C5-C6
27	k	306	CLA	C4-C3-C5-C6
30	A	846	WVN	C01-C02-C11-C19
37	c	610	KC2	C1A-C2A-CAA-CBA
37	k	312	KC2	C1A-C2A-CAA-CBA
37	k	312	KC2	C3A-C2A-CAA-CBA
37	j	610	KC2	C1A-C2A-CAA-CBA
37	d	309	KC2	C1A-C2A-CAA-CBA
37	d	309	KC2	C3A-C2A-CAA-CBA
37	g	312	KC2	C1A-C2A-CAA-CBA
37	n	612	KC2	C1A-C2A-CAA-CBA
29	c	618	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	A	828	CLA	CAA-CBA-CGA-O1A
34	s	210	LMG	C14-C15-C16-C17
27	g	322	CLA	C4C-C3C-CAC-CBC
29	e	617	LHG	O1-C1-C2-O2
29	m	617	LHG	C31-C32-C33-C34
27	n	601	CLA	CAA-CBA-CGA-O2A
37	g	314	KC2	CBD-CGD-O2D-CED
30	F	204	WVN	C30-C33-C34-C37
27	A	816	CLA	CBA-CGA-O2A-C1
27	L	202	CLA	CAA-CBA-CGA-O1A
27	O	206	CLA	CAA-CBA-CGA-O1A
27	c	606	CLA	CAA-CBA-CGA-O1A
27	c	612	CLA	CAA-CBA-CGA-O1A
27	m	604	CLA	CAA-CBA-CGA-O1A
27	n	610	CLA	CAA-CBA-CGA-O1A
29	A	845	LHG	O9-C7-C8-C9
29	f	619	LHG	O9-C7-C8-C9
27	A	810	CLA	C10-C11-C12-C13
27	m	606	CLA	C15-C16-C17-C18
27	B	808	CLA	O1A-CGA-O2A-C1
27	e	601	CLA	CAA-CBA-CGA-O2A
27	B	827	CLA	O2A-C1-C2-C3
27	e	607	CLA	CAA-CBA-CGA-O1A
27	j	604	CLA	CAA-CBA-CGA-O1A
27	A	839	CLA	CAA-CBA-CGA-O2A
27	e	604	CLA	CAA-CBA-CGA-O2A
34	s	210	LMG	C16-C17-C18-C19
27	A	836	CLA	CAA-CBA-CGA-O1A
27	B	835	CLA	CAA-CBA-CGA-O1A
27	B	849	CLA	CAA-CBA-CGA-O1A
27	e	603	CLA	CAA-CBA-CGA-O1A
27	f	603	CLA	CAA-CBA-CGA-O1A
27	i	311	CLA	CAA-CBA-CGA-O1A
27	f	603	CLA	CAA-CBA-CGA-O2A
29	c	618	LHG	O7-C7-C8-C9
37	d	310	KC2	C2B-C3B-CAB-CBB
27	B	831	CLA	CBD-CGD-O2D-CED
29	a	301	LHG	C26-C27-C28-C29
27	B	838	CLA	CAA-CBA-CGA-O1A
27	s	203	CLA	CAA-CBA-CGA-O1A
34	s	210	LMG	C29-C30-C31-C32
27	A	806	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	A	810	CLA	CAD-CBD-CGD-O2D
27	A	835	CLA	CAD-CBD-CGD-O2D
27	B	825	CLA	CAD-CBD-CGD-O2D
27	B	834	CLA	CAD-CBD-CGD-O2D
27	F	203	CLA	CAD-CBD-CGD-O2D
27	L	202	CLA	CAD-CBD-CGD-O2D
27	l	309	CLA	CAD-CBD-CGD-O2D
27	k	301	CLA	CAD-CBD-CGD-O2D
27	k	313	CLA	CAD-CBD-CGD-O2D
27	f	608	CLA	CAD-CBD-CGD-O2D
27	i	305	CLA	CAD-CBD-CGD-O2D
27	i	309	CLA	CAD-CBD-CGD-O2D
27	g	304	CLA	CAD-CBD-CGD-O2D
27	g	310	CLA	CAD-CBD-CGD-O2D
27	d	302	CLA	CAA-CBA-CGA-O2A
27	e	604	CLA	O1A-CGA-O2A-C1
27	A	802	CLA	C2-C1-O2A-CGA
27	B	835	CLA	C2-C1-O2A-CGA
27	L	204	CLA	C2-C1-O2A-CGA
27	a	311	CLA	C2-C1-O2A-CGA
27	k	309	CLA	C2-C1-O2A-CGA
27	d	302	CLA	C2-C1-O2A-CGA
27	B	826	CLA	CAA-CBA-CGA-O1A
27	h	308	CLA	CAA-CBA-CGA-O1A
27	g	315	CLA	CAA-CBA-CGA-O1A
27	s	206	CLA	CAA-CBA-CGA-O2A
27	a	306	CLA	CAA-CBA-CGA-O2A
27	A	815	CLA	CAA-CBA-CGA-O2A
27	e	601	CLA	CAA-CBA-CGA-O1A
34	J	106	LMG	O10-C28-C29-C30
27	B	834	CLA	C15-C16-C17-C18
27	e	605	CLA	C10-C11-C12-C13
27	m	609	CLA	CAA-CBA-CGA-O2A
27	g	308	CLA	C16-C17-C18-C19
27	m	609	CLA	CAA-CBA-CGA-O1A
27	d	302	CLA	CAA-CBA-CGA-O1A
27	B	831	CLA	O1D-CGD-O2D-CED
27	b	603	CLA	CBD-CGD-O2D-CED
27	A	833	CLA	CAA-CBA-CGA-O2A
27	B	829	CLA	CAA-CBA-CGA-O2A
27	c	605	CLA	CAA-CBA-CGA-O2A
27	e	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	j	601	CLA	CAA-CBA-CGA-O2A
29	b	618	LHG	O9-C7-C8-C9

There are no ring outliers.

227 monomers are involved in 408 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	n	614	II0	1	0
37	f	611	KC2	2	0
27	f	604	CLA	4	0
27	B	824	CLA	1	0
27	l	310	CLA	1	0
27	a	310	CLA	1	0
36	f	617	IHT	2	0
27	A	856	CLA	3	0
27	A	821	CLA	2	0
27	B	826	CLA	1	0
36	c	620	IHT	1	0
35	m	615	II0	1	0
27	B	810	CLA	1	0
27	g	309	CLA	1	0
27	g	302	CLA	2	0
27	B	822	CLA	1	0
27	A	832	CLA	1	0
27	B	825	CLA	1	0
27	n	603	CLA	2	0
27	g	308	CLA	3	0
37	l	311	KC2	1	0
27	f	610	CLA	4	0
35	b	613	II0	1	0
35	f	616	II0	1	0
29	g	301	LHG	4	0
38	i	301	LMU	1	0
27	A	812	CLA	1	0
33	B	842	DGD	2	0
27	L	202	CLA	2	0
29	c	621	LHG	6	0
35	i	318	II0	1	0
29	A	850	LHG	4	0
27	A	838	CLA	2	0
27	A	824	CLA	3	0
27	A	828	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	m	609	CLA	6	0
27	d	305	CLA	2	0
27	h	306	CLA	6	0
36	g	319	IHT	1	0
27	h	305	CLA	1	0
27	B	840	CLA	1	0
27	A	807	CLA	1	0
27	A	822	CLA	2	0
27	j	606	CLA	2	0
27	g	303	CLA	2	0
27	A	808	CLA	2	0
31	a	320	LMT	1	0
27	k	307	CLA	2	0
27	i	302	CLA	2	0
27	A	801	CLA	2	0
27	d	301	CLA	1	0
27	a	311	CLA	1	0
27	A	815	CLA	1	0
29	a	319	LHG	1	0
27	m	601	CLA	2	0
27	m	606	CLA	2	0
27	F	201	CLA	1	0
27	B	821	CLA	1	0
27	b	608	CLA	5	0
27	a	308	CLA	2	0
27	k	304	CLA	3	0
27	i	306	CLA	1	0
27	s	206	CLA	2	0
35	l	313	II0	2	0
27	c	604	CLA	1	0
27	j	607	CLA	3	0
27	A	826	CLA	2	0
27	c	608	CLA	3	0
27	B	802	CLA	2	0
27	i	311	CLA	1	0
34	s	210	LMG	3	0
27	l	312	CLA	1	0
27	b	606	CLA	3	0
27	A	841	CLA	1	0
27	e	605	CLA	2	0
27	f	607	CLA	2	0
27	k	309	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	e	604	CLA	4	0
27	e	610	CLA	3	0
27	A	811	CLA	2	0
27	F	203	CLA	1	0
27	A	820	CLA	2	0
27	B	803	CLA	2	0
27	b	603	CLA	3	0
27	n	610	CLA	4	0
27	h	301	CLA	2	0
29	f	619	LHG	3	0
27	s	208	CLA	2	0
27	b	610	CLA	5	0
27	a	304	CLA	1	0
27	B	838	CLA	5	0
27	A	827	CLA	2	0
28	B	841	PQN	1	0
27	a	303	CLA	2	0
29	a	301	LHG	1	0
27	B	849	CLA	2	0
31	b	616	LMT	1	0
27	B	804	CLA	3	0
27	A	830	CLA	2	0
34	L	208	LMG	2	0
27	A	853	CLA	2	0
27	B	837	CLA	1	0
27	f	601	CLA	2	0
29	J	107	LHG	6	0
27	h	307	CLA	1	0
35	k	315	II0	1	0
27	A	809	CLA	3	0
27	A	803	CLA	1	0
27	e	607	CLA	5	0
27	j	604	CLA	1	0
27	B	816	CLA	2	0
27	A	842	CLA	4	0
36	j	616	IHT	2	0
27	B	801	CLA	2	0
27	h	308	CLA	2	0
29	b	617	LHG	5	0
37	k	311	KC2	3	0
27	b	601	CLA	1	0
27	A	814	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	j	610	KC2	1	0
27	L	203	CLA	2	0
27	A	806	CLA	1	0
27	j	603	CLA	1	0
27	A	829	CLA	2	0
27	B	815	CLA	1	0
27	c	601	CLA	1	0
27	b	611	CLA	3	0
34	b	619	LMG	2	0
27	l	309	CLA	1	0
27	g	322	CLA	4	0
27	j	602	CLA	2	0
27	n	609	CLA	2	0
27	s	202	CLA	3	0
34	c	619	LMG	3	0
27	n	608	CLA	1	0
27	i	305	CLA	1	0
27	A	835	CLA	1	0
27	A	855	CLA	4	0
27	f	609	CLA	1	0
27	F	202	CLA	5	0
27	c	603	CLA	1	0
27	k	305	CLA	1	0
27	f	608	CLA	7	0
27	n	613	CLA	1	0
27	A	831	CLA	2	0
27	k	301	CLA	2	0
27	m	604	CLA	1	0
37	i	317	KC2	1	0
27	b	607	CLA	1	0
27	B	812	CLA	1	0
27	c	602	CLA	2	0
29	b	618	LHG	1	0
30	s	205	WVN	1	0
27	f	606	CLA	2	0
27	a	312	CLA	3	0
27	a	306	CLA	1	0
27	c	607	CLA	1	0
27	O	202	CLA	2	0
27	i	303	CLA	2	0
27	l	303	CLA	1	0
27	e	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	831	CLA	1	0
27	n	607	CLA	1	0
27	A	816	CLA	1	0
27	B	814	CLA	2	0
27	B	830	CLA	1	0
27	l	304	CLA	3	0
32	A	854	SF4	5	0
27	j	605	CLA	1	0
27	A	852	CLA	4	0
27	A	837	CLA	4	0
35	j	615	II0	1	0
27	B	834	CLA	3	0
27	A	802	CLA	7	0
27	B	836	CLA	4	0
27	B	808	CLA	1	0
37	k	310	KC2	1	0
27	l	307	CLA	2	0
28	A	843	PQN	2	0
27	B	809	CLA	2	0
27	s	203	CLA	1	0
27	b	605	CLA	1	0
27	m	612	CLA	1	0
27	B	829	CLA	1	0
27	k	306	CLA	1	0
27	J	105	CLA	2	0
34	F	206	LMG	1	0
27	d	304	CLA	1	0
29	l	318	LHG	2	0
27	A	818	CLA	3	0
27	e	611	CLA	4	0
27	d	303	CLA	2	0
29	j	617	LHG	2	0
37	m	610	KC2	7	0
29	L	207	LHG	2	0
27	L	206	CLA	1	0
27	A	840	CLA	2	0
27	A	836	CLA	2	0
27	B	805	CLA	1	0
29	i	316	LHG	1	0
27	j	609	CLA	4	0
27	m	603	CLA	6	0
27	A	804	CLA	2	0

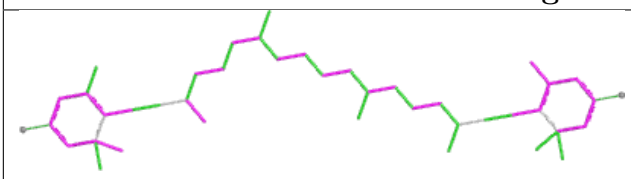
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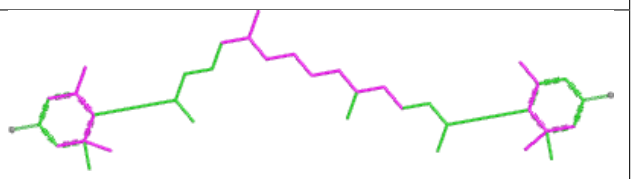
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	m	602	CLA	4	0
27	A	839	CLA	8	0
27	n	604	CLA	2	0
27	B	835	CLA	5	0
27	c	606	CLA	1	0
31	A	851	LMT	1	0
27	i	308	CLA	2	0
27	e	602	CLA	1	0
29	n	619	LHG	1	0
35	h	312	II0	1	0
27	A	823	CLA	1	0
27	f	602	CLA	3	0
36	b	614	IHT	3	0
27	j	601	CLA	2	0
34	J	106	LMG	3	0
29	e	617	LHG	1	0
27	n	602	CLA	1	0
27	i	309	CLA	2	0
27	k	308	CLA	3	0
27	A	817	CLA	2	0
27	g	311	CLA	2	0
27	l	308	CLA	3	0
27	e	606	CLA	4	0
27	B	820	CLA	3	0

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

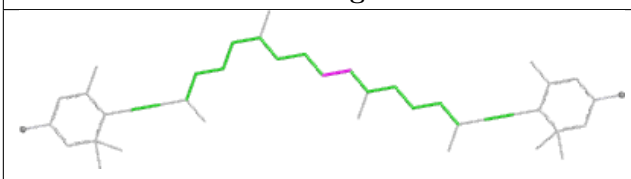
Ligand II0 n 614



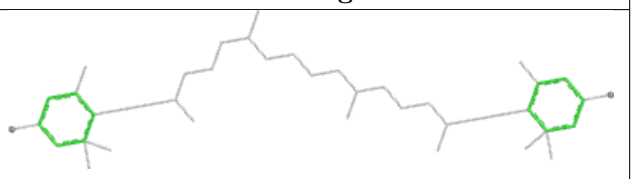
Bond lengths



Bond angles

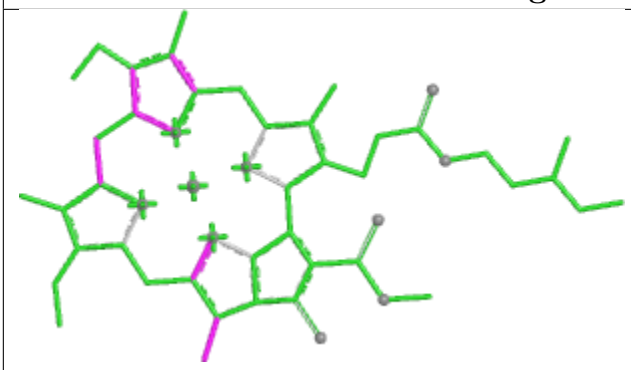


Torsions

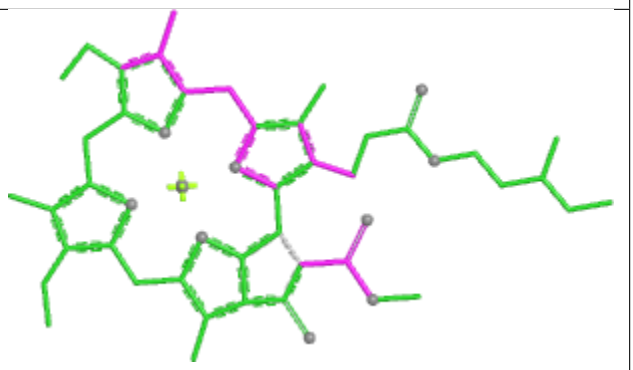


Rings

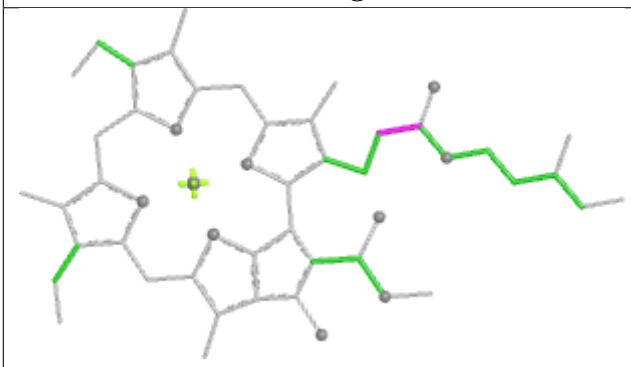
Ligand CLA e 603



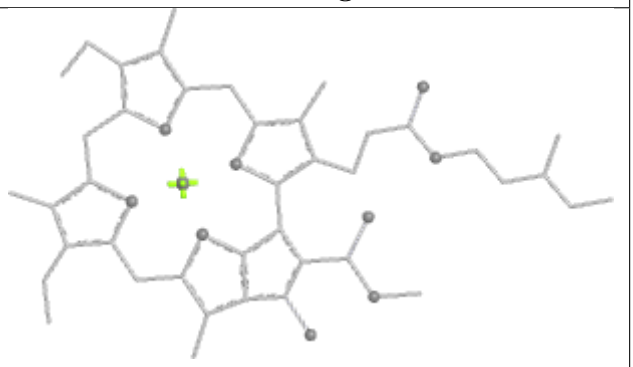
Bond lengths



Bond angles

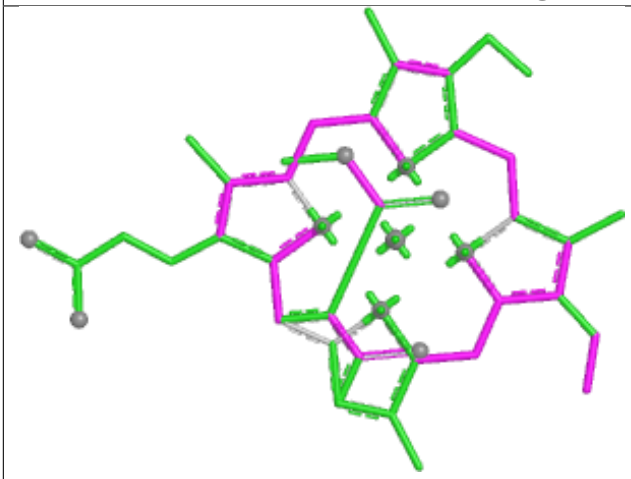


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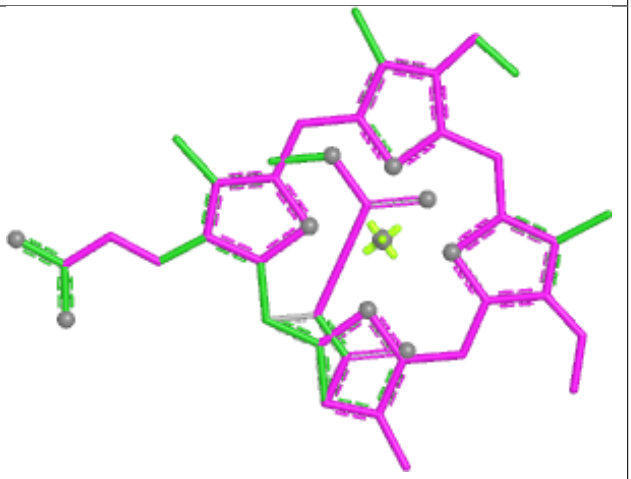


Rings

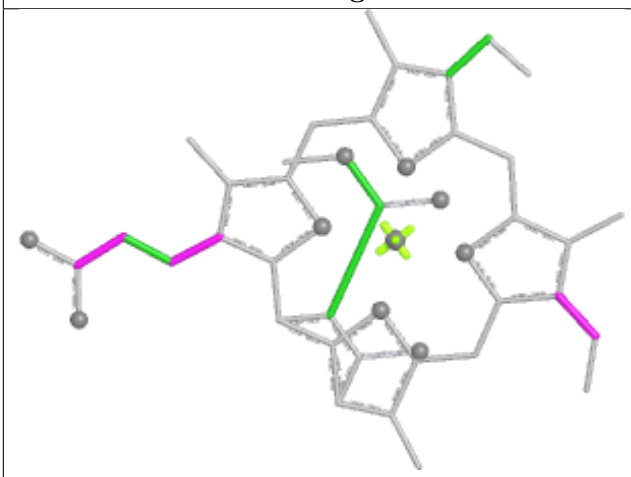
Ligand KC2 f 611



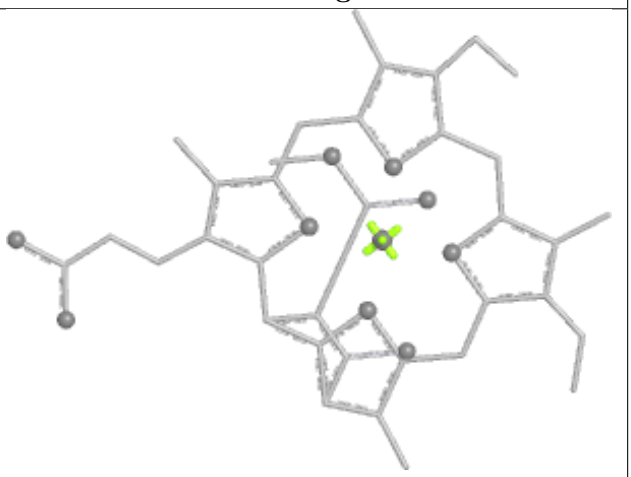
Bond lengths



Bond angles

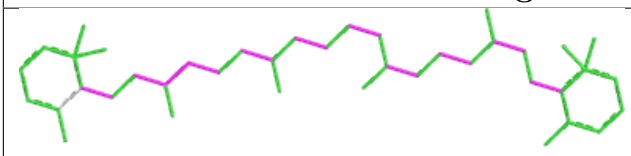


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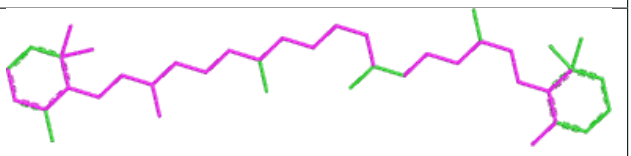


Rings

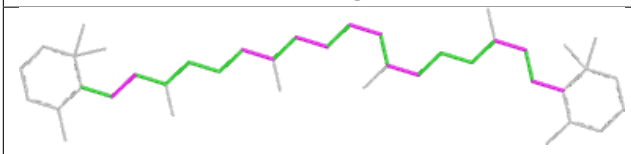
Ligand WVN B 843



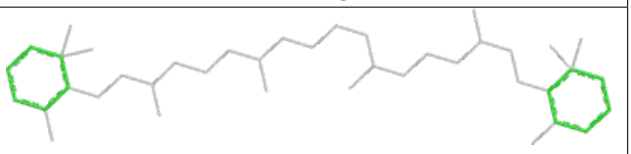
Bond lengths



Bond angles

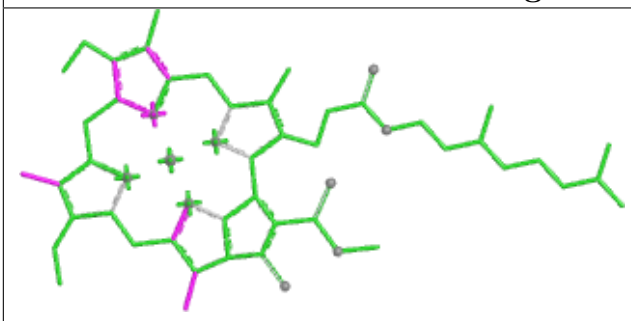


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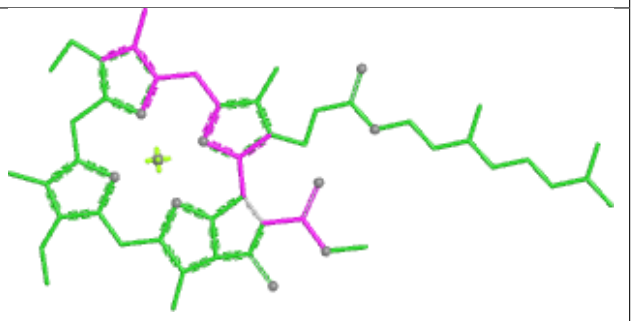


Rings

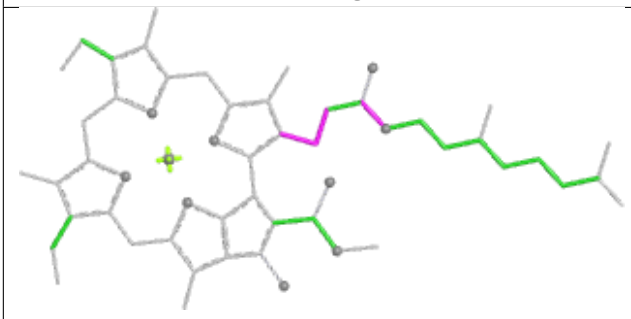
Ligand CLA B 813



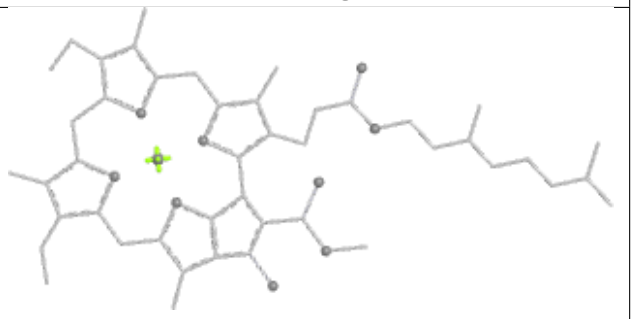
Bond lengths



Bond angles

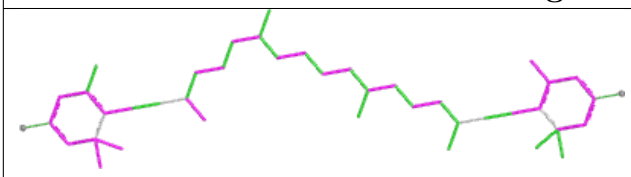


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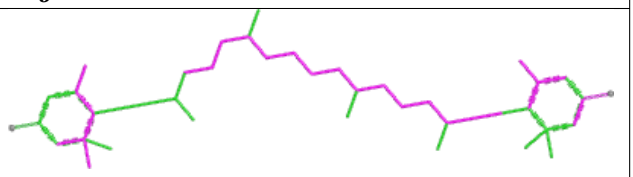


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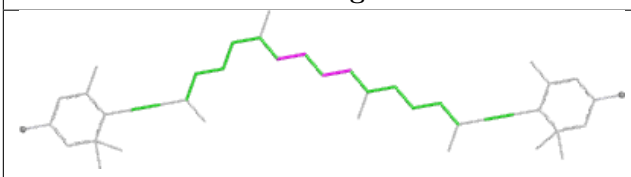
Ligand II0 j 614



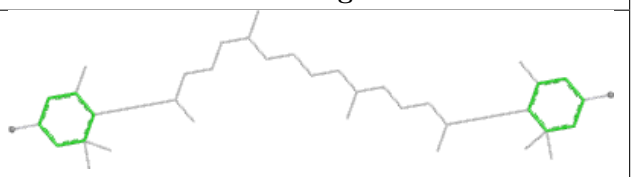
Bond lengths



Bond angles

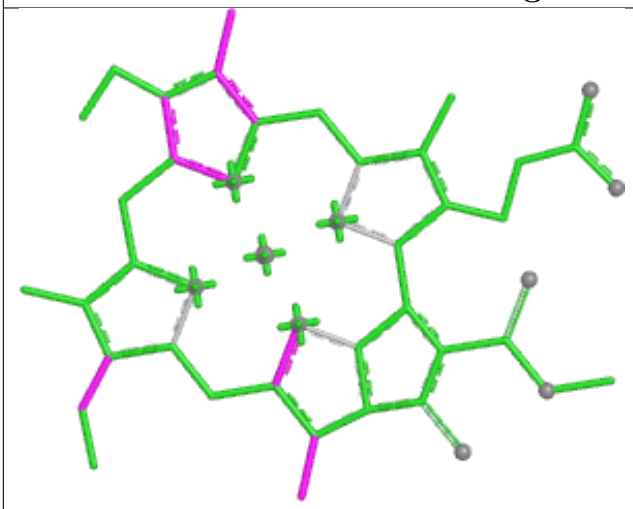


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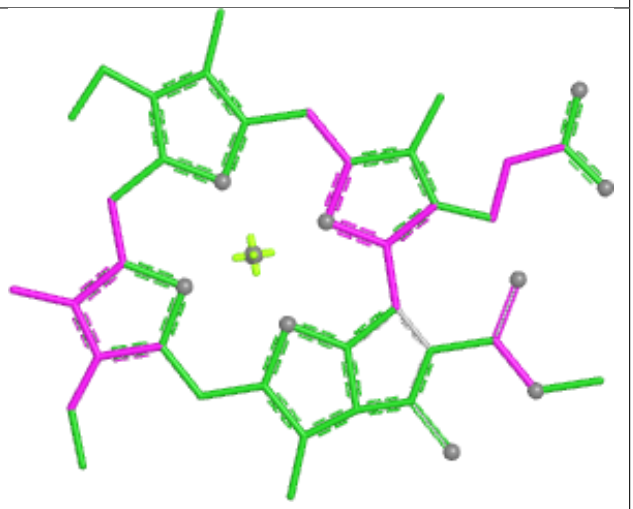


Rings

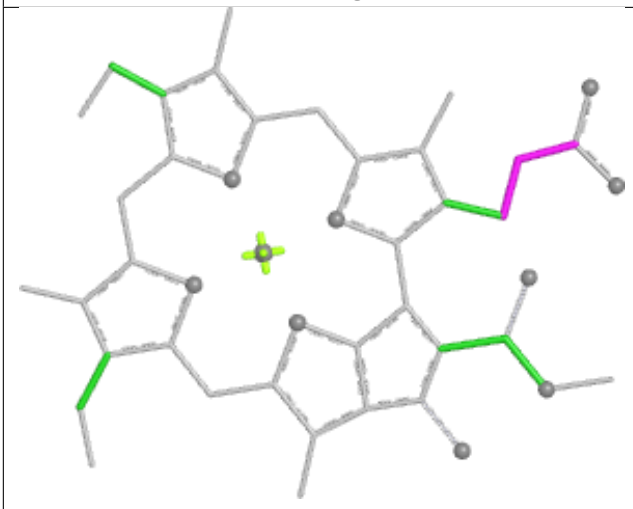
Ligand CLA A 819



Bond lengths



Bond angles

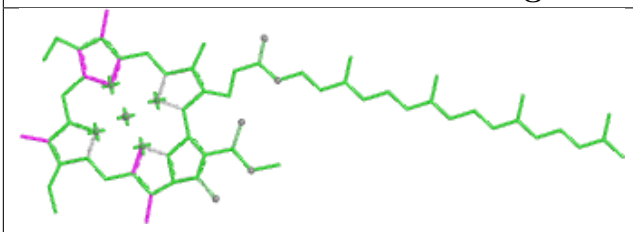


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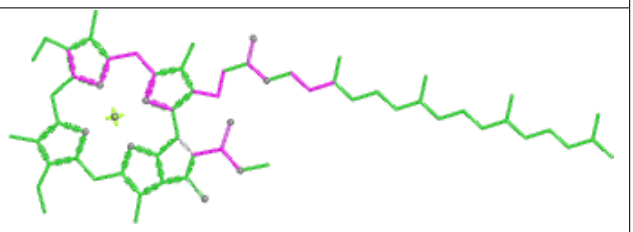


Rings

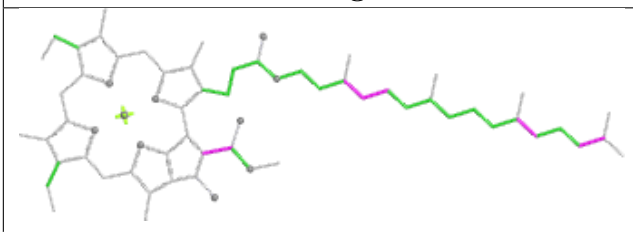
Ligand CLA B 806



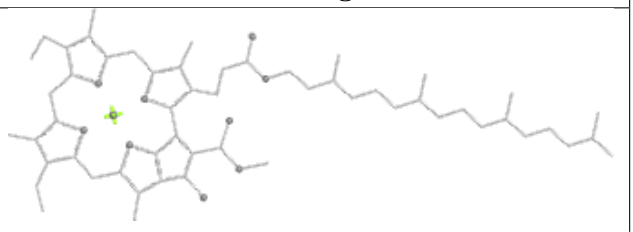
Bond lengths



Bond angles

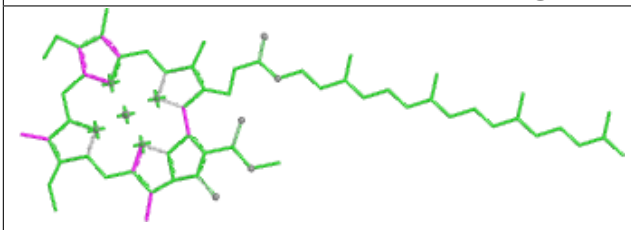


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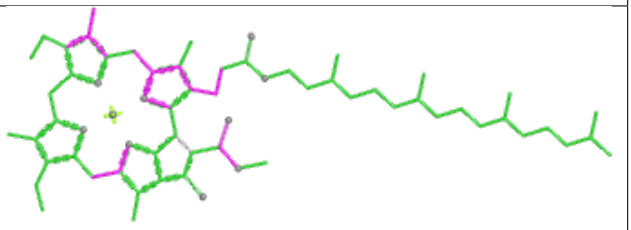


Rings

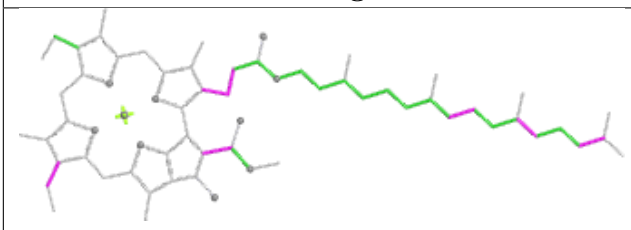
Ligand CLA f 604



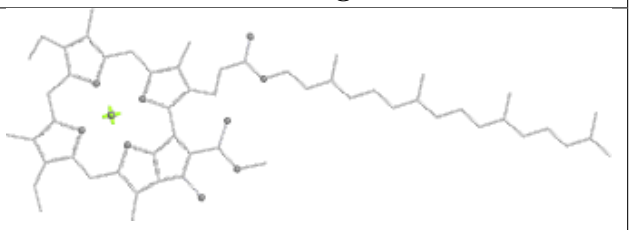
Bond lengths



Bond angles

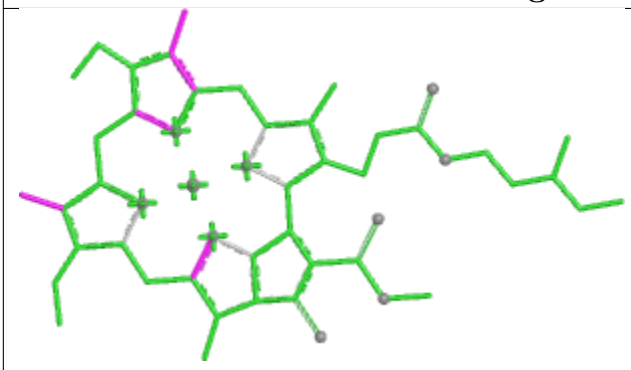


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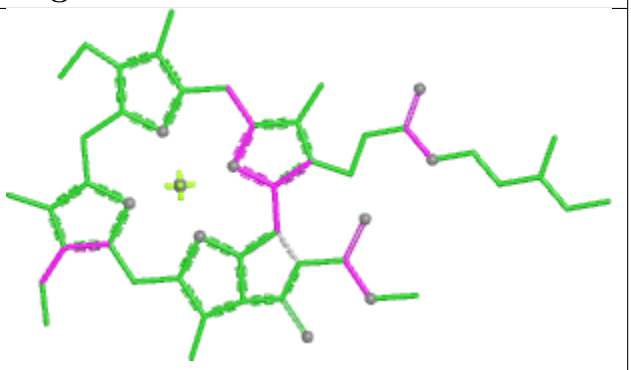


Rings

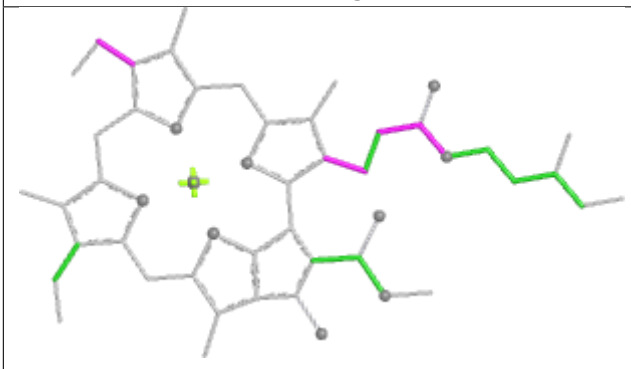
Ligand CLA g 306



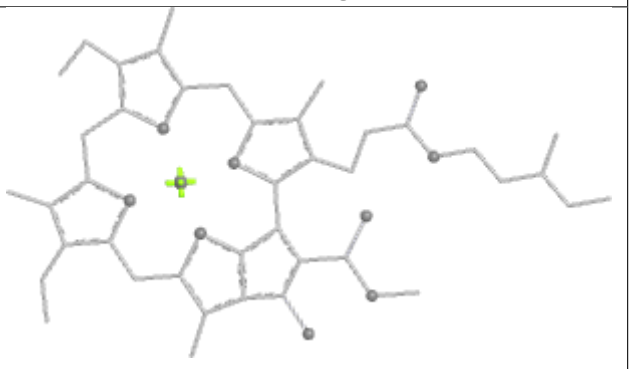
Bond lengths



Bond angles

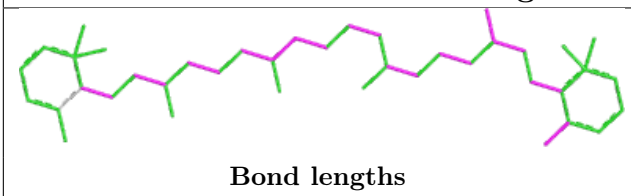


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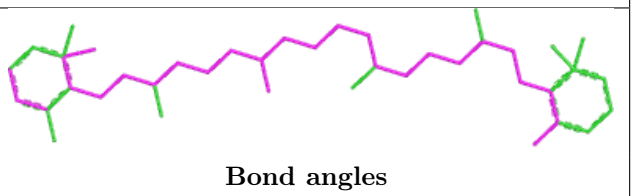


Rings

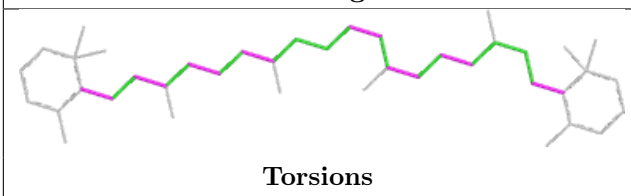
Ligand WVN F 205



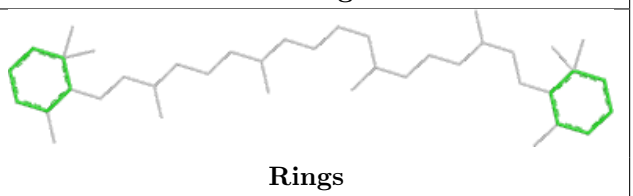
Bond lengths



Bond angles

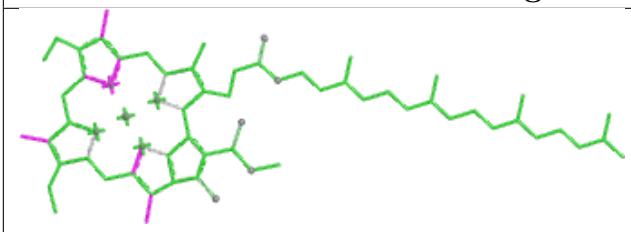


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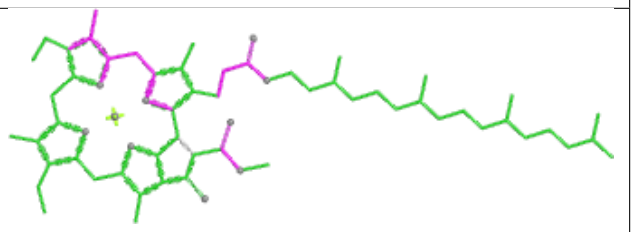


Rings

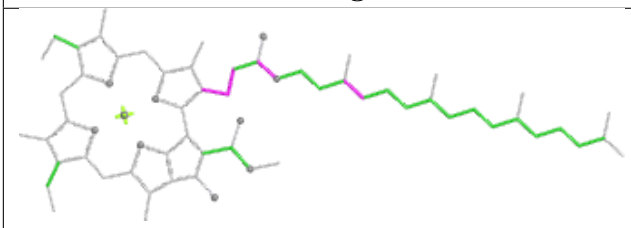
Ligand CLA B 824



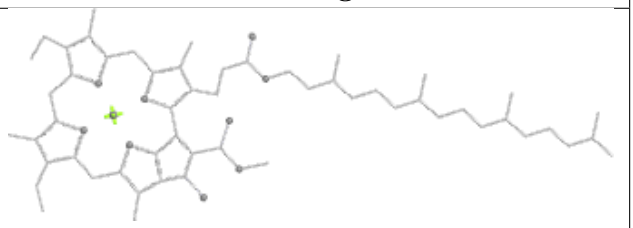
Bond lengths



Bond angles

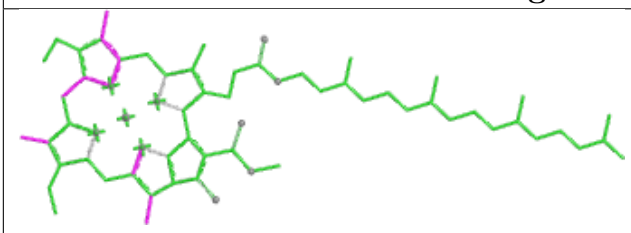


Torsions

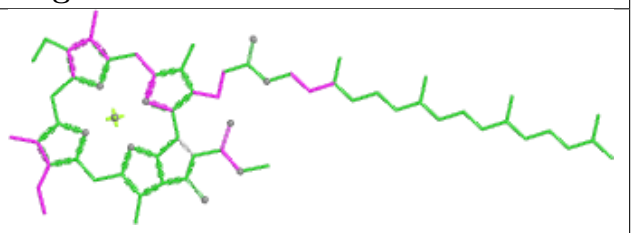


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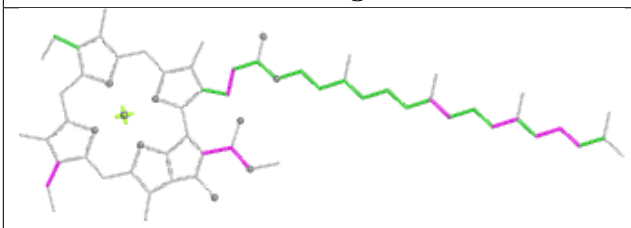
Ligand CLA g 305



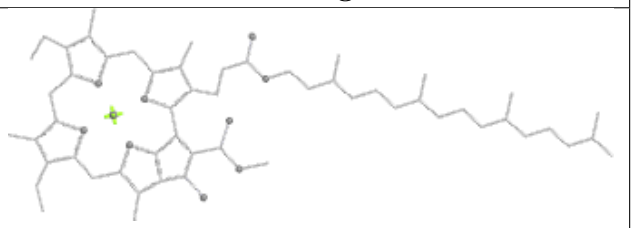
Bond lengths



Bond angles

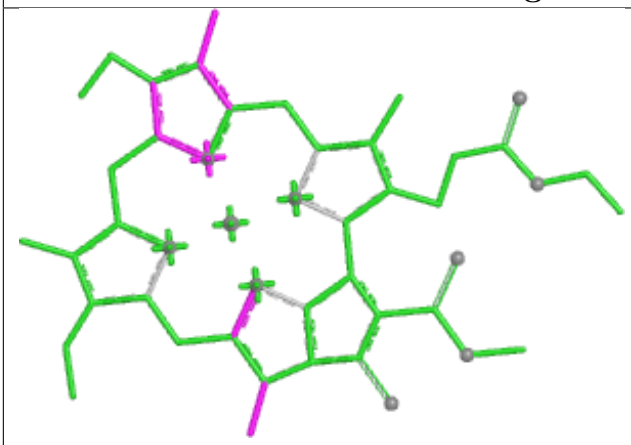


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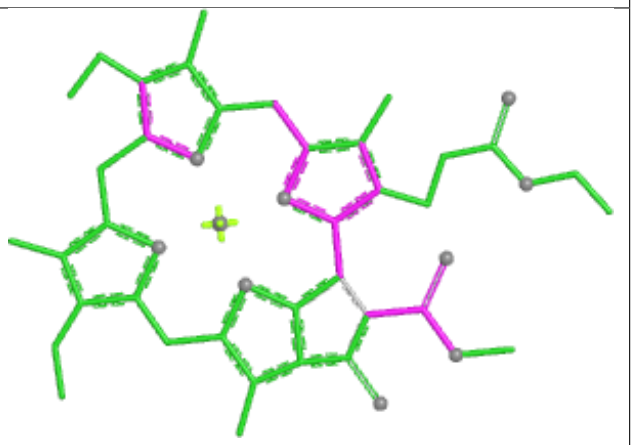


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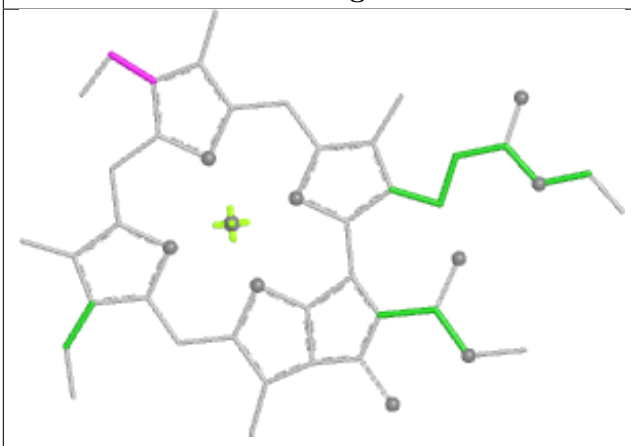
Ligand CLA B 833



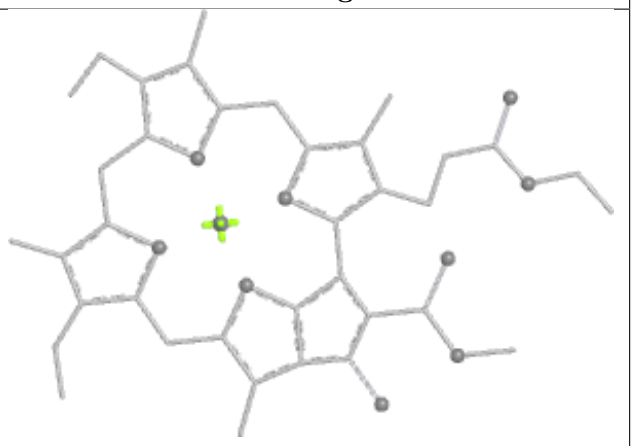
Bond lengths



Bond angles

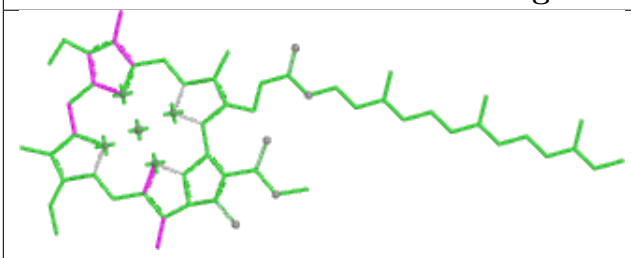


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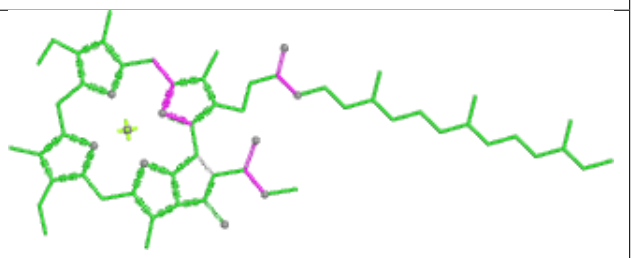


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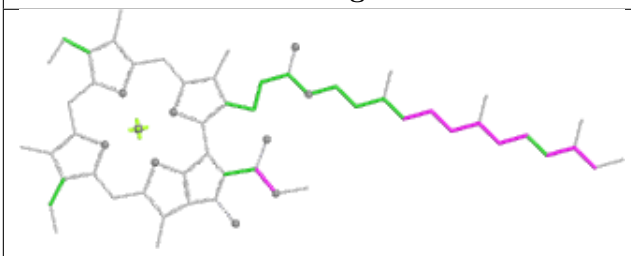
Ligand CLA l 310



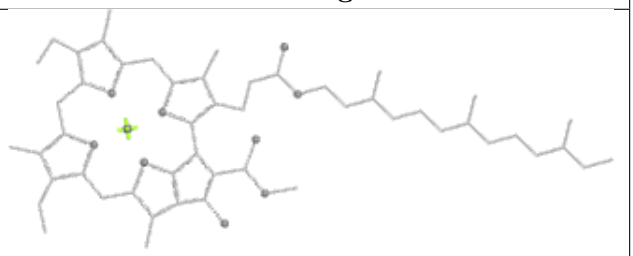
Bond lengths



Bond angles

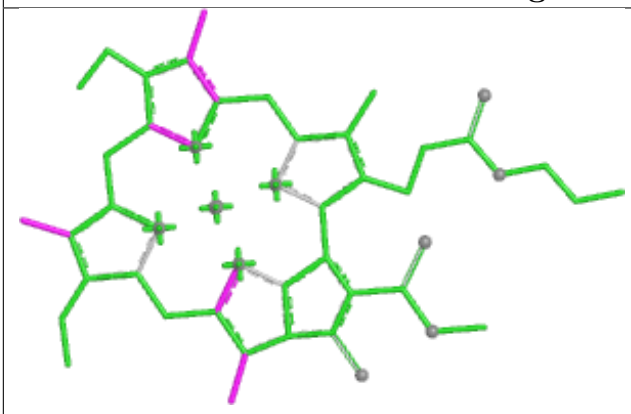


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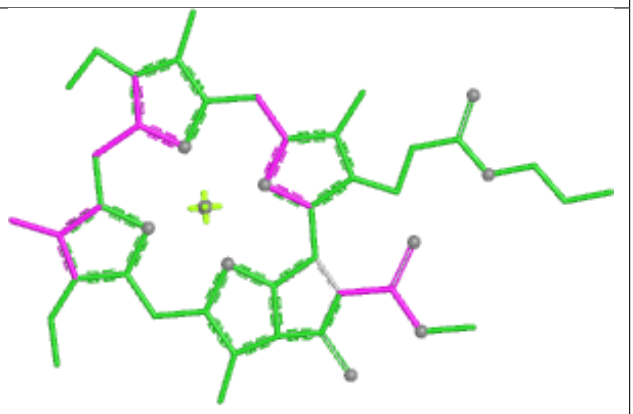


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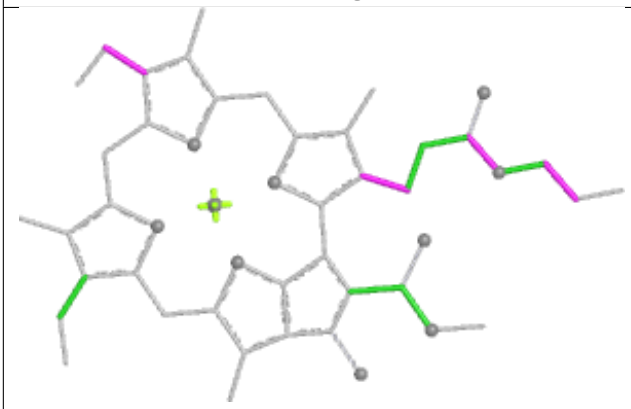
Ligand CLA a 310



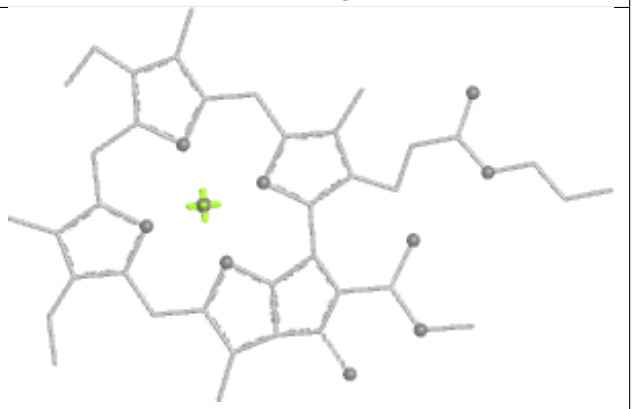
Bond lengths



Bond angles

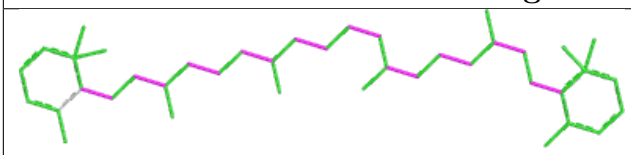


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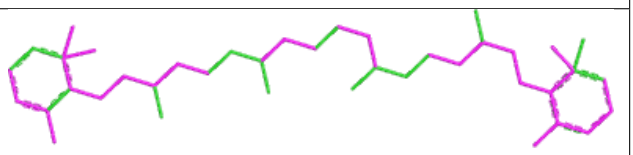


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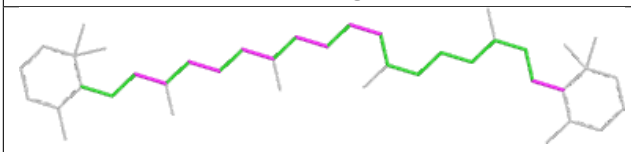
Ligand WVN l 316



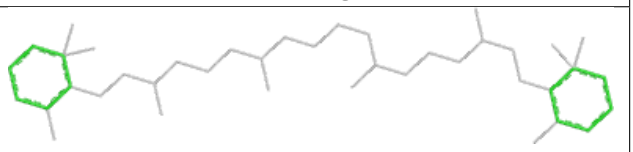
Bond lengths



Bond angles

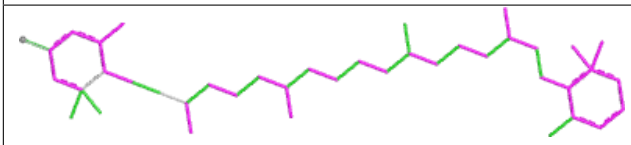


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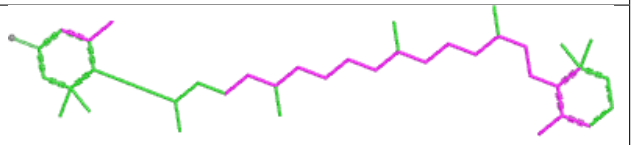


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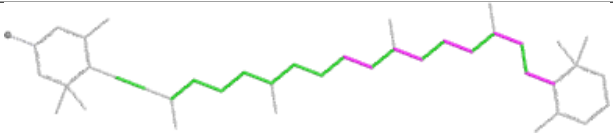
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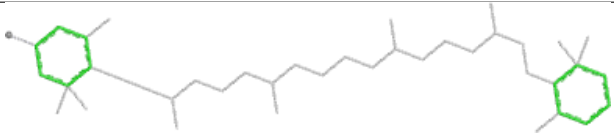
Bond lengths



Bond angles

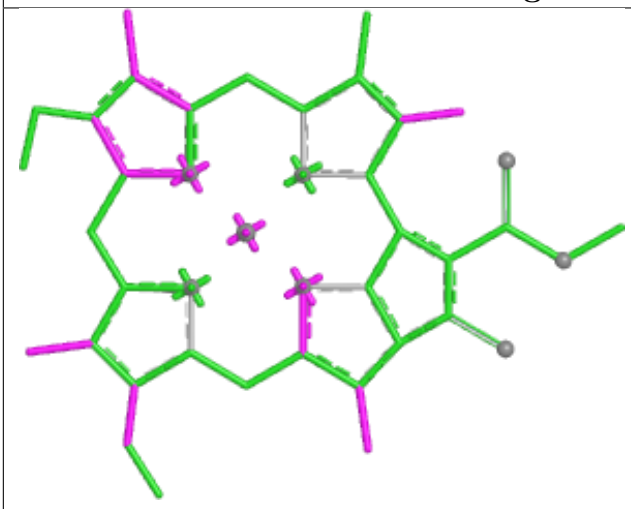


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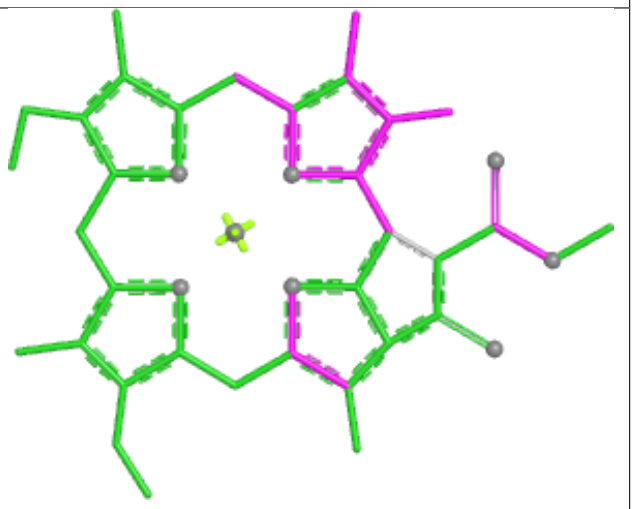


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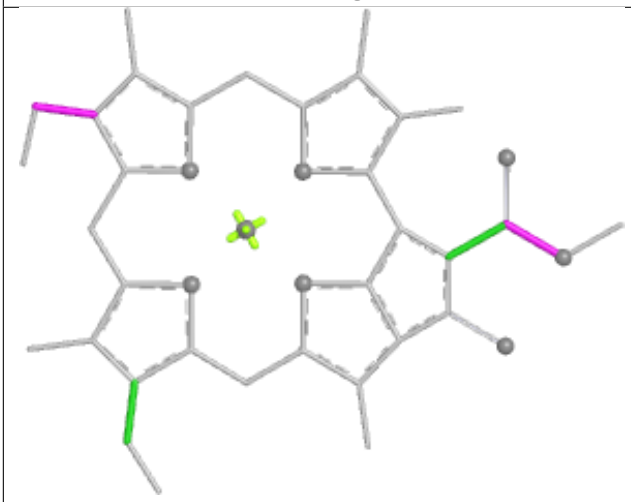
Ligand CLA A 856



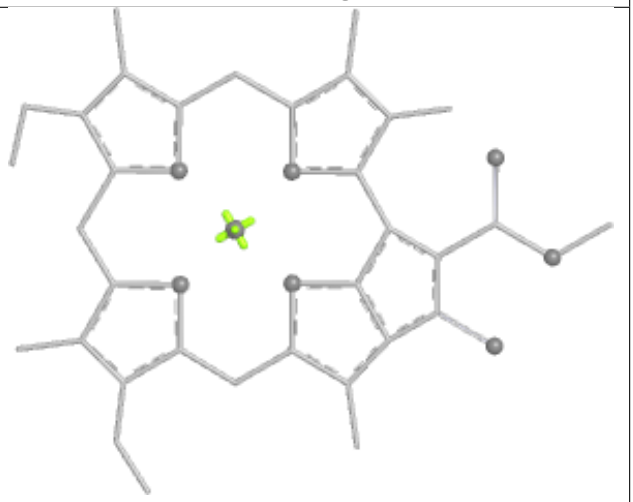
Bond lengths



Bond angles

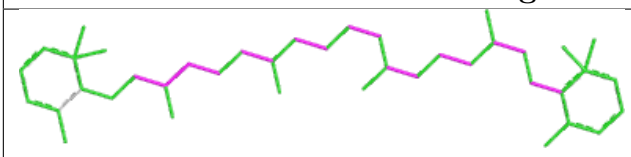


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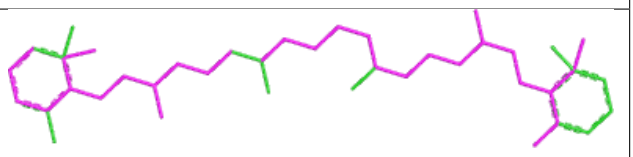


Rings

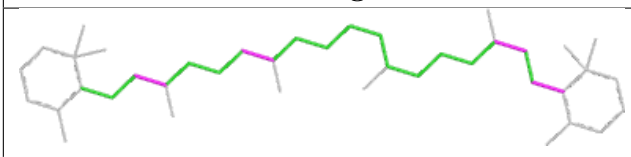
Ligand WVN J 101



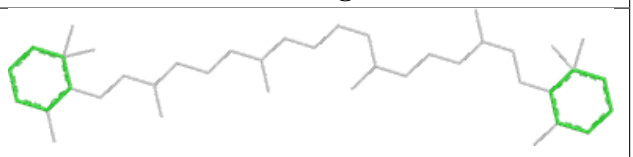
Bond lengths



Bond angles

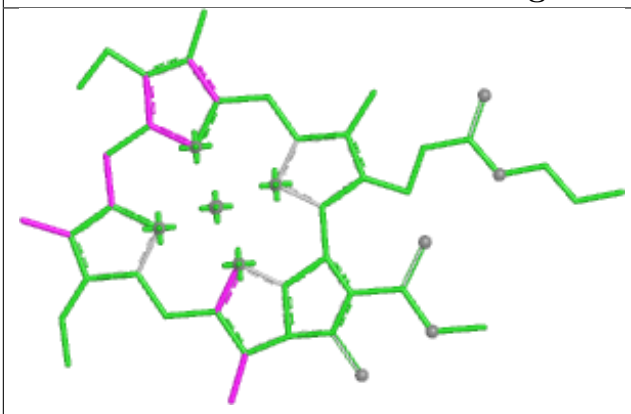


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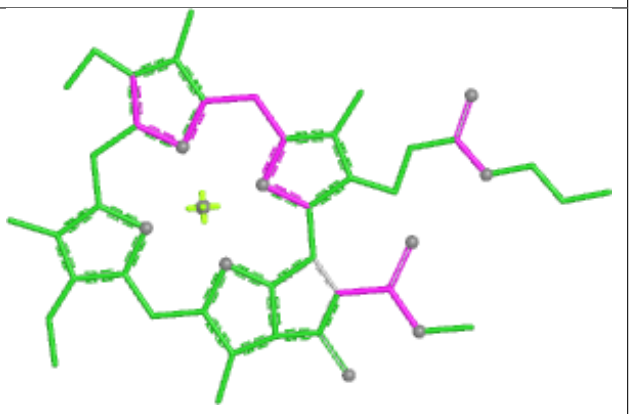


Rings

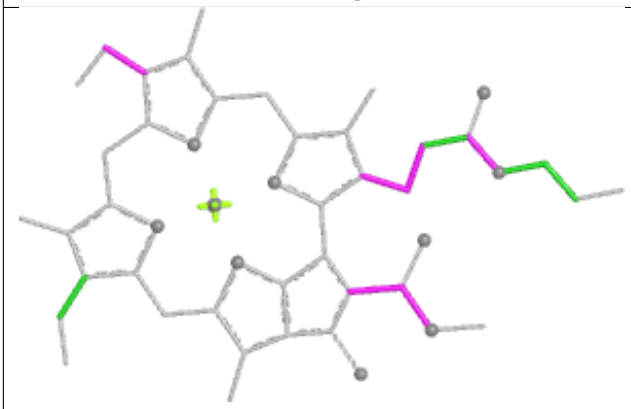
Ligand CLA a 313



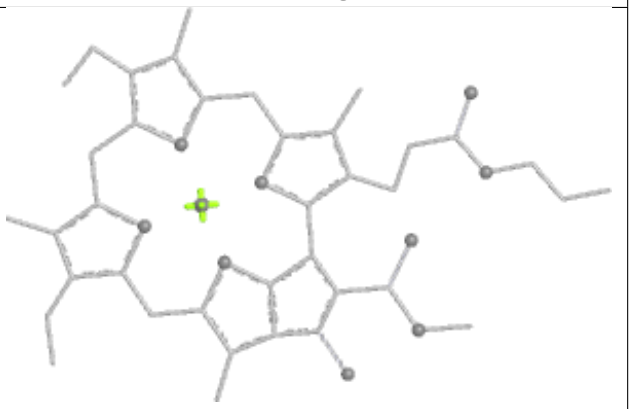
Bond lengths



Bond angles

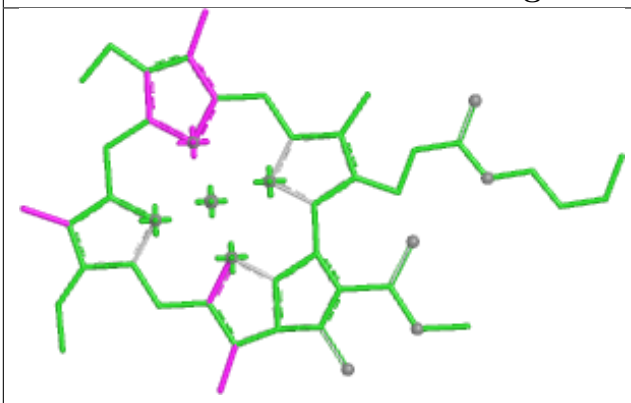


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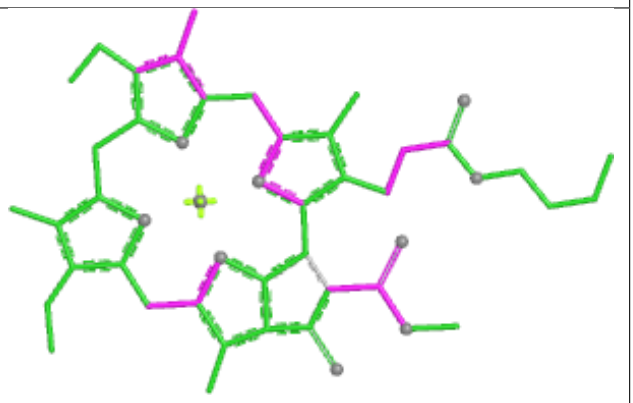


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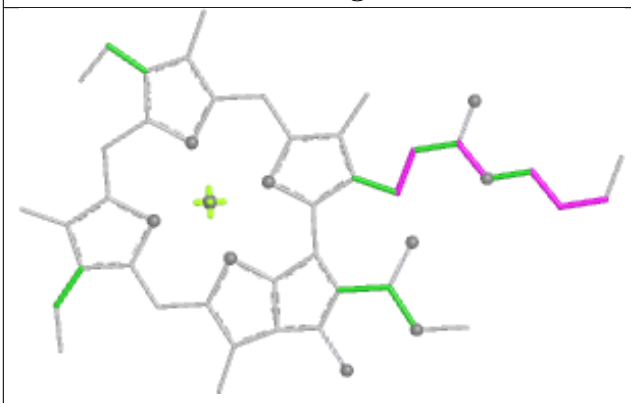
Ligand CLA A 821



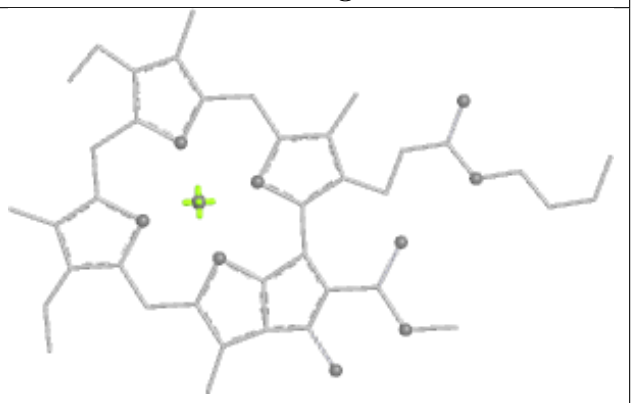
Bond lengths



Bond angles

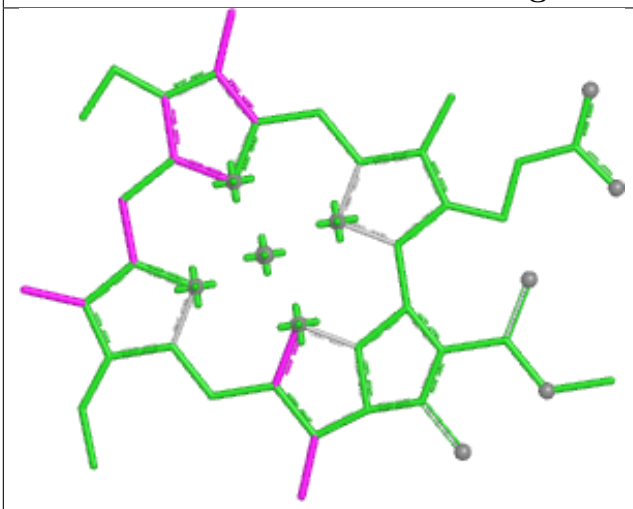


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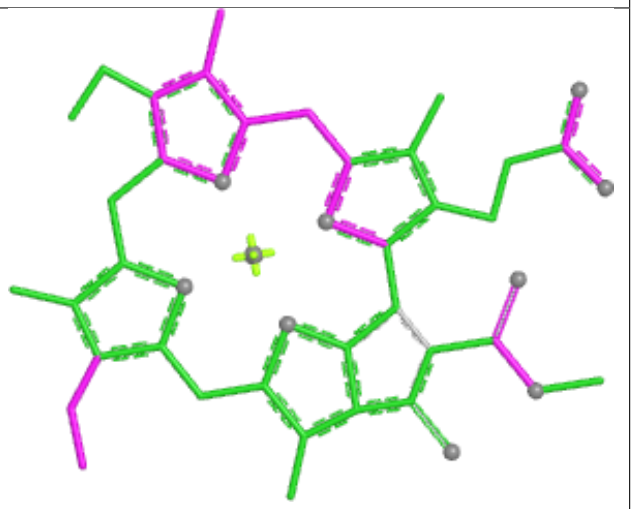


Rings

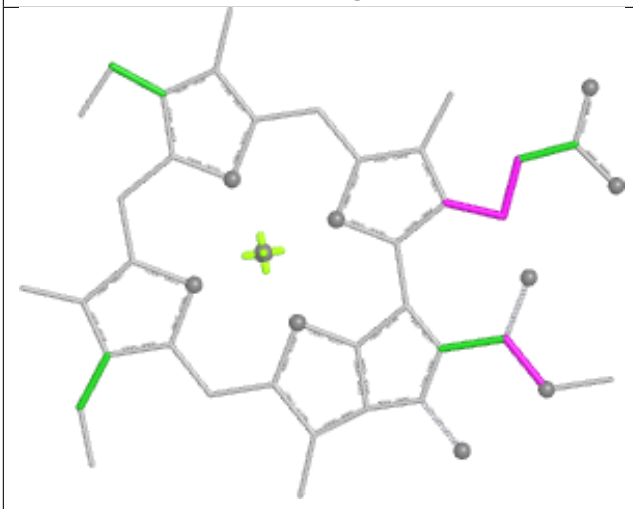
Ligand CLA c 611



Bond lengths



Bond angles

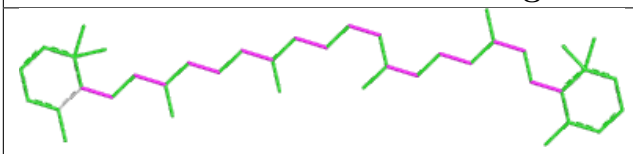


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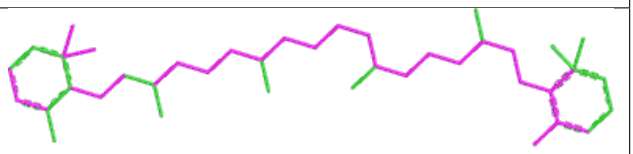


Rings

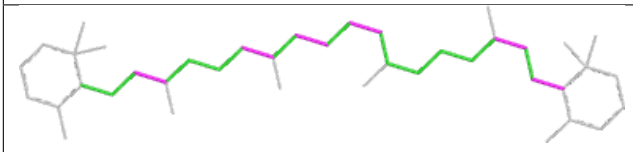
Ligand WVN i 315



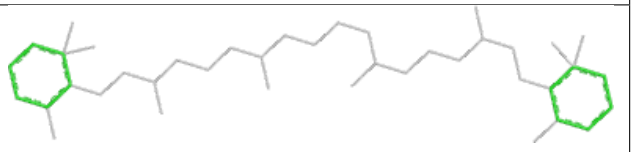
Bond lengths



Bond angles

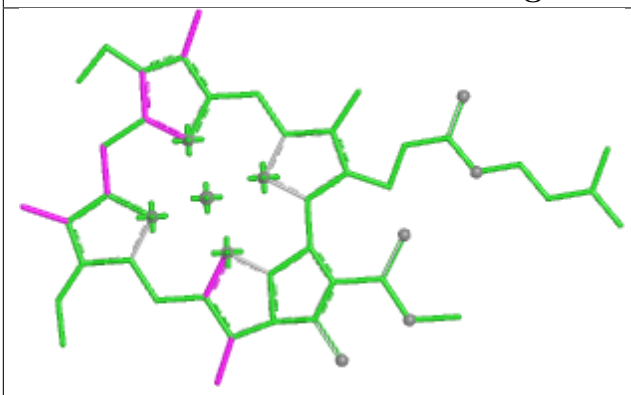


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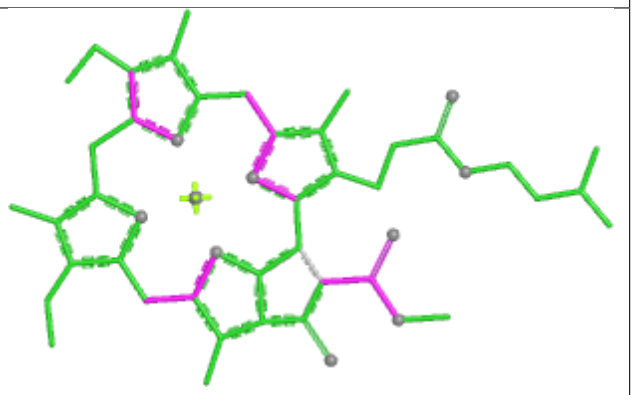


Rings

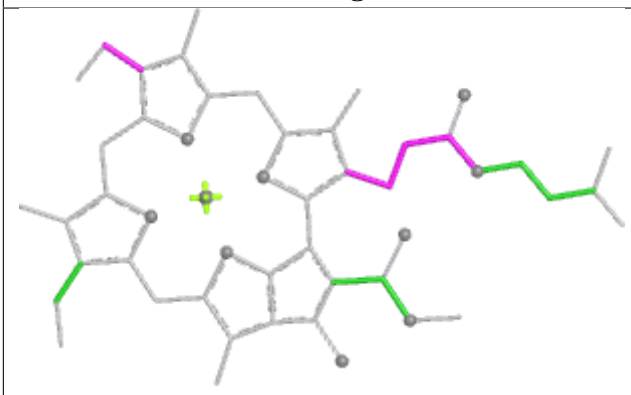
Ligand CLA B 826



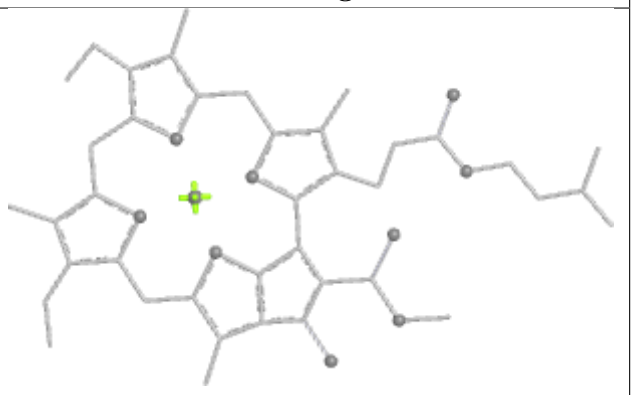
Bond lengths



Bond angles

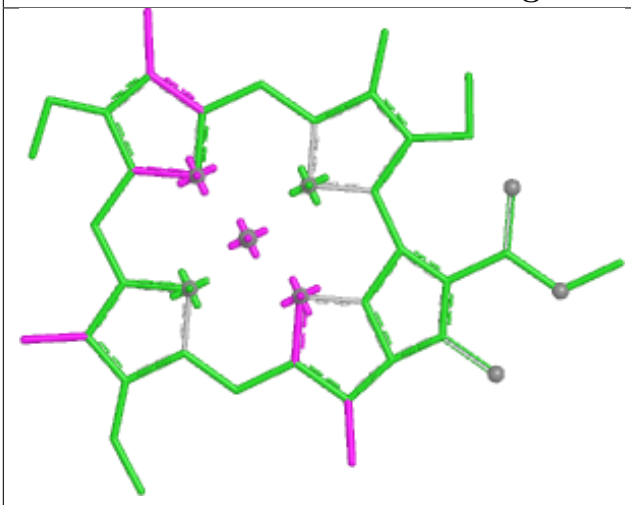


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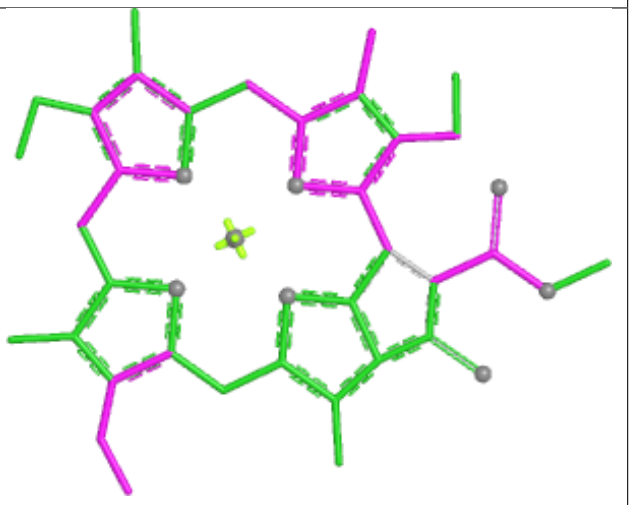


Rings

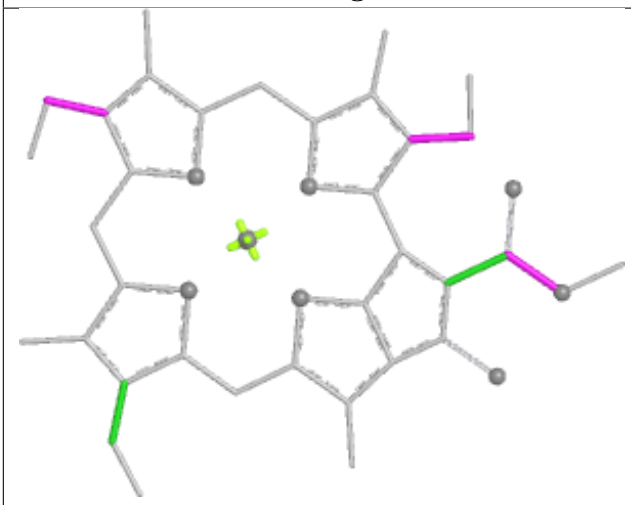
Ligand CLA m 605



Bond lengths



Bond angles

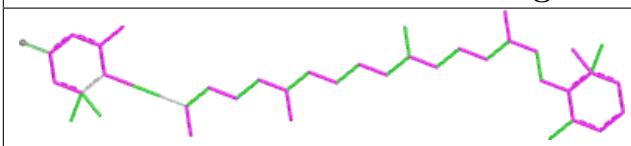


Torsions

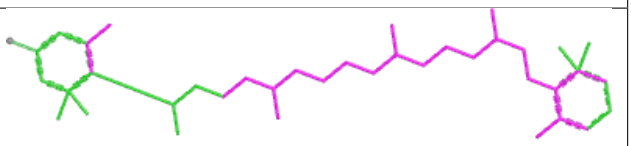


Rings

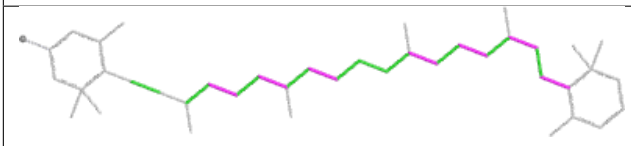
Ligand IHT c 620



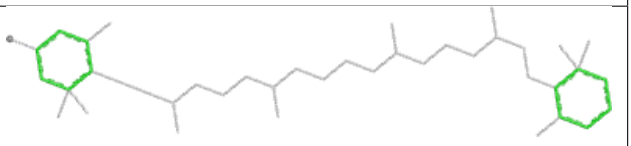
Bond lengths



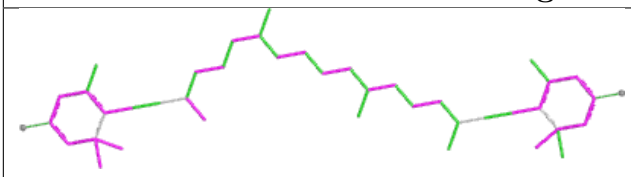
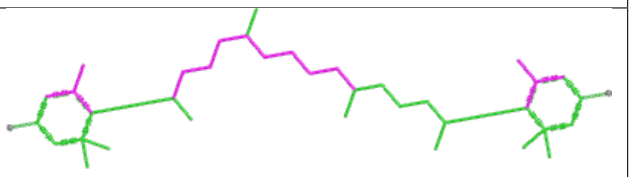
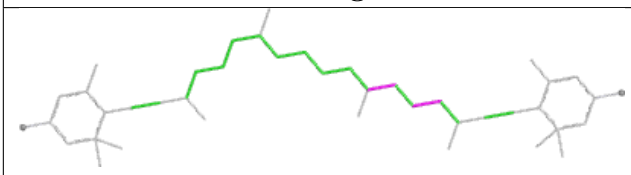
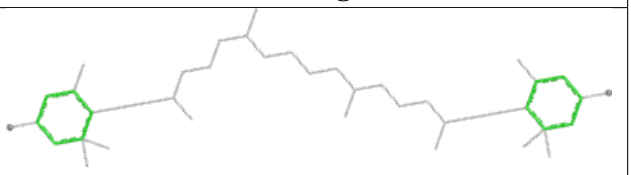
Bond angles

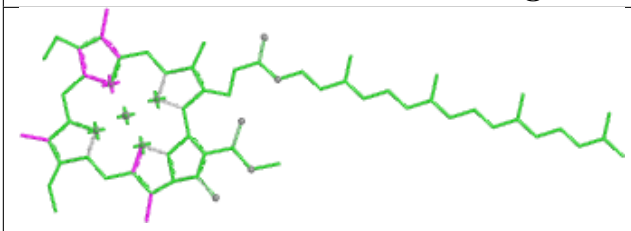
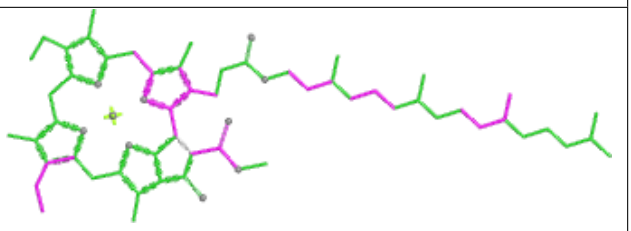
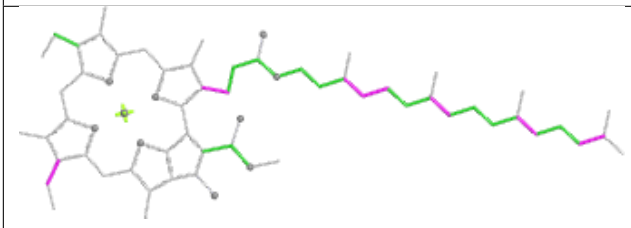
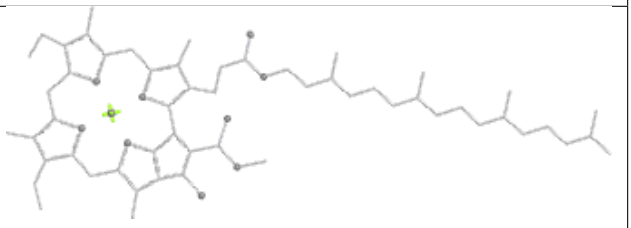


Torsions

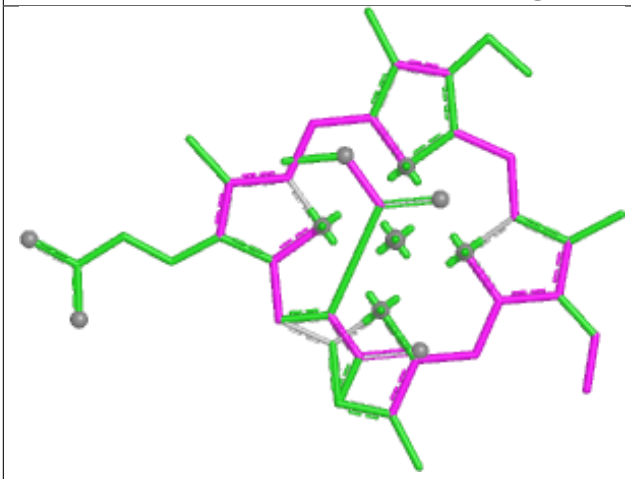


Rings

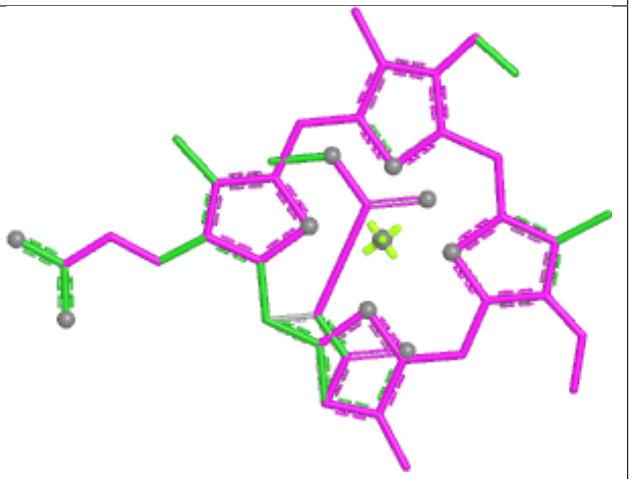
Ligand II0 m 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

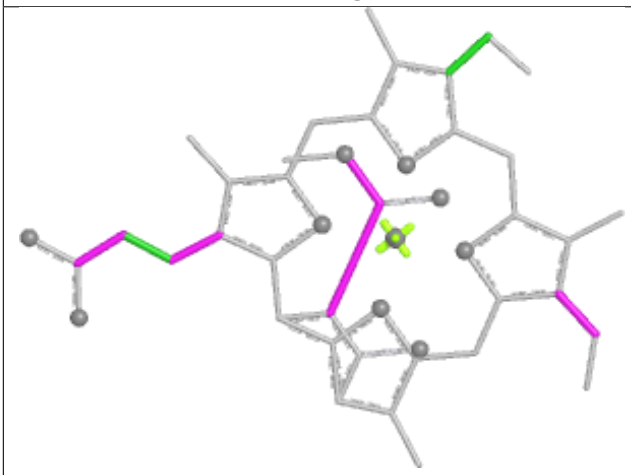
Ligand KC2 d 309



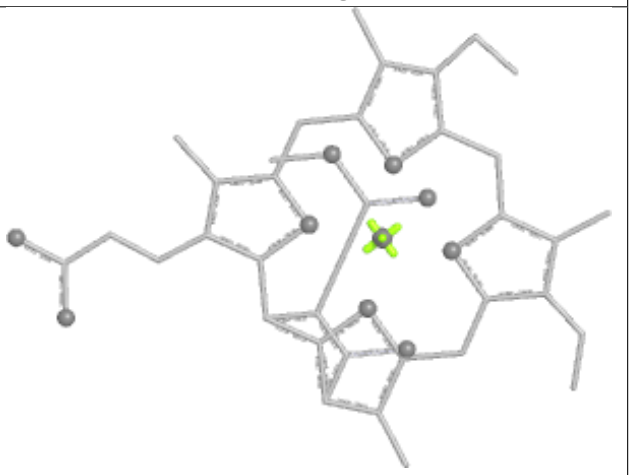
Bond lengths



Bond angles

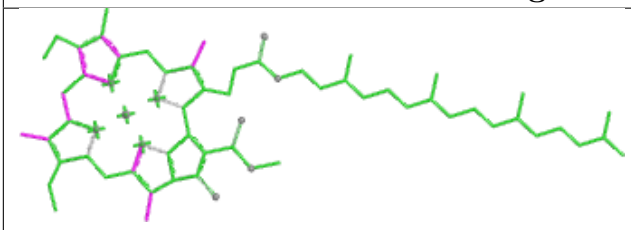


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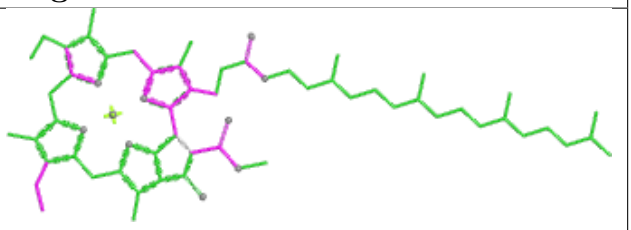


Rings

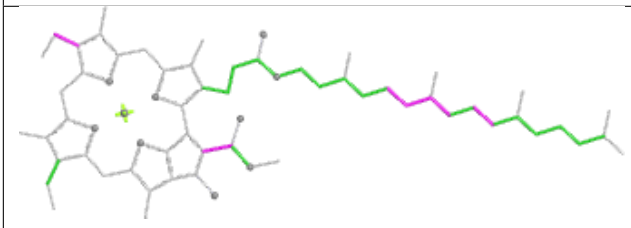
Ligand CLA g 309



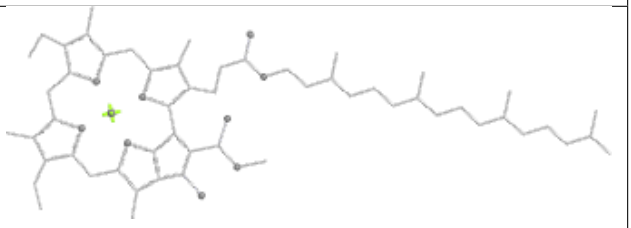
Bond lengths



Bond angles

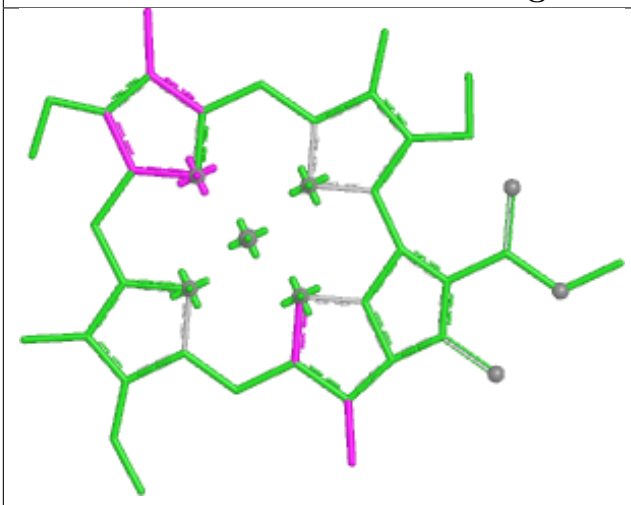


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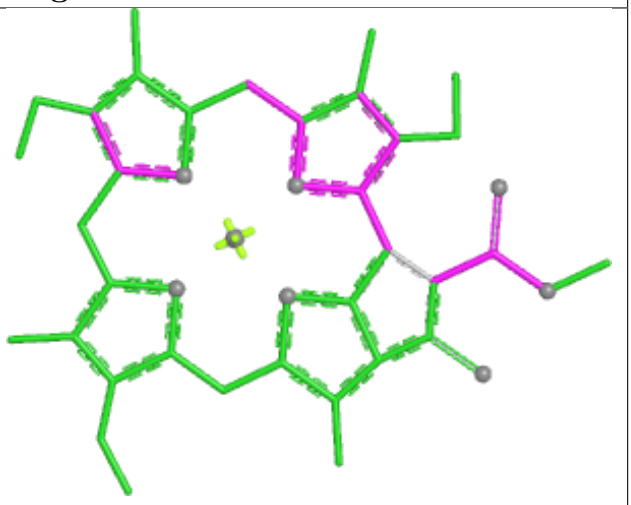


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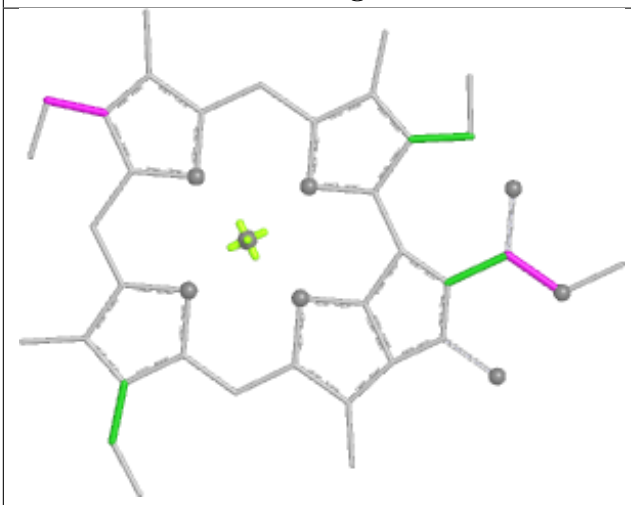
Ligand CLA g 302



Bond lengths



Bond angles

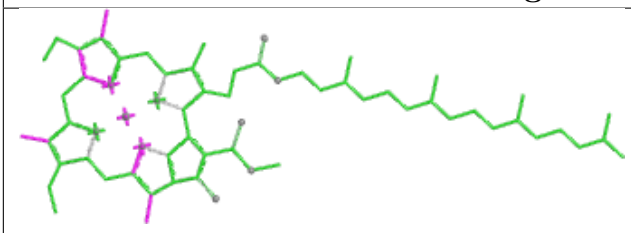


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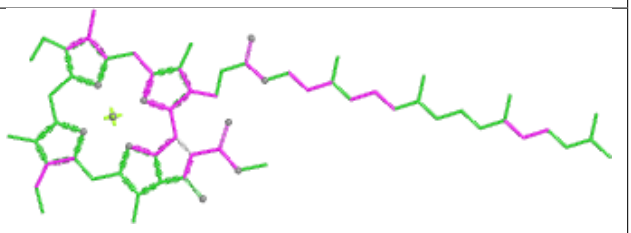


Rings

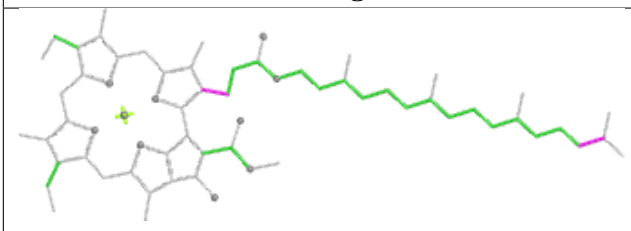
Ligand CLA B 822



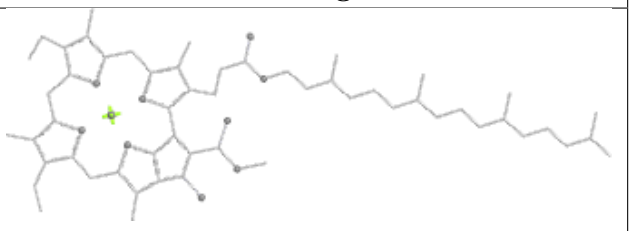
Bond lengths



Bond angles

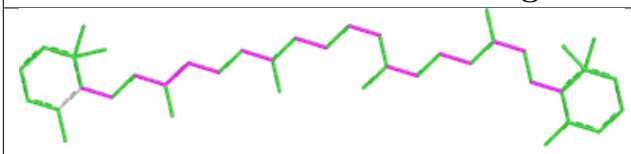


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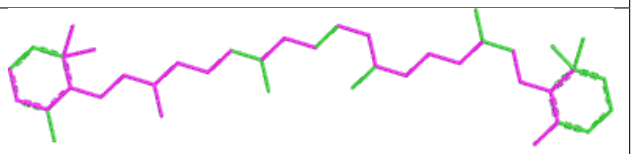


Rings

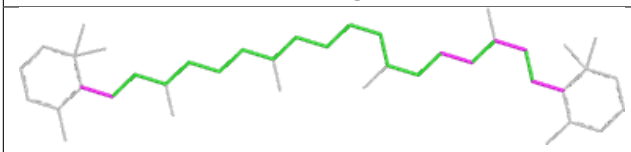
Ligand WVN s 207



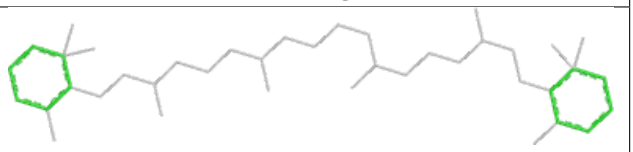
Bond lengths



Bond angles

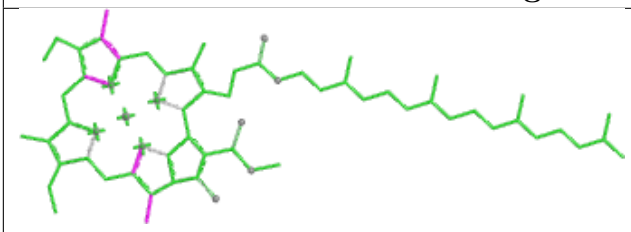


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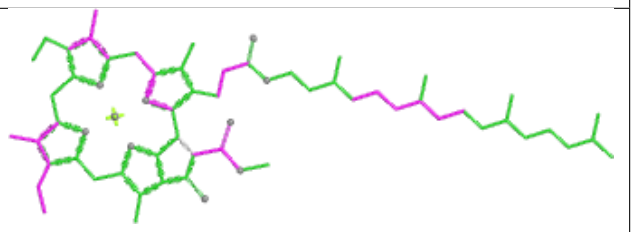


Rings

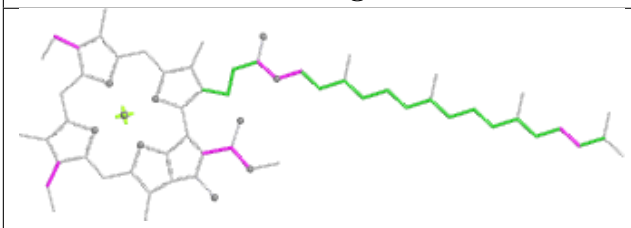
Ligand CLA A 832



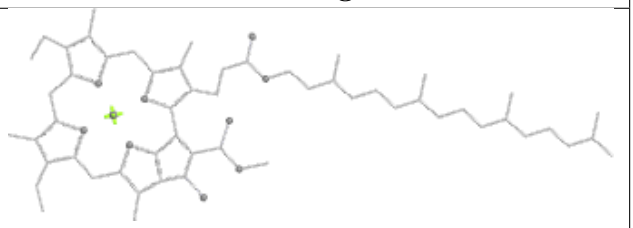
Bond lengths



Bond angles

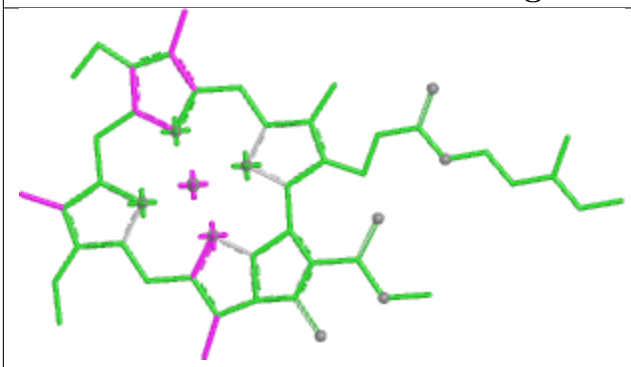


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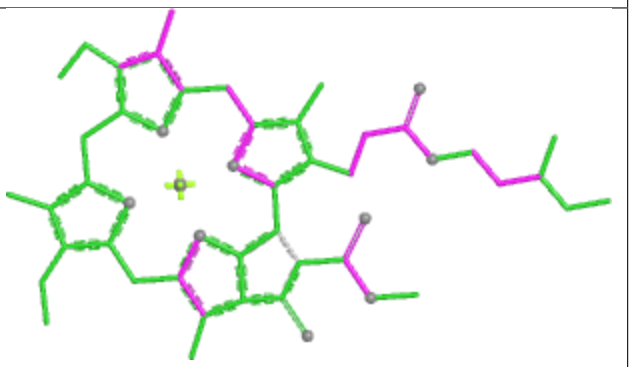


Rings

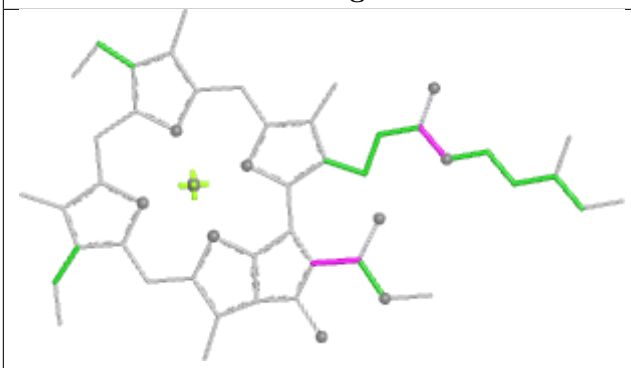
Ligand CLA B 825



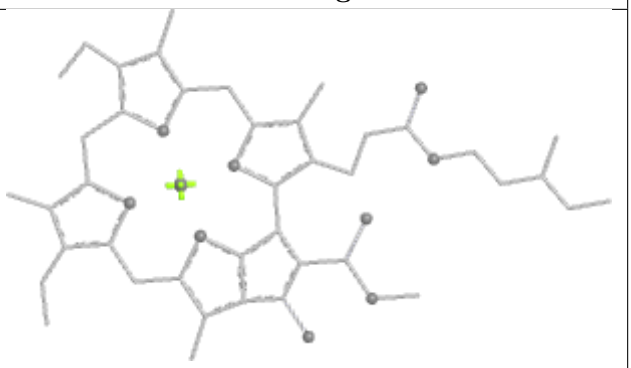
Bond lengths



Bond angles

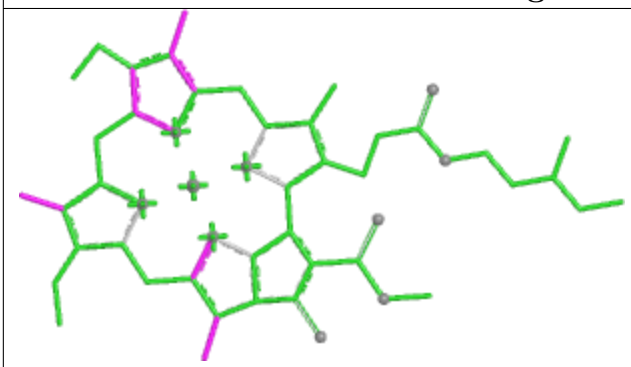


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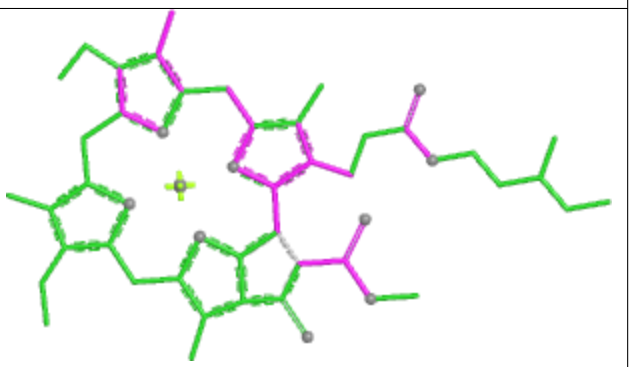


Rings

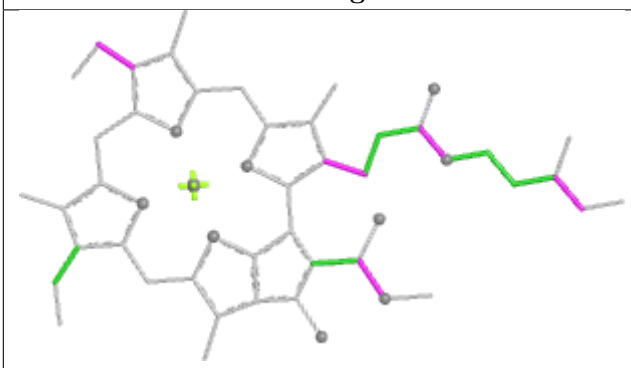
Ligand CLA n 603



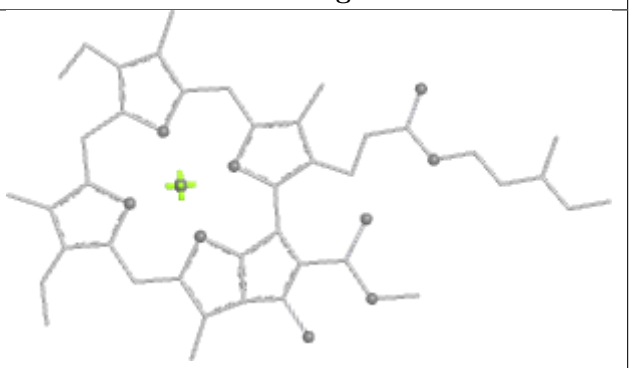
Bond lengths



Bond angles

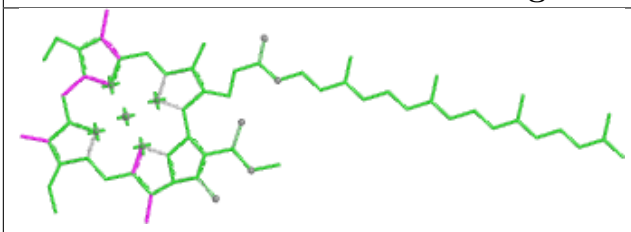


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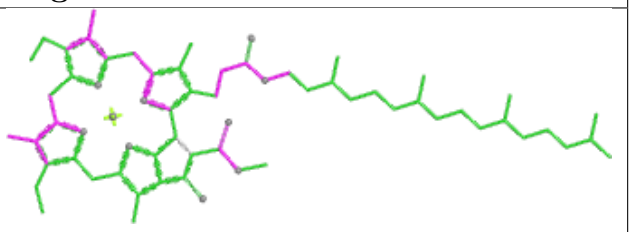


Rings

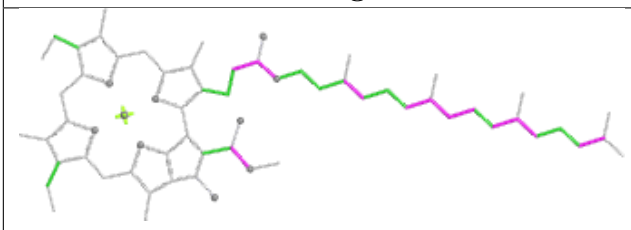
Ligand CLA g 308



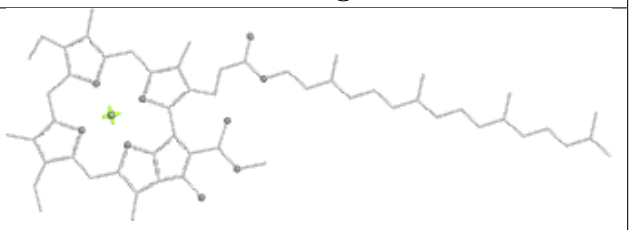
Bond lengths



Bond angles

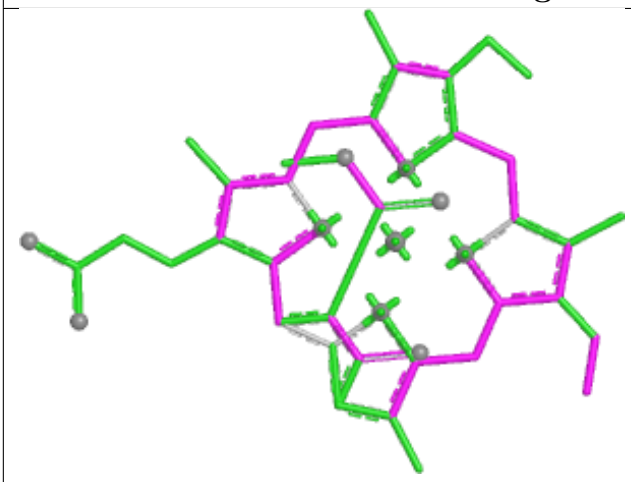


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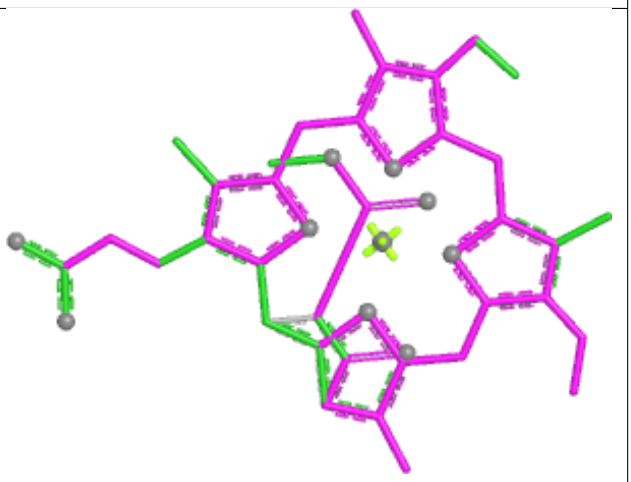


Rings

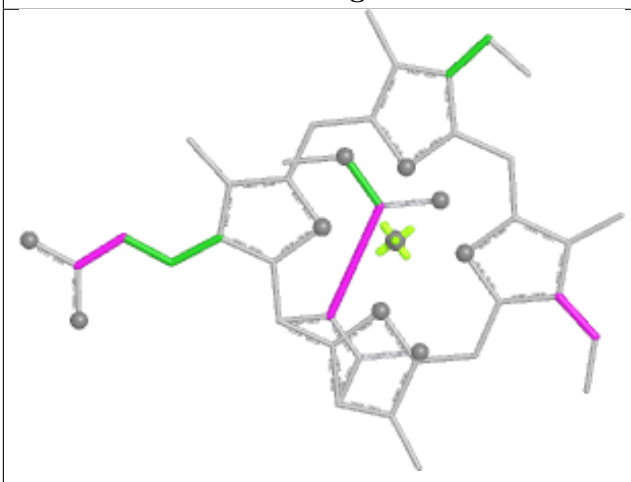
Ligand KC2 l 311



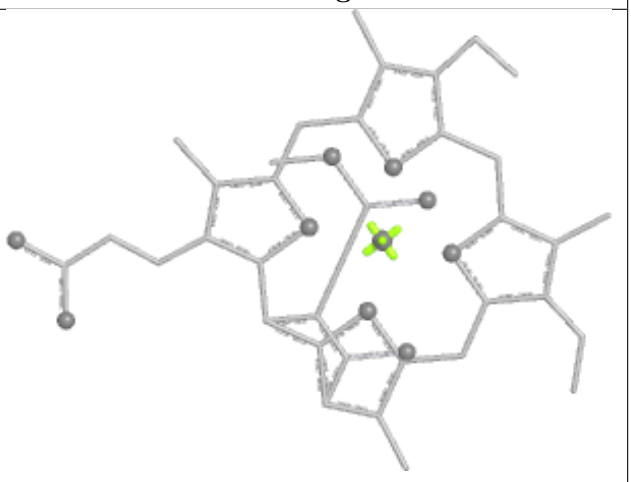
Bond lengths



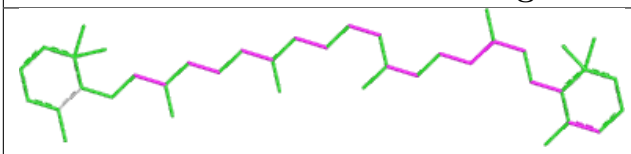
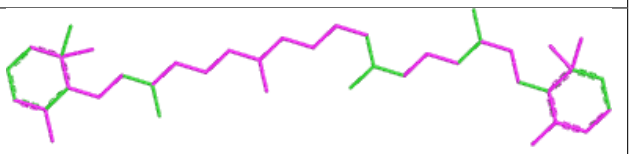
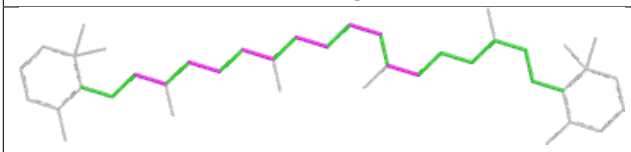
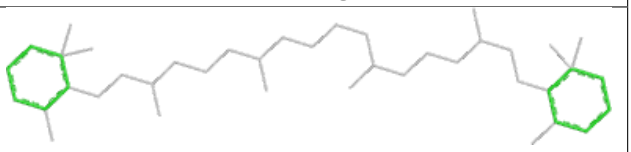
Bond angles

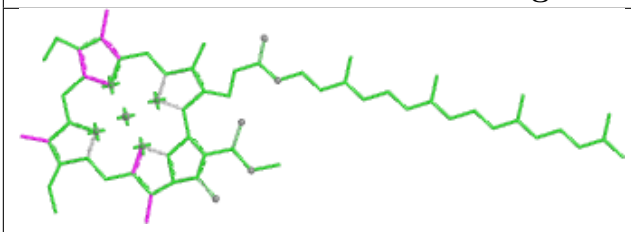
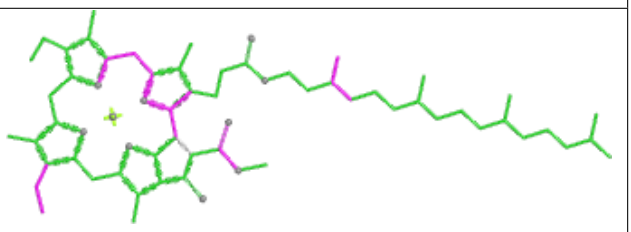
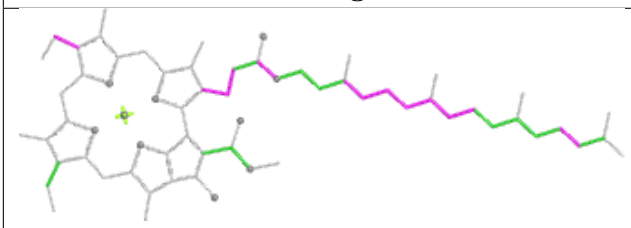
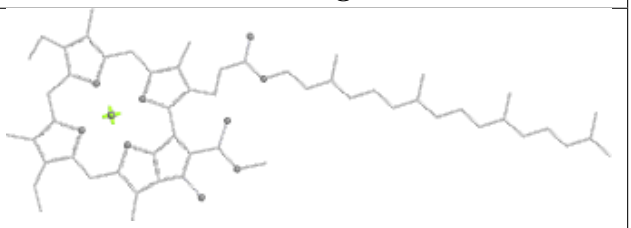


Torsions

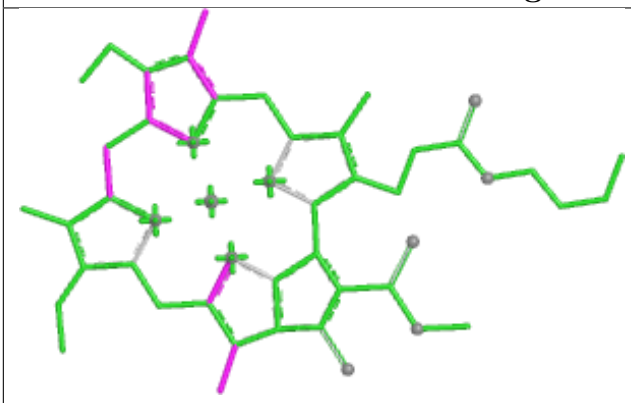


Rings

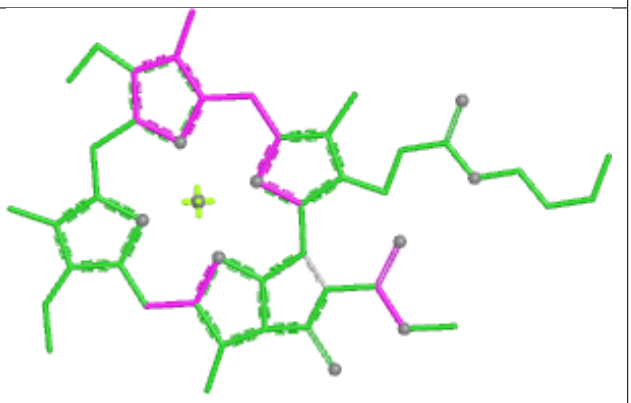
Ligand WVN F 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

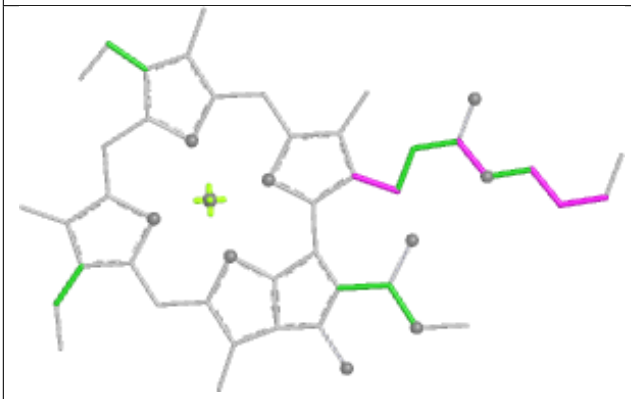
Ligand CLA B 827



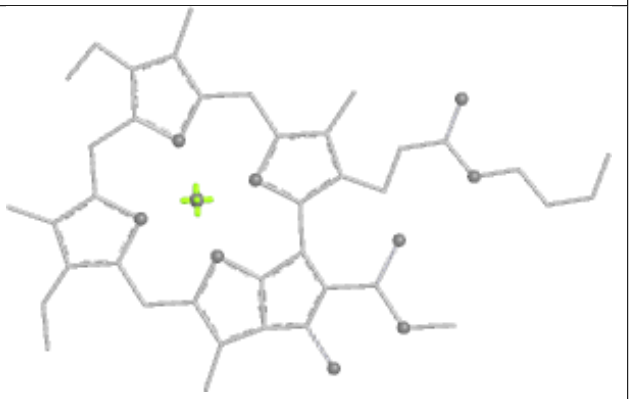
Bond lengths



Bond angles

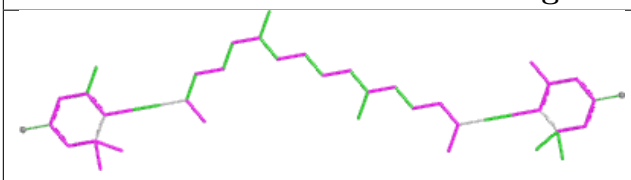


Torsions

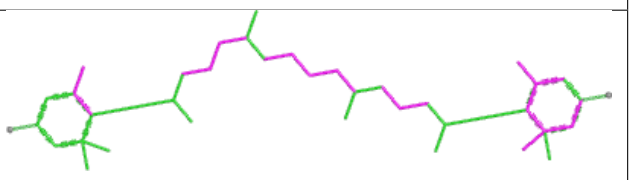


Rings

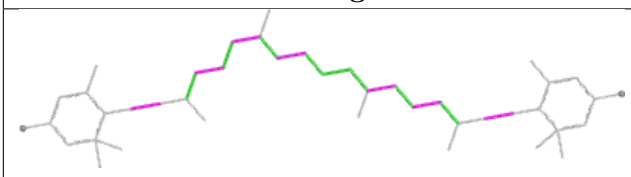
Ligand II0 b 613



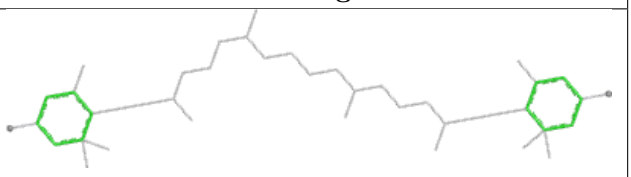
Bond lengths



Bond angles

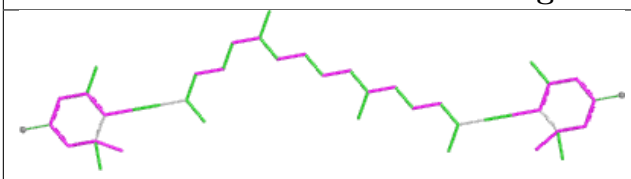


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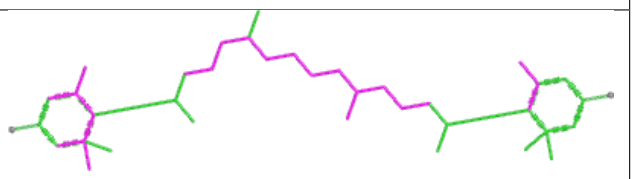


Rings

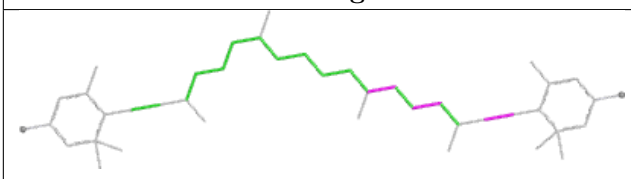
Ligand II0 m 613



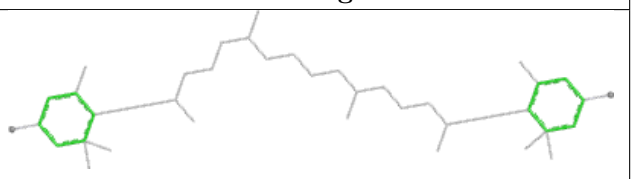
Bond lengths



Bond angles

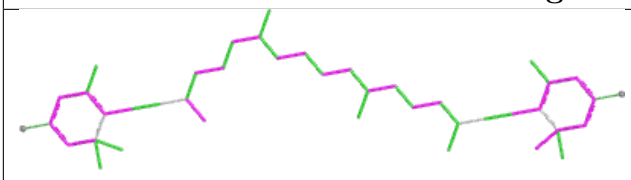


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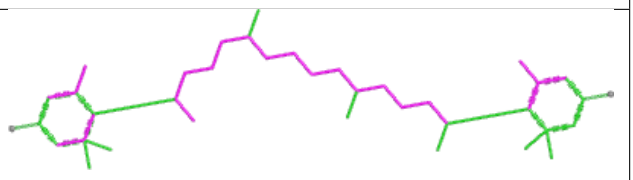


Rings

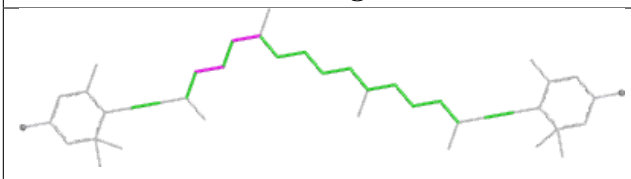
Ligand II0 f 616



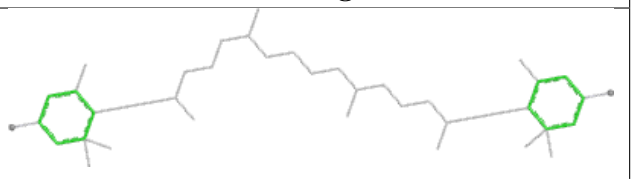
Bond lengths



Bond angles

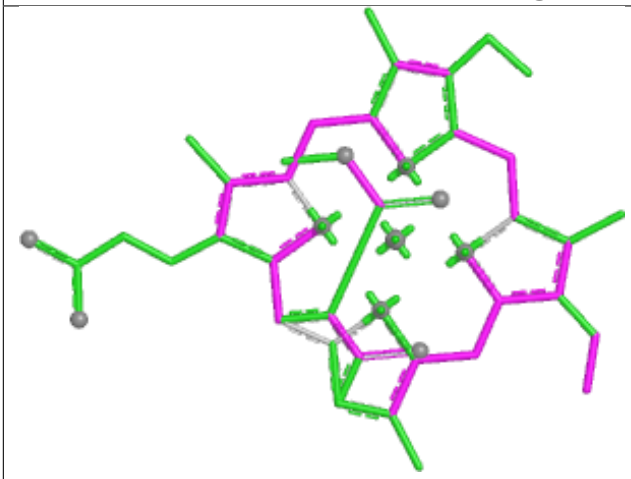


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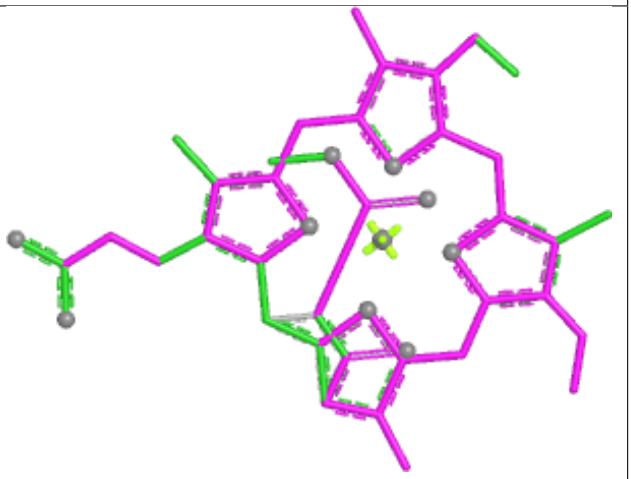


Rings

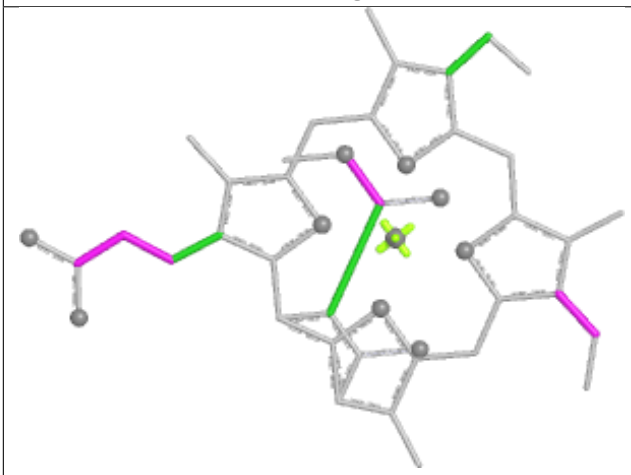
Ligand KC2 e 609



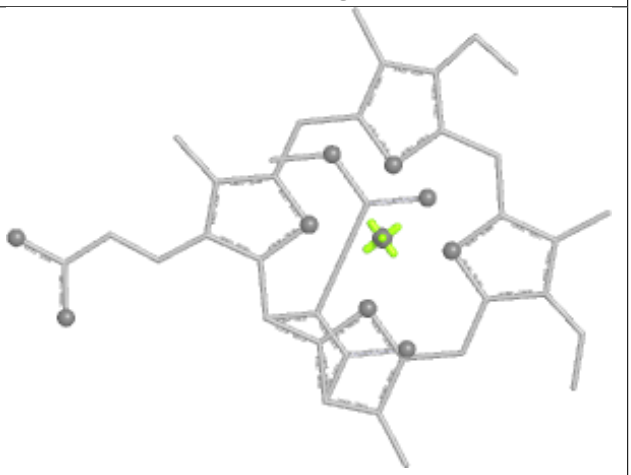
Bond lengths



Bond angles

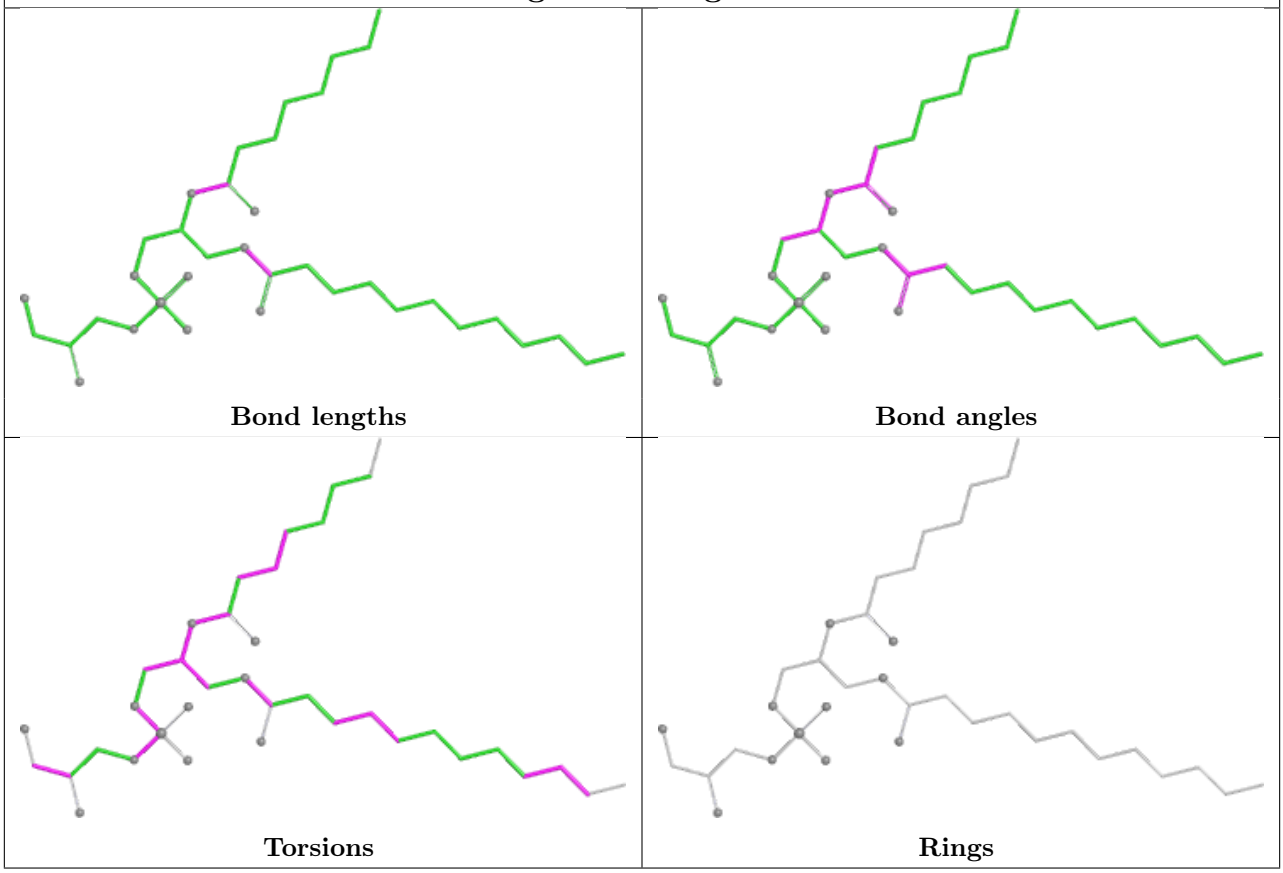


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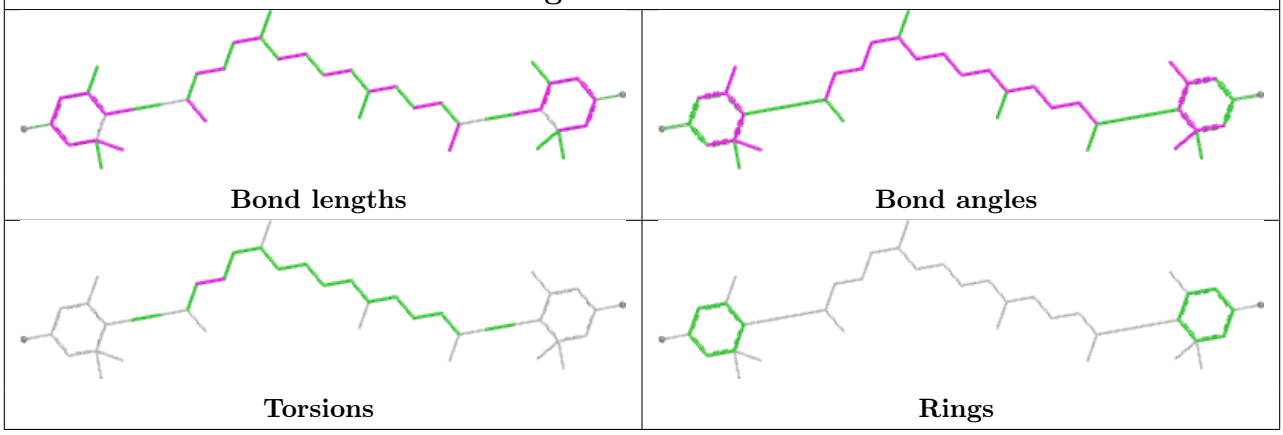


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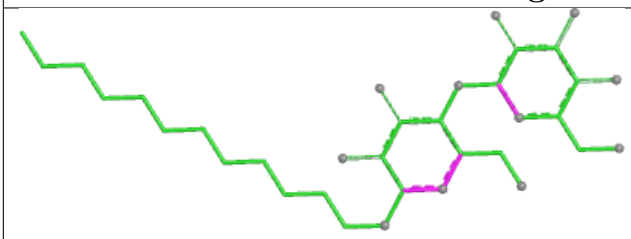
Ligand LHG g 301



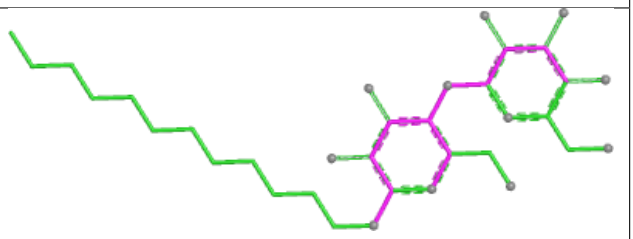
Ligand II0 c 614



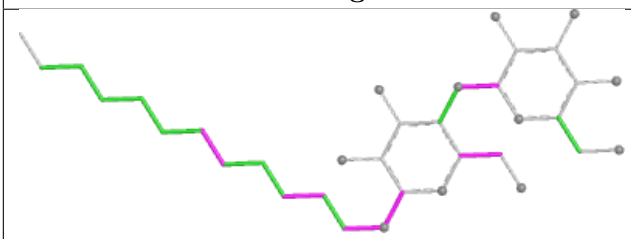
Ligand LMU i 301



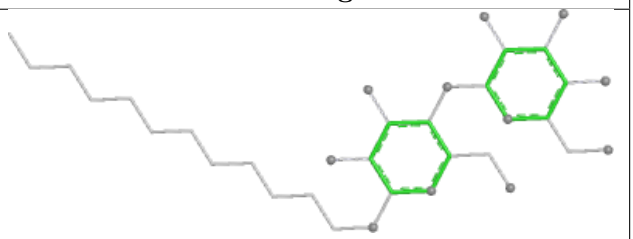
Bond lengths



Bond angles

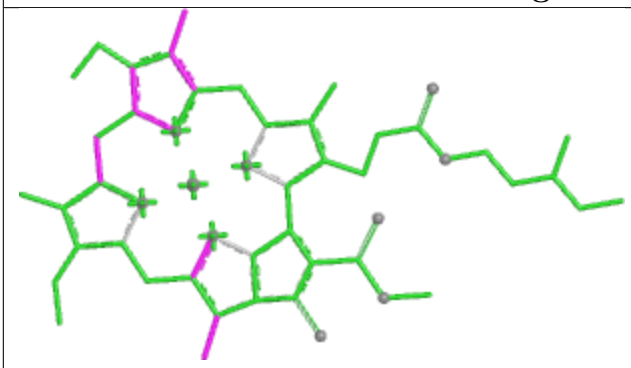


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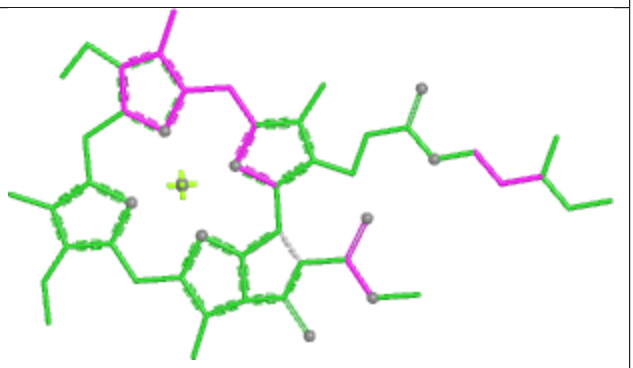


Rings

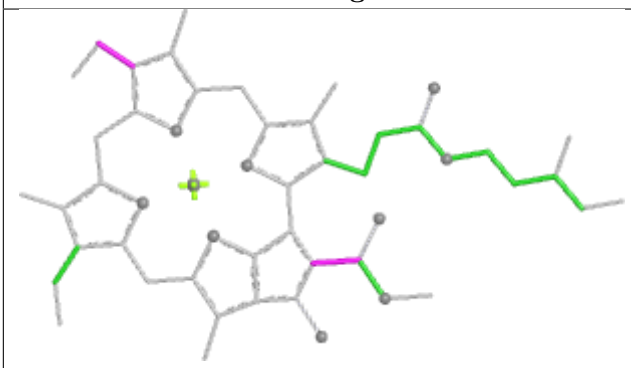
Ligand CLA i 304



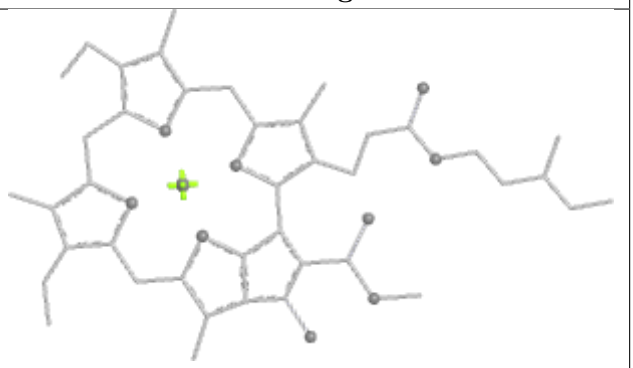
Bond lengths



Bond angles

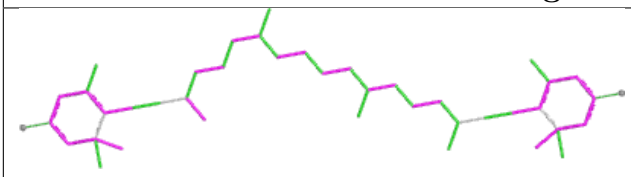


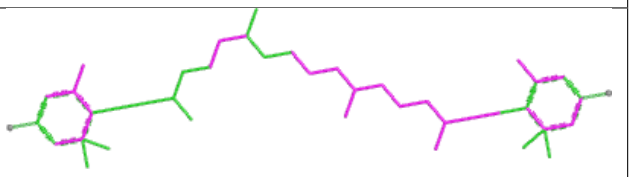
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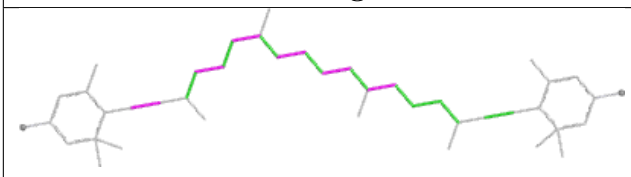


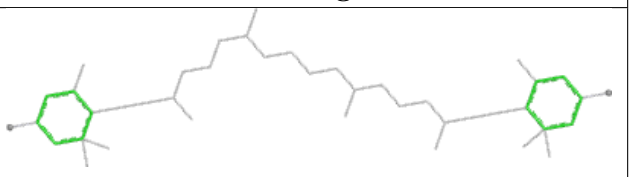
Rings

Ligand II0 a 318

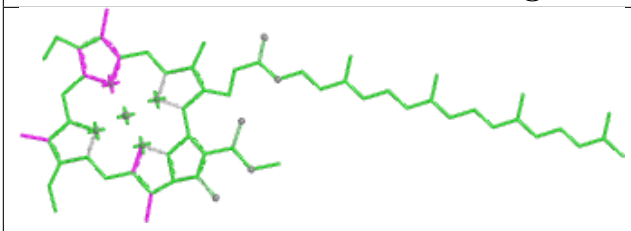

Bond lengths

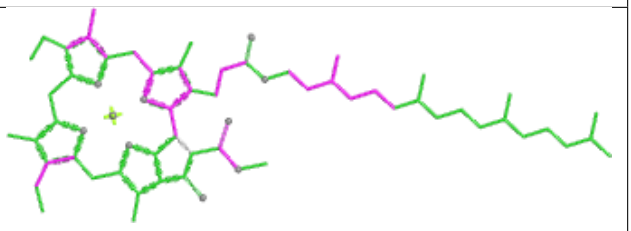

Bond angles

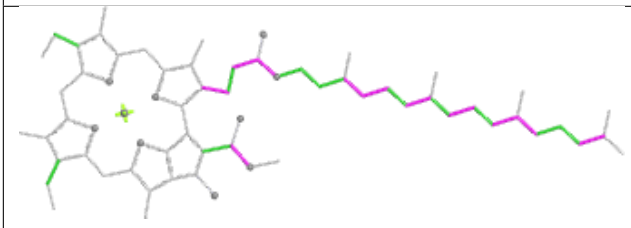

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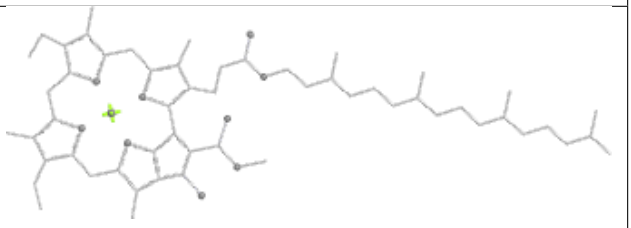

Rings

Ligand CLA A 812

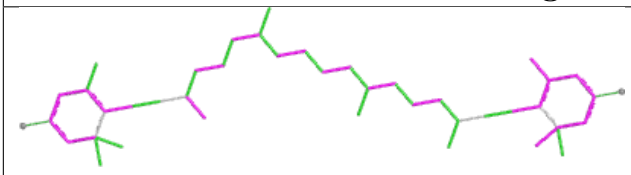

Bond lengths

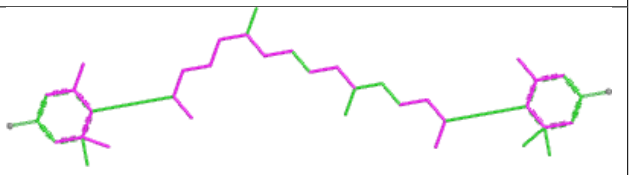

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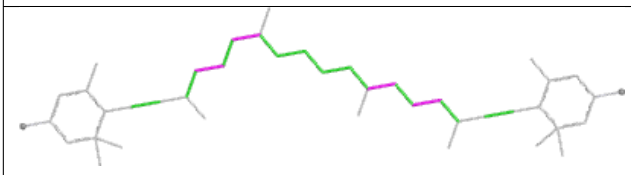

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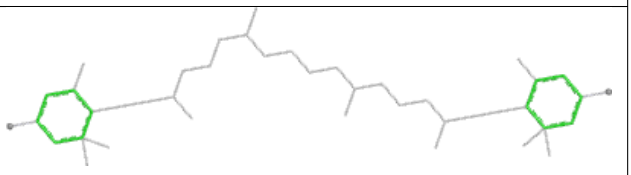

Rings

Ligand II0 d 313

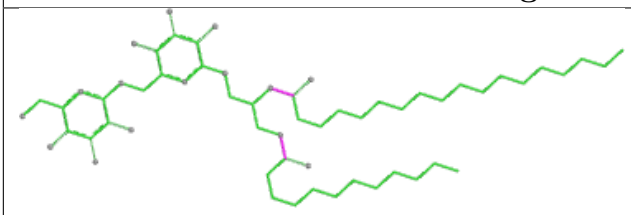

Bond lengths


Bond angles

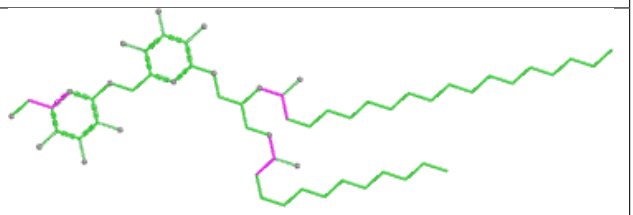

Torsions


Rings

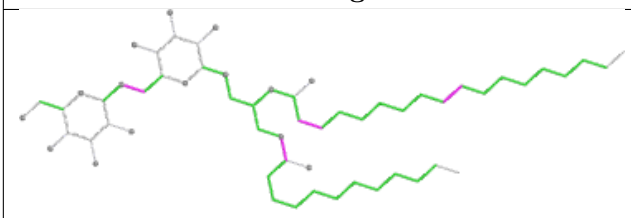
Ligand DGD B 842



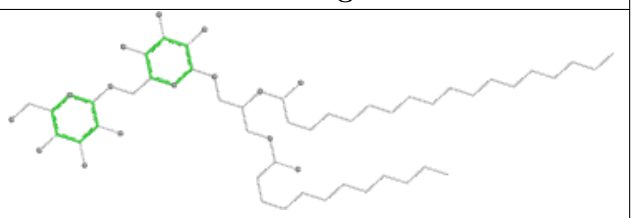
Bond lengths



Bond angles

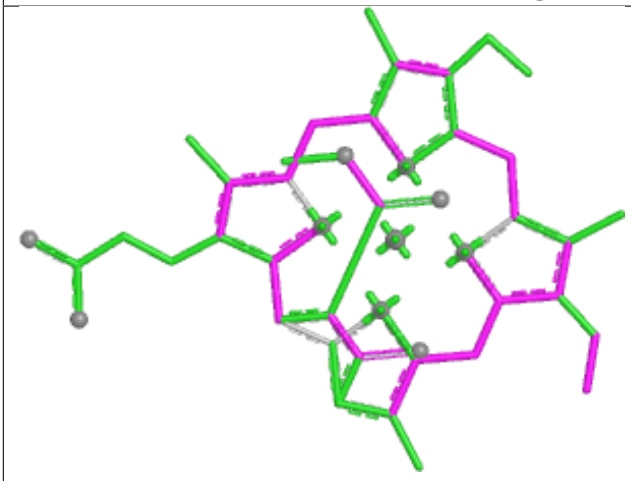


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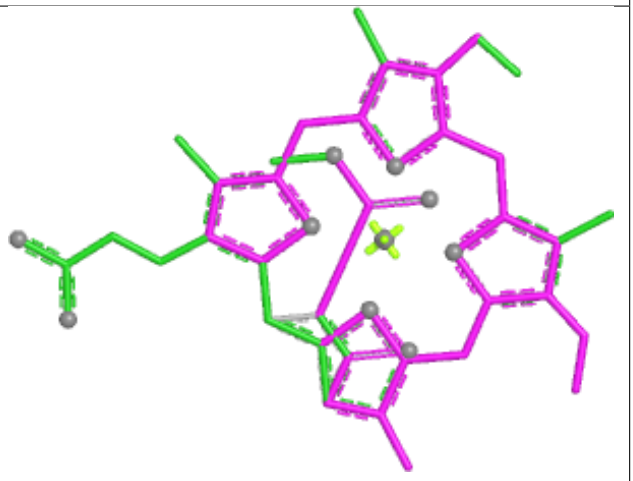


Rings

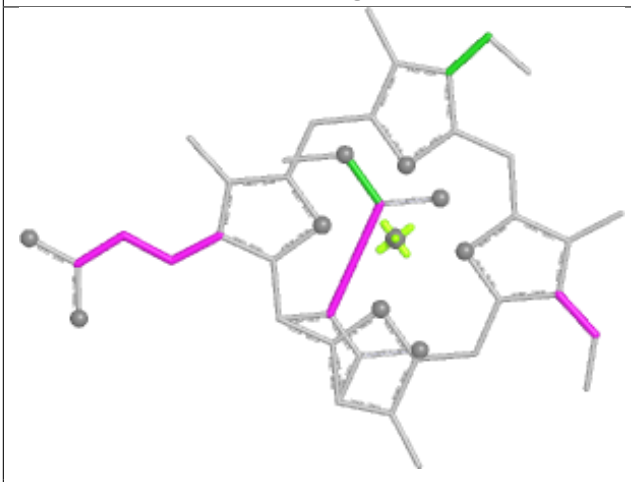
Ligand KC2 c 610



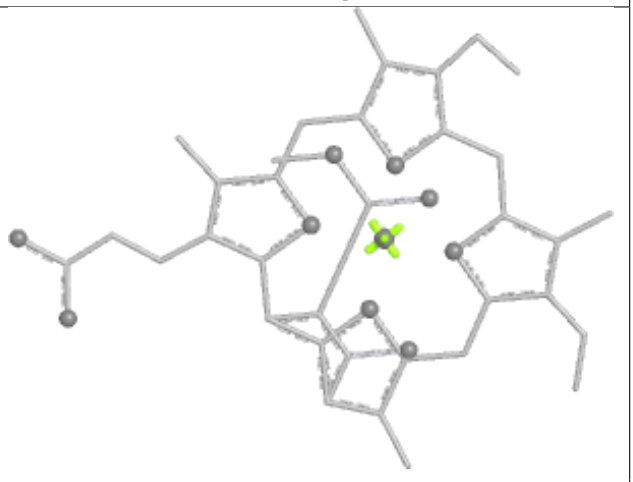
Bond lengths



Bond angles

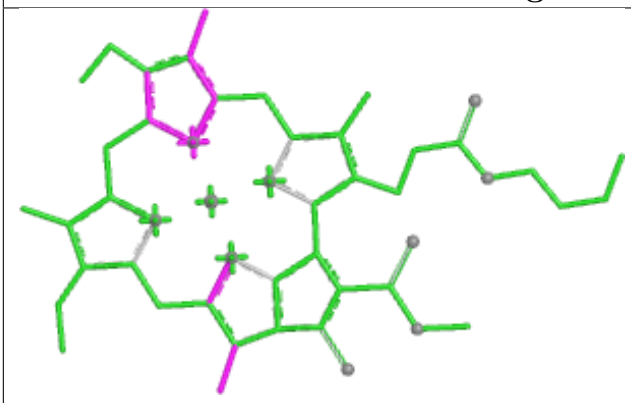


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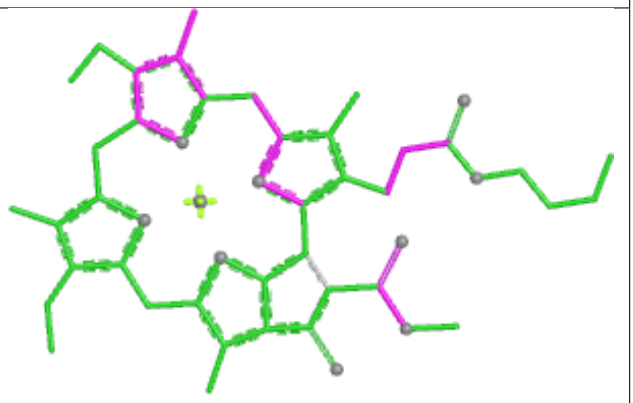


Rings

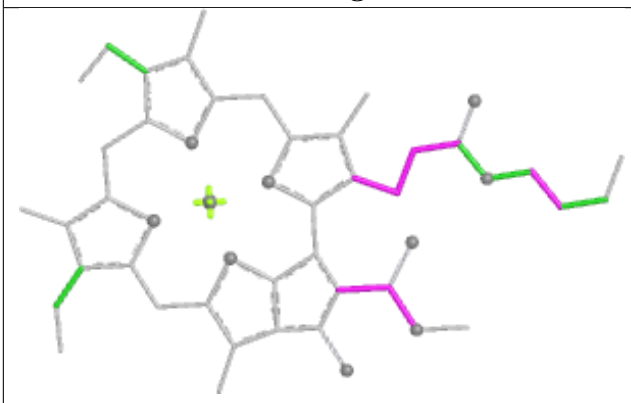
Ligand CLA L 202



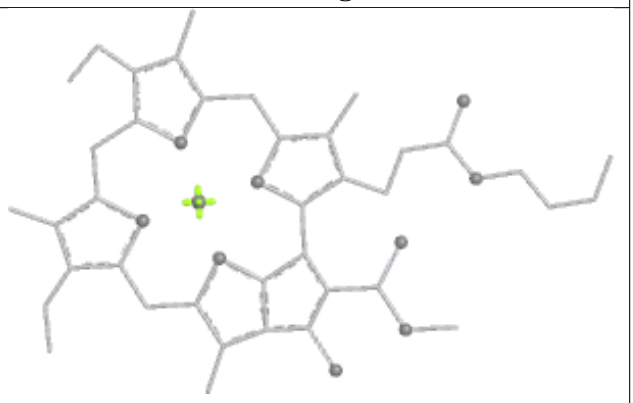
Bond lengths



Bond angles

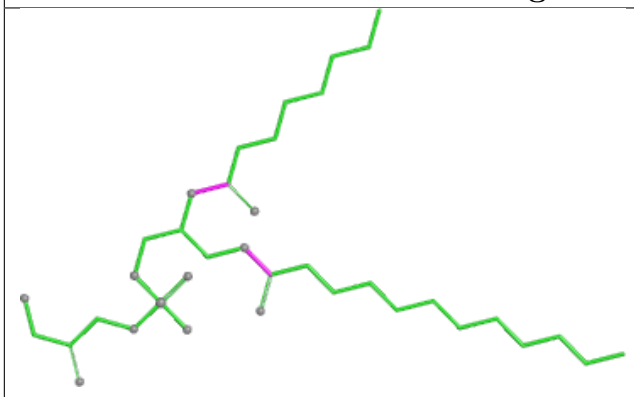


Torsions

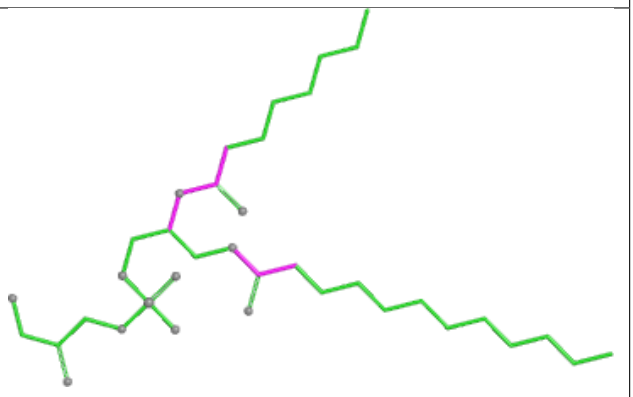


Rings

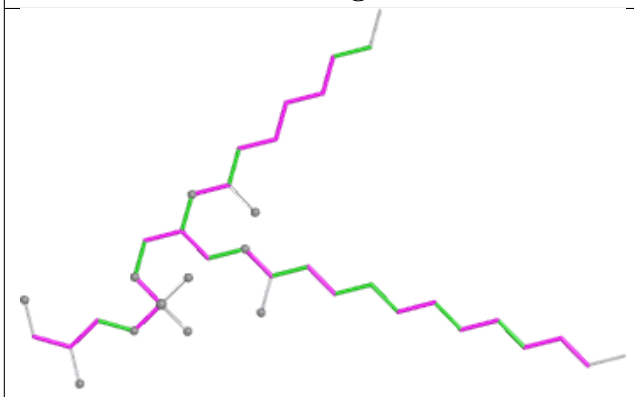
Ligand LHG c 621



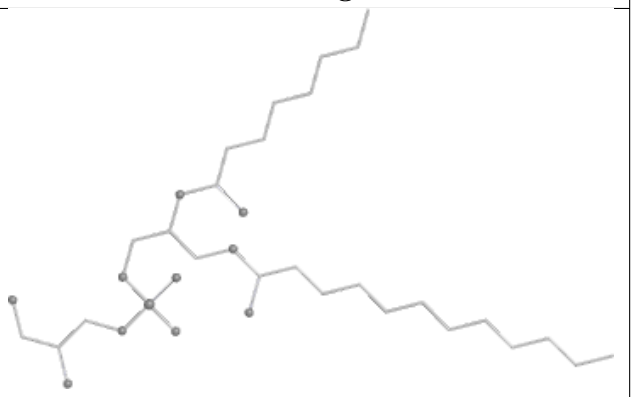
Bond lengths



Bond angles

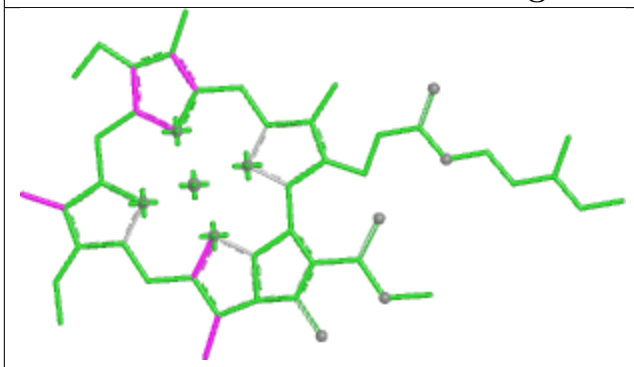


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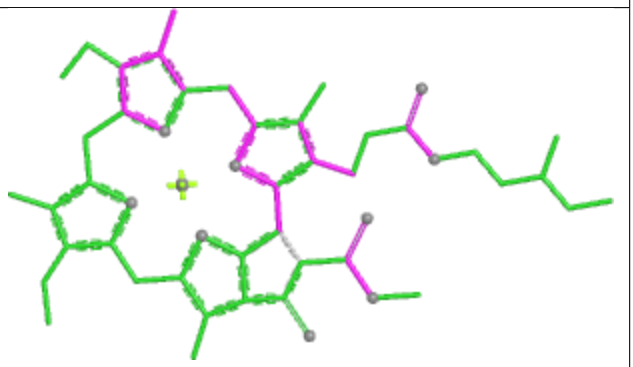


Rings

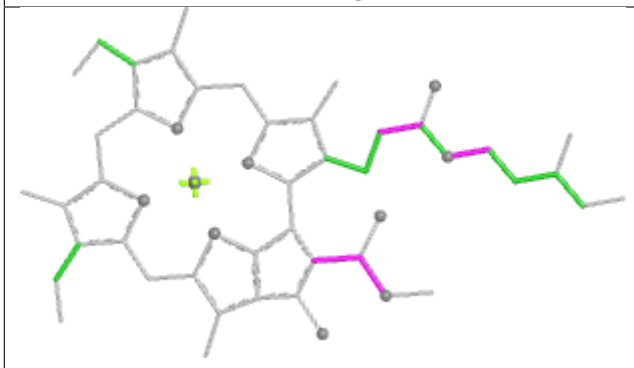
Ligand CLA d 302



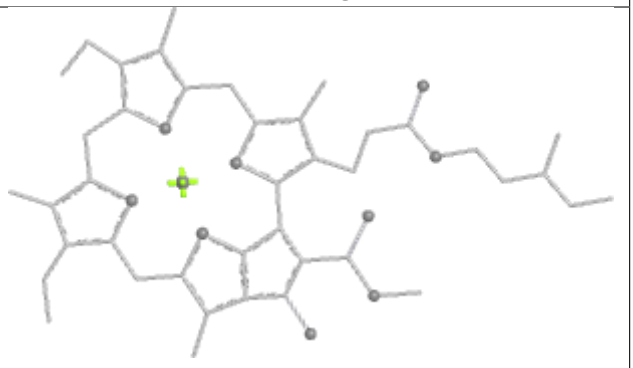
Bond lengths



Bond angles

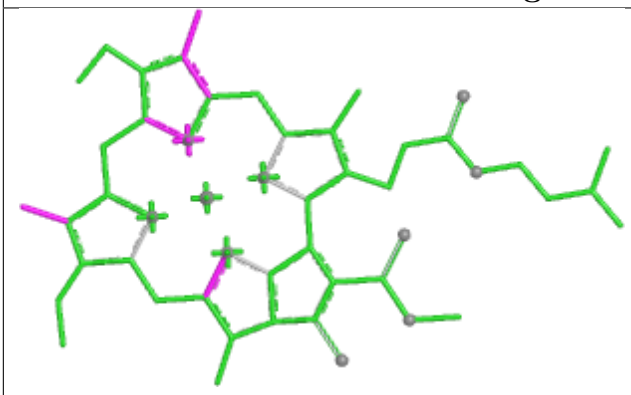


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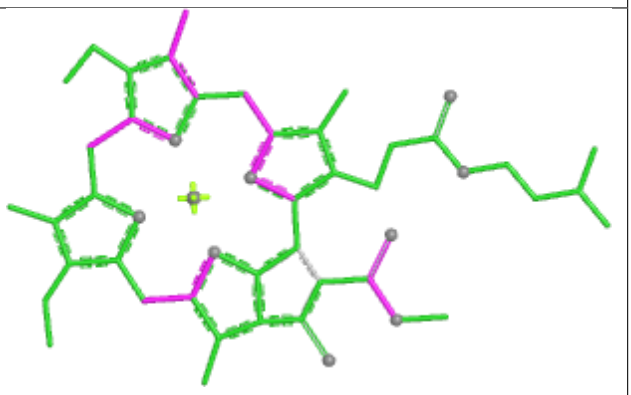


Rings

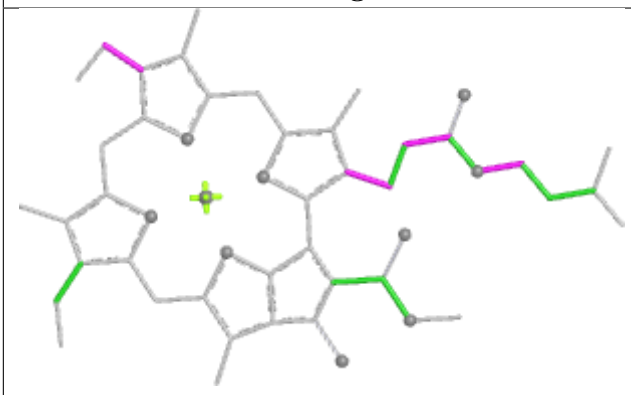
Ligand CLA A 833



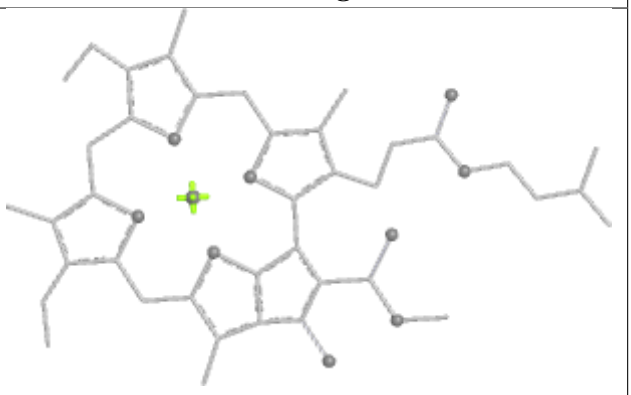
Bond lengths



Bond angles

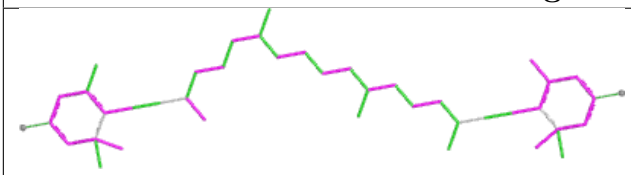


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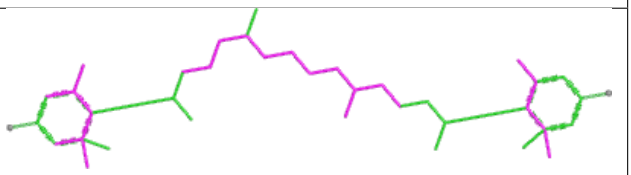


Rings

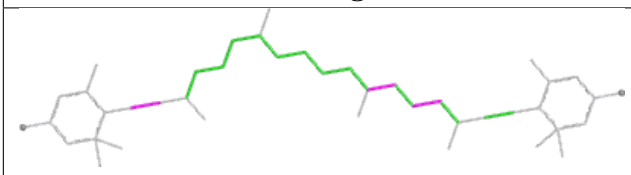
Ligand II0 c 613



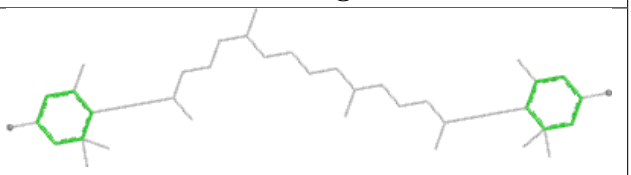
Bond lengths



Bond angles

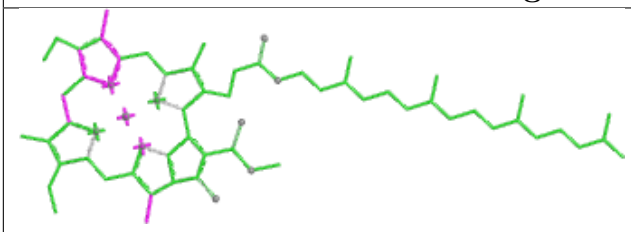


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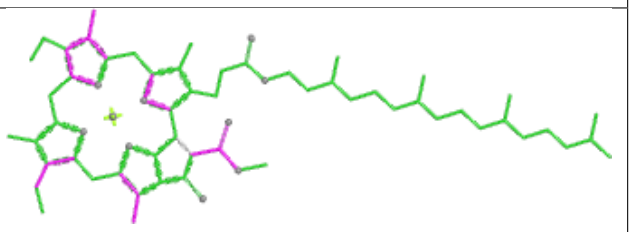


Rings

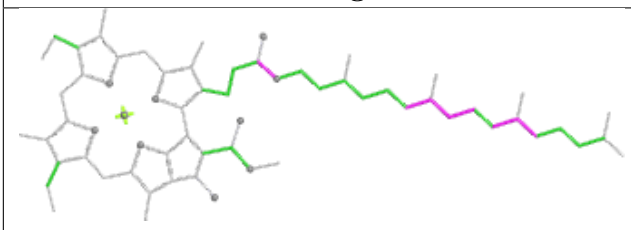
Ligand CLA A 825



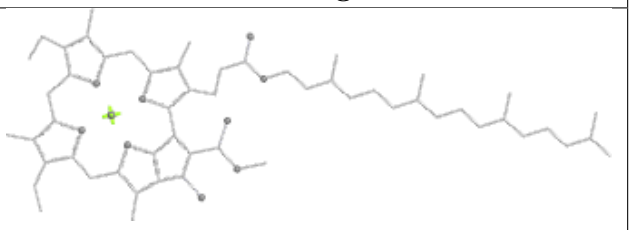
Bond lengths



Bond angles

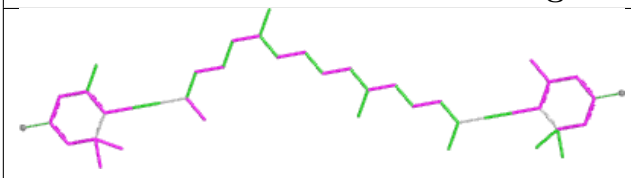


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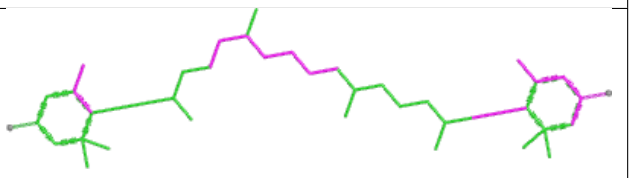


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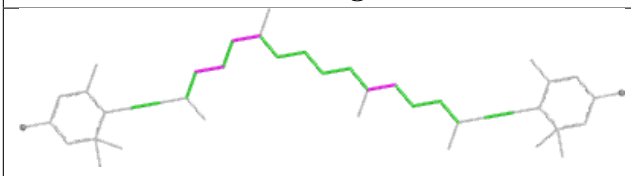
Ligand II0 i 318



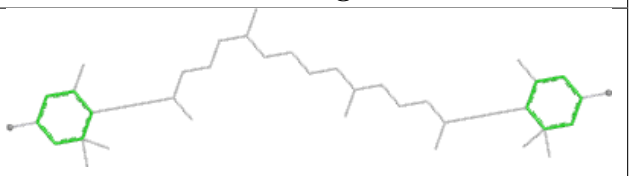
Bond lengths



Bond angles

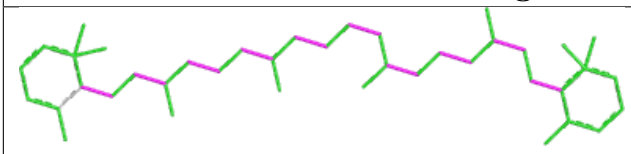


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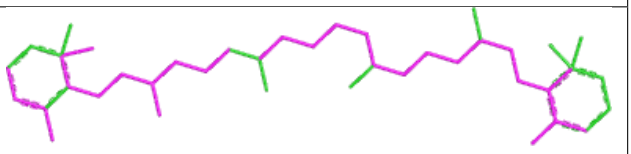


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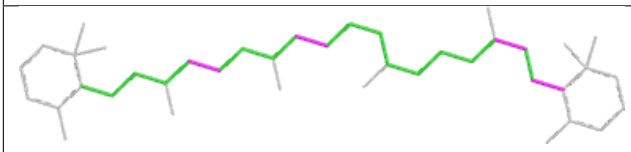
Ligand WVN K 103



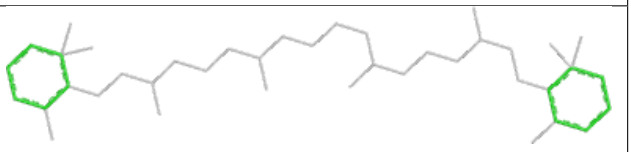
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Bond angles

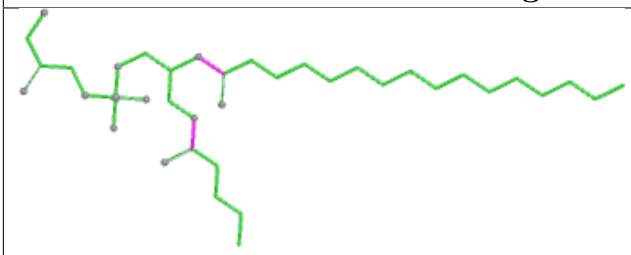


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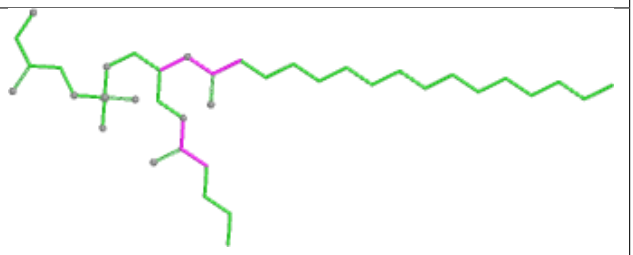


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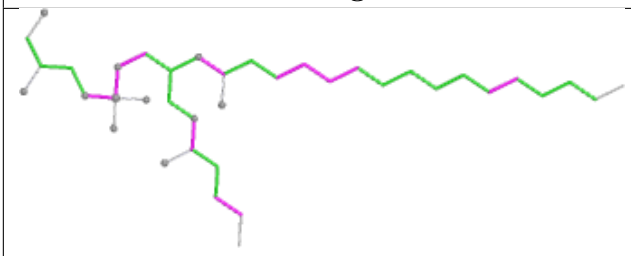
Ligand LHG A 850



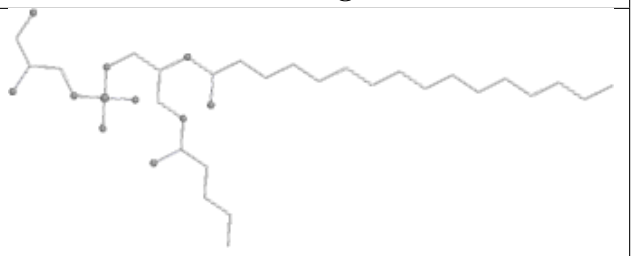
Bond lengths



Bond angles

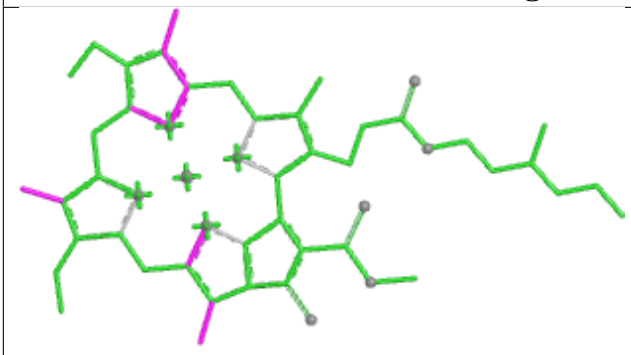


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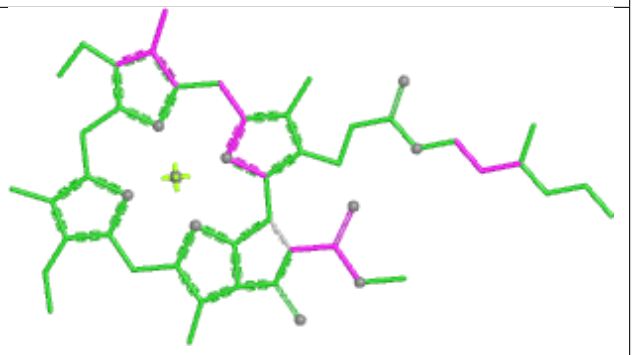


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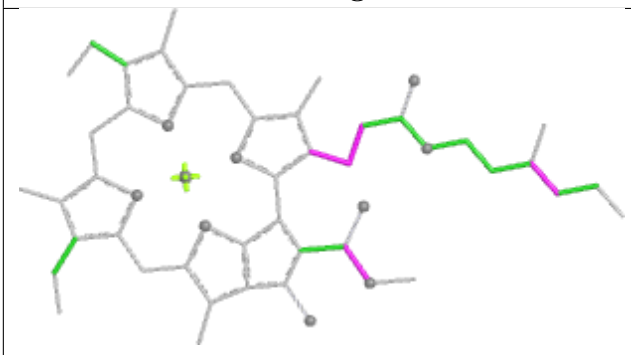
Ligand CLA A 838



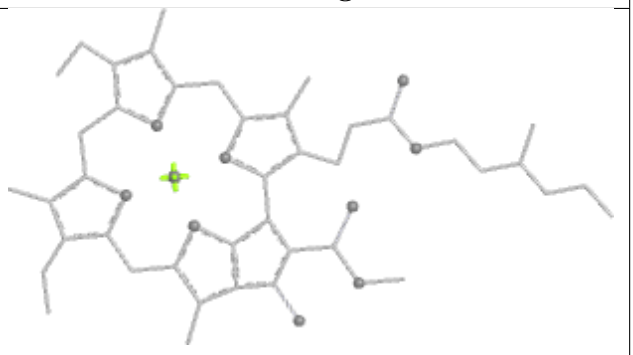
Bond lengths



Bond angles

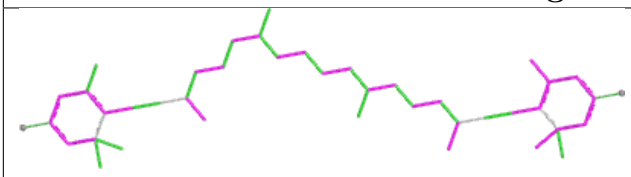


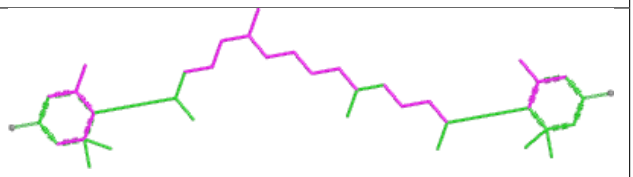
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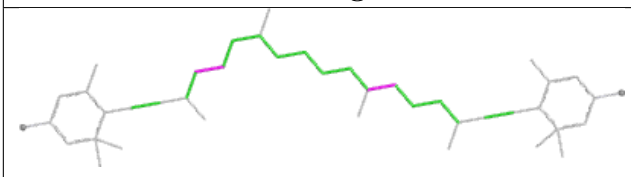


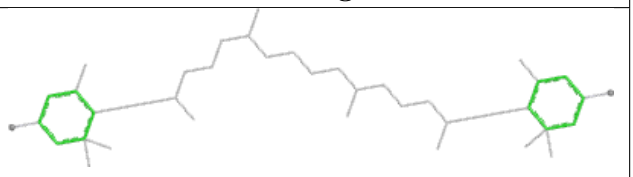
Rings

Ligand II0 i 314

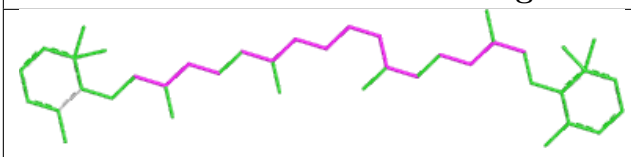

Bond lengths

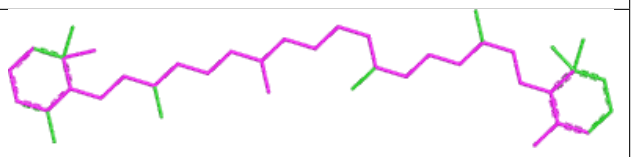

Bond angles

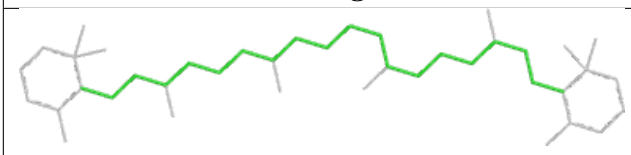

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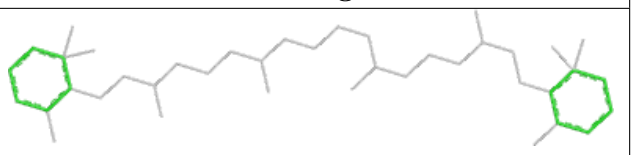

Rings

Ligand WVN B 844

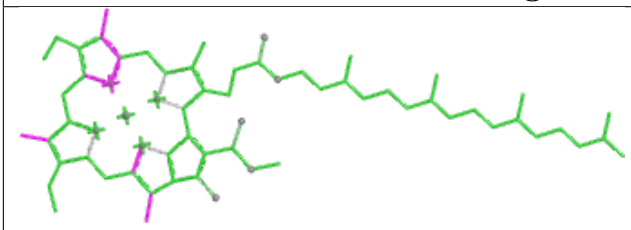

Bond lengths

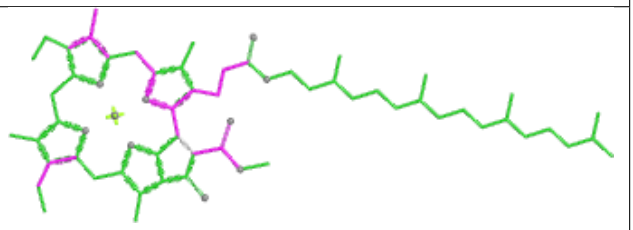

Bond angles

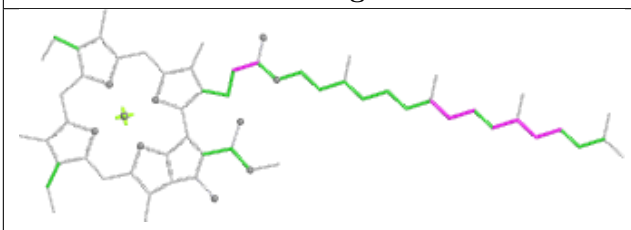

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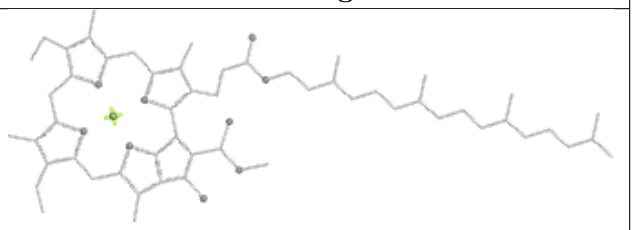

Rings

Ligand CLA A 824

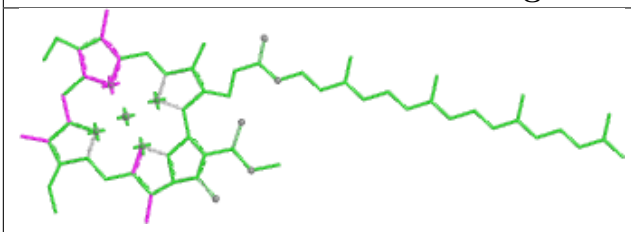

Bond lengths


Bond angles

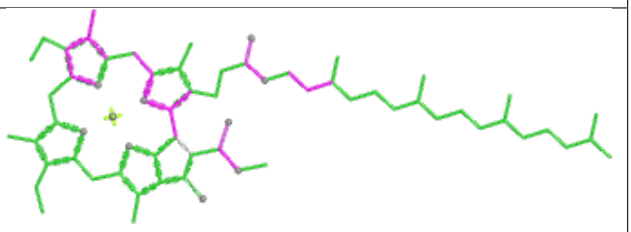

Torsions


Rings

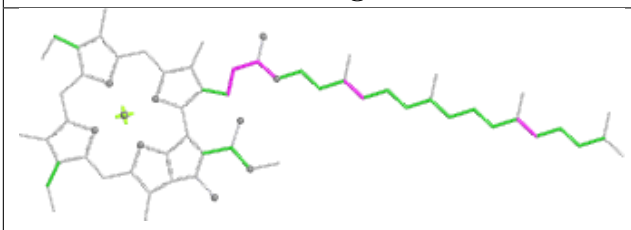
Ligand CLA A 828



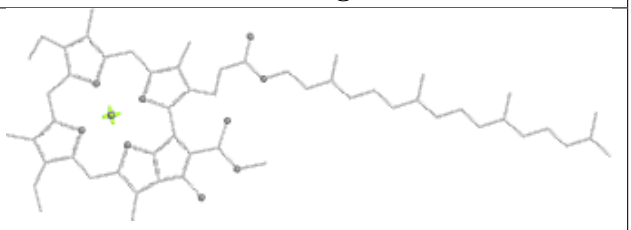
Bond lengths



Bond angles

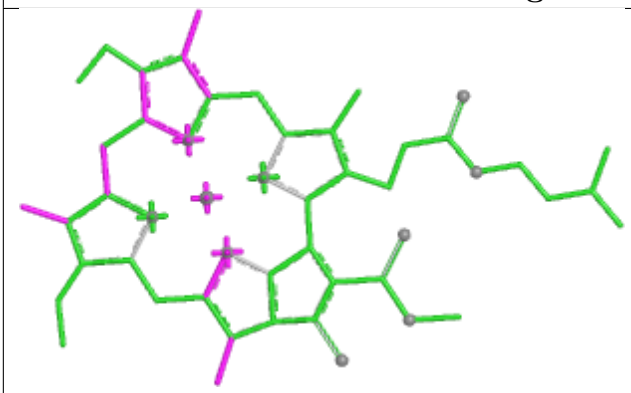


Torsions

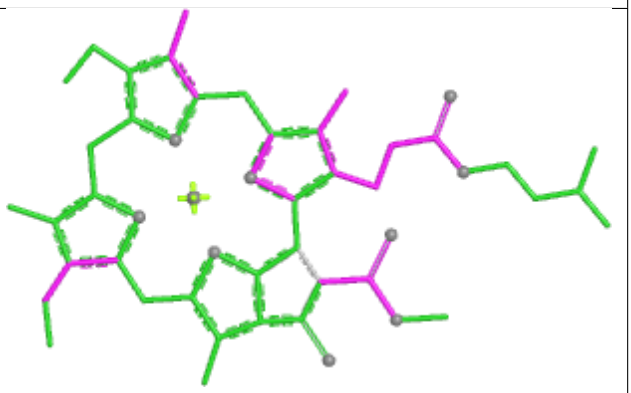


Rings

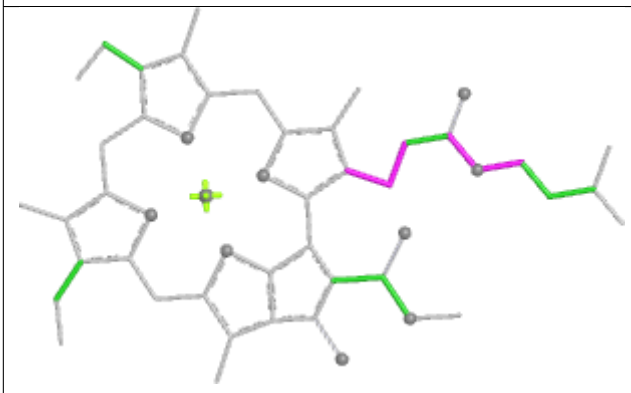
Ligand CLA L 204



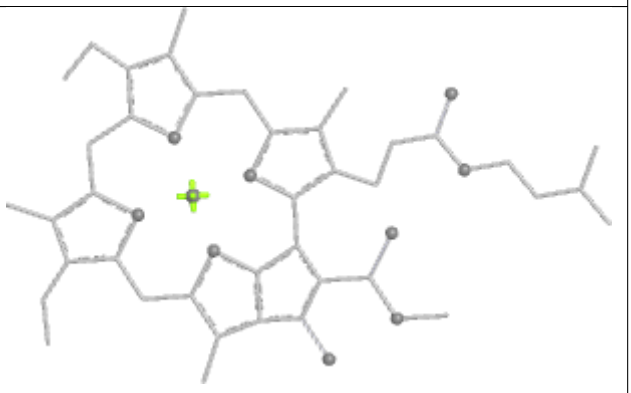
Bond lengths



Bond angles

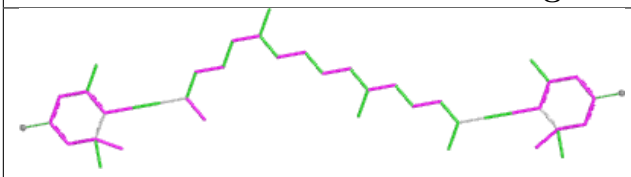


Torsions

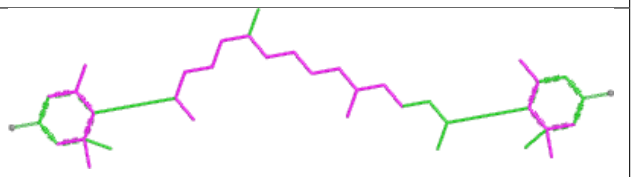


Rings

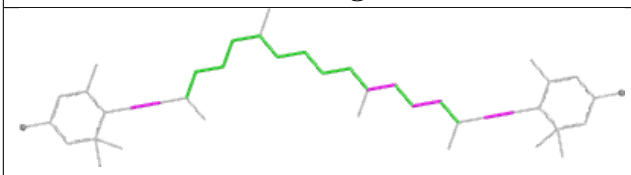
Ligand II0 c 617



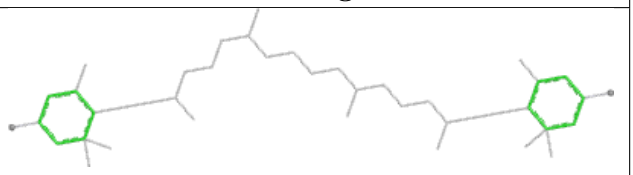
Bond lengths



Bond angles

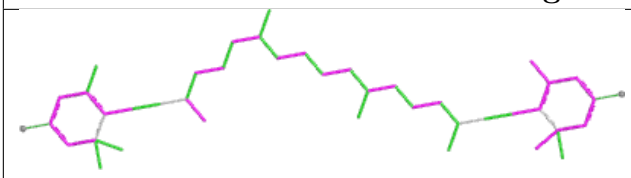


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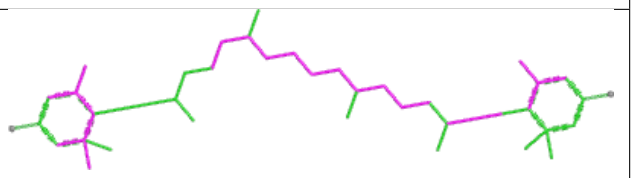


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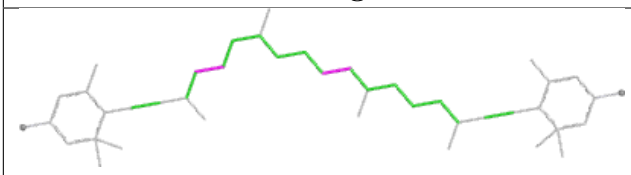
Ligand II0 a 316



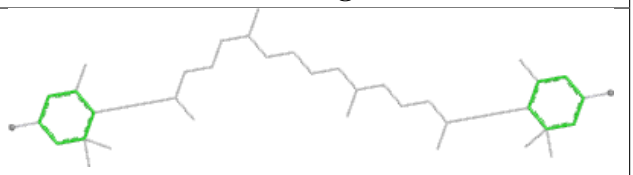
Bond lengths



Bond angles

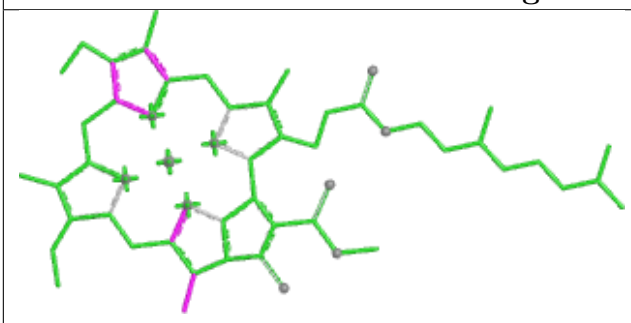


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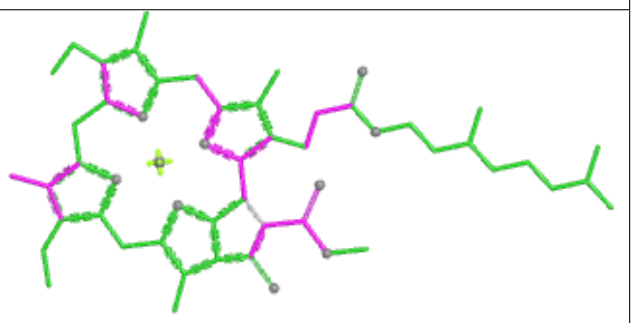


Rings

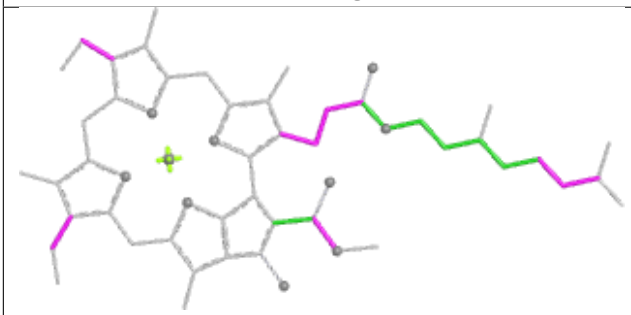
Ligand CLA m 609



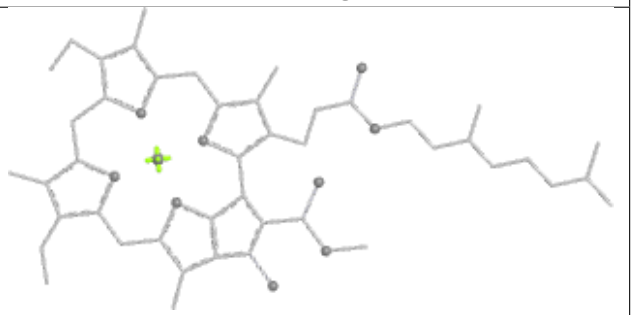
Bond lengths



Bond angles

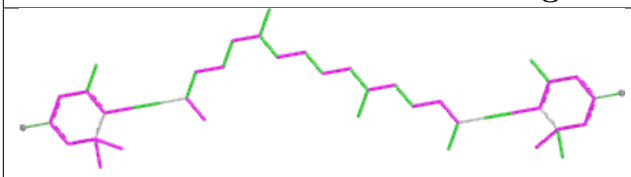


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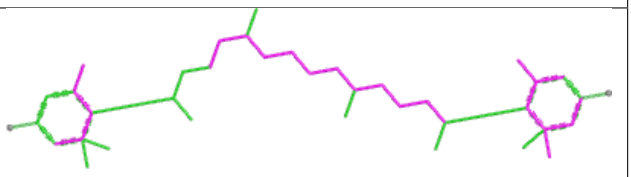


Rings

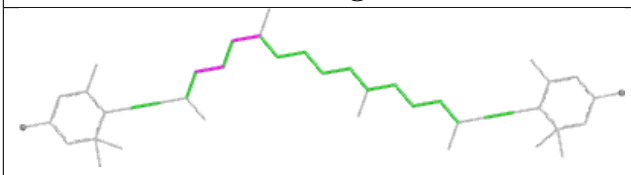
Ligand II0 n 615



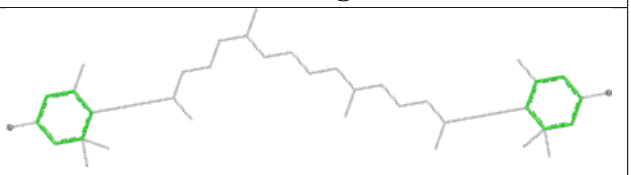
Bond lengths



Bond angles

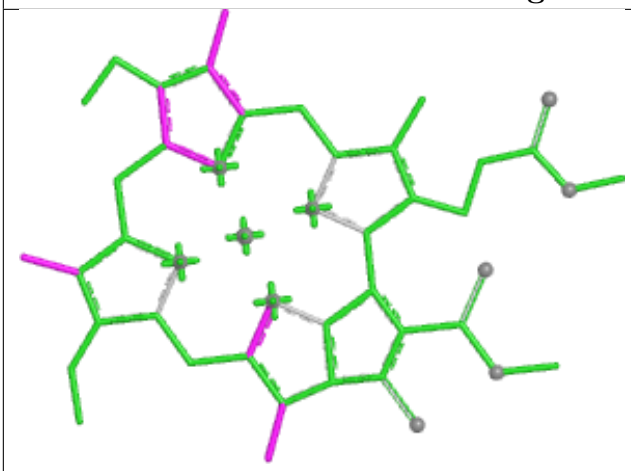


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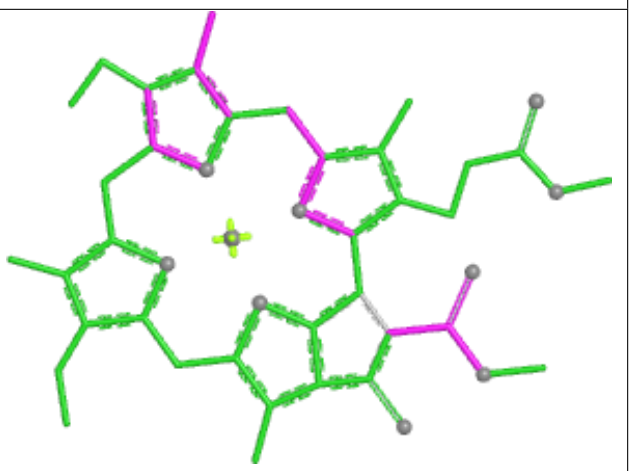


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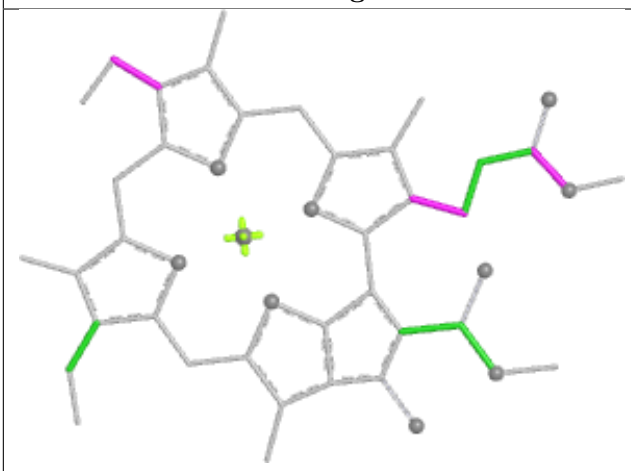
Ligand CLA d 306



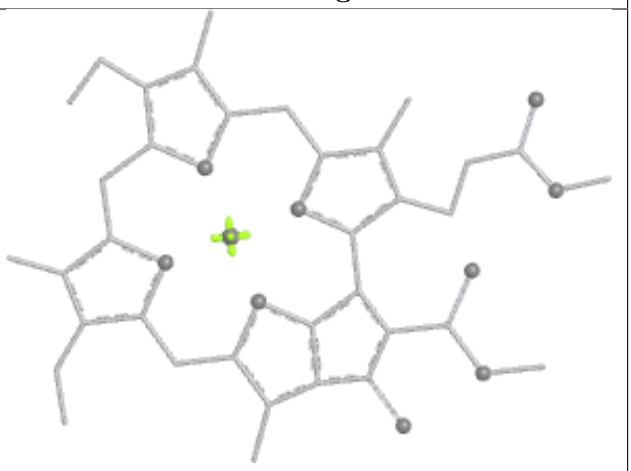
Bond lengths



Bond angles

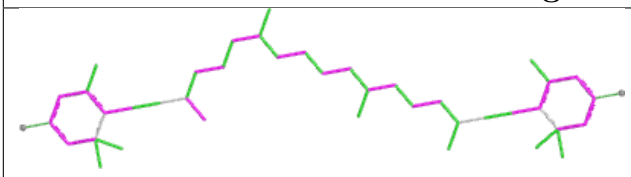


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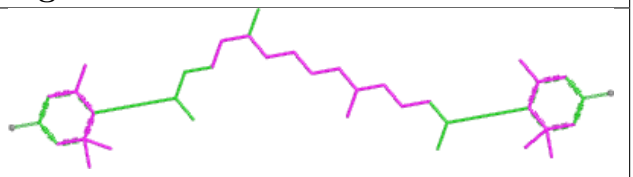


Rings

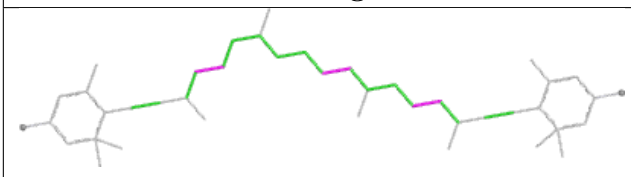
Ligand II0 g 318



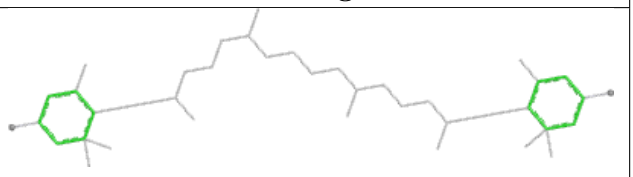
Bond lengths



Bond angles

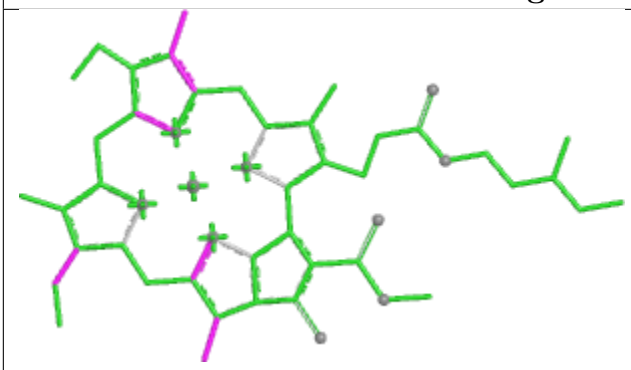


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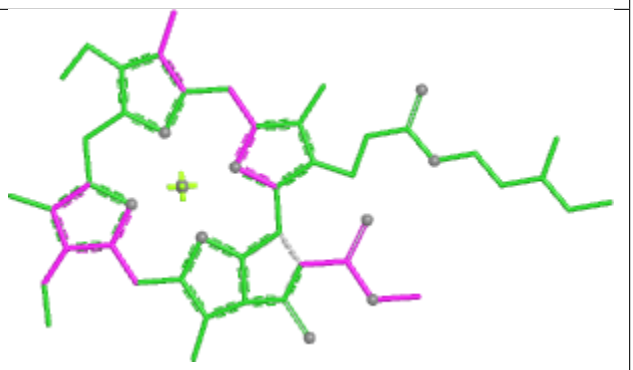


Rings

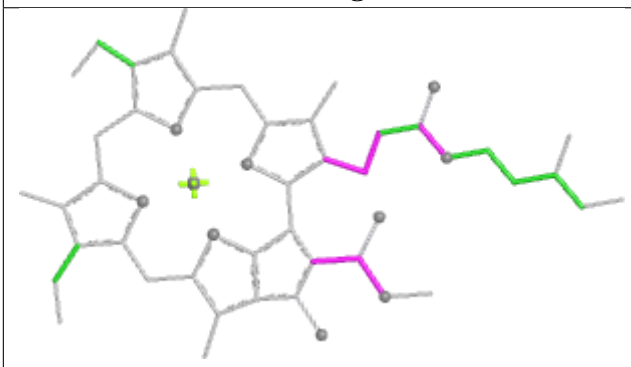
Ligand CLA d 305



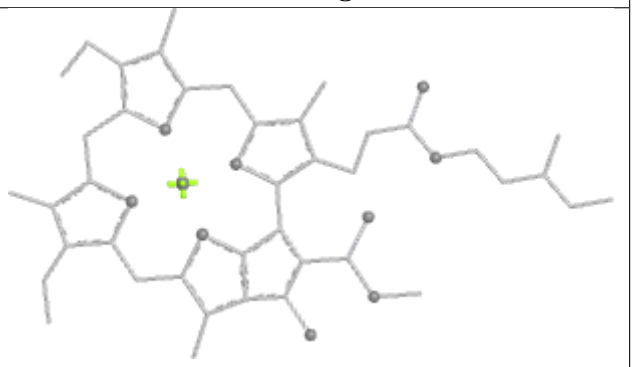
Bond lengths



Bond angles

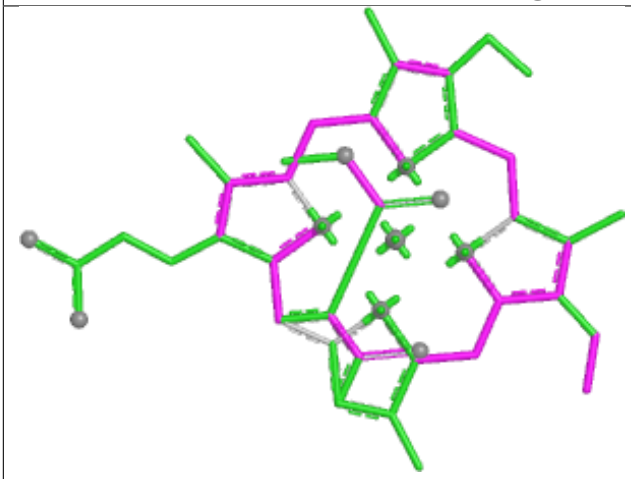


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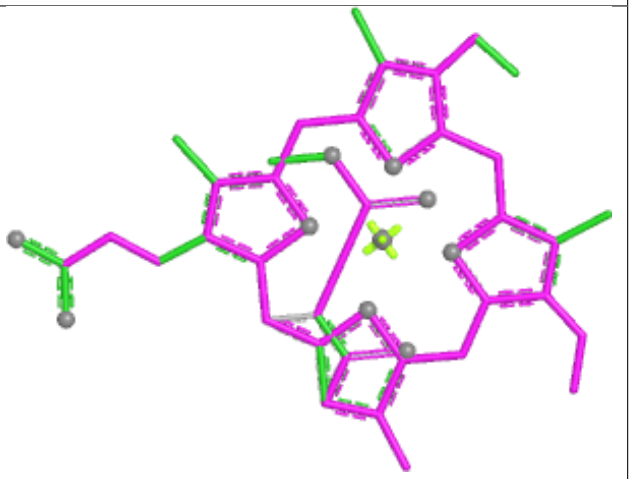


Rings

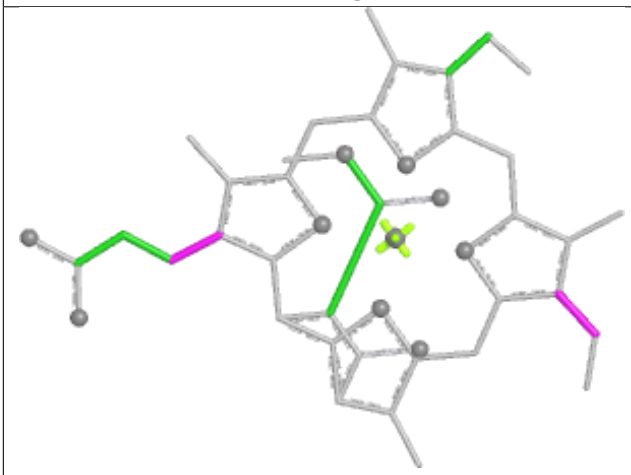
Ligand KC2 n 611



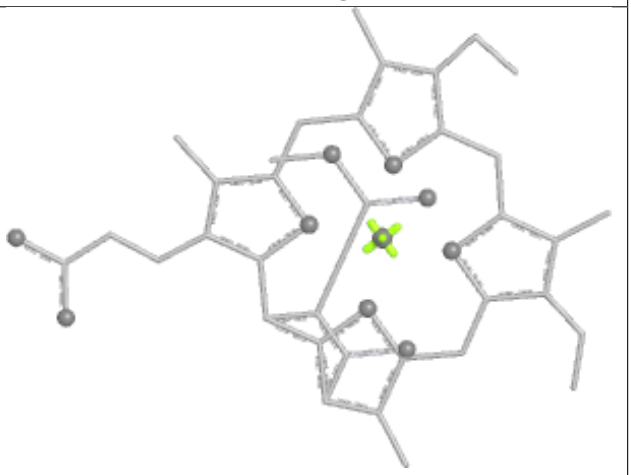
Bond lengths



Bond angles

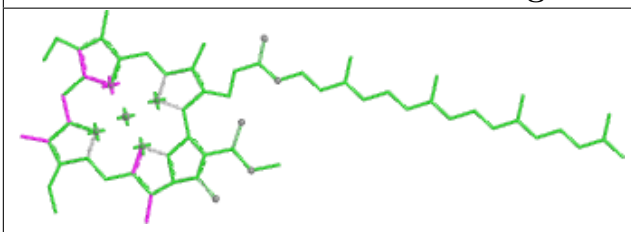


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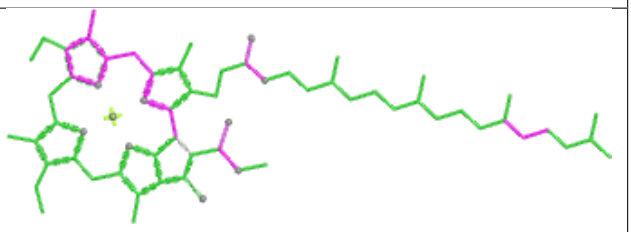


Rings

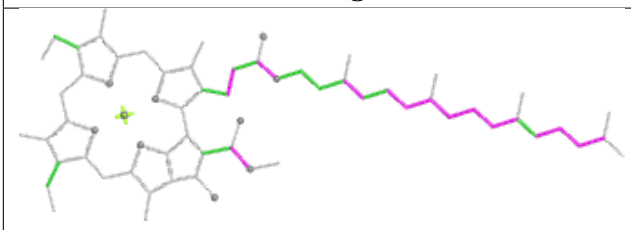
Ligand CLA h 306



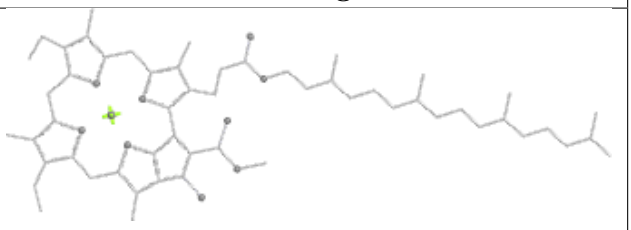
Bond lengths



Bond angles

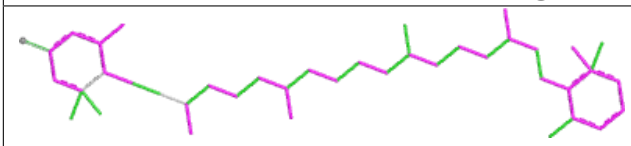


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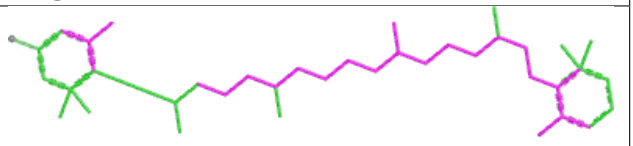


Rings

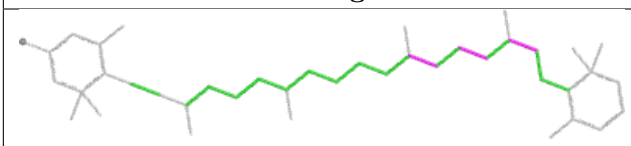
Ligand IHT g 319



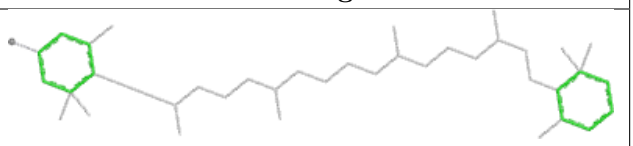
Bond lengths



Bond angles

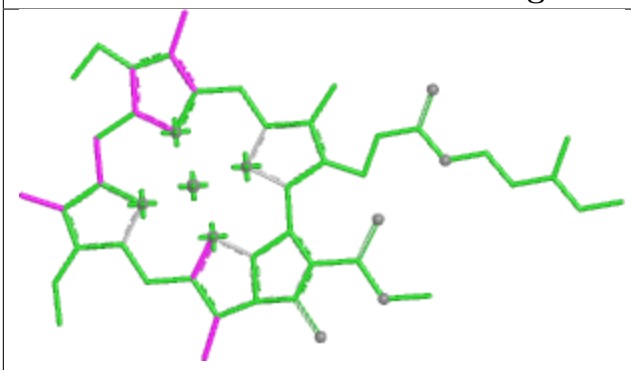


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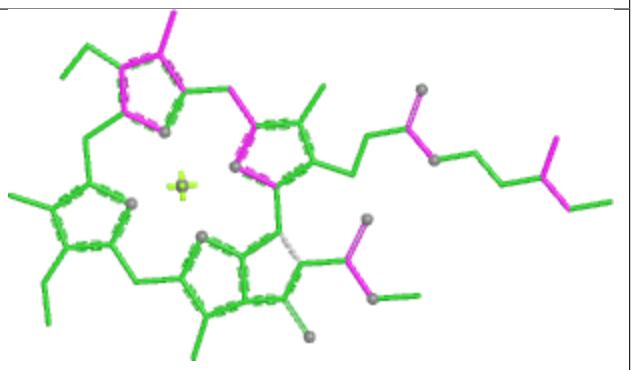


Rings

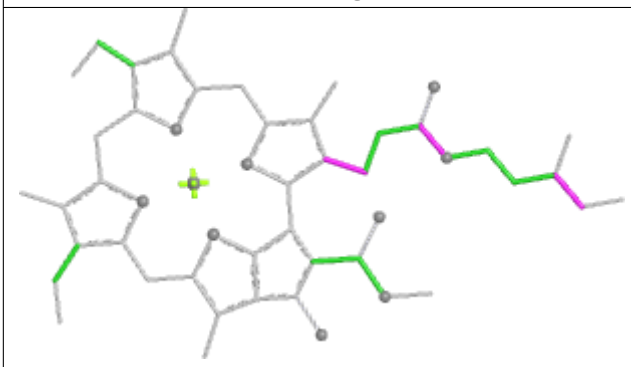
Ligand CLA h 305



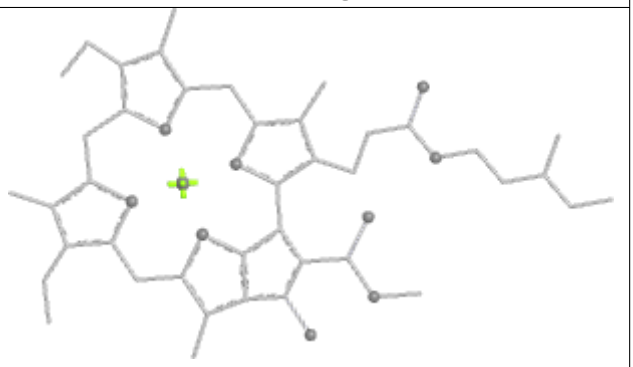
Bond lengths



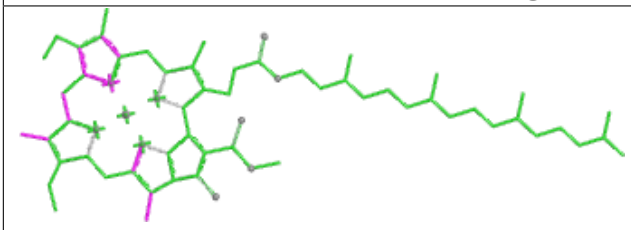
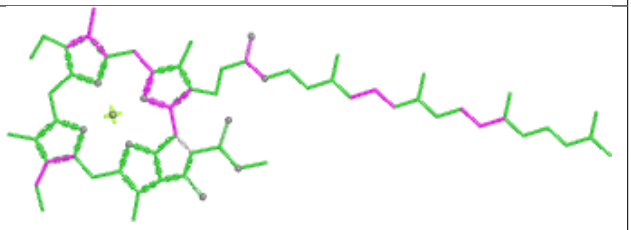
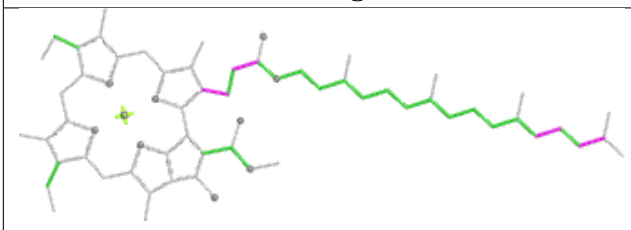
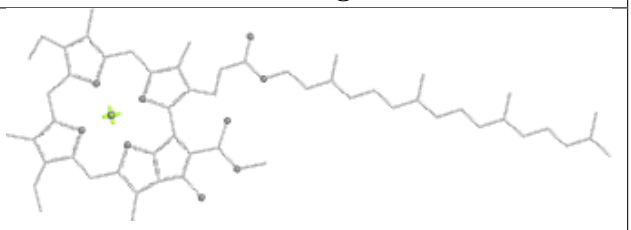
Bond angles

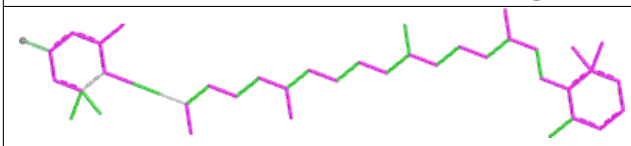
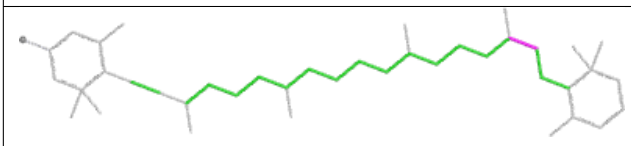
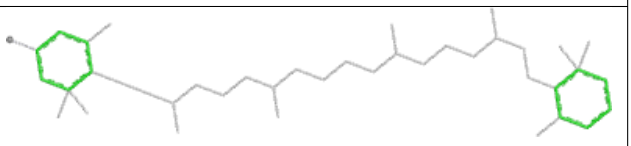


Torsions

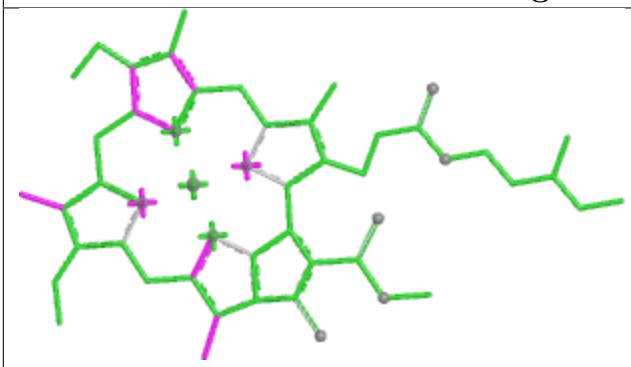


Rings

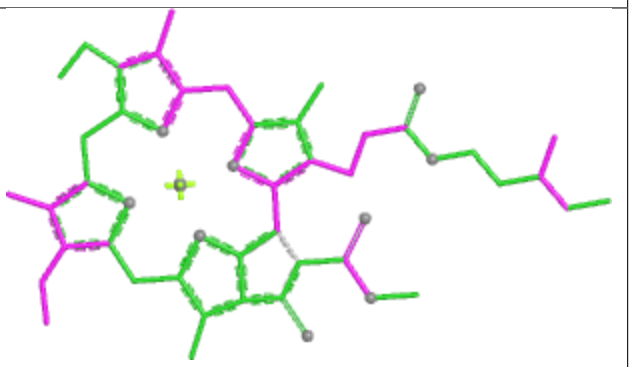
Ligand CLA B 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHT R 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

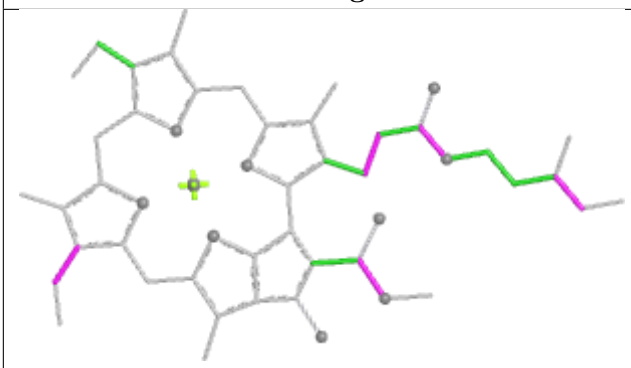
Ligand CLA f 612



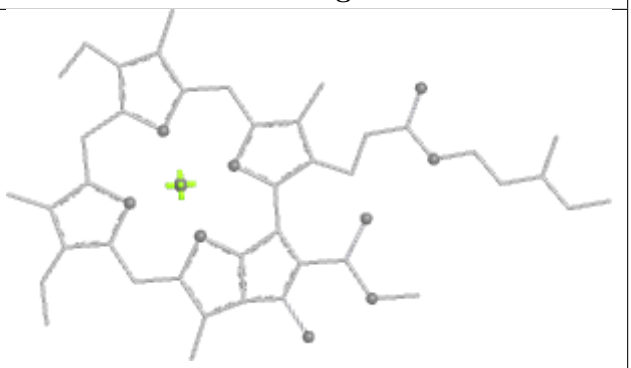
Bond lengths



Bond angles

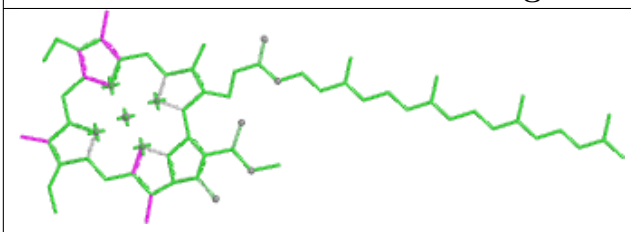


Torsions

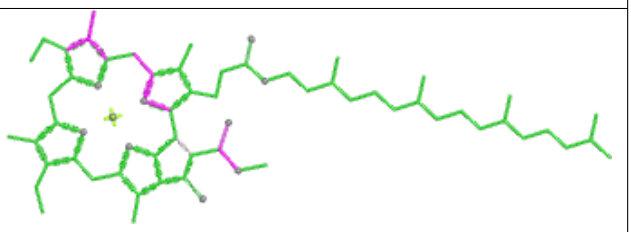


Rings

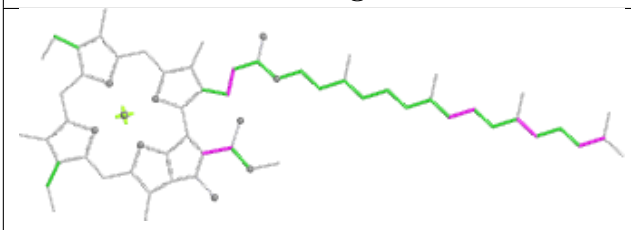
Ligand CLA A 807



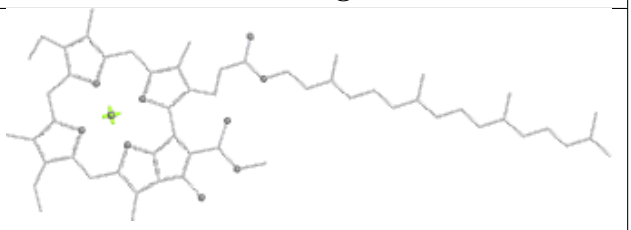
Bond lengths



Bond angles

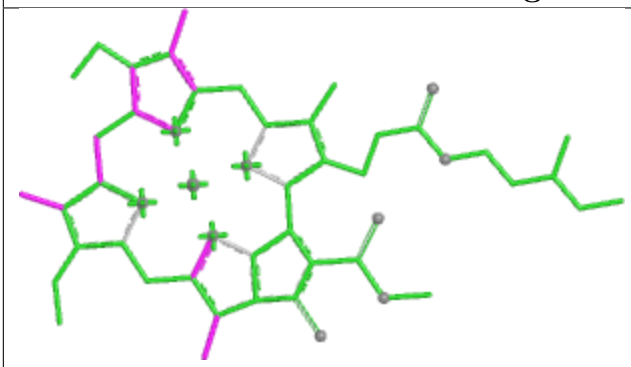


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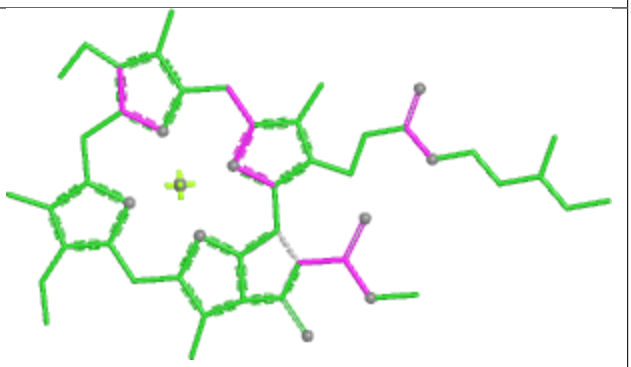


Rings

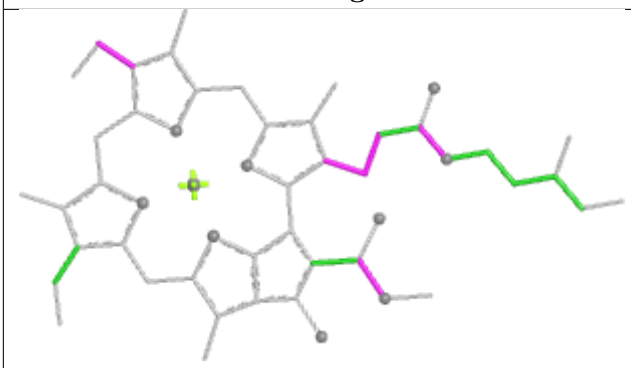
Ligand CLA A 822



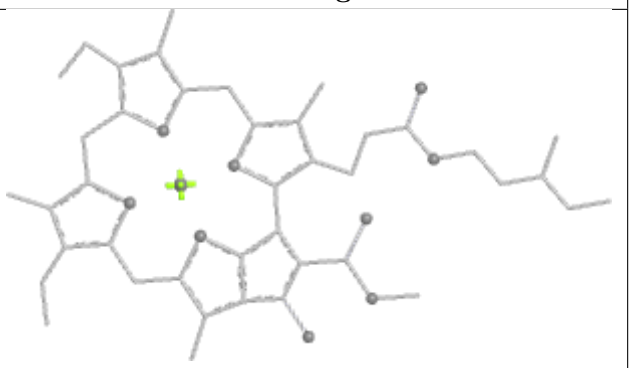
Bond lengths



Bond angles

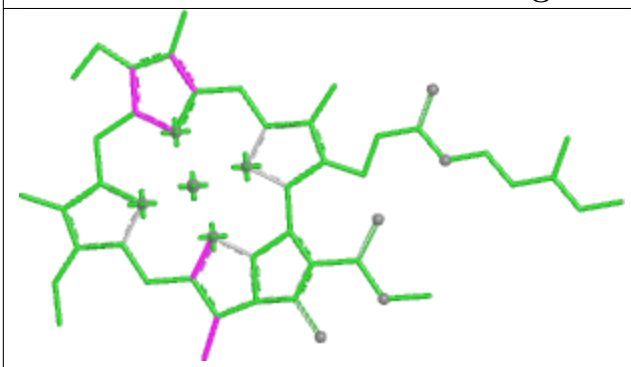


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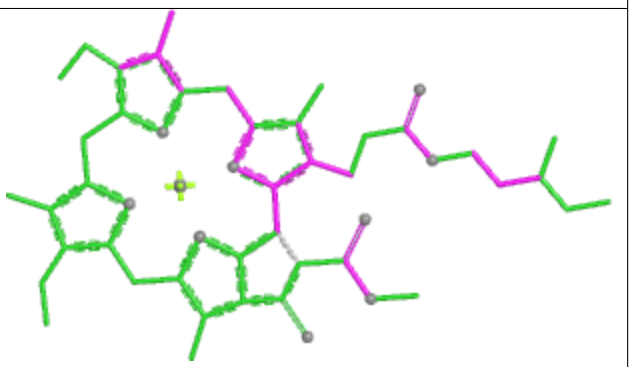


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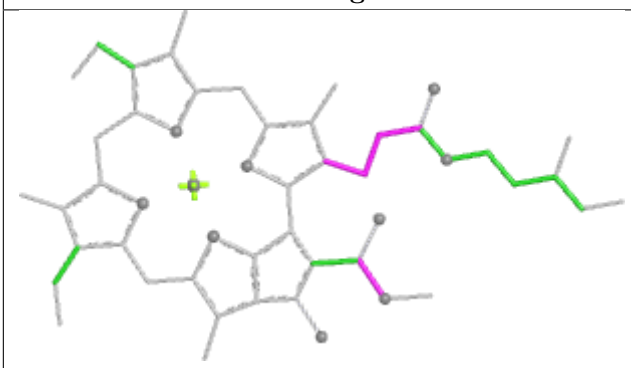
Ligand CLA i 312



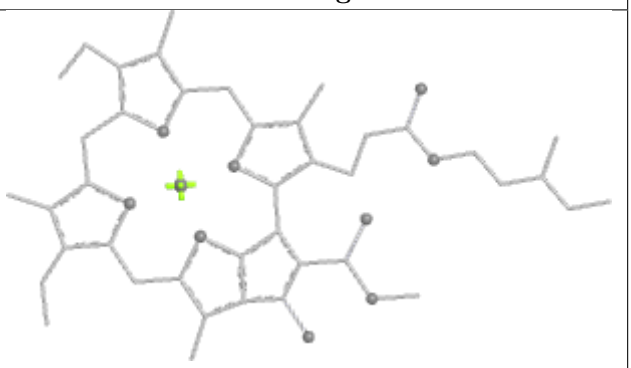
Bond lengths



Bond angles

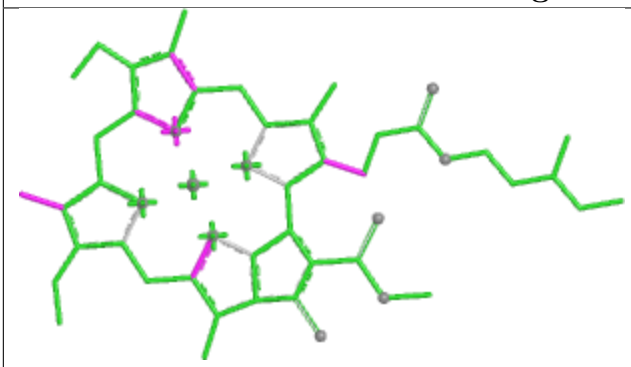


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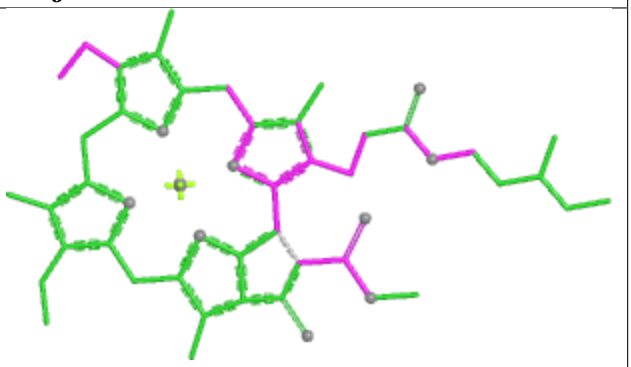


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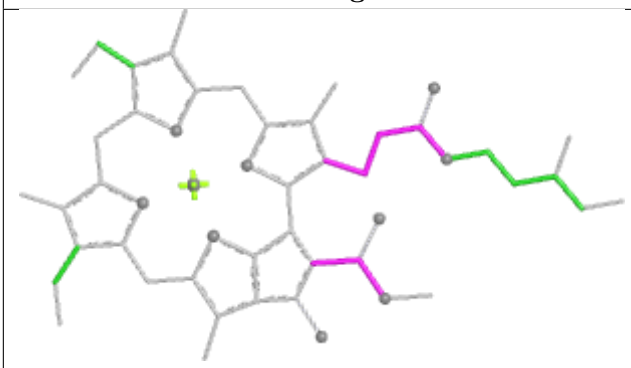
Ligand CLA j 606



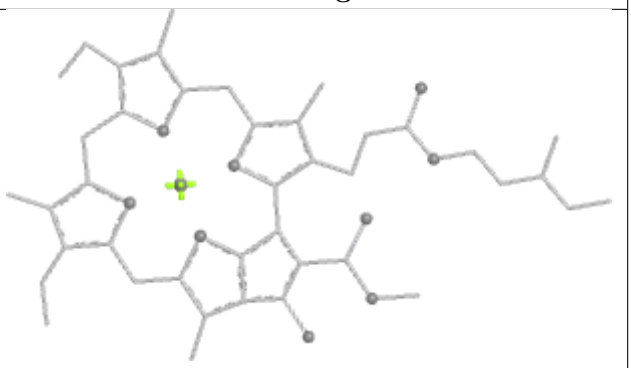
Bond lengths



Bond angles

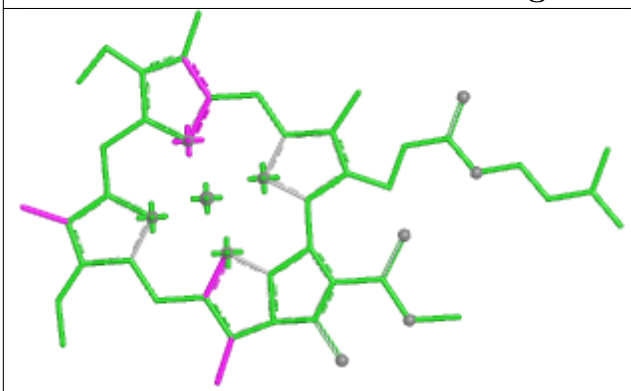


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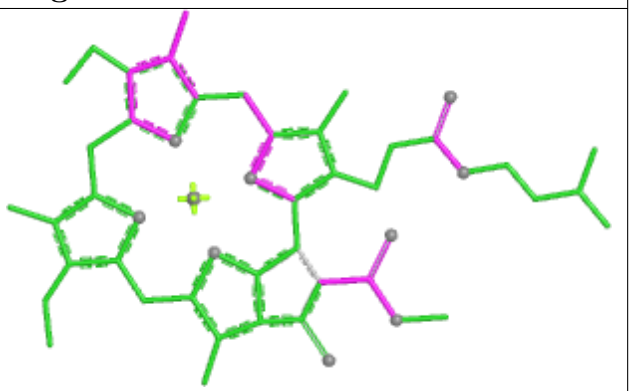


Rings

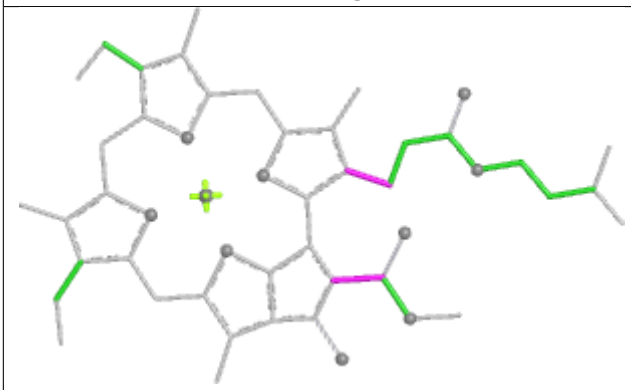
Ligand CLA g 303



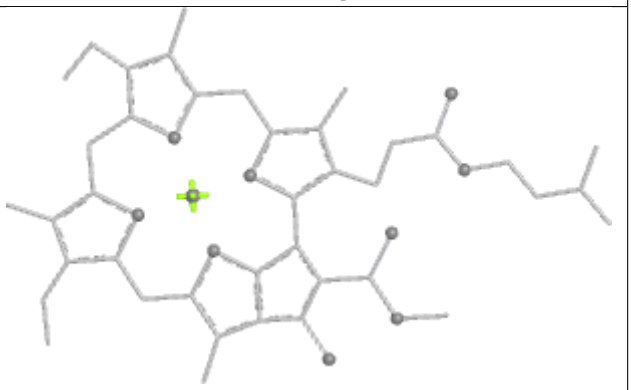
Bond lengths



Bond angles

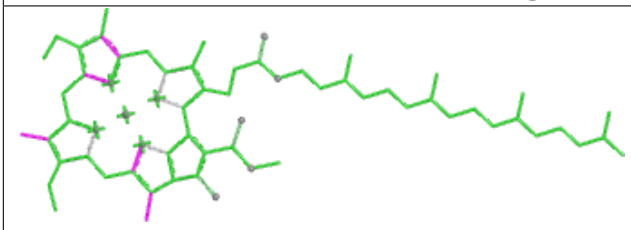


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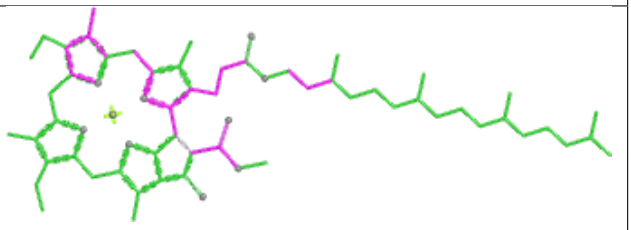


Rings

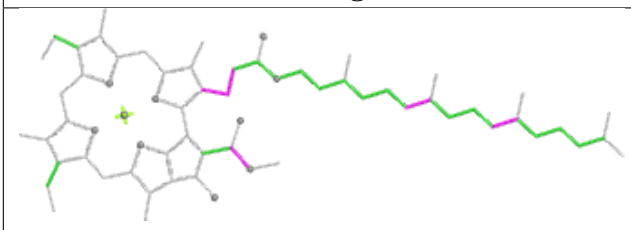
Ligand CLA A 808



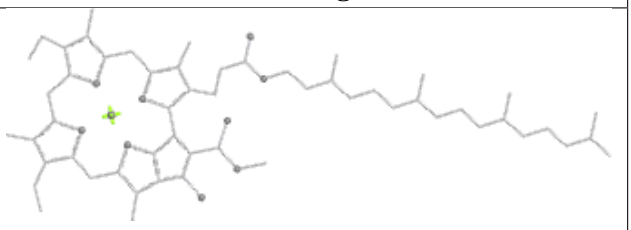
Bond lengths



Bond angles

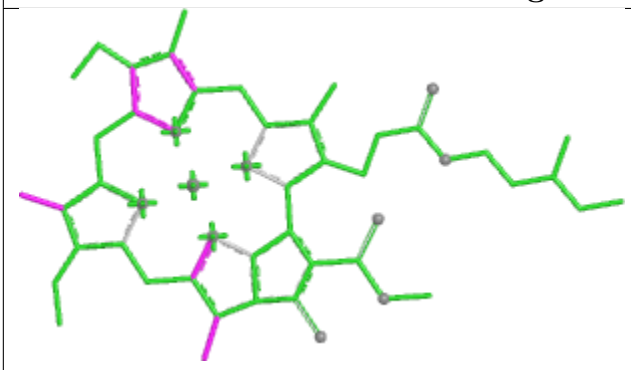


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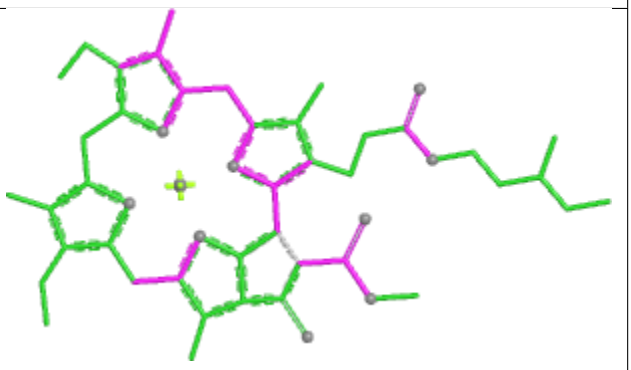


Rings

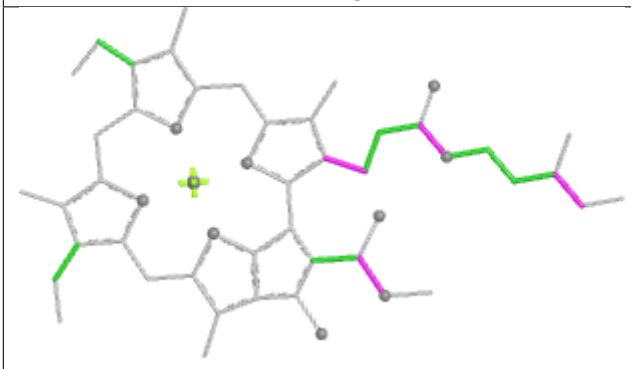
Ligand CLA d 311



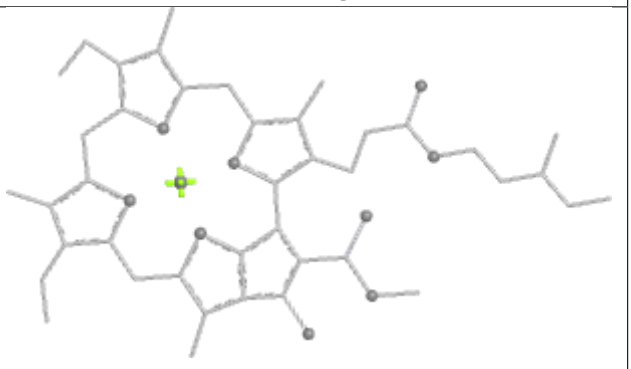
Bond lengths



Bond angles

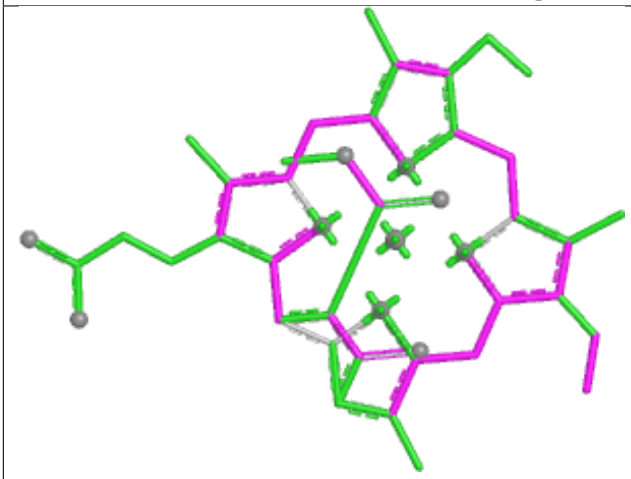


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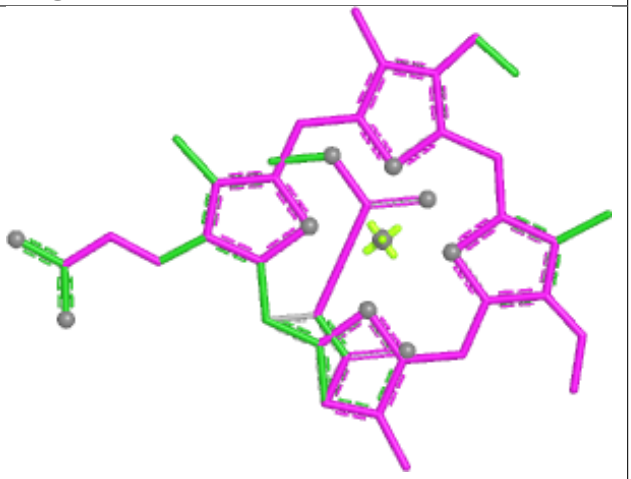


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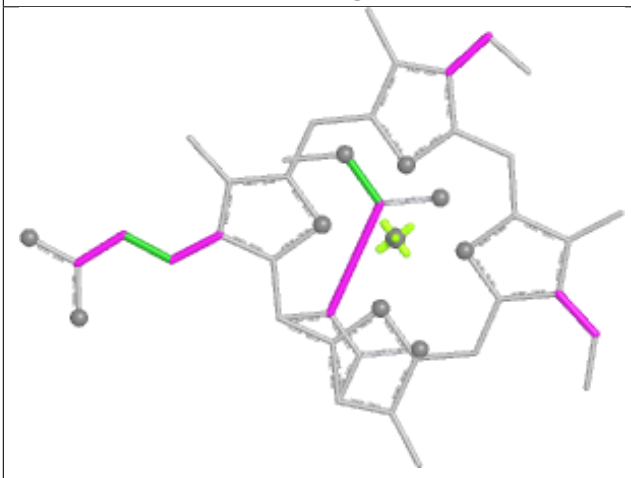
Ligand KC2 g 312



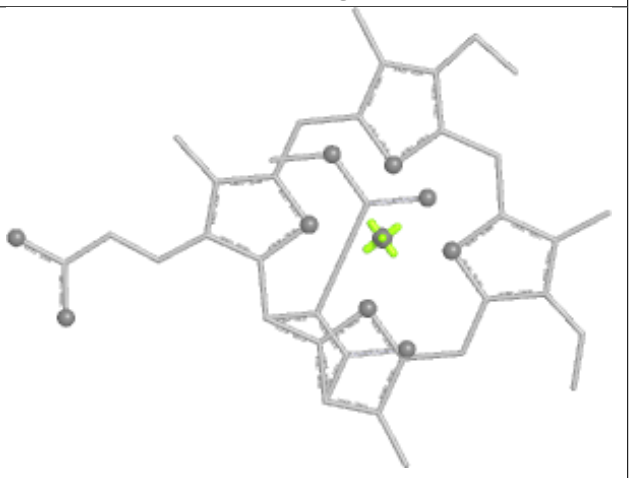
Bond lengths



Bond angles

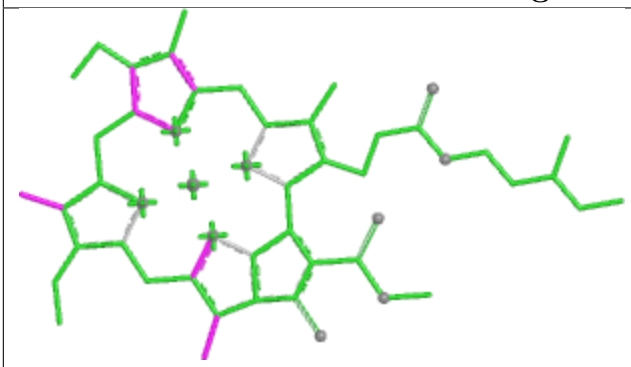


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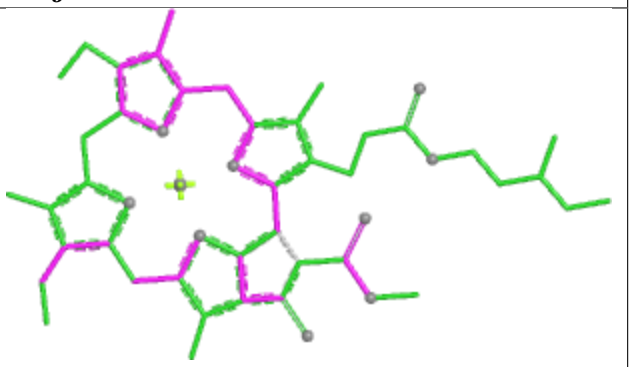


Rings

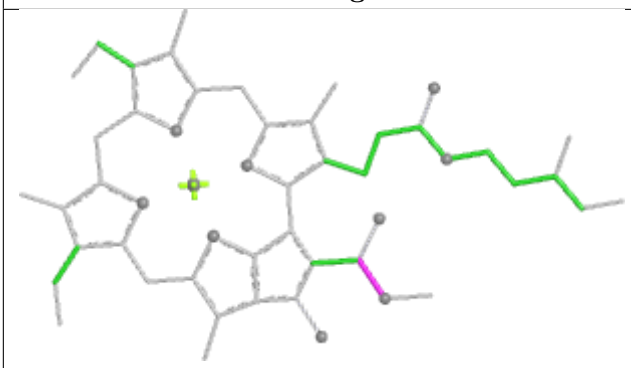
Ligand CLA j 608



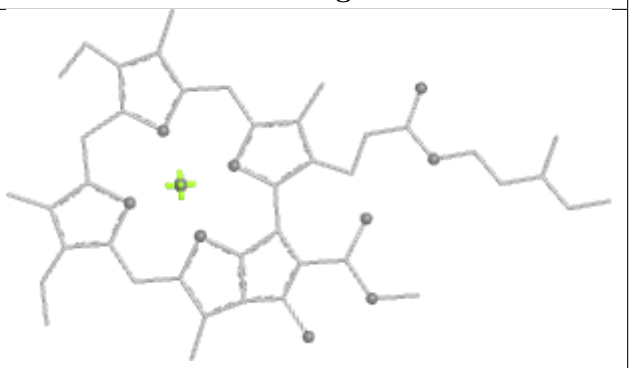
Bond lengths



Bond angles

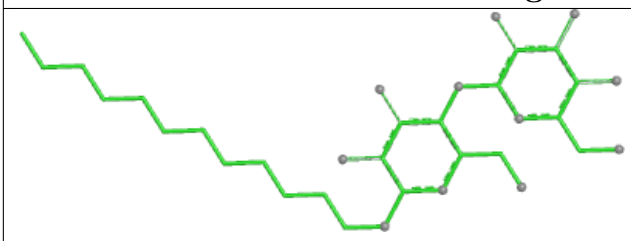


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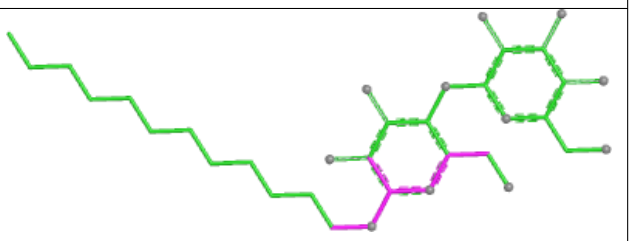


Rings

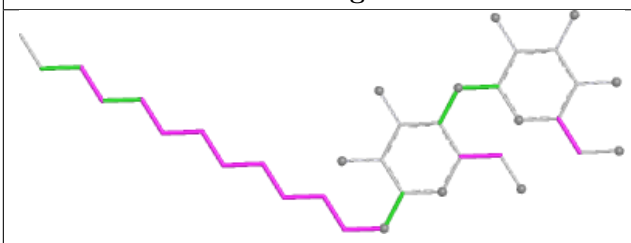
Ligand LMT a 320



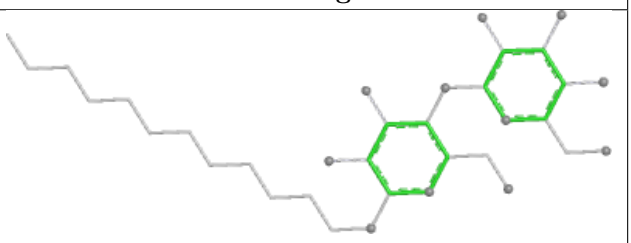
Bond lengths



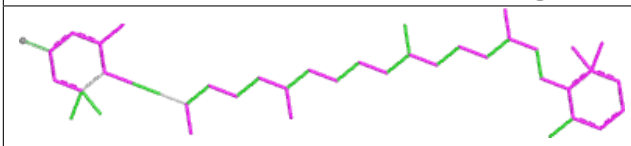
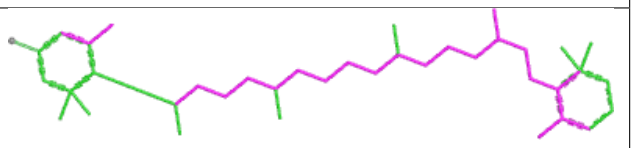
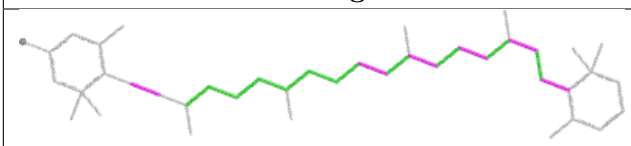
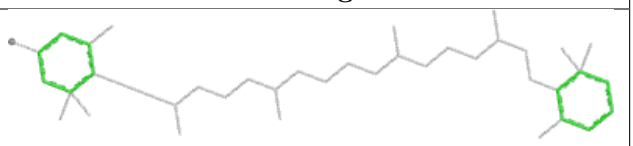
Bond angles

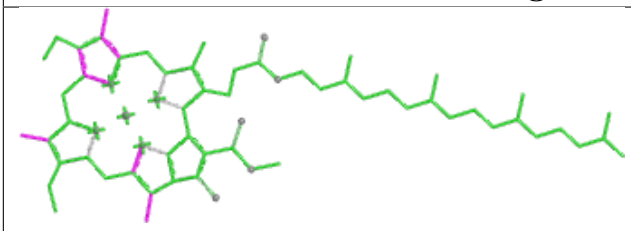
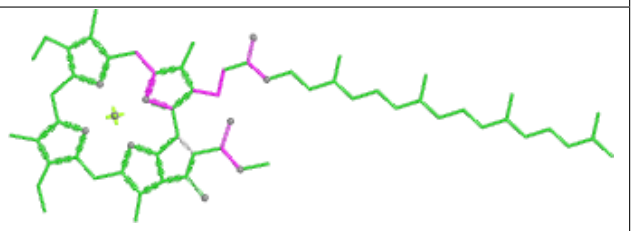
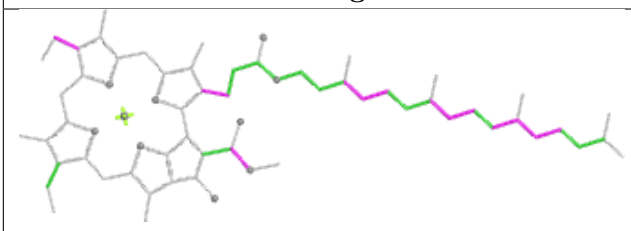
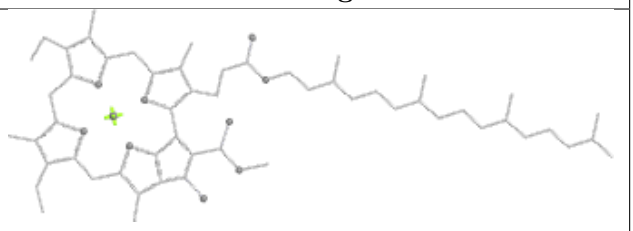


Torsions

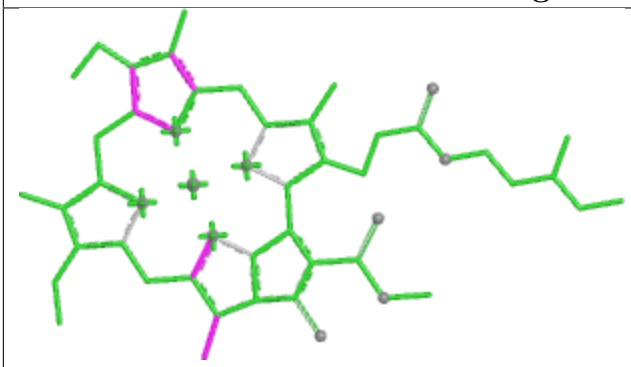


Rings

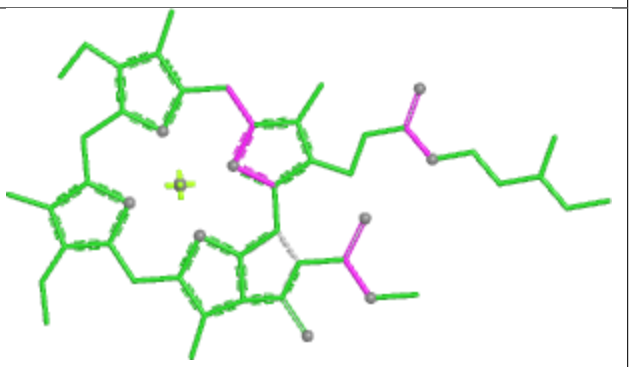
Ligand IHT n 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

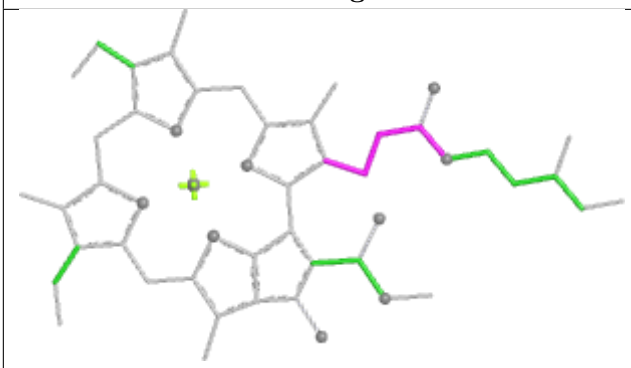
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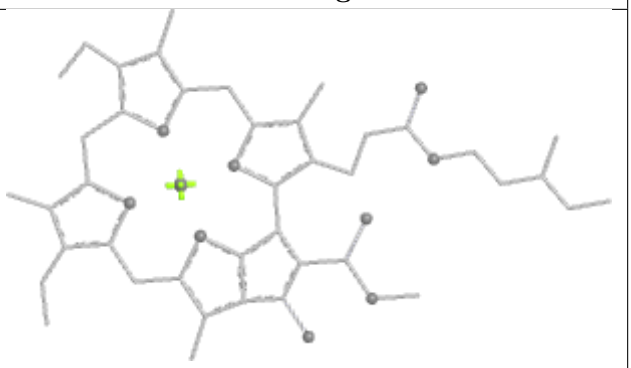
Bond lengths



Bond angles

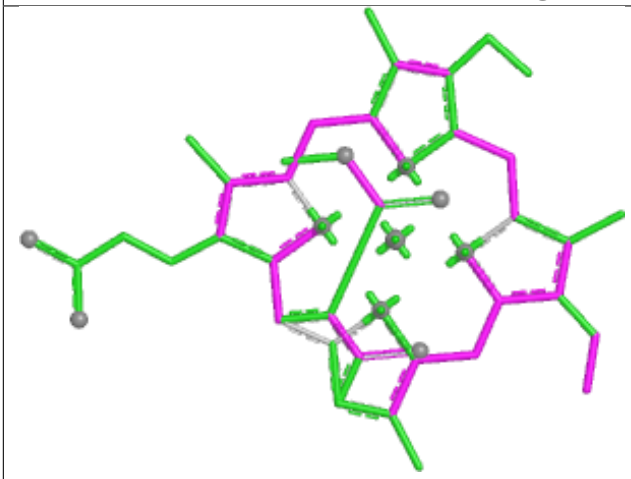


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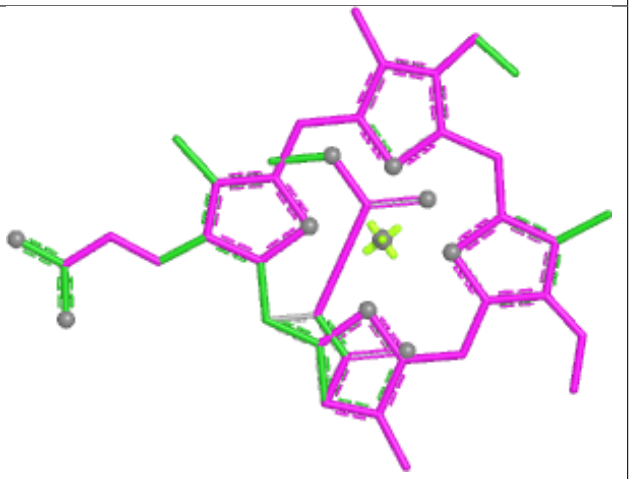


Rings

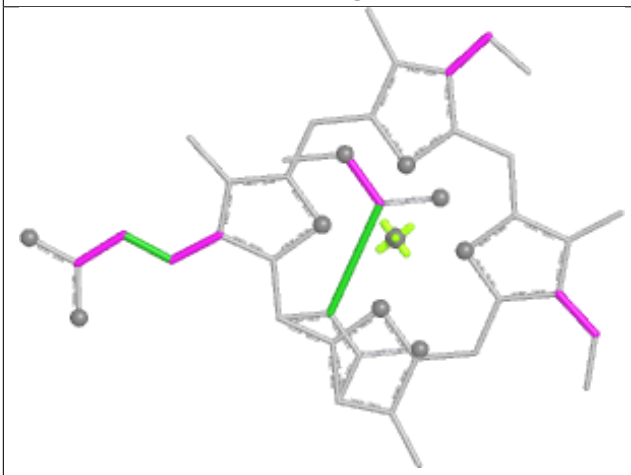
Ligand KC2 i 310



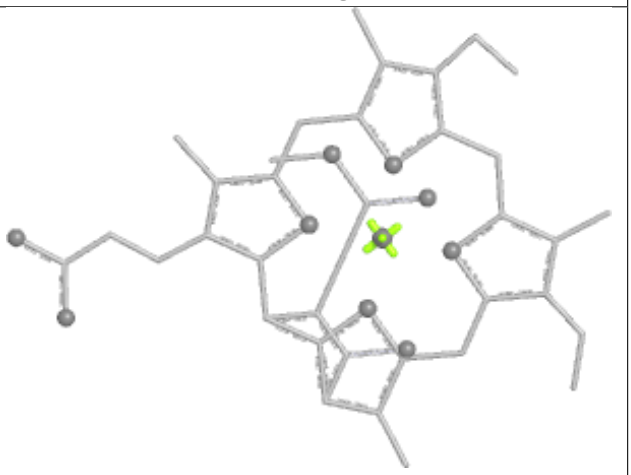
Bond lengths



Bond angles

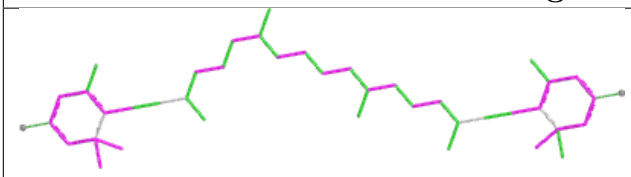


Torsions

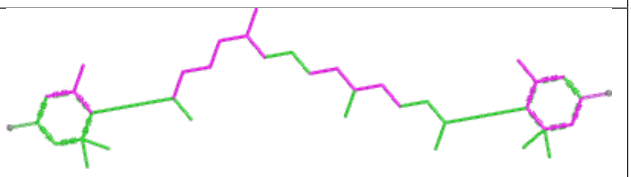


Rings

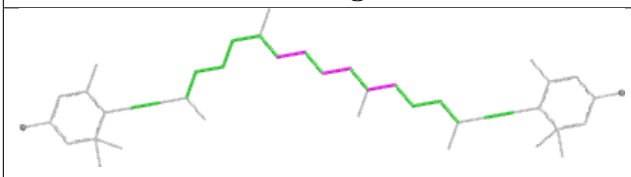
Ligand II0 l 317



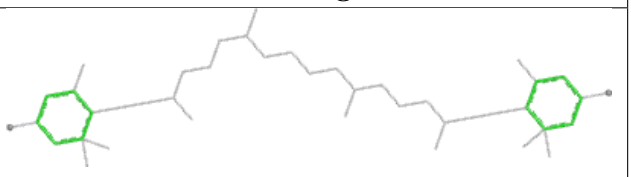
Bond lengths



Bond angles

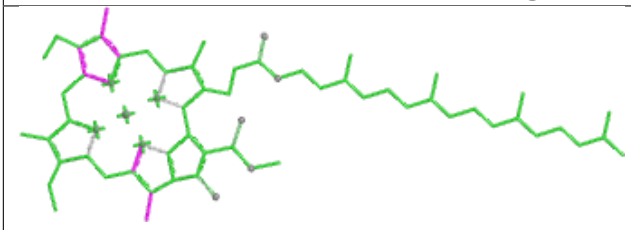


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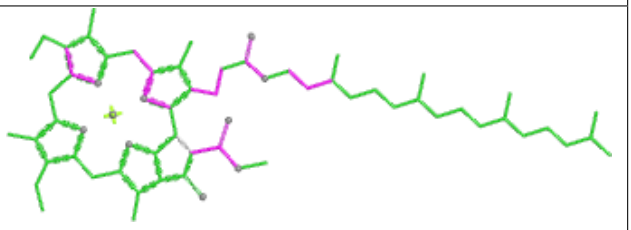


Rings

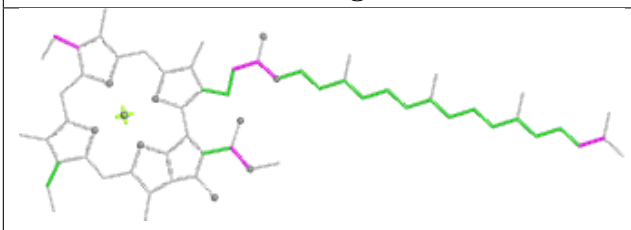
Ligand CLA A 801



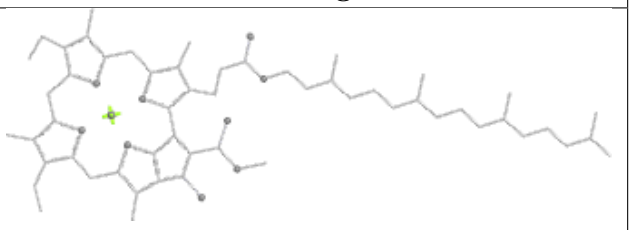
Bond lengths



Bond angles

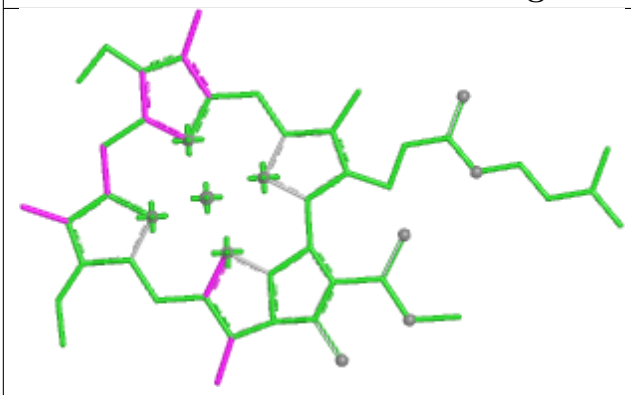


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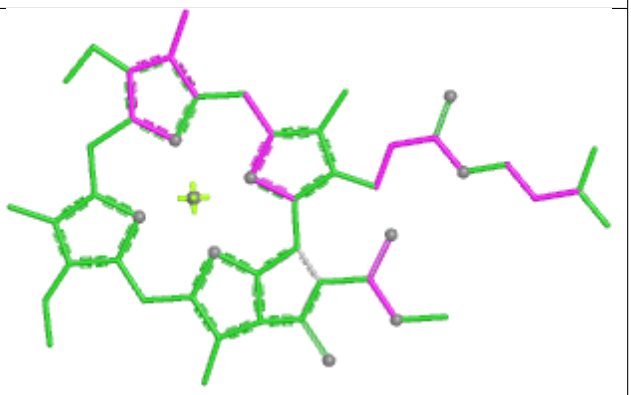


Rings

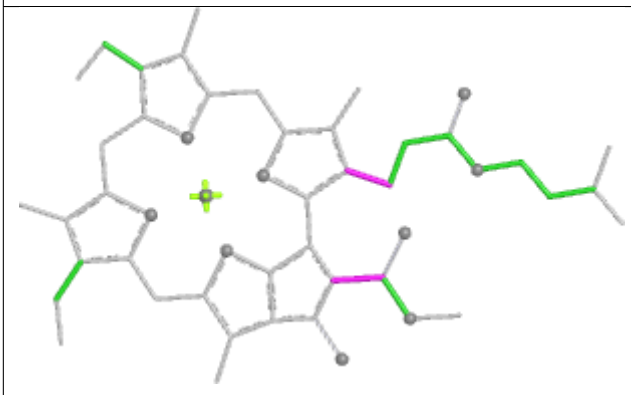
Ligand CLA d 301



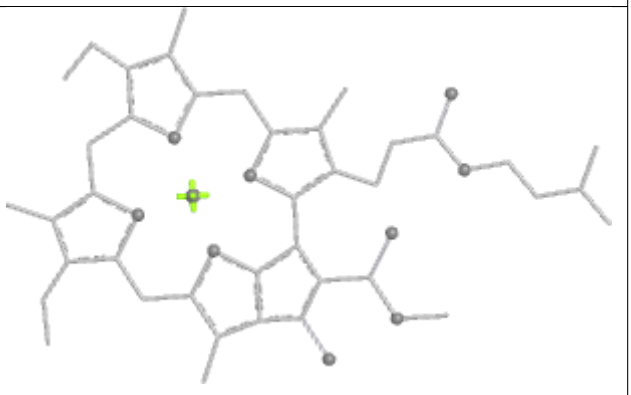
Bond lengths



Bond angles

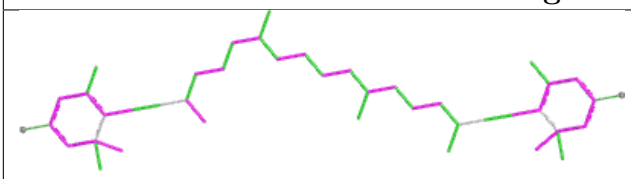


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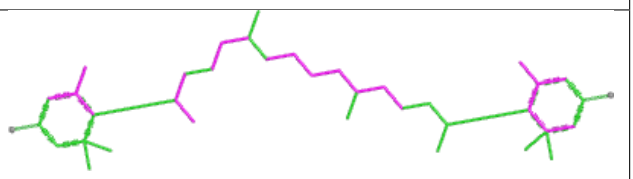


Rings

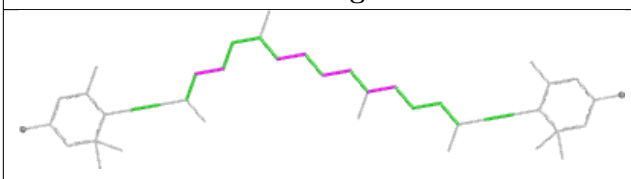
Ligand II0 e 616



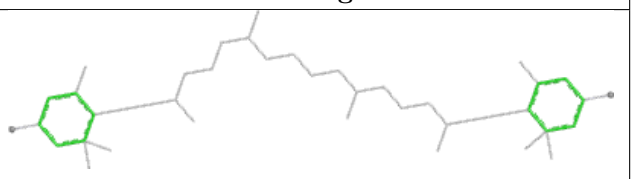
Bond lengths



Bond angles

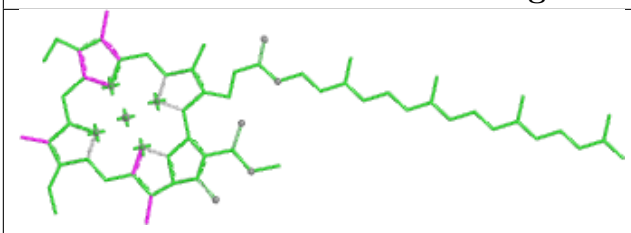


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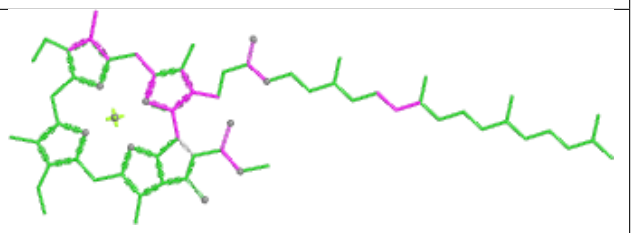


Rings

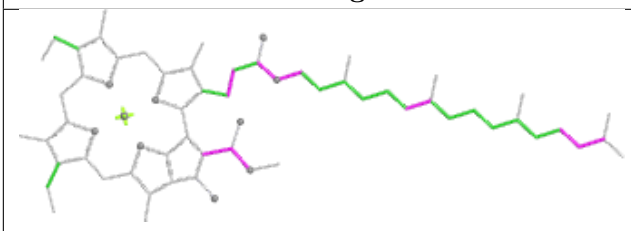
Ligand CLA a 311



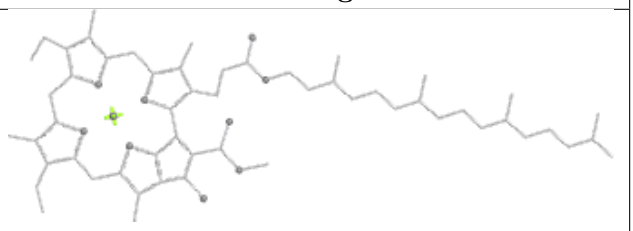
Bond lengths



Bond angles

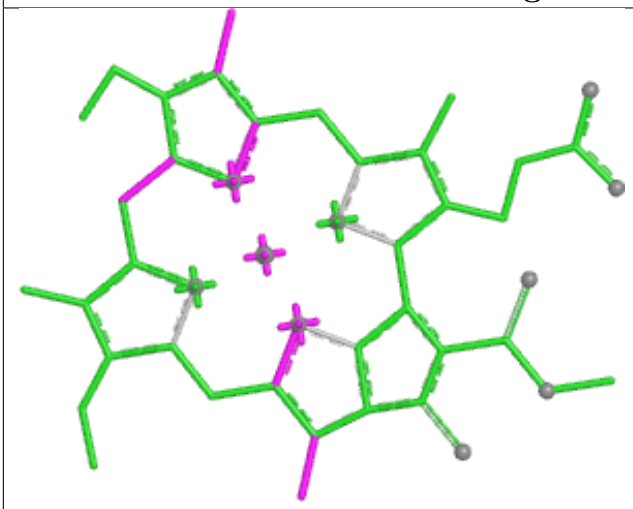


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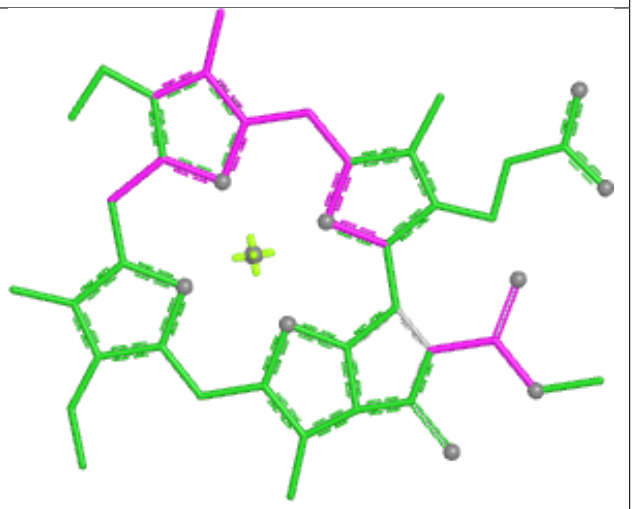


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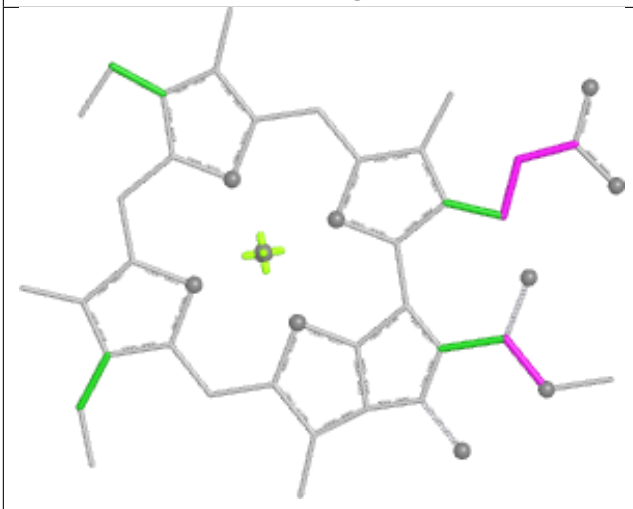
Ligand CLA A 815



Bond lengths



Bond angles

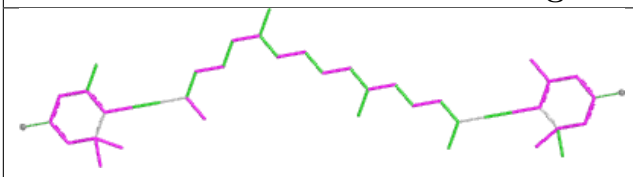


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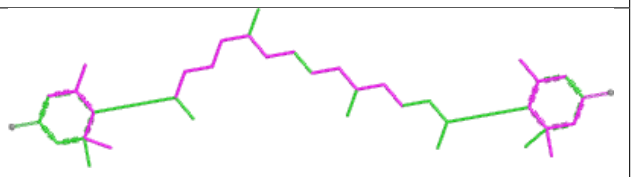


Rings

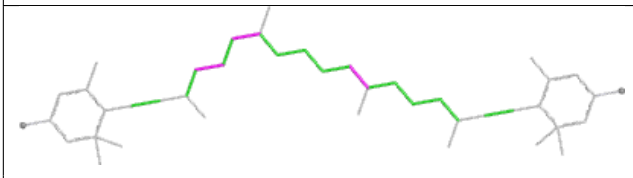
Ligand II0 l 314



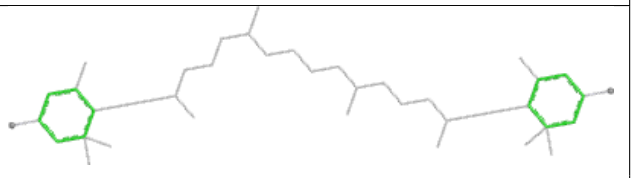
Bond lengths



Bond angles

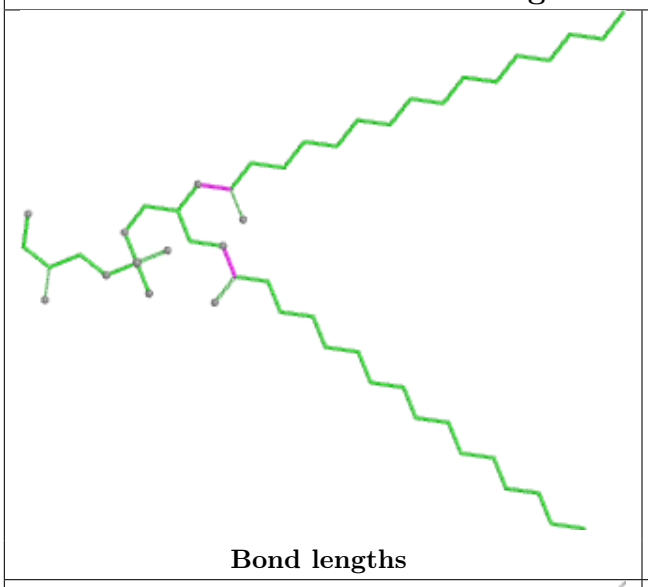


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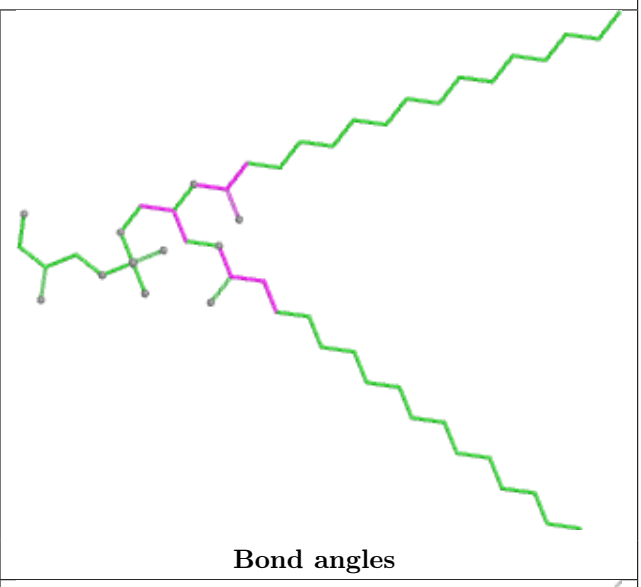


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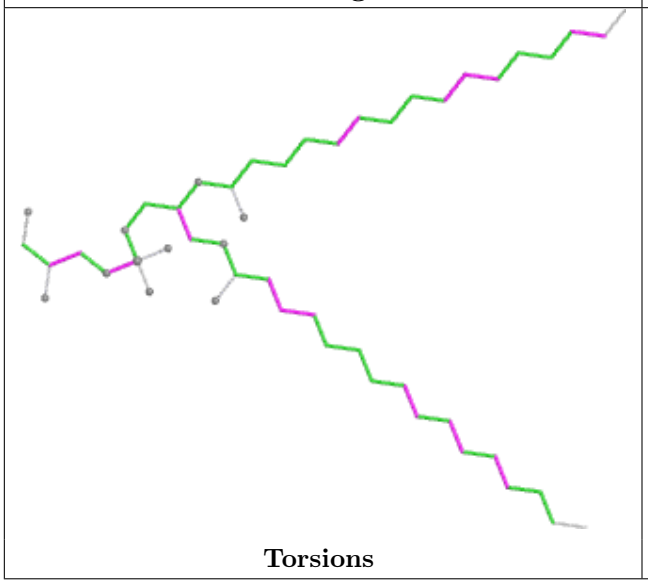
Ligand LHG a 319



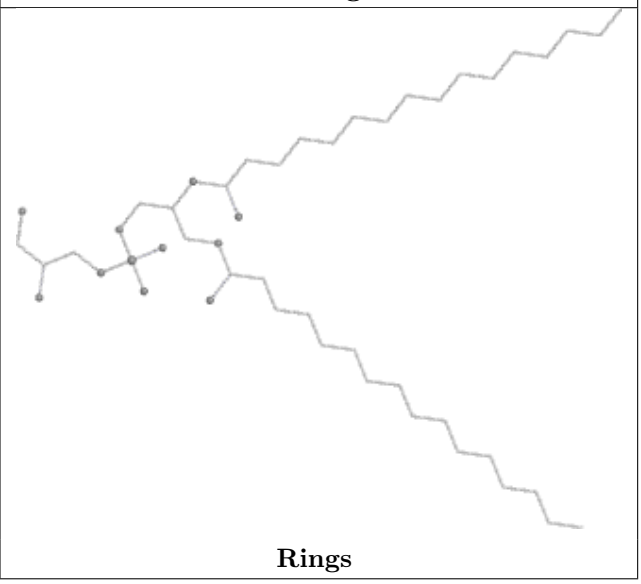
Bond lengths



Bond angles

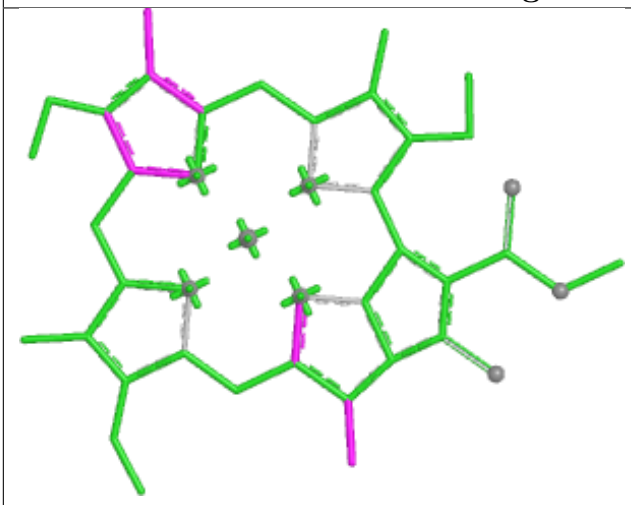


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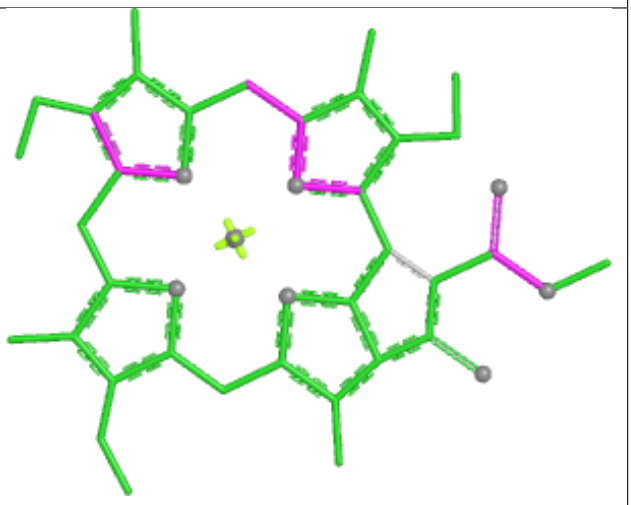


Rings

Ligand CLA m 601



Bond lengths



Bond angles

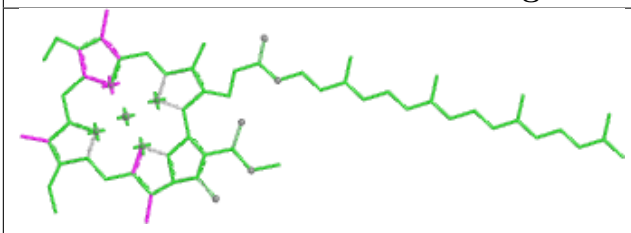


Torsions

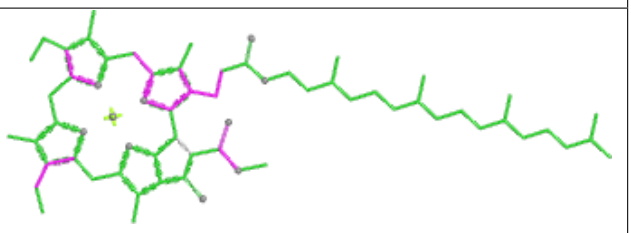


Rings

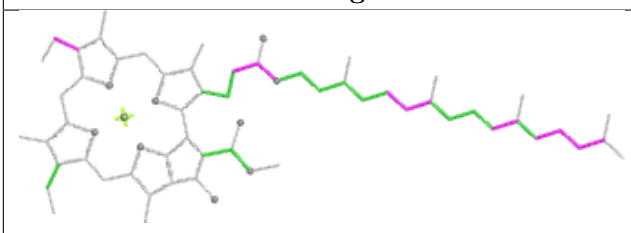
Ligand CLA m 606



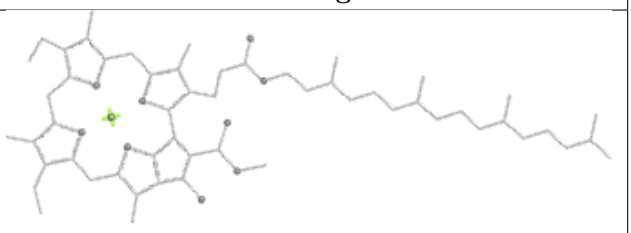
Bond lengths



Bond angles

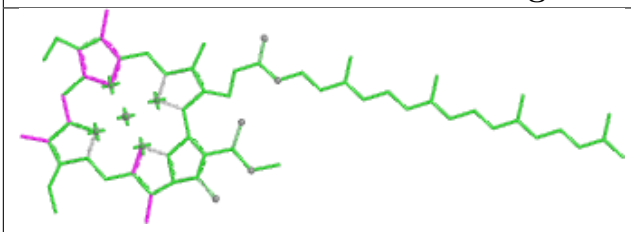


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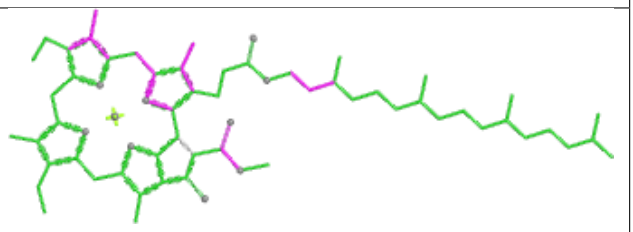


Rings

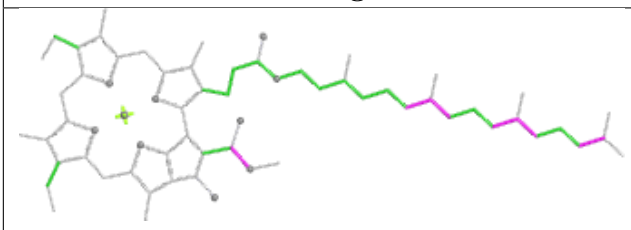
Ligand CLA a 309



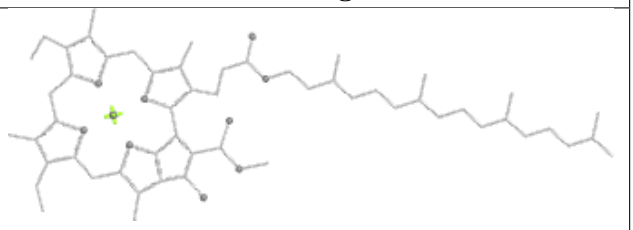
Bond lengths



Bond angles

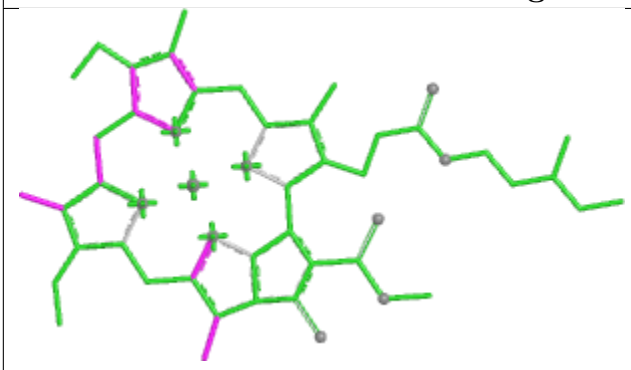


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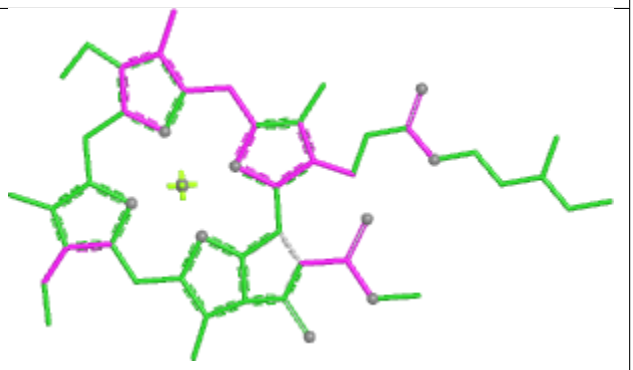


Rings

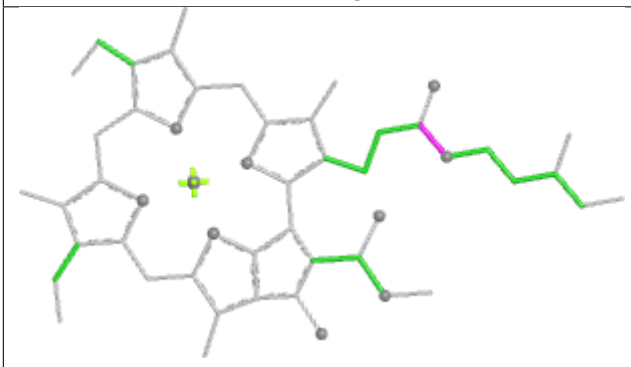
Ligand CLA k 302



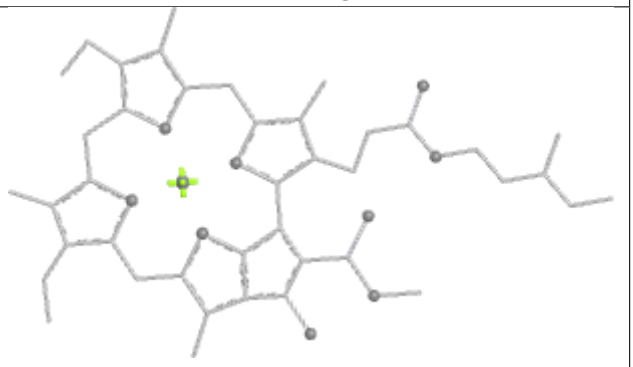
Bond lengths



Bond angles

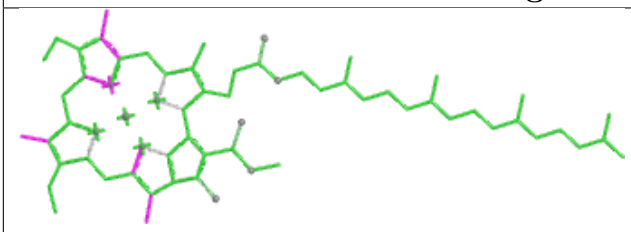


Torsions

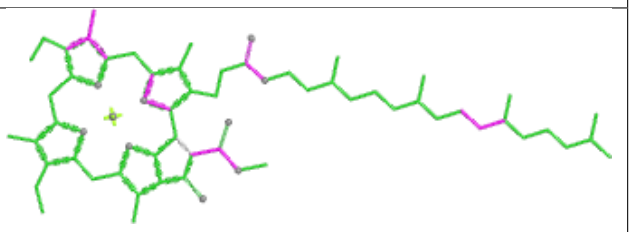


Rings

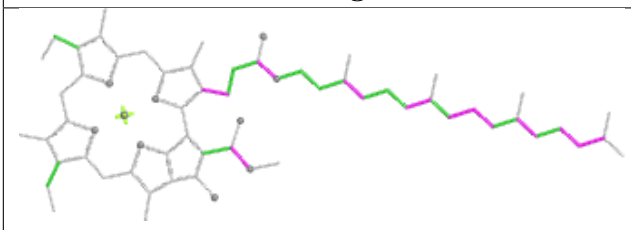
Ligand CLA F 201



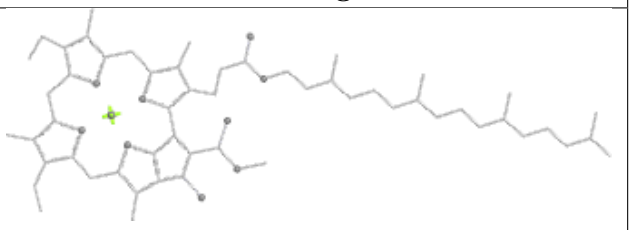
Bond lengths



Bond angles

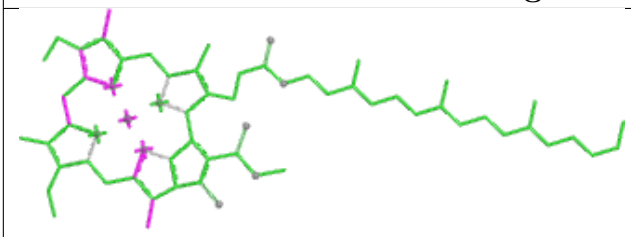


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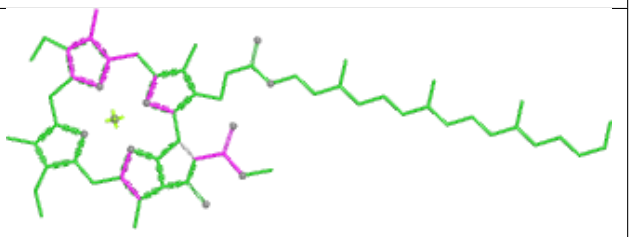


Rings

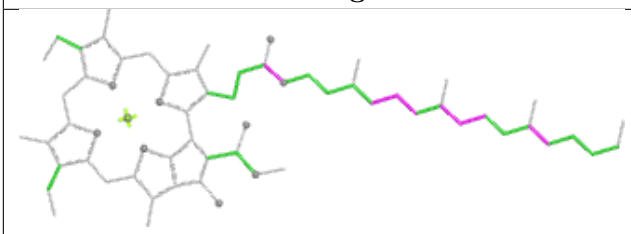
Ligand CLA B 821



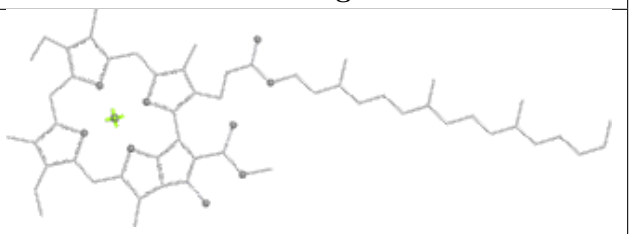
Bond lengths



Bond angles

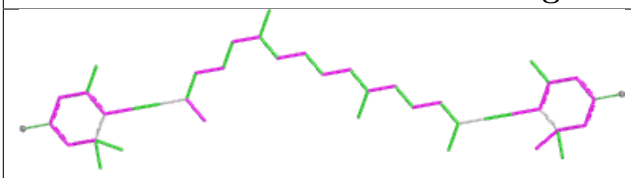


Torsions

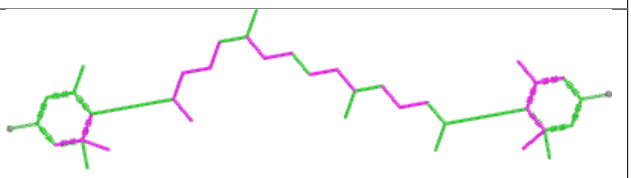


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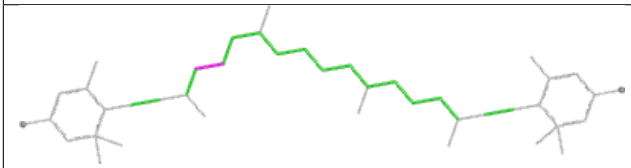
Ligand II0 k 316



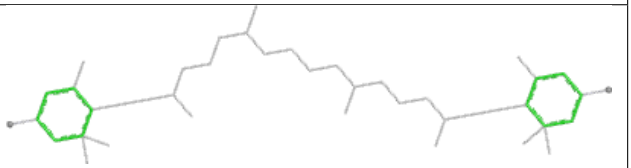
Bond lengths



Bond angles

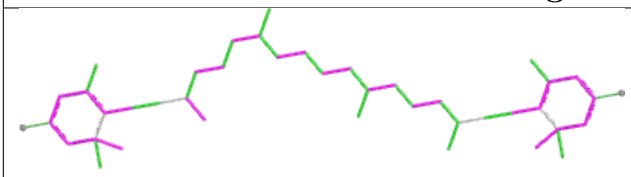


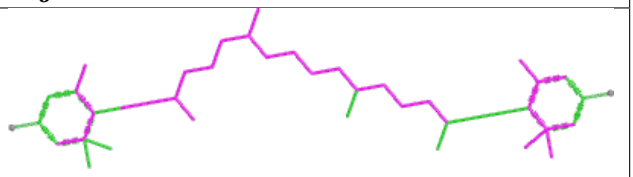
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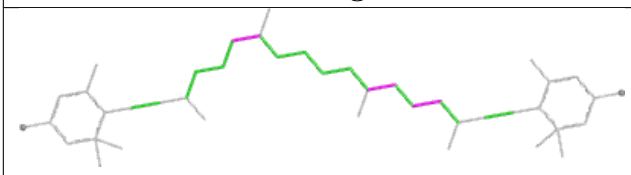


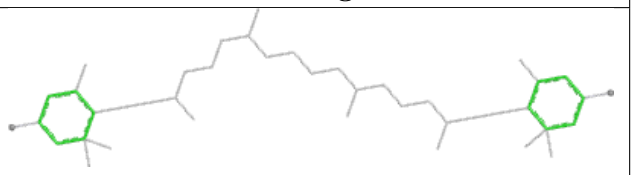
Rings

Ligand II0 j 613

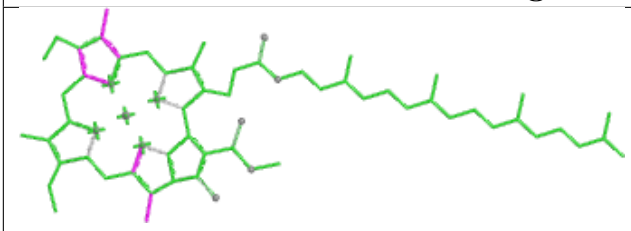

Bond lengths

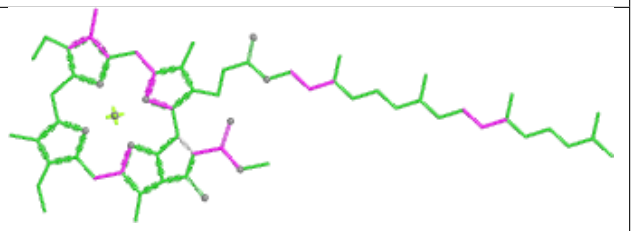

Bond angles

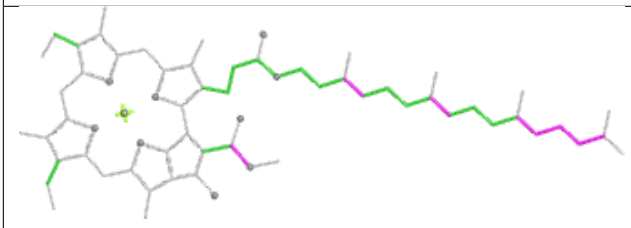

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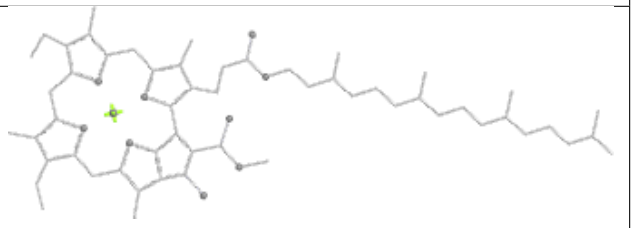

Rings

Ligand CLA b 608

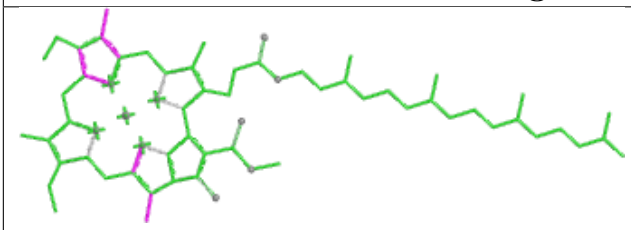

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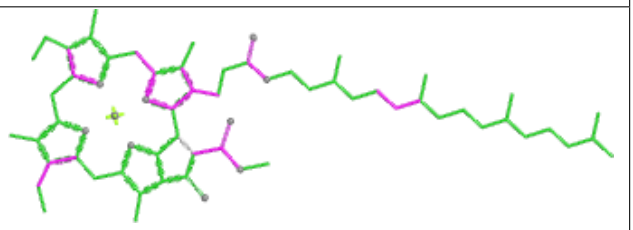

Bond angles

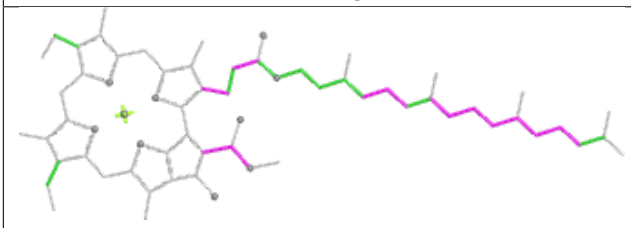

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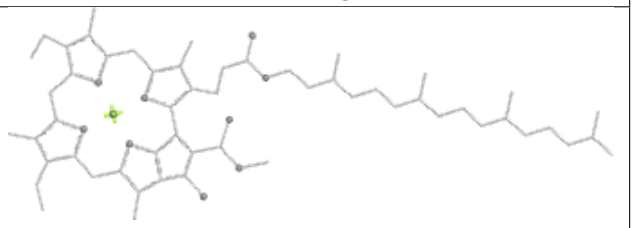

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Ligand CLA a 308

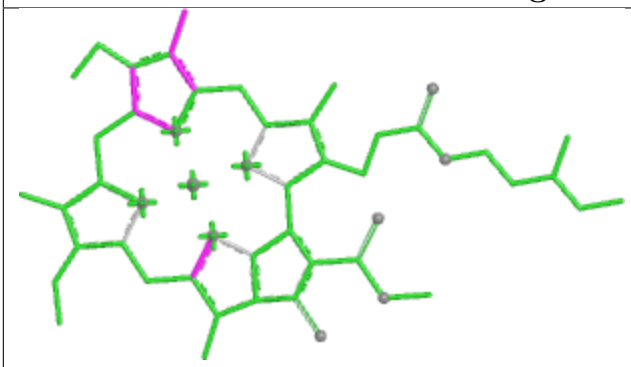

Bond lengths


Bond angles

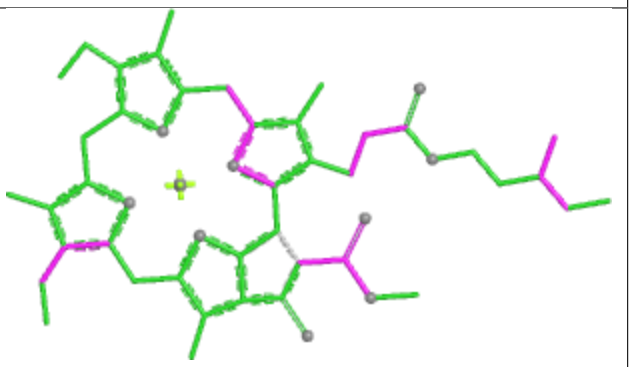

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Rings

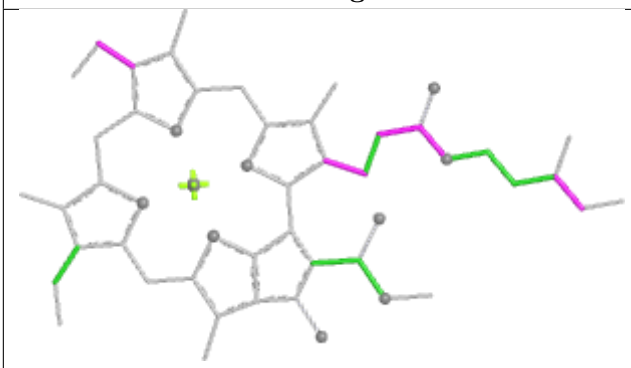
Ligand CLA c 605



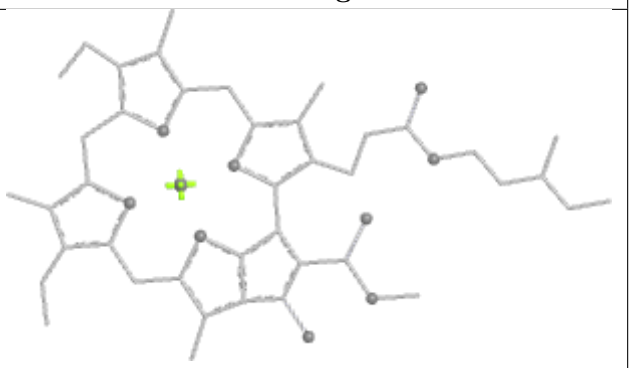
Bond lengths



Bond angles

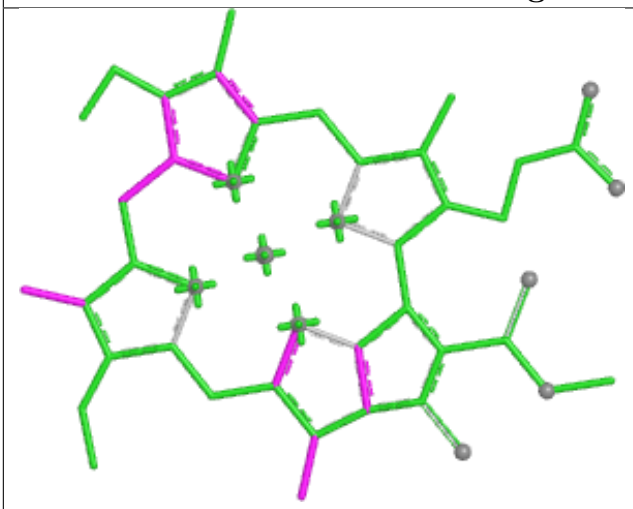


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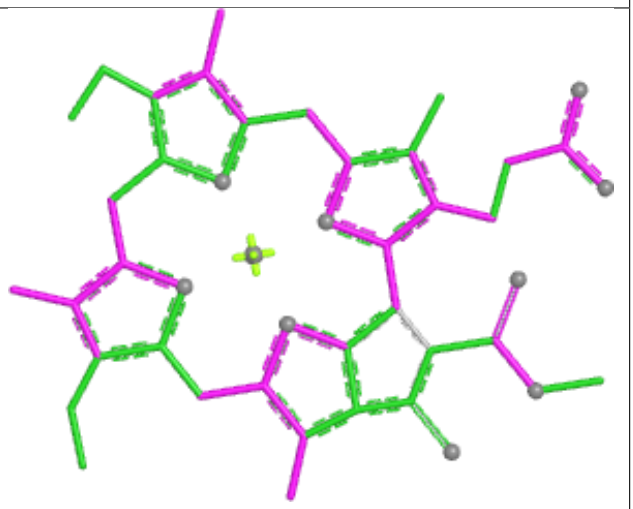


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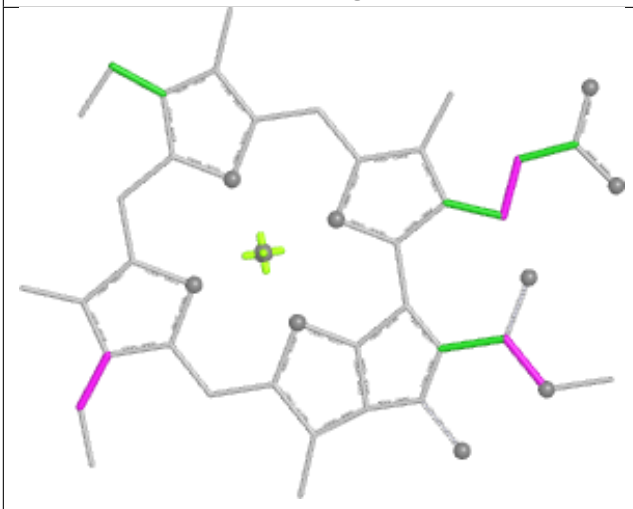
Ligand CLA k 304



Bond lengths



Bond angles

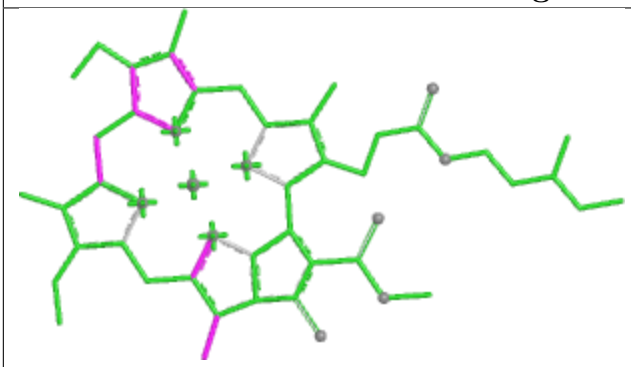


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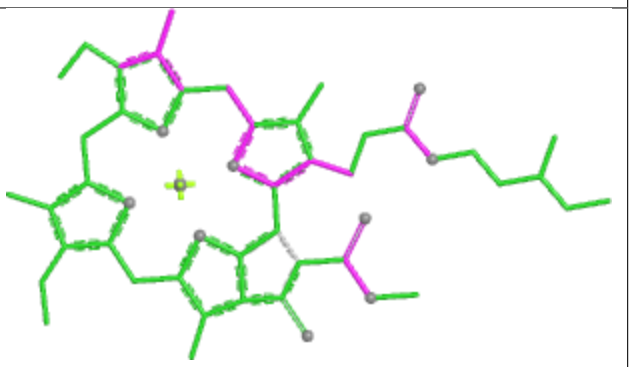


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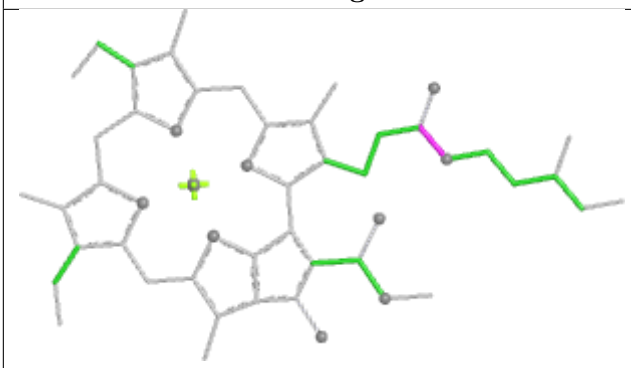
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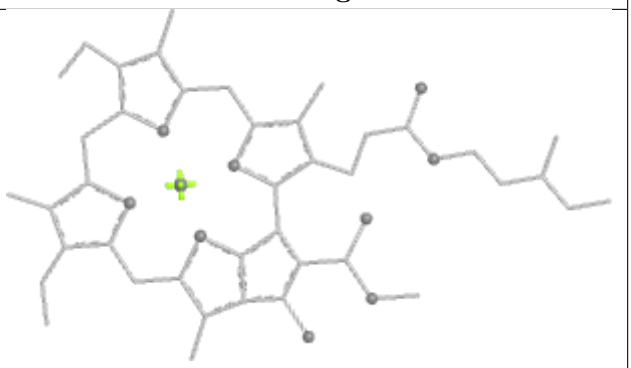
Bond lengths



Bond angles

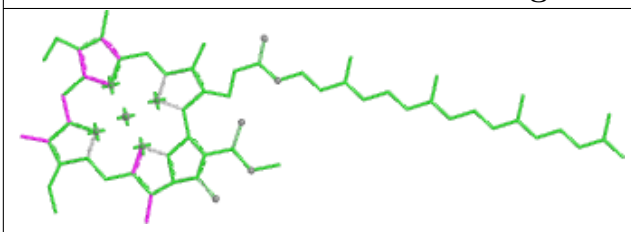


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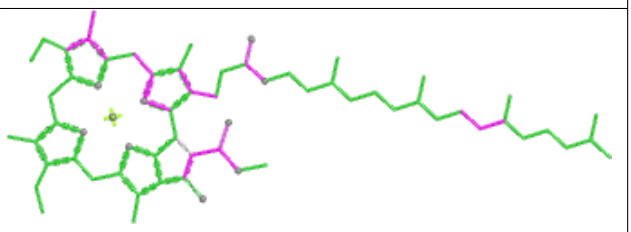


Rings

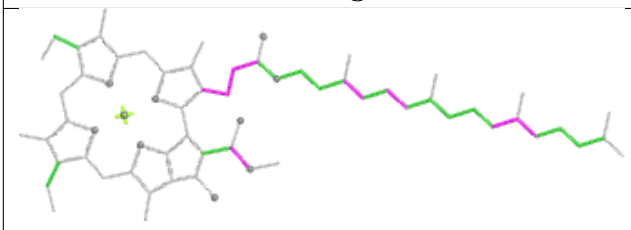
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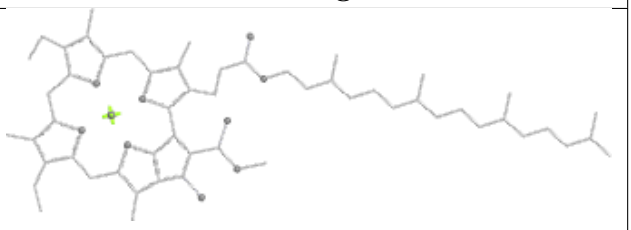
Bond lengths



Bond angles

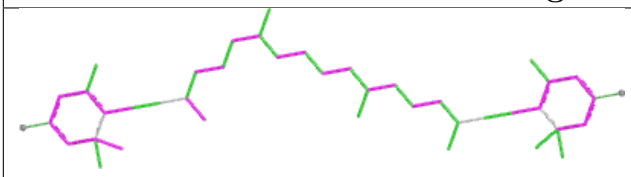


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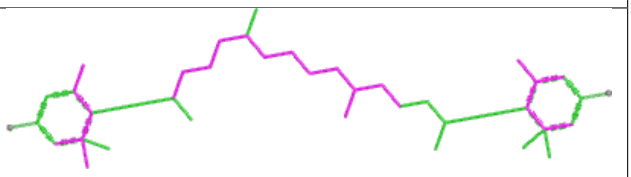


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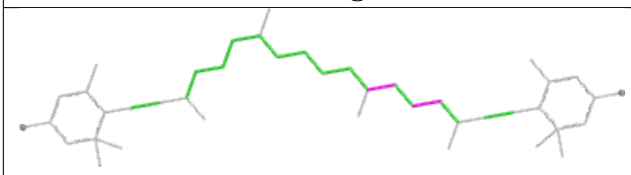
Ligand II0 l 313



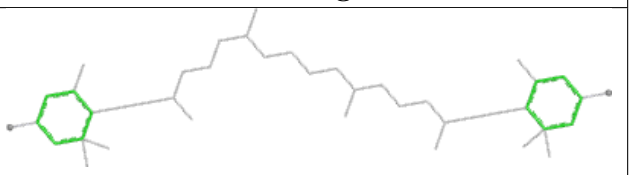
Bond lengths



Bond angles

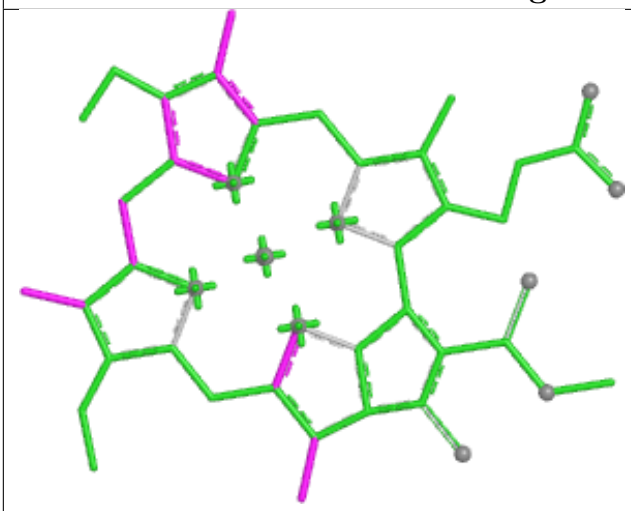


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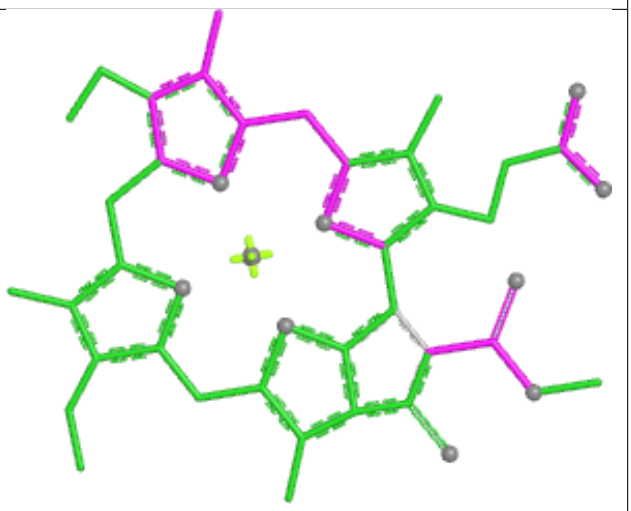


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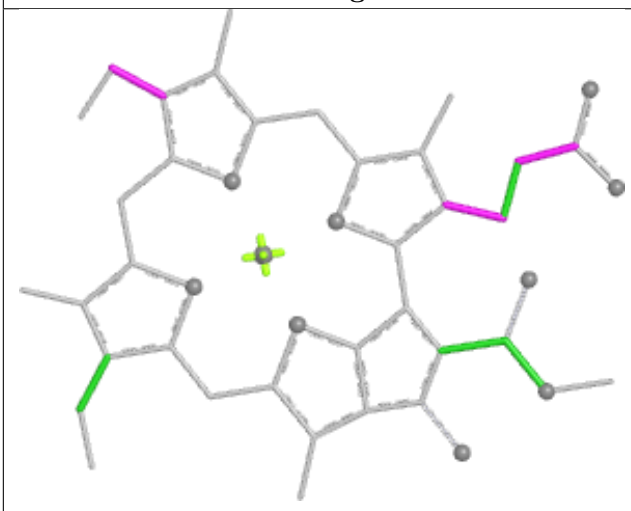
Ligand CLA c 609



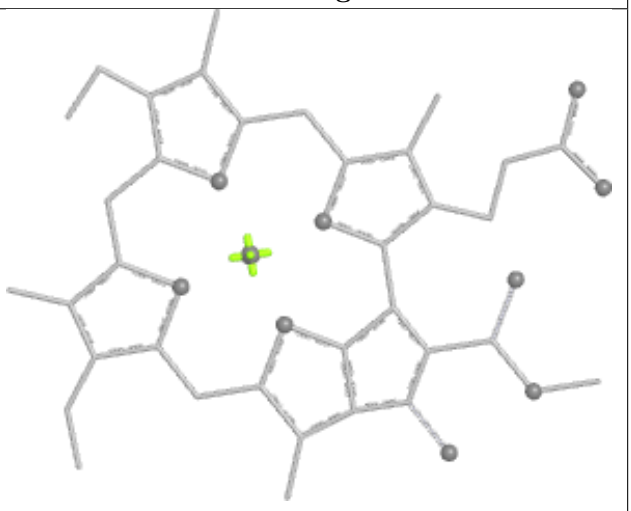
Bond lengths



Bond angles

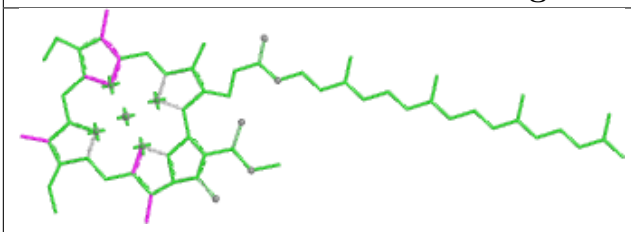


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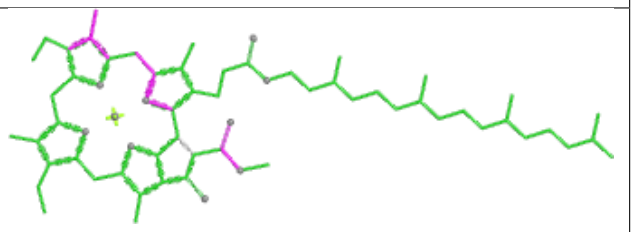


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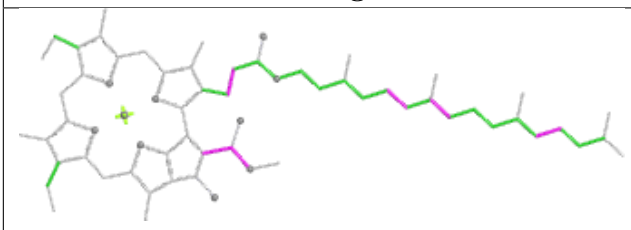
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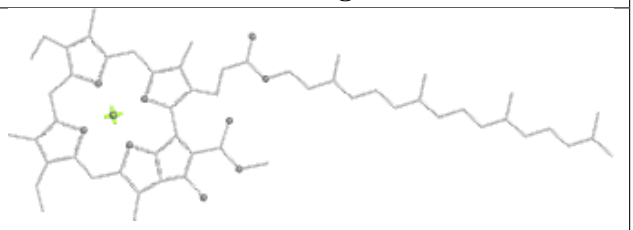
Bond lengths



Bond angles

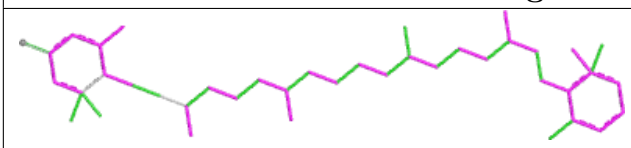


Torsions



Rings

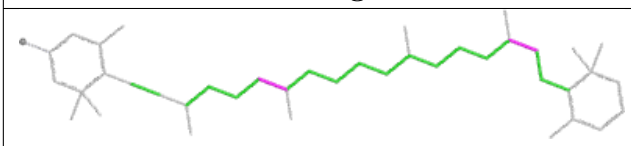
Ligand IHT m 616



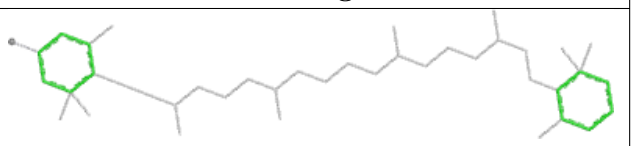
Bond lengths



Bond angles

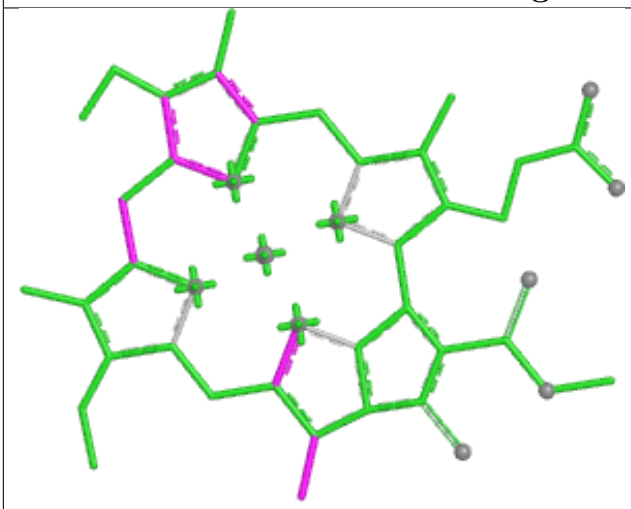


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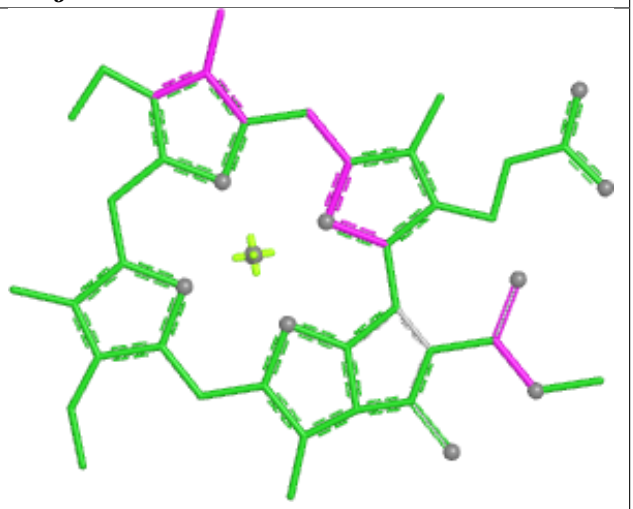


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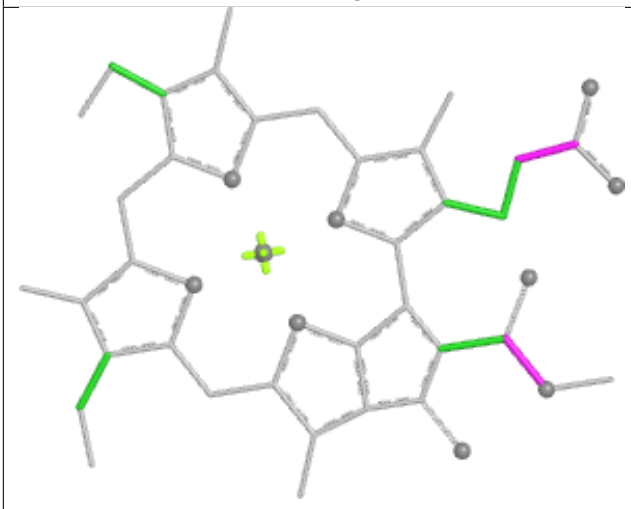
Ligand CLA j 607



Bond lengths



Bond angles

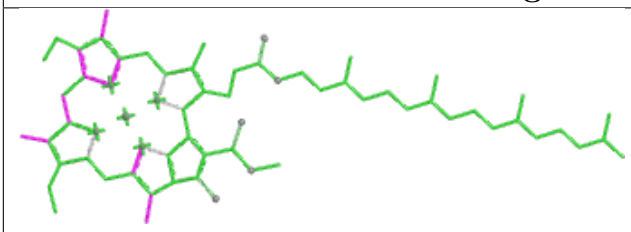


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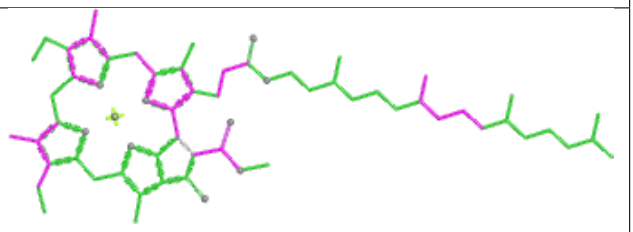


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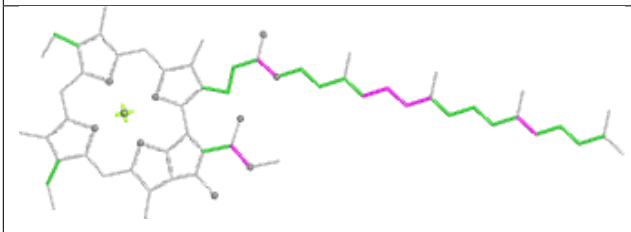
Ligand CLA A 826



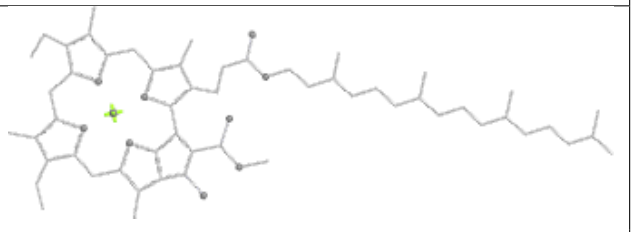
Bond lengths



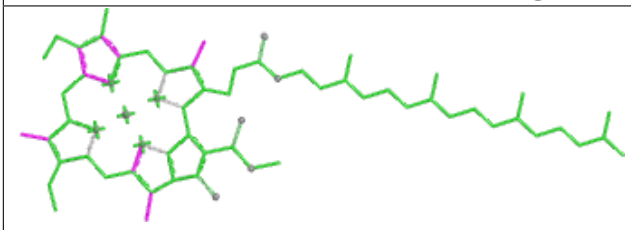
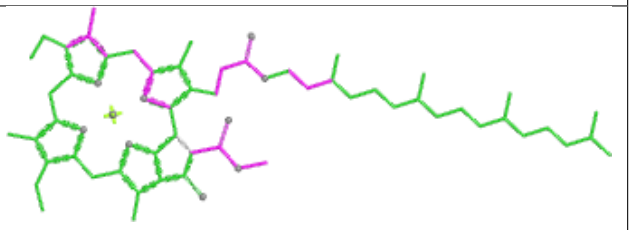
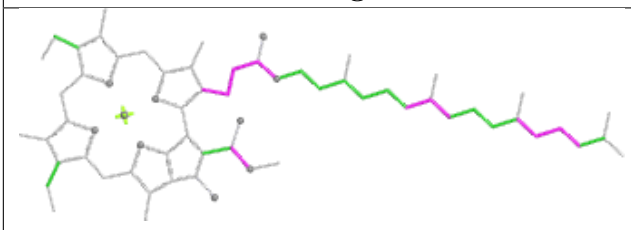
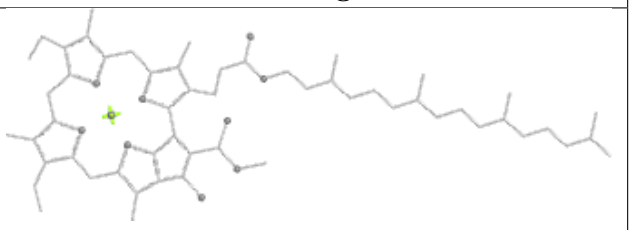
Bond angles

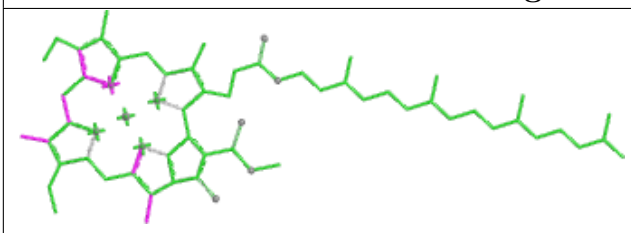
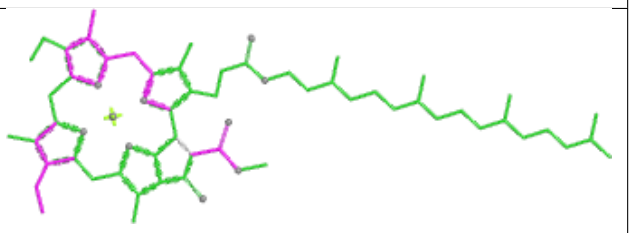
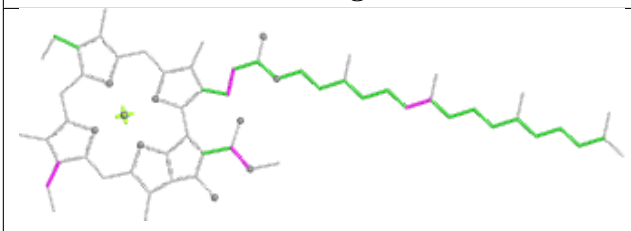
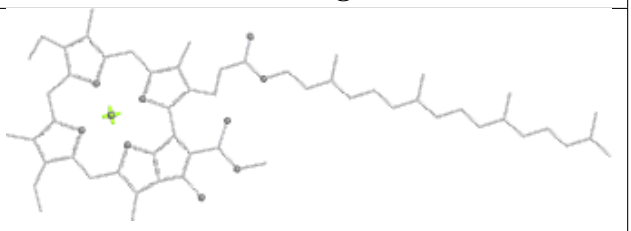


Torsions

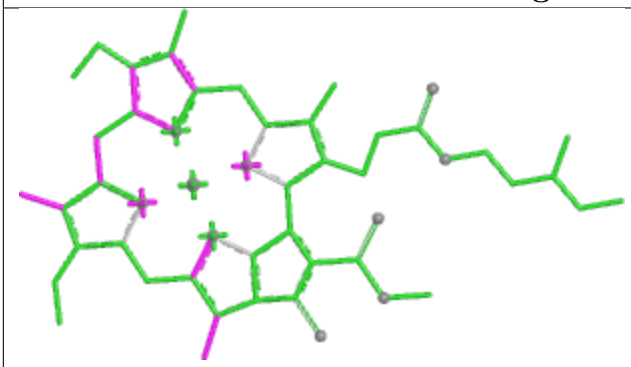


Rings

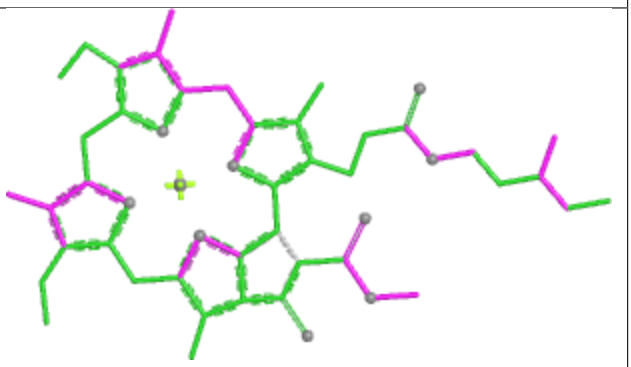
Ligand CLA c 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

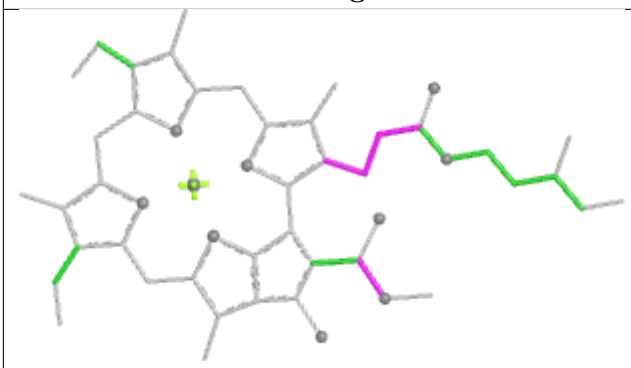
Ligand CLA i 311



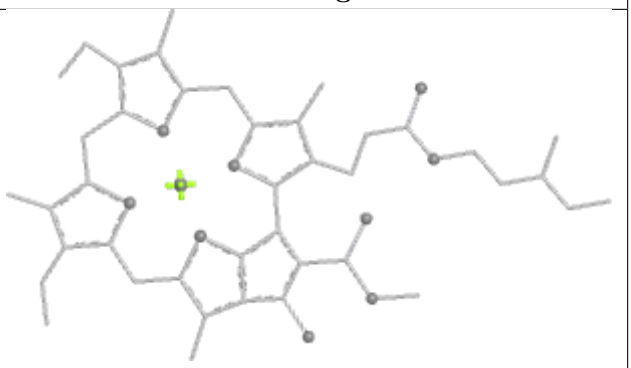
Bond lengths



Bond angles

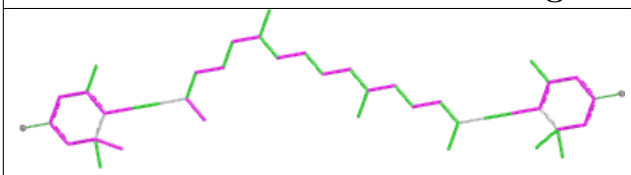


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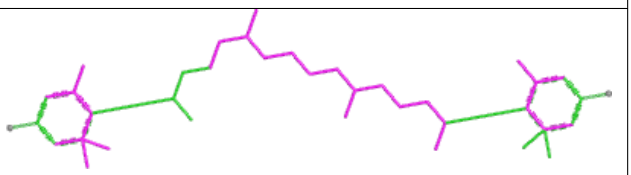


Rings

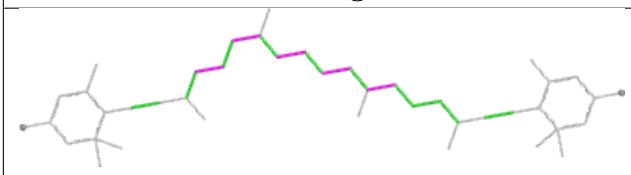
Ligand II0 f 618



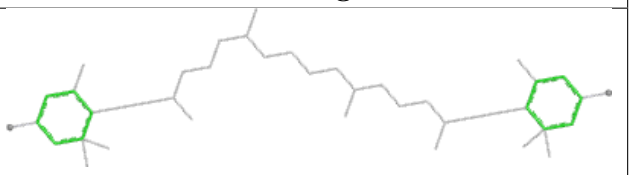
Bond lengths



Bond angles

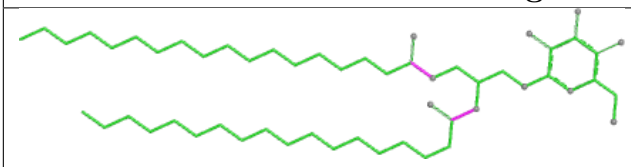


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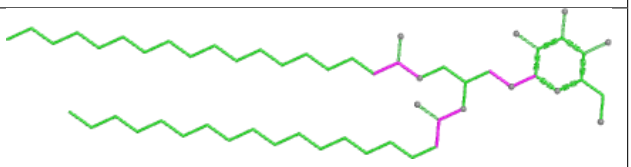


Rings

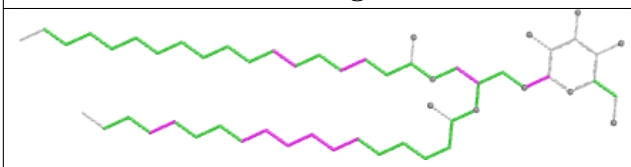
Ligand LMG s 210



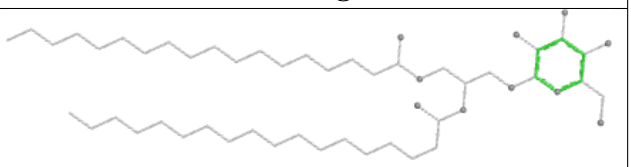
Bond lengths



Bond angles

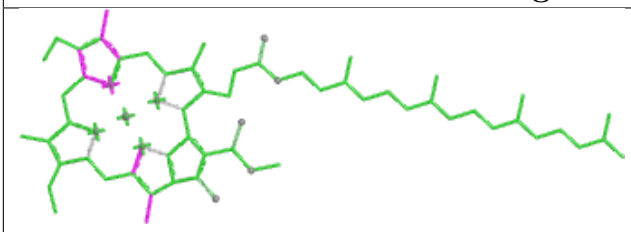


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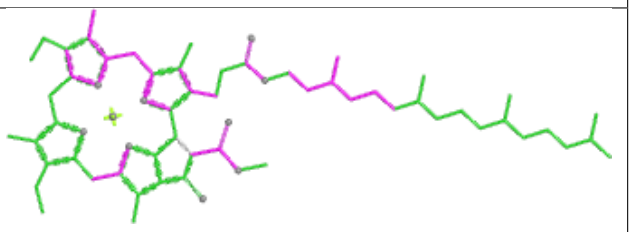


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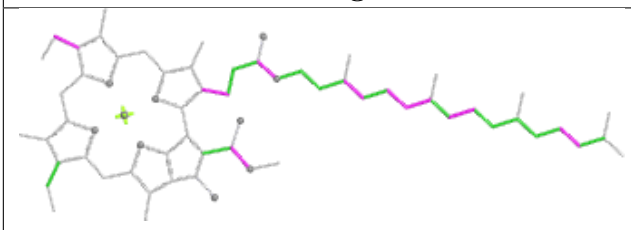
Ligand CLA l 312



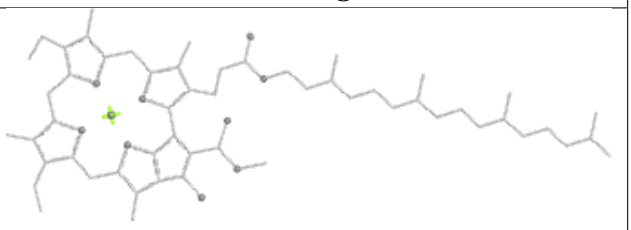
Bond lengths



Bond angles

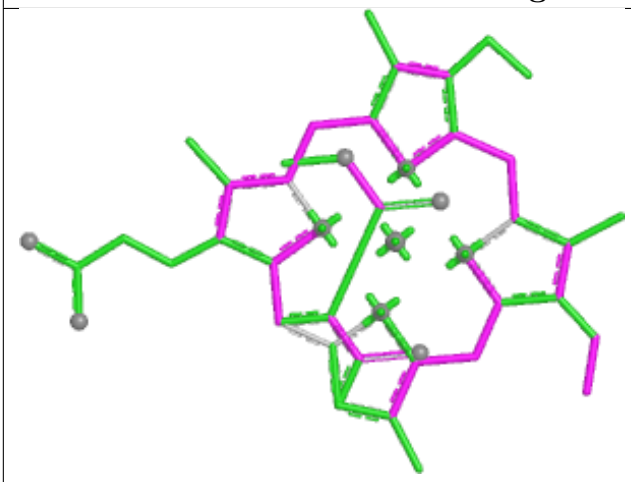


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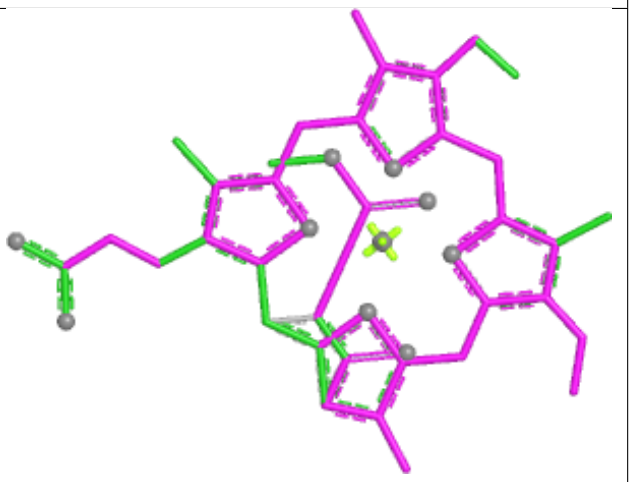


Rings

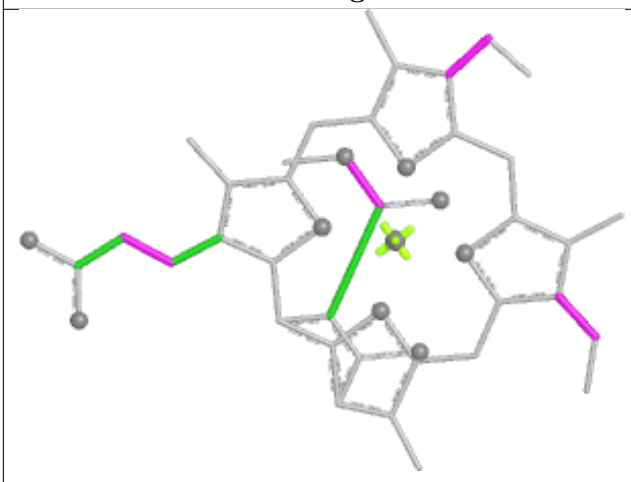
Ligand KC2 d 310



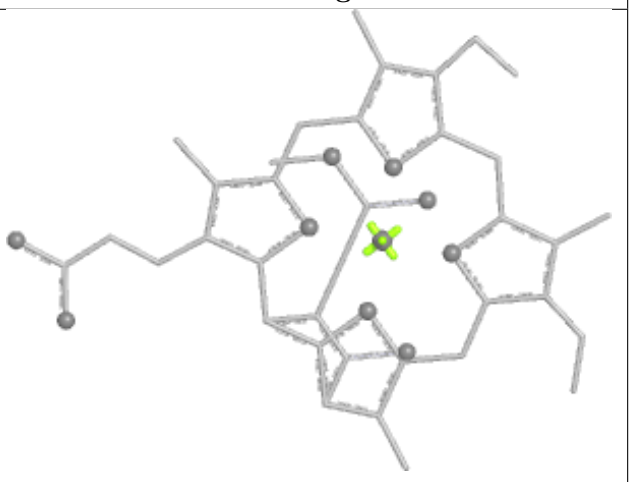
Bond lengths



Bond angles

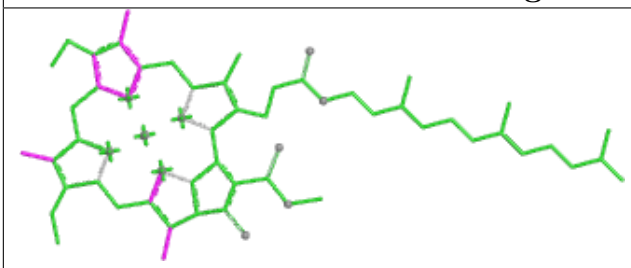


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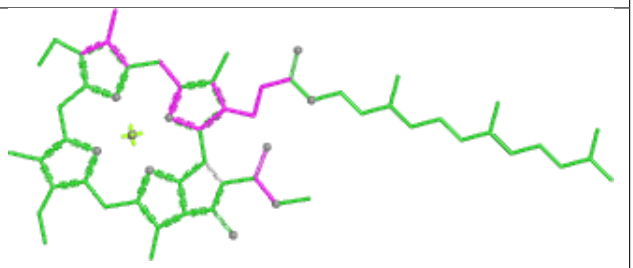


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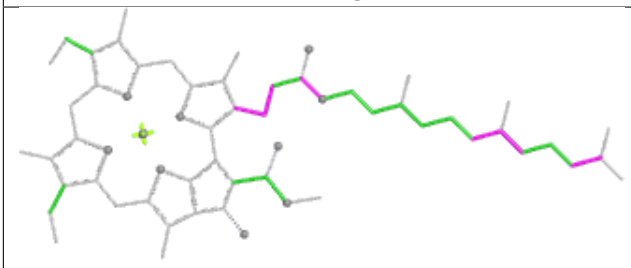
Ligand CLA B 811



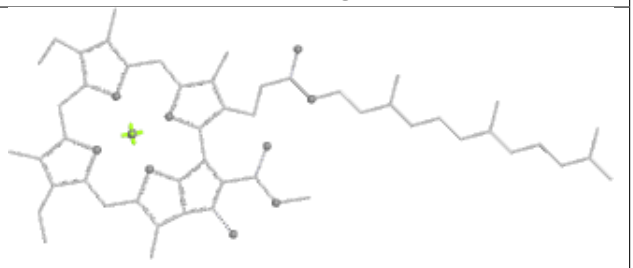
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Bond angles

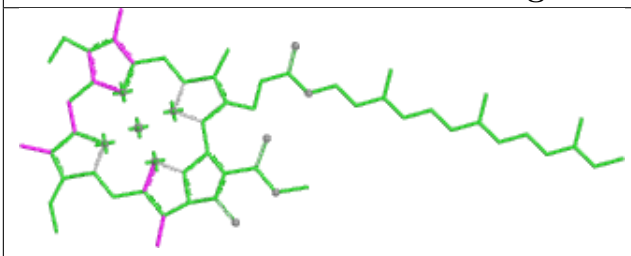


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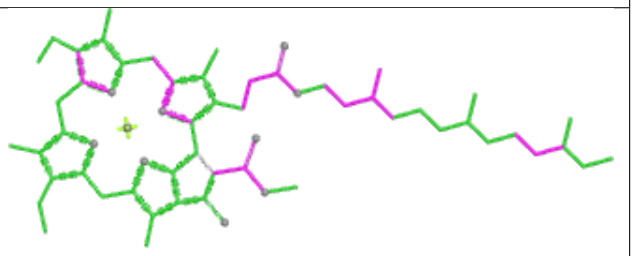


Rings

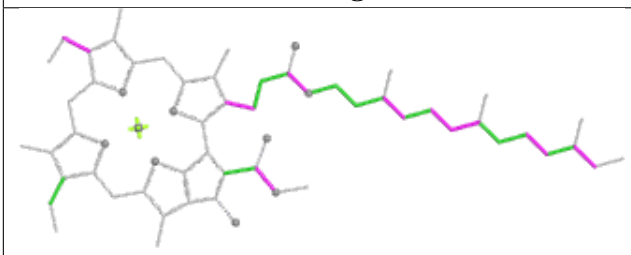
Ligand CLA b 606



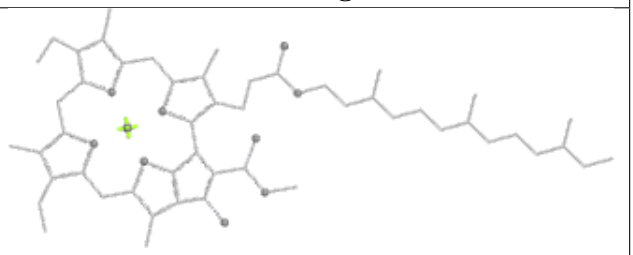
Bond lengths



Bond angles

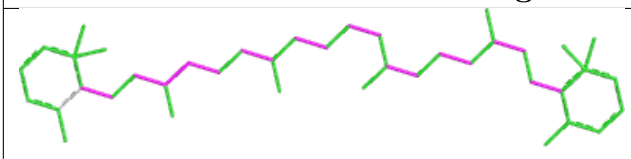


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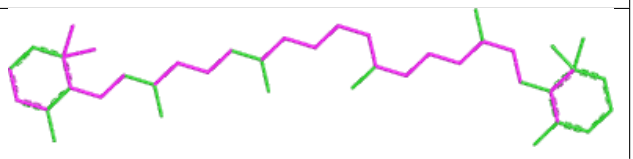


Rings

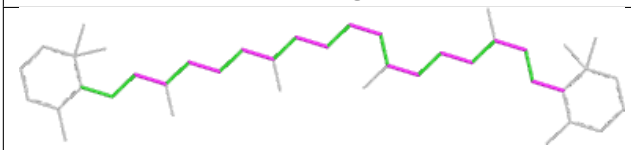
Ligand WVN A 849



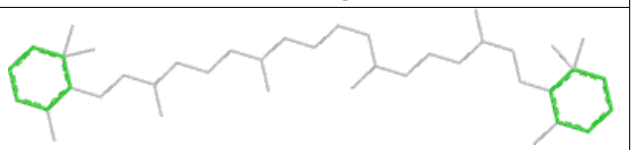
Bond lengths



Bond angles

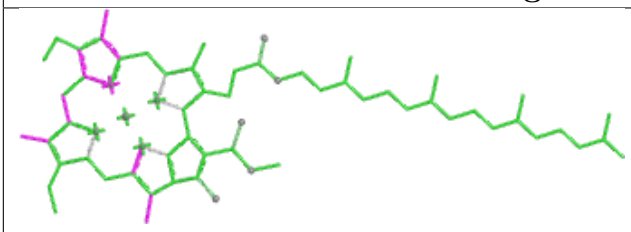


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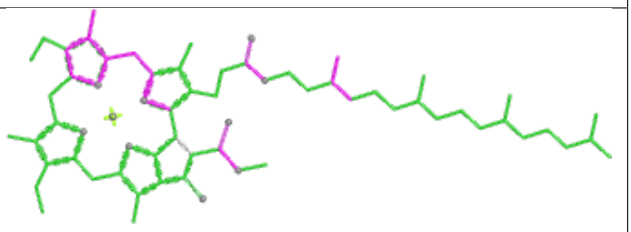


Rings

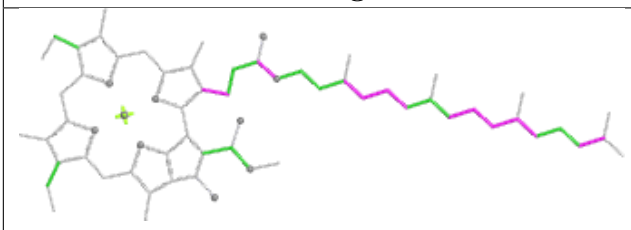
Ligand CLA A 841



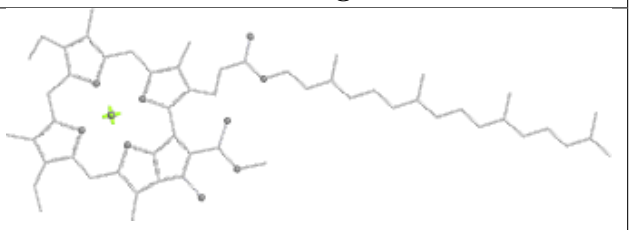
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Bond angles

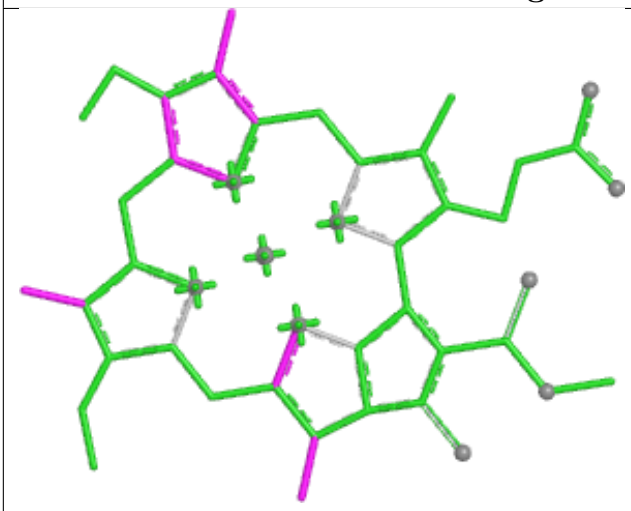


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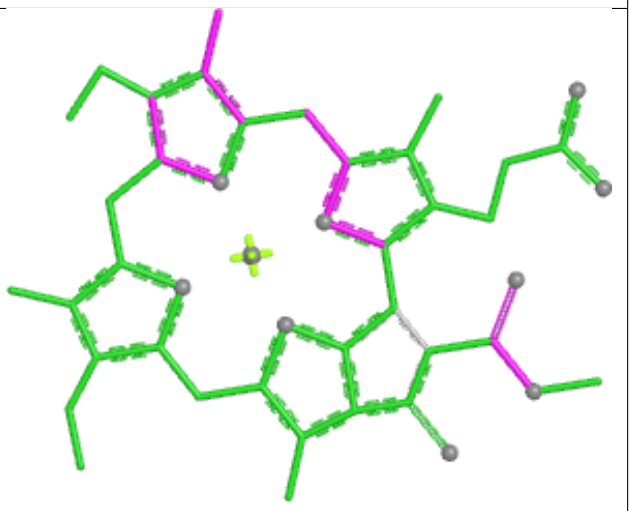


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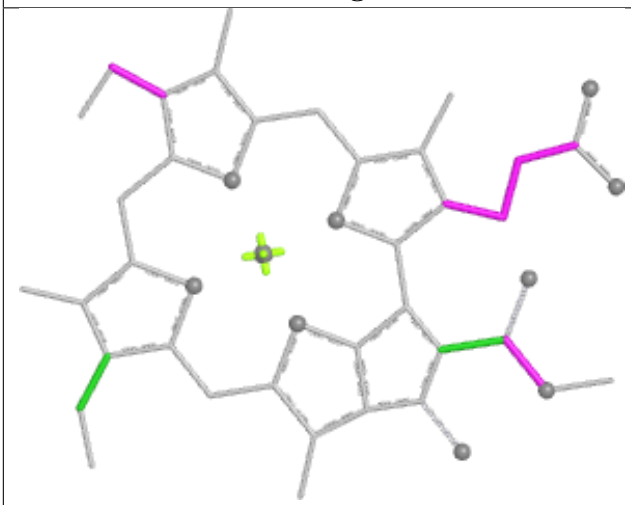
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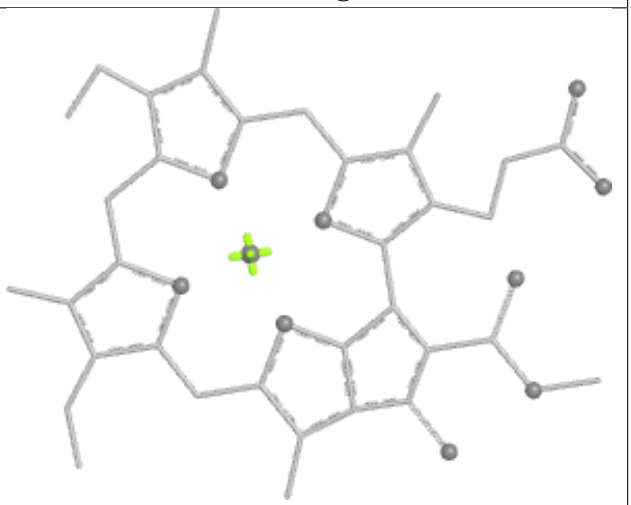
Bond lengths



Bond angles

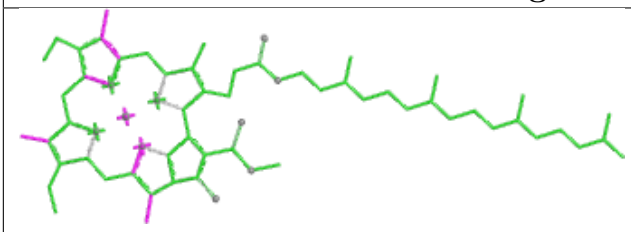


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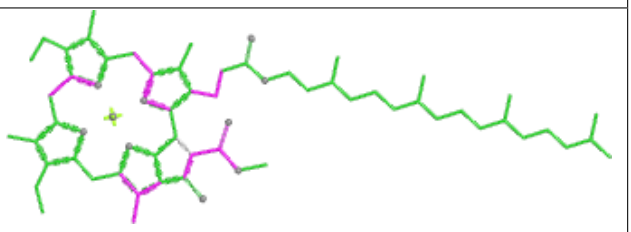


Rings

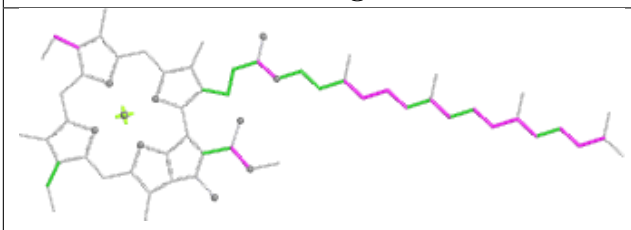
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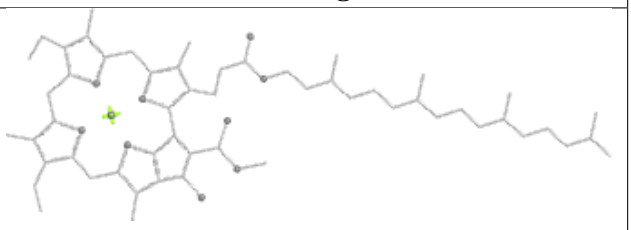
Bond lengths



Bond angles

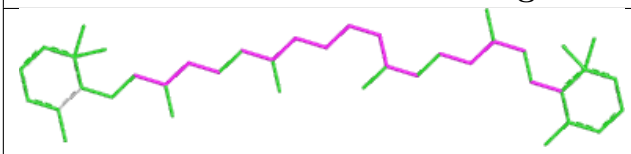


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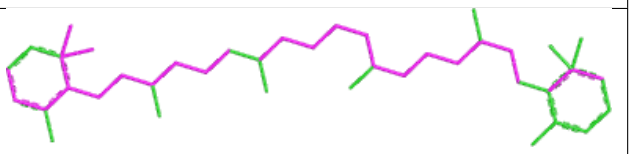


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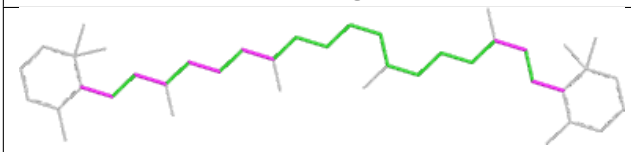
Ligand WVN L 201



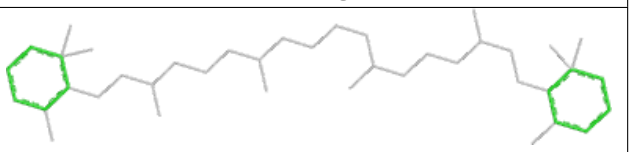
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Bond angles

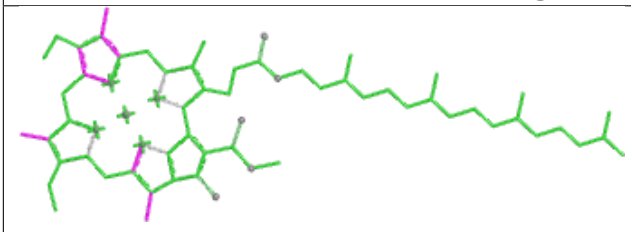


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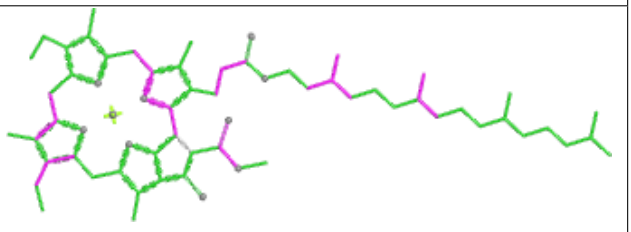


Rings

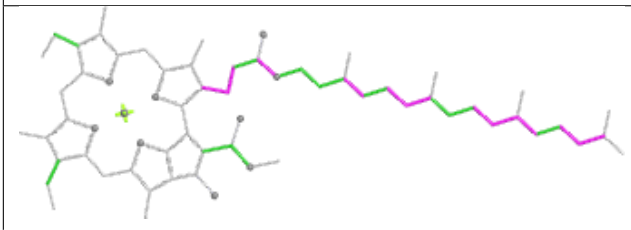
Ligand CLA f 607



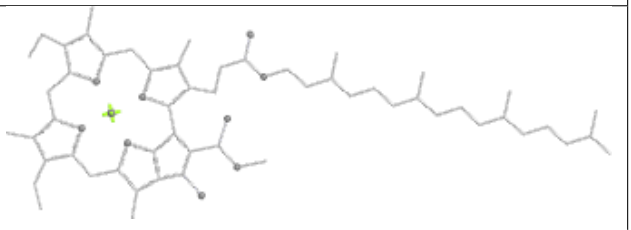
Bond lengths



Bond angles

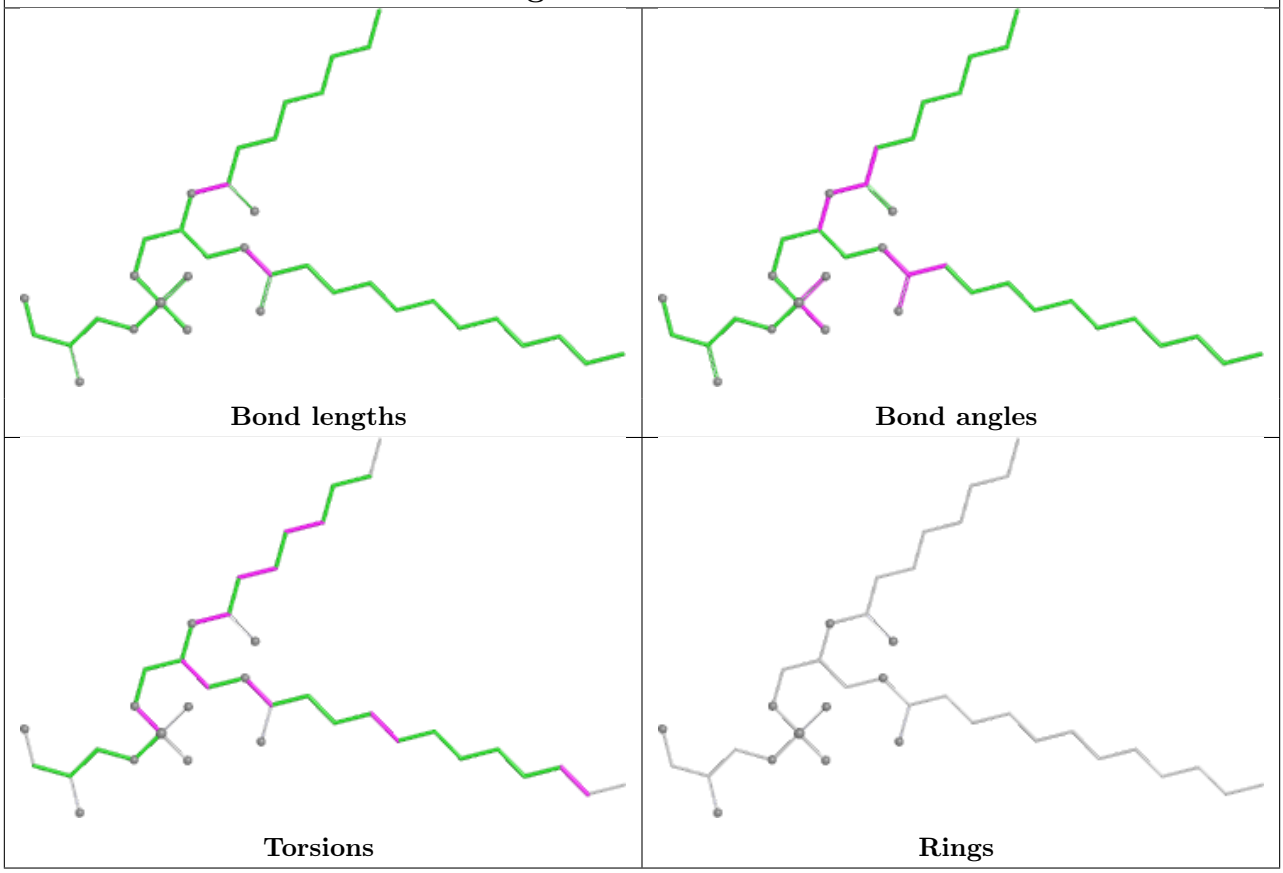


Torsions

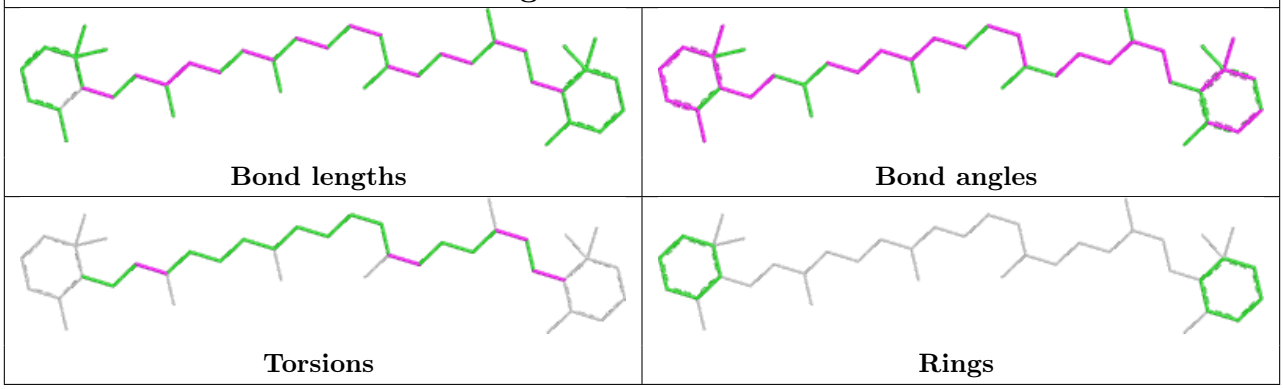


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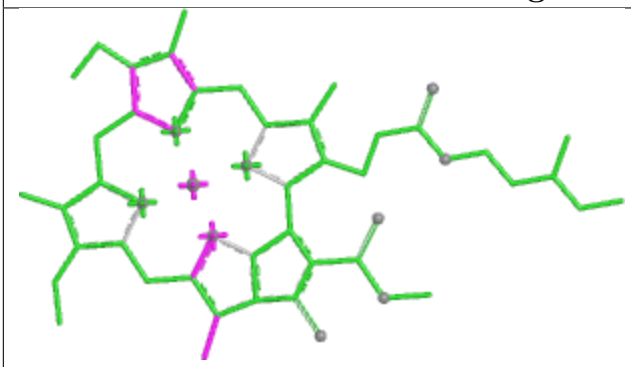
Ligand LHG k 319



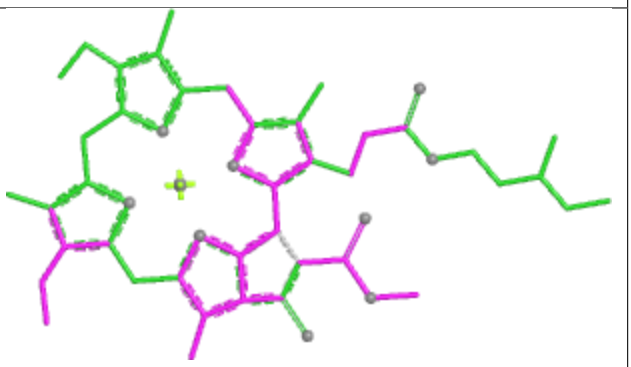
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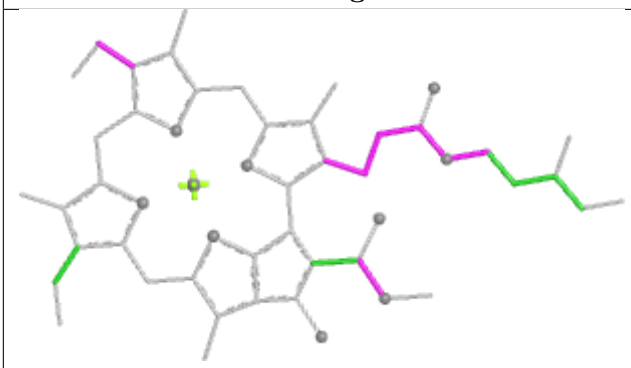
Ligand CLA k 309



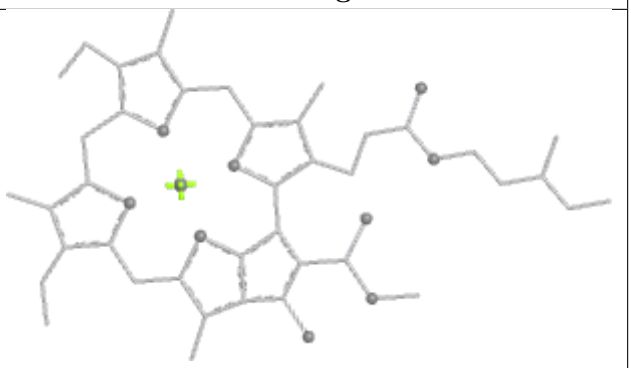
Bond lengths



Bond angles

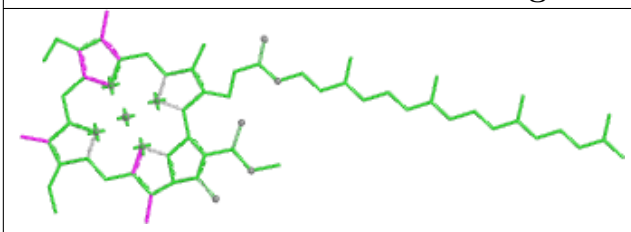


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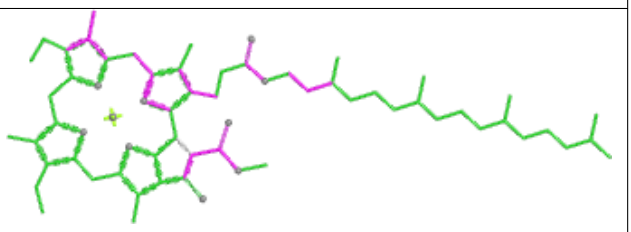


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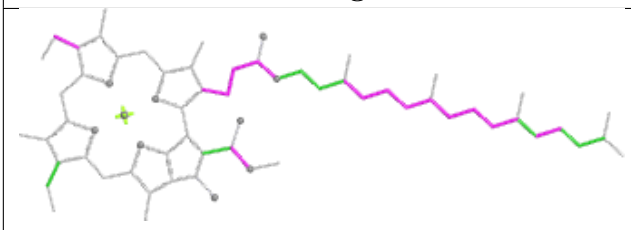
Ligand CLA e 604



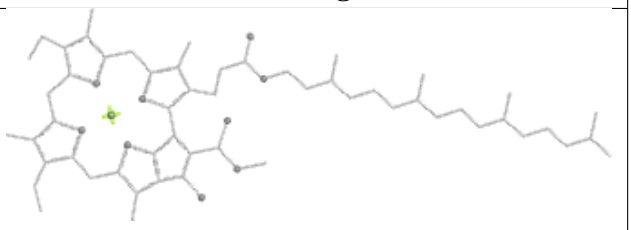
Bond lengths



Bond angles

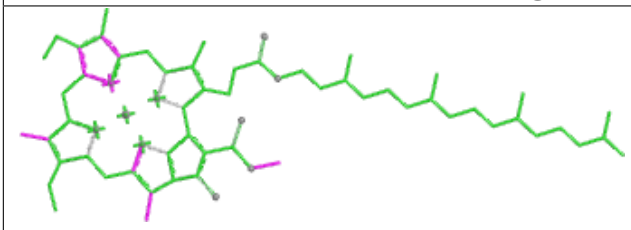


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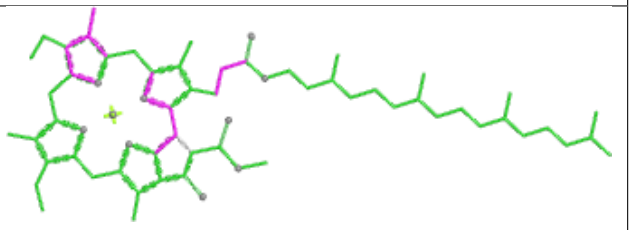


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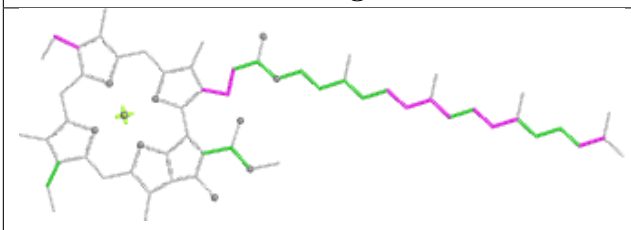
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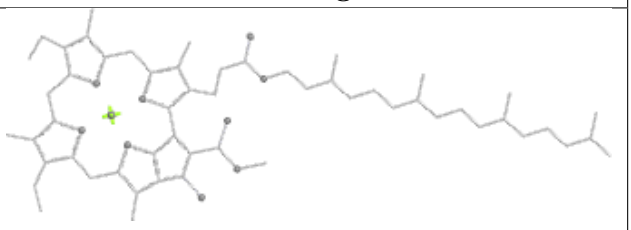
Bond lengths



Bond angles

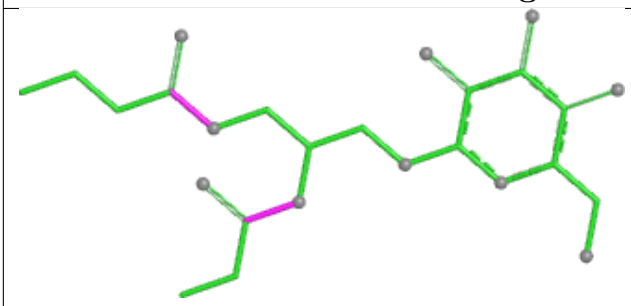


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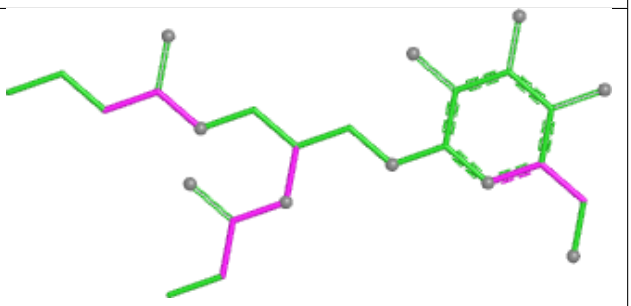


Rings

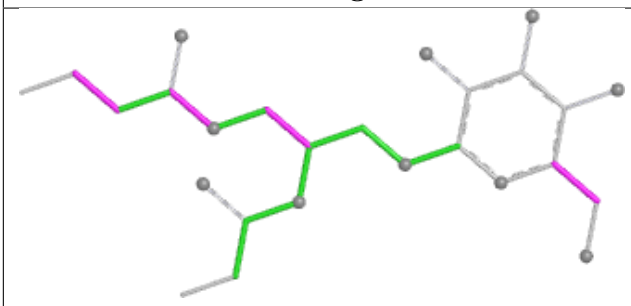
Ligand LMG O 205



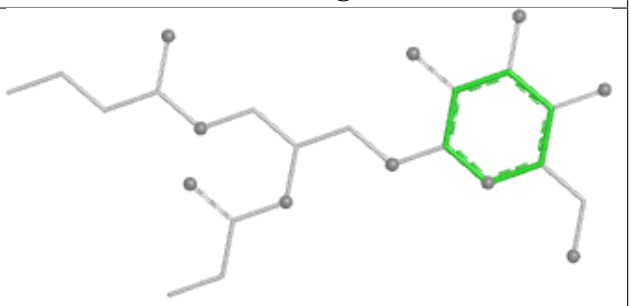
Bond lengths



Bond angles

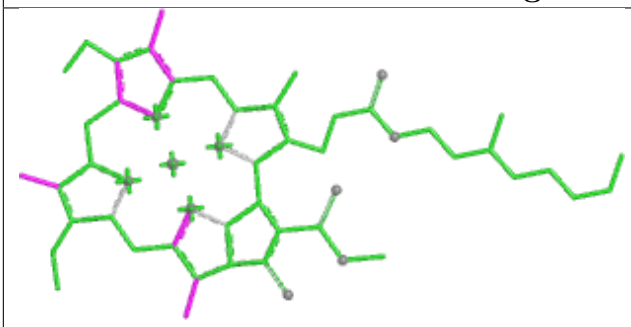


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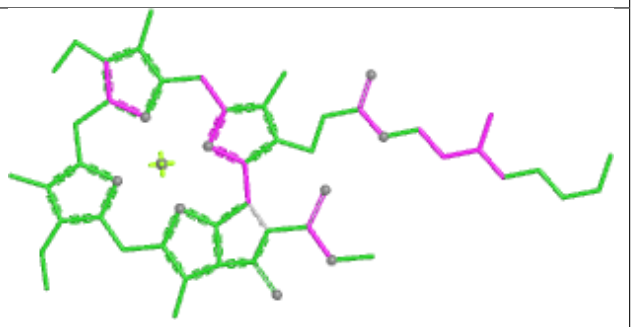


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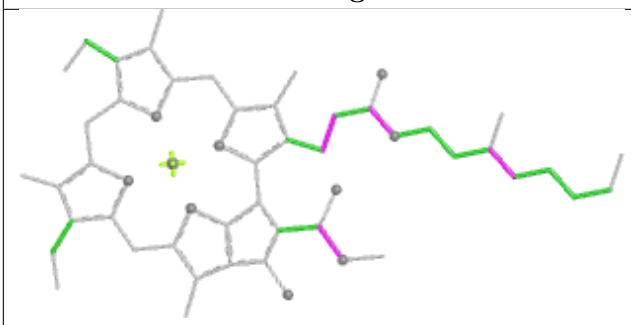
Ligand CLA A 811



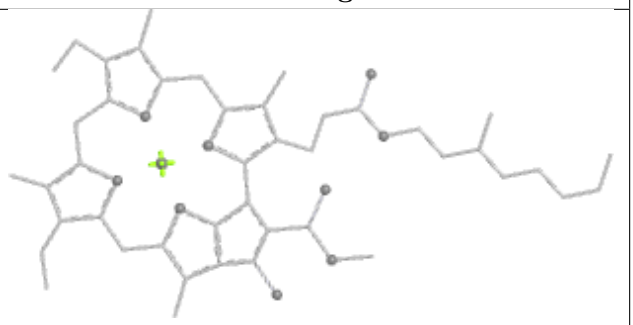
Bond lengths



Bond angles

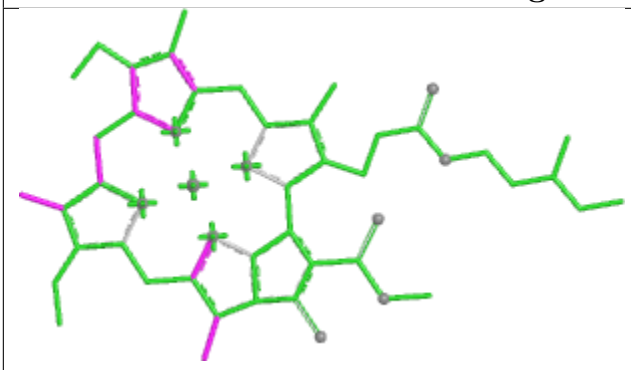


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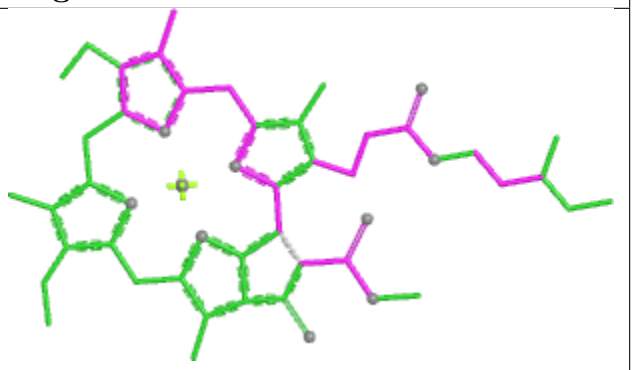


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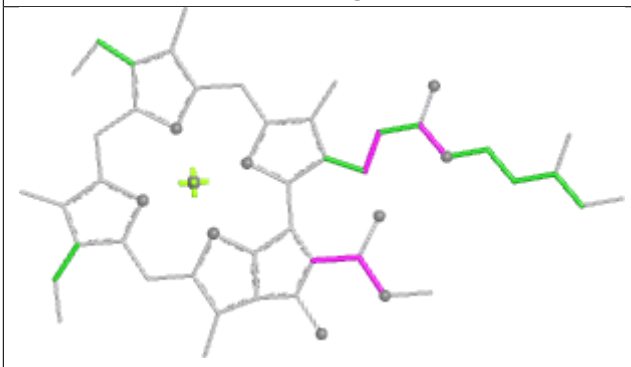
Ligand CLA g 310



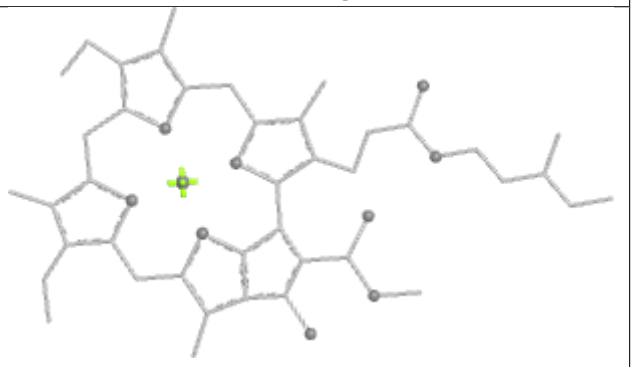
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Bond angles

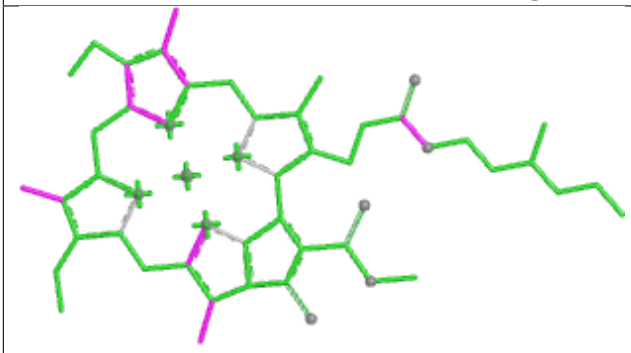


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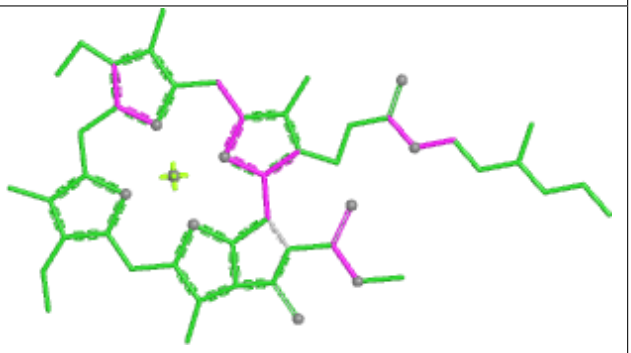


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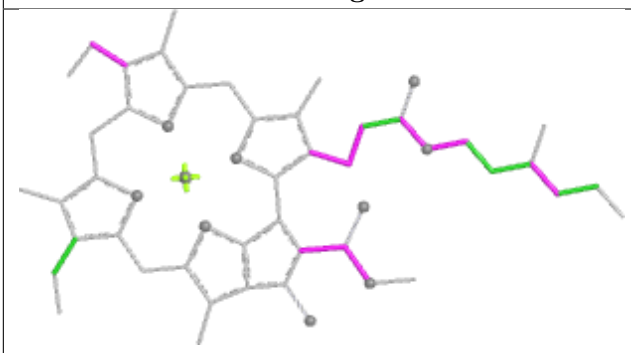
Ligand CLA F 203



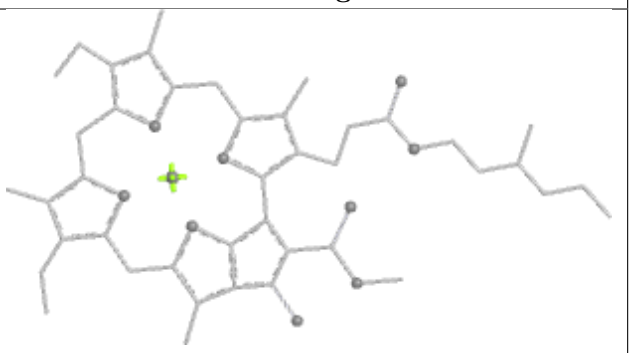
Bond lengths



Bond angles

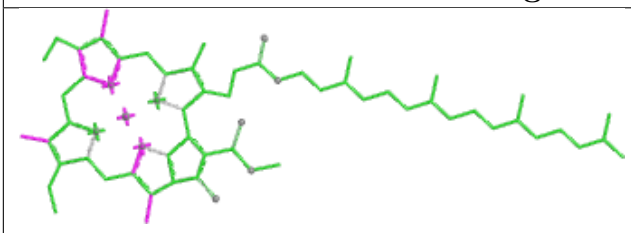


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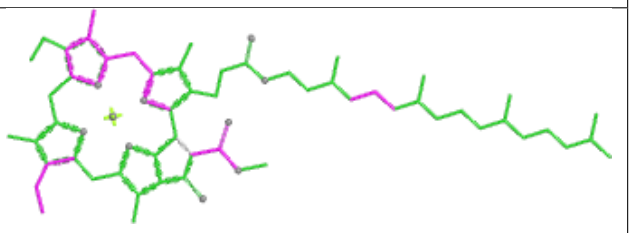


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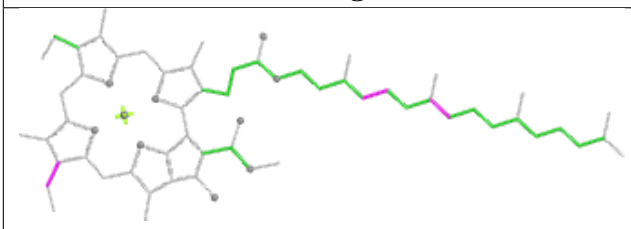
Ligand CLA A 820



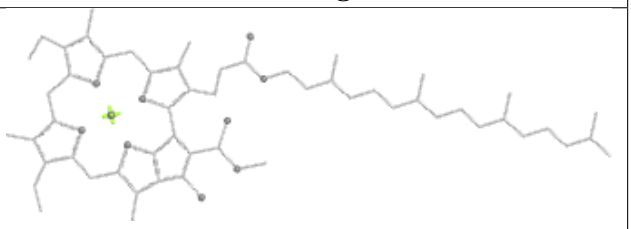
Bond lengths



Bond angles

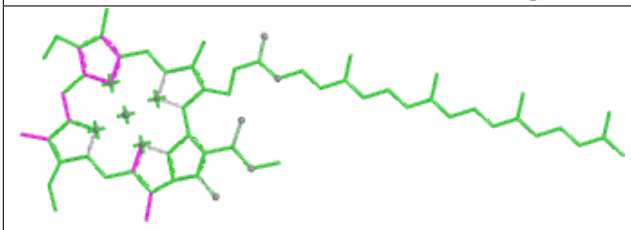


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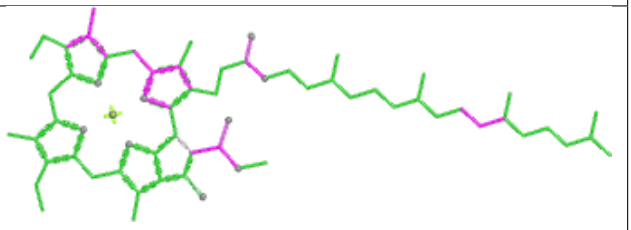


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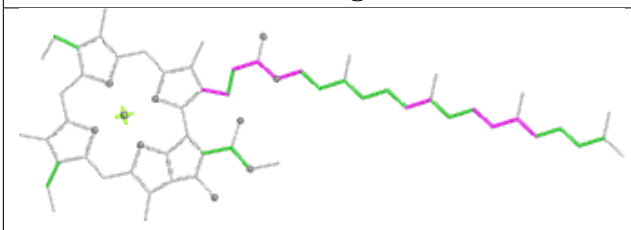
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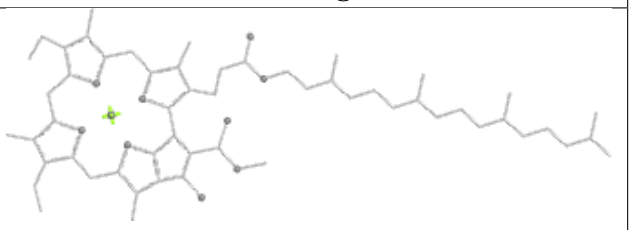
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Bond angles

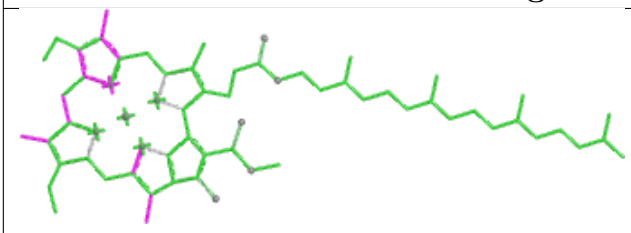


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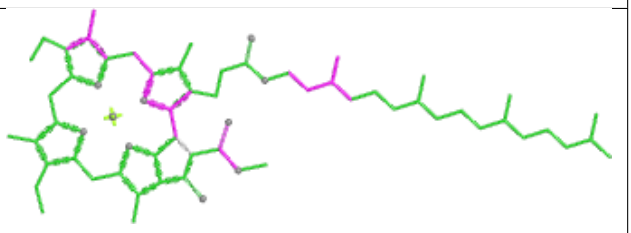


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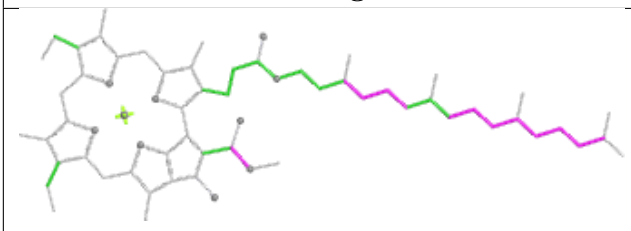
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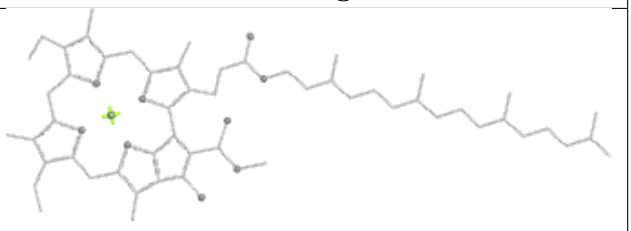
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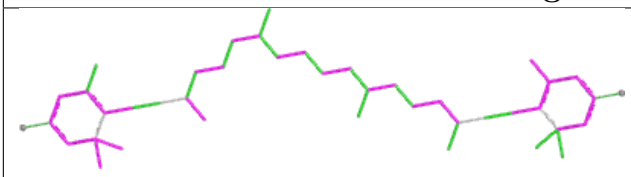


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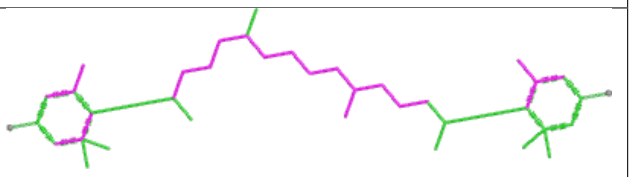


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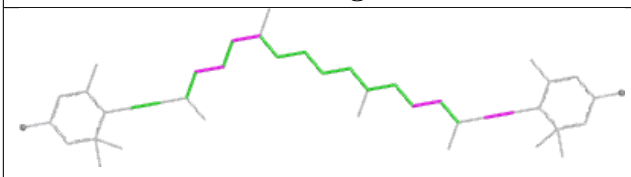
Ligand II0 e 613



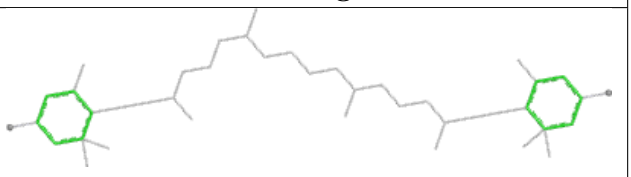
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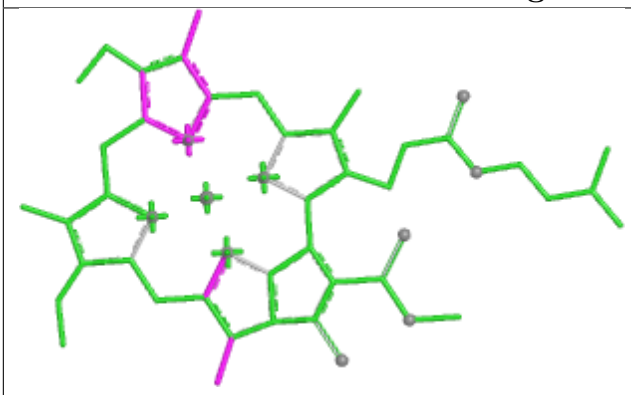


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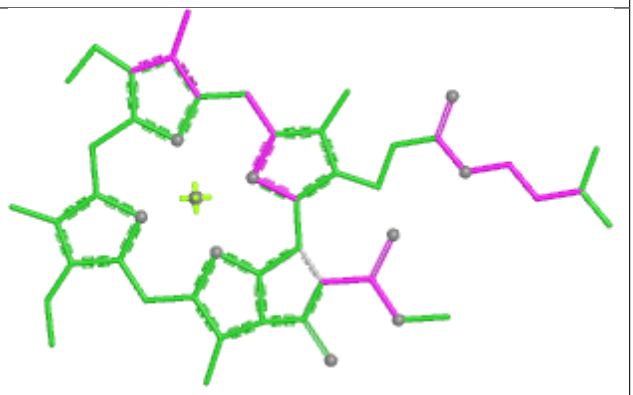


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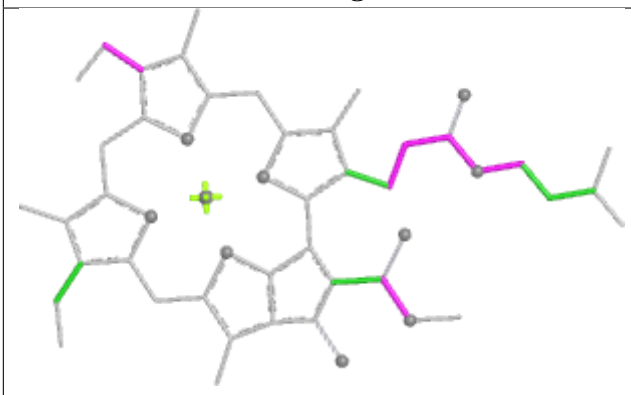
Ligand CLA h 303



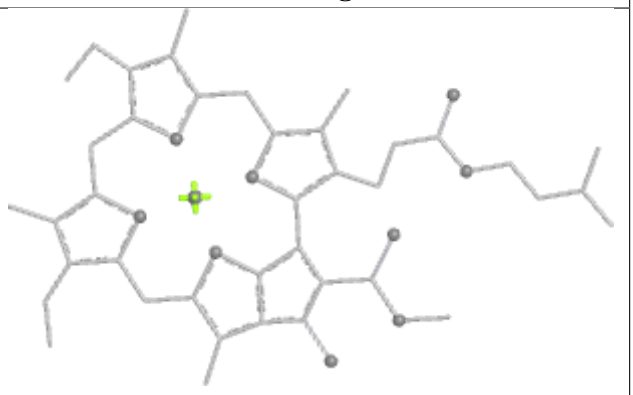
Bond lengths



Bond angles

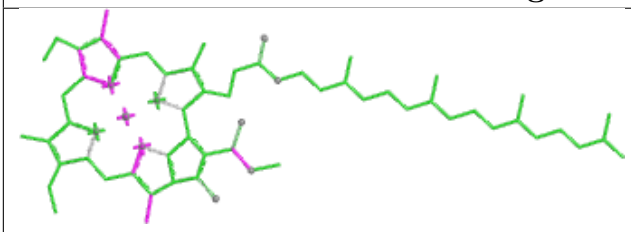


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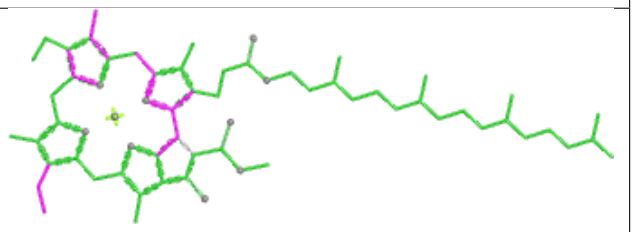


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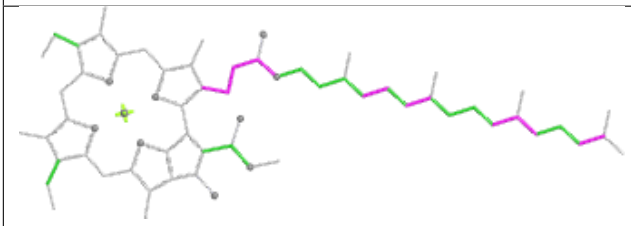
Ligand CLA n 610



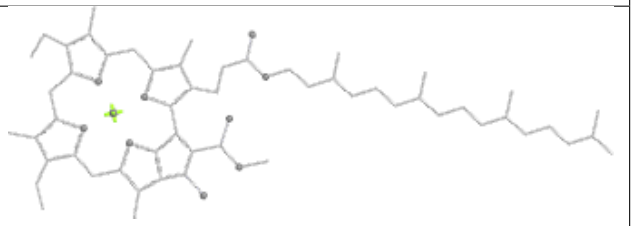
Bond lengths



Bond angles

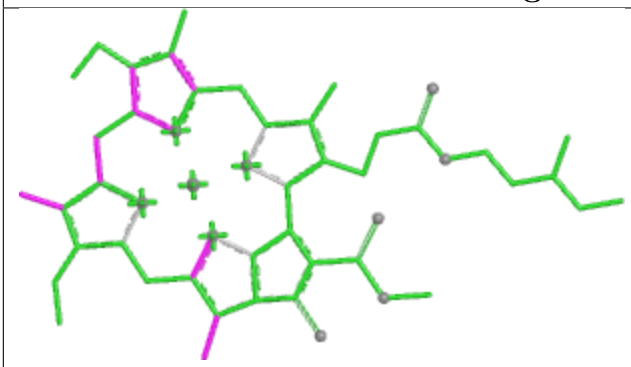


Torsions

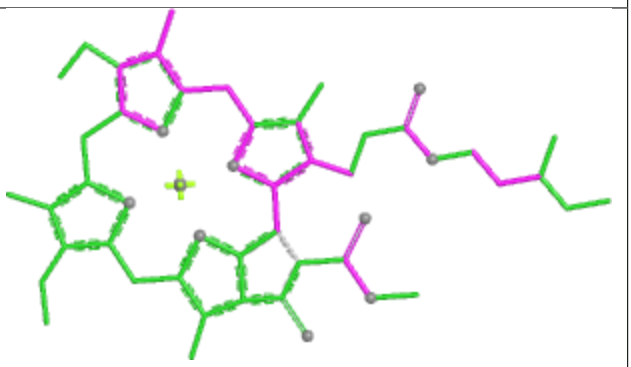


Rings

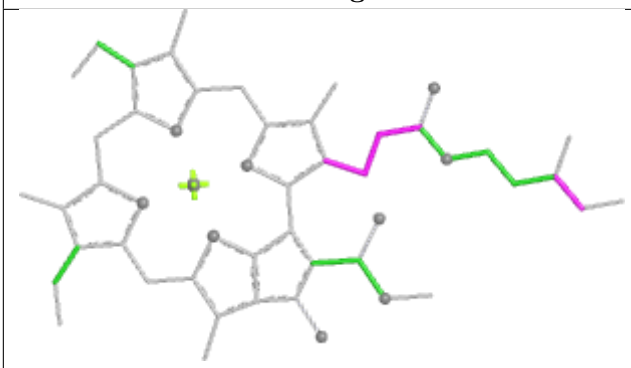
Ligand CLA R 203



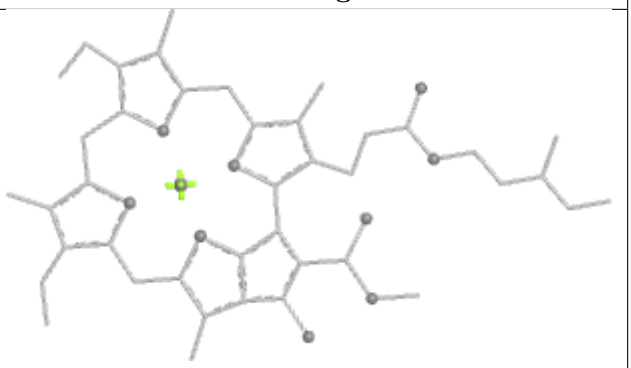
Bond lengths



Bond angles

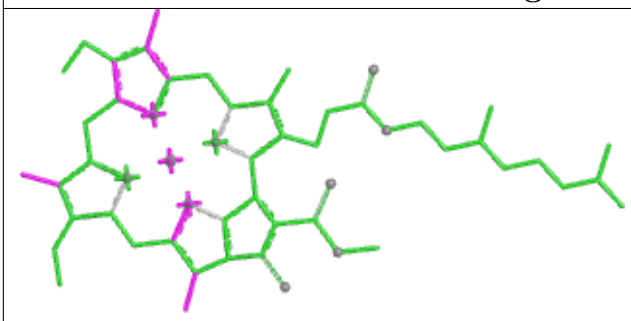


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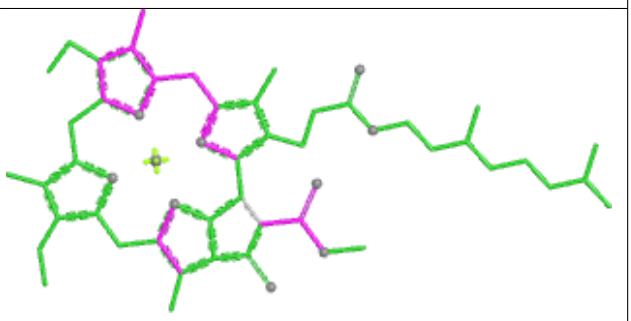


Rings

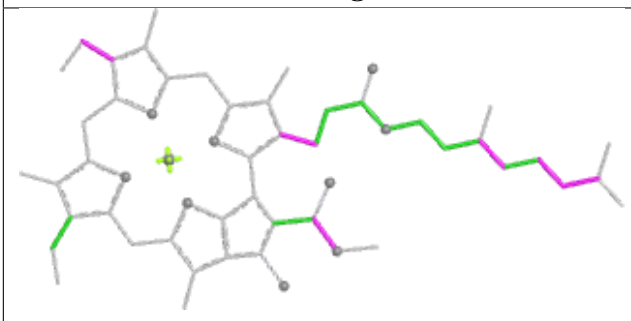
Ligand CLA B 818



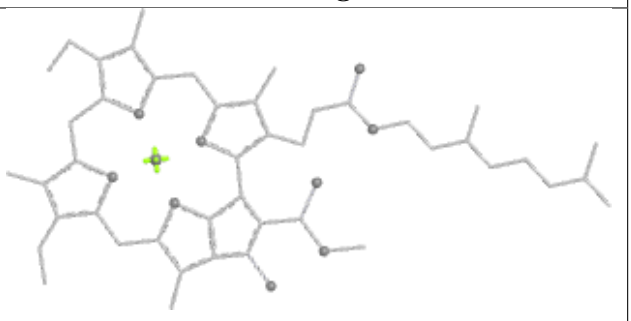
Bond lengths



Bond angles

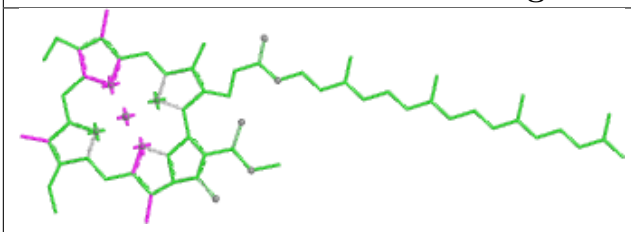


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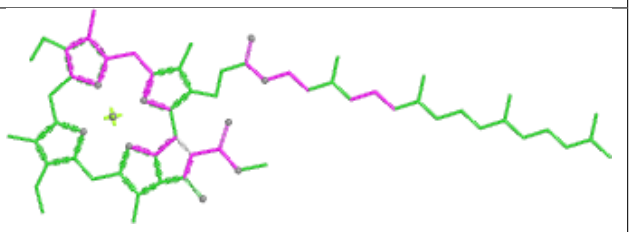


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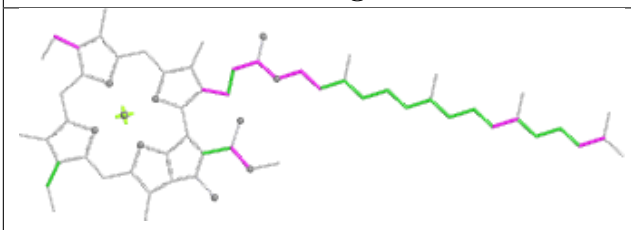
Ligand CLA h 301



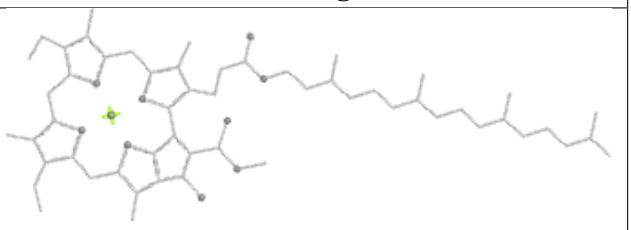
Bond lengths



Bond angles

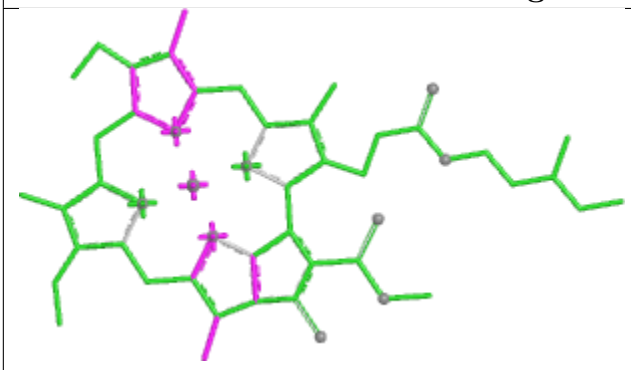


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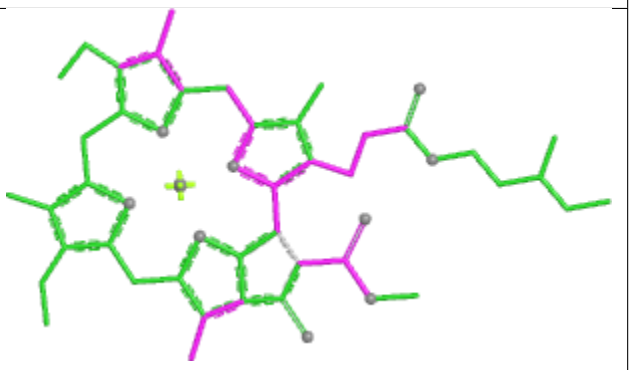


Rings

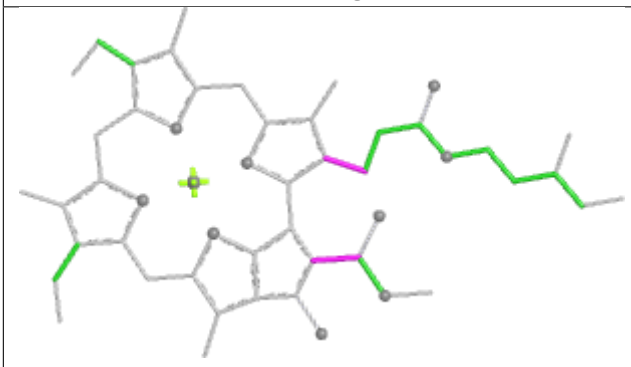
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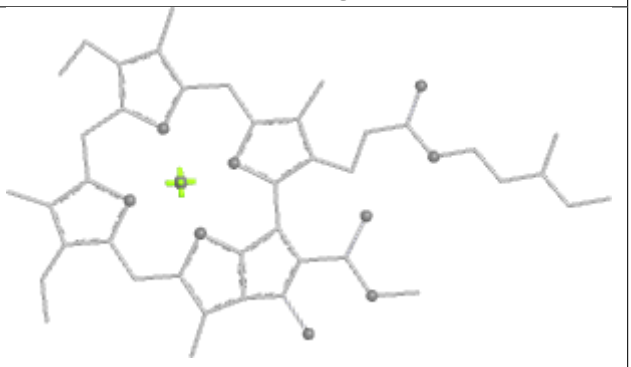
Bond lengths



Bond angles

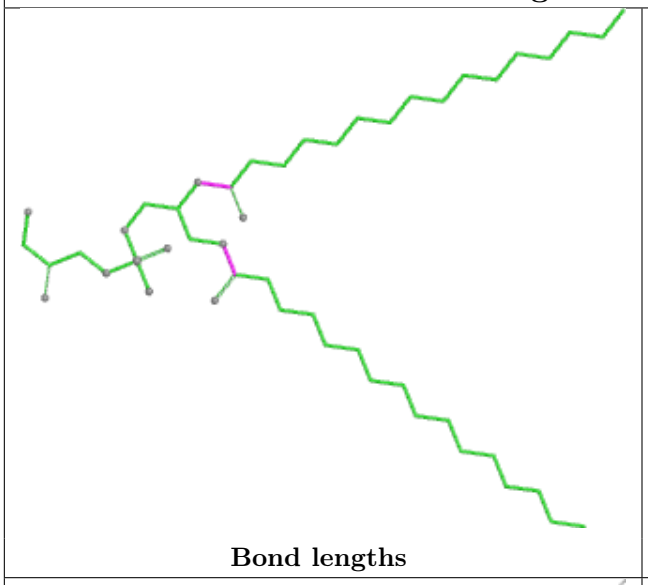


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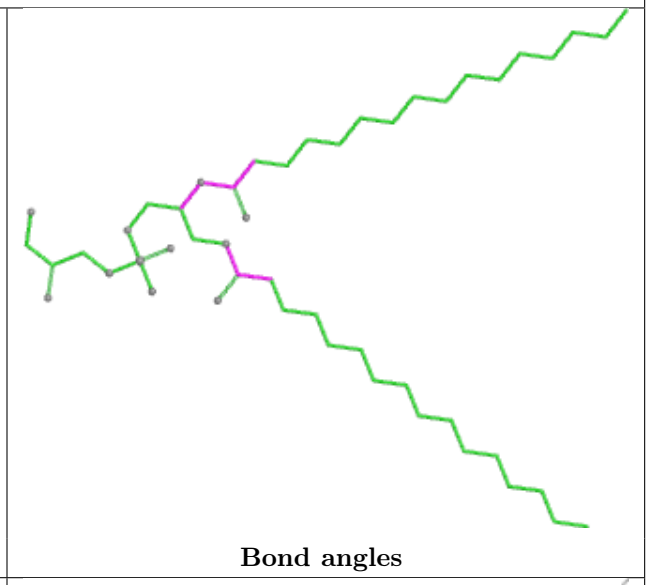


Rings

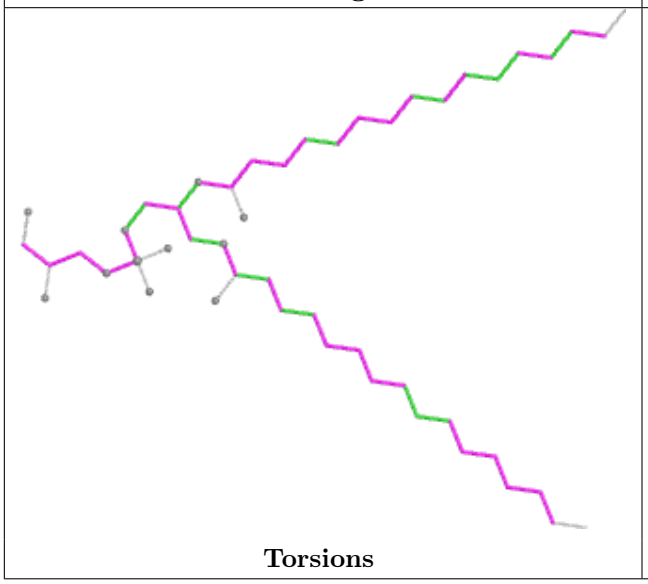
Ligand LHG f 619



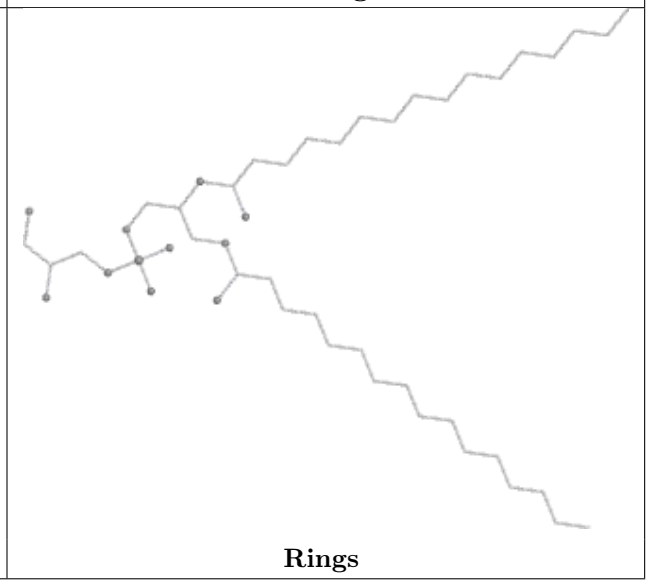
Bond lengths



Bond angles

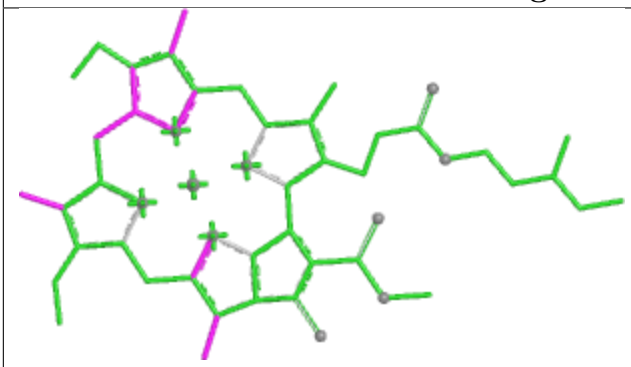


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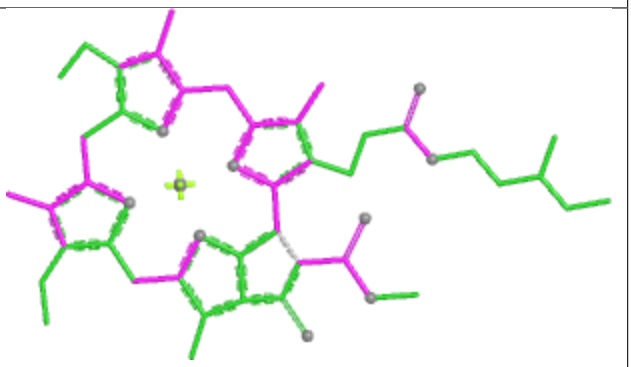


Rings

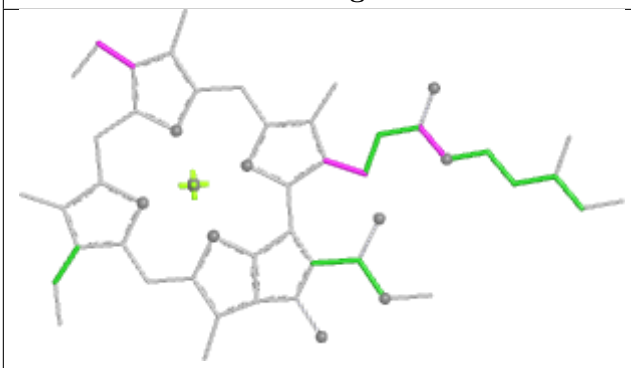
Ligand CLA s 208



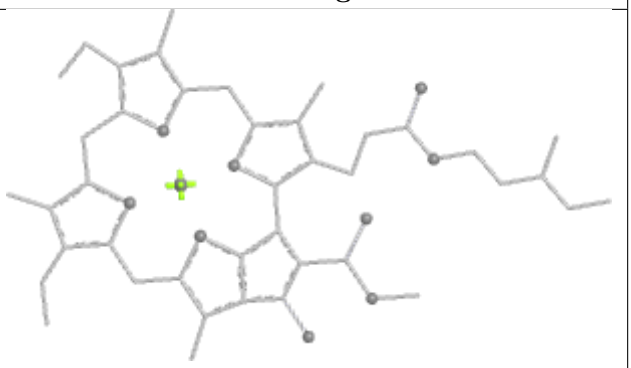
Bond lengths



Bond angles

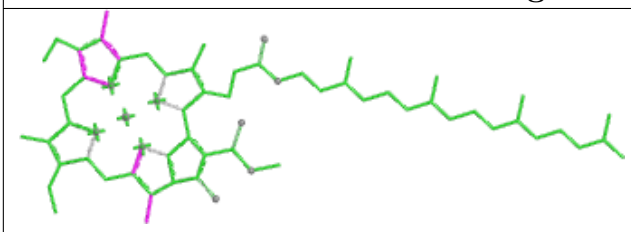


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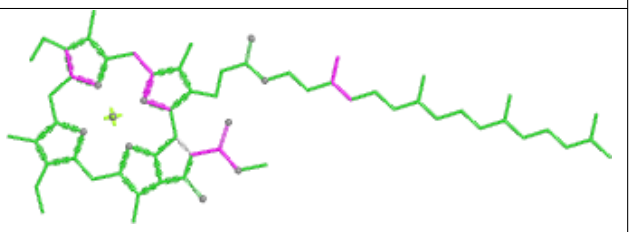


Rings

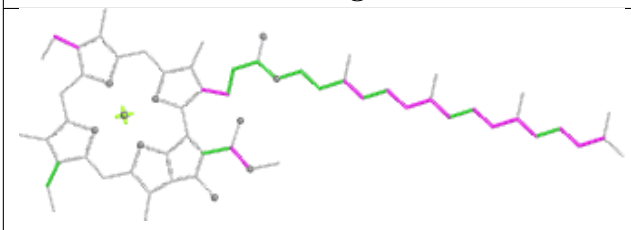
Ligand CLA b 610



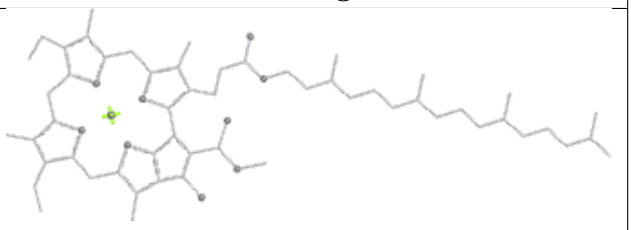
Bond lengths



Bond angles

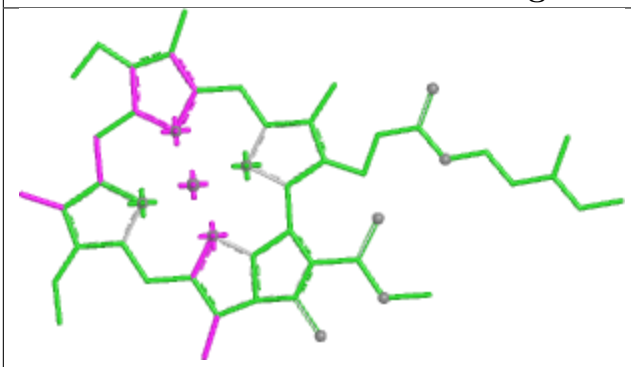


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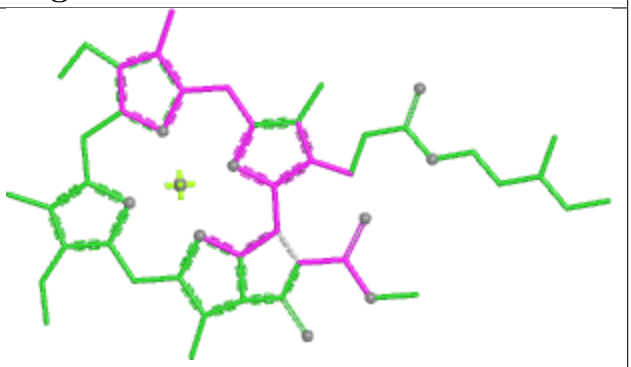


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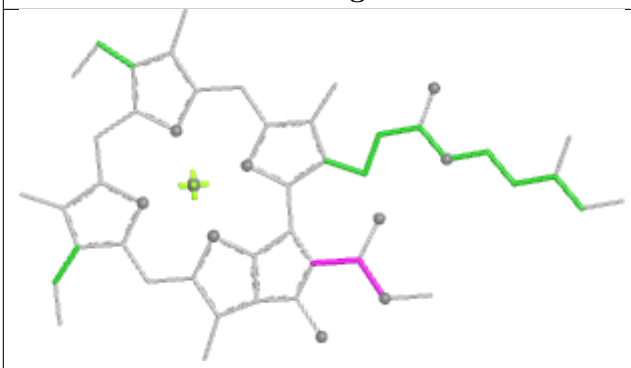
Ligand CLA g 304



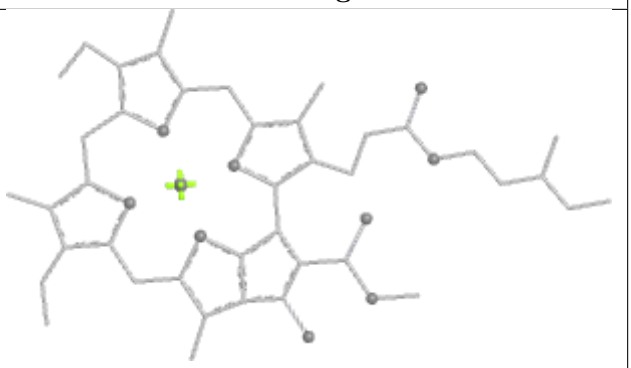
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Bond angles

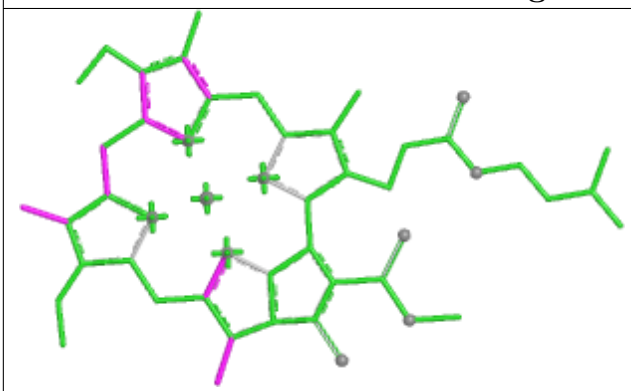


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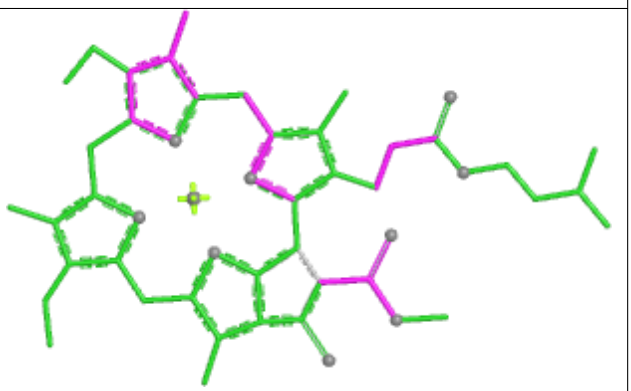


Rings

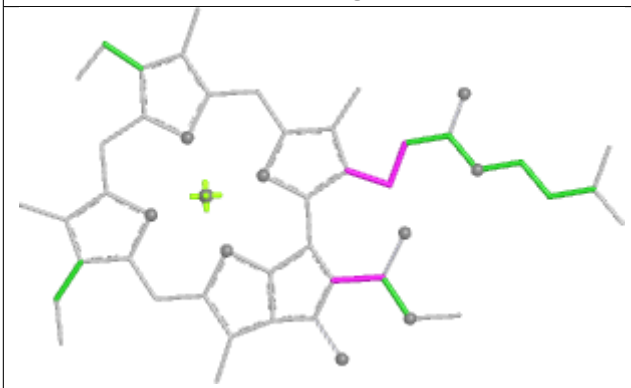
Ligand CLA a 304



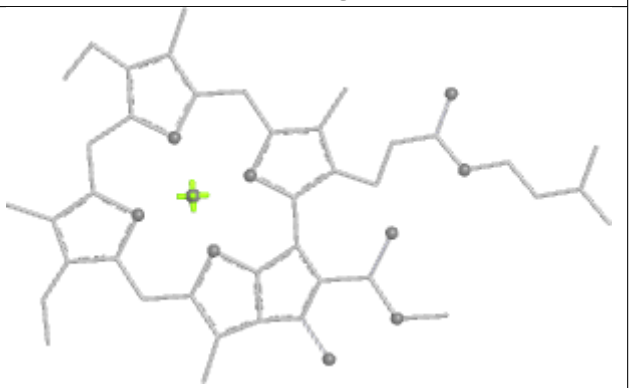
Bond lengths



Bond angles

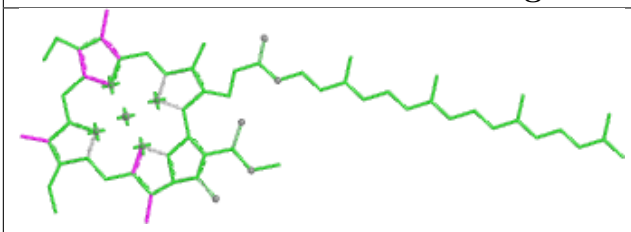


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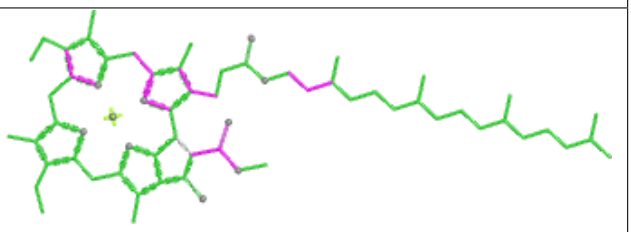


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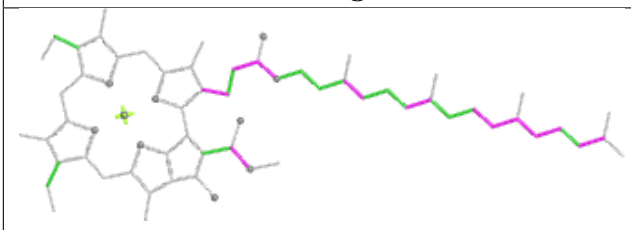
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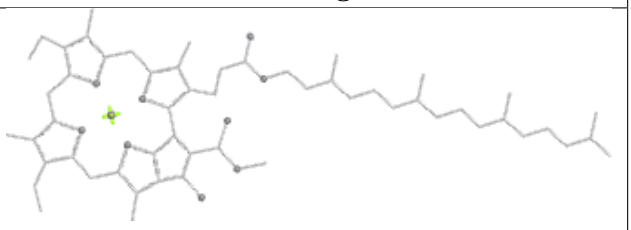
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Bond angles

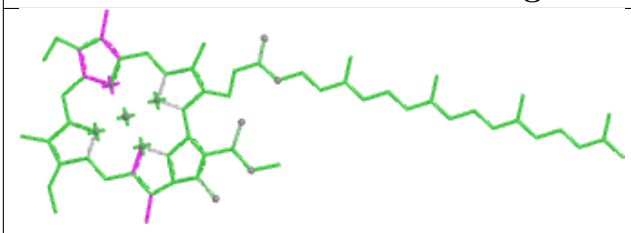


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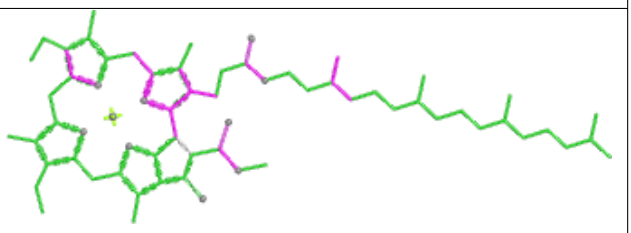


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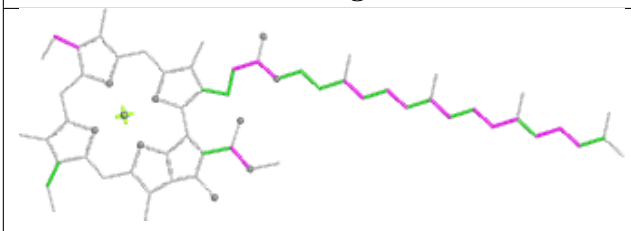
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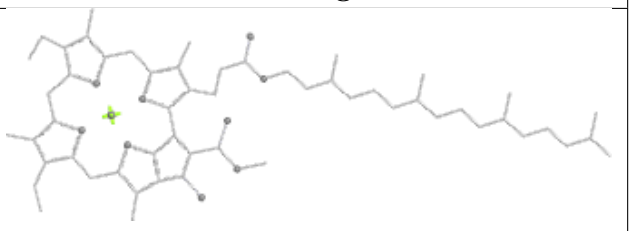
Bond lengths



Bond angles

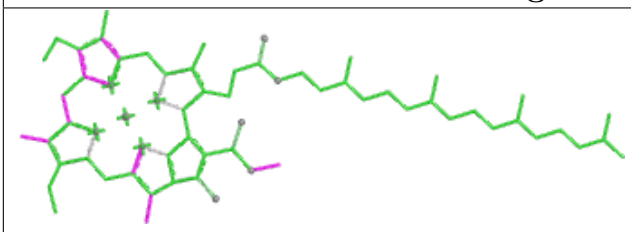


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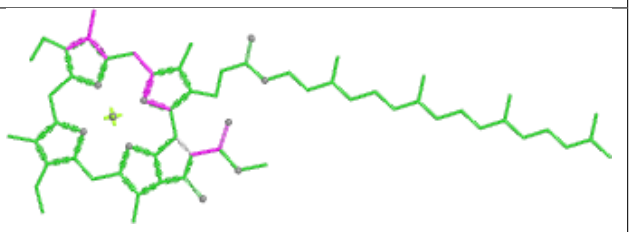


Rings

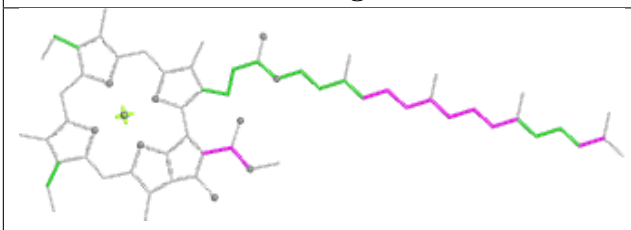
Ligand CLA b 604



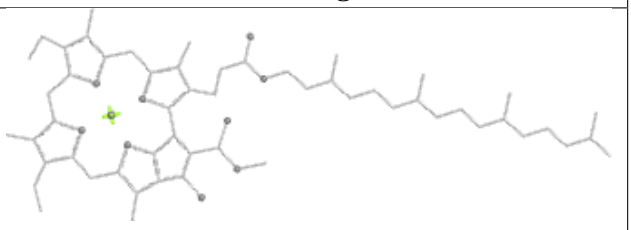
Bond lengths



Bond angles

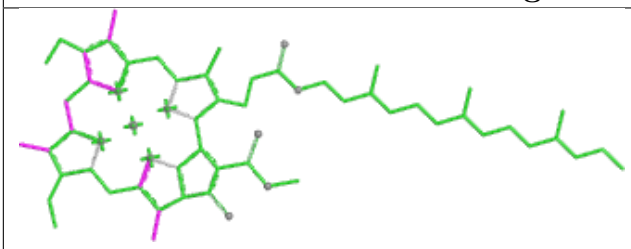


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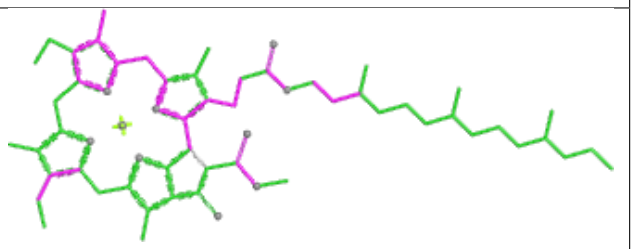


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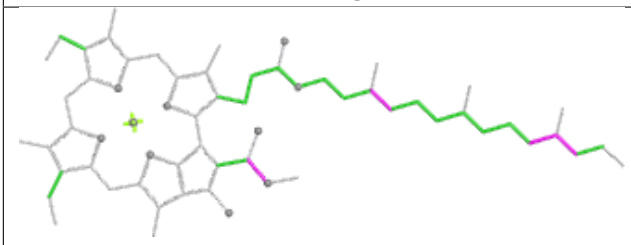
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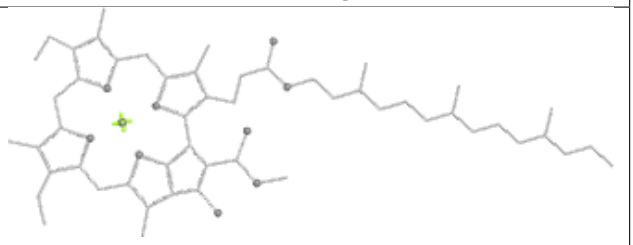
Bond lengths



Bond angles

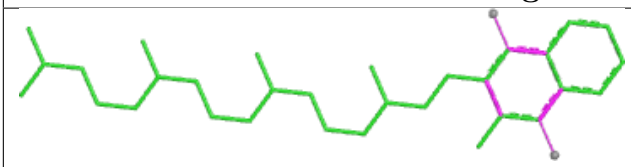


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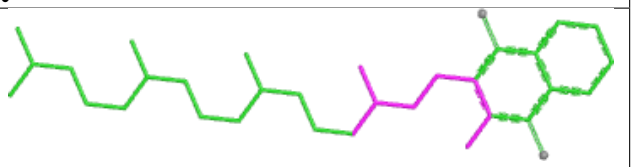


Rings

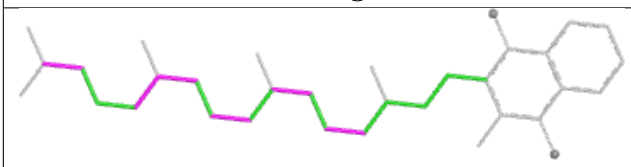
Ligand PQN B 841



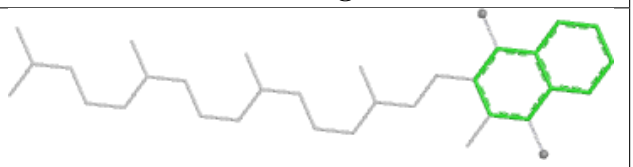
Bond lengths



Bond angles

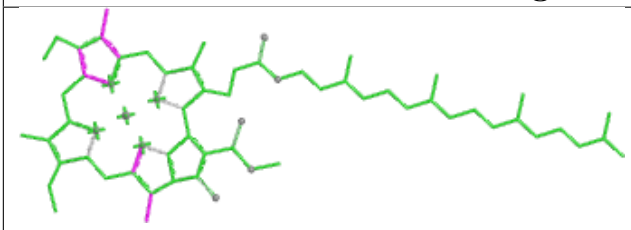


Torsions

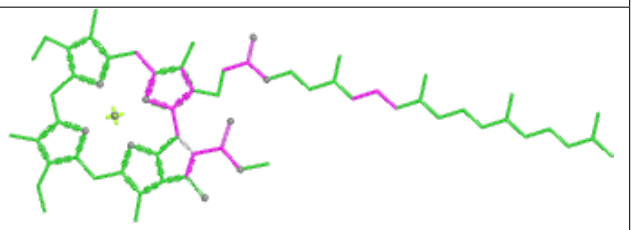


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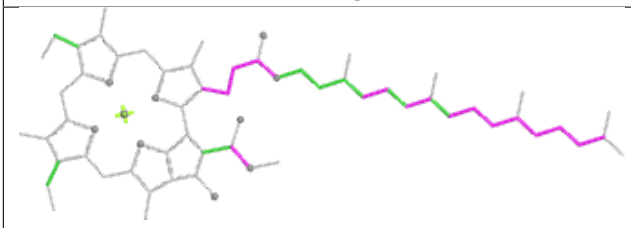
Ligand CLA f 613



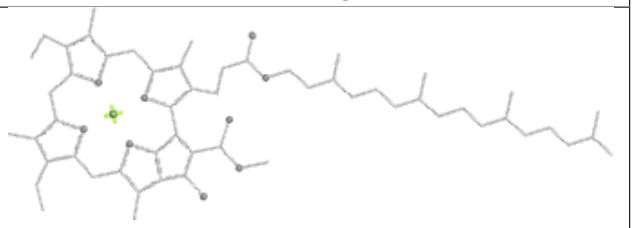
Bond lengths



Bond angles

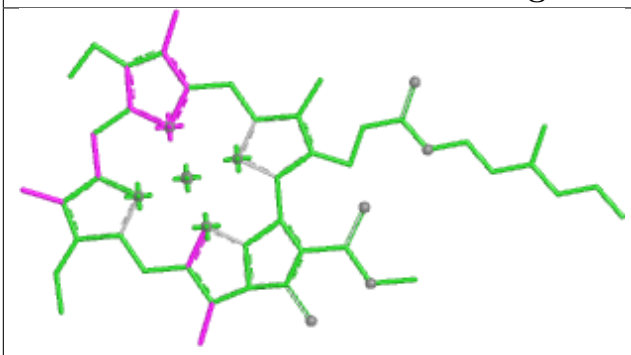


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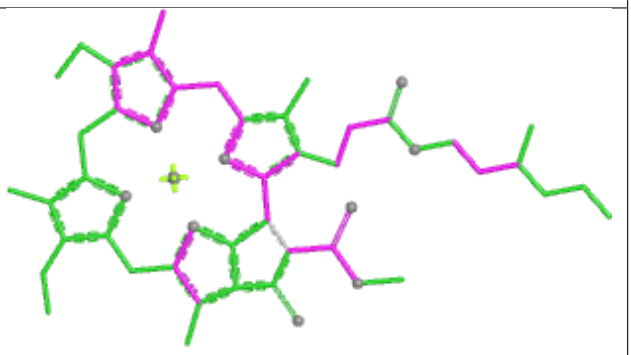


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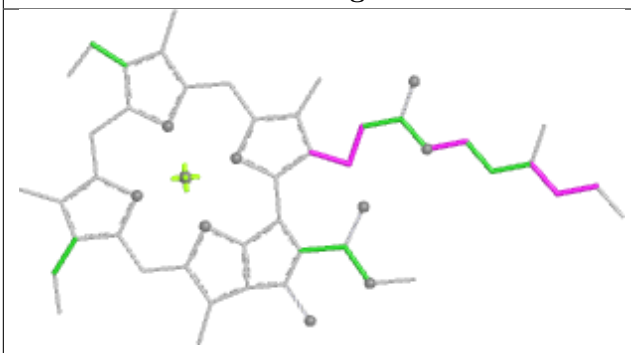
Ligand CLA a 303



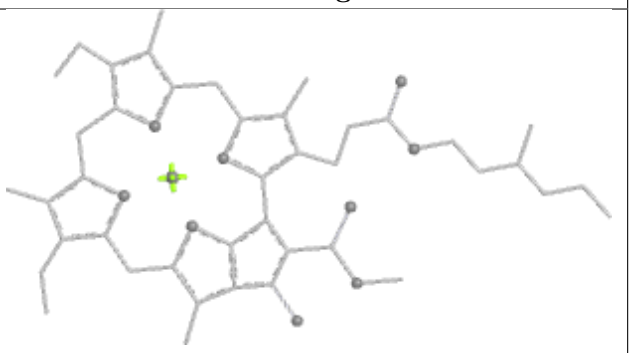
Bond lengths



Bond angles

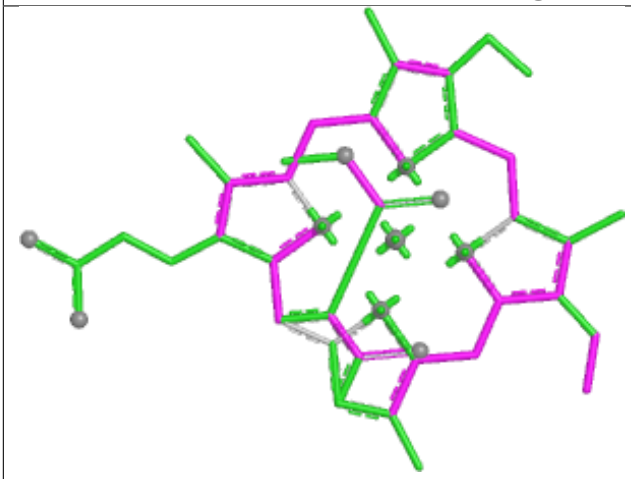


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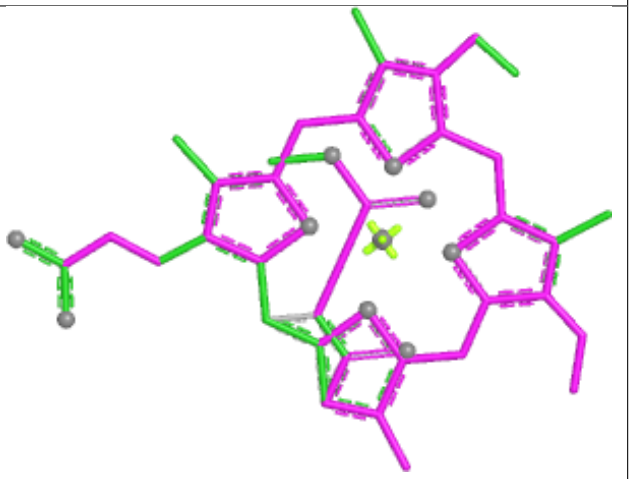


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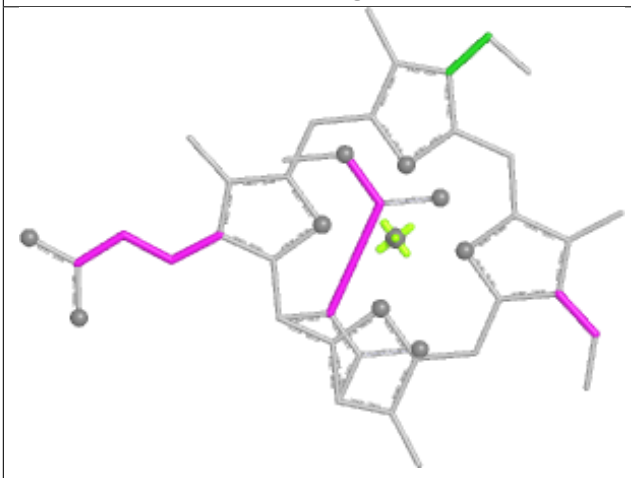
Ligand KC2 k 312



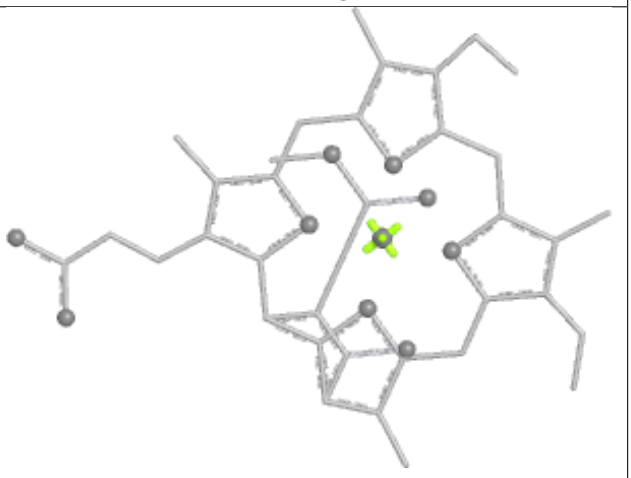
Bond lengths



Bond angles

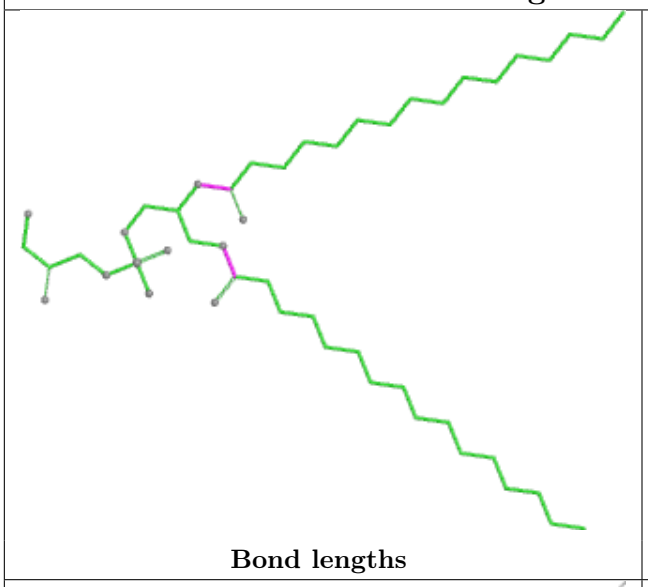


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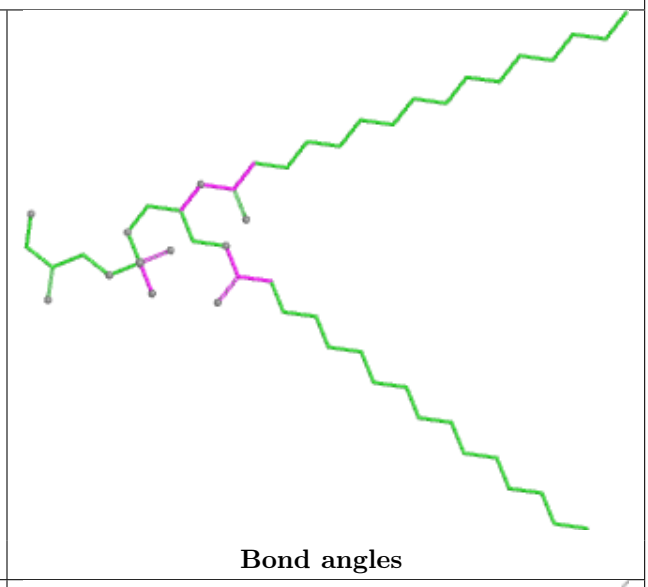


Rings

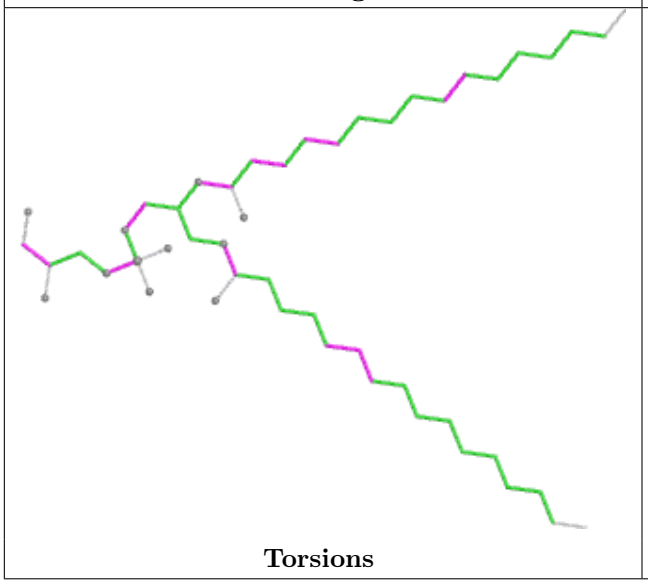
Ligand LHG a 301



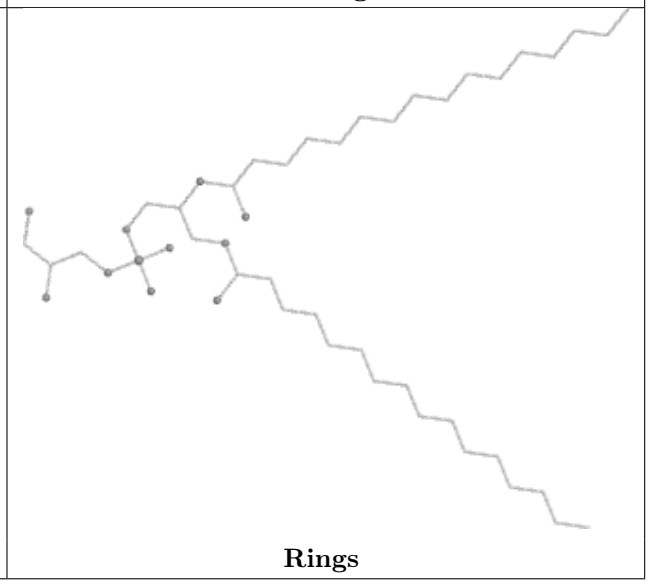
Bond lengths



Bond angles

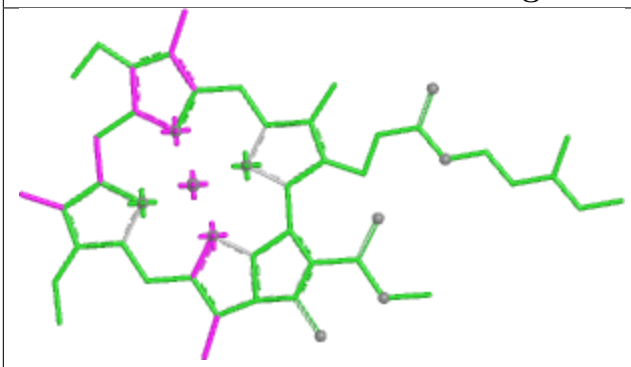


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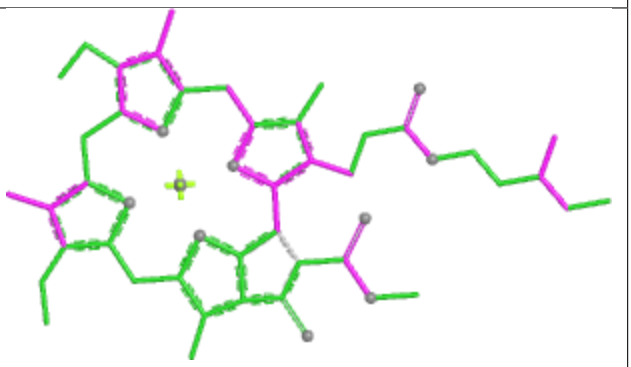


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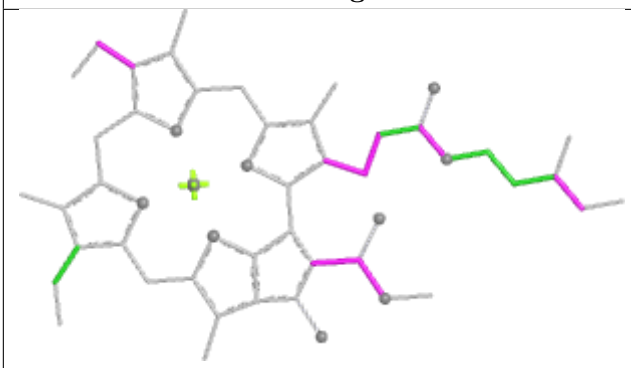
Ligand CLA m 611



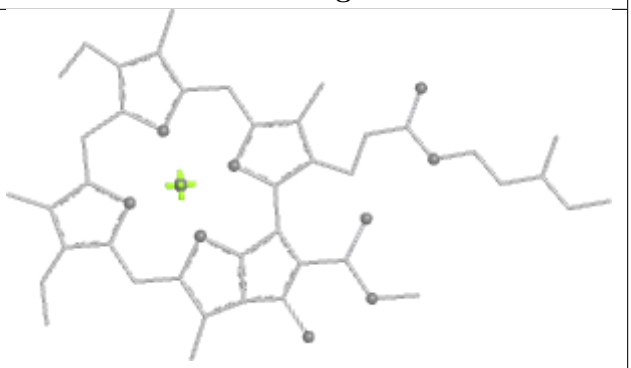
Bond lengths



Bond angles

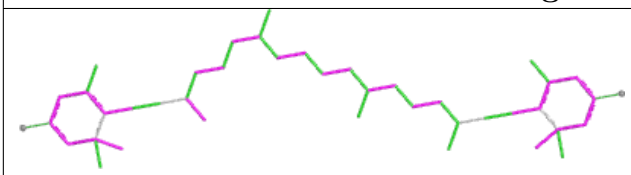


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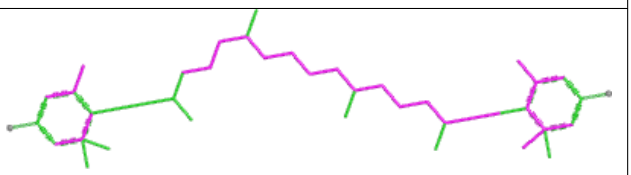


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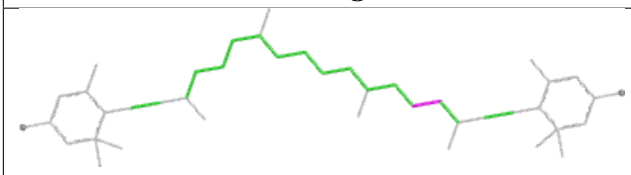
Ligand II0 b 612



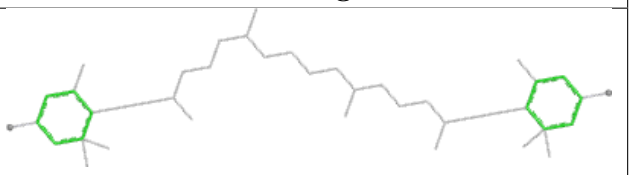
Bond lengths



Bond angles

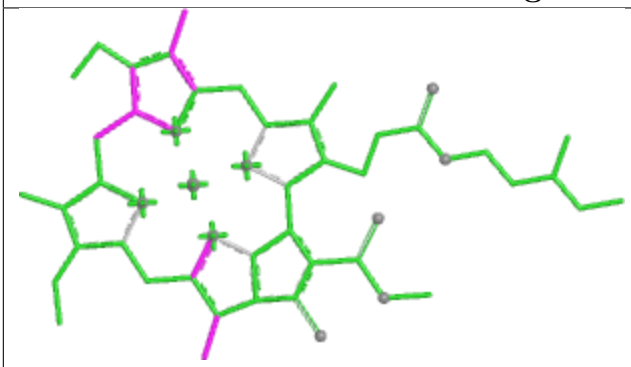


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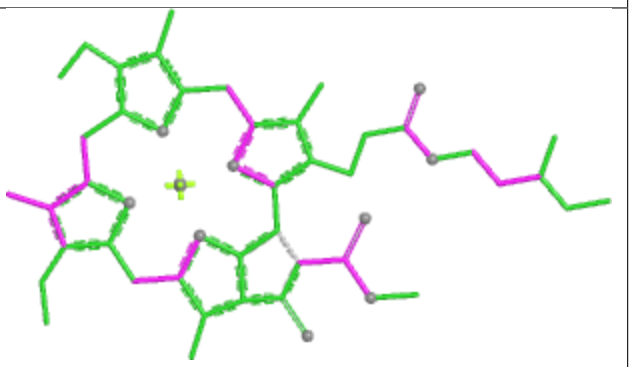


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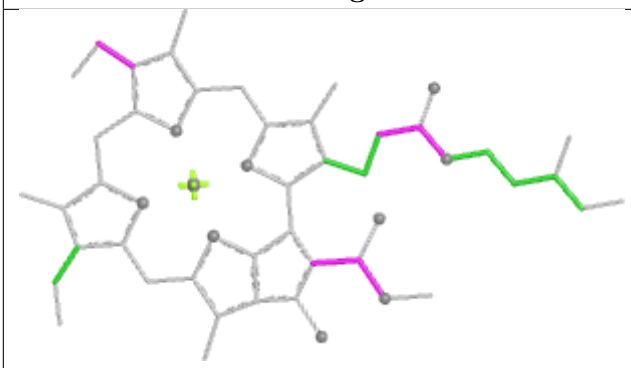
Ligand CLA B 849



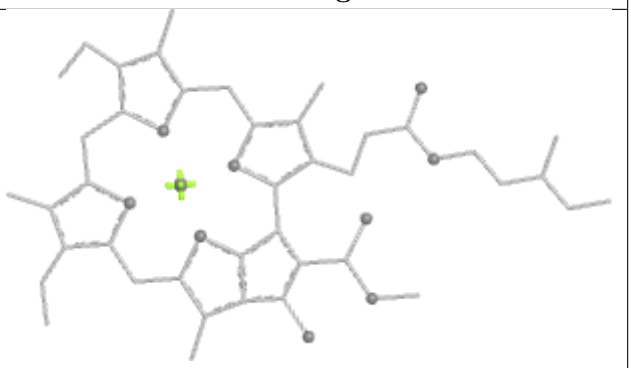
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Bond angles

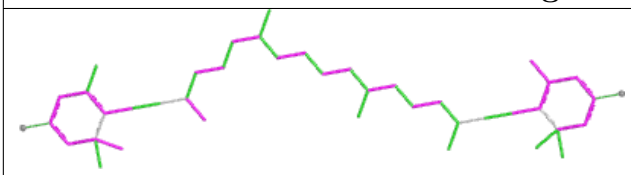


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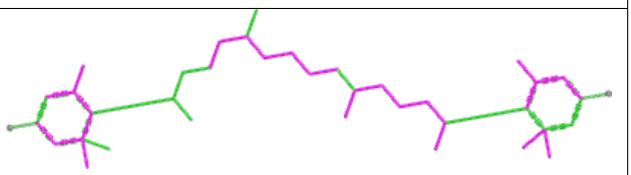


Rings

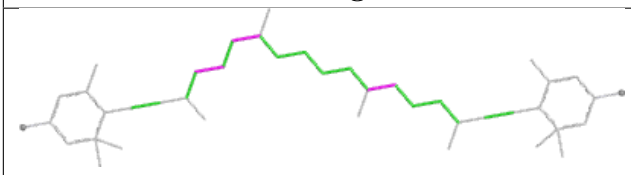
Ligand II0 n 618



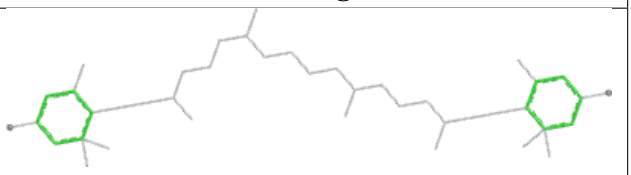
Bond lengths



Bond angles

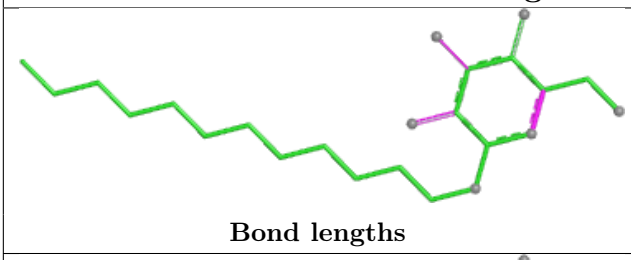


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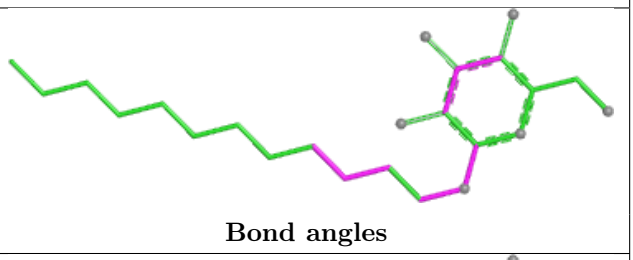


Rings

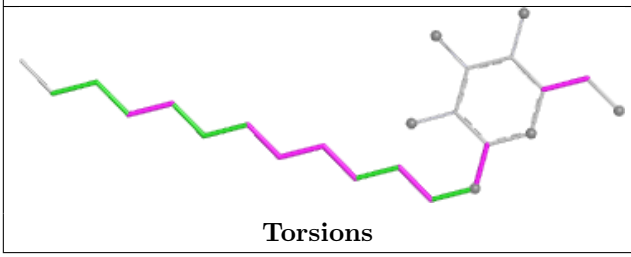
Ligand LMT b 616



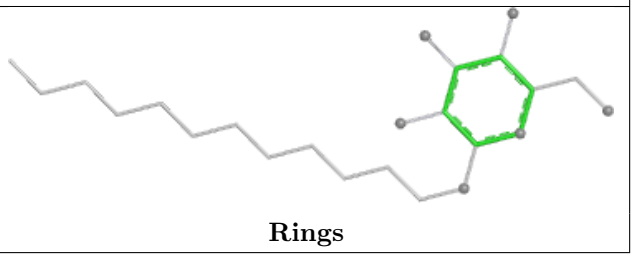
Bond lengths



Bond angles

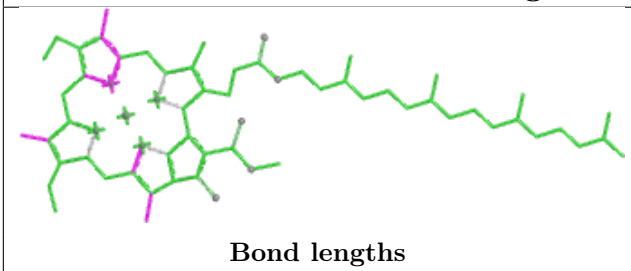


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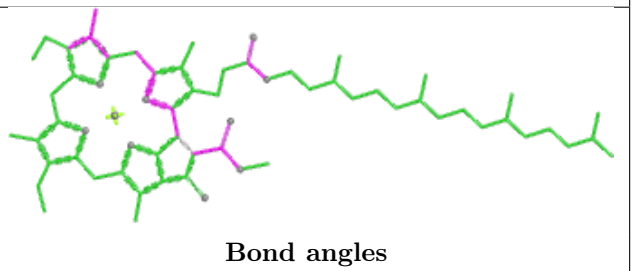


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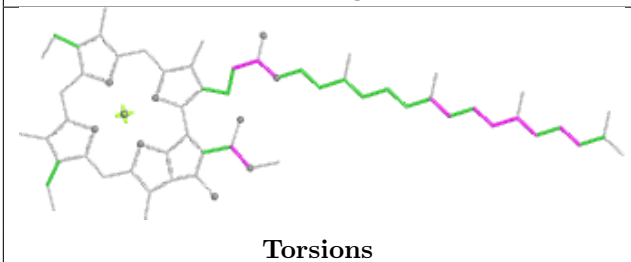
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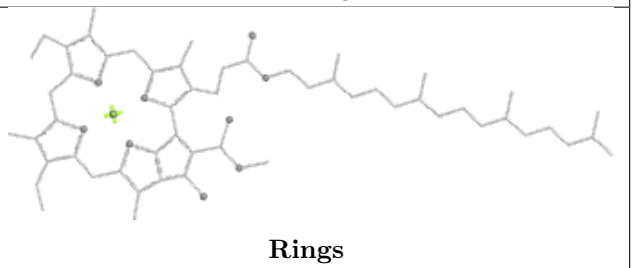
Bond lengths



Bond angles

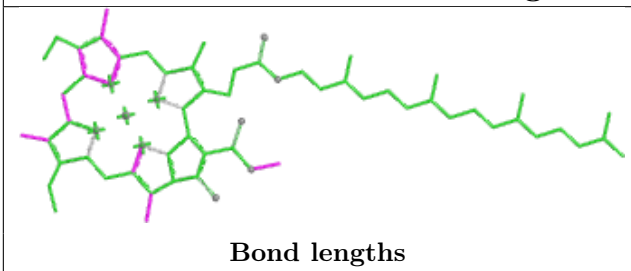


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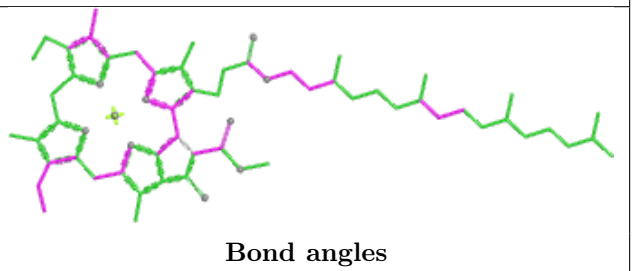


Rings

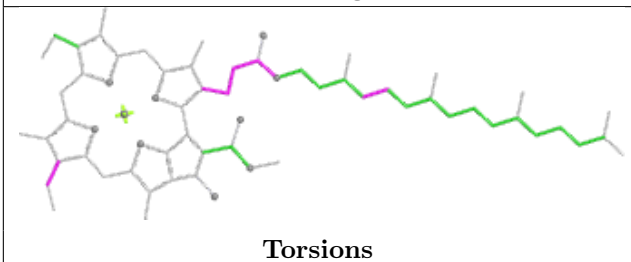
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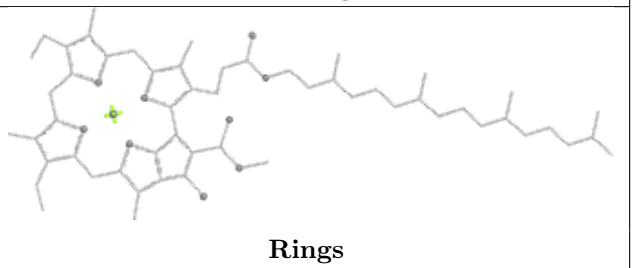
Bond lengths



Bond angles

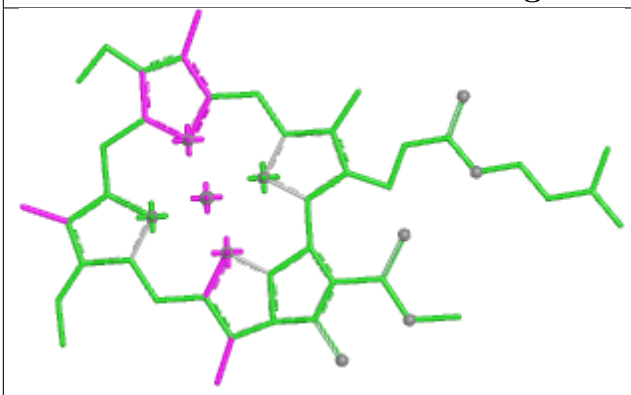


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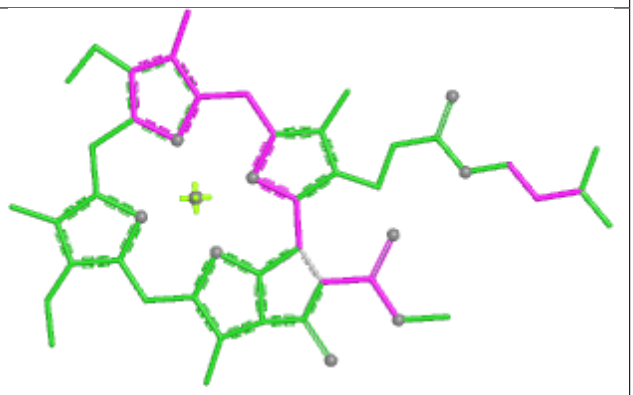


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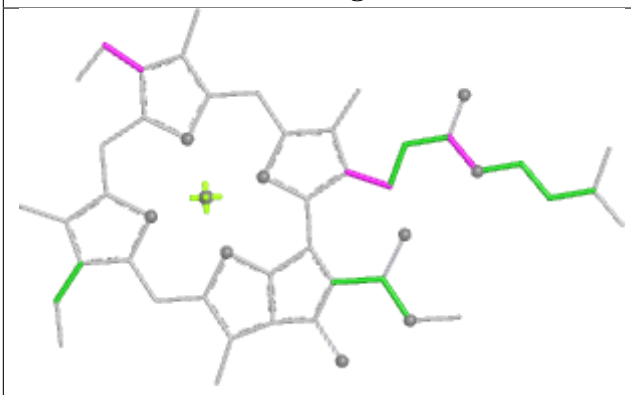
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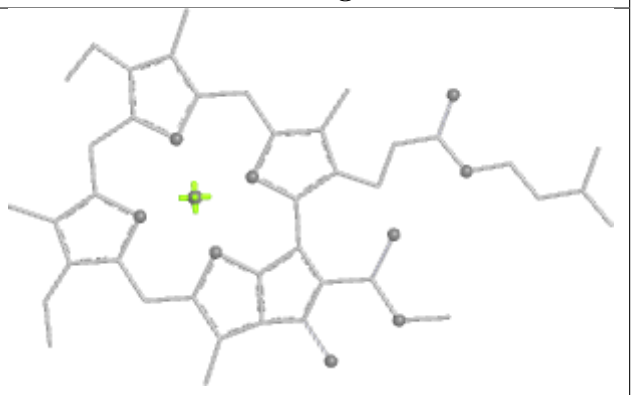
Bond lengths



Bond angles

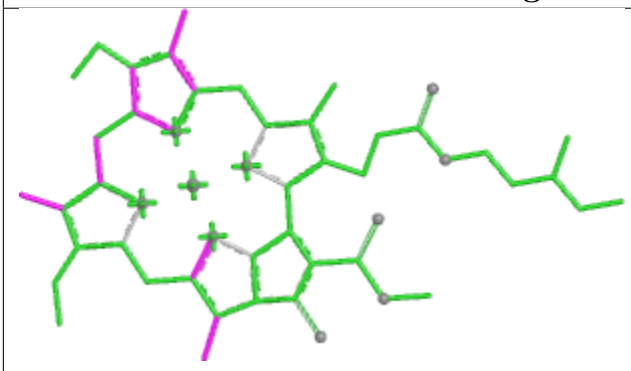


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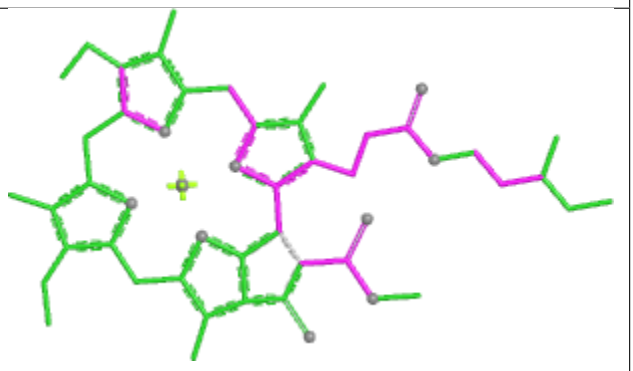


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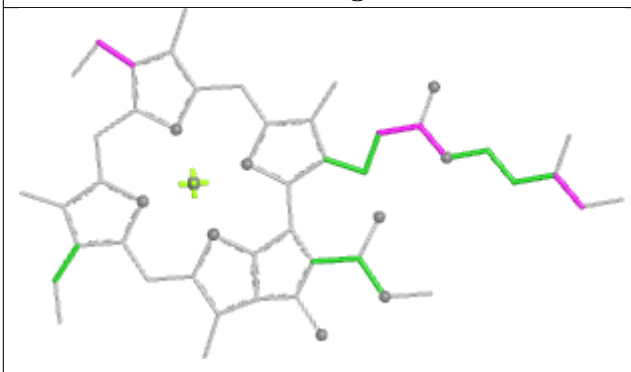
Ligand CLA K 101



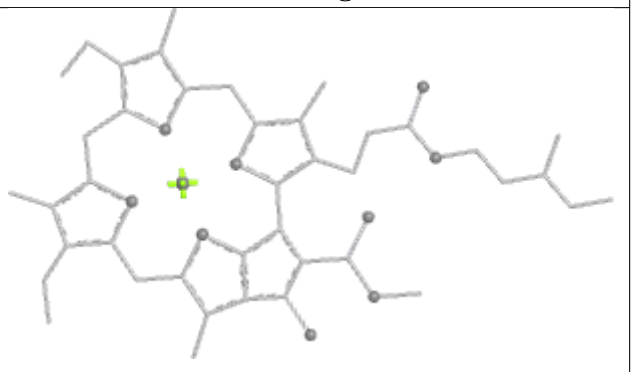
Bond lengths



Bond angles

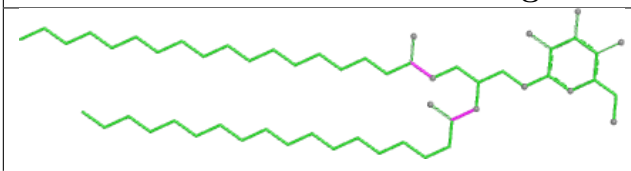


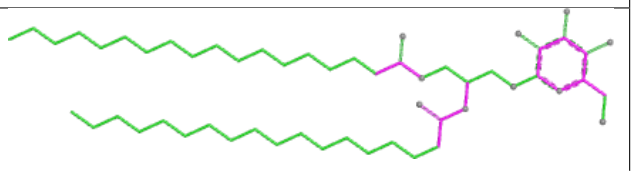
Torsions

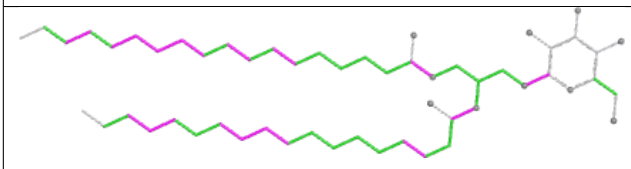


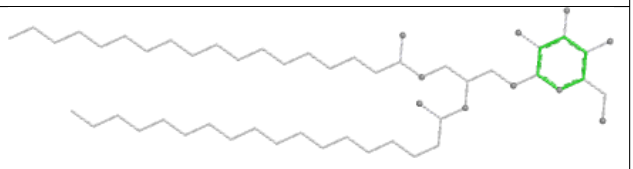
Rings

Ligand LMG L 208

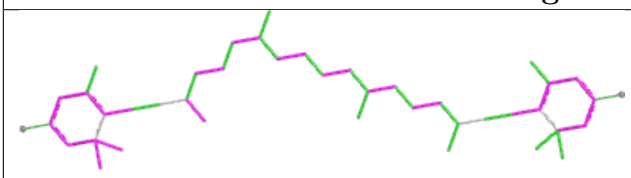

Bond lengths

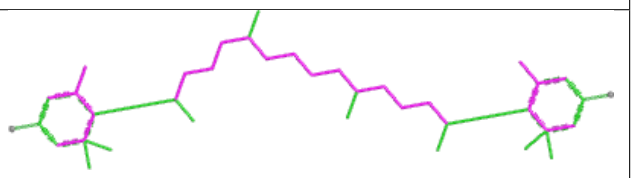

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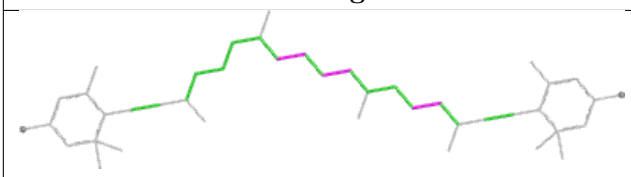

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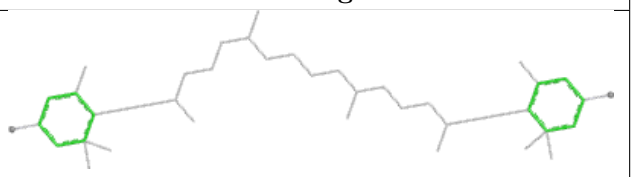

Rings

Ligand II0 n 616

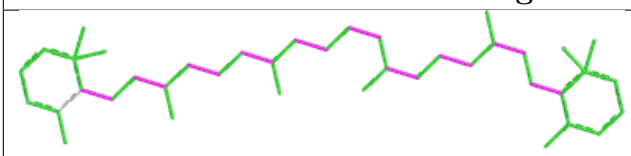

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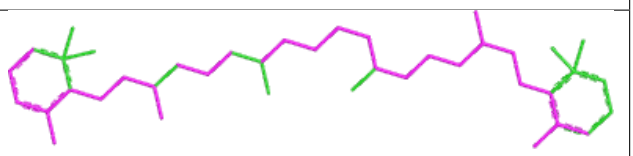

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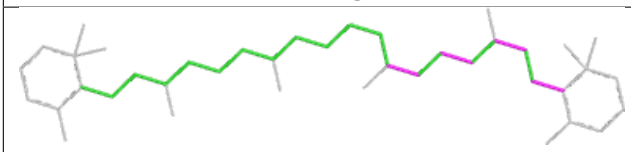

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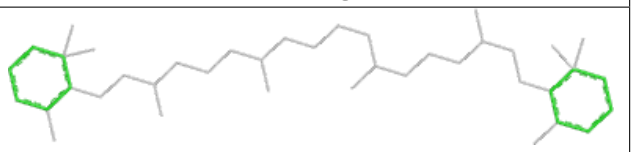

Rings

Ligand WVN B 846

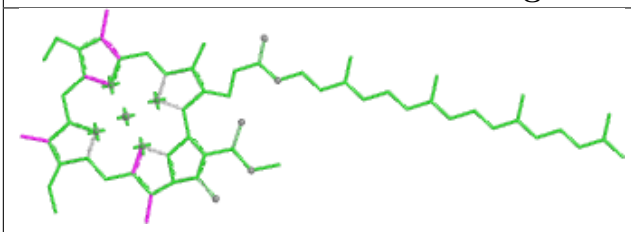

Bond lengths


Bond angles

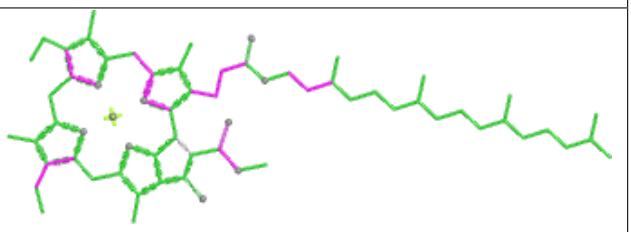

Torsions


Rings

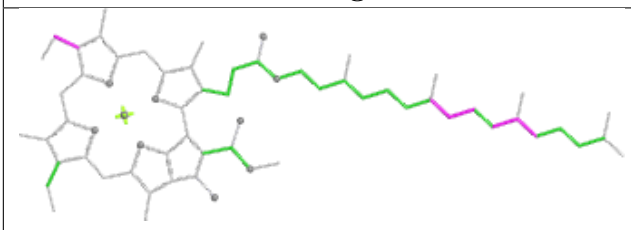
Ligand CLA A 853



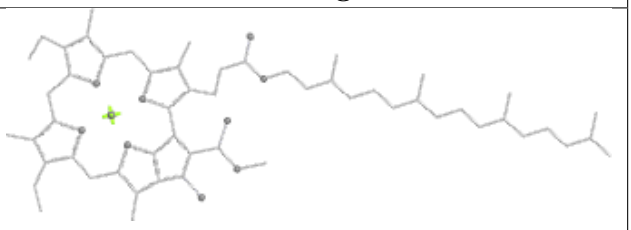
Bond lengths



Bond angles

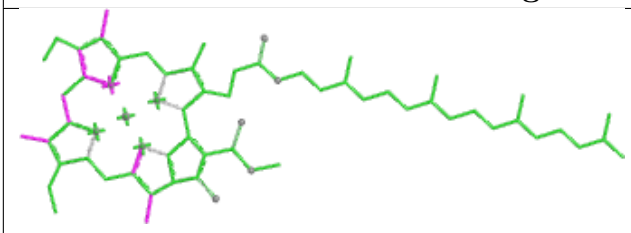


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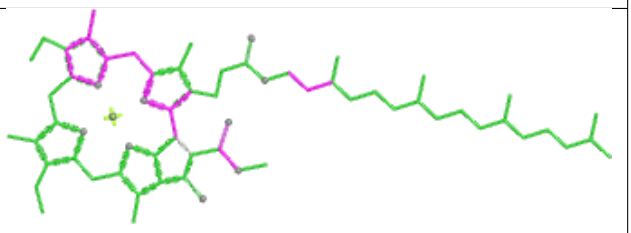


Rings

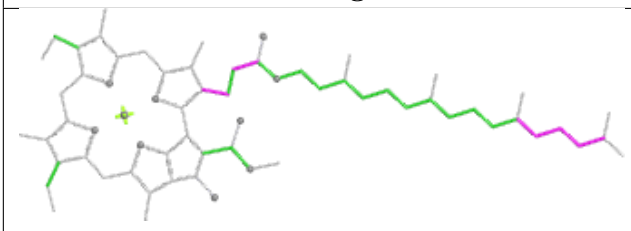
Ligand CLA m 607



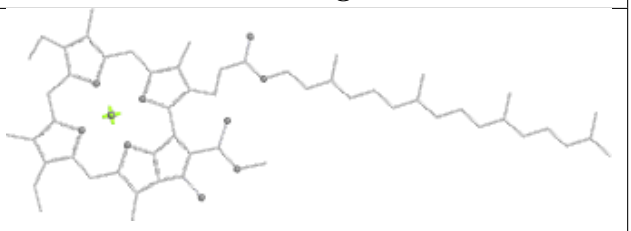
Bond lengths



Bond angles

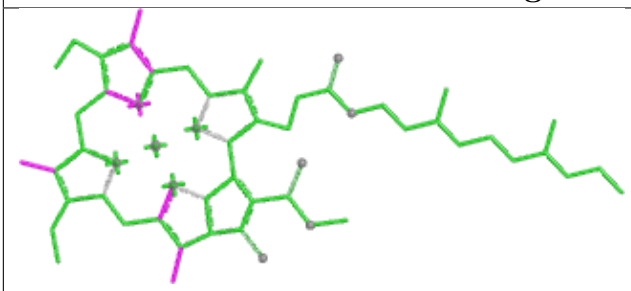


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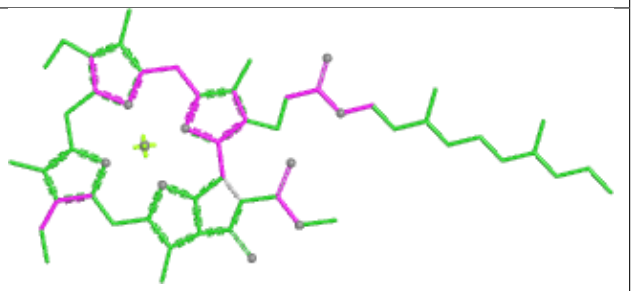


Rings

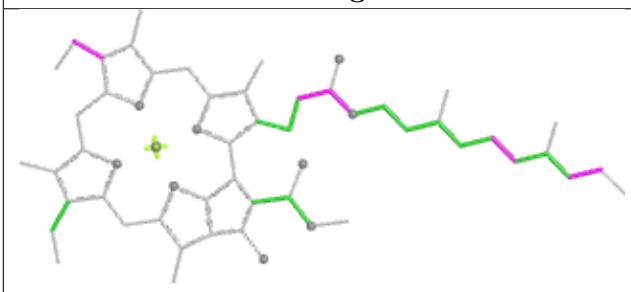
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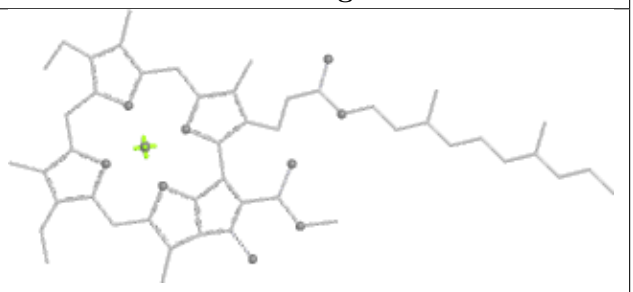
Bond lengths



Bond angles

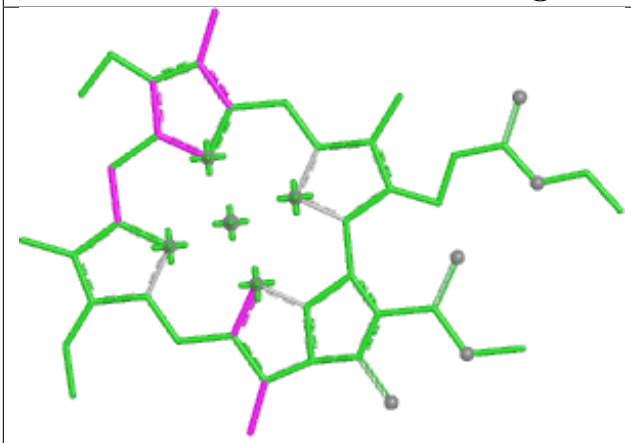


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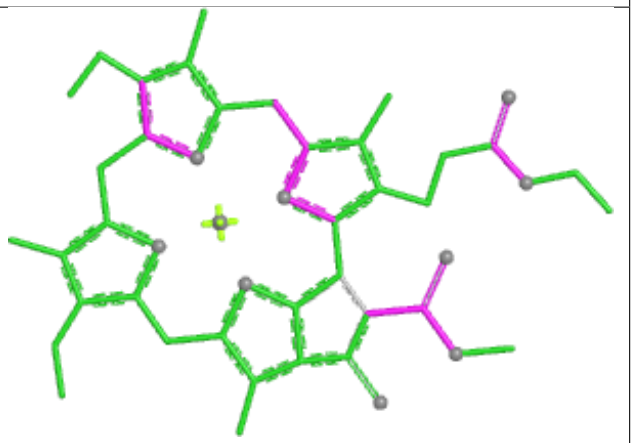


Rings

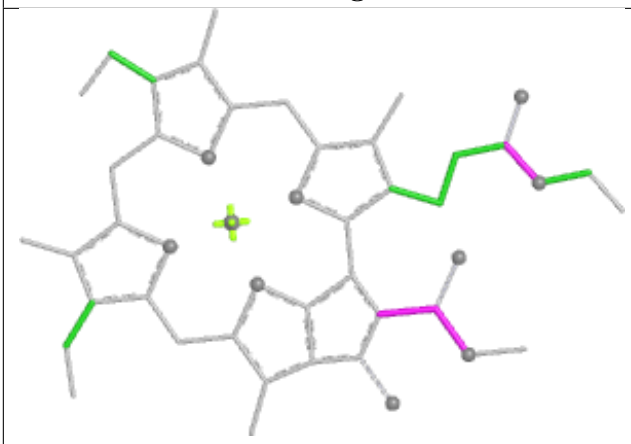
Ligand CLA f 601



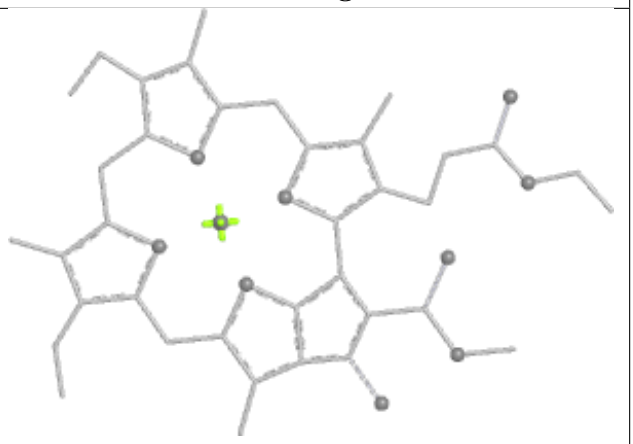
Bond lengths



Bond angles

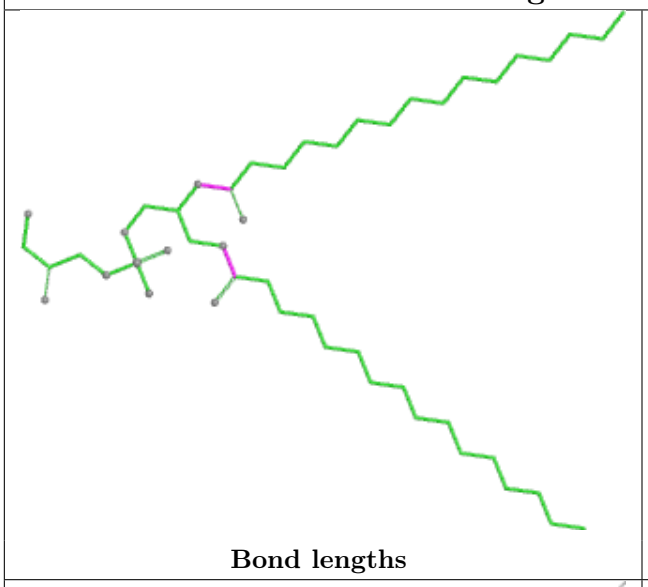


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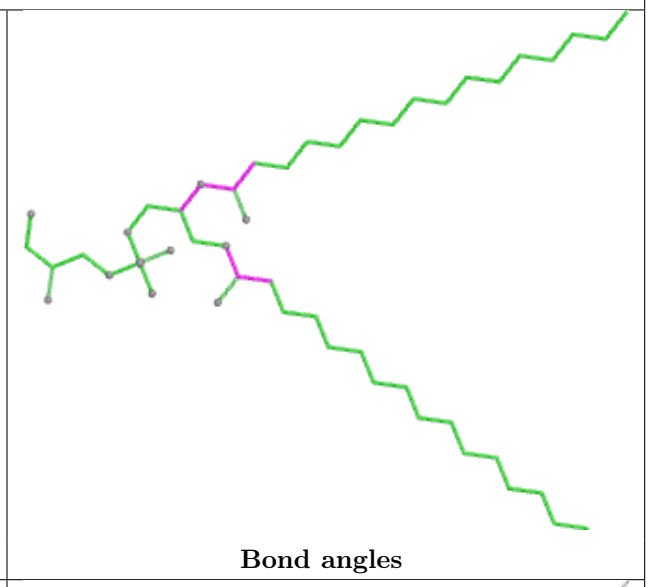


Rings

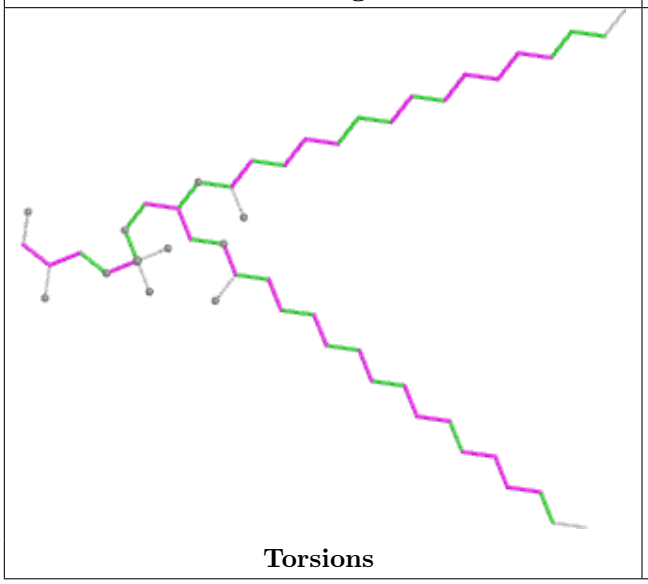
Ligand LHG J 107



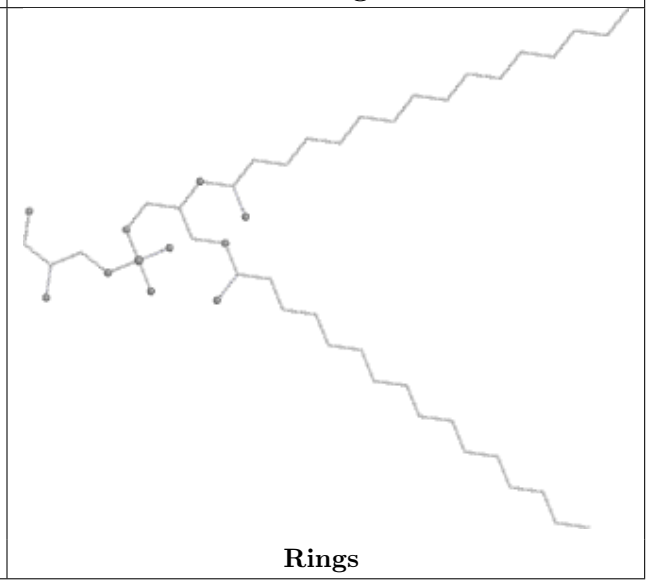
Bond lengths



Bond angles

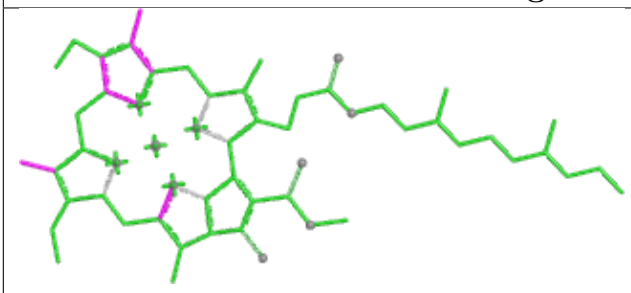


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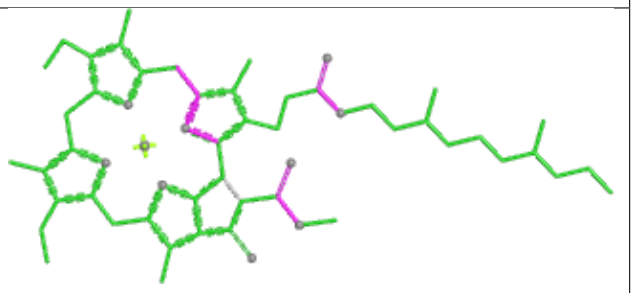


Rings

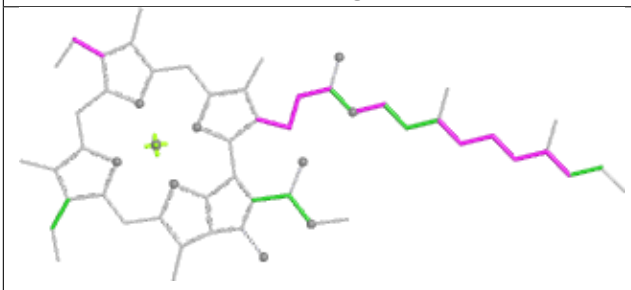
Ligand CLA h 307



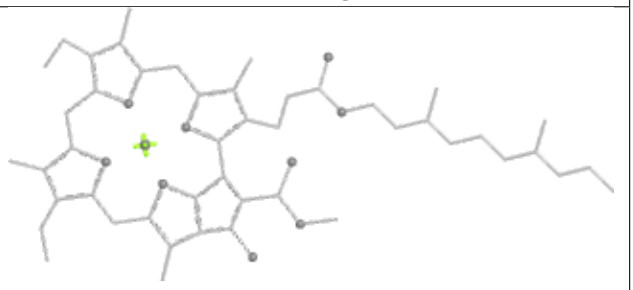
Bond lengths



Bond angles

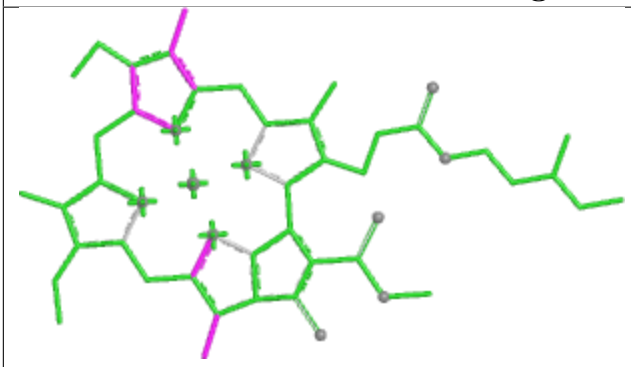


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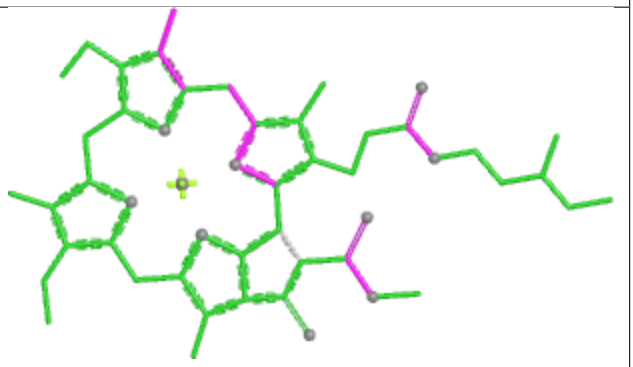


Rings

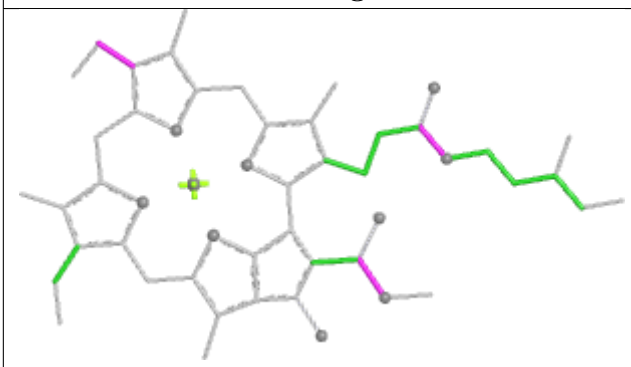
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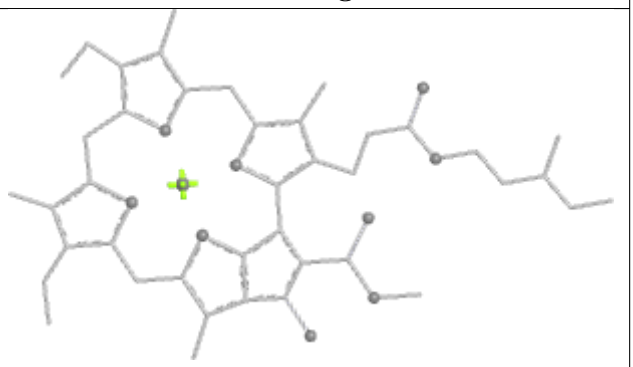
Bond lengths



Bond angles

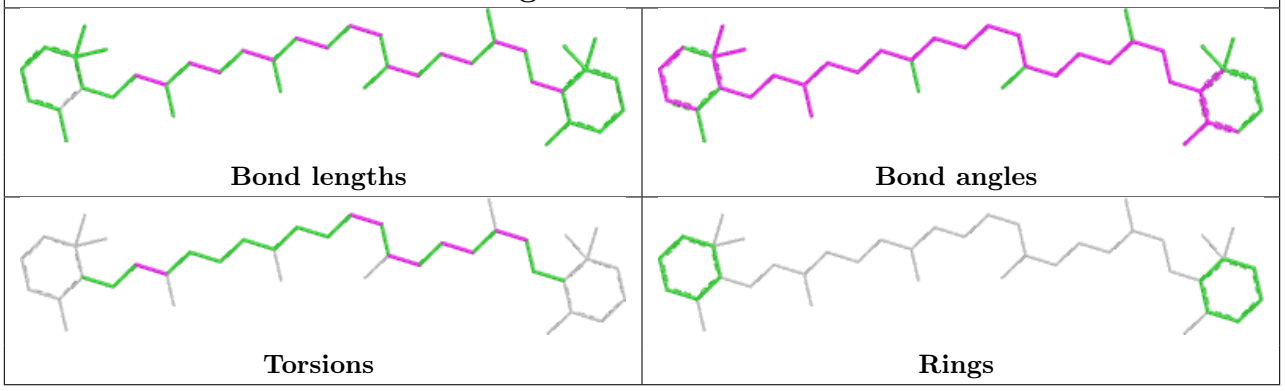


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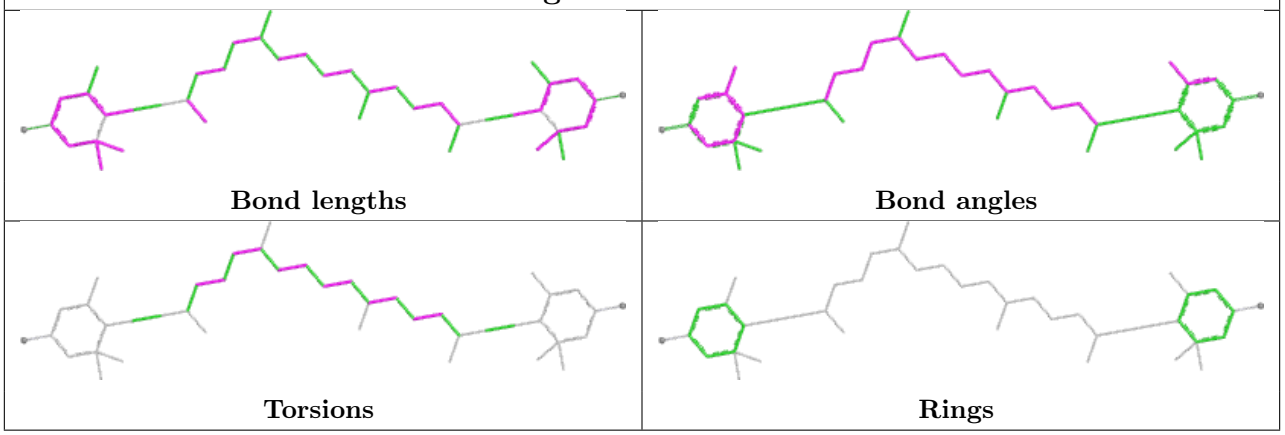


Rings

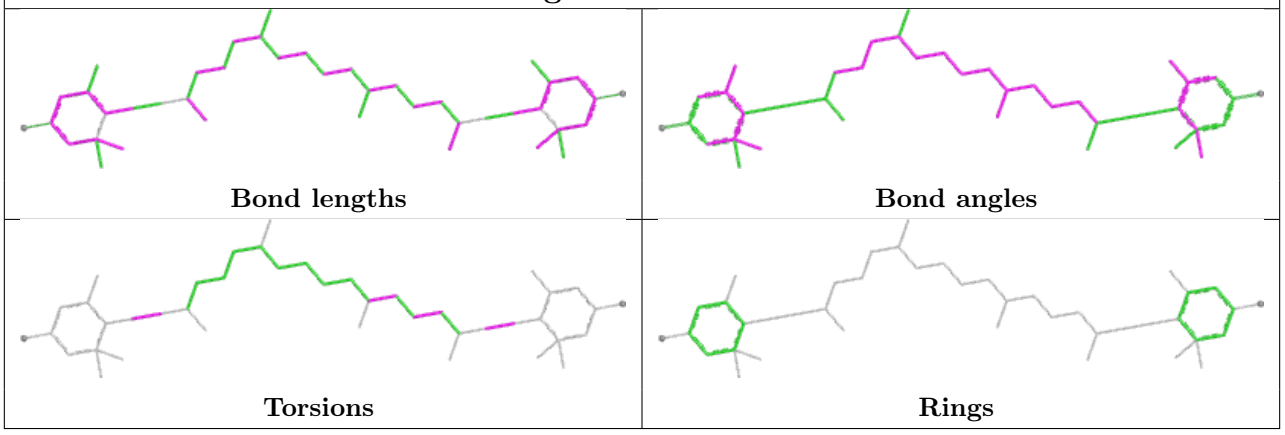
Ligand WVN h 309



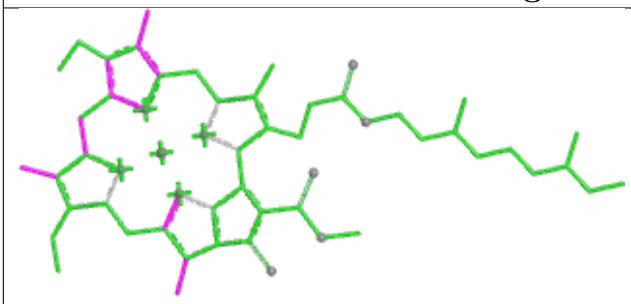
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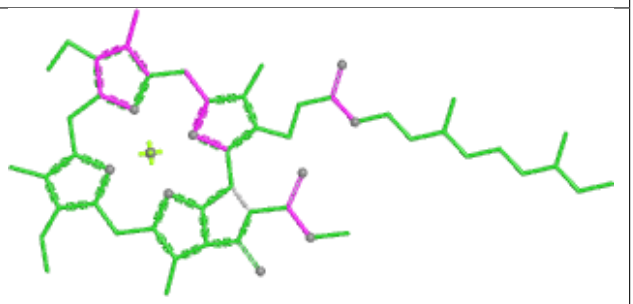
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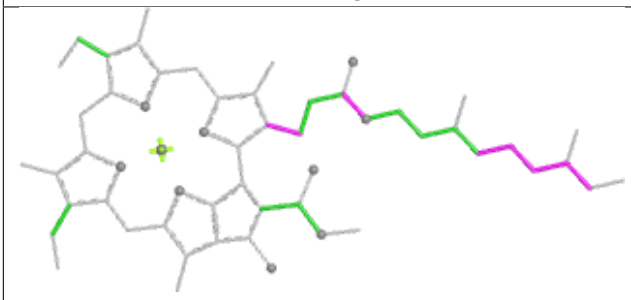
Ligand CLA A 809



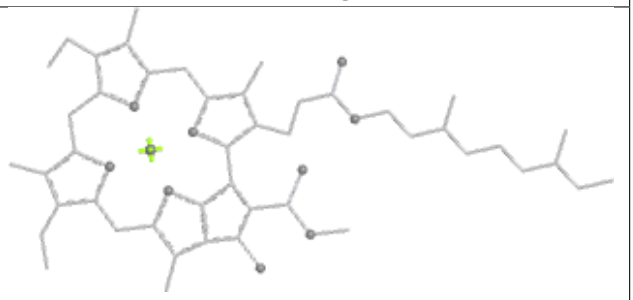
Bond lengths



Bond angles

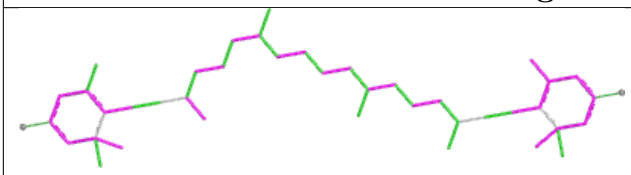


Torsions

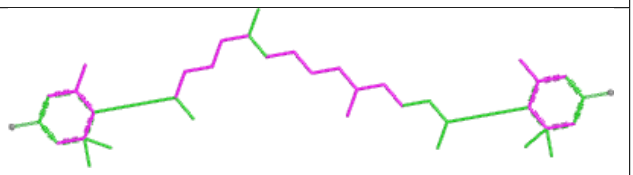


Rings

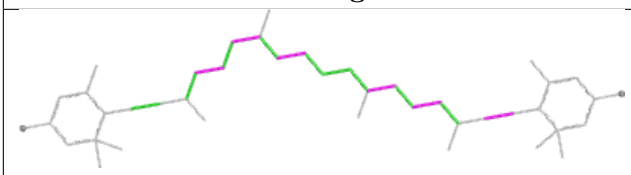
Ligand II0 m 614



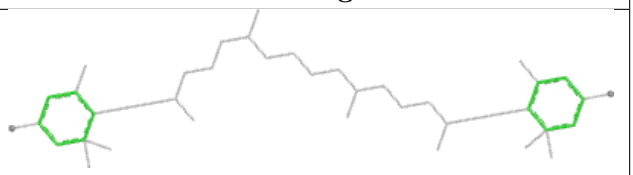
Bond lengths



Bond angles

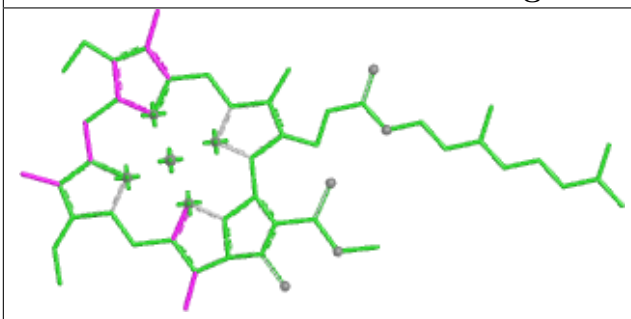


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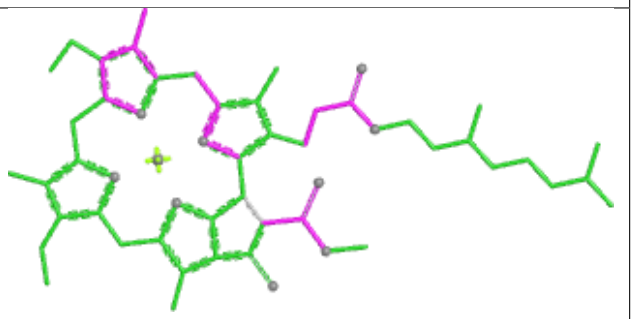


Rings

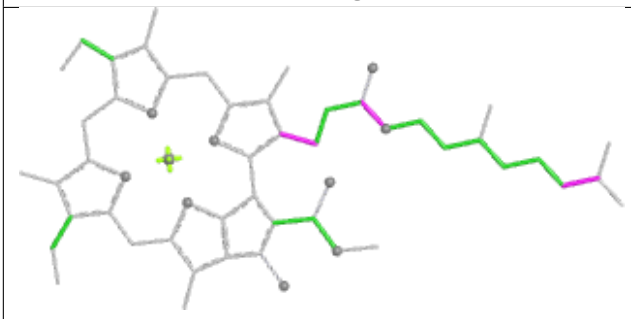
Ligand CLA A 803



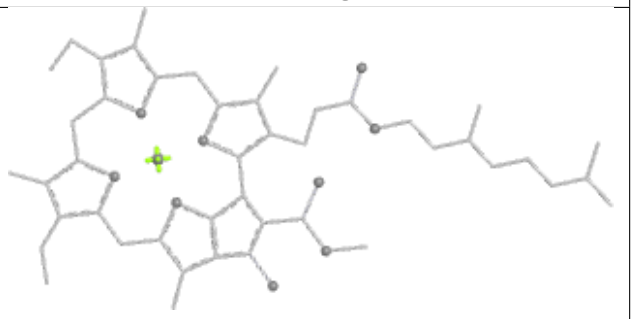
Bond lengths



Bond angles

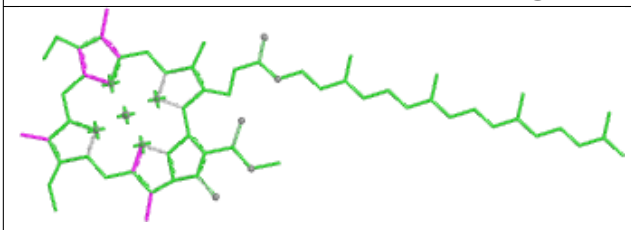


Torsions

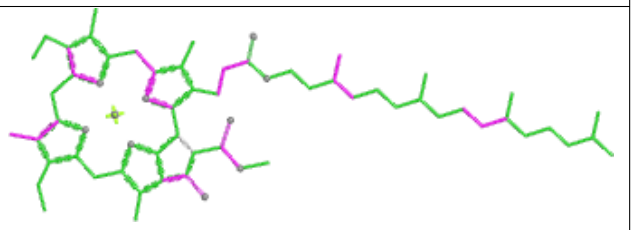


Rings

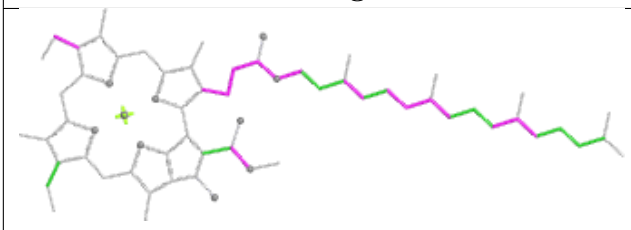
Ligand CLA e 607



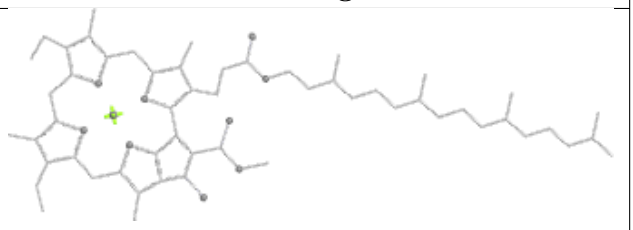
Bond lengths



Bond angles

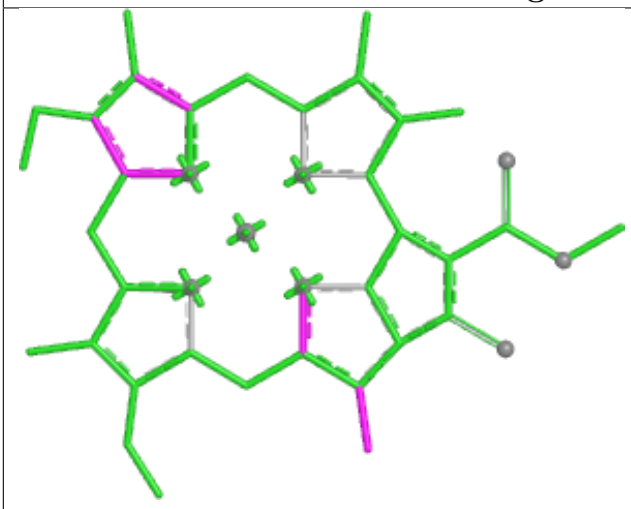


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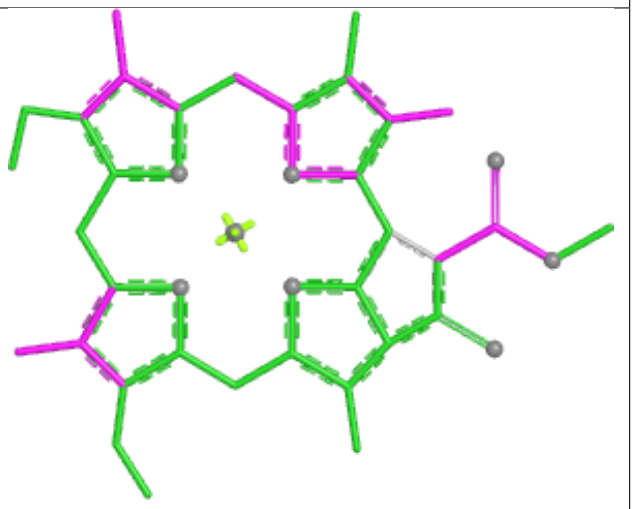


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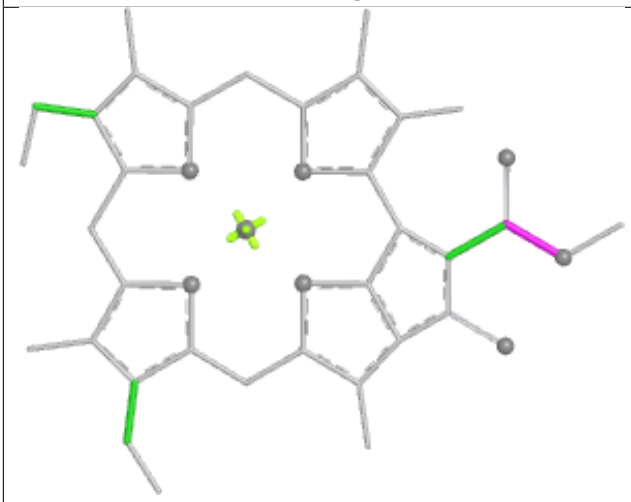
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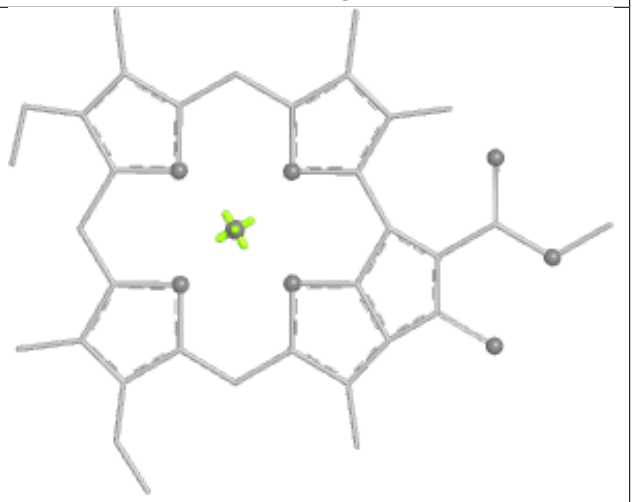
Bond lengths



Bond angles

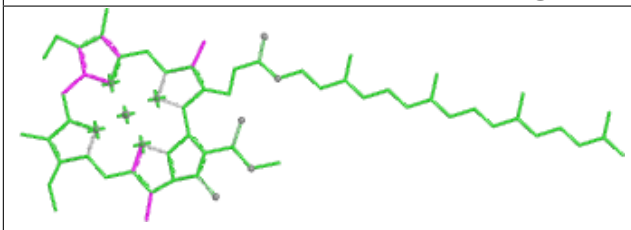


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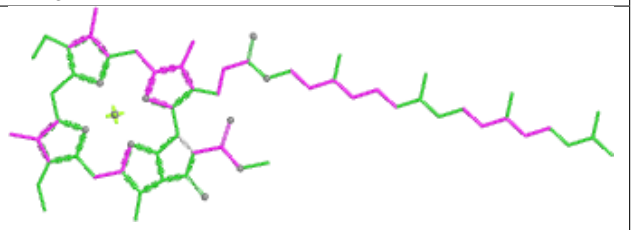


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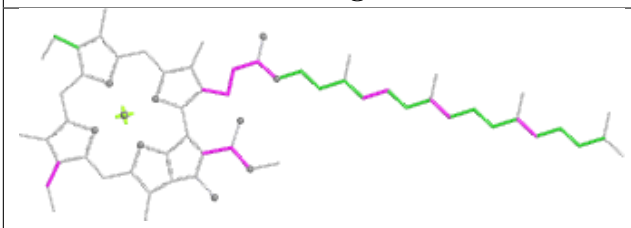
Ligand CLA j 604



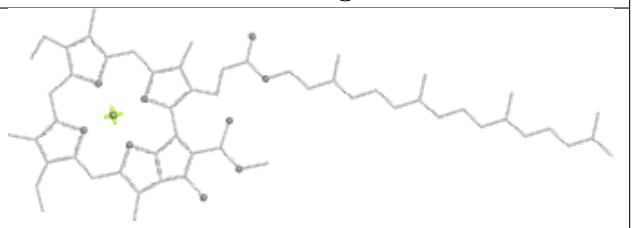
Bond lengths



Bond angles

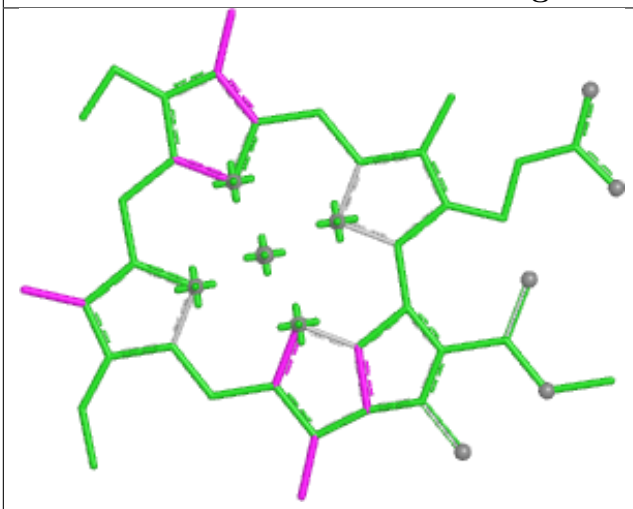


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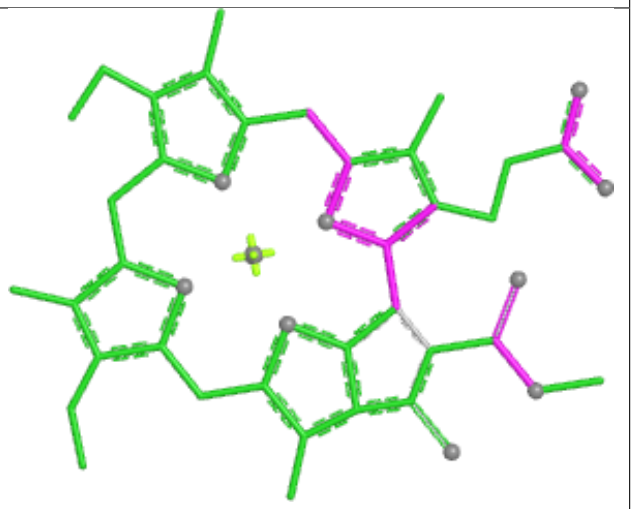


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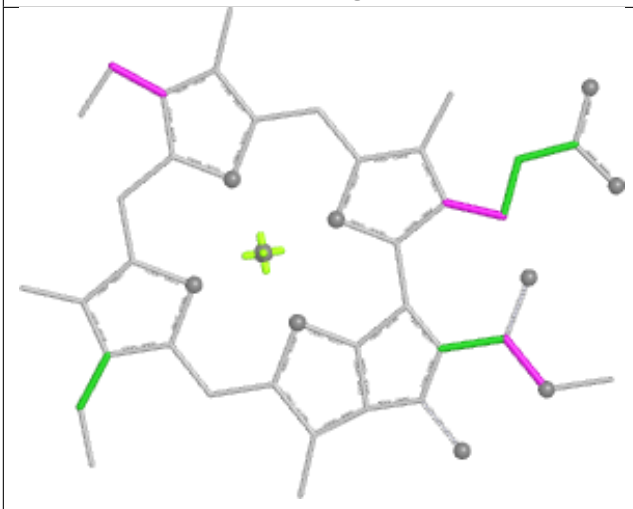
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Bond lengths



Bond angles

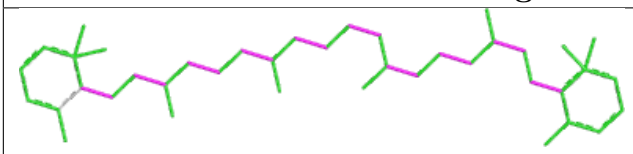


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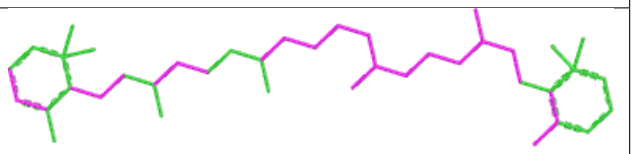


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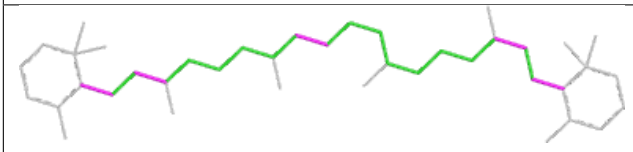
Ligand WVN A 846



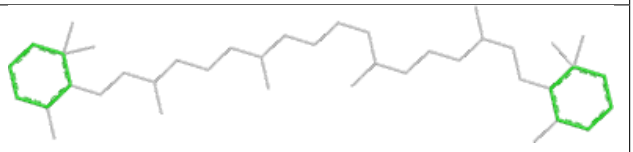
Bond lengths



Bond angles

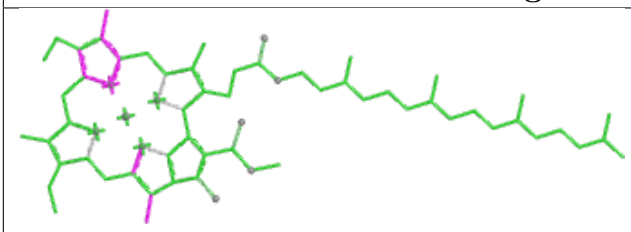


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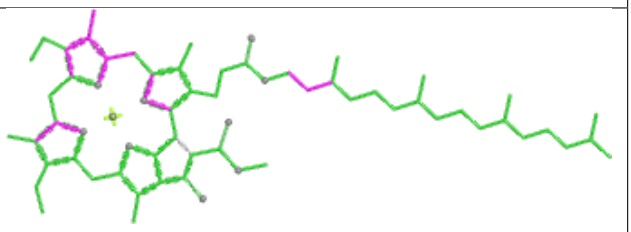


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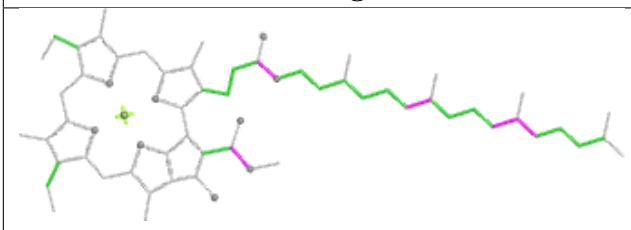
Ligand CLA B 816



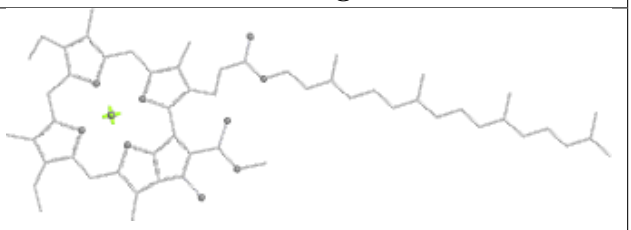
Bond lengths



Bond angles

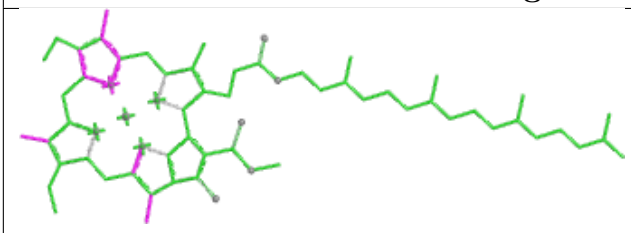


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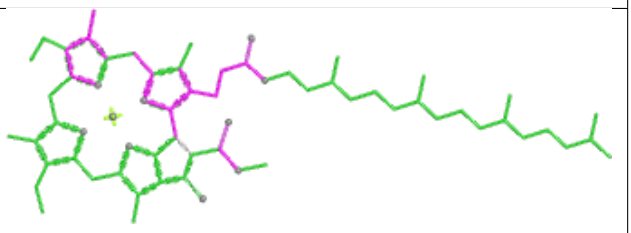


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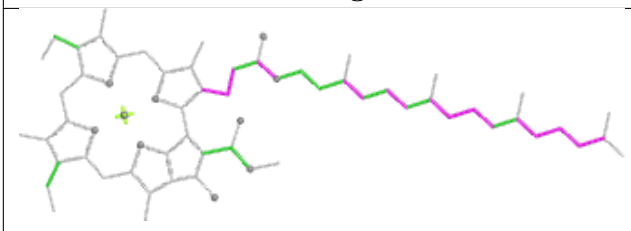
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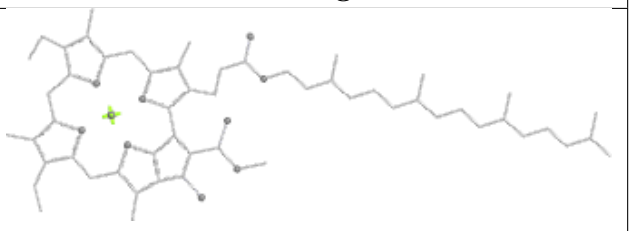
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Bond angles

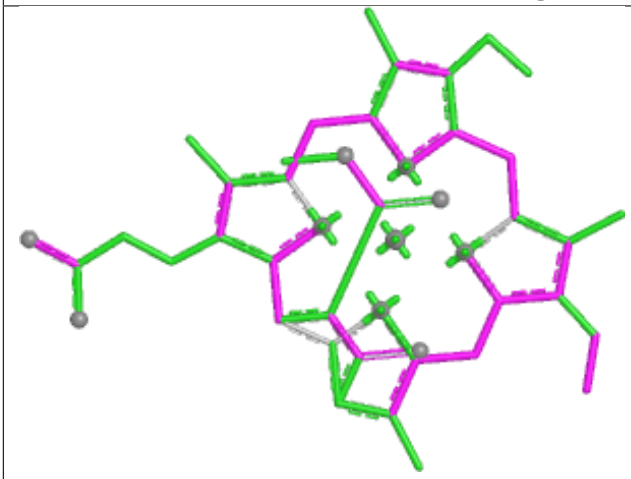


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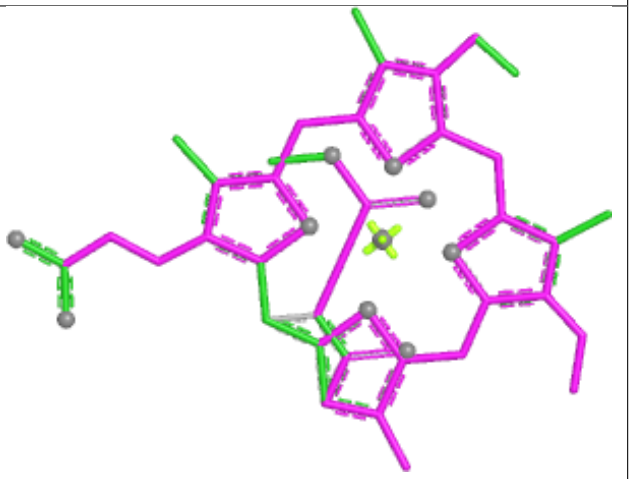


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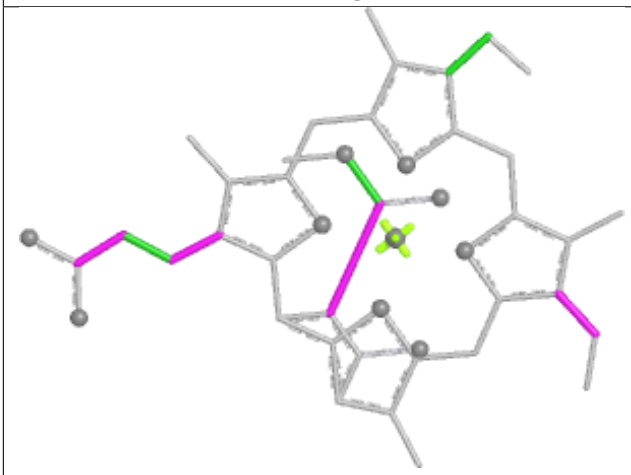
Ligand KC2 s 204



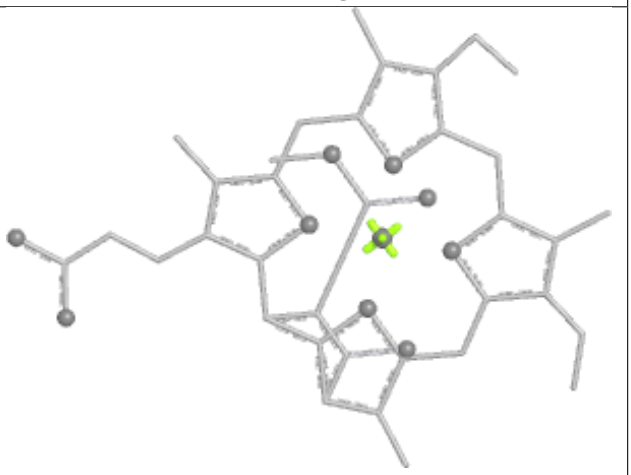
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Bond angles

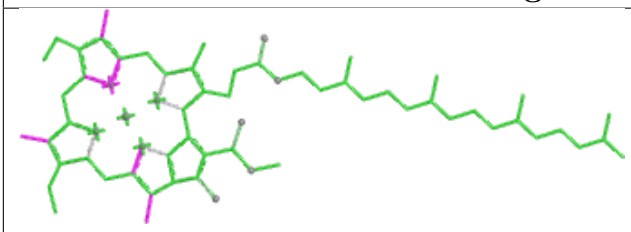


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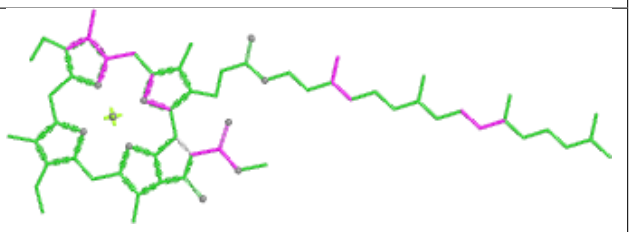


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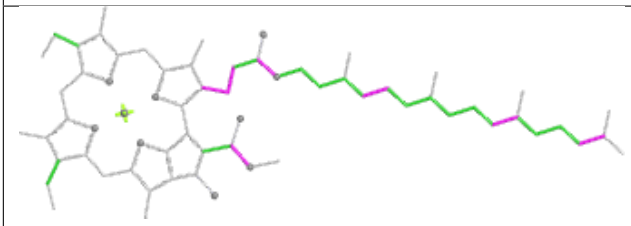
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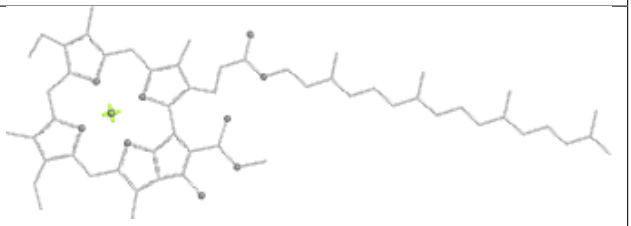
Bond lengths



Bond angles

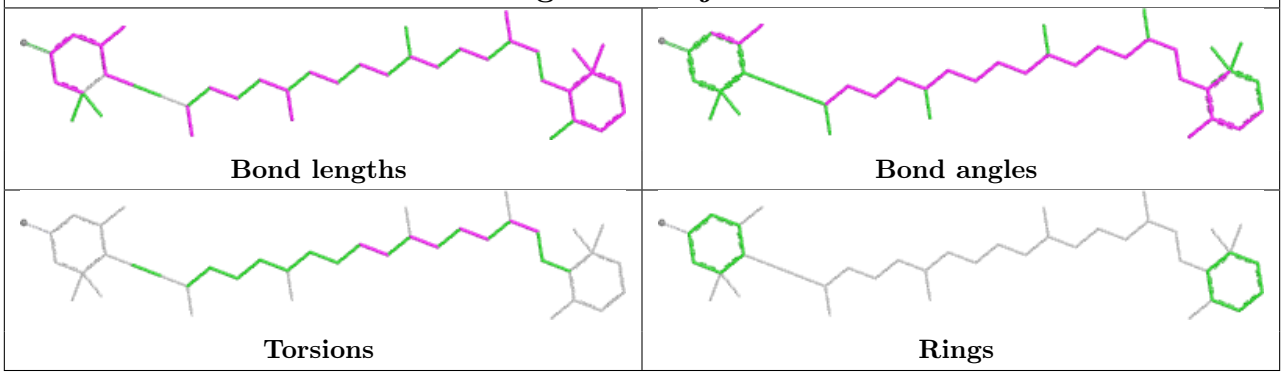


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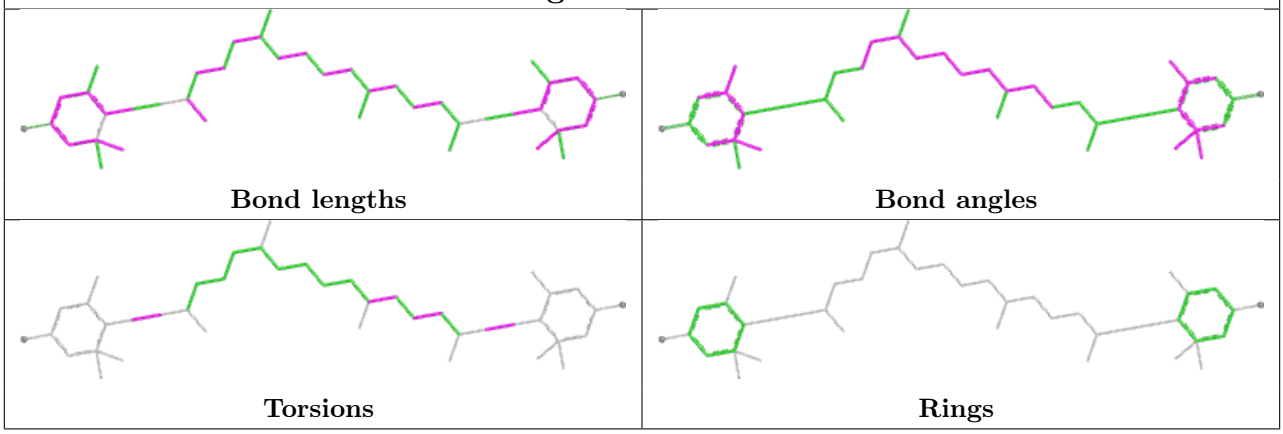


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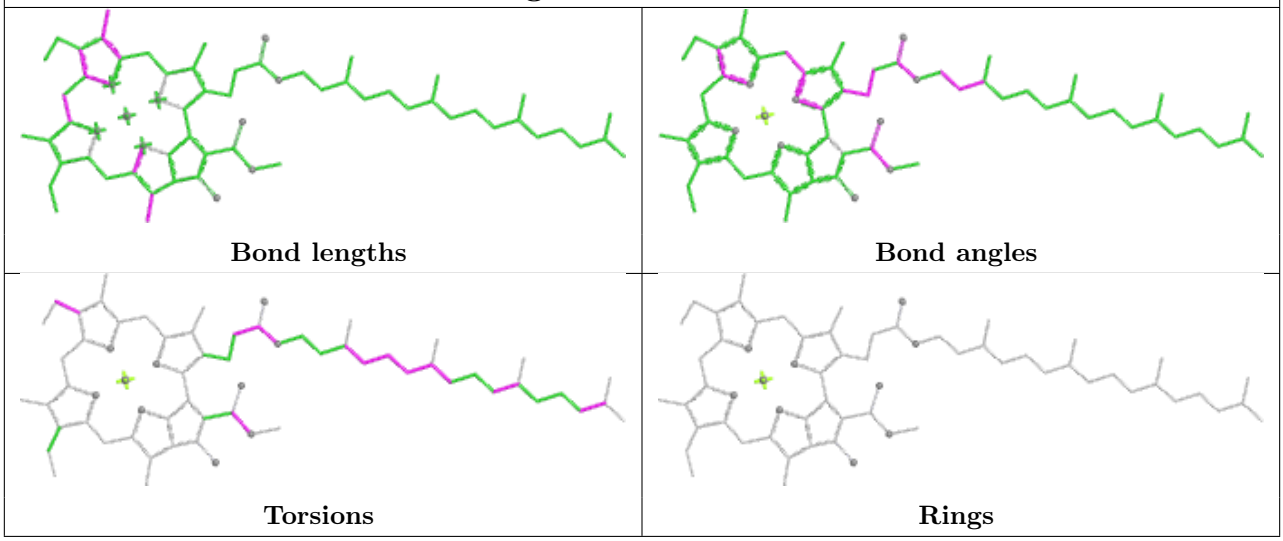
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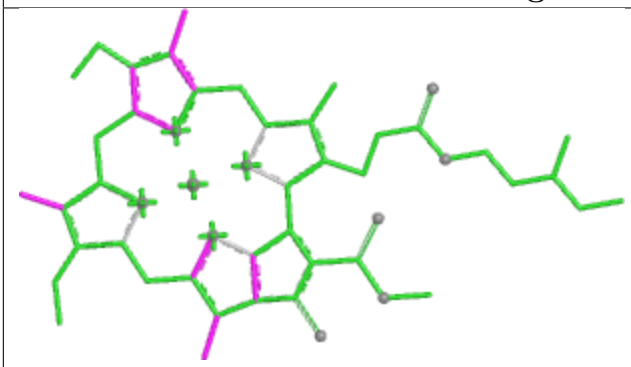
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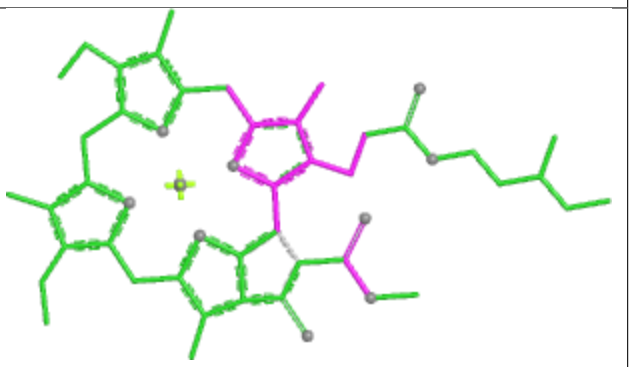
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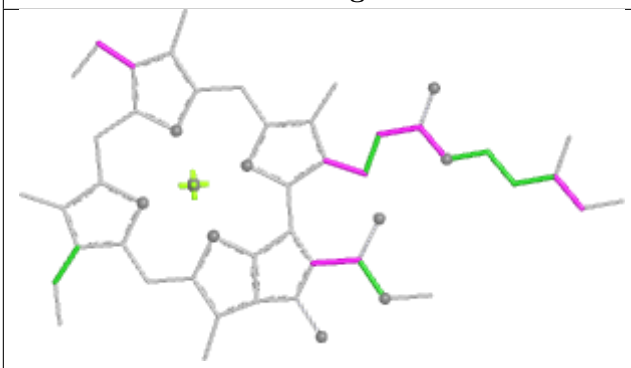
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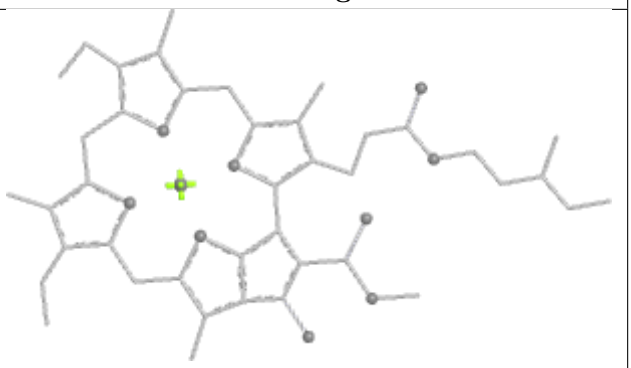
Bond lengths



Bond angles

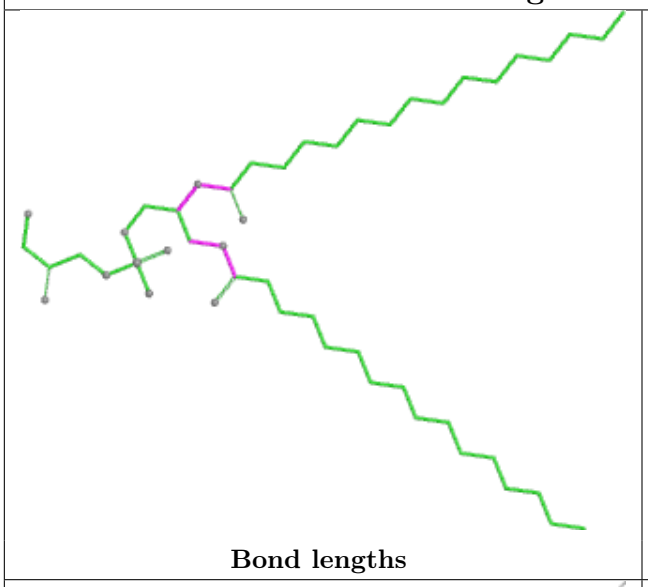


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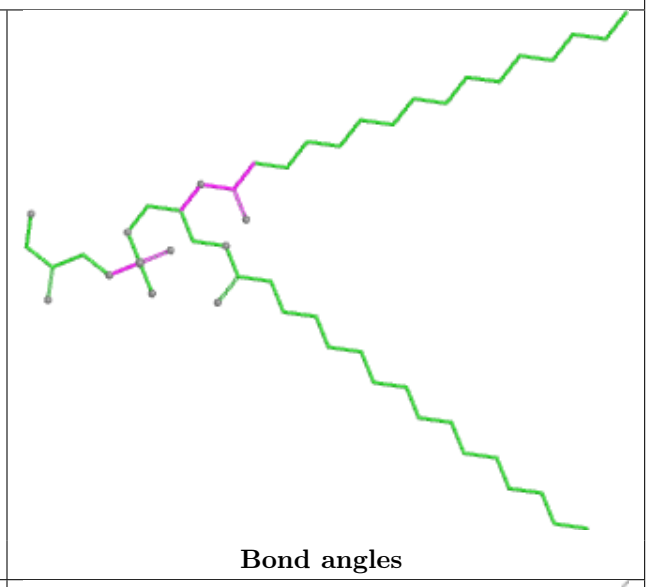


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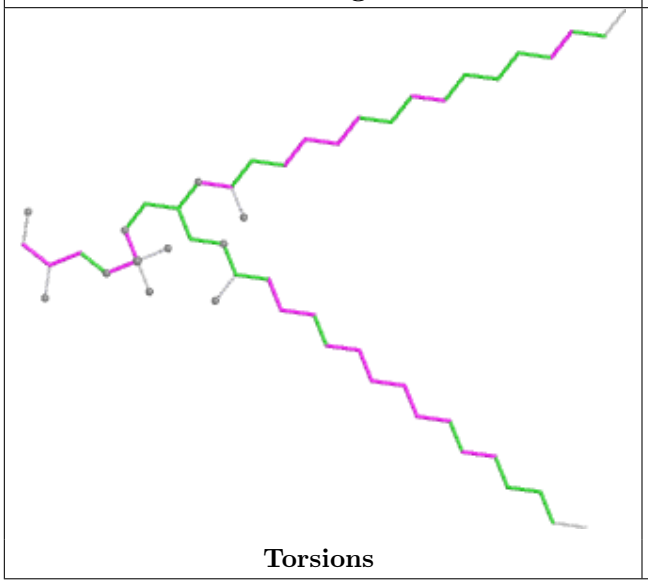
Ligand LHG b 617



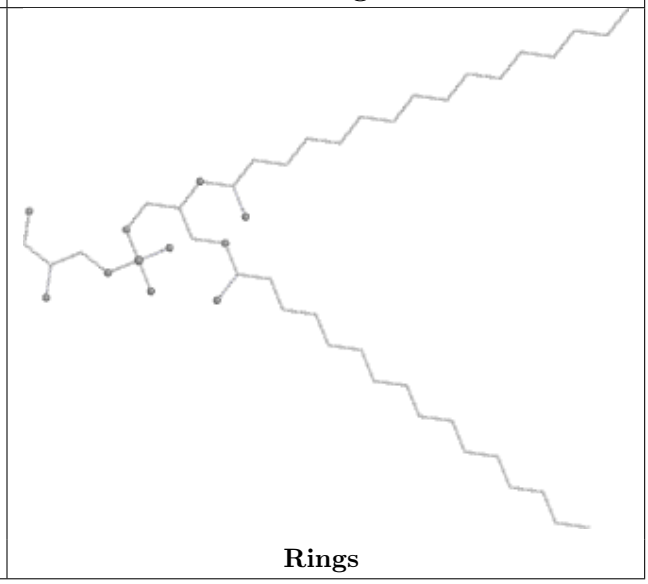
Bond lengths



Bond angles

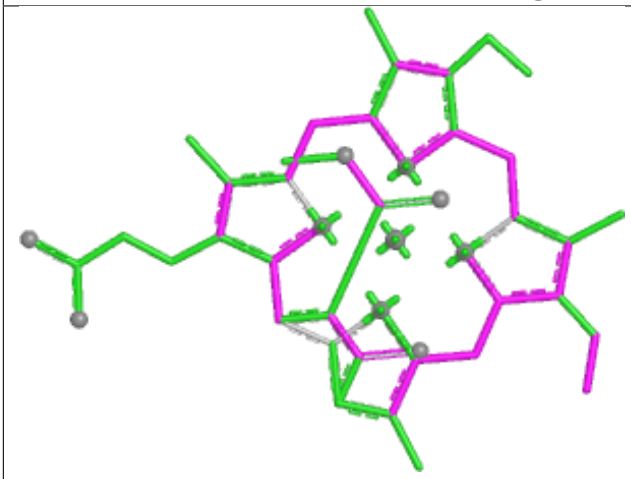


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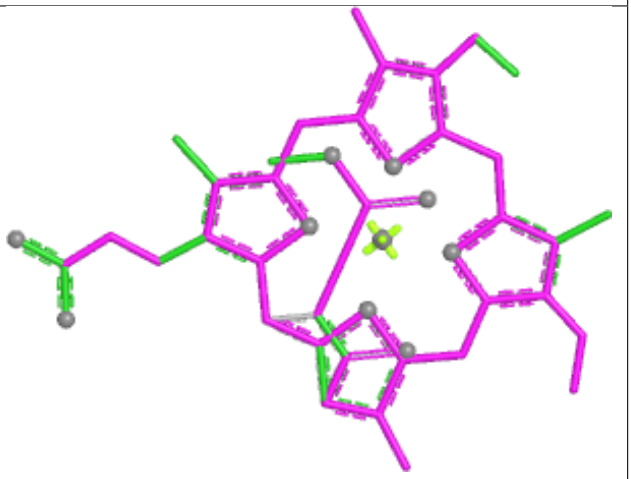


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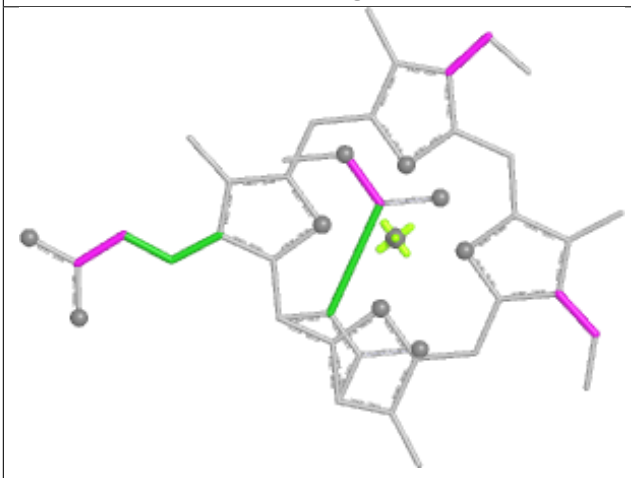
Ligand KC2 k 311



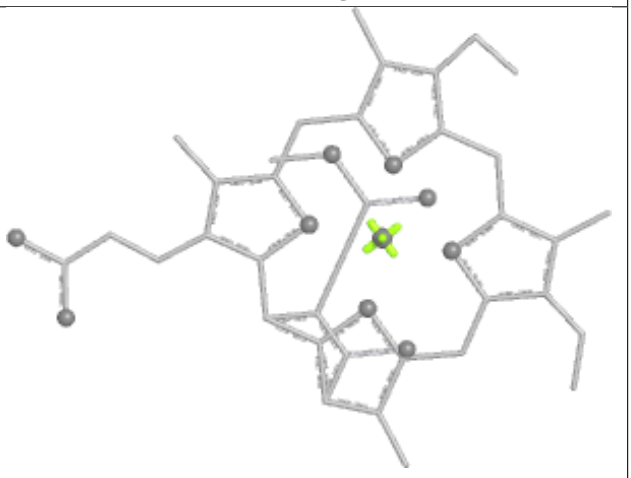
Bond lengths



Bond angles

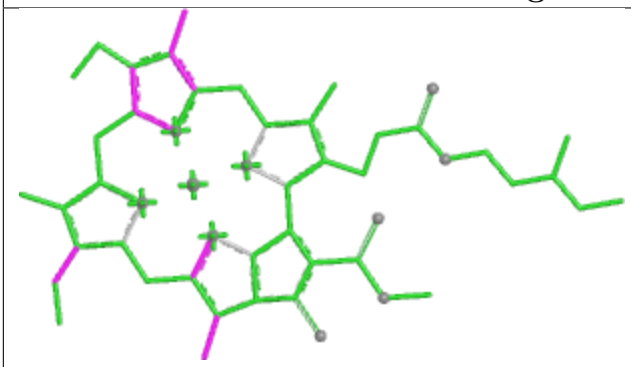


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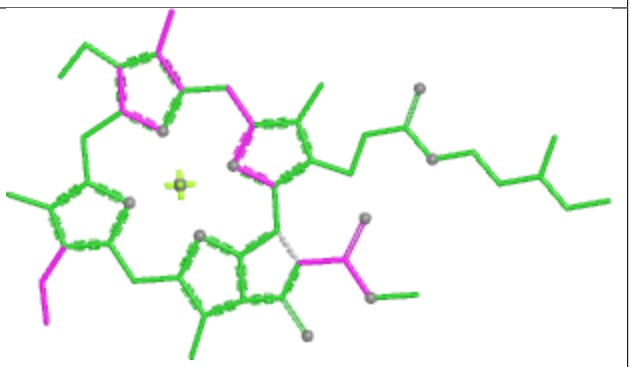


Rings

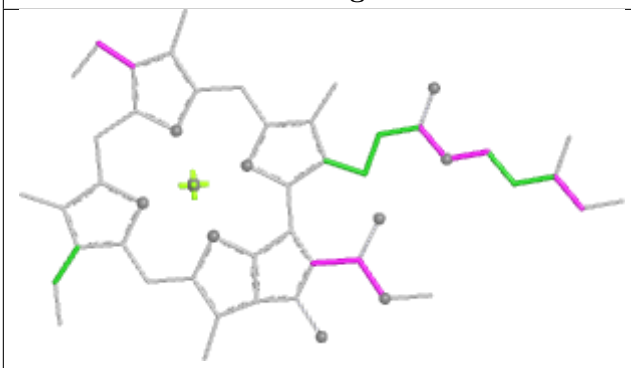
Ligand CLA b 601



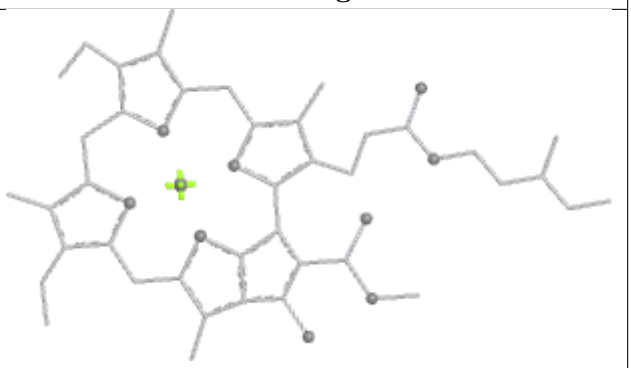
Bond lengths



Bond angles

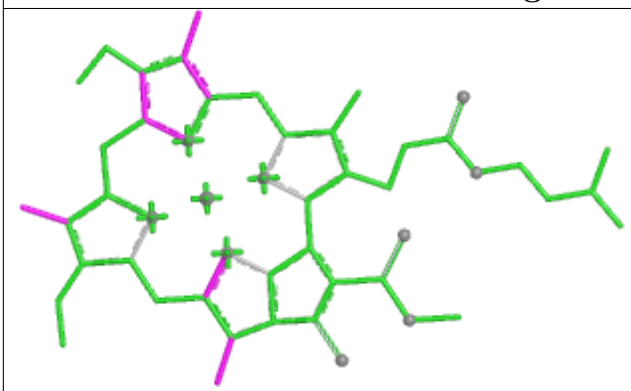


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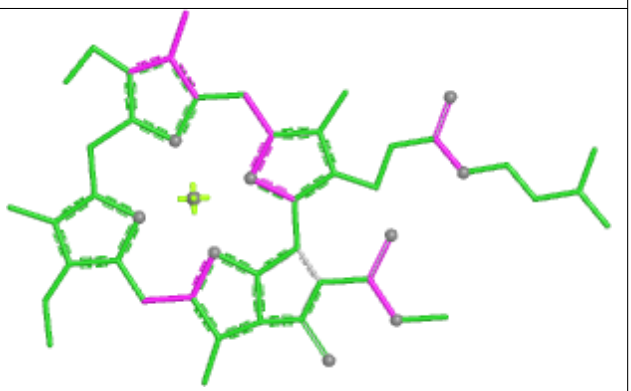


Rings

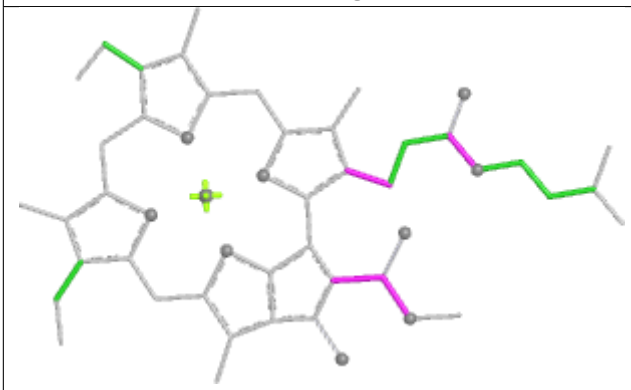
Ligand CLA A 814



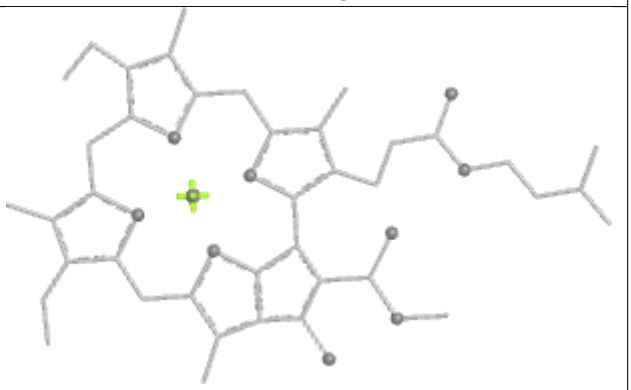
Bond lengths



Bond angles

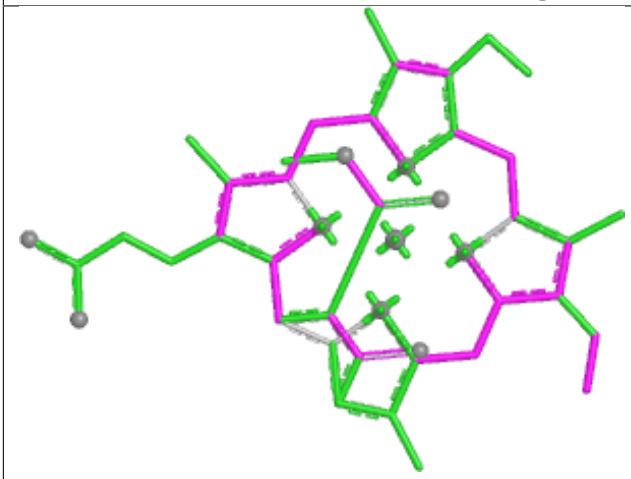


Torsions

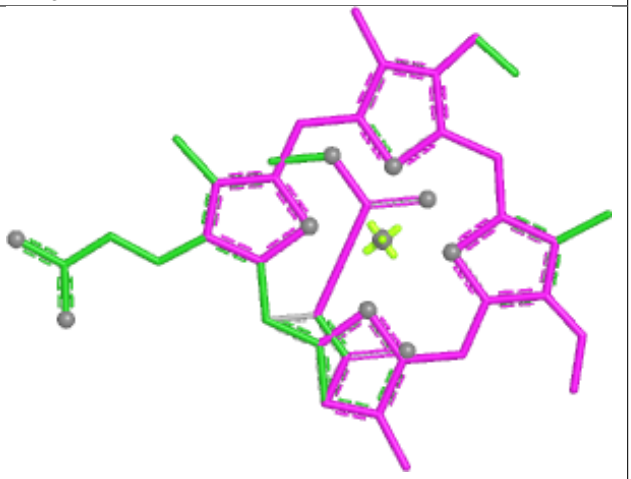


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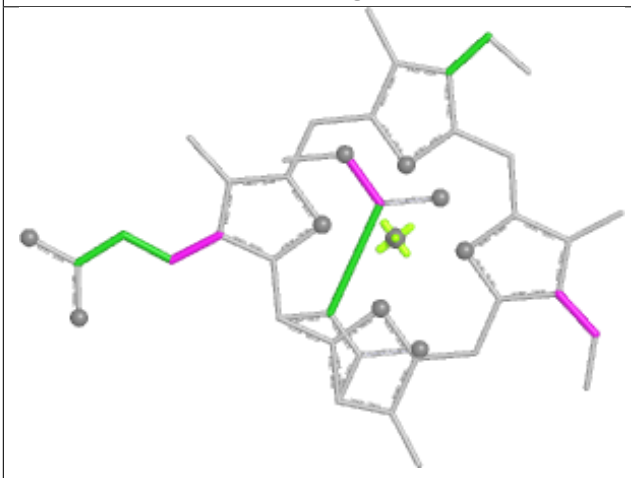
Ligand KC2 j 610



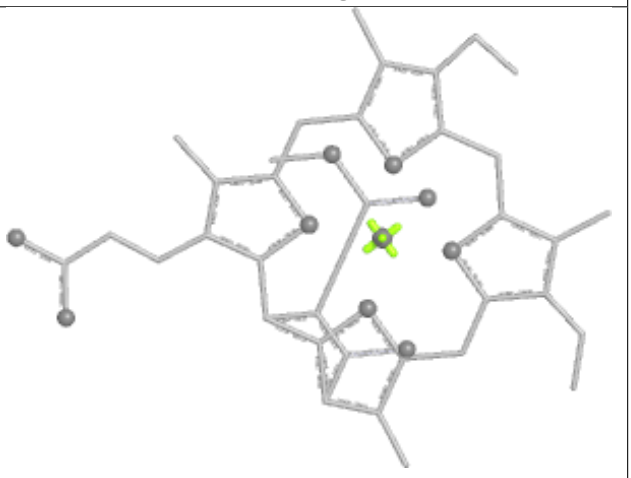
Bond lengths



Bond angles

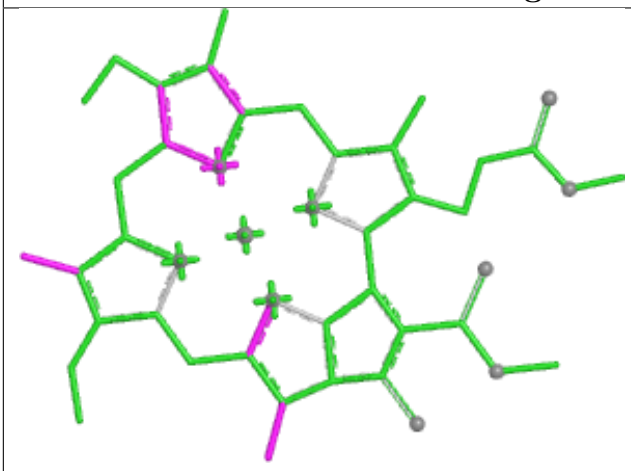


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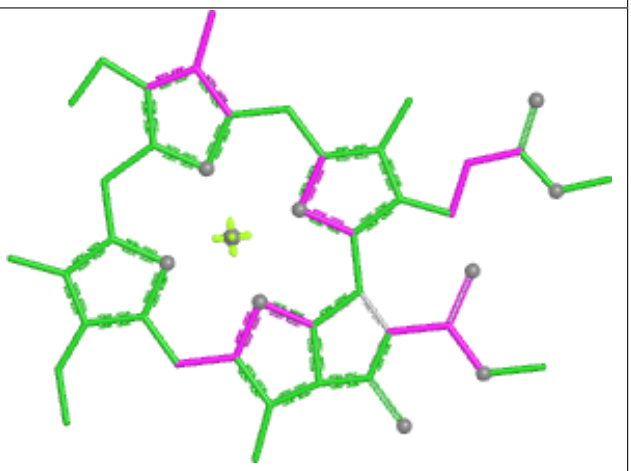


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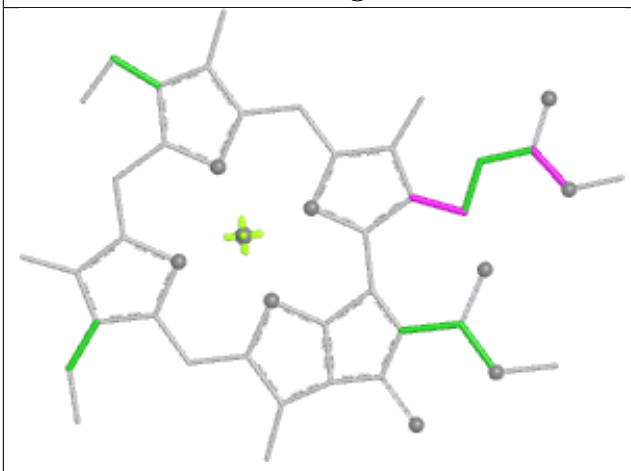
Ligand CLA B 817



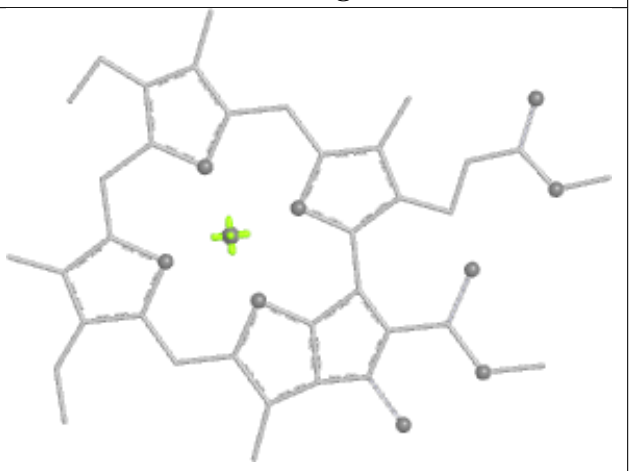
Bond lengths



Bond angles

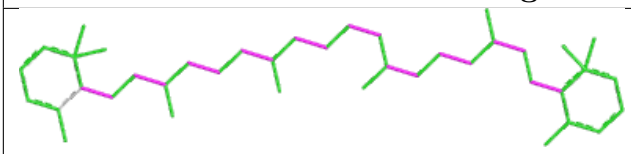


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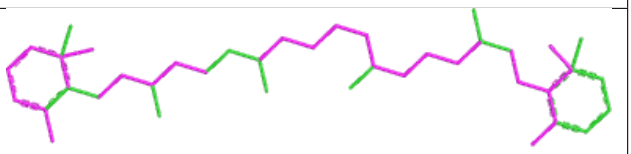


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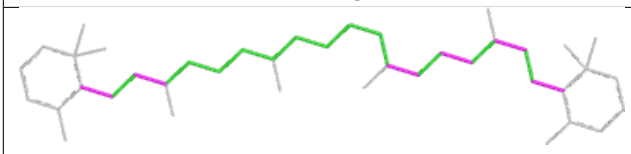
Ligand WVN e 615



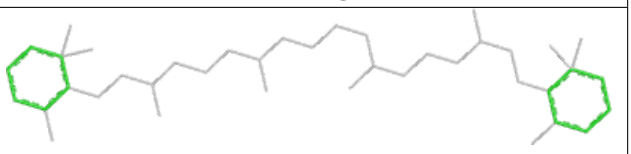
Bond lengths



Bond angles

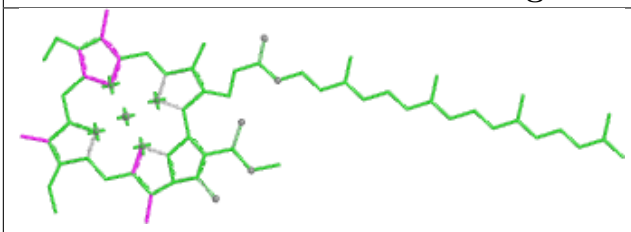


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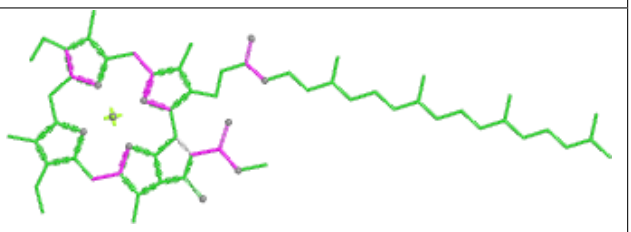


Rings

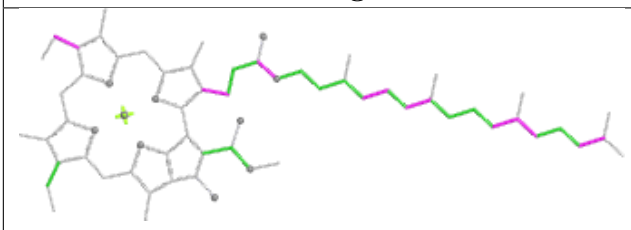
Ligand CLA L 203



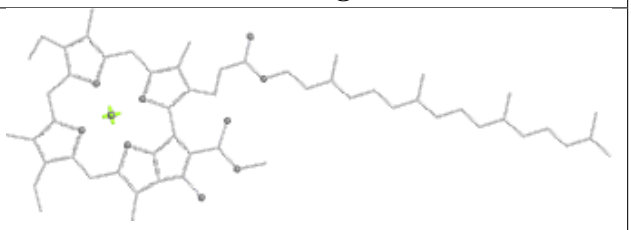
Bond lengths



Bond angles

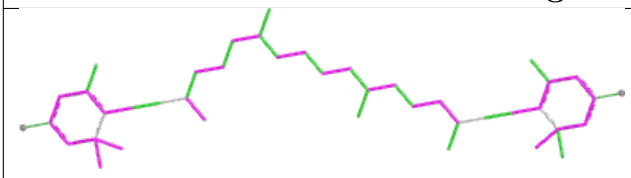


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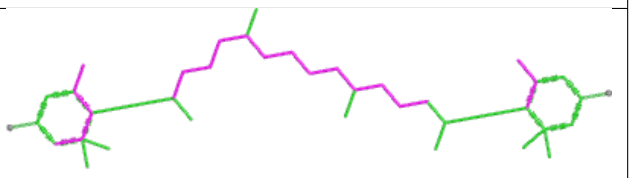


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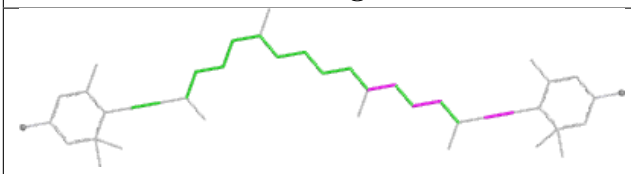
Ligand II0 i 313



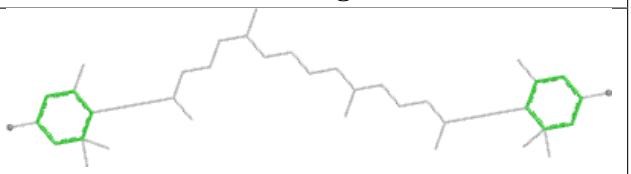
Bond lengths



Bond angles

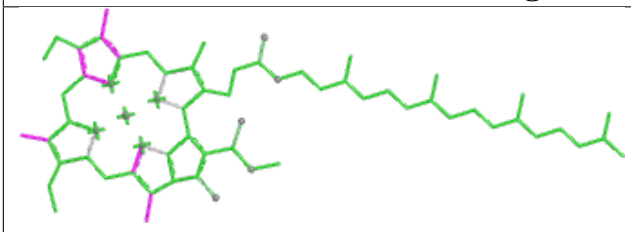


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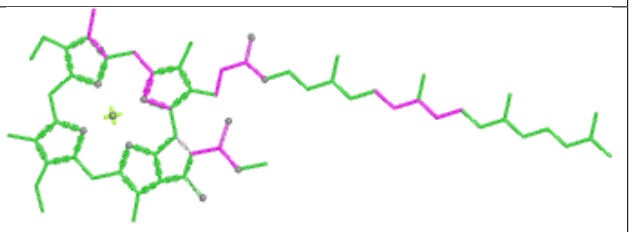


Rings

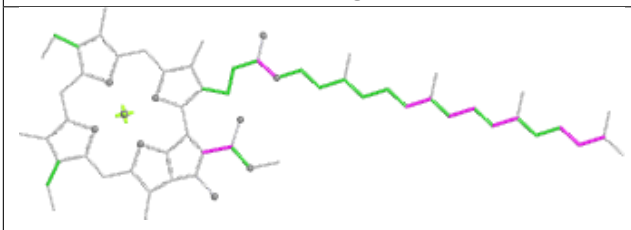
Ligand CLA A 806



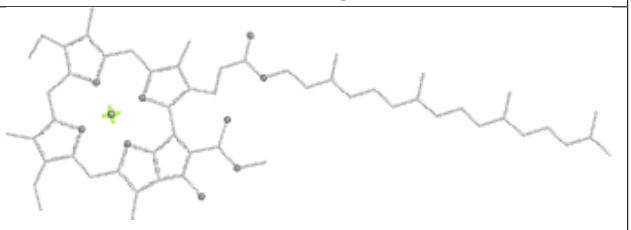
Bond lengths



Bond angles

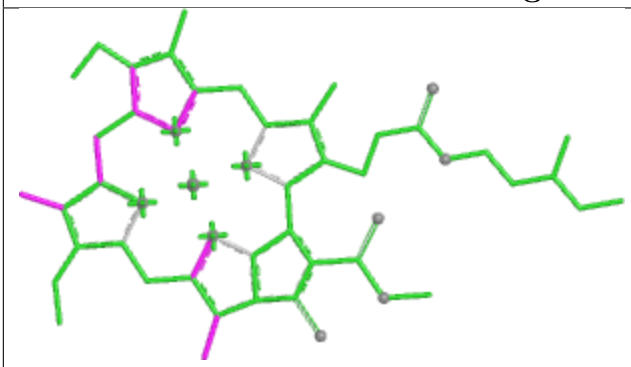


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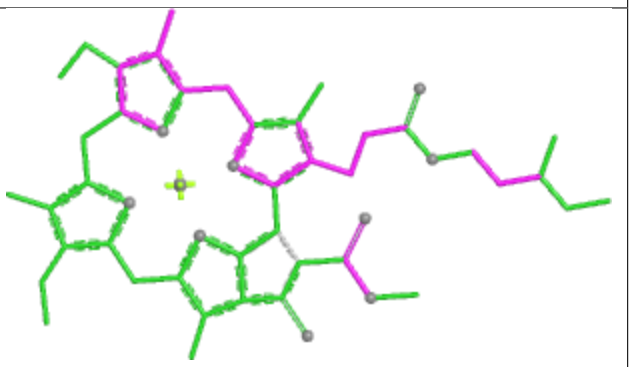


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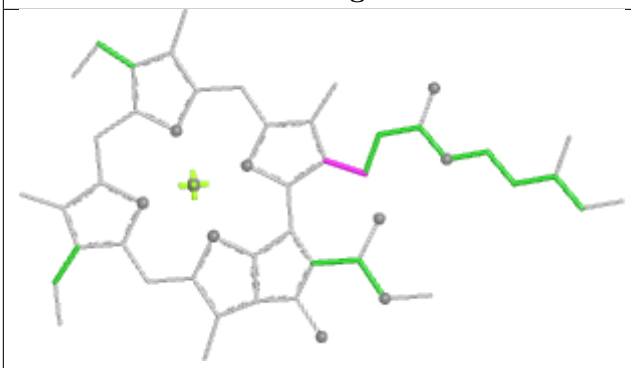
Ligand CLA A 834



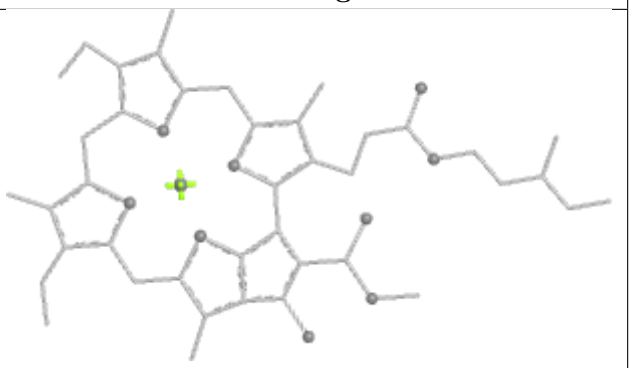
Bond lengths



Bond angles

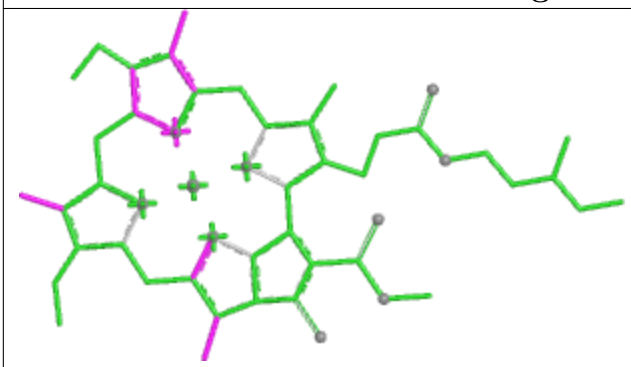


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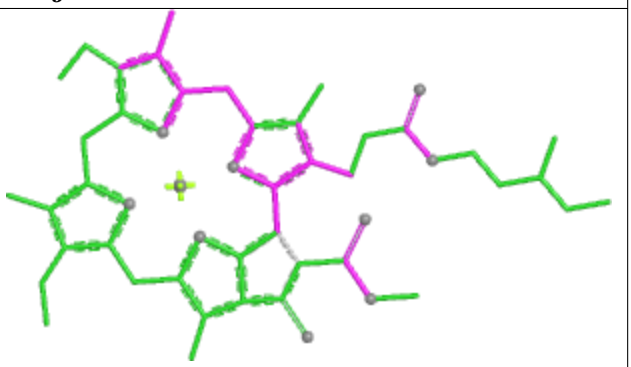


Rings

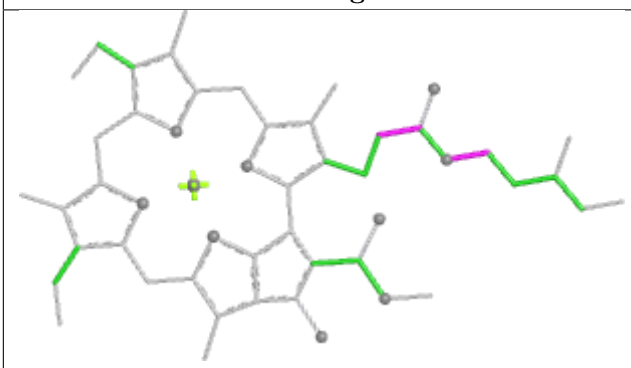
Ligand CLA j 603



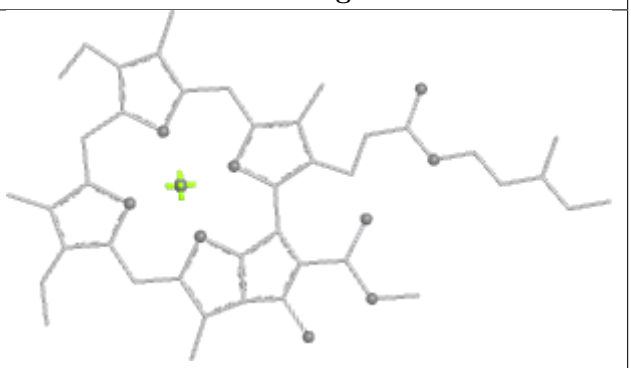
Bond lengths



Bond angles

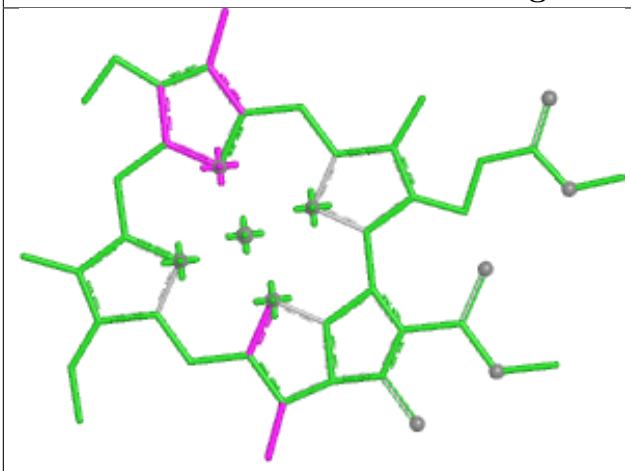


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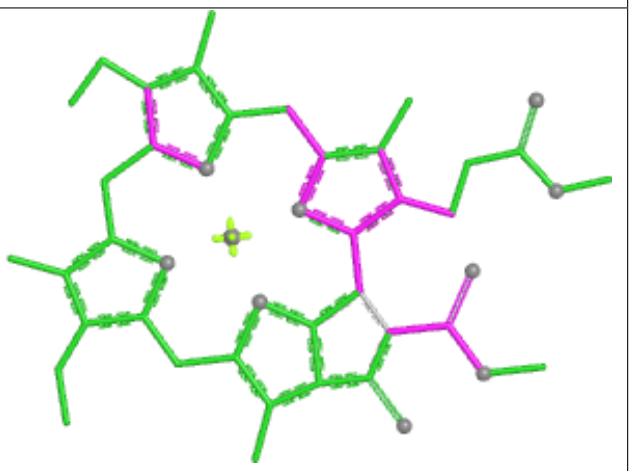


Rings

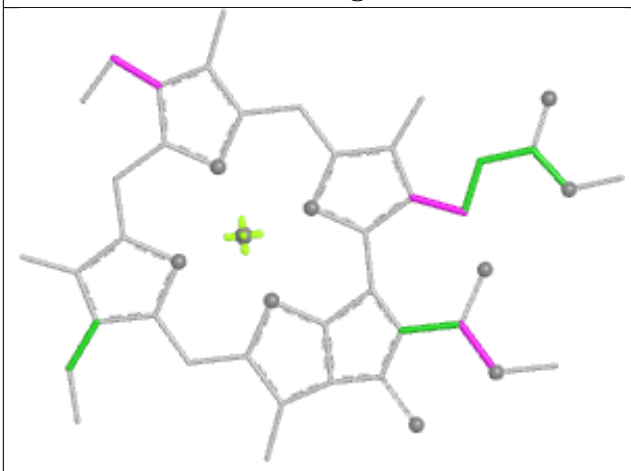
Ligand CLA e 608



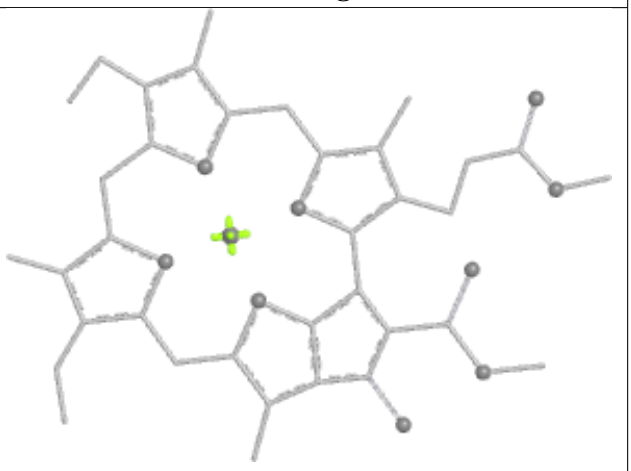
Bond lengths



Bond angles

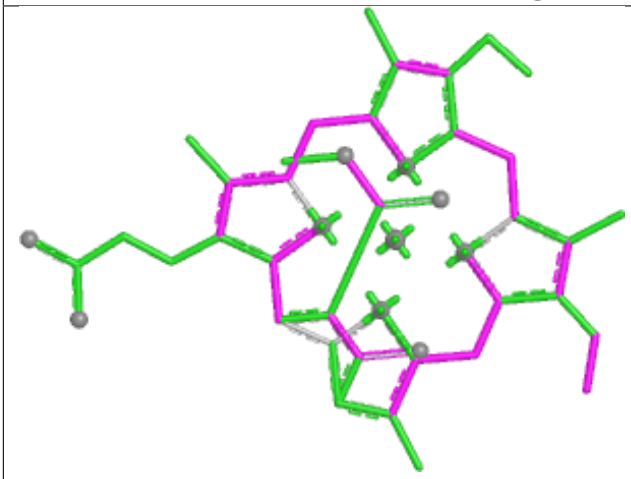


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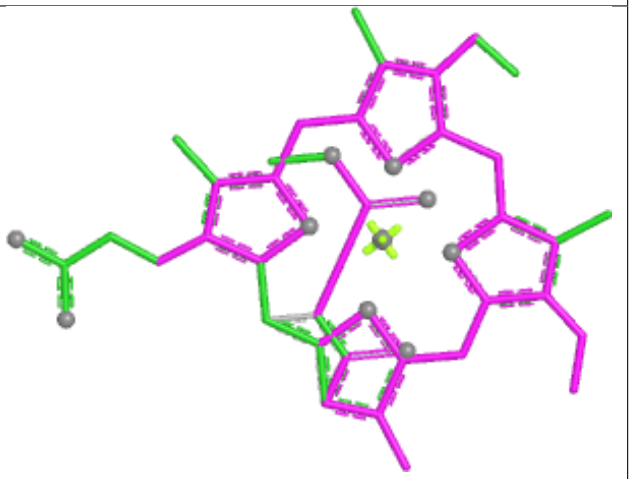


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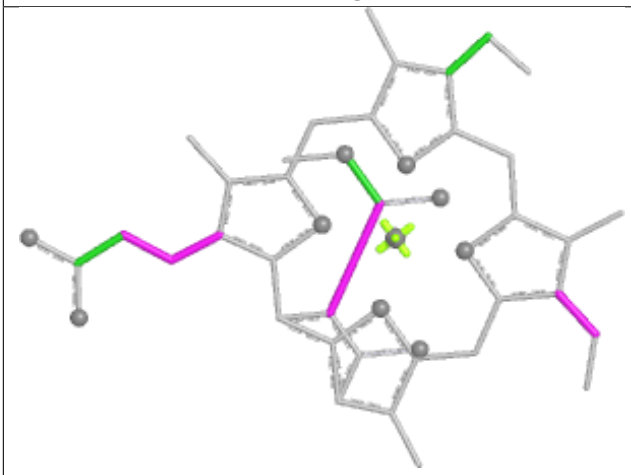
Ligand KC2 n 612



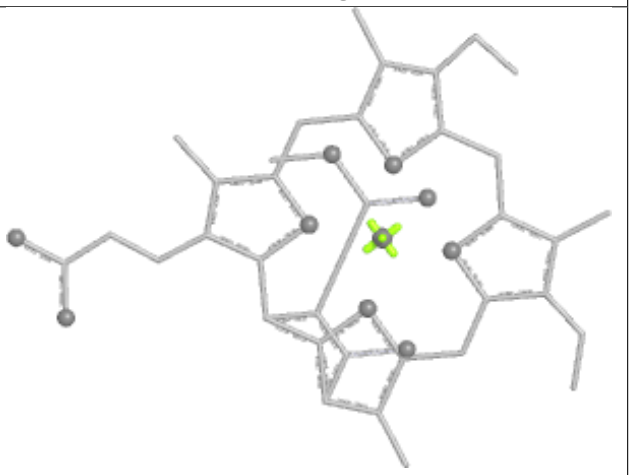
Bond lengths



Bond angles

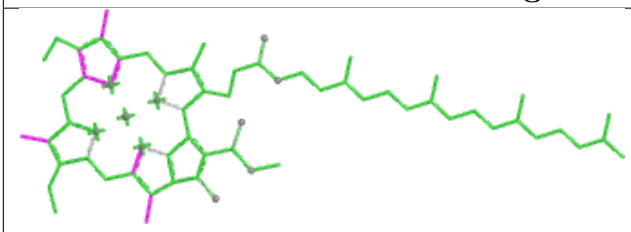


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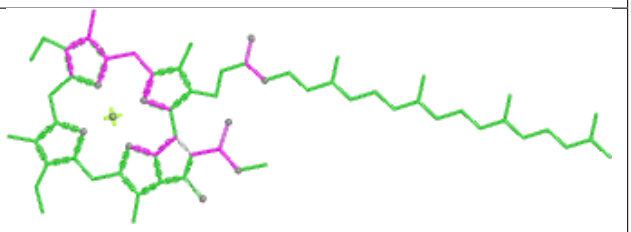


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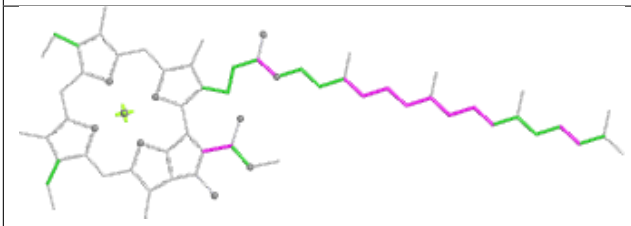
Ligand CLA A 829



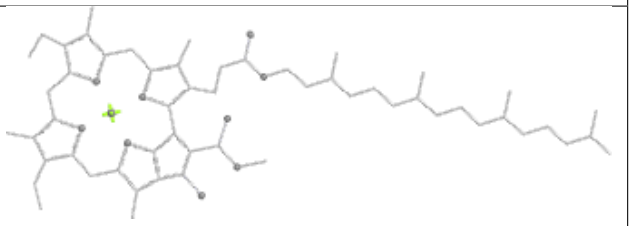
Bond lengths



Bond angles

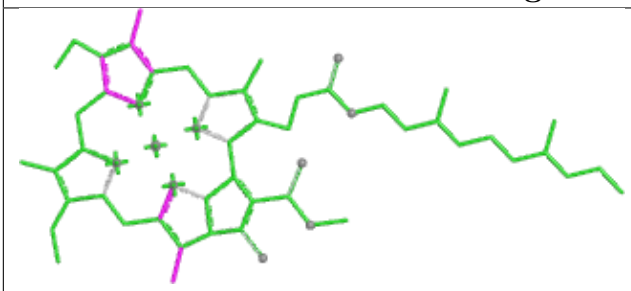


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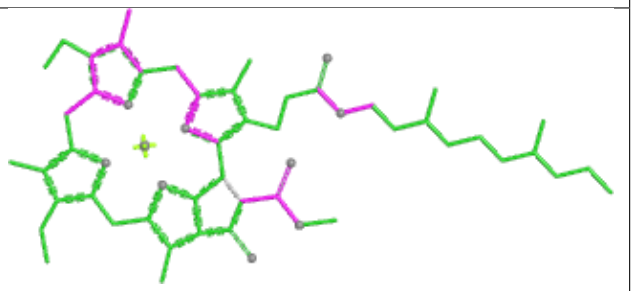


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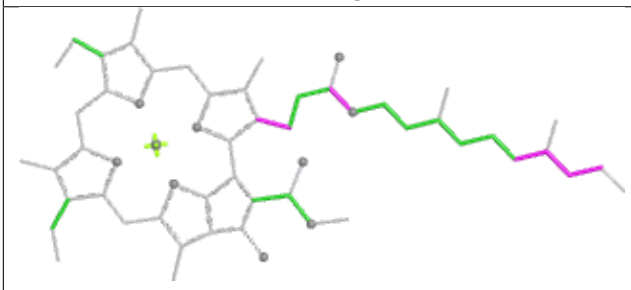
Ligand CLA B 815



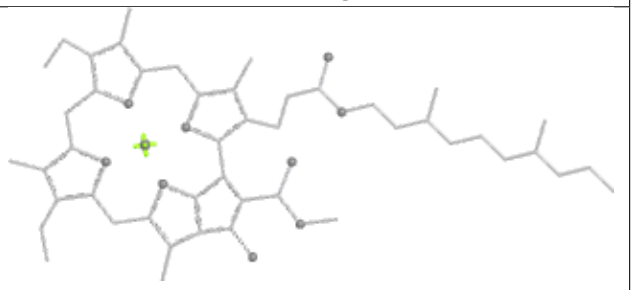
Bond lengths



Bond angles

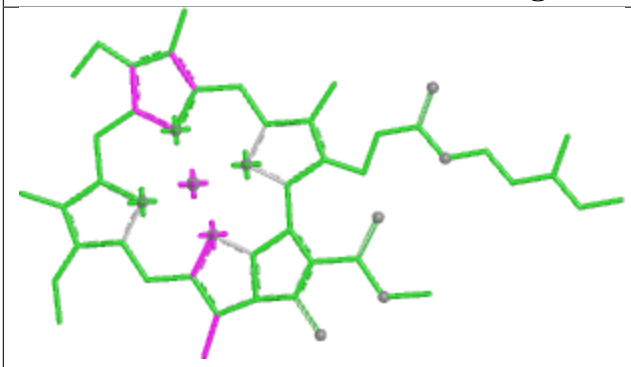


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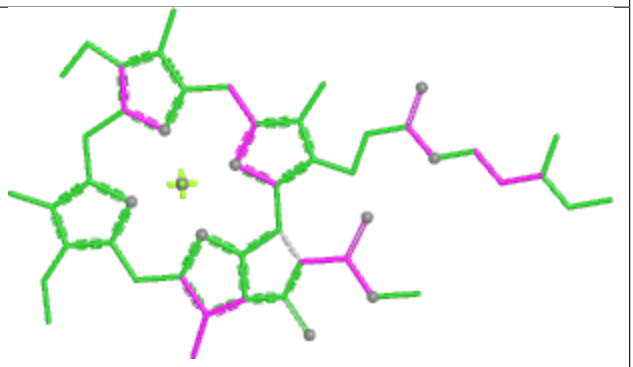


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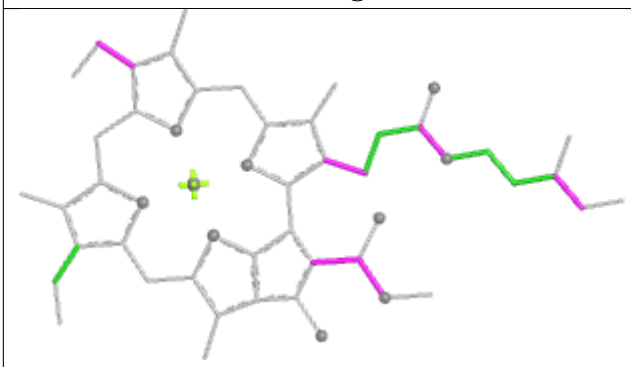
Ligand CLA c 601



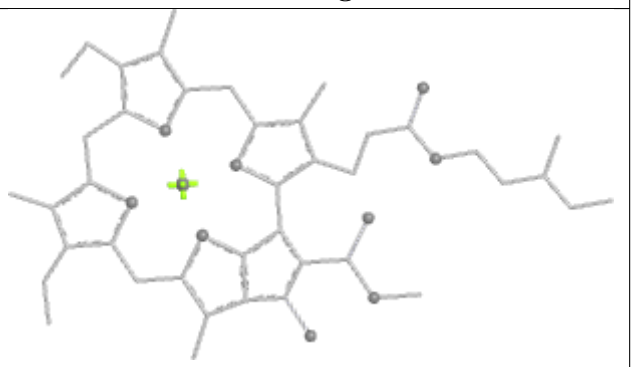
Bond lengths



Bond angles

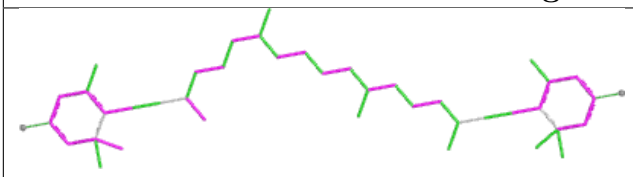


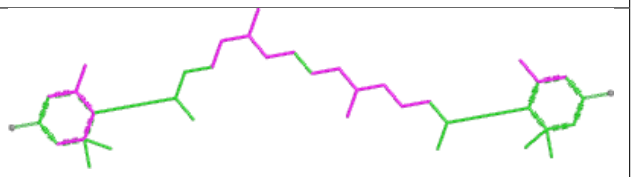
Torsions

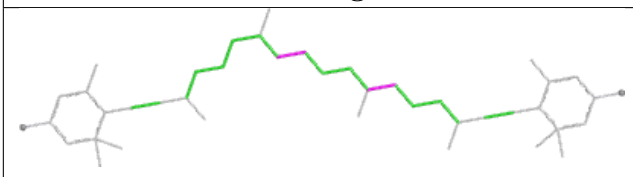


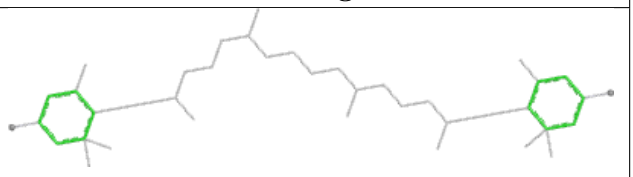
Rings

Ligand II0 k 314

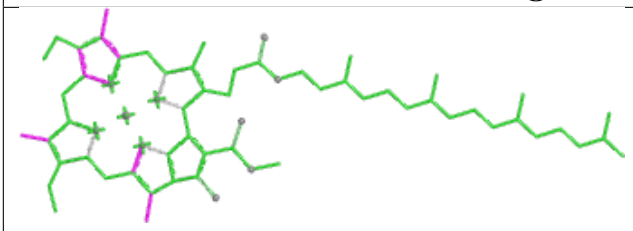

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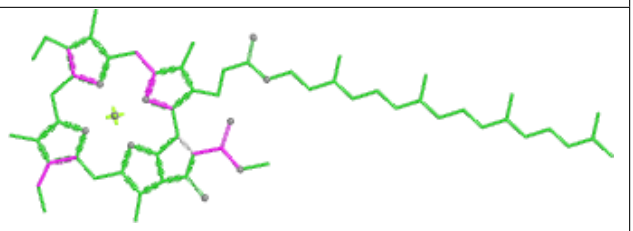

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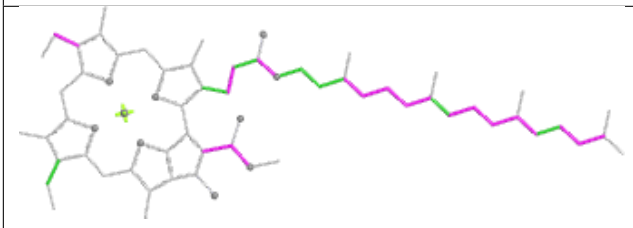

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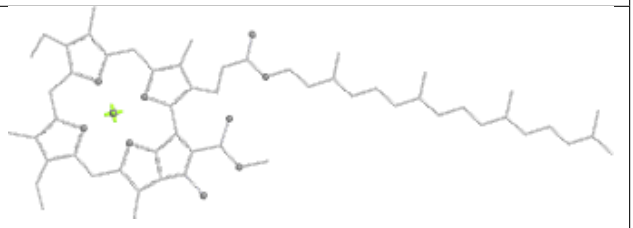

Rings

Ligand CLA b 611

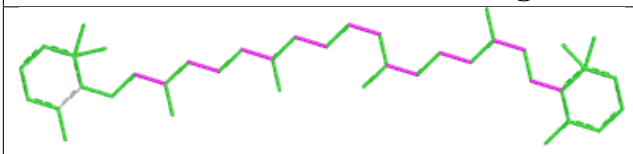

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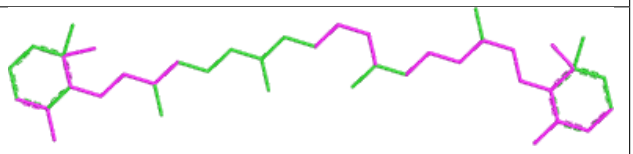

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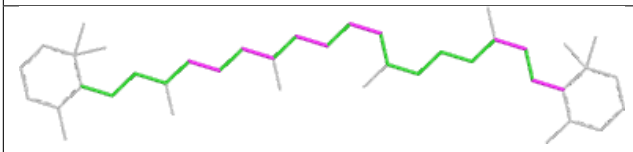

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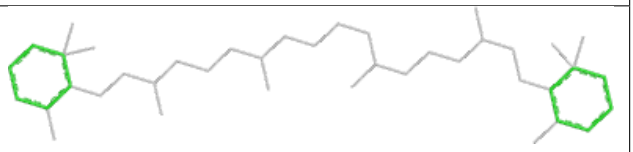

Rings

Ligand WVN O 201

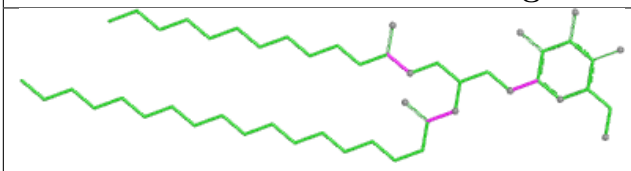

Bond lengths


Bond angles

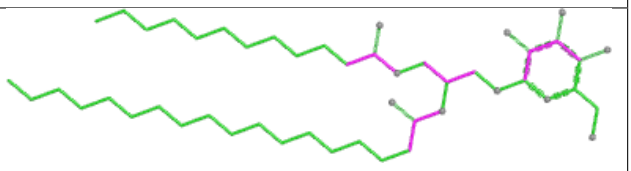

Torsions


Rings

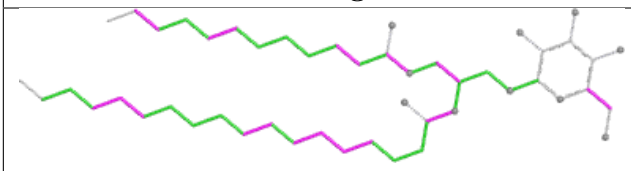
Ligand LMG b 619



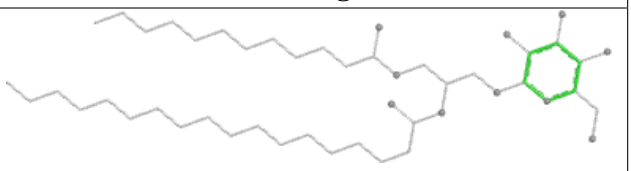
Bond lengths



Bond angles

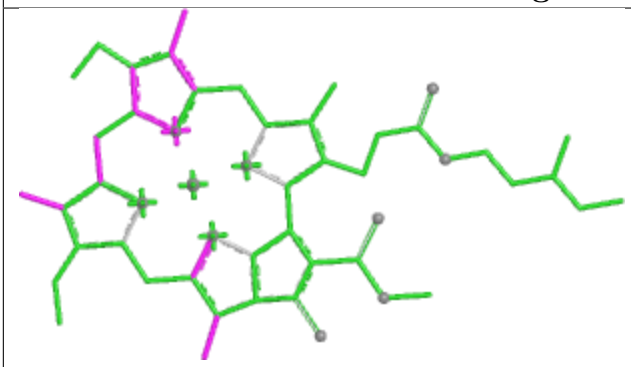


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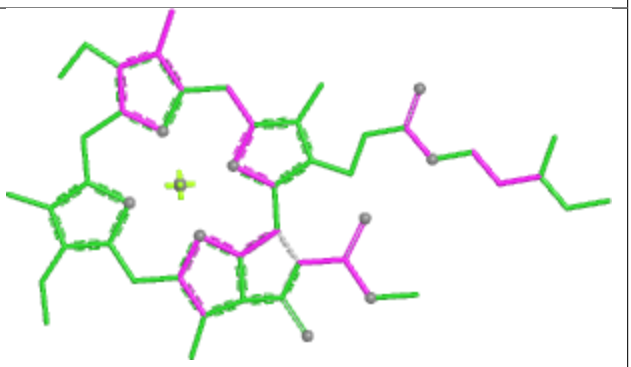


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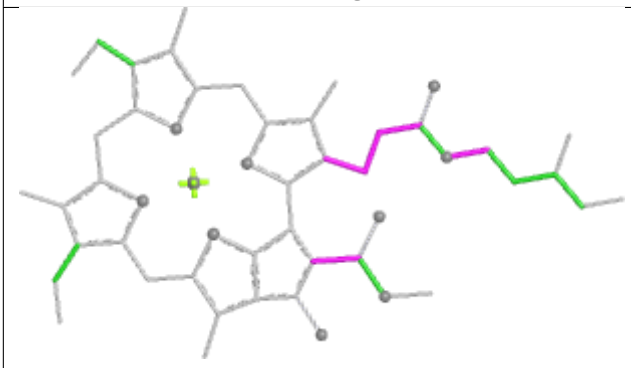
Ligand CLA l 309



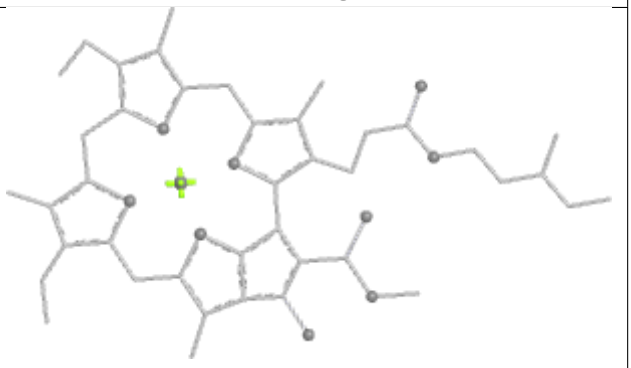
Bond lengths



Bond angles

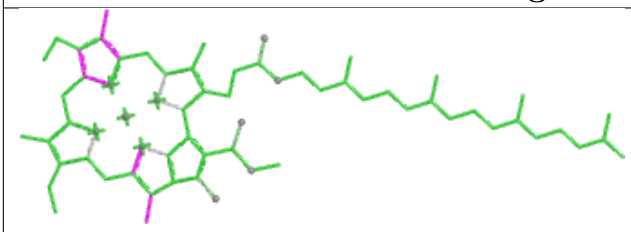


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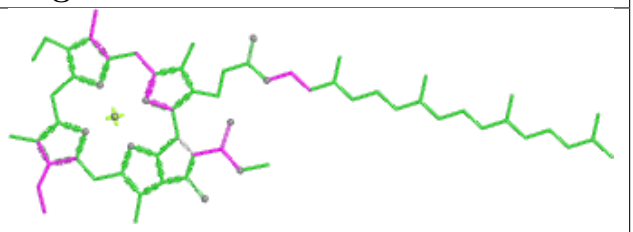


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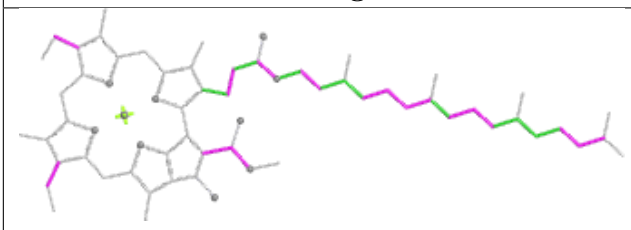
Ligand CLA g 322



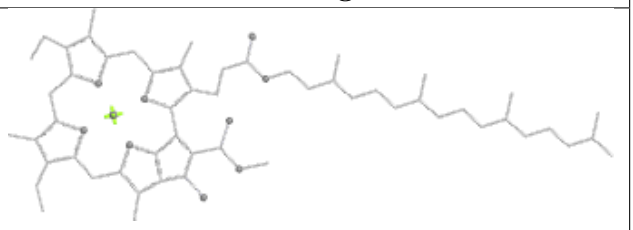
Bond lengths



Bond angles

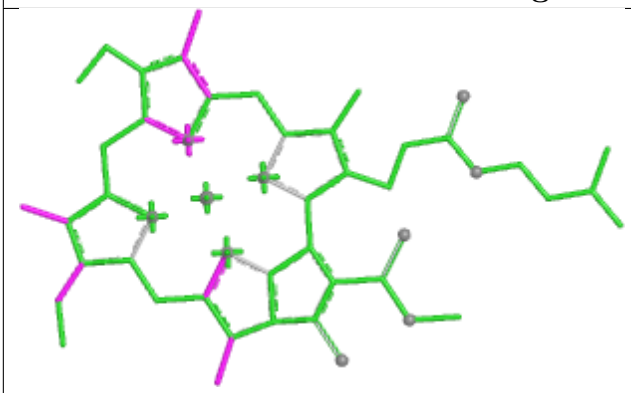


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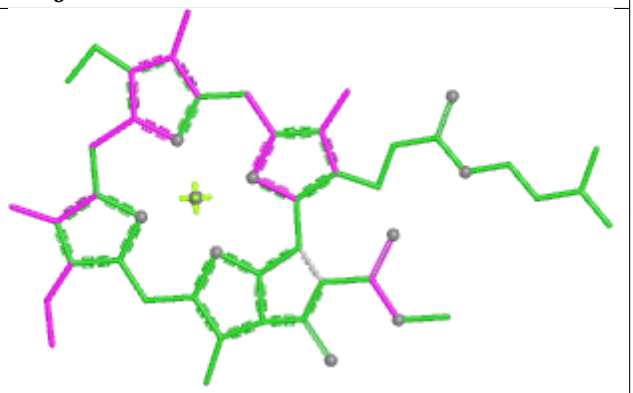


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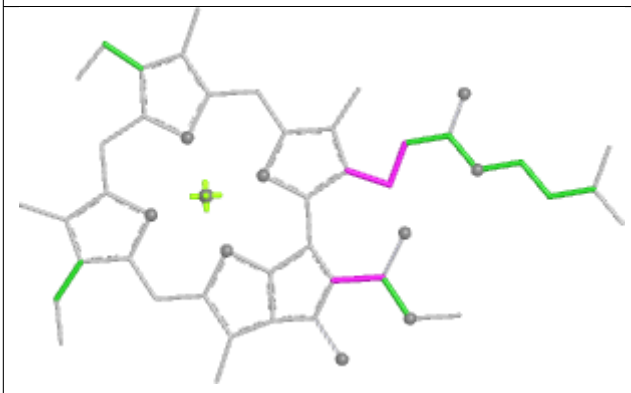
Ligand CLA j 602



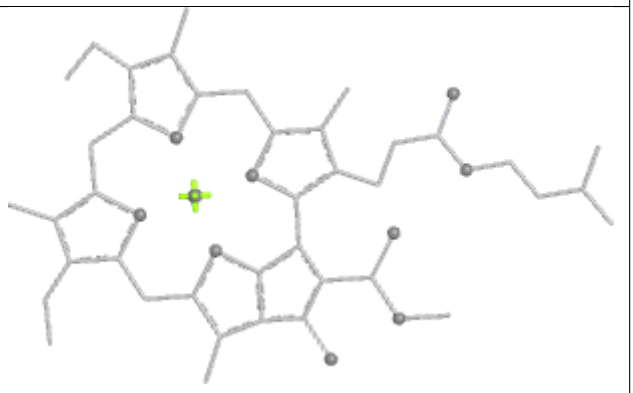
Bond lengths



Bond angles

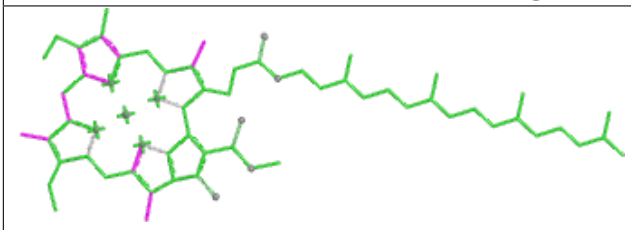


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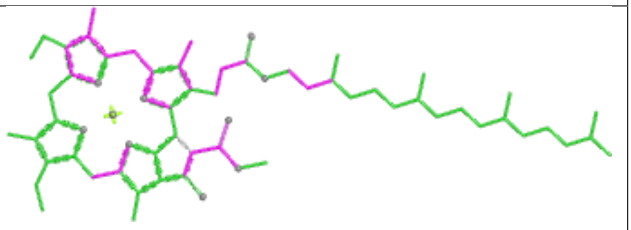


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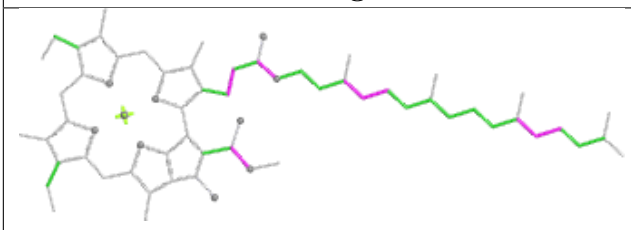
Ligand CLA n 609



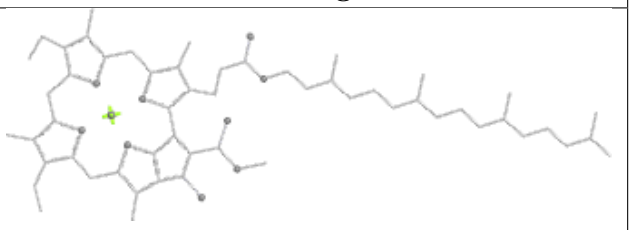
Bond lengths



Bond angles

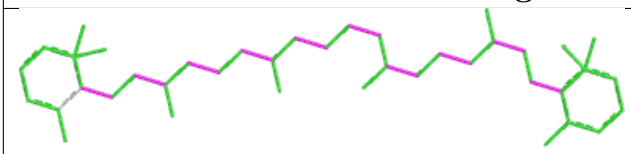


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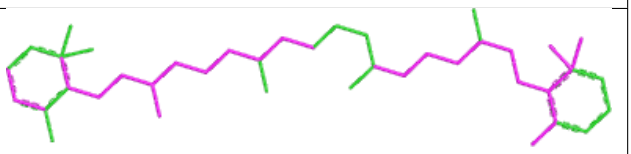


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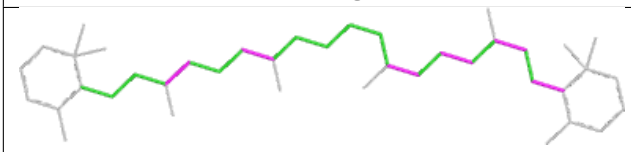
Ligand WVN A 847



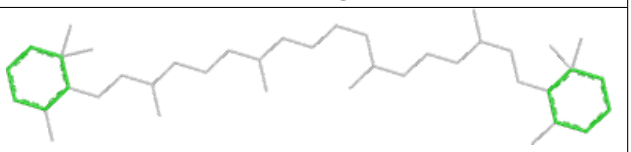
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Bond angles

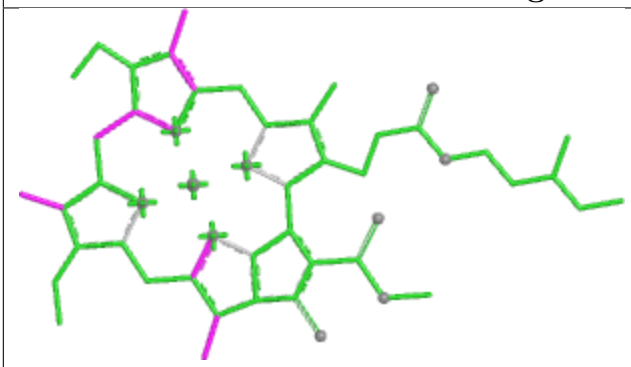


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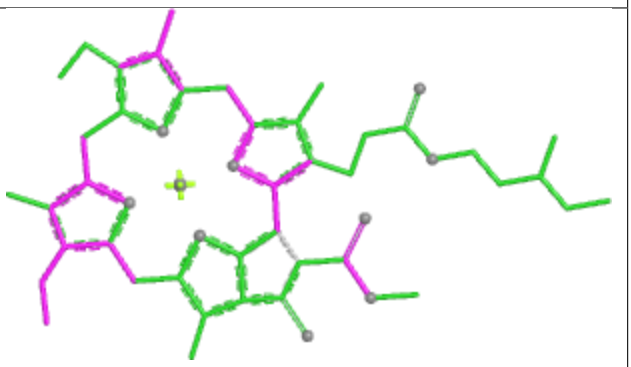


Rings

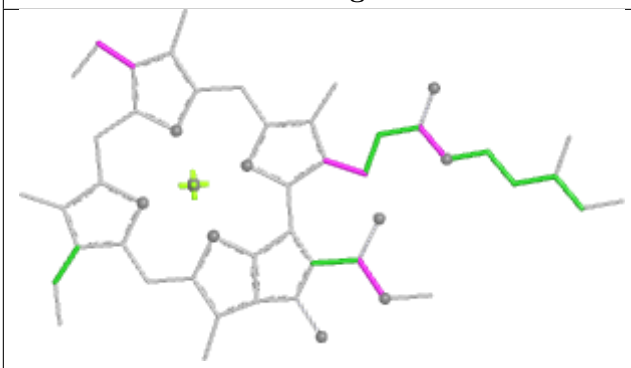
Ligand CLA n 605



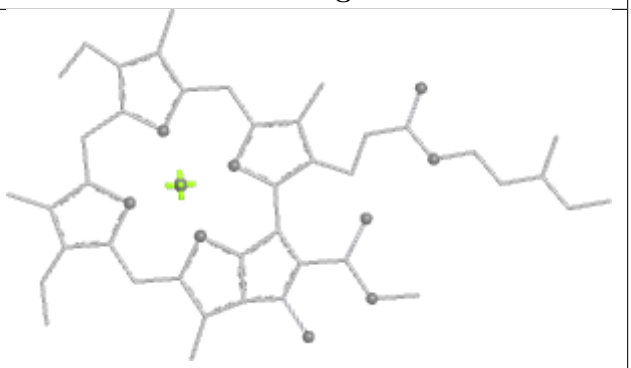
Bond lengths



Bond angles

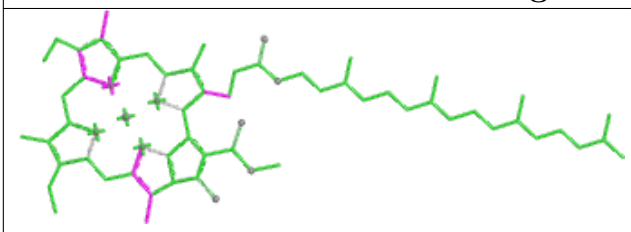


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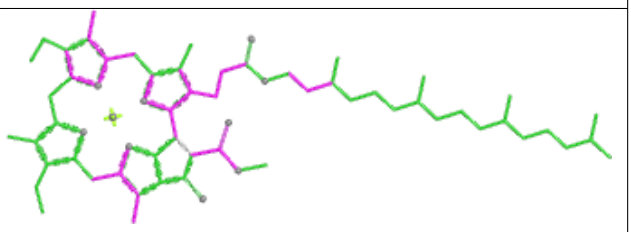


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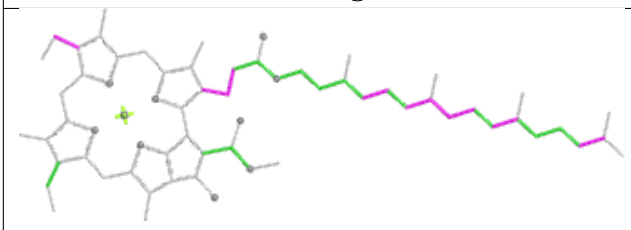
Ligand CLA s 202



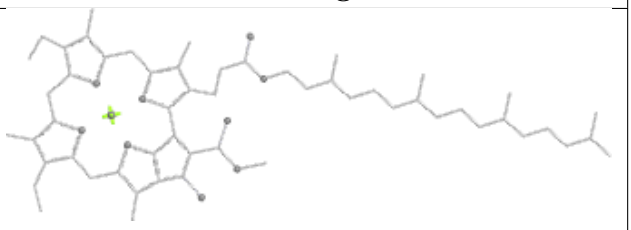
Bond lengths



Bond angles

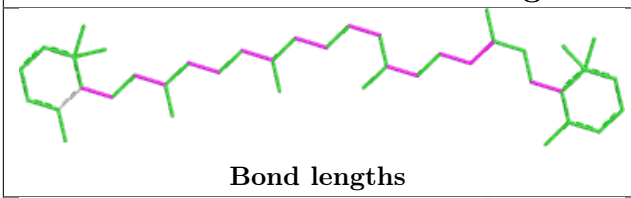


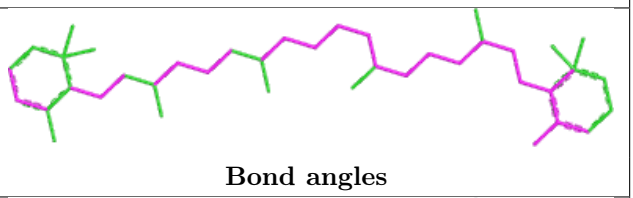
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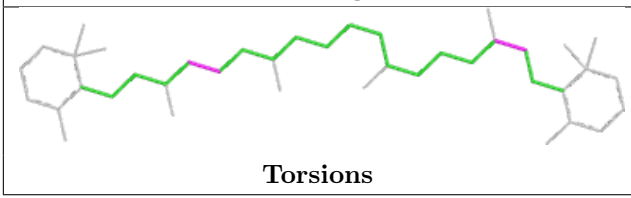


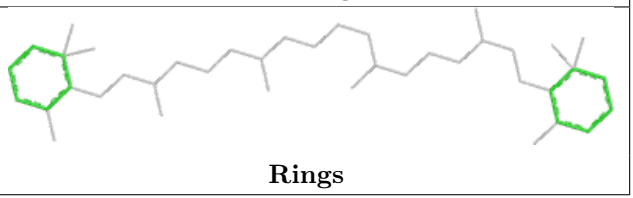
Rings

Ligand WVN l 301

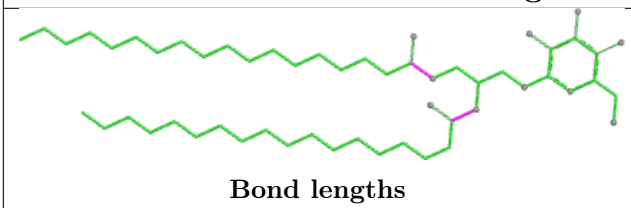

Bond lengths

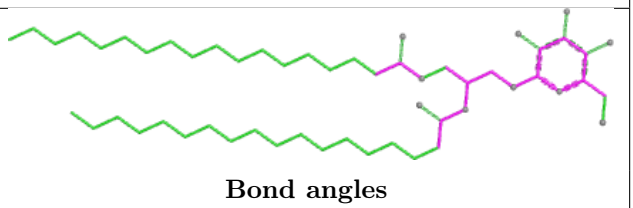

Bond angles

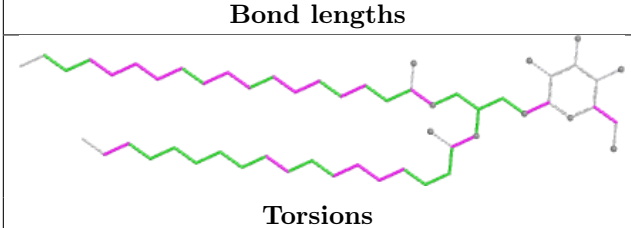

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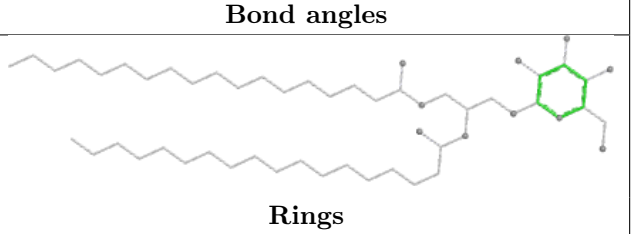

Rings

Ligand LMG c 619

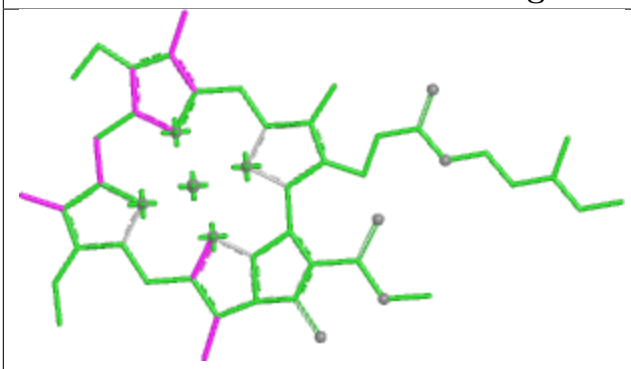

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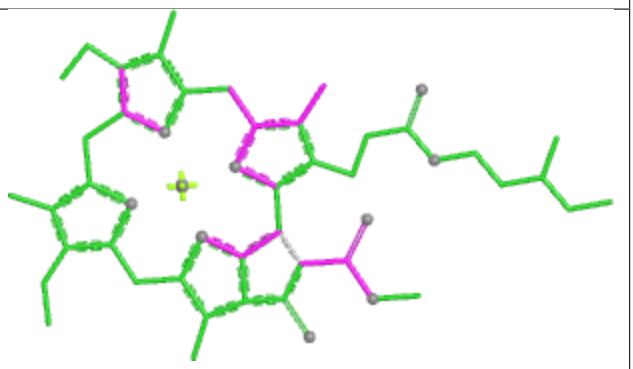

Bond angles

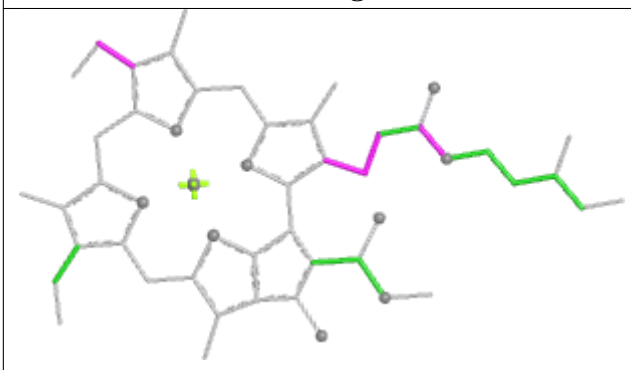

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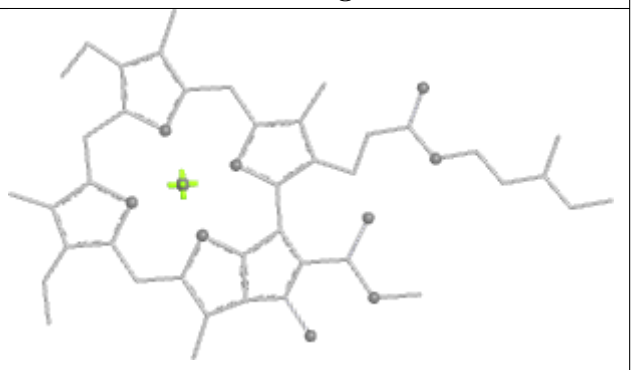

Rings

Ligand CLA n 608

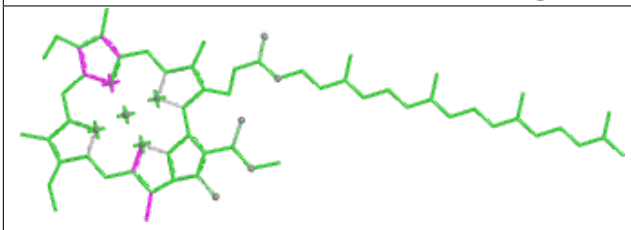

Bond lengths


Bond angles

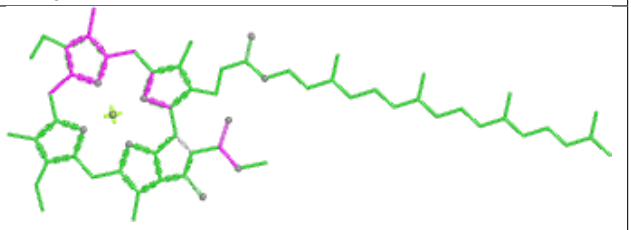

Torsions


Rings

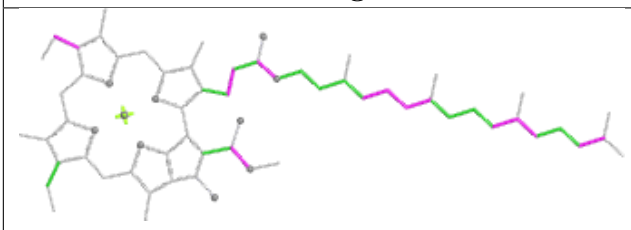
Ligand CLA j 612



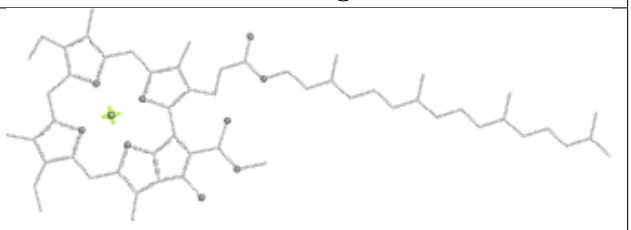
Bond lengths



Bond angles

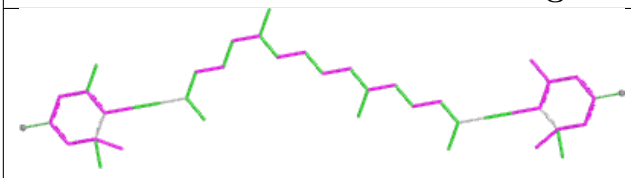


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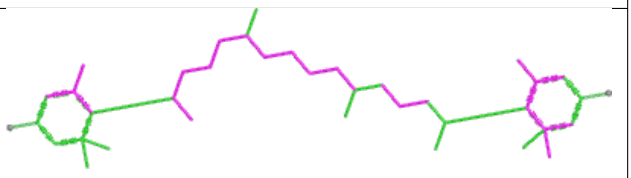


Rings

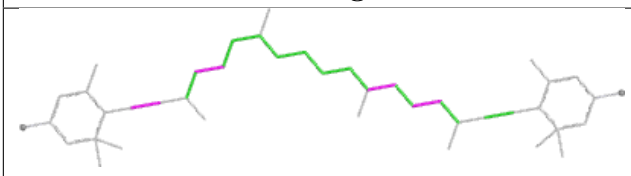
Ligand II0 l 315



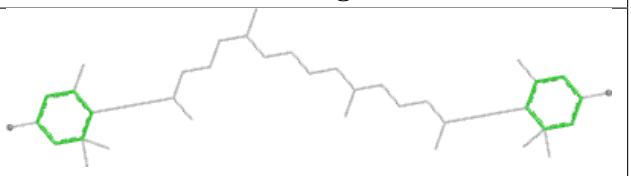
Bond lengths



Bond angles

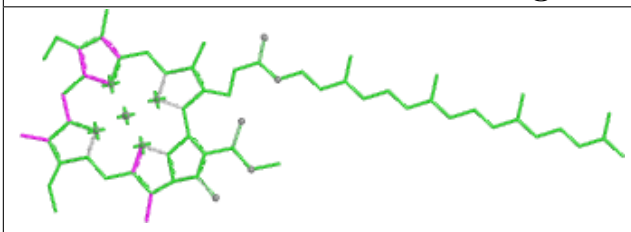


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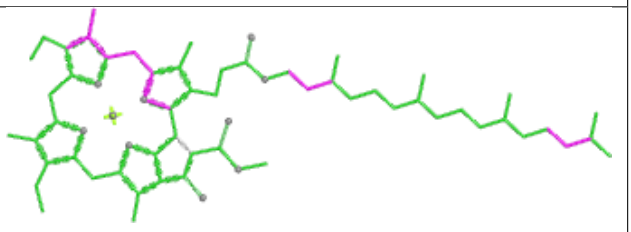


Rings

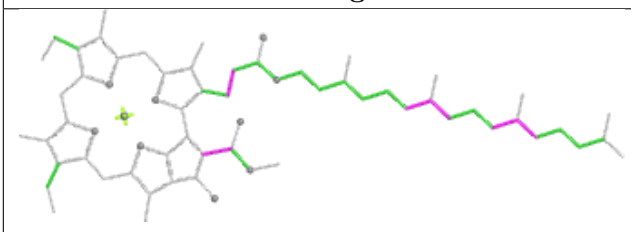
Ligand CLA i 305



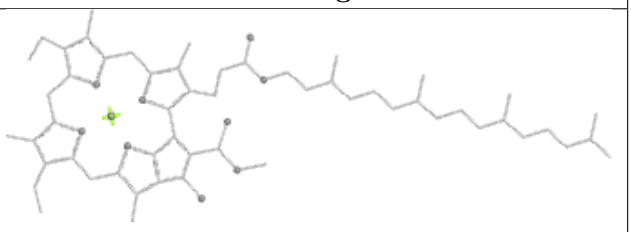
Bond lengths



Bond angles

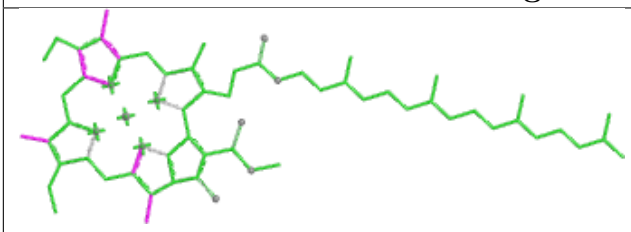


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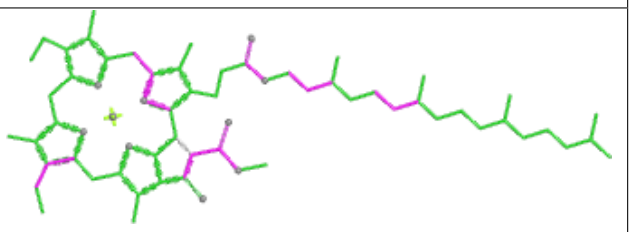


Rings

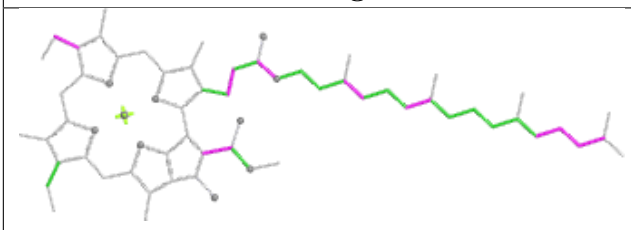
Ligand CLA A 835



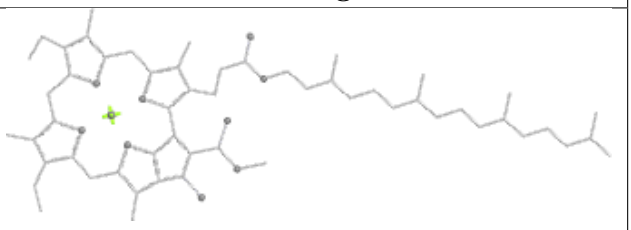
Bond lengths



Bond angles

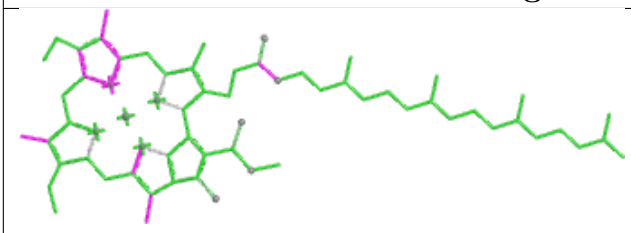


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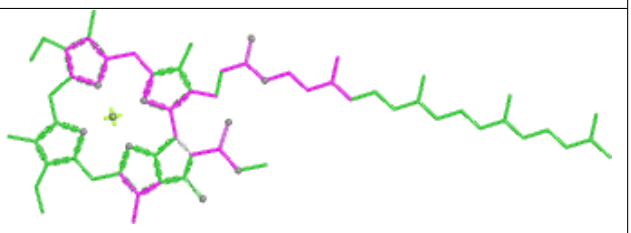


Rings

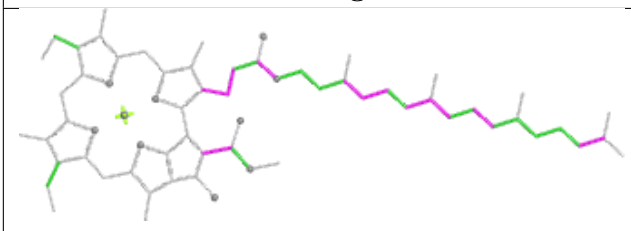
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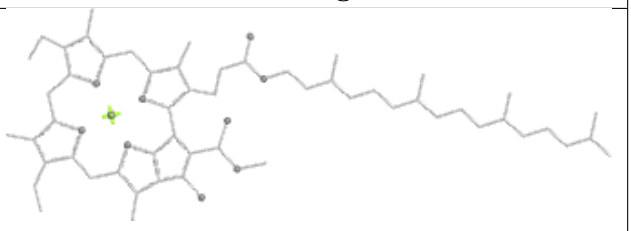
Bond lengths



Bond angles

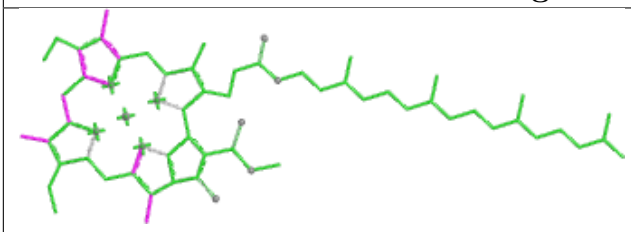


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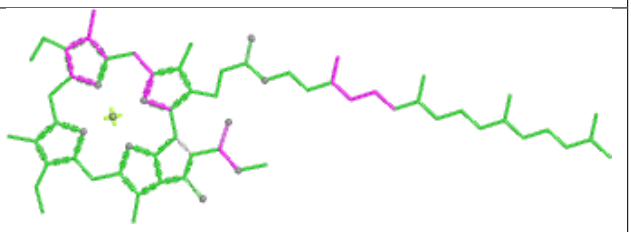


Rings

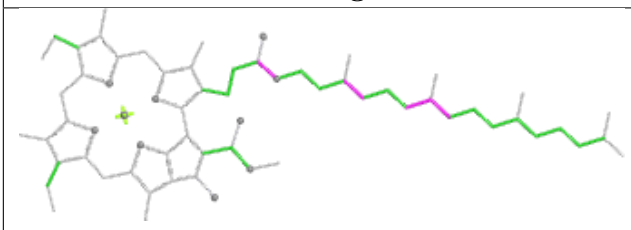
Ligand CLA f 609



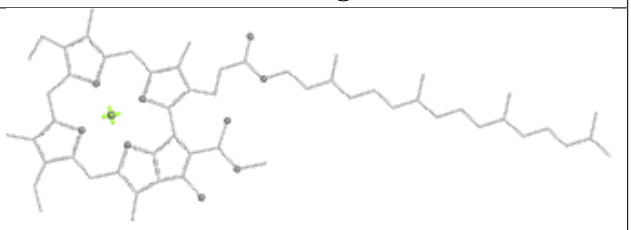
Bond lengths



Bond angles

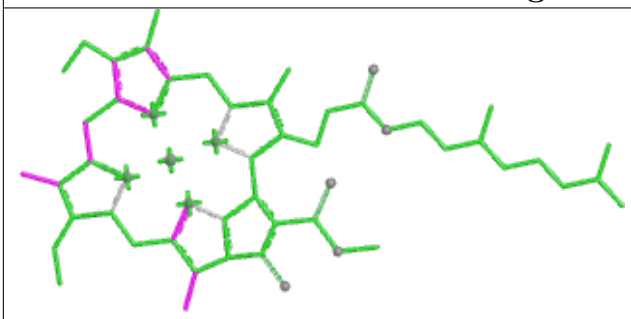


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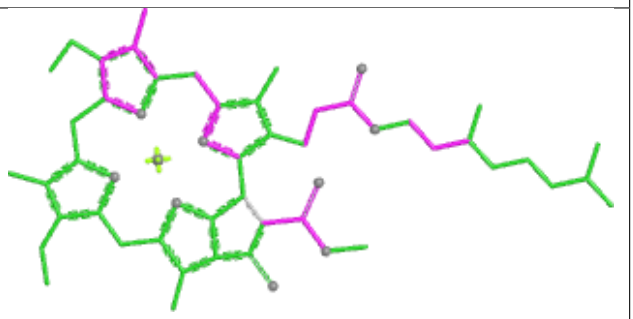


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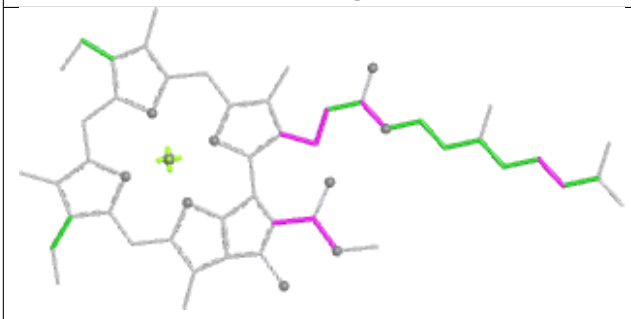
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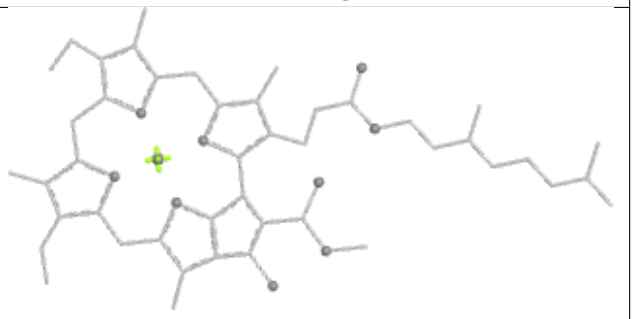
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Bond angles

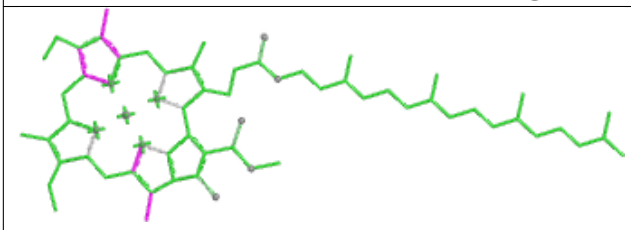


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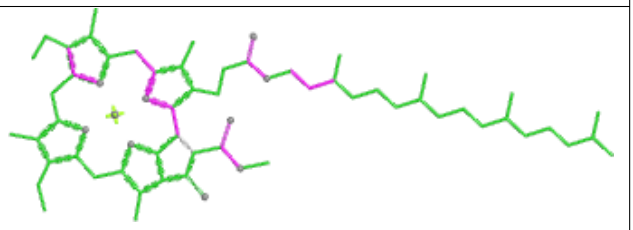


Rings

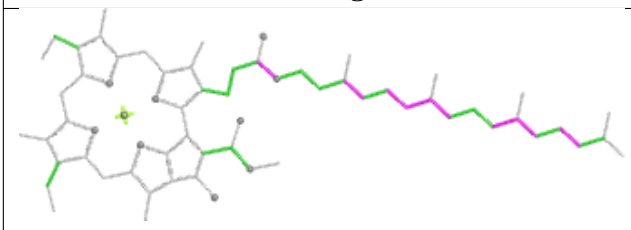
Ligand CLA F 202



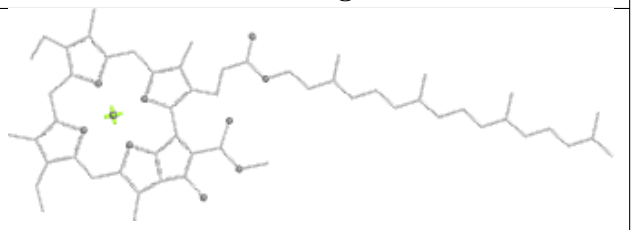
Bond lengths



Bond angles

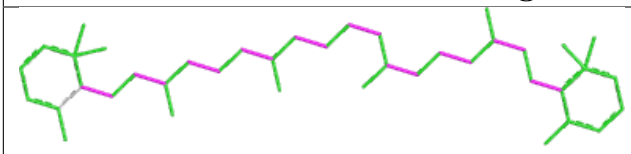


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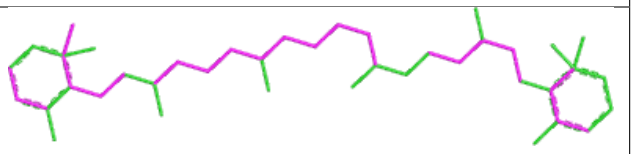


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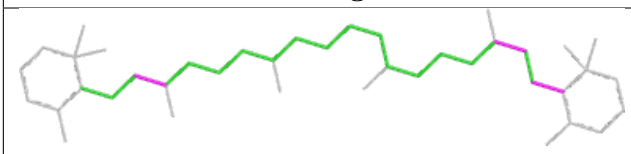
Ligand WVN L 205



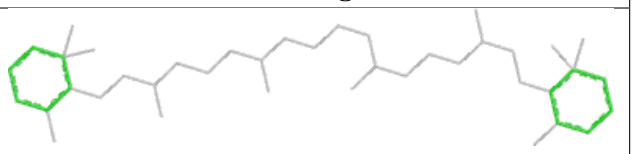
Bond lengths



Bond angles

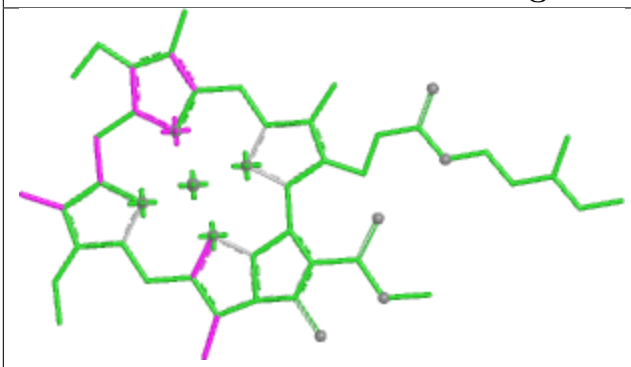


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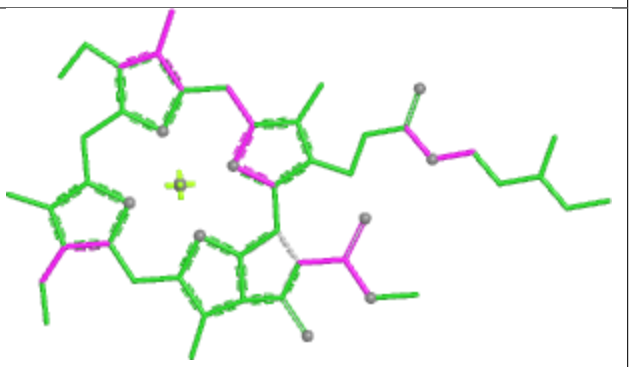


Rings

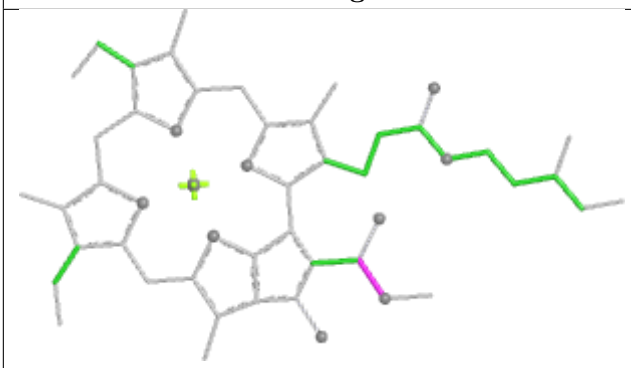
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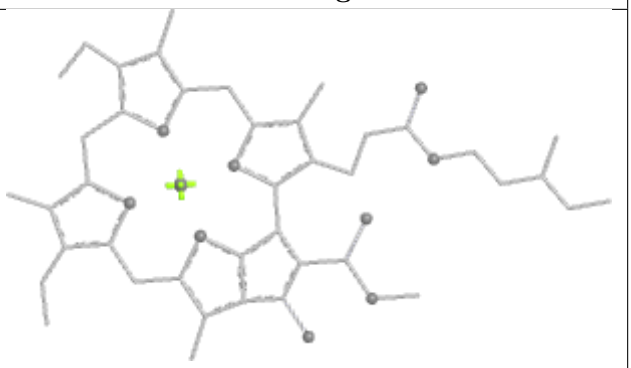
Bond lengths



Bond angles

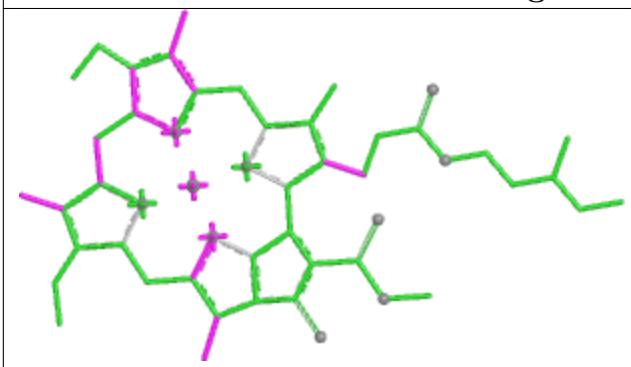


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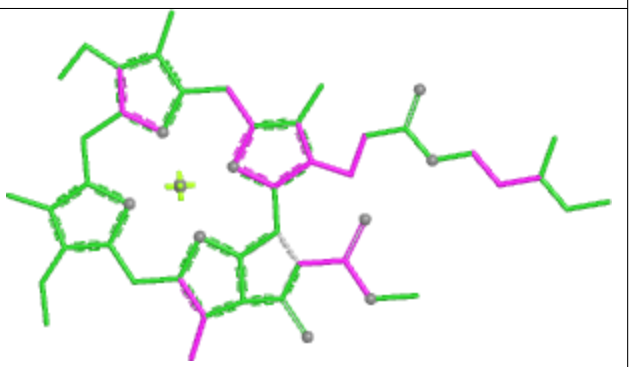


Rings

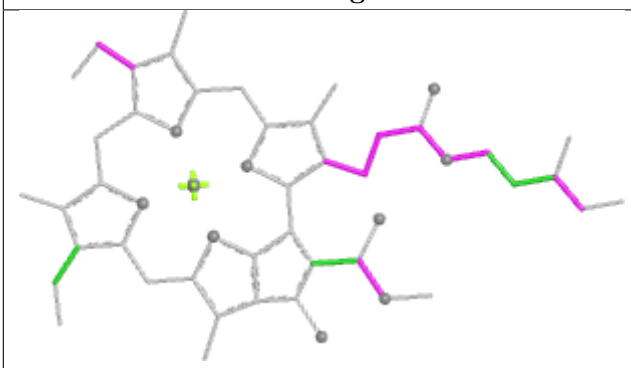
Ligand CLA k 305



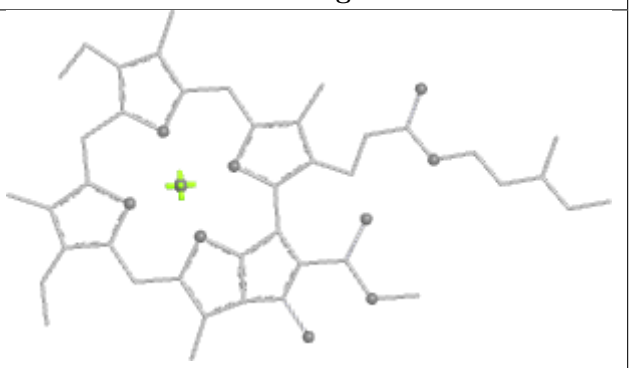
Bond lengths



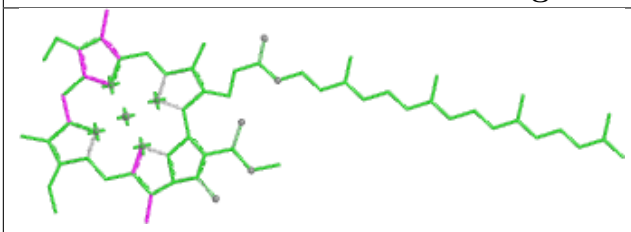
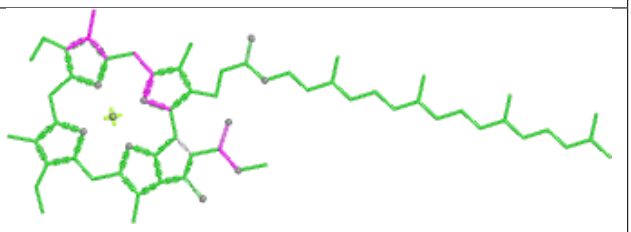
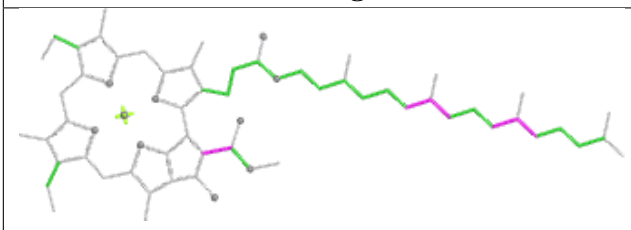
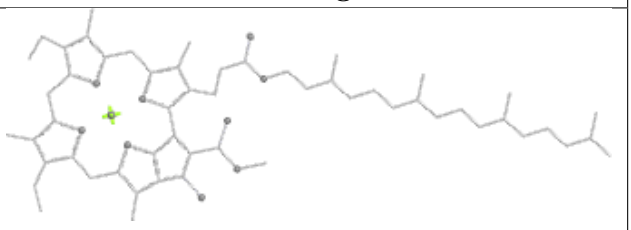
Bond angles

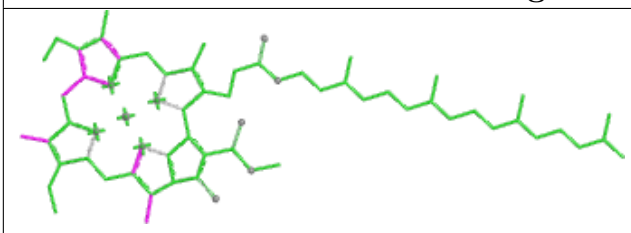
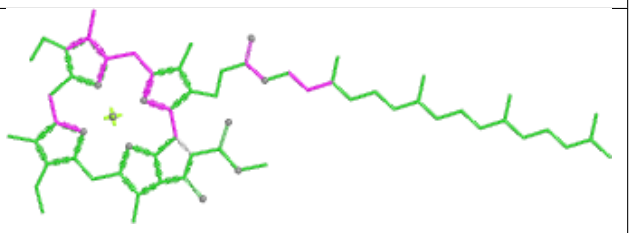
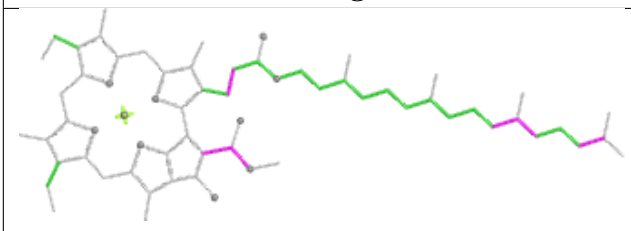
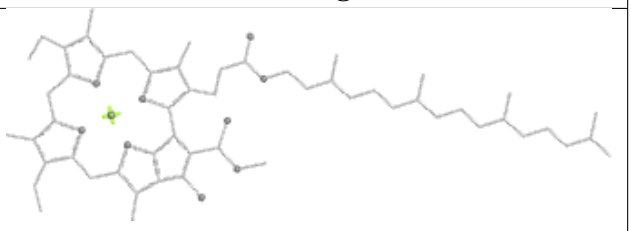


Torsions

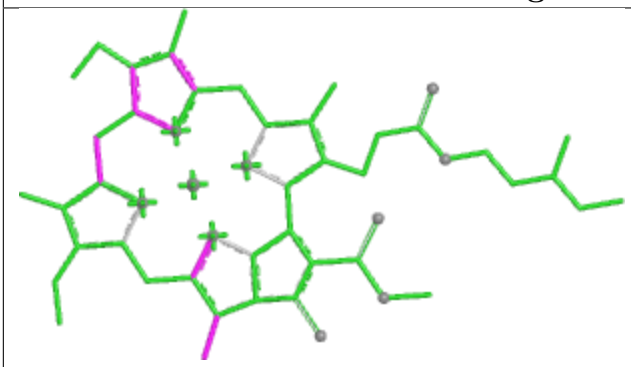


Rings

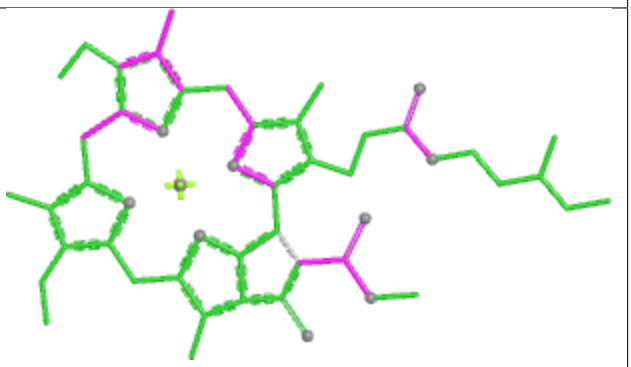
Ligand CLA f 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA k 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

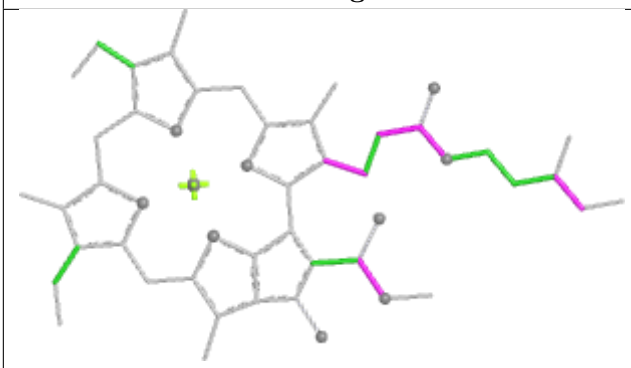
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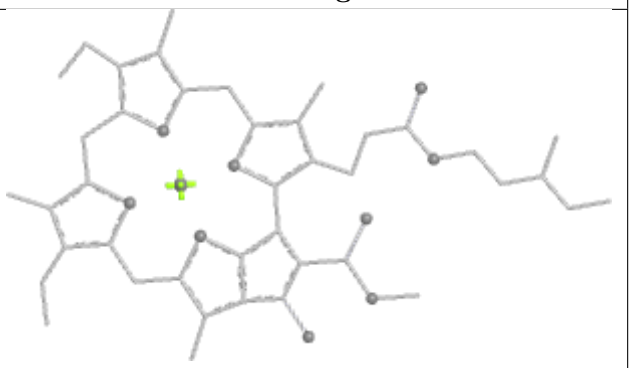
Bond lengths



Bond angles

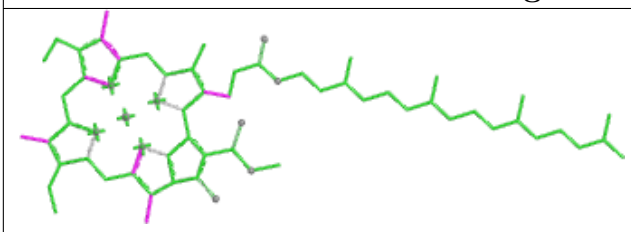


Torsions

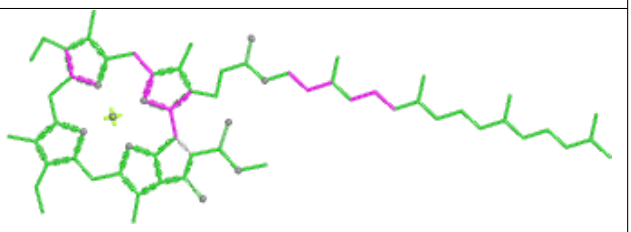


Rings

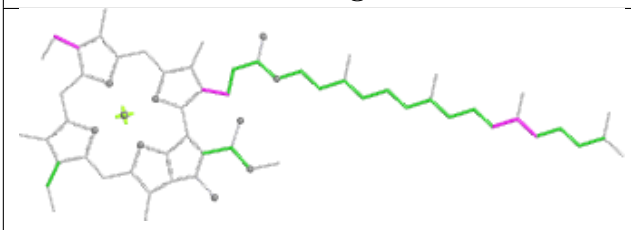
Ligand CLA A 831



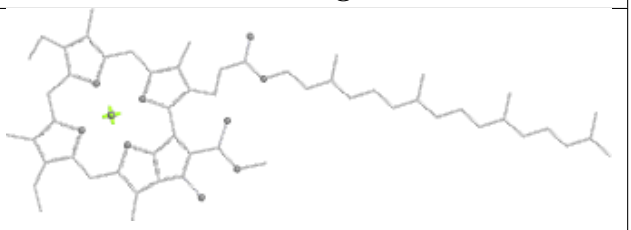
Bond lengths



Bond angles

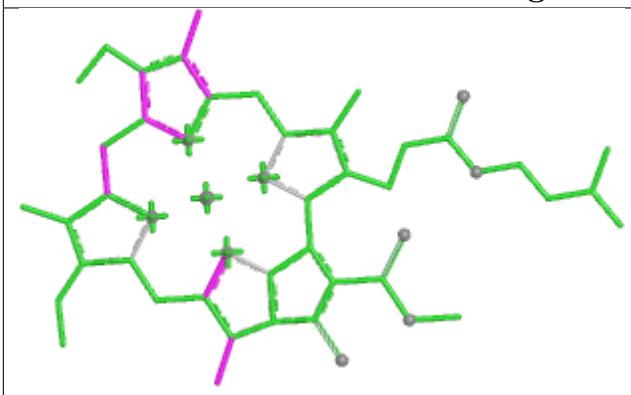


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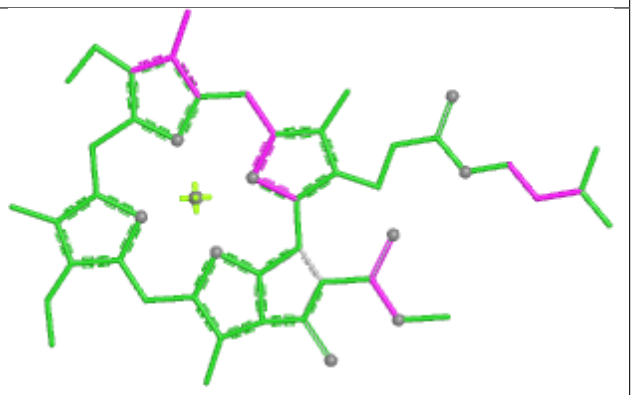


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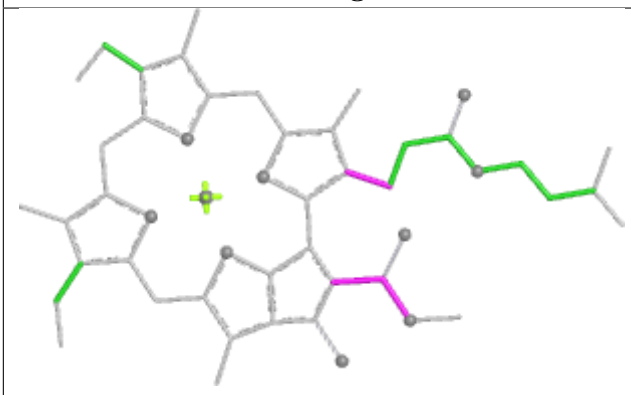
Ligand CLA k 301



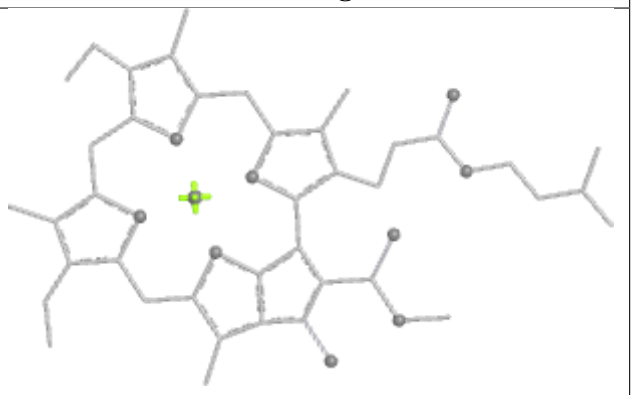
Bond lengths



Bond angles

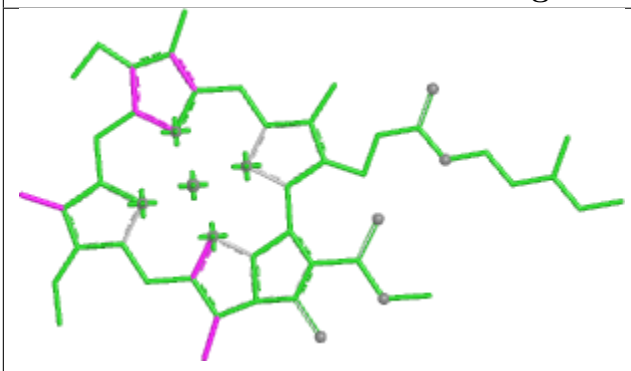


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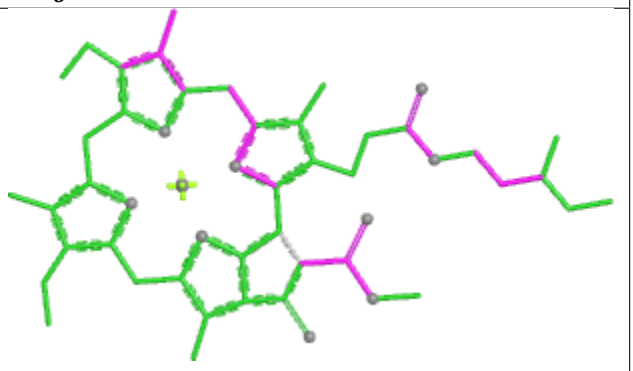


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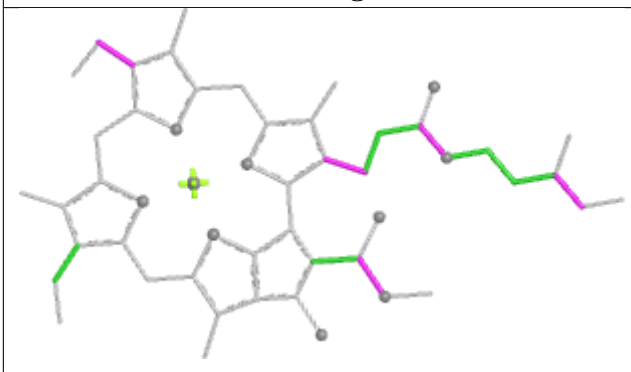
Ligand CLA j 611



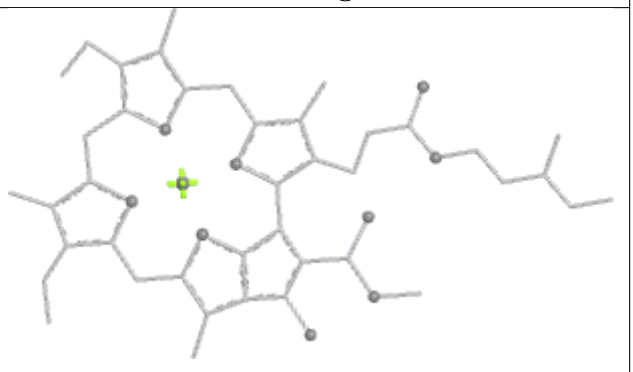
Bond lengths



Bond angles

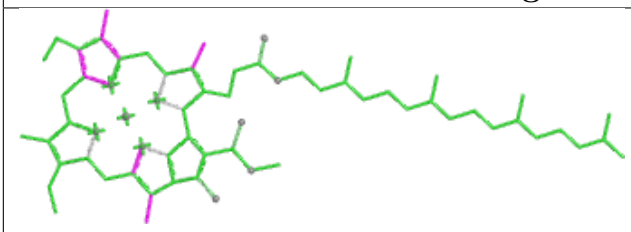


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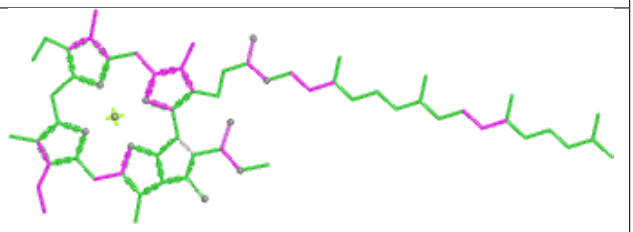


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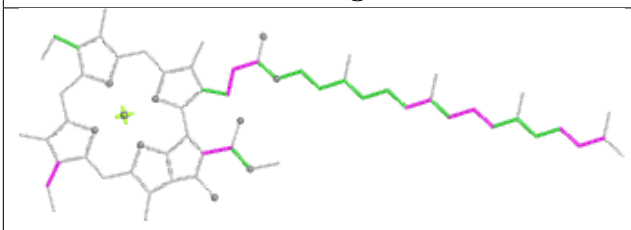
Ligand CLA m 604



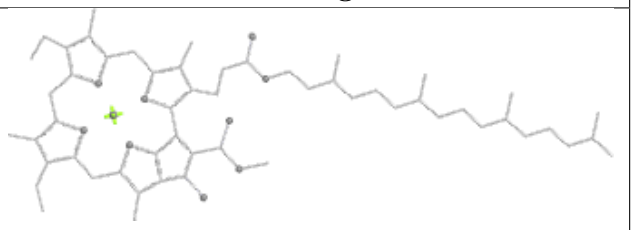
Bond lengths



Bond angles

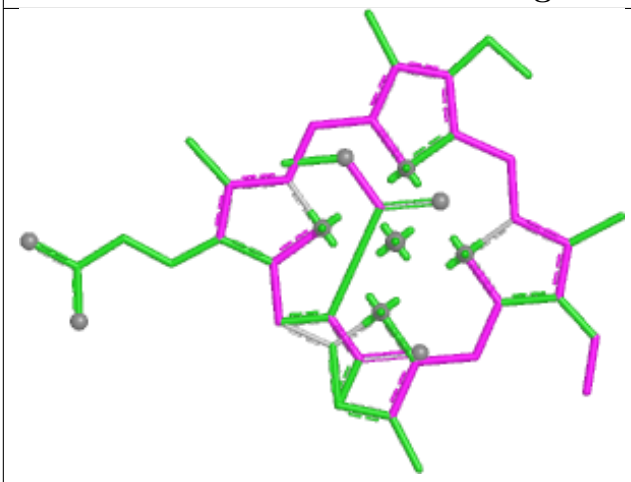


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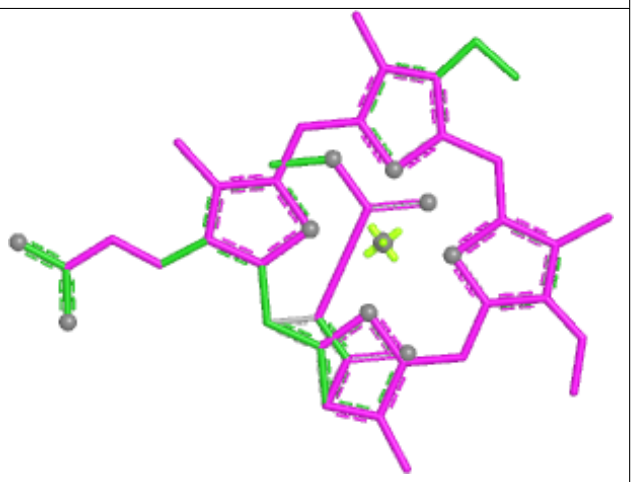


Rings

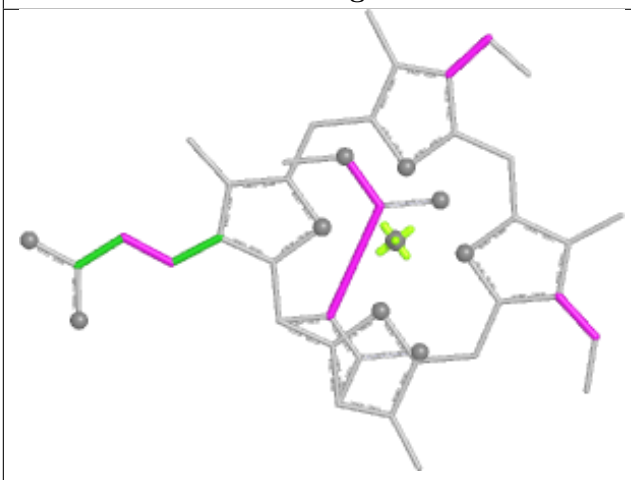
Ligand KC2 i 317



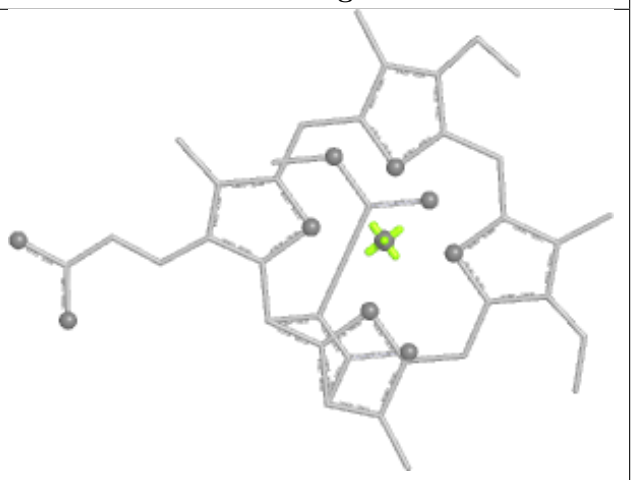
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Bond angles

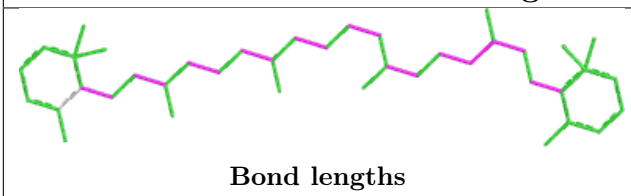


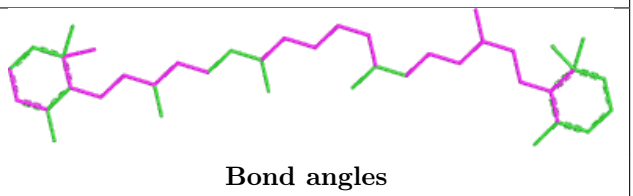
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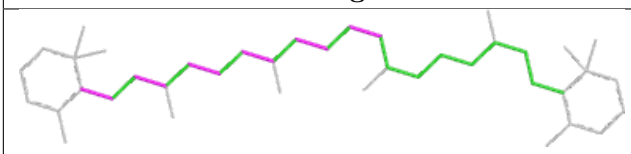


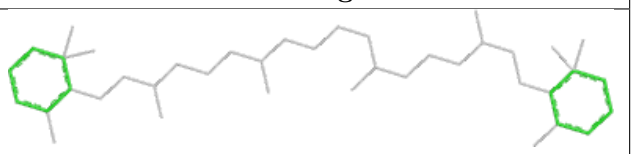
Rings

Ligand WVN I 101

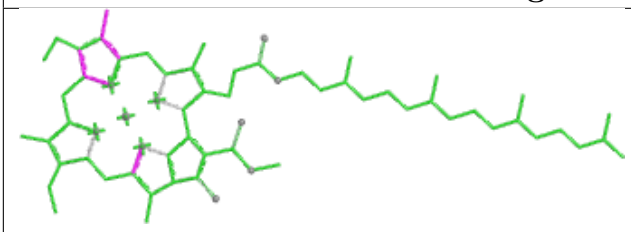

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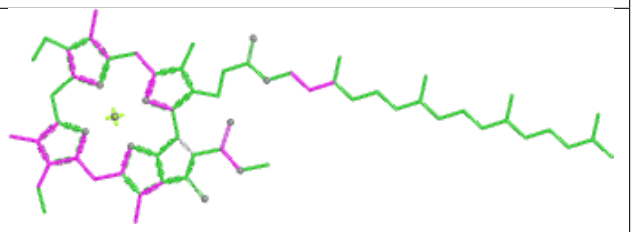

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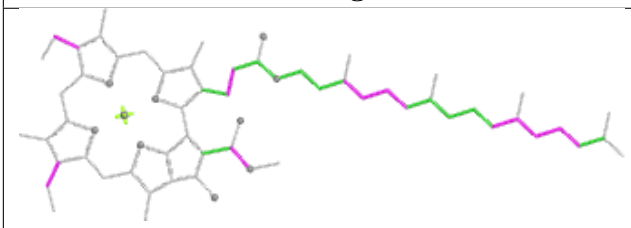

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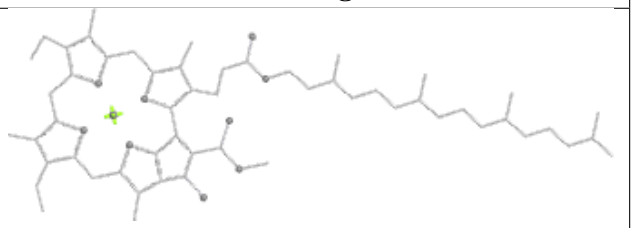

Rings

Ligand CLA b 607

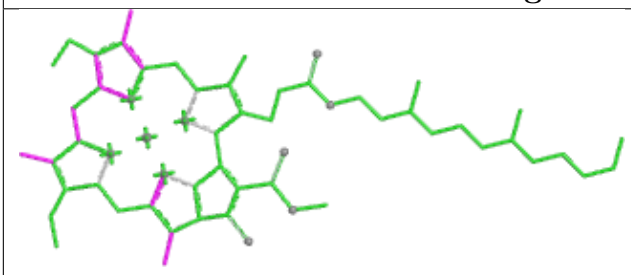

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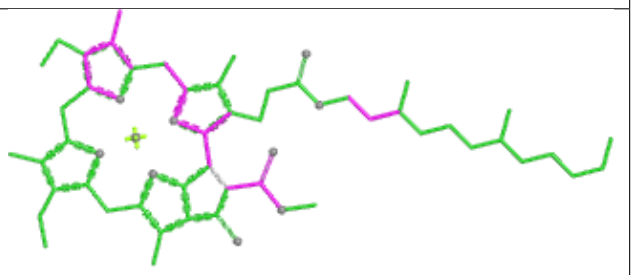

Bond angles

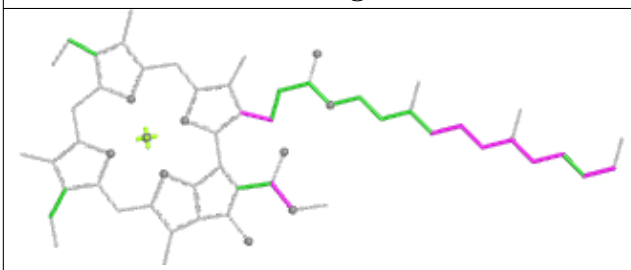

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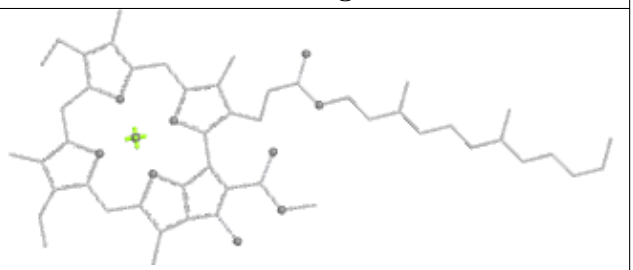

Rings

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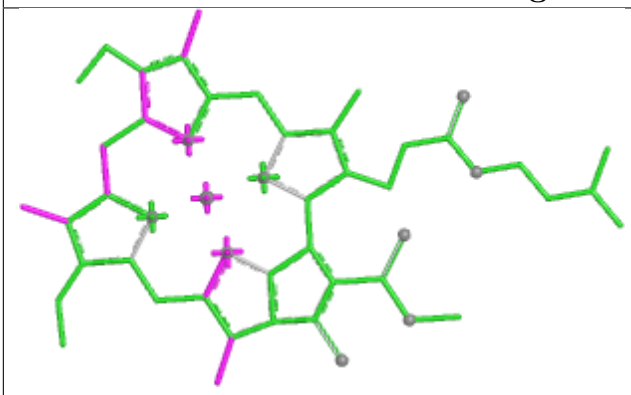

Bond lengths


Bond angles

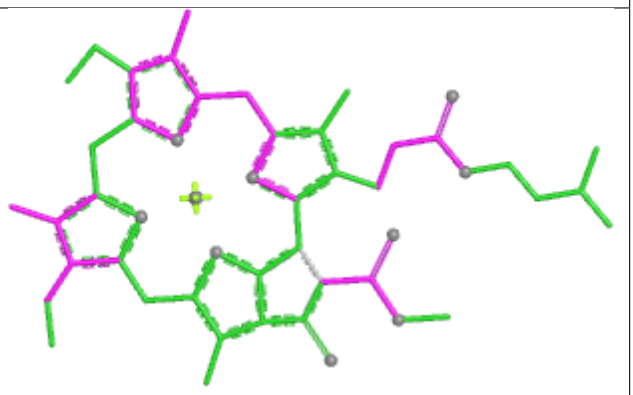

Torsions


Rings

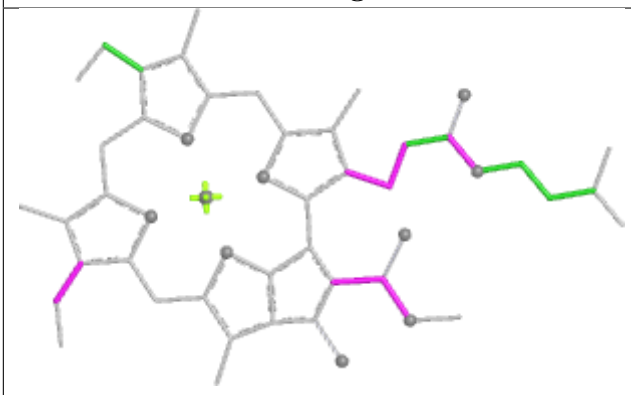
Ligand CLA c 602



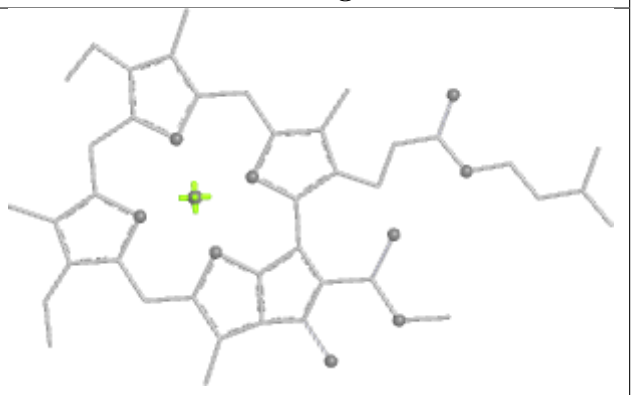
Bond lengths



Bond angles

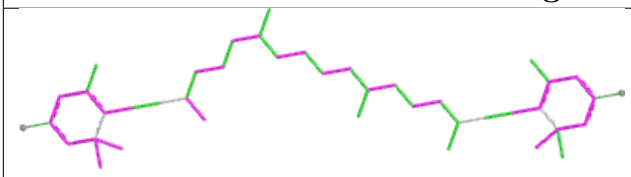


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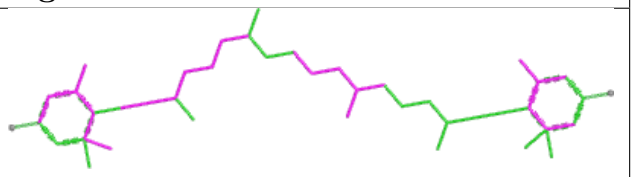


Rings

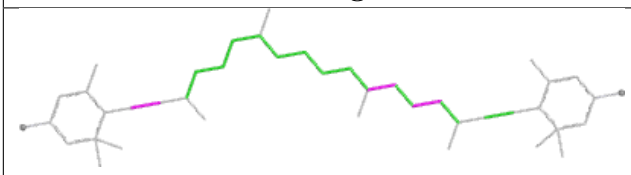
Ligand II0 g 316



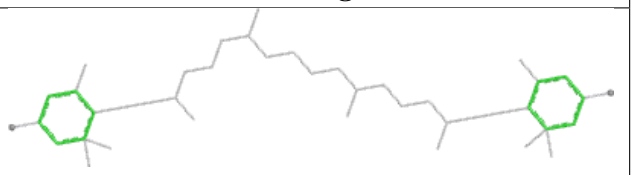
Bond lengths



Bond angles

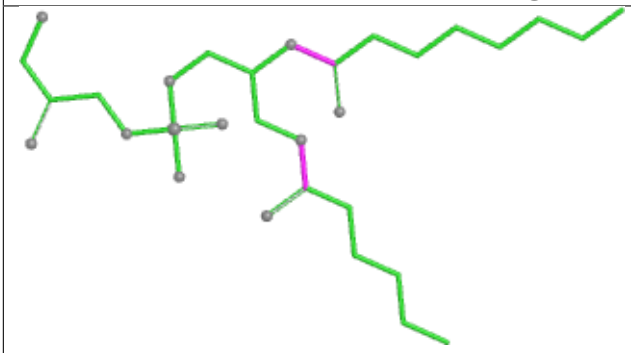


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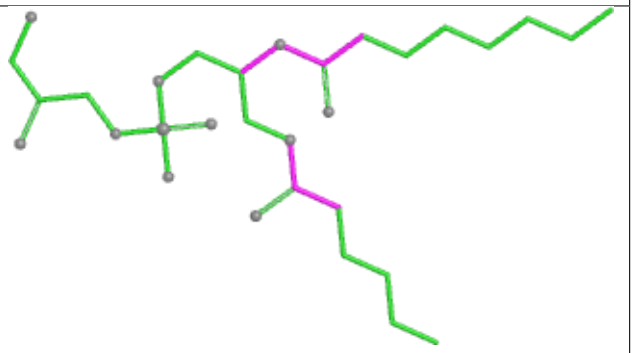


Rings

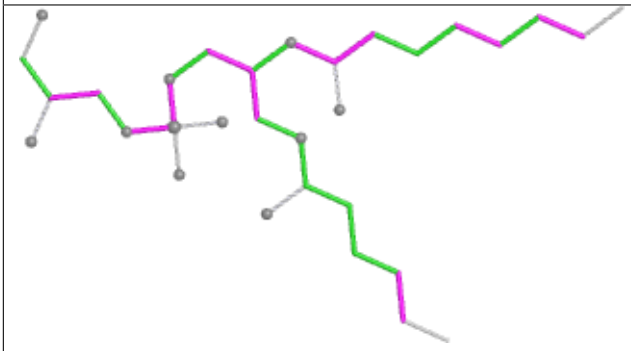
Ligand LHG b 618



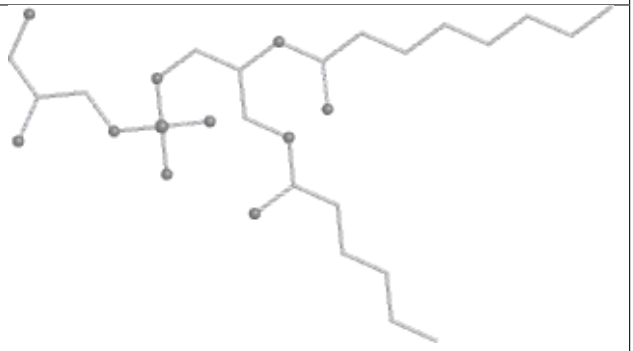
Bond lengths



Bond angles

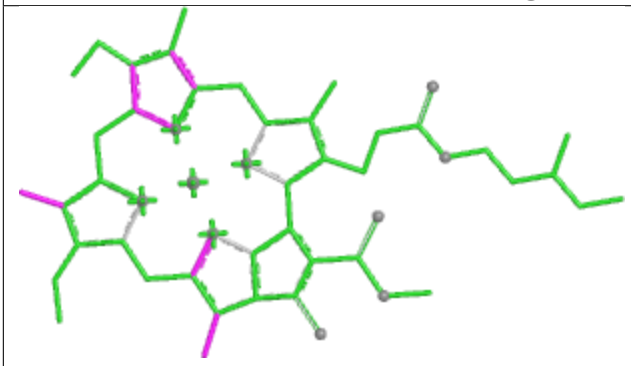


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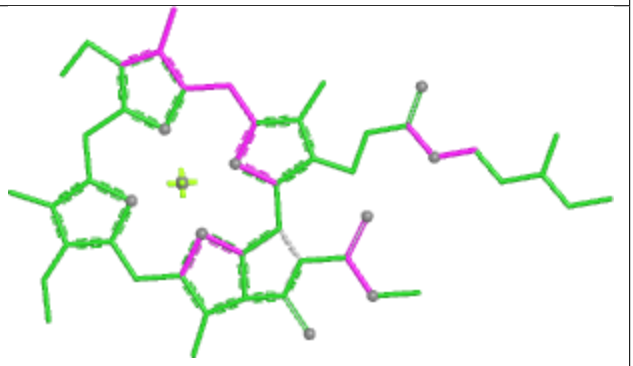


Rings

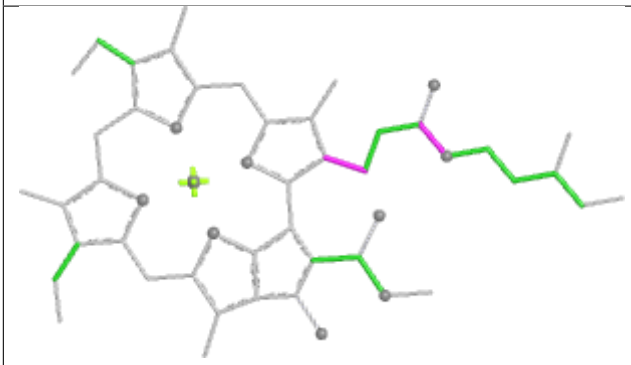
Ligand CLA m 608



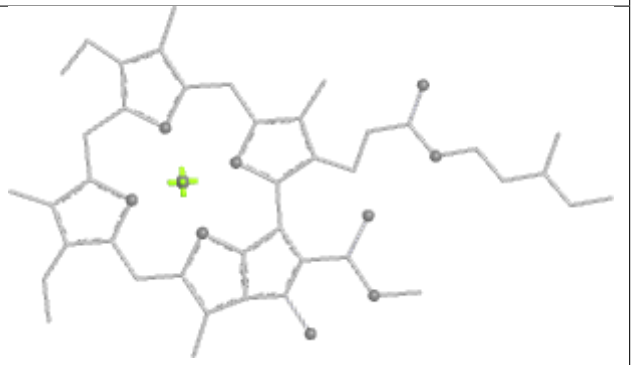
Bond lengths



Bond angles

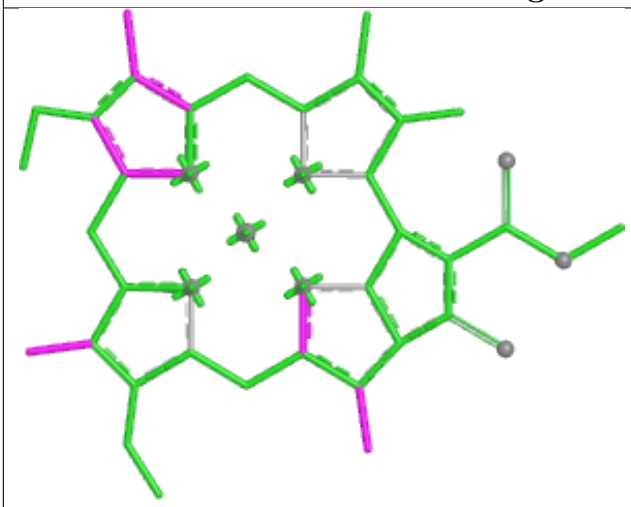


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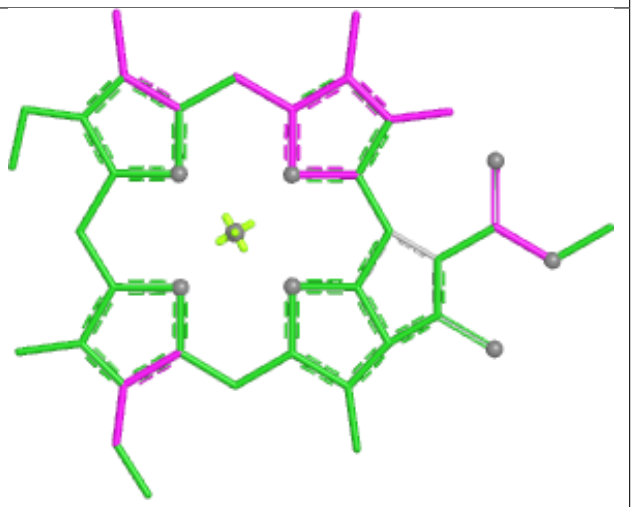


Rings

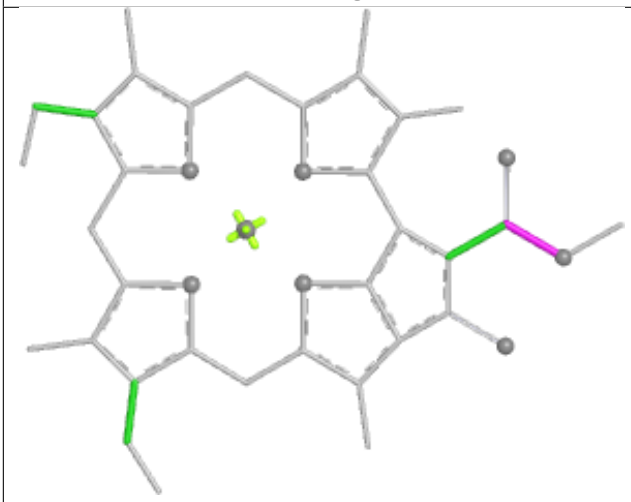
Ligand CLA d 307



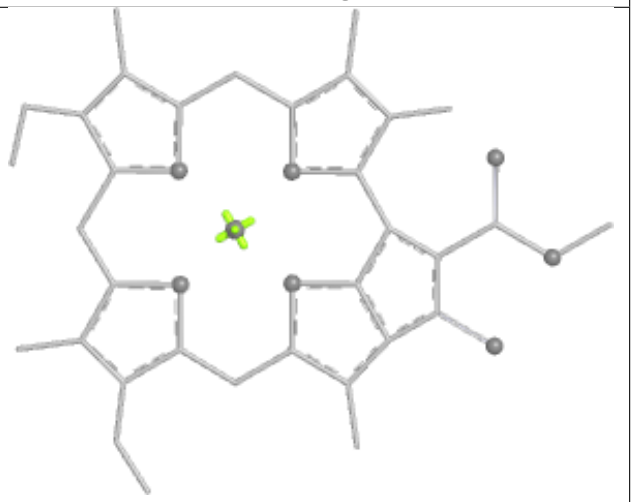
Bond lengths



Bond angles

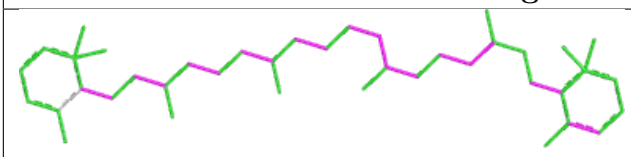


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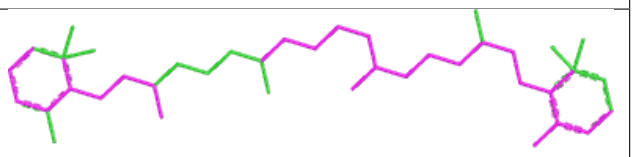


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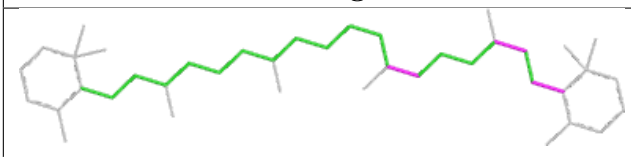
Ligand WVN s 205



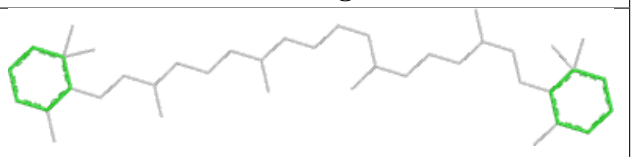
Bond lengths



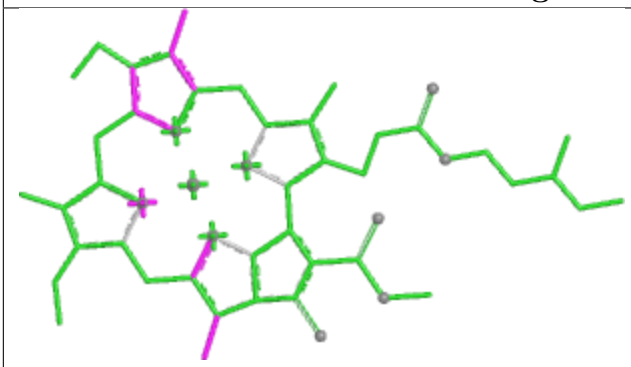
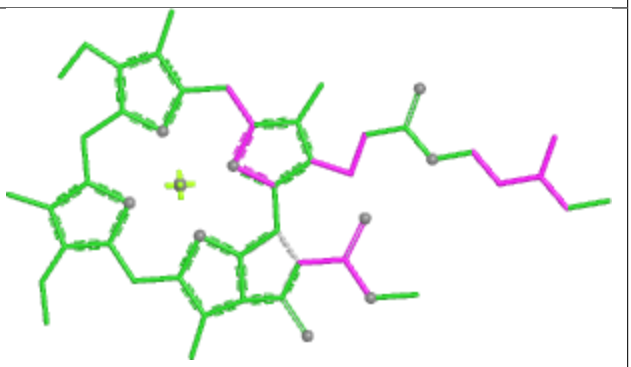
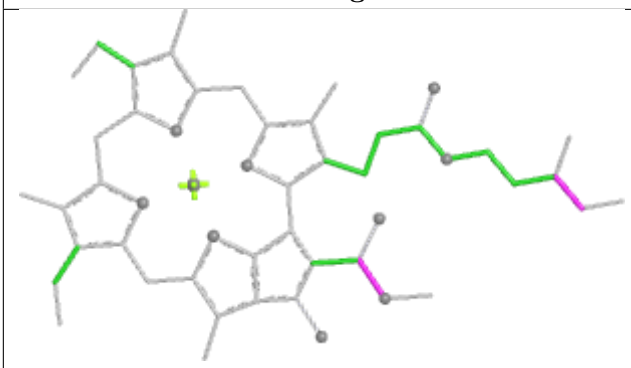
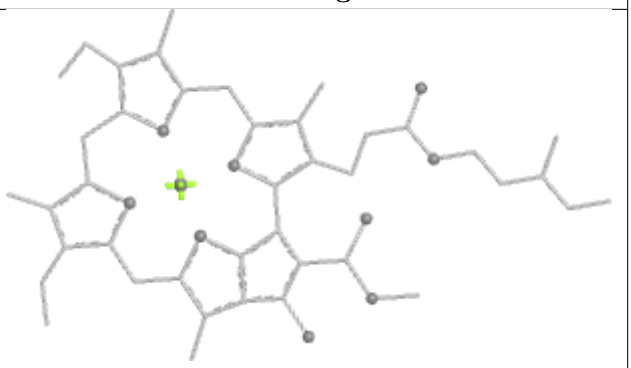
Bond angles

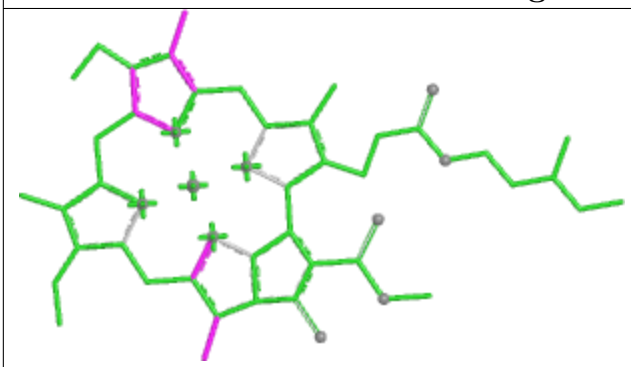
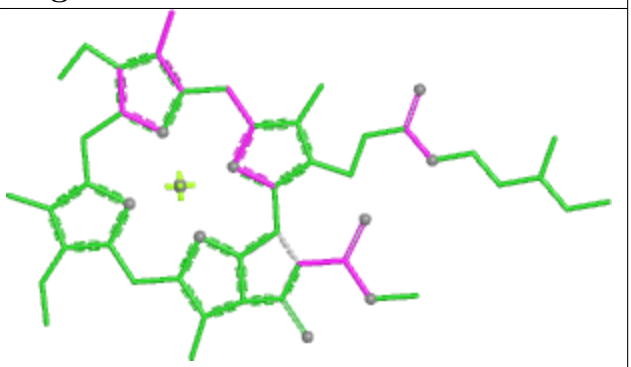
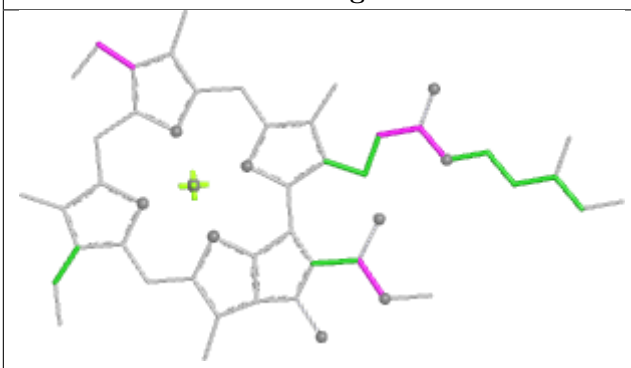
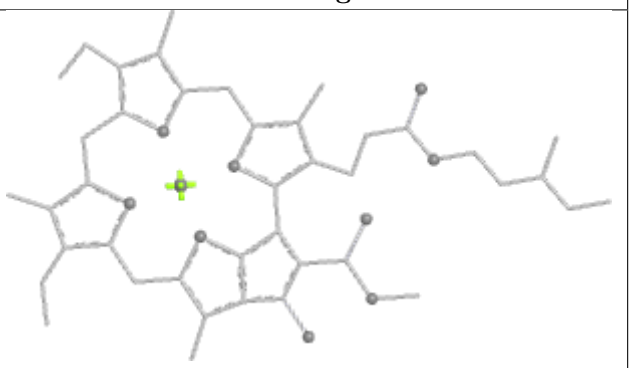


Torsions

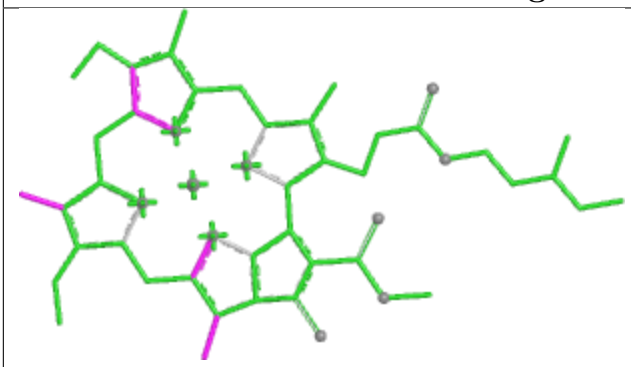


Rings

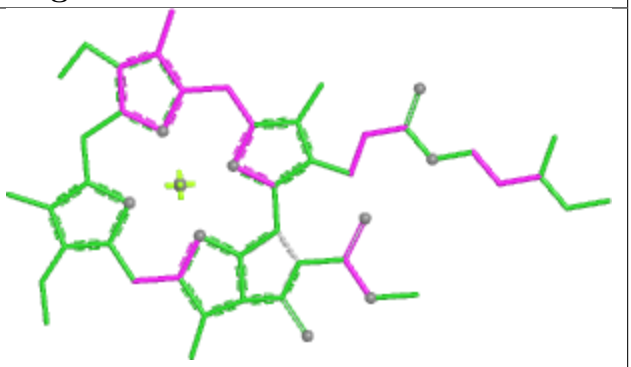
Ligand CLA f 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

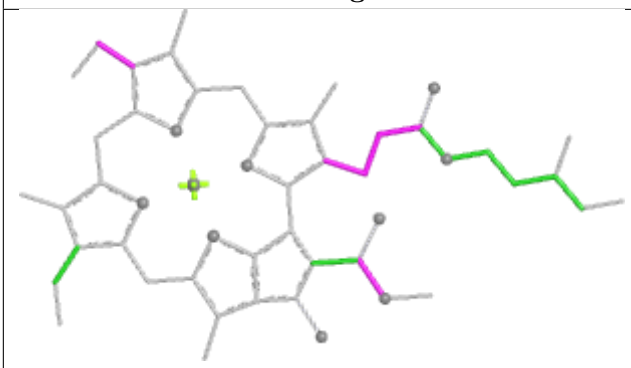
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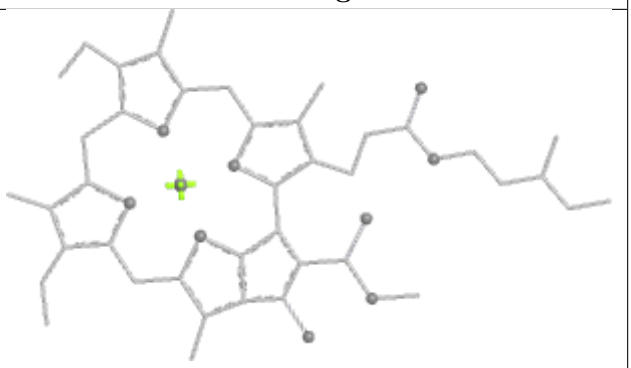
Bond lengths



Bond angles

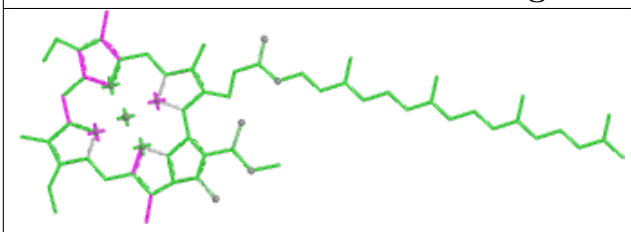


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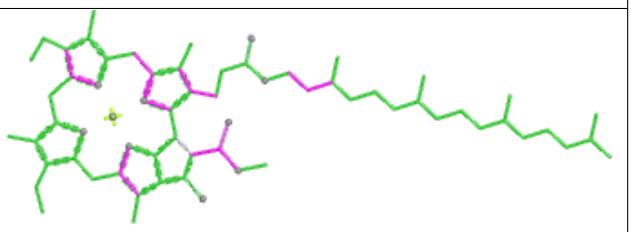


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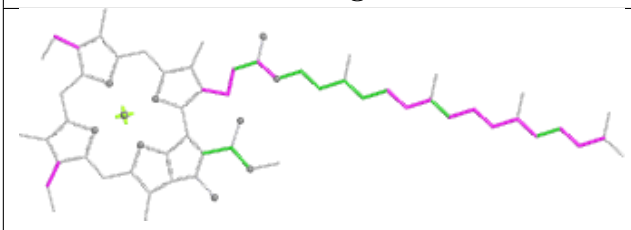
Ligand CLA a 312



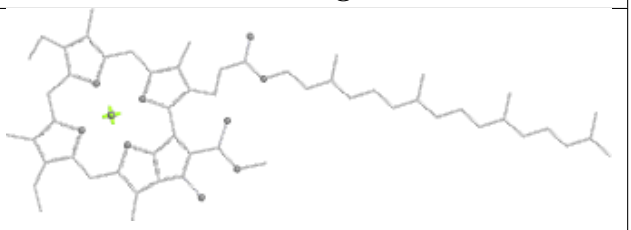
Bond lengths



Bond angles

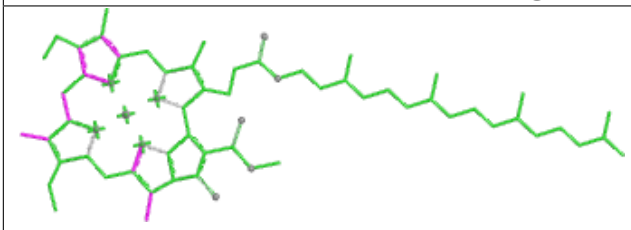


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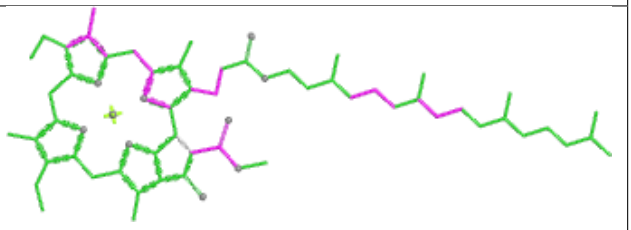


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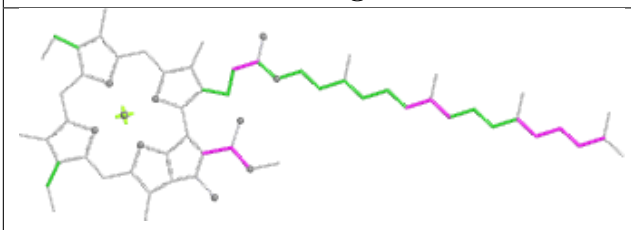
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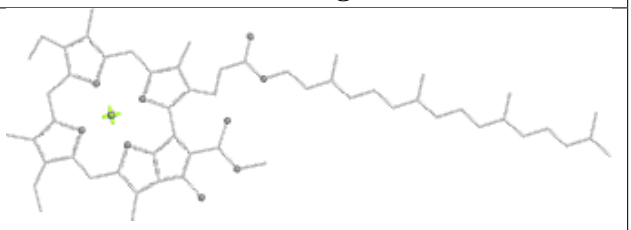
Bond lengths



Bond angles

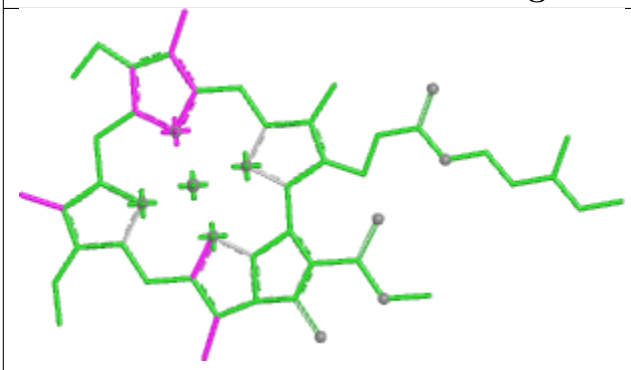


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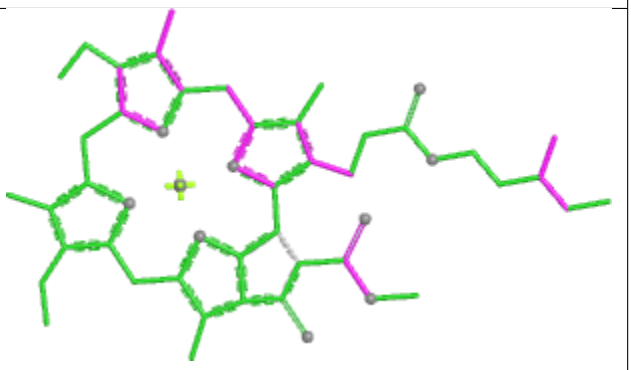


Rings

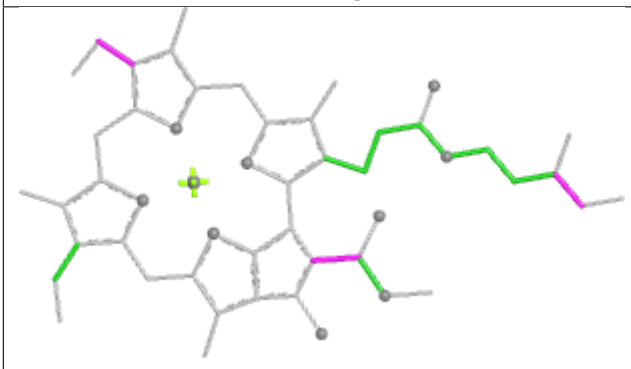
Ligand CLA a 305



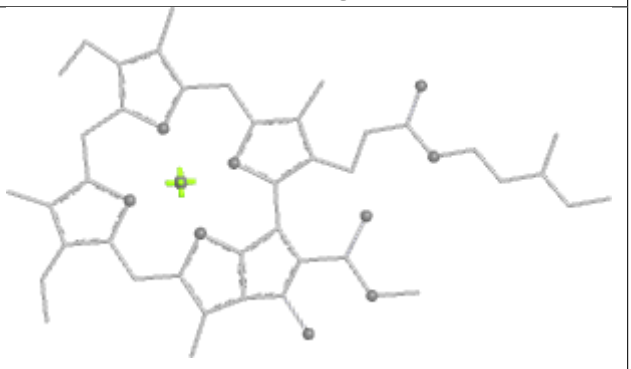
Bond lengths



Bond angles

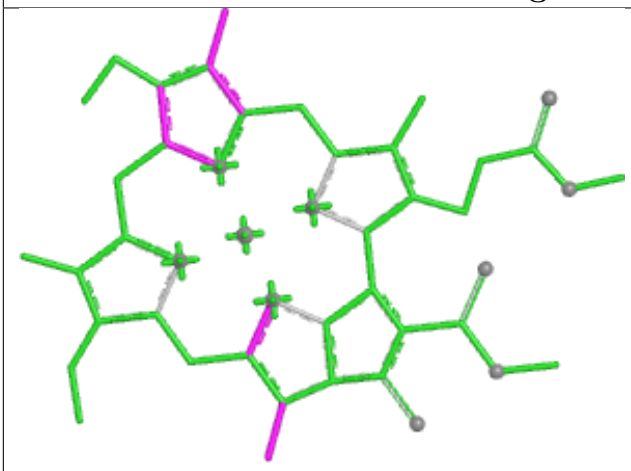


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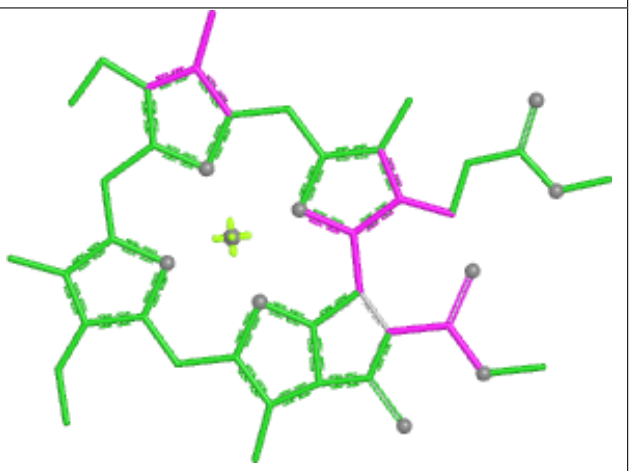


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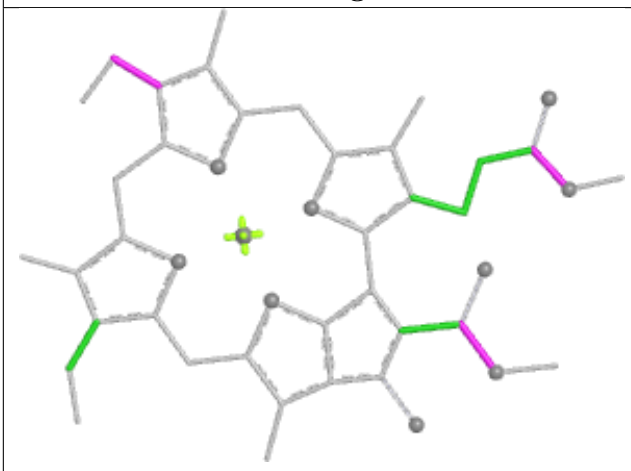
Ligand CLA c 607



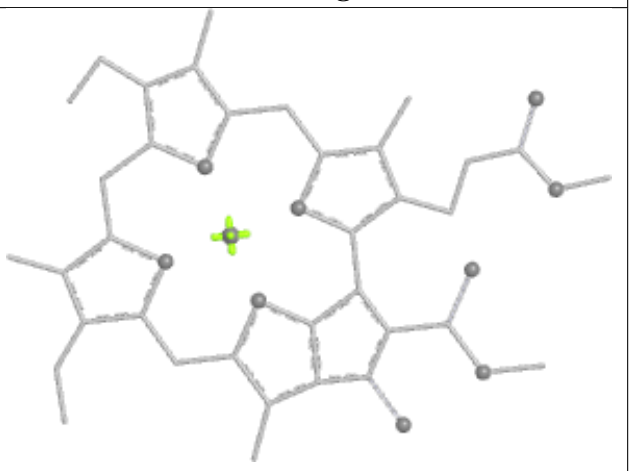
Bond lengths



Bond angles

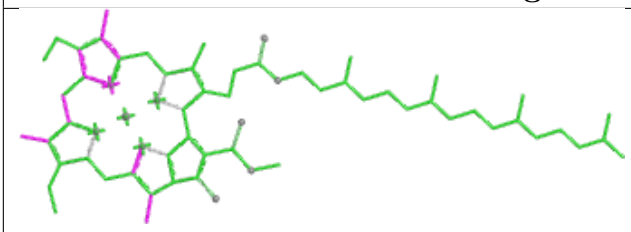


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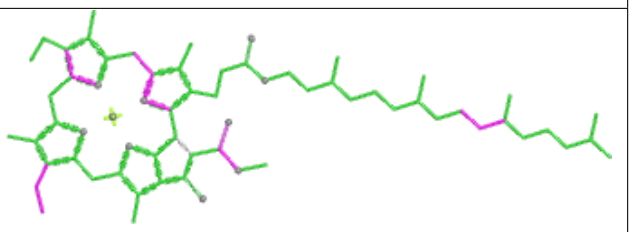


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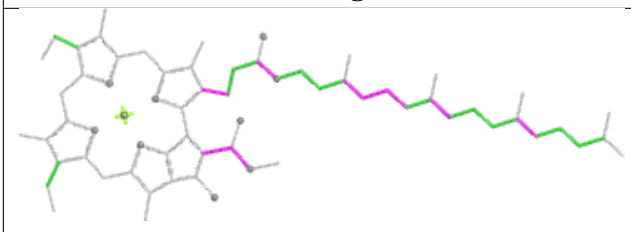
Ligand CLA O 202



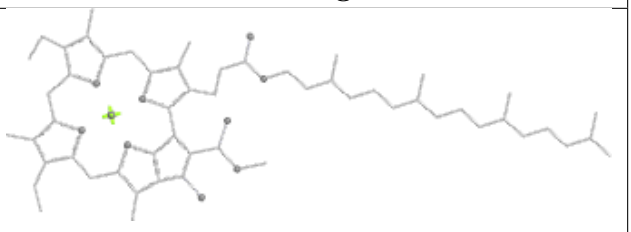
Bond lengths



Bond angles

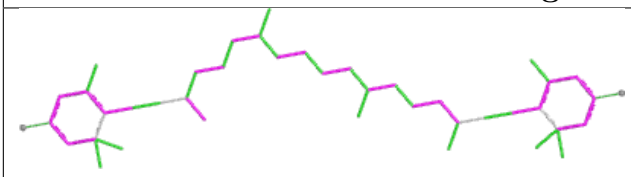


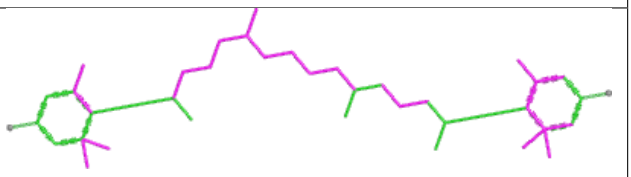
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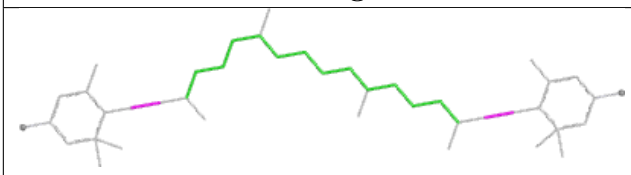


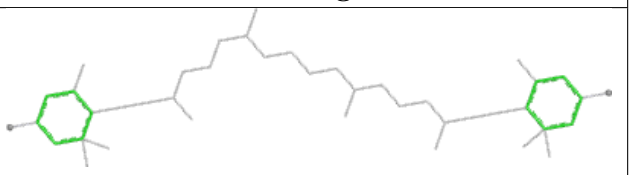
Rings

Ligand II0 b 615

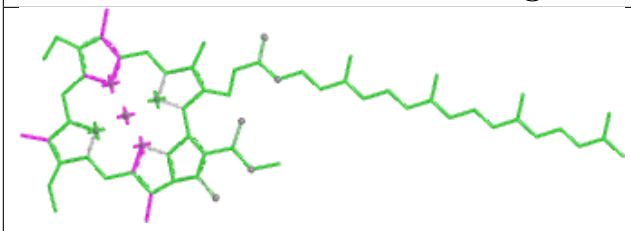

Bond lengths

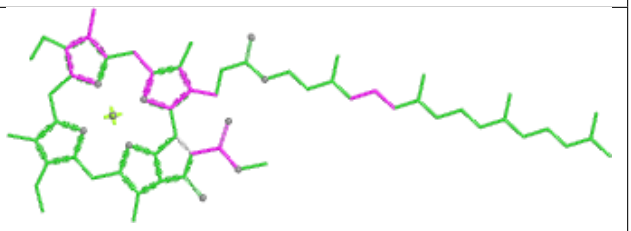

Bond angles

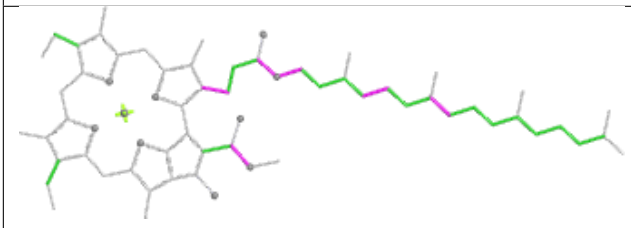

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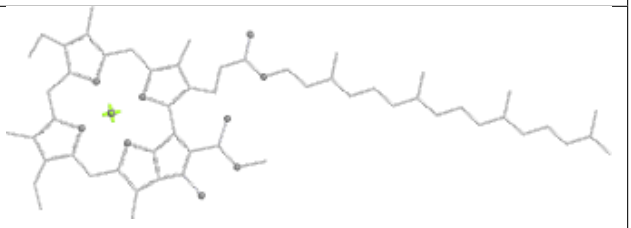

Rings

Ligand CLA A 805

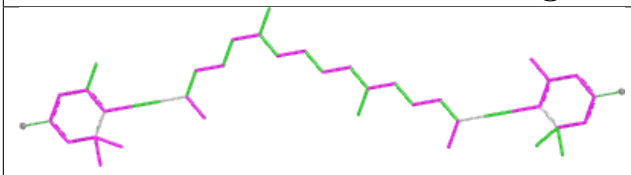

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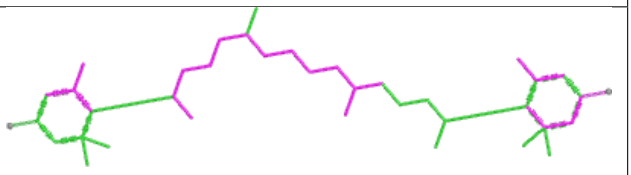

Bond angles

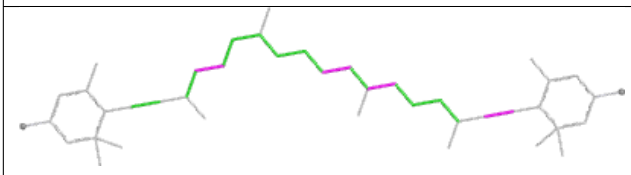

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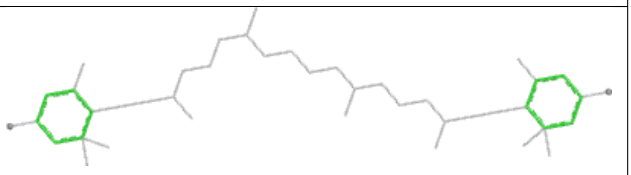

Rings

Ligand II0 d 312

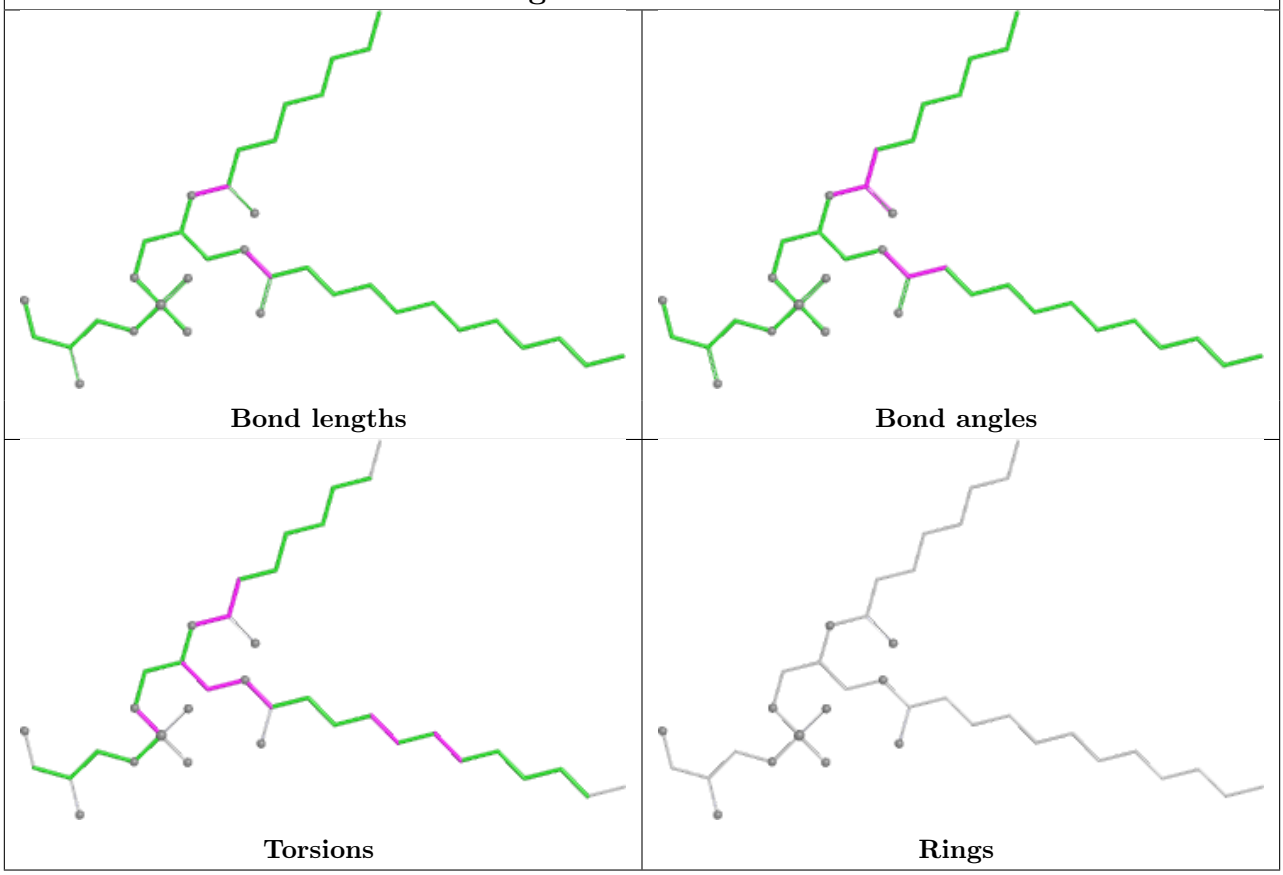

Bond lengths


Bond angles

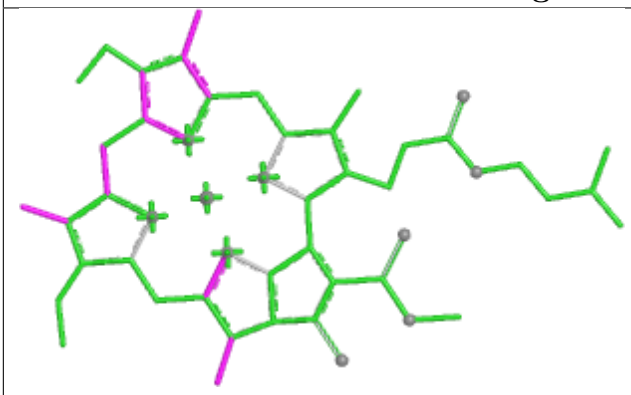

Torsions


Rings

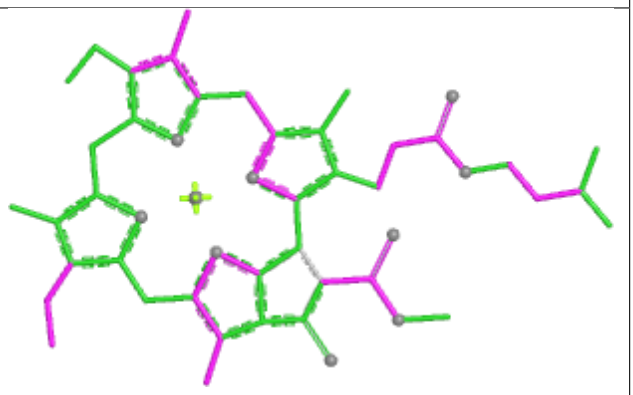
Ligand LHG c 618



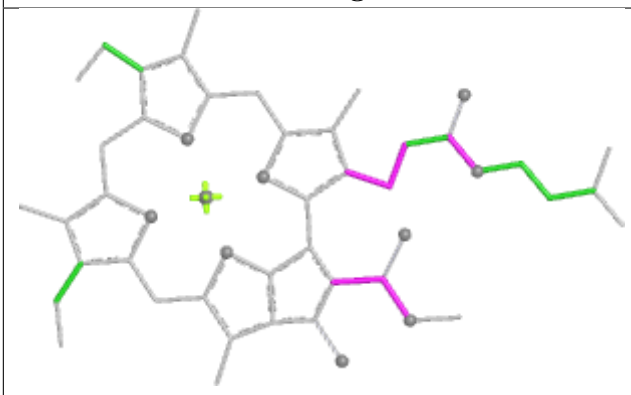
Ligand CLA i 303



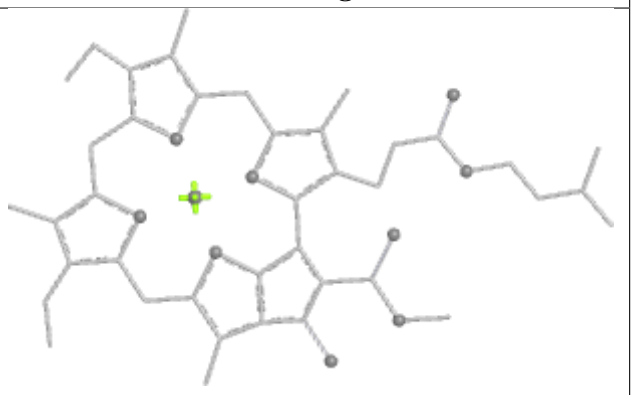
Bond lengths



Bond angles

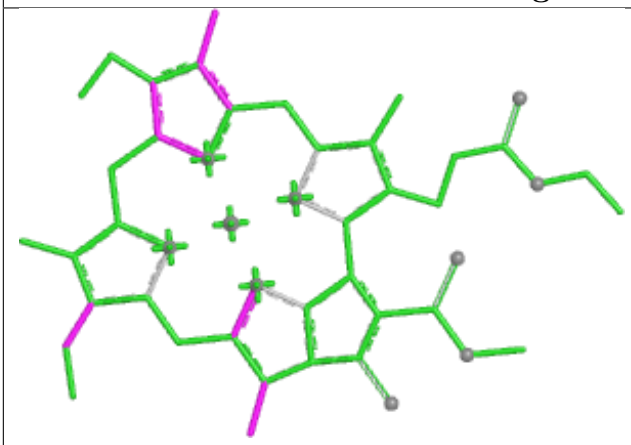


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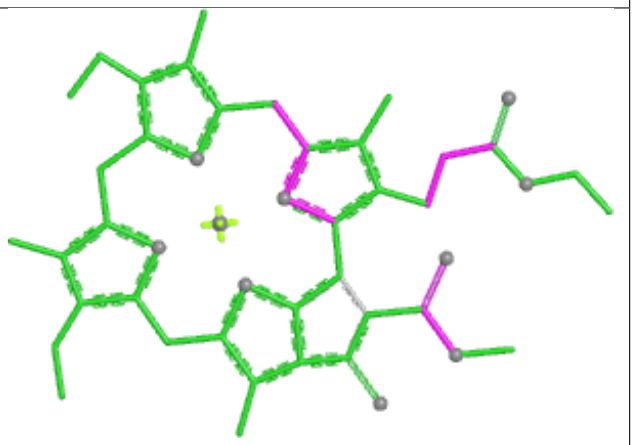


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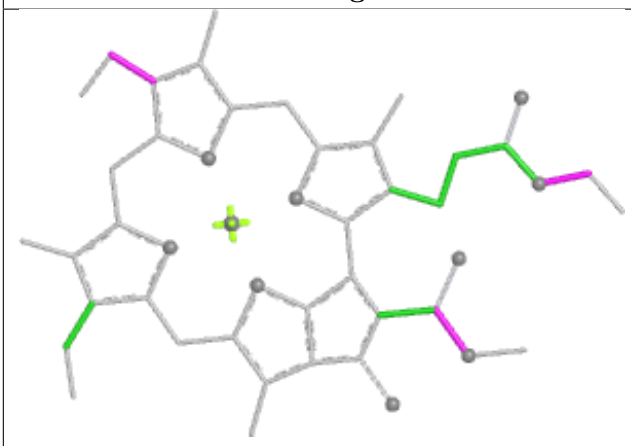
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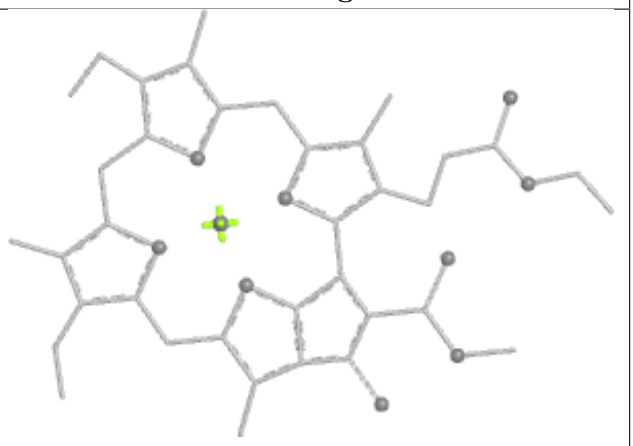
Bond lengths



Bond angles

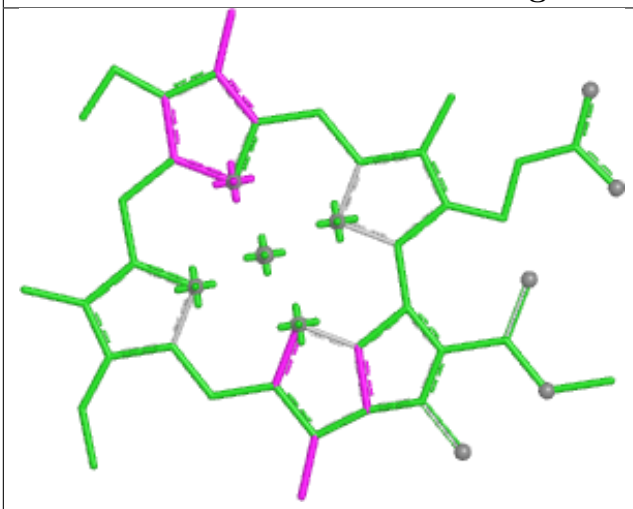


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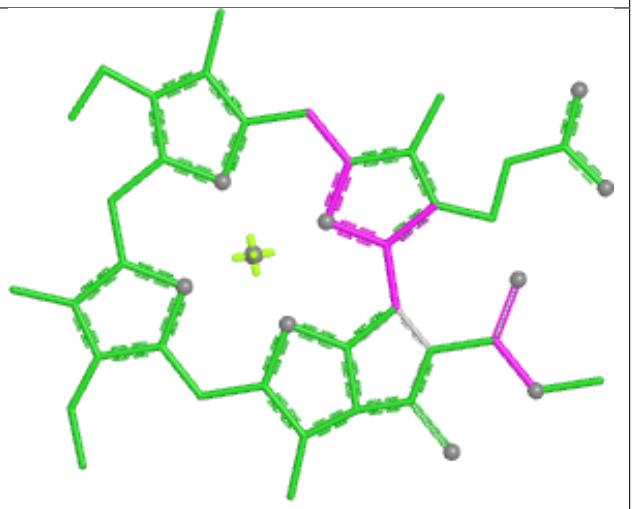


Rings

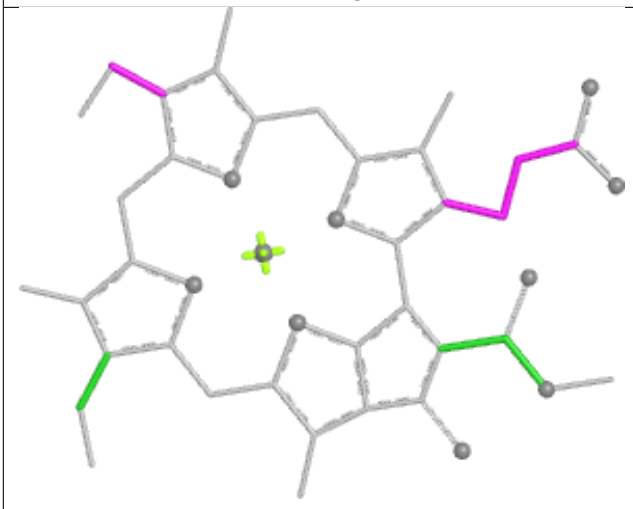
Ligand CLA e 601



Bond lengths



Bond angles

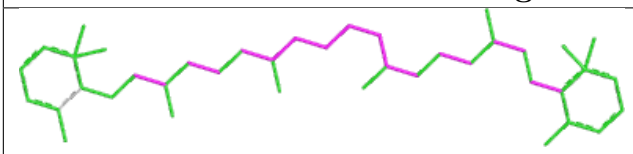


Torsions

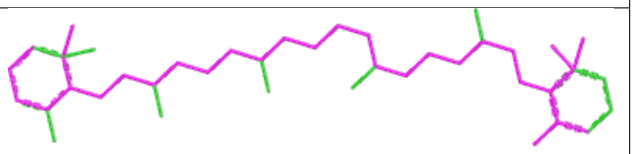


Rings

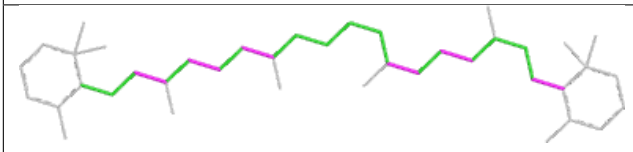
Ligand WVN R 202



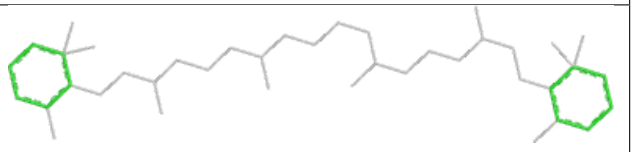
Bond lengths



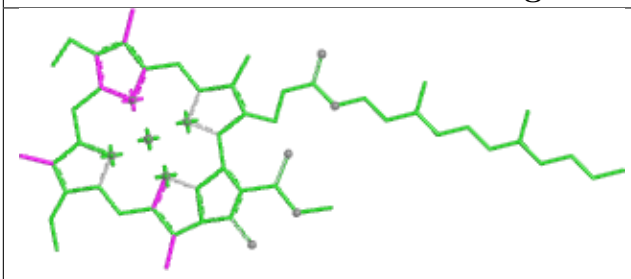
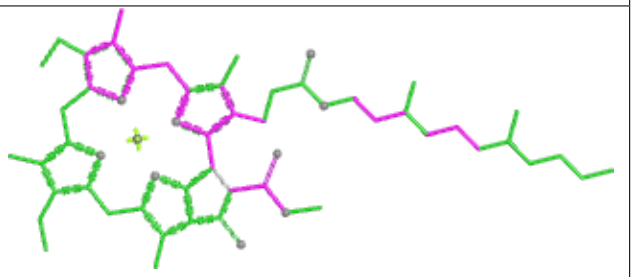
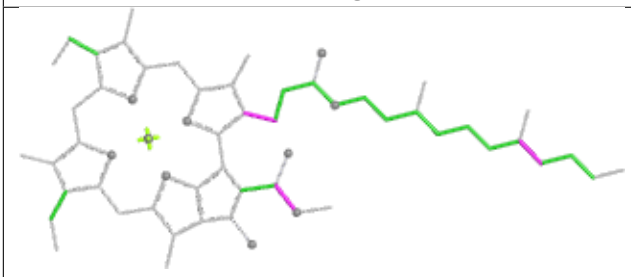
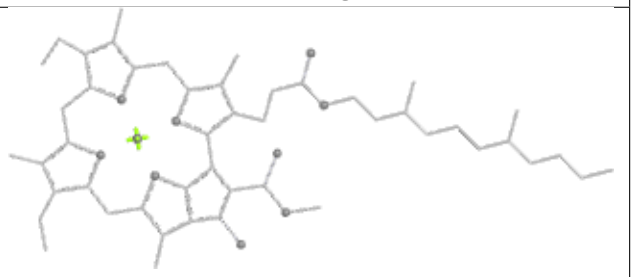
Bond angles

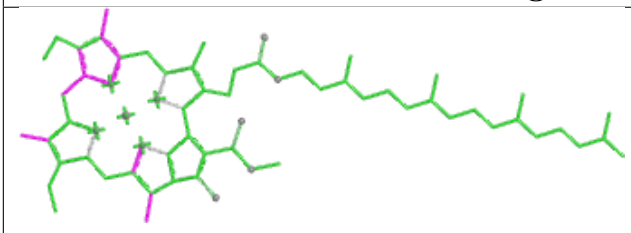
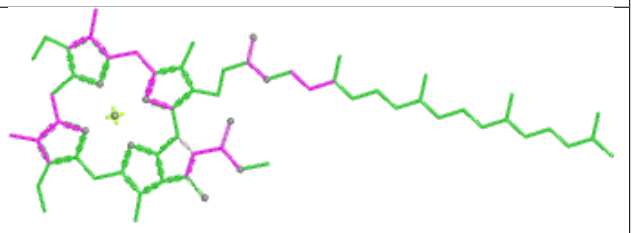
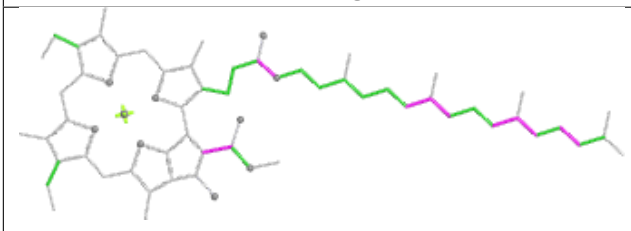
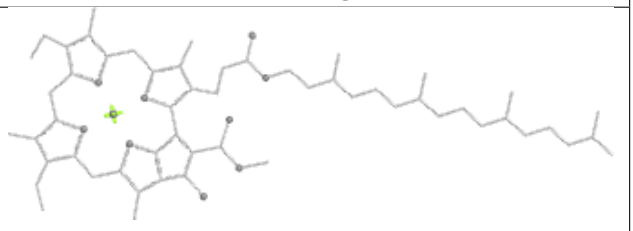


Torsions

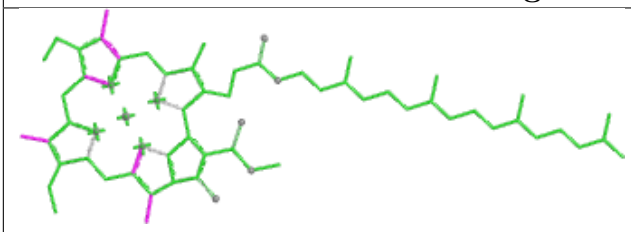


Rings

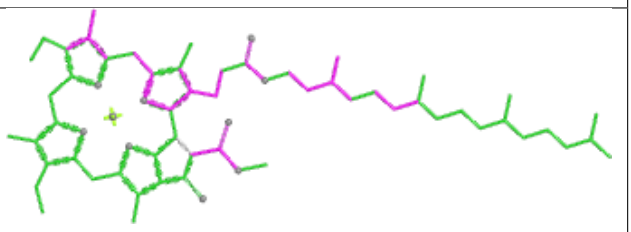
Ligand CLA B 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

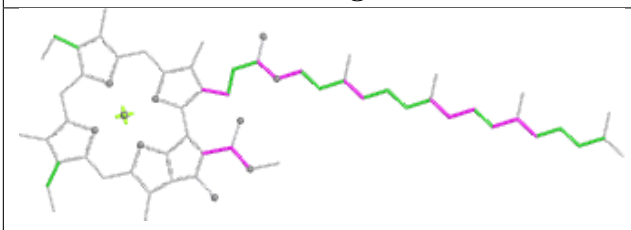
Ligand CLA A 816



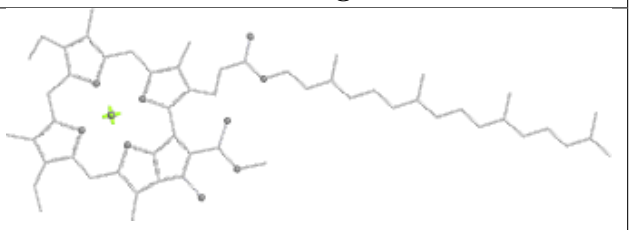
Bond lengths



Bond angles

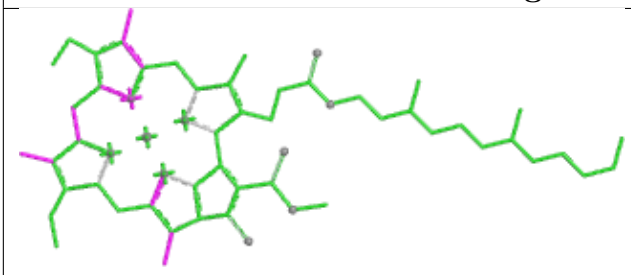


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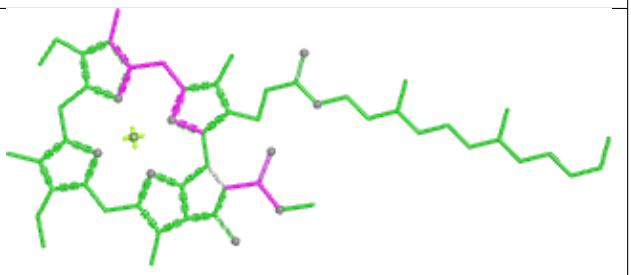


Rings

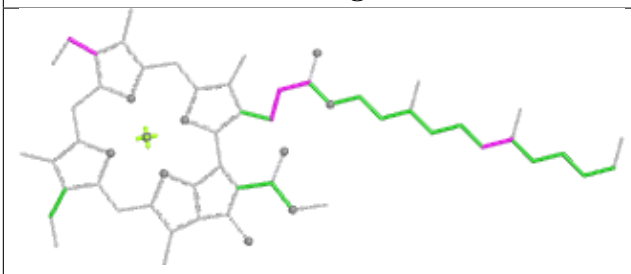
Ligand CLA B 814



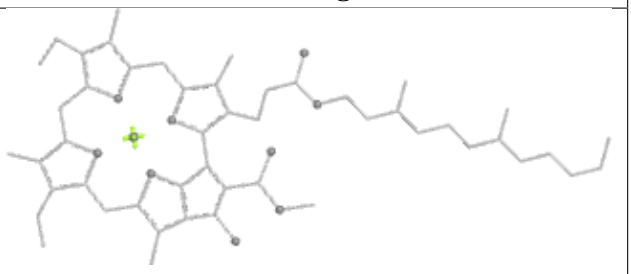
Bond lengths



Bond angles

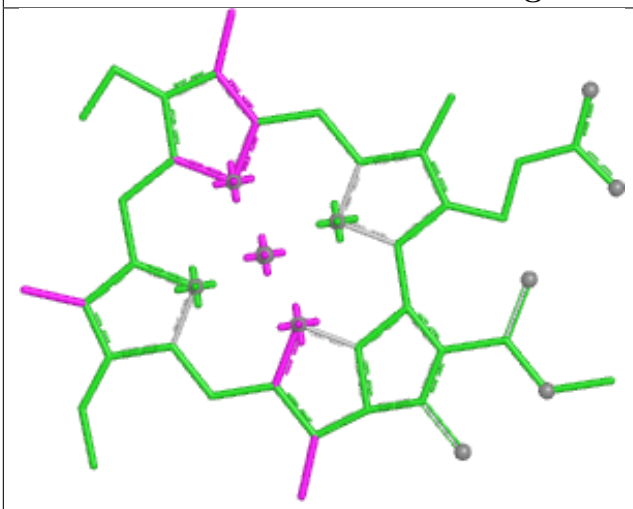


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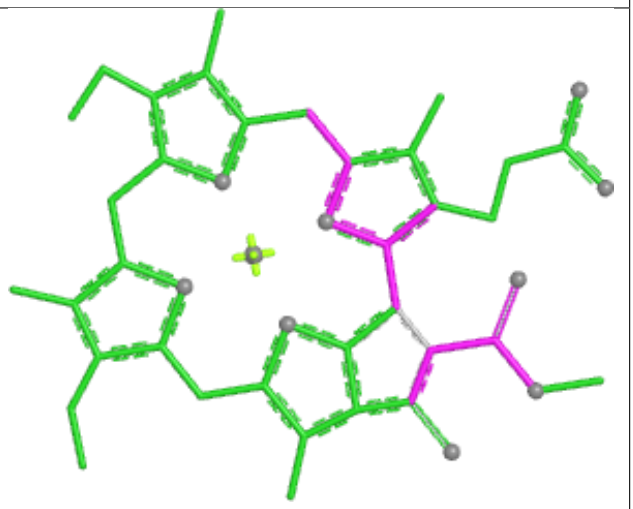


Rings

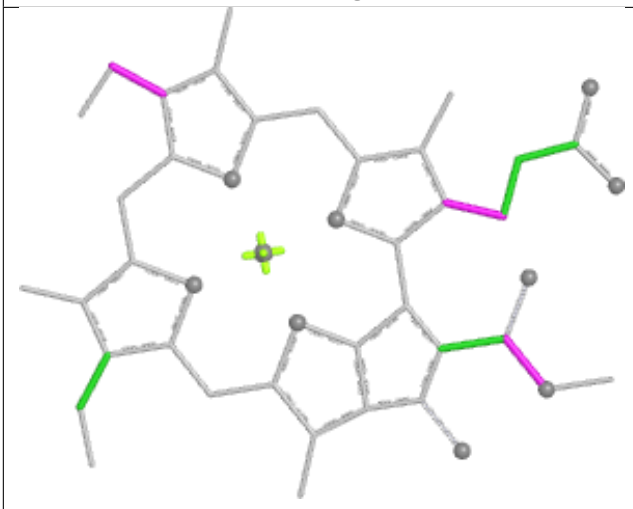
Ligand CLA B 830



Bond lengths



Bond angles

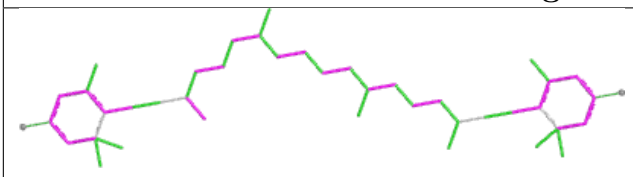


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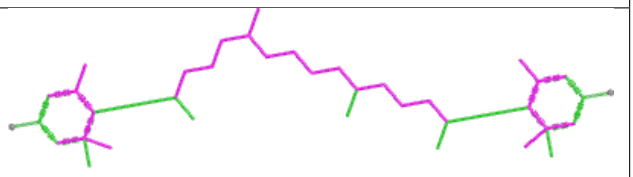


Rings

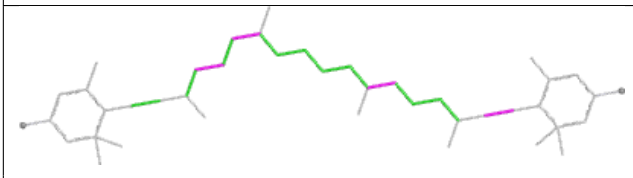
Ligand II0 k 318



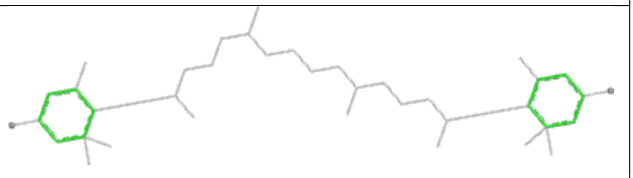
Bond lengths



Bond angles

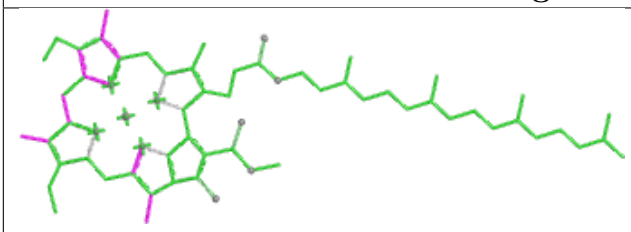


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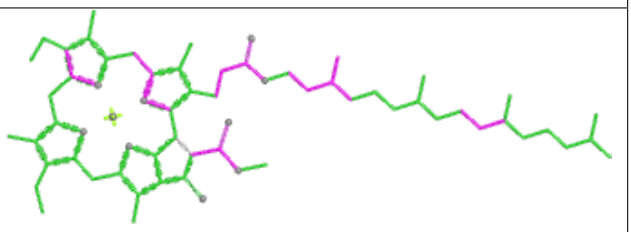


Rings

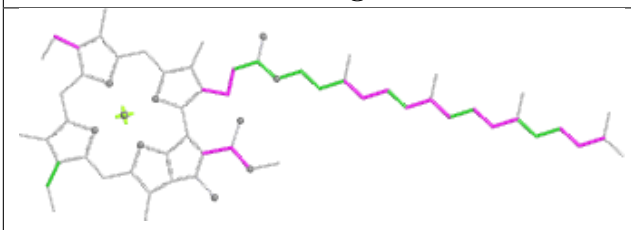
Ligand CLA l 304



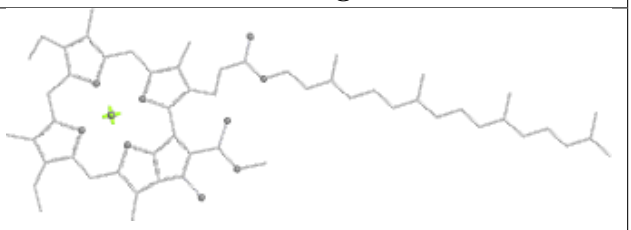
Bond lengths



Bond angles

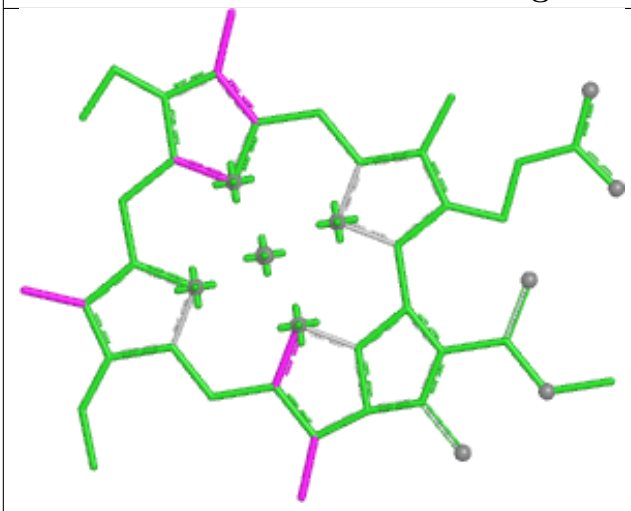


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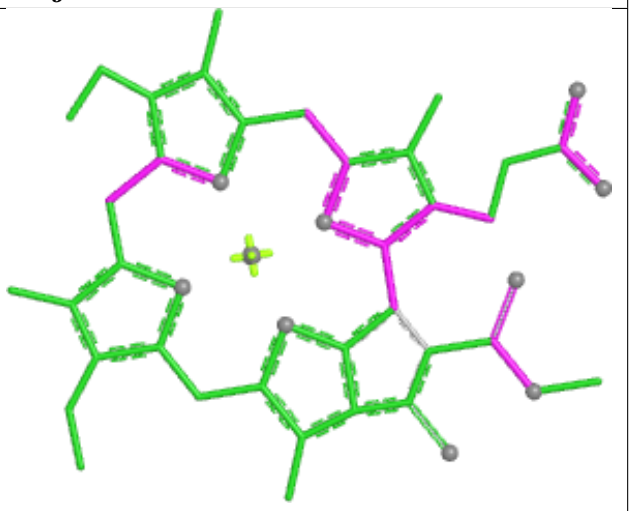


Rings

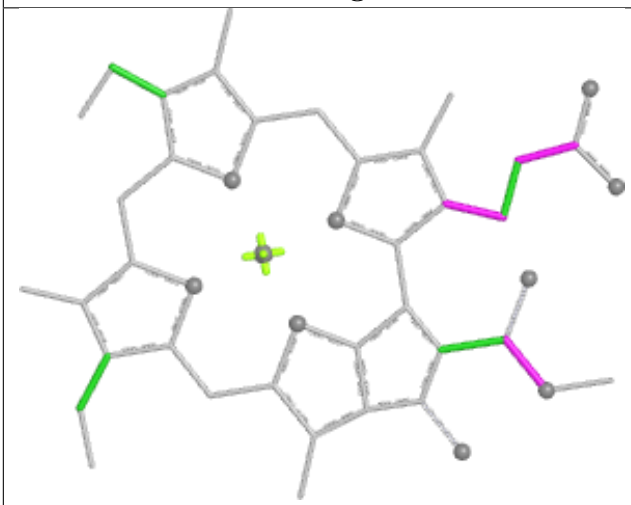
Ligand CLA j 605



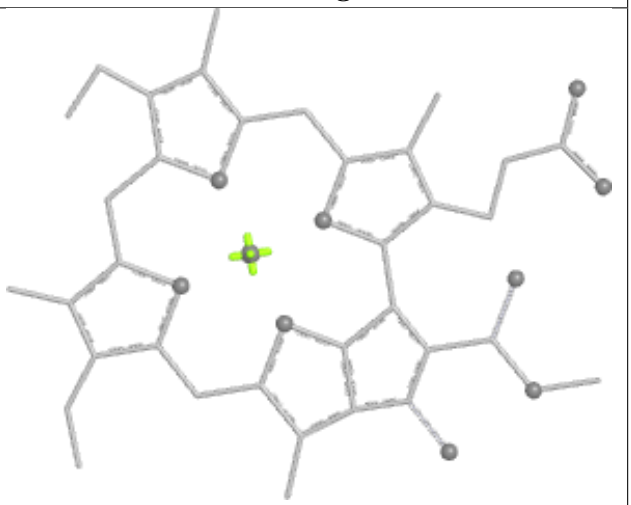
Bond lengths



Bond angles

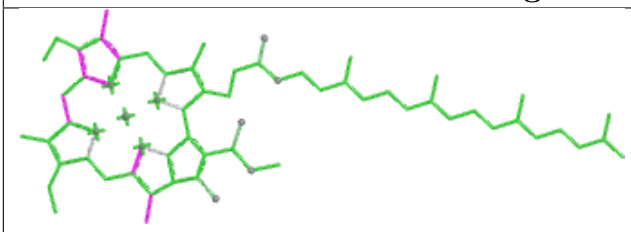


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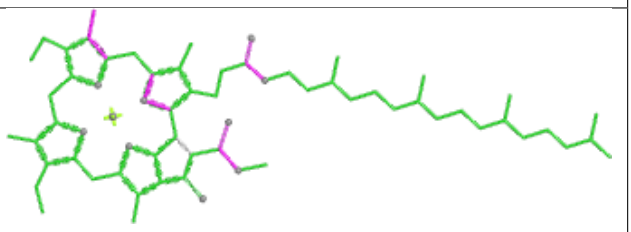


Rings

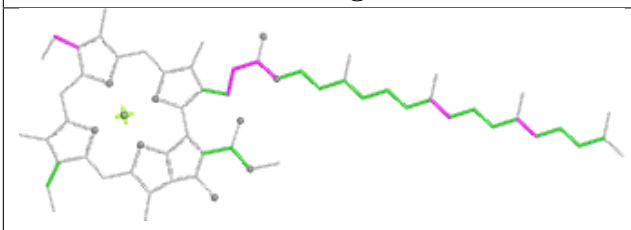
Ligand CLA A 852



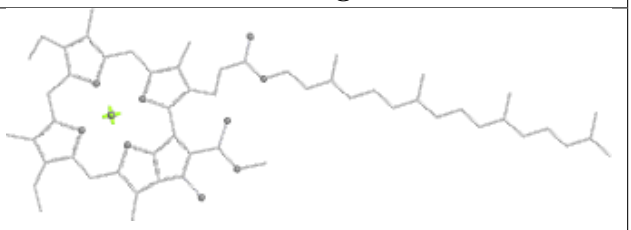
Bond lengths



Bond angles

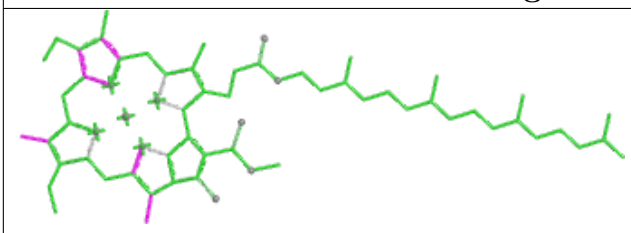


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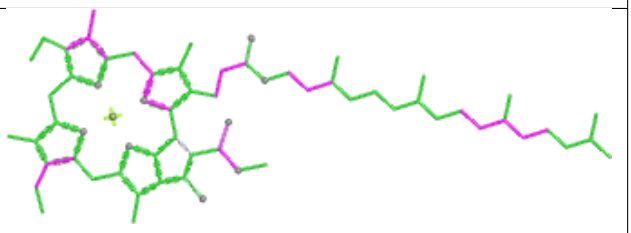


Rings

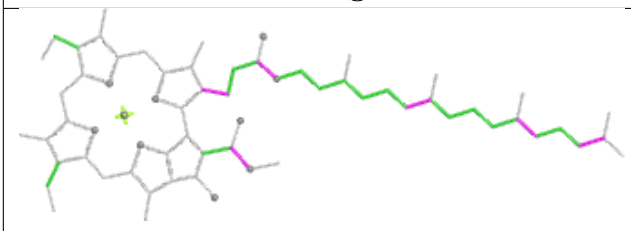
Ligand CLA A 837



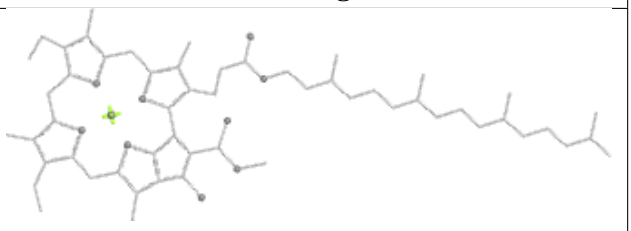
Bond lengths



Bond angles

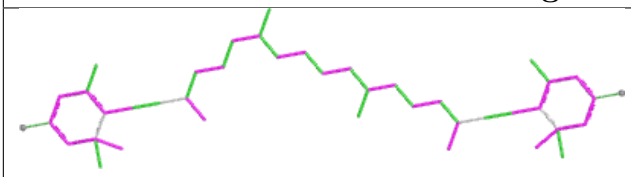


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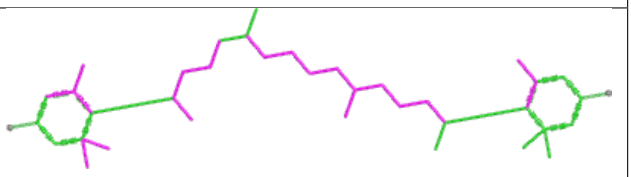


Rings

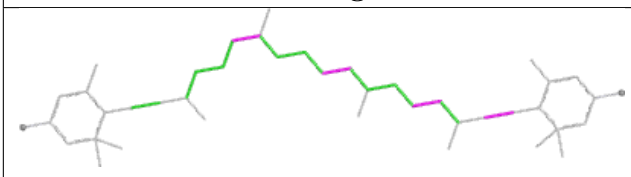
Ligand II0 d 314



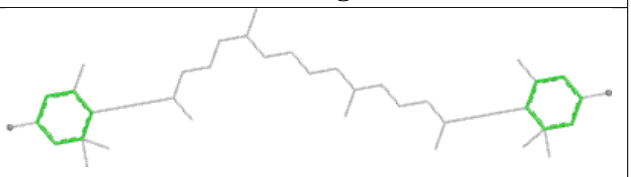
Bond lengths



Bond angles

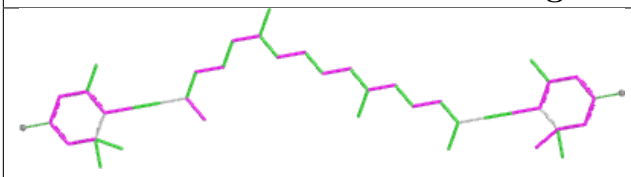


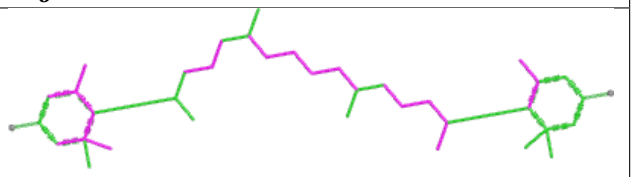
Torsions

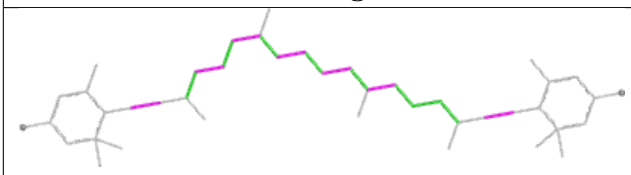


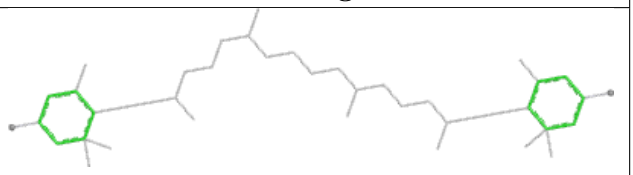
Rings

Ligand II0 j 615

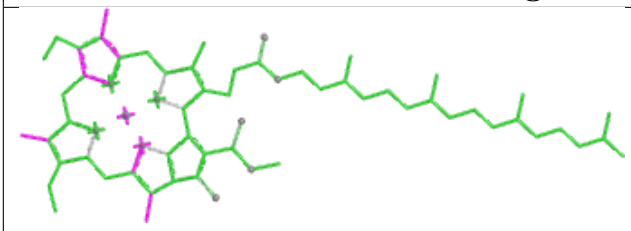

Bond lengths

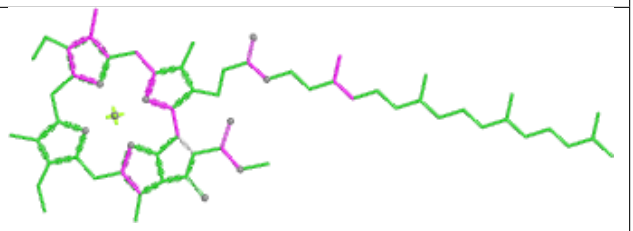

Bond angles

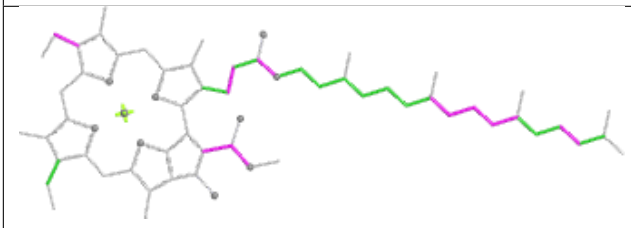

Torsions

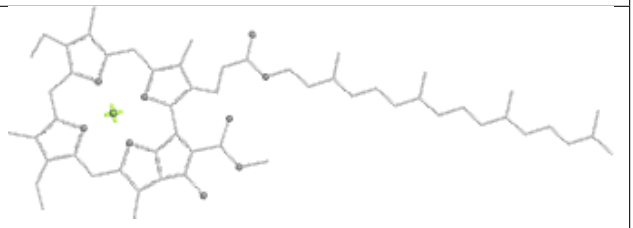

Rings

Ligand CLA B 834

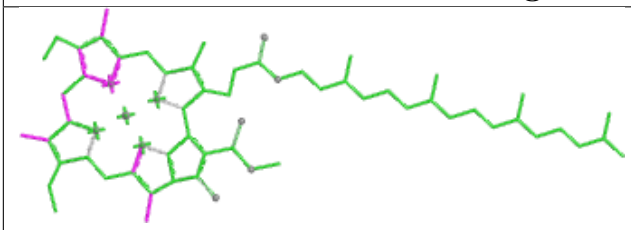

Bond lengths

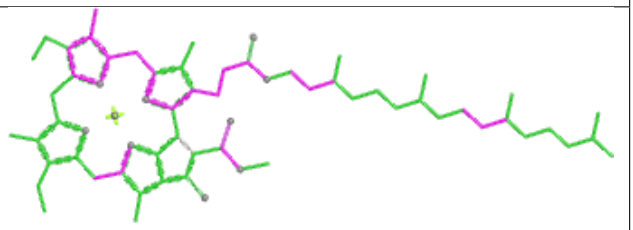

Bond angles

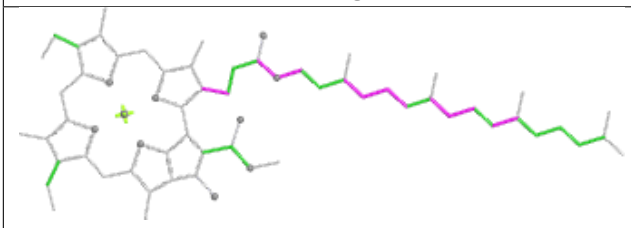

Torsions

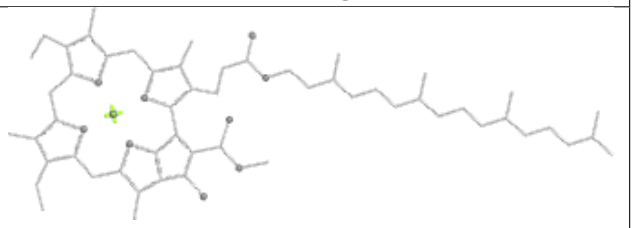

Rings

Ligand CLA A 802

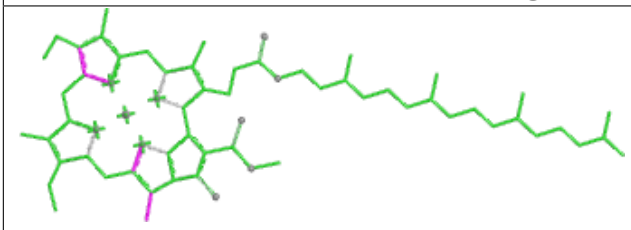

Bond lengths


Bond angles

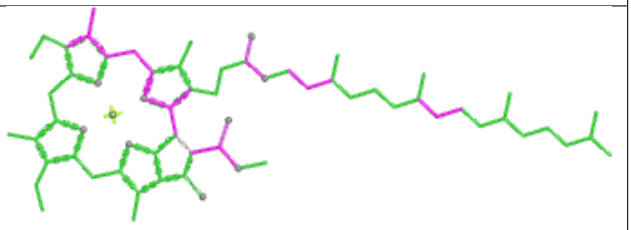

Torsions


Rings

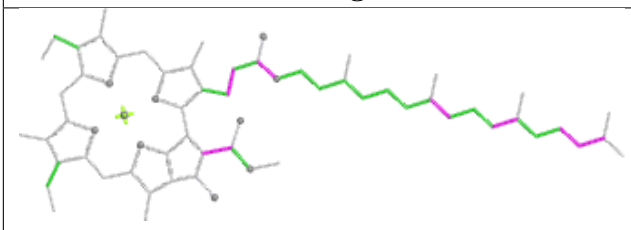
Ligand CLA B 836



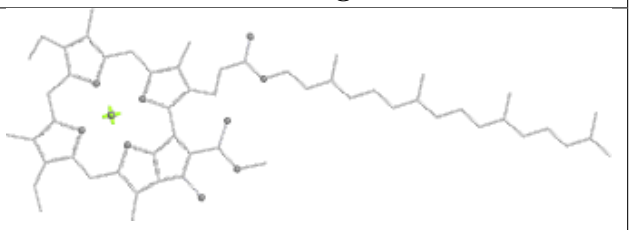
Bond lengths



Bond angles

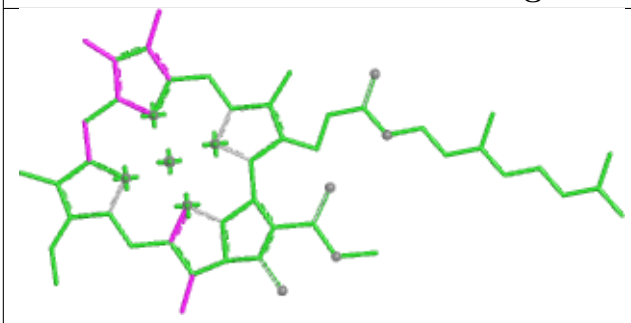


Torsions

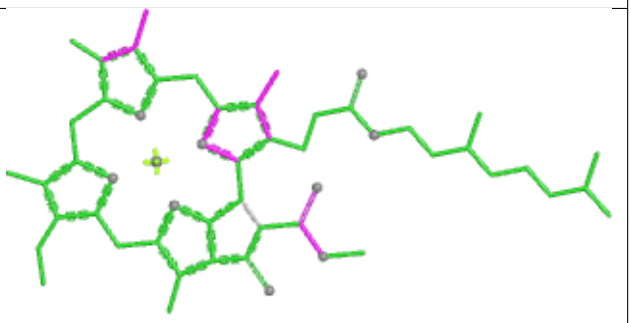


Rings

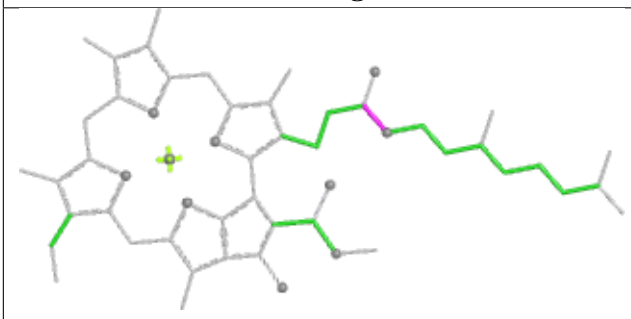
Ligand CLA B 808



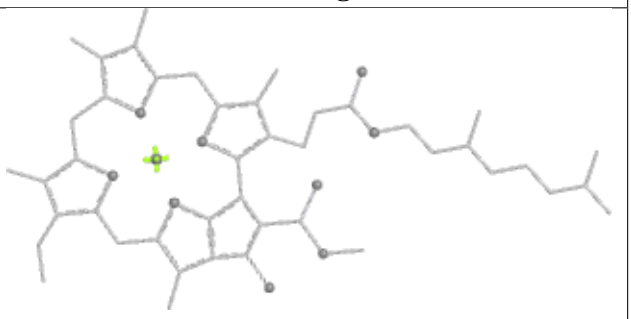
Bond lengths



Bond angles

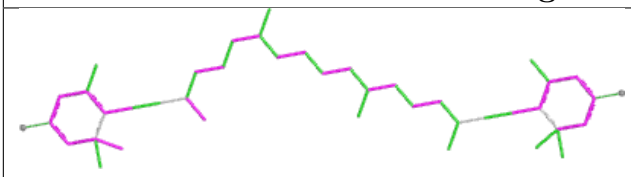


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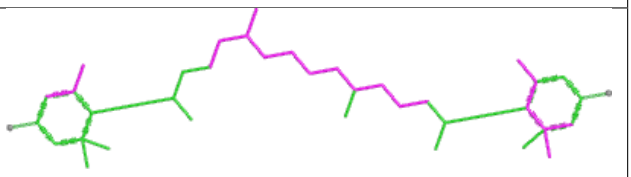


Rings

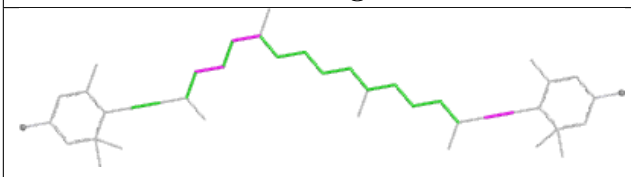
Ligand II0 O 203



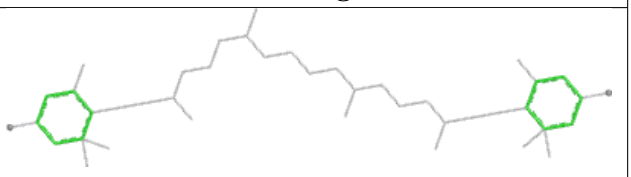
Bond lengths



Bond angles

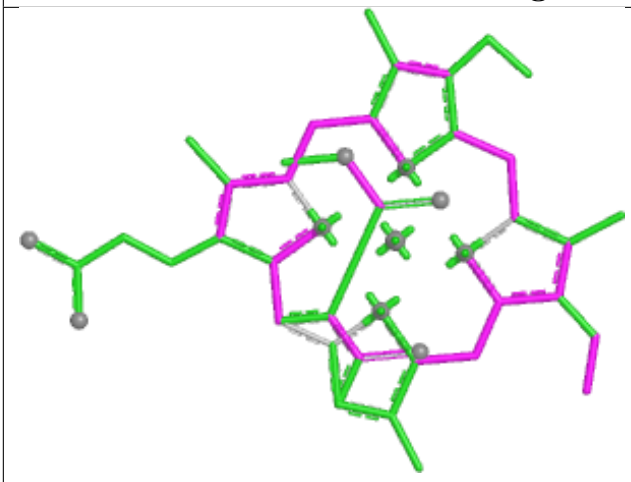


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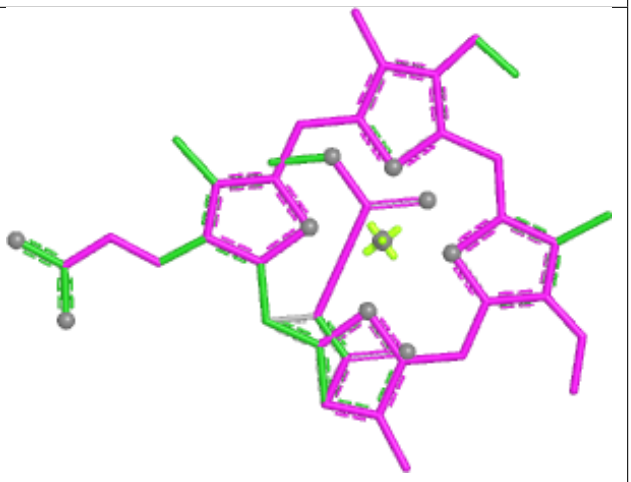


Rings

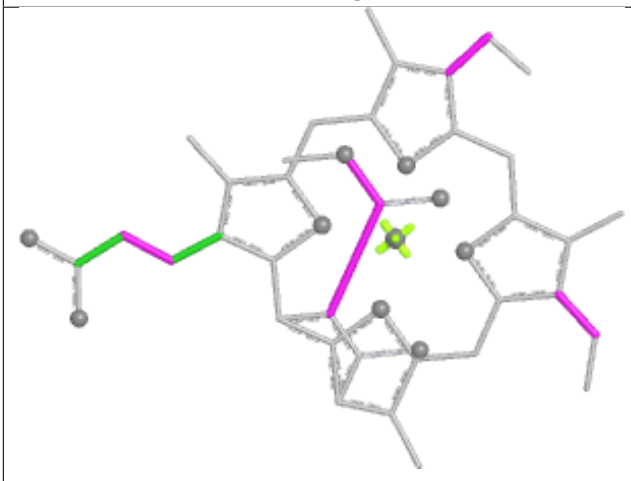
Ligand KC2 k 310



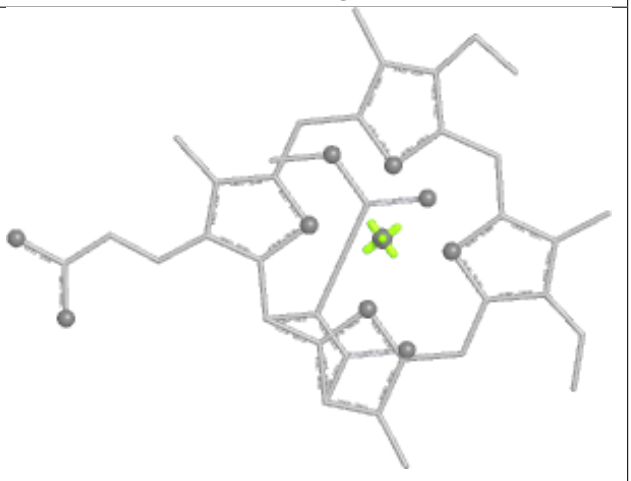
Bond lengths



Bond angles

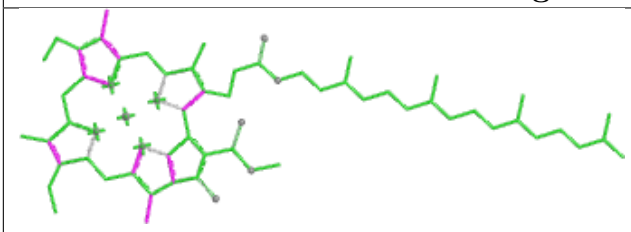


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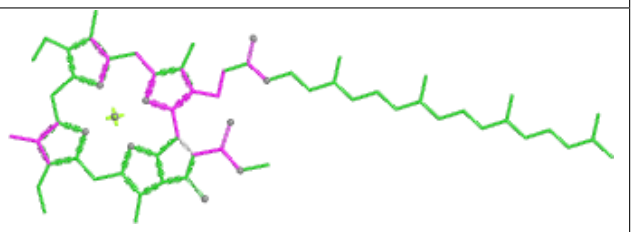


Rings

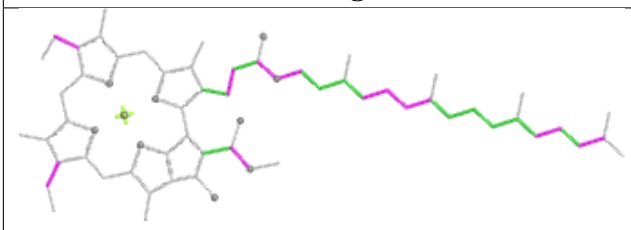
Ligand CLA l 307



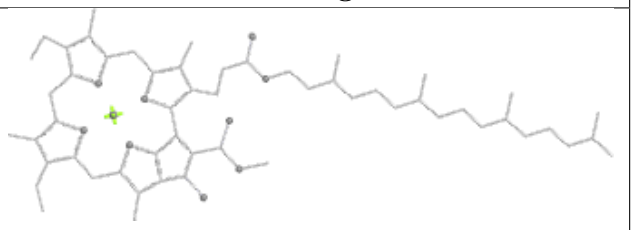
Bond lengths



Bond angles

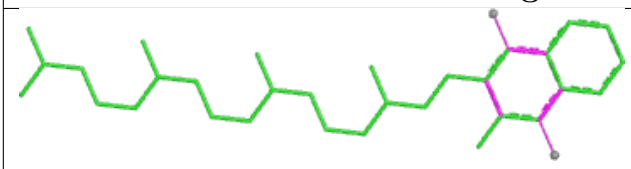


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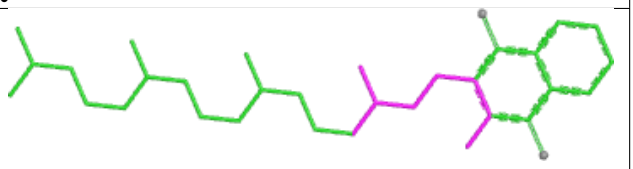


Rings

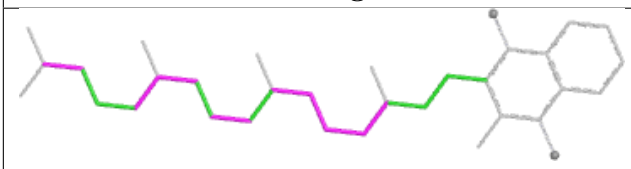
Ligand PQN A 843



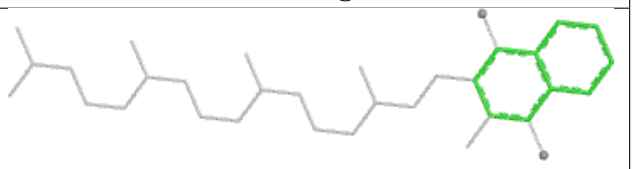
Bond lengths



Bond angles

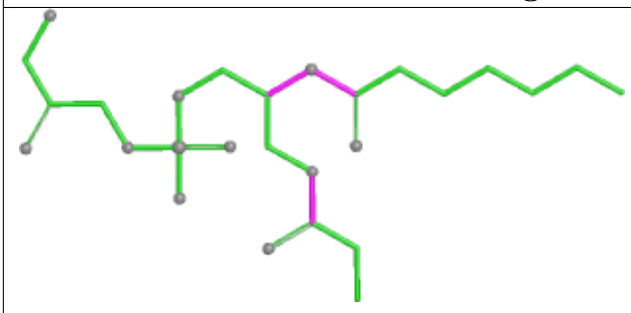


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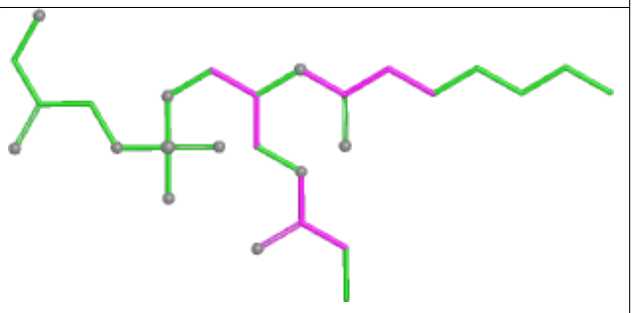


Rings

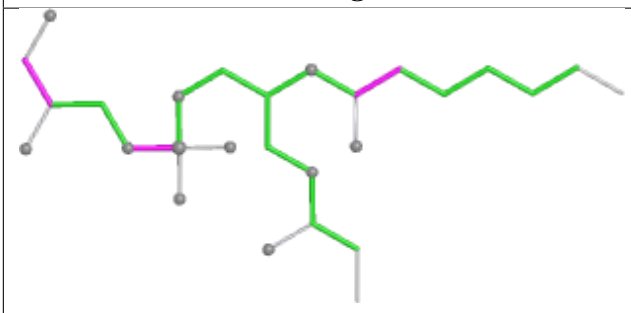
Ligand LHG A 845



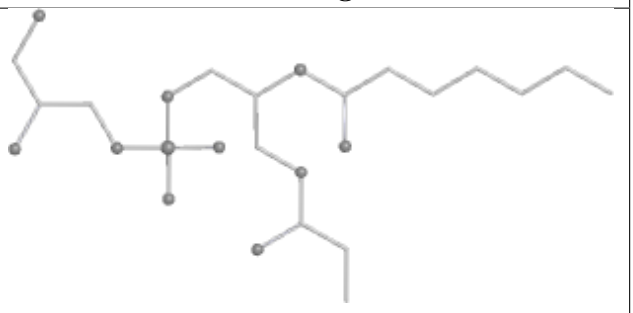
Bond lengths



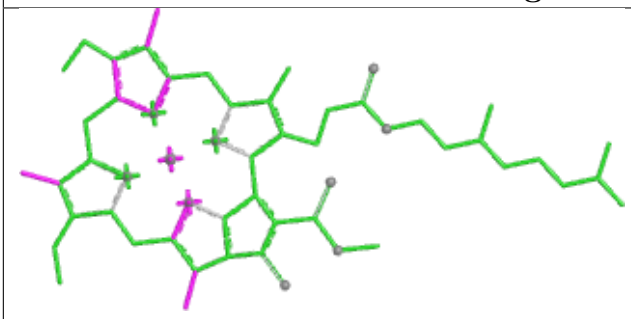
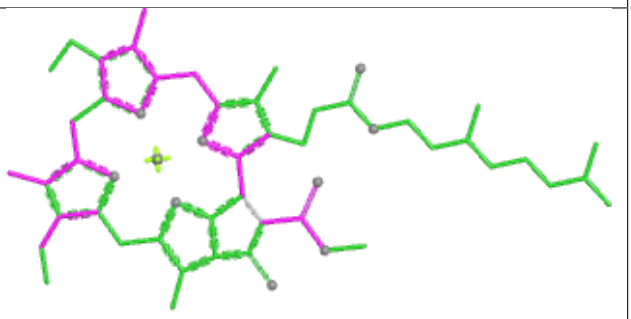
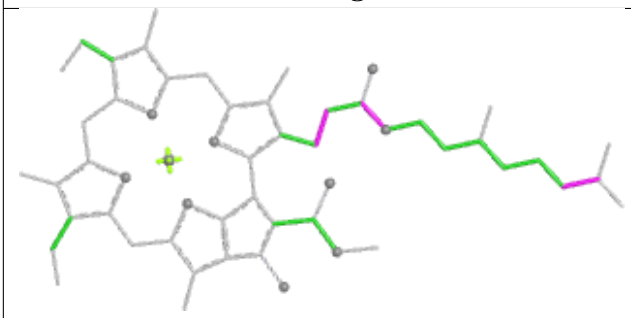
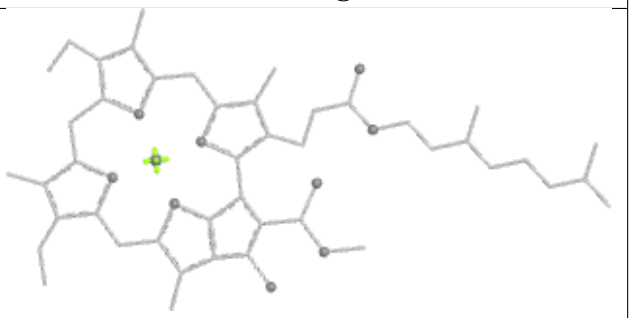
Bond angles

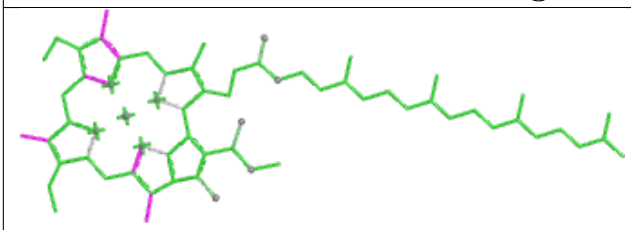
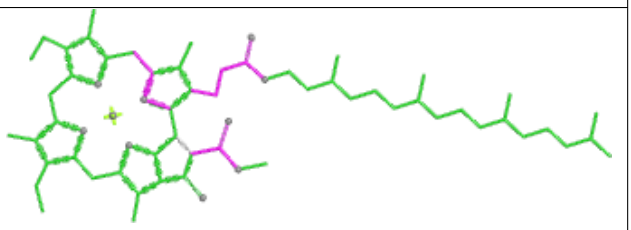
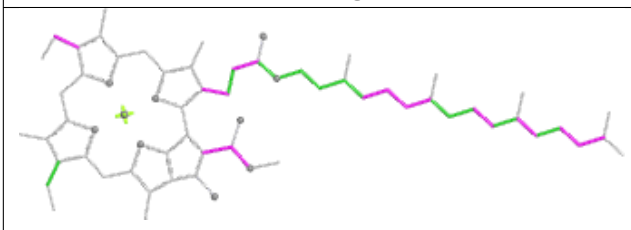
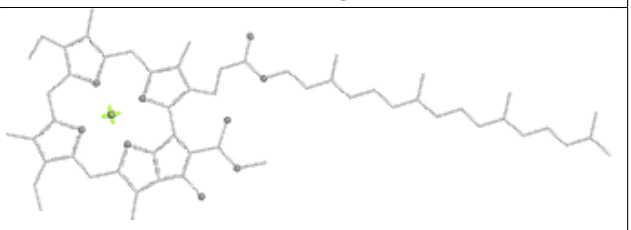


Torsions

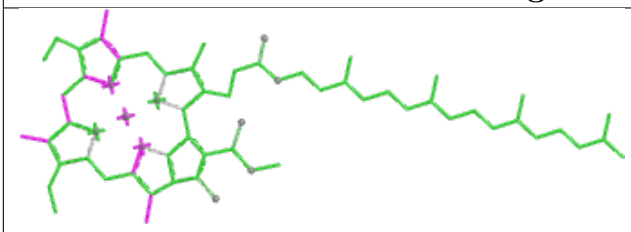


Rings

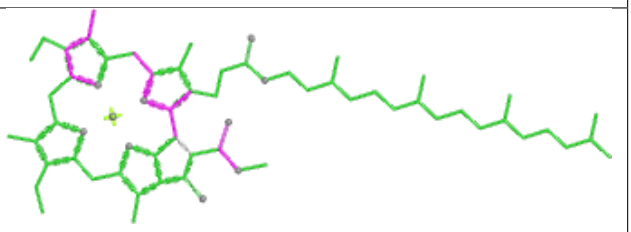
Ligand CLA B 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

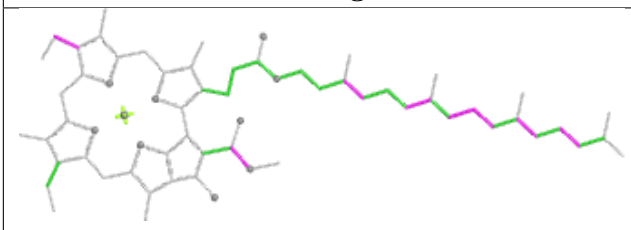
Ligand CLA b 605



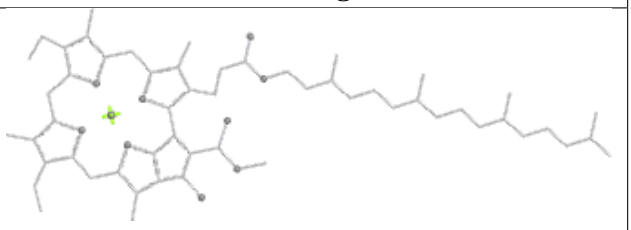
Bond lengths



Bond angles

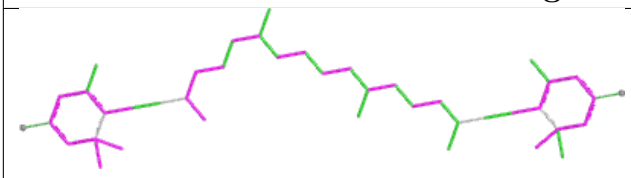


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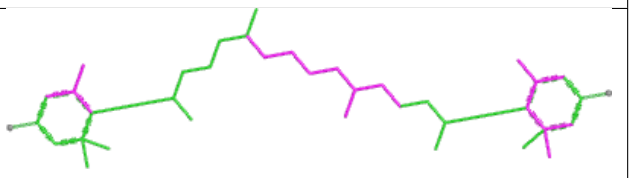


Rings

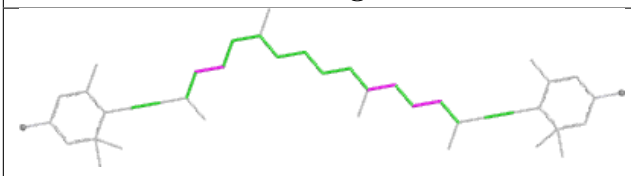
Ligand II0 e 612



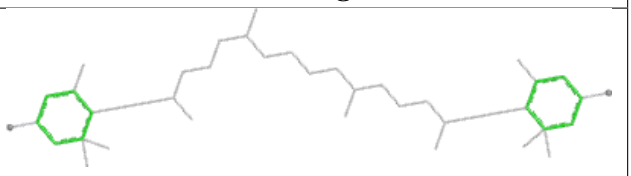
Bond lengths



Bond angles

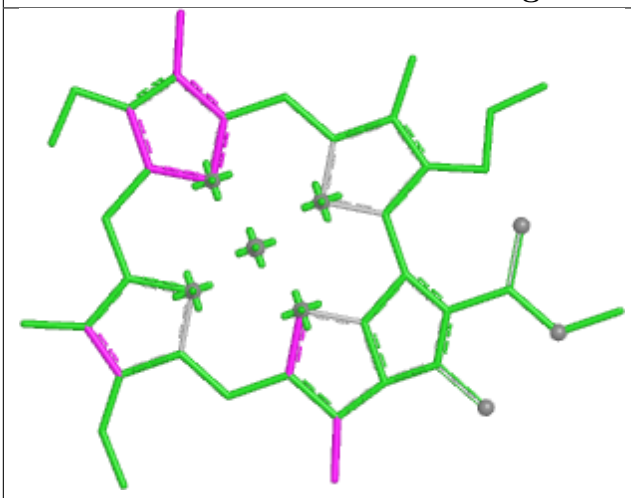


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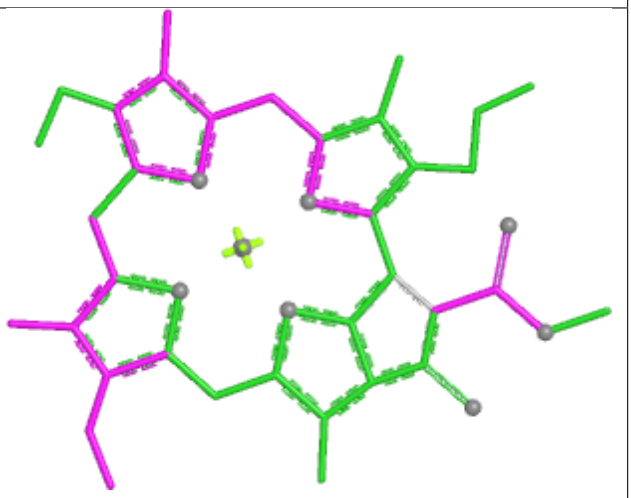


Rings

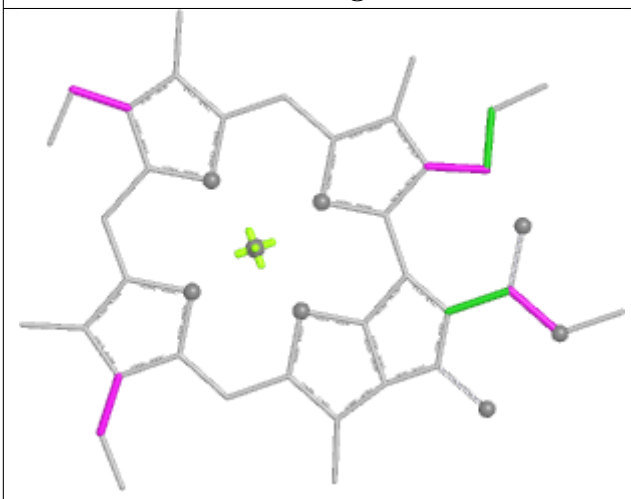
Ligand CLA m 612



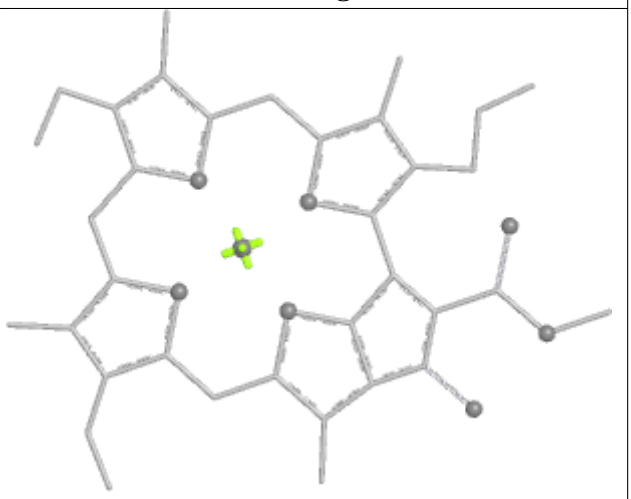
Bond lengths



Bond angles

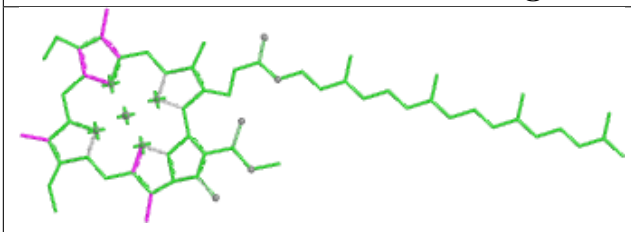


Torsions

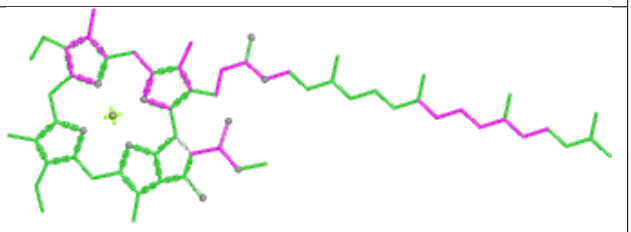


Rings

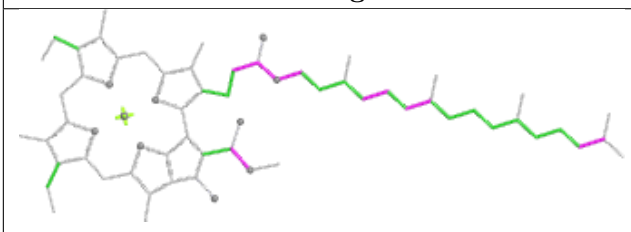
Ligand CLA B 829



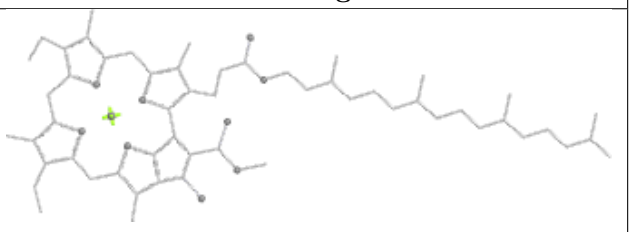
Bond lengths



Bond angles

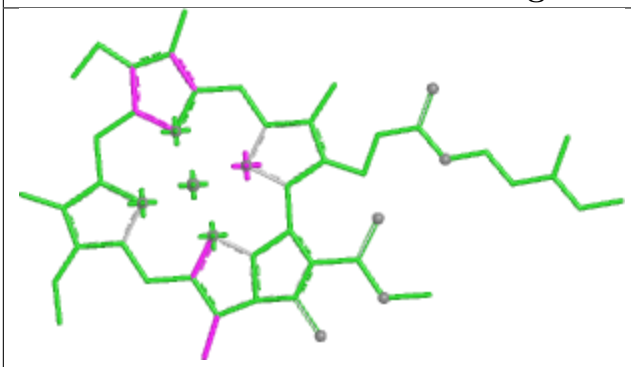


Torsions

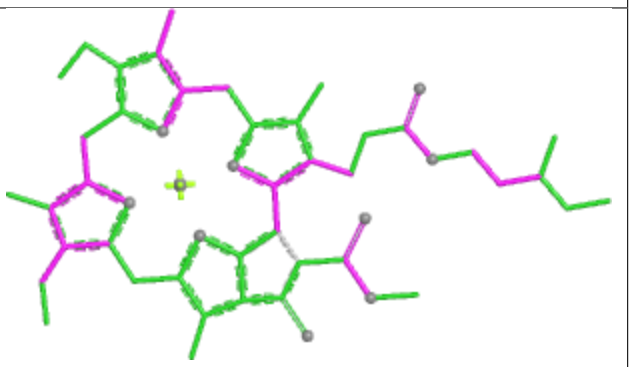


Rings

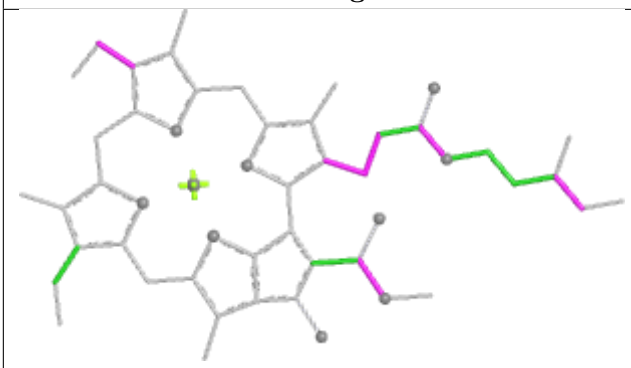
Ligand CLA k 306



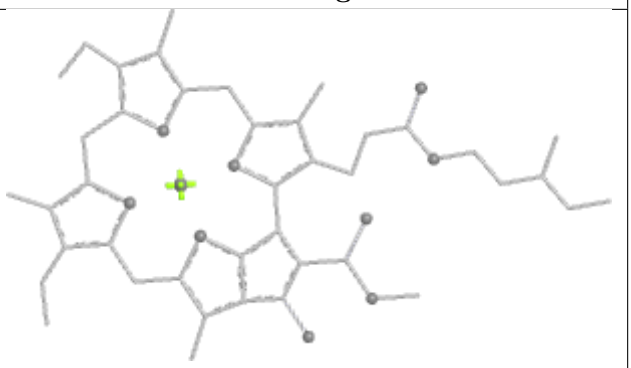
Bond lengths



Bond angles

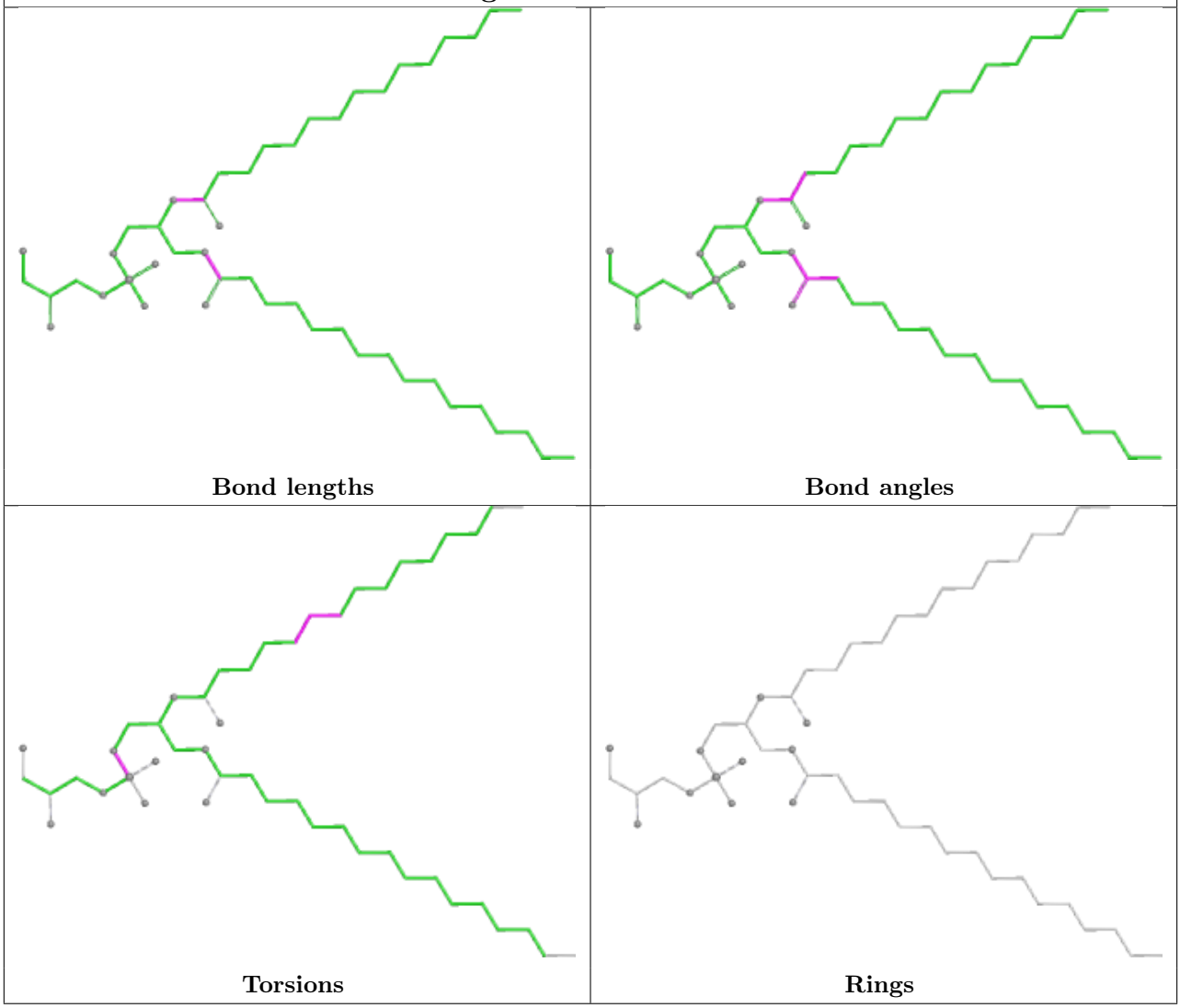


Torsions

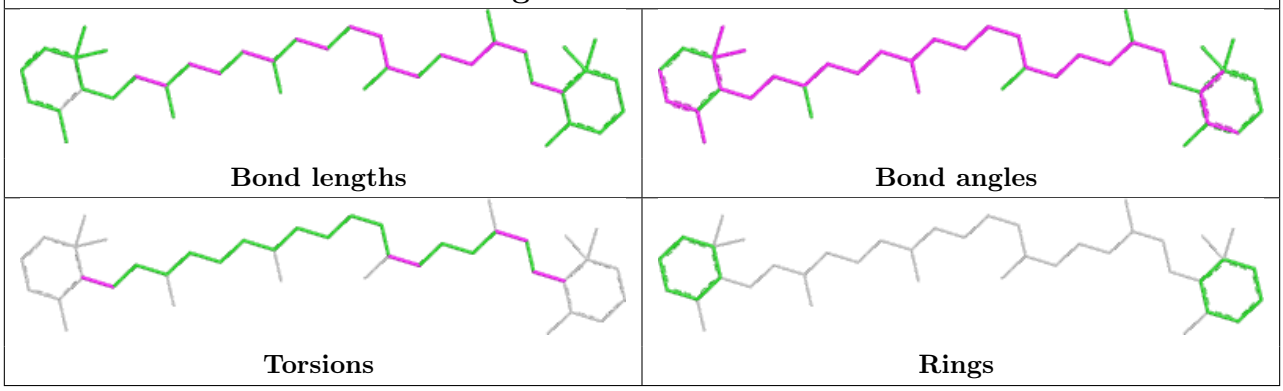


Rings

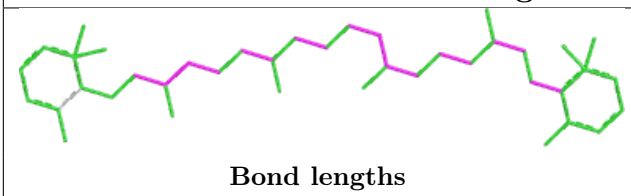
Ligand LHG A 844



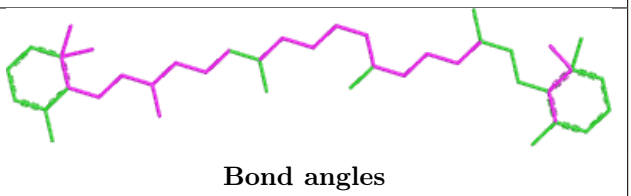
Ligand WVN M 101



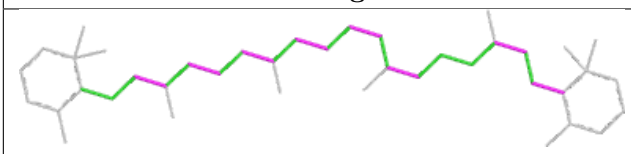
Ligand WVN B 847



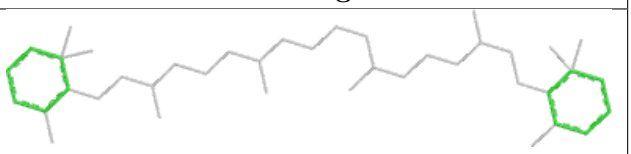
Bond lengths



Bond angles

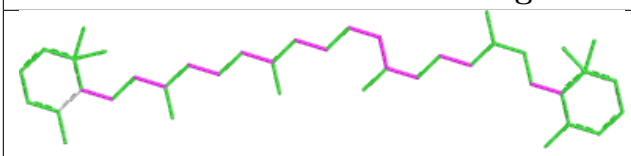


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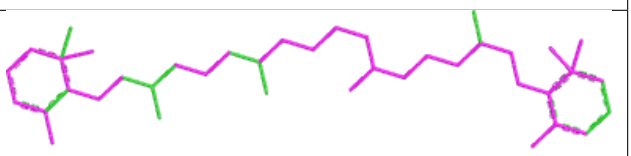


Rings

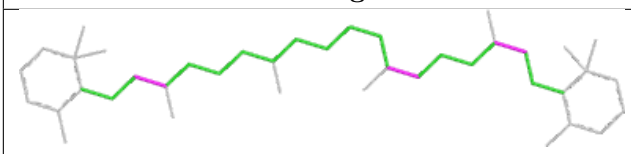
Ligand WVN R 201



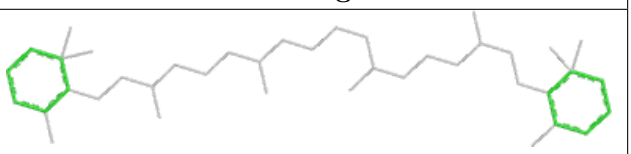
Bond lengths



Bond angles

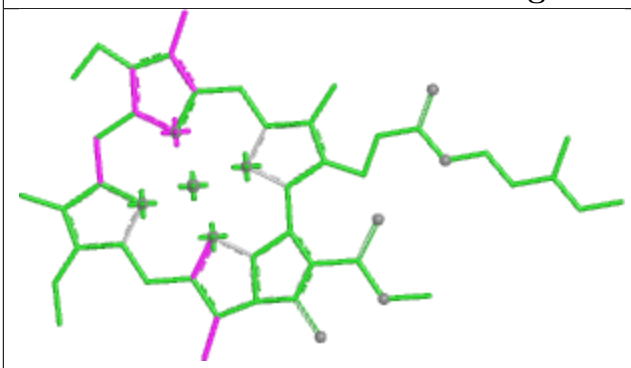


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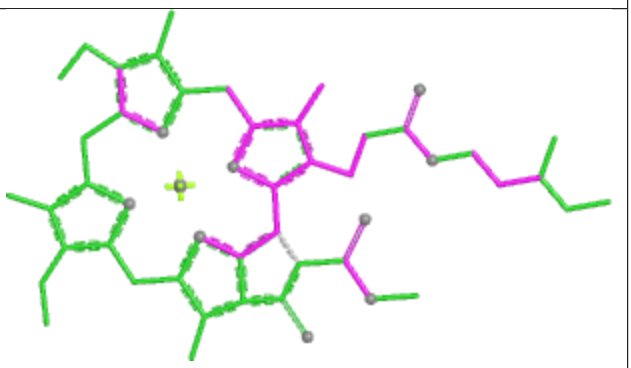


Rings

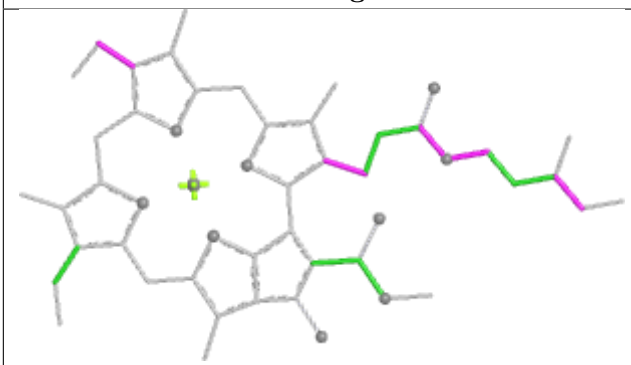
Ligand CLA J 105



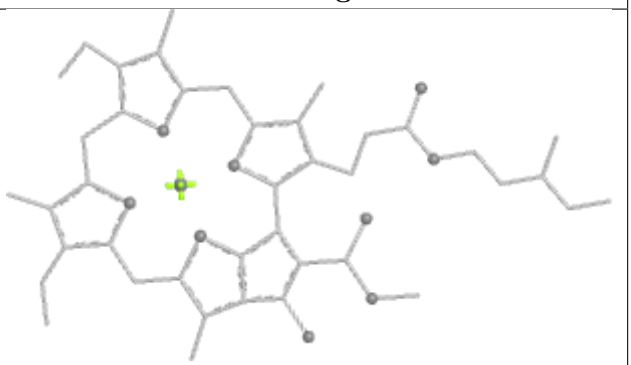
Bond lengths



Bond angles

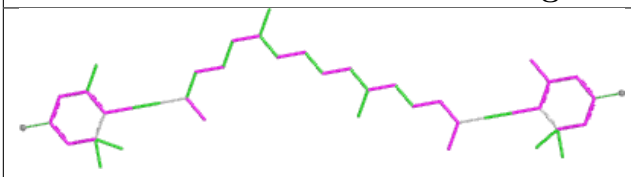


Torsions

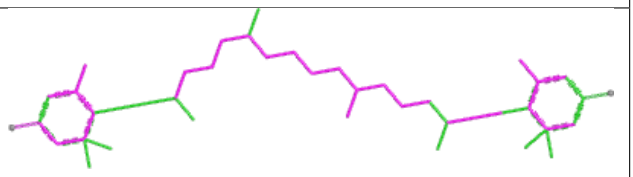


Rings

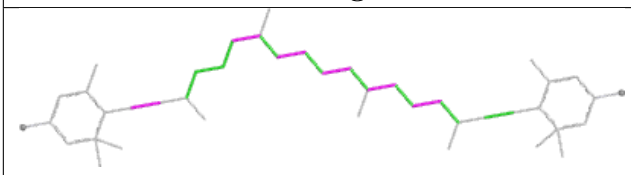
Ligand II0 h 311



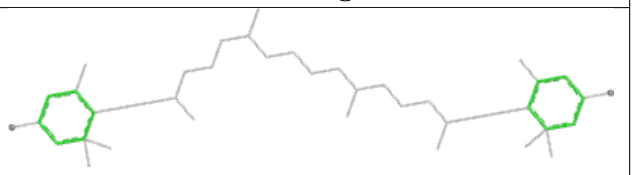
Bond lengths



Bond angles

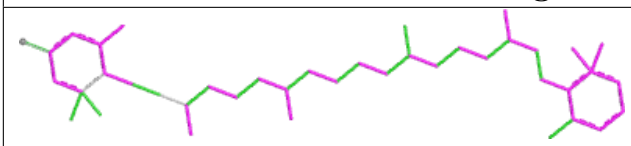


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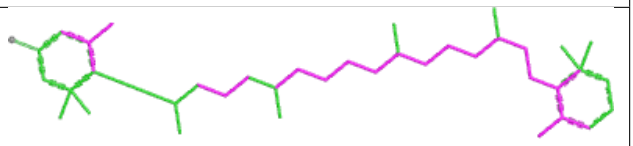


Rings

Ligand IHT a 317



Bond lengths



Bond angles

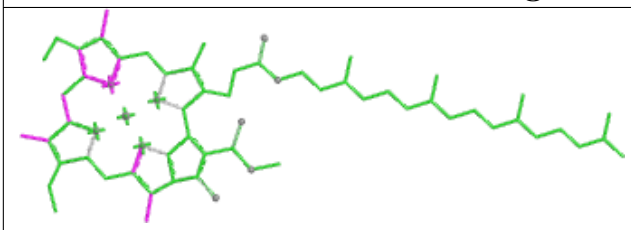


Torsions

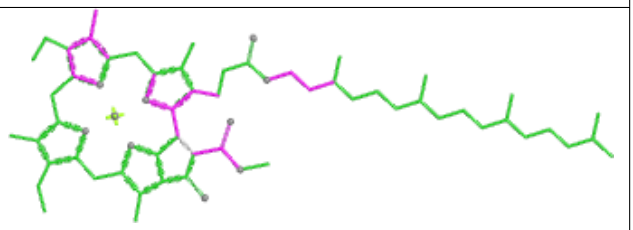


Rings

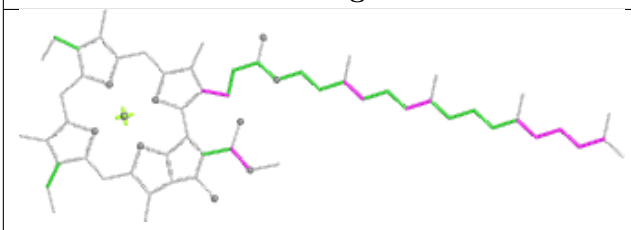
Ligand CLA B 823



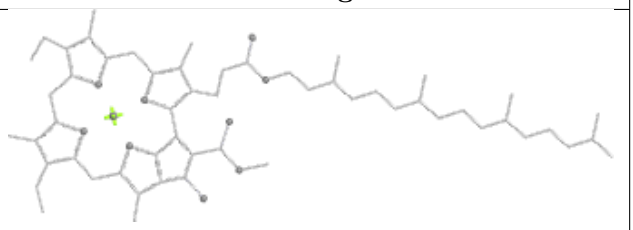
Bond lengths



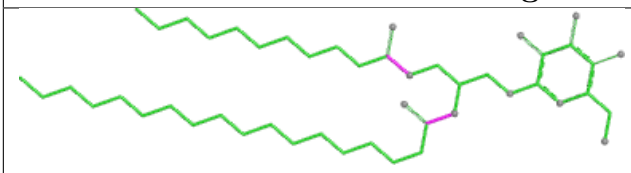
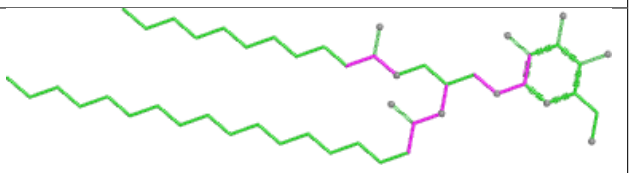
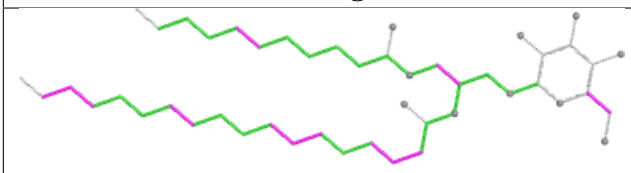
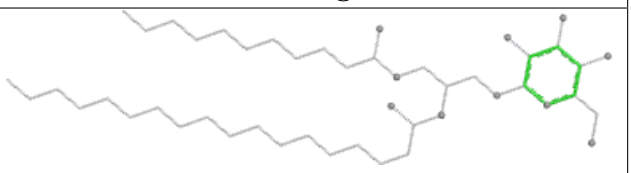
Bond angles

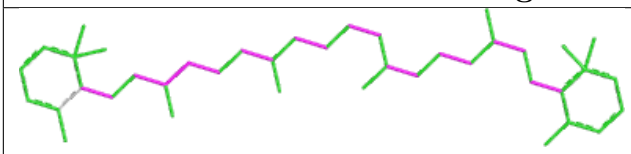
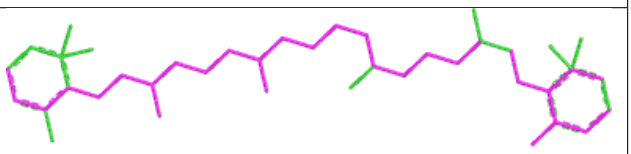
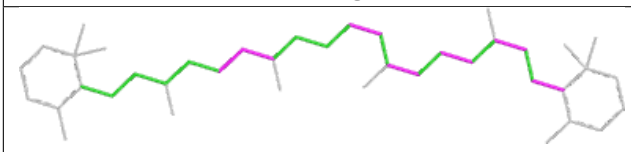
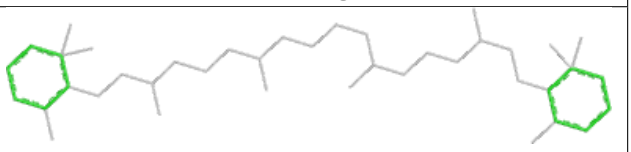


Torsions

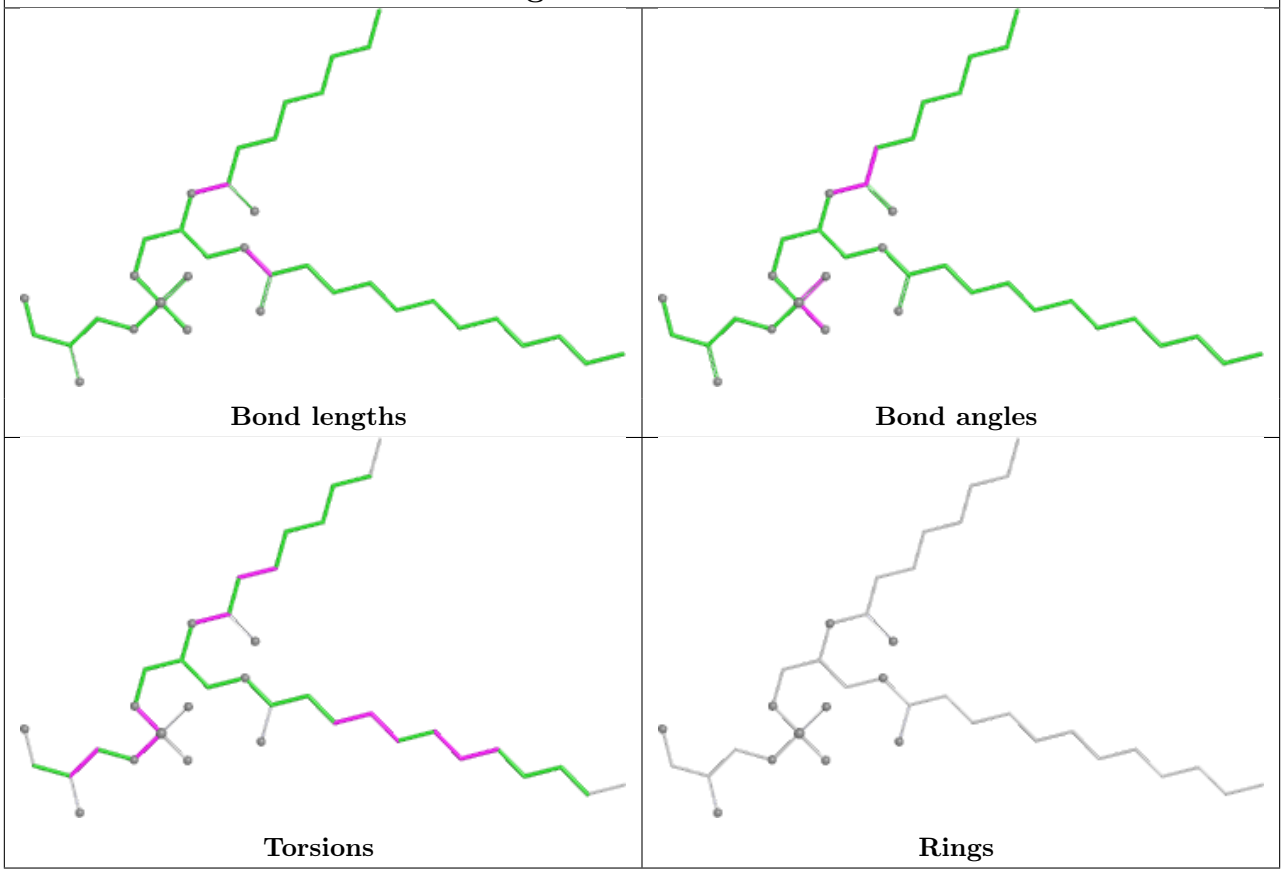


Rings

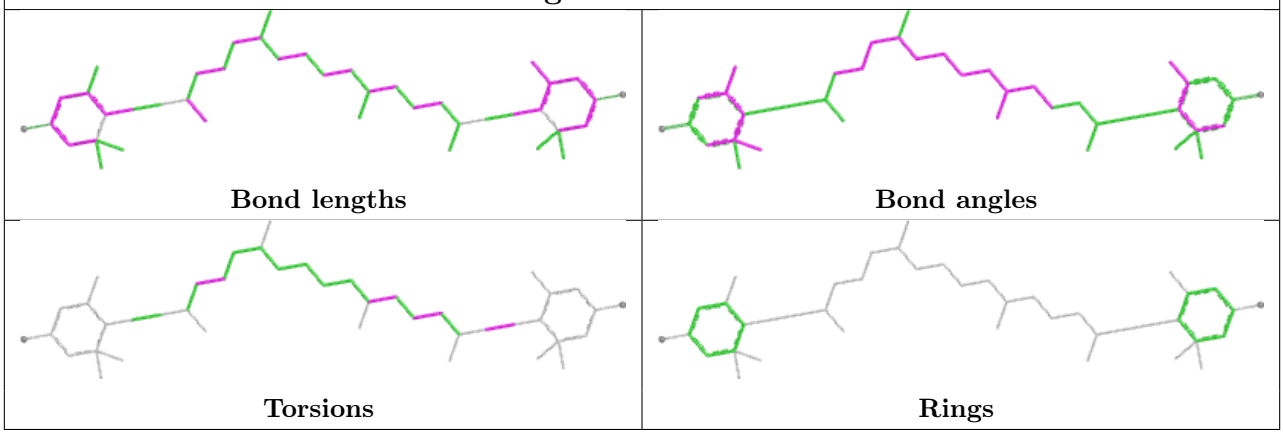
Ligand LMG F 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand WVN B 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

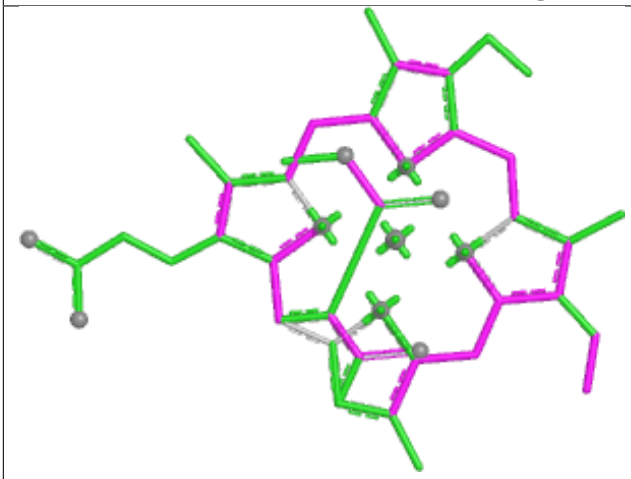
Ligand LHG d 315



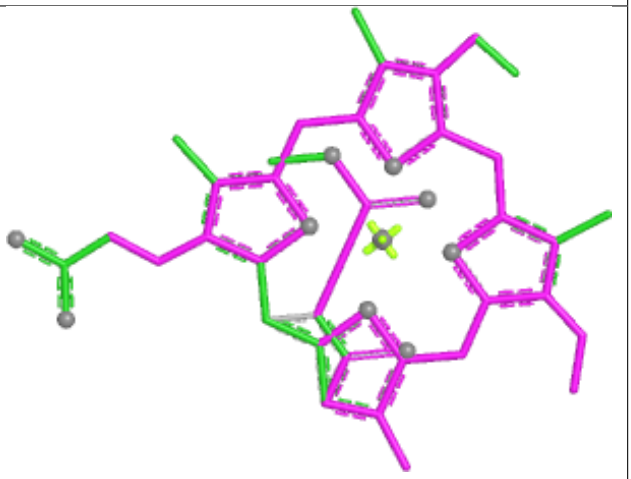
Ligand II0 e 614



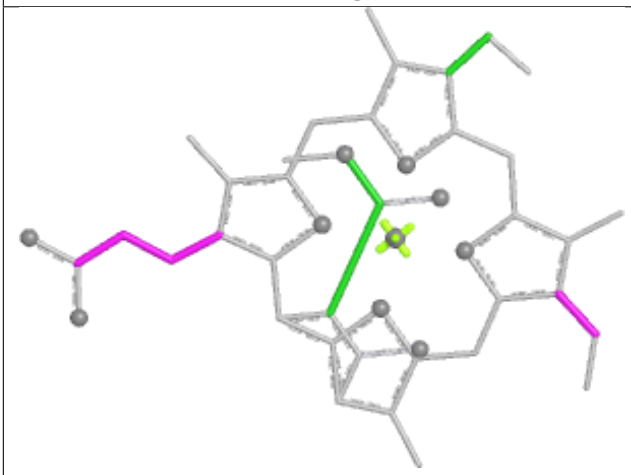
Ligand KC2 s 201



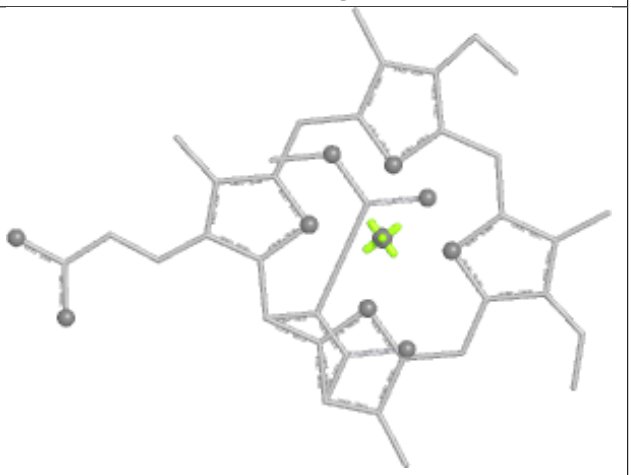
Bond lengths



Bond angles

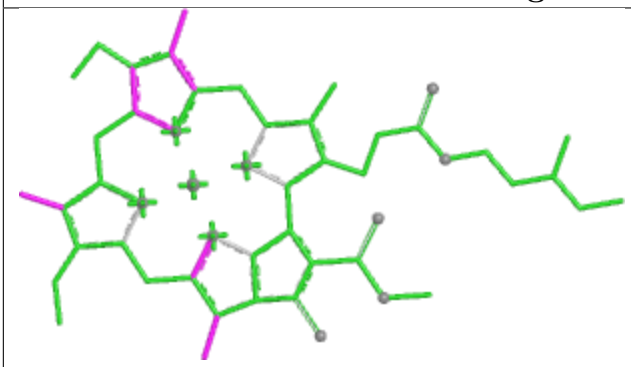


Torsions

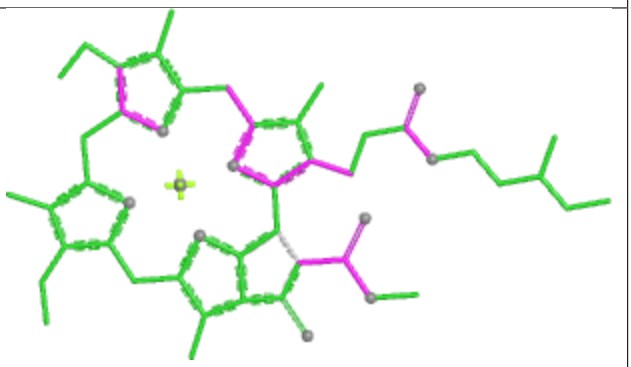


Rings

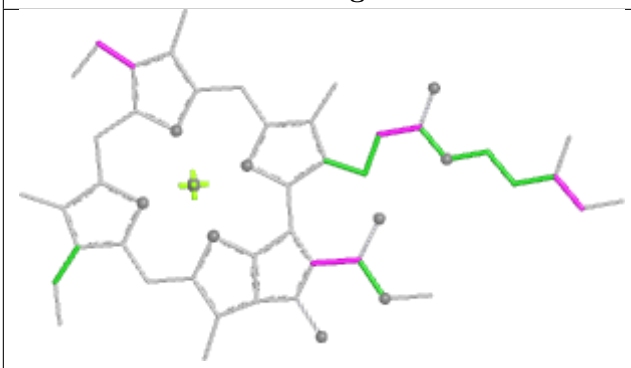
Ligand CLA d 304



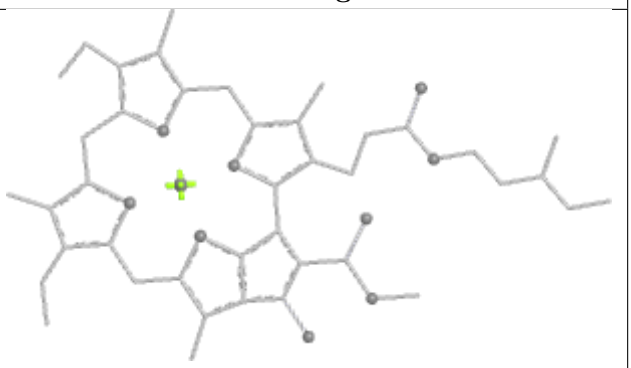
Bond lengths



Bond angles

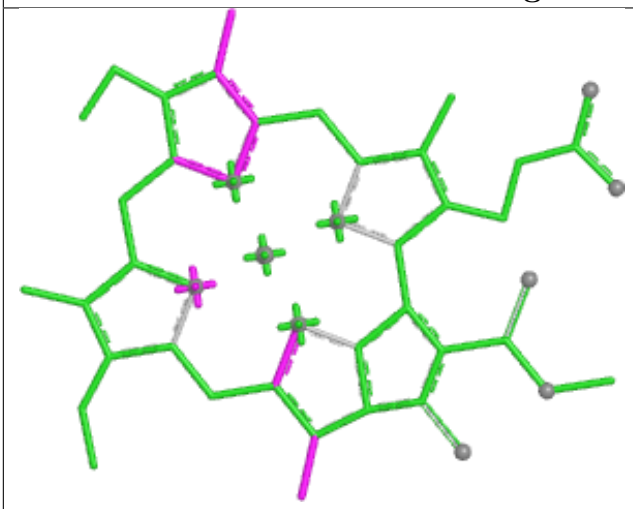


Torsions

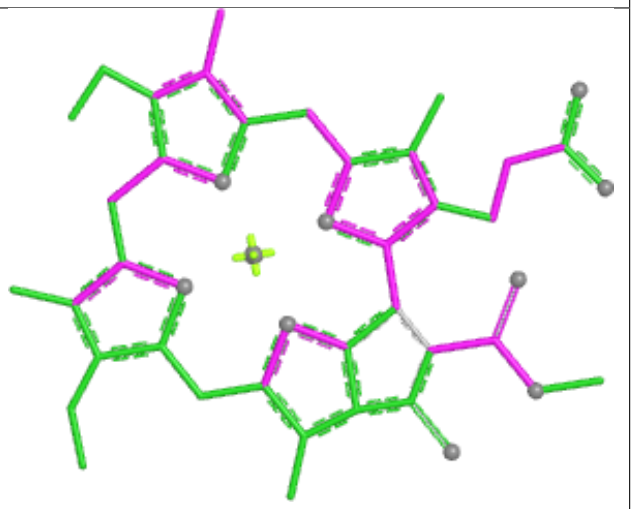


Rings

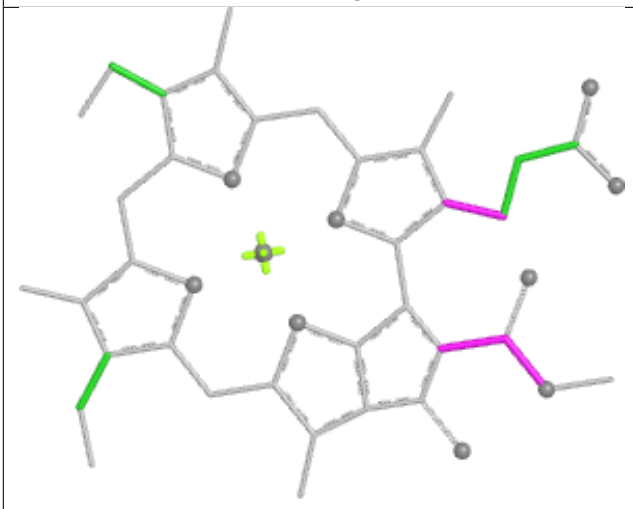
Ligand CLA A 813



Bond lengths



Bond angles

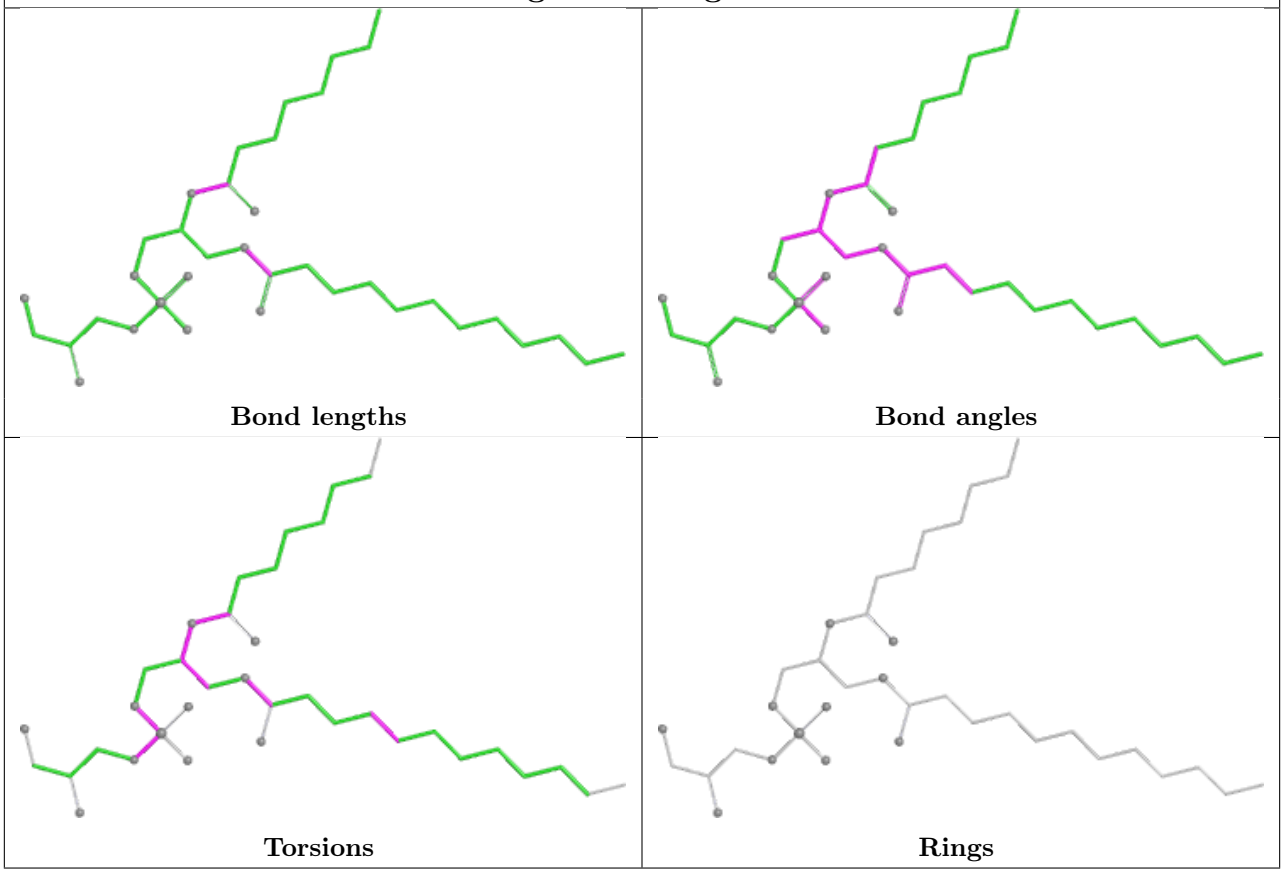


Torsions

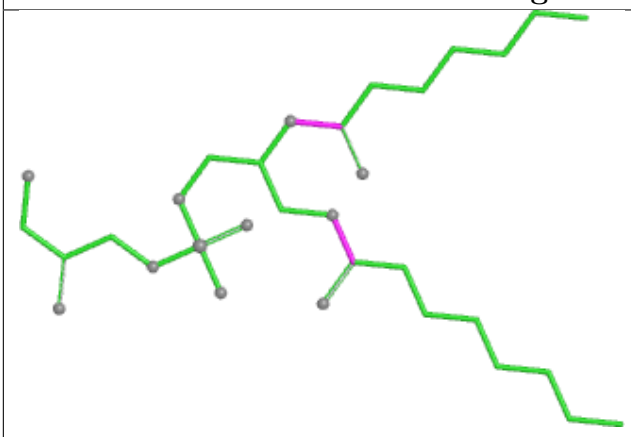


Rings

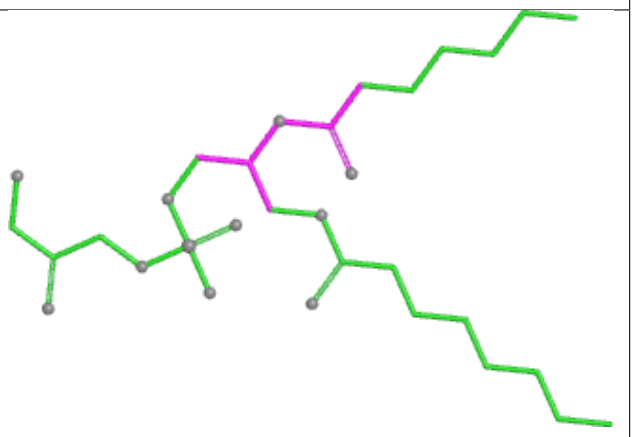
Ligand LHG g 321



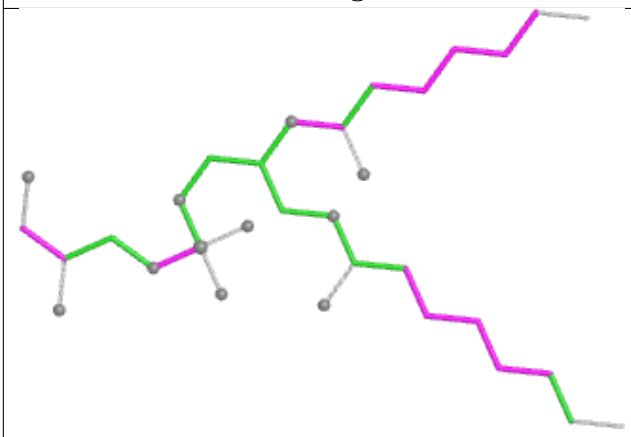
Ligand LHG l 318



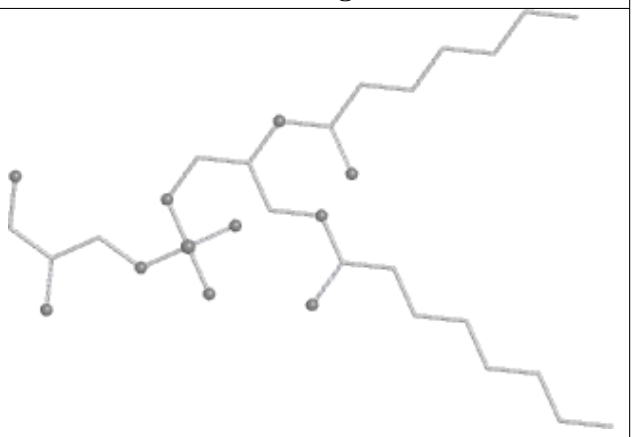
Bond lengths



Bond angles

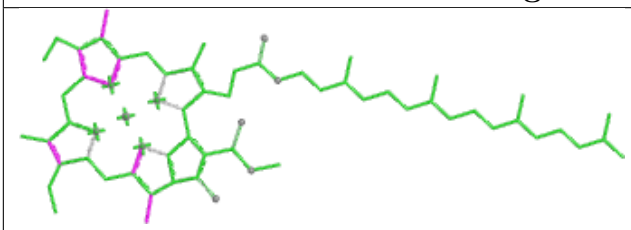


Torsions

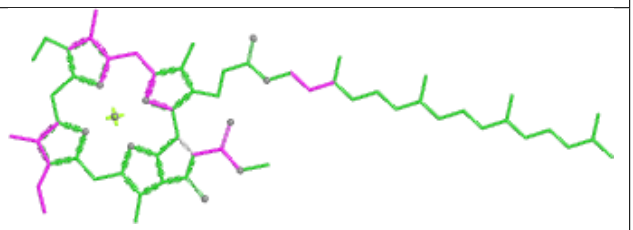


Rings

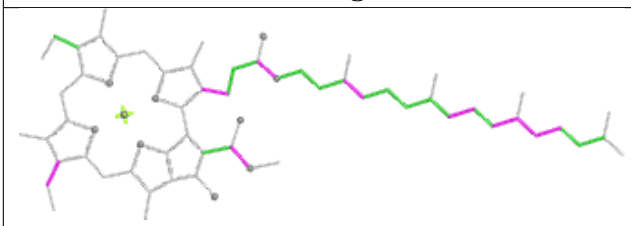
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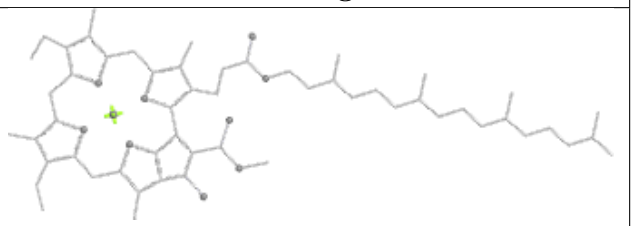
Bond lengths



Bond angles

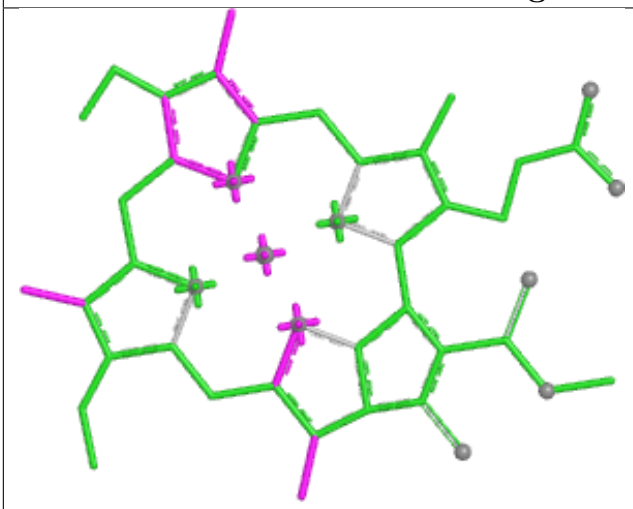


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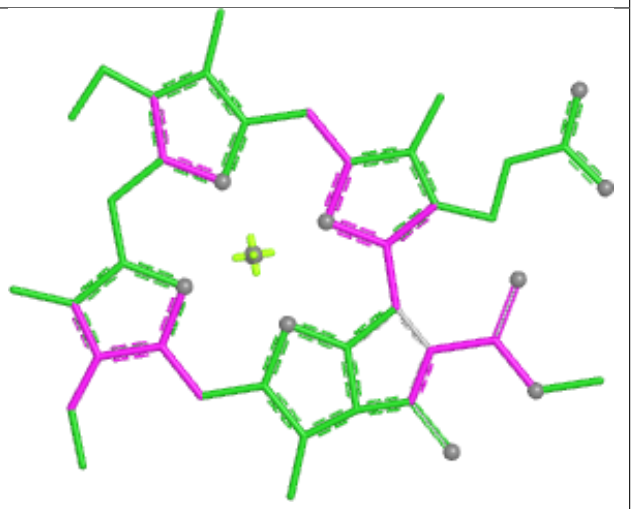


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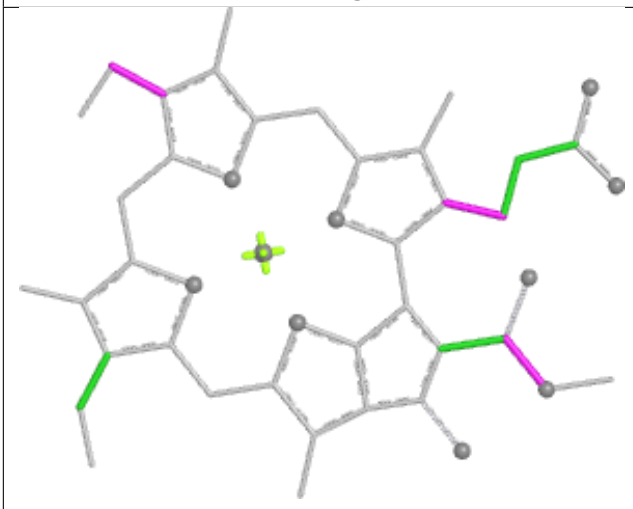
Ligand CLA a 307



Bond lengths



Bond angles

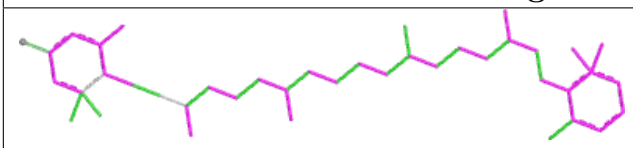


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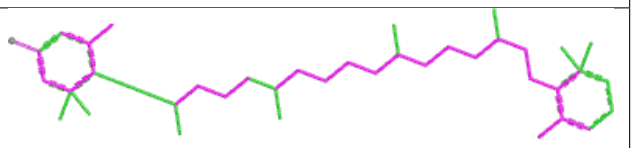


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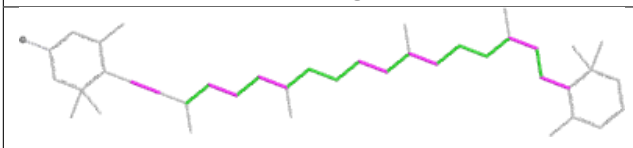
Ligand IHT O 204



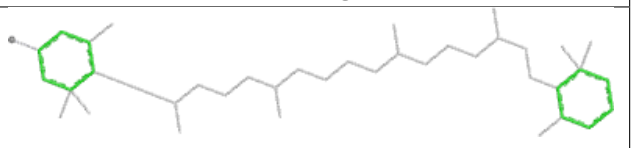
Bond lengths



Bond angles

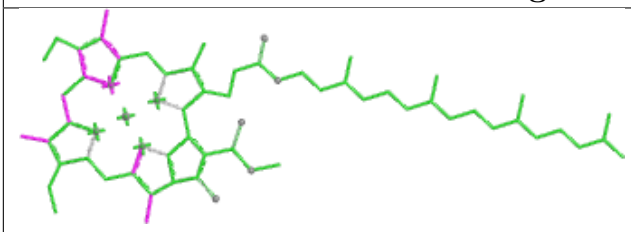


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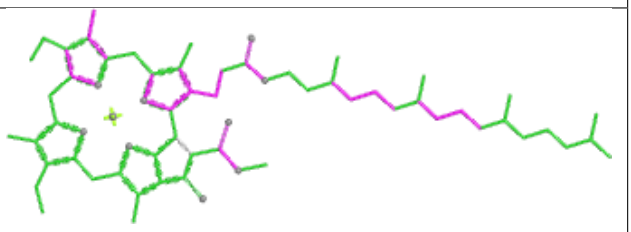


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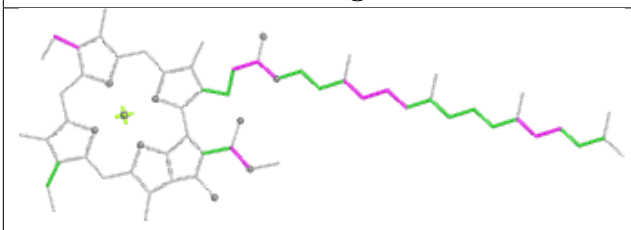
Ligand CLA e 611



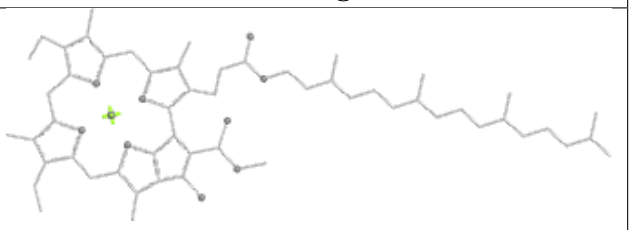
Bond lengths



Bond angles

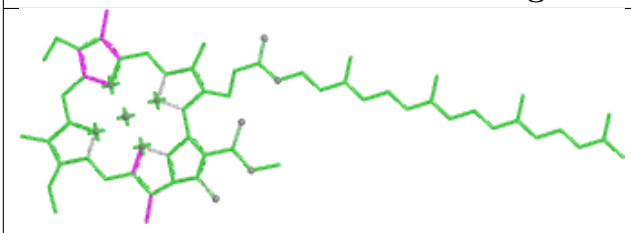


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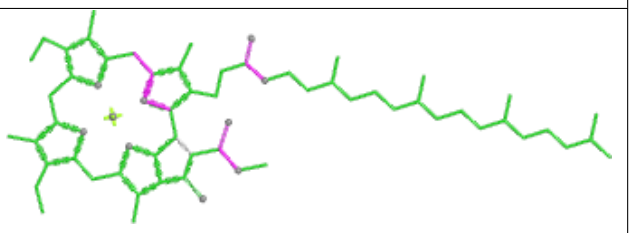


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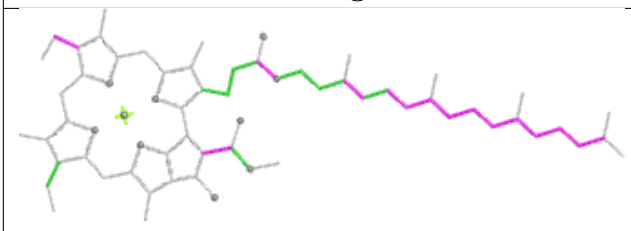
Ligand CLA d 303



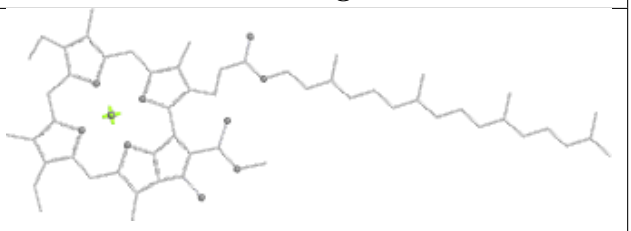
Bond lengths



Bond angles

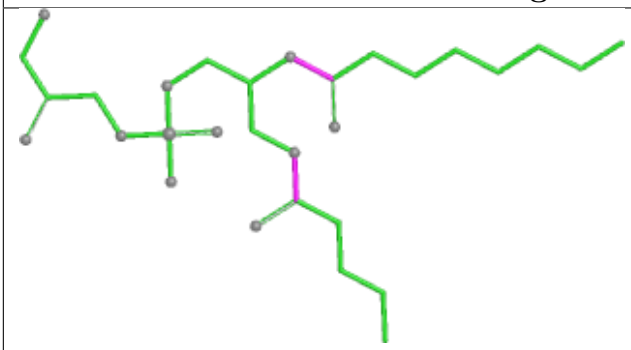


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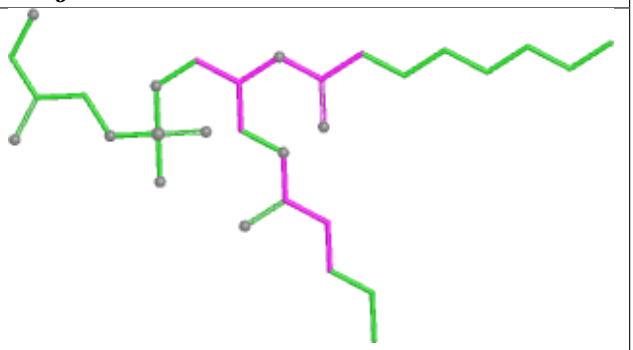


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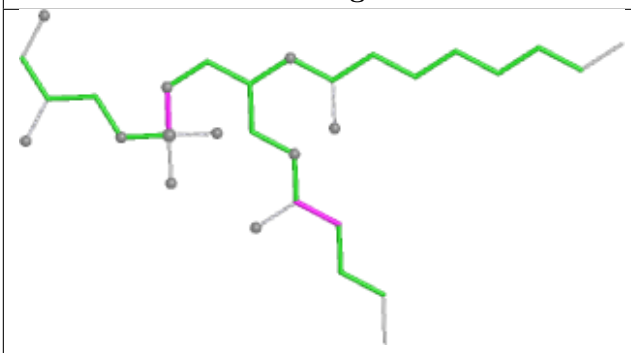
Ligand LHG j 617



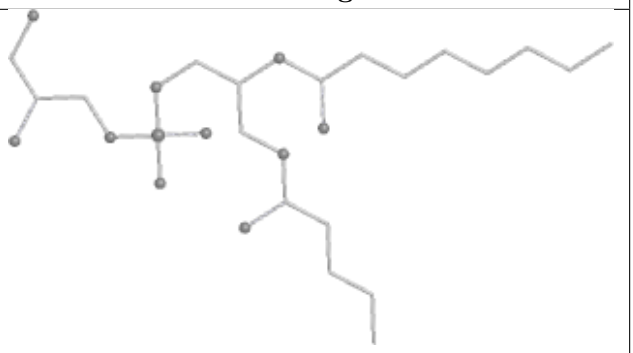
Bond lengths



Bond angles

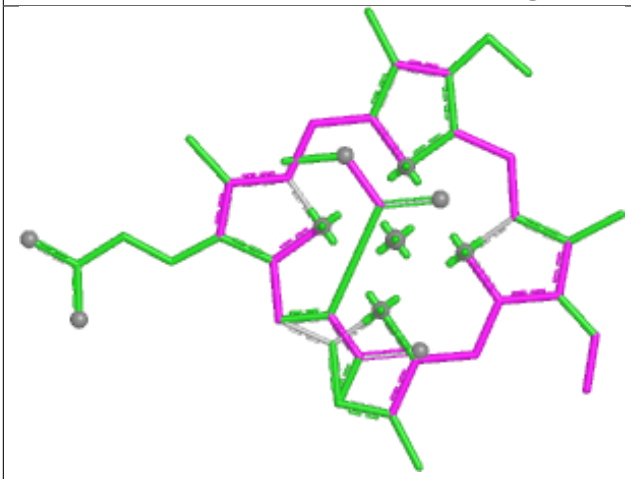


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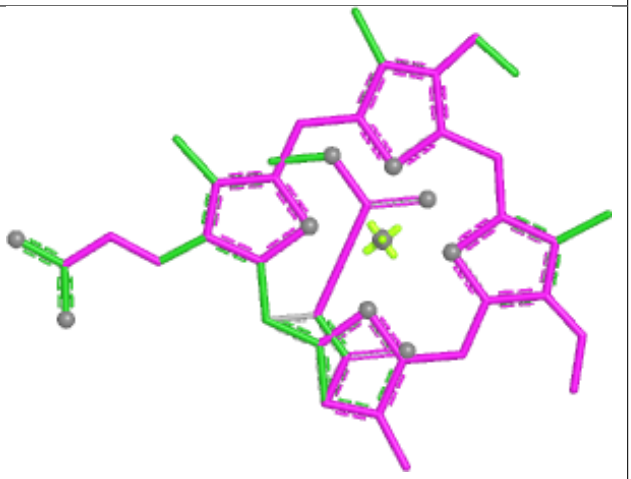


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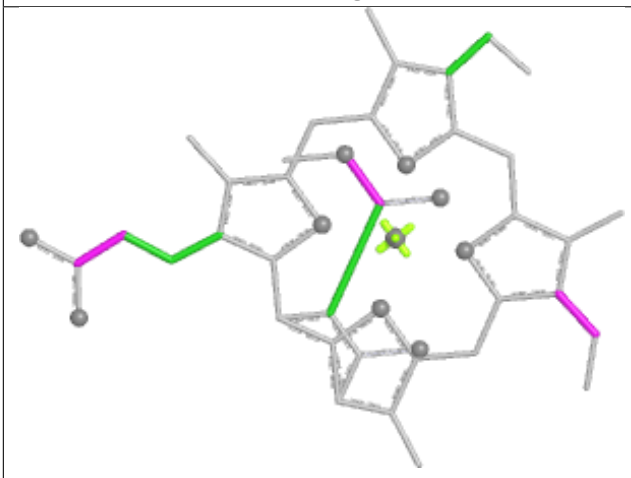
Ligand KC2 m 610



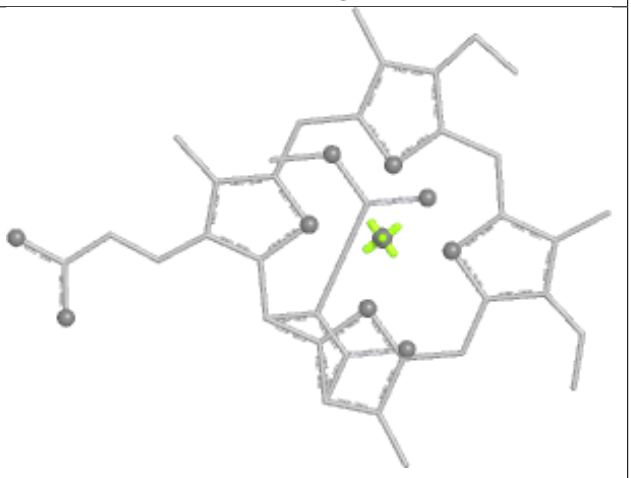
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Bond angles

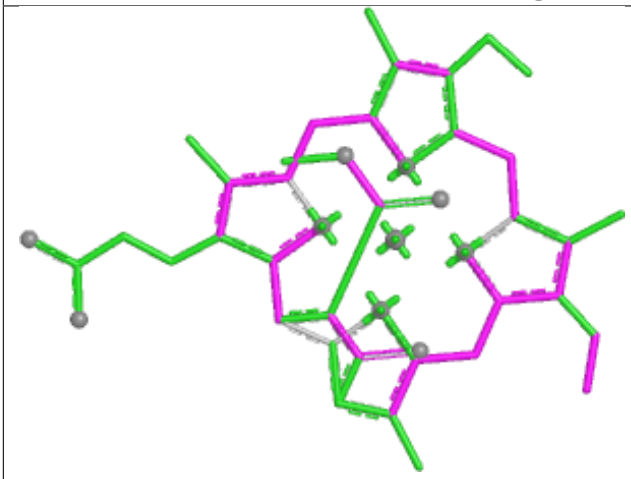


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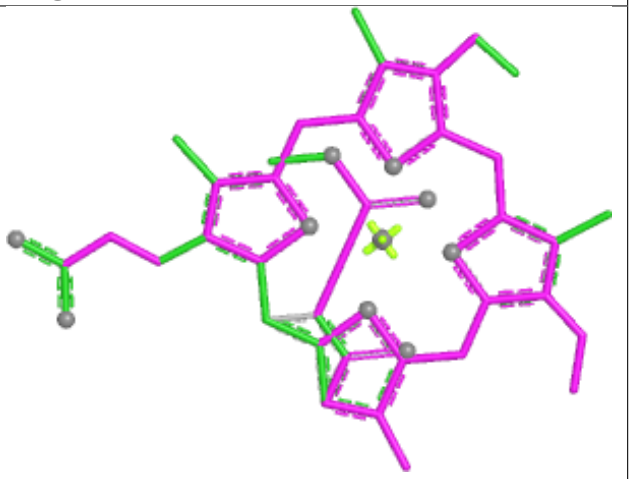


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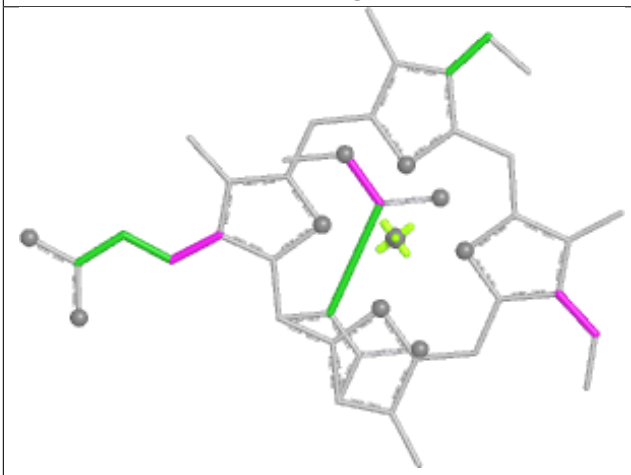
Ligand KC2 g 314



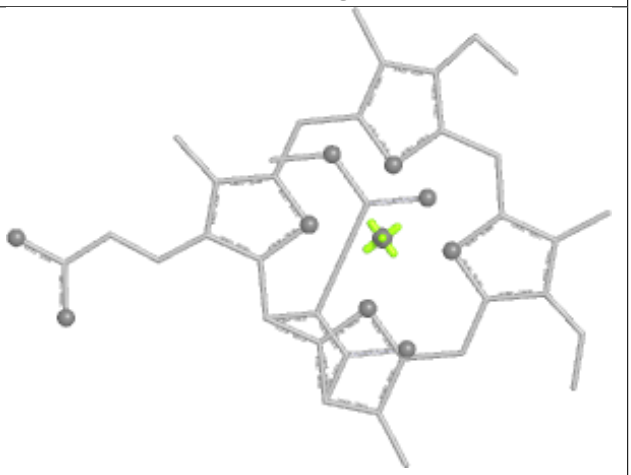
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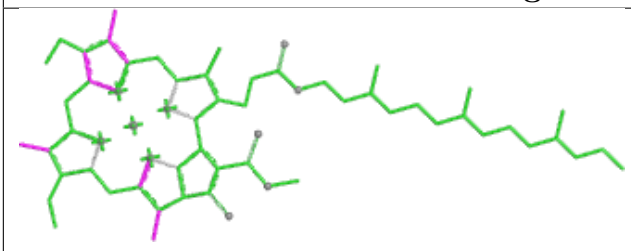


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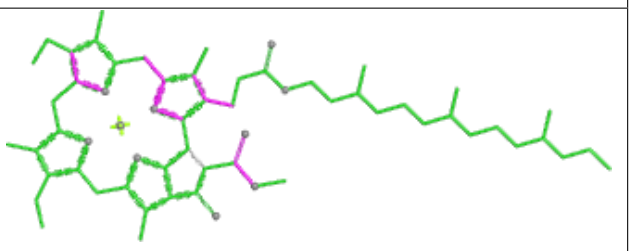


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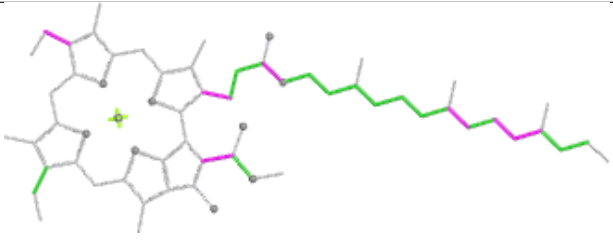
Ligand CLA A 810



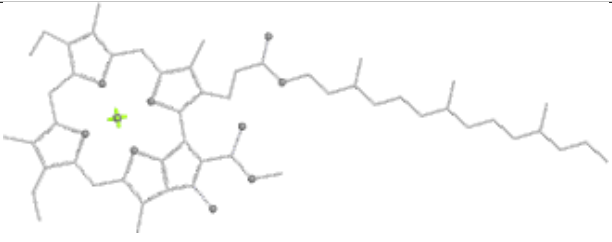
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Bond angles

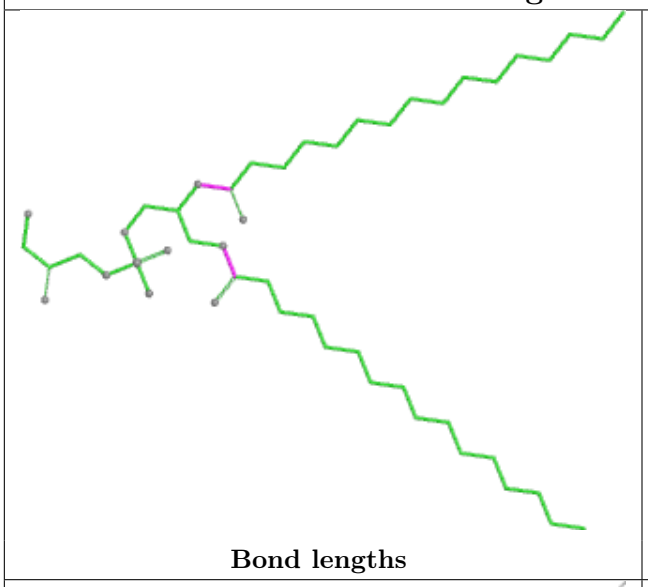


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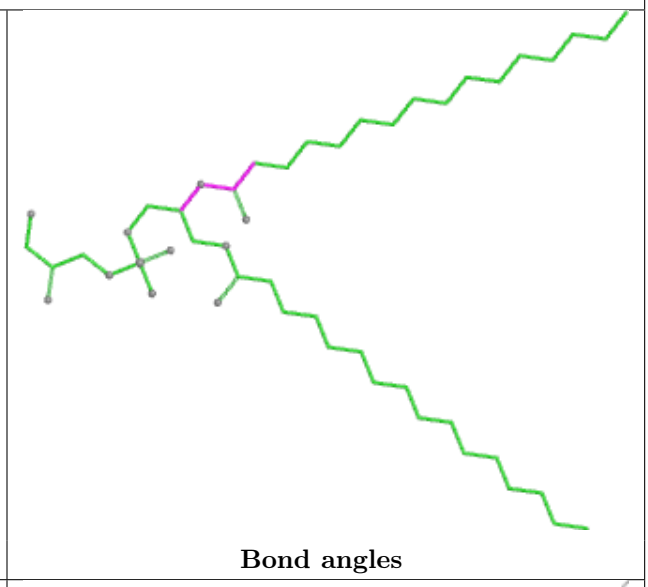


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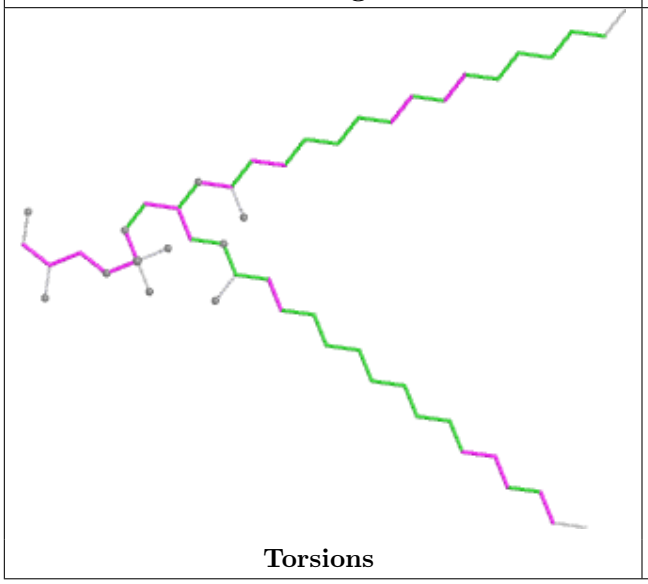
Ligand LHG L 207



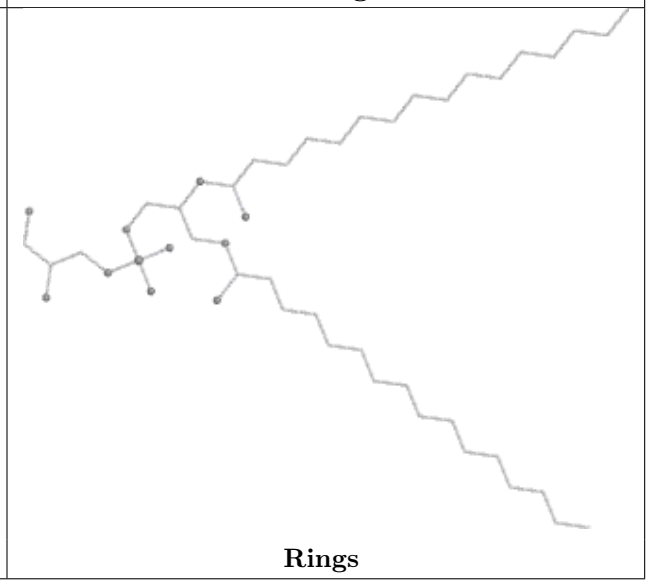
Bond lengths



Bond angles

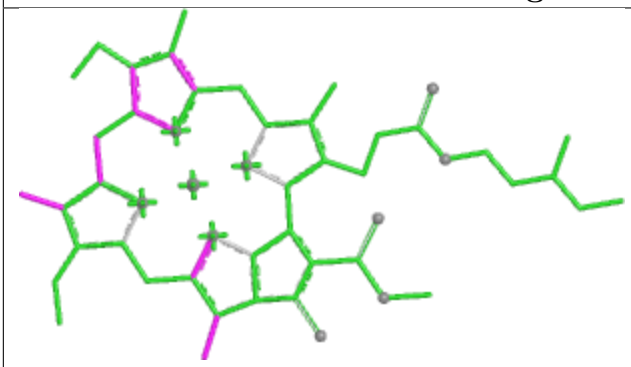


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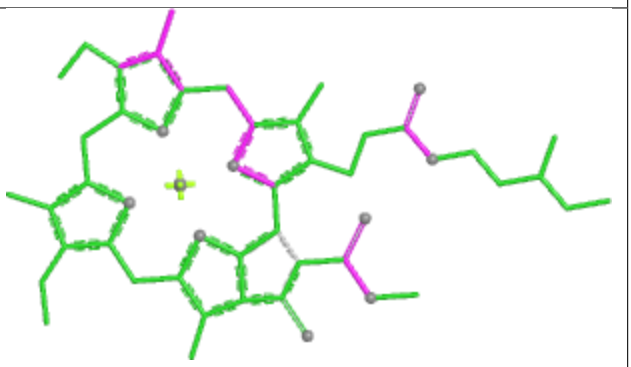


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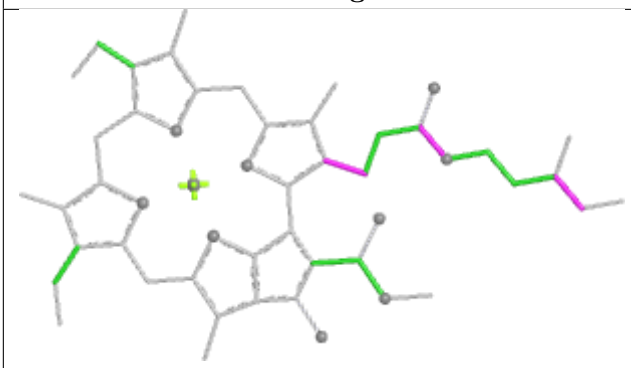
Ligand CLA L 206



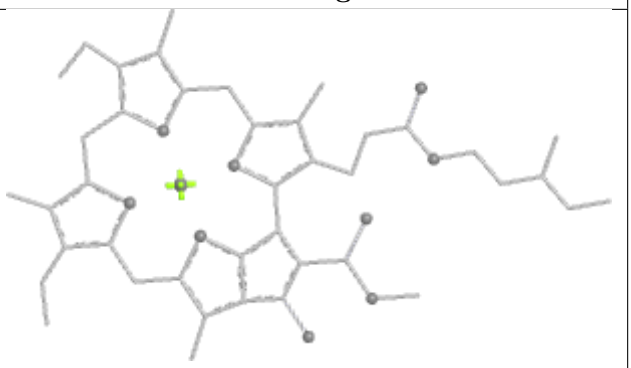
Bond lengths



Bond angles

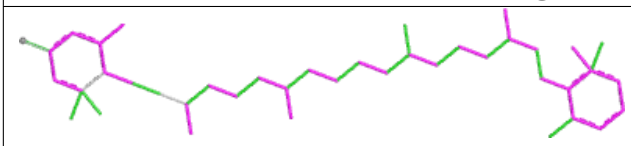


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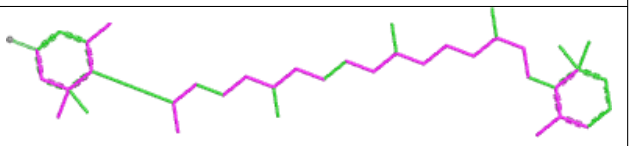


Rings

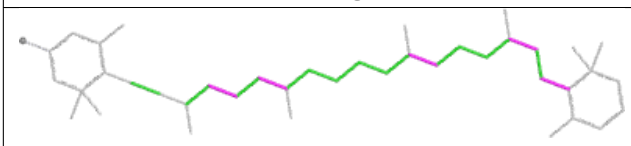
Ligand IHT c 616



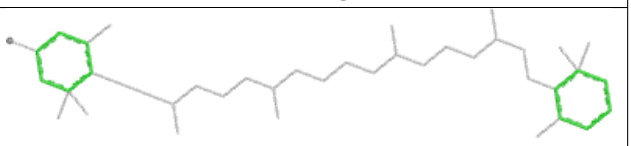
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Bond angles

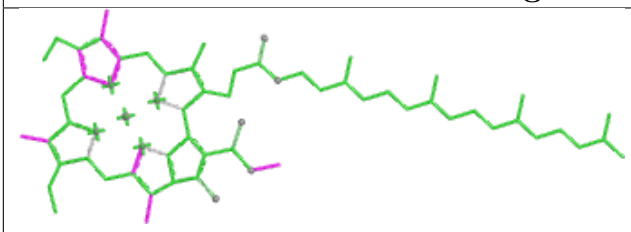


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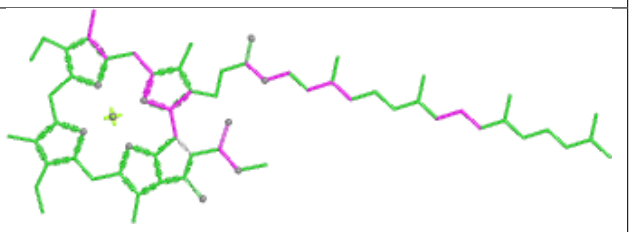


Rings

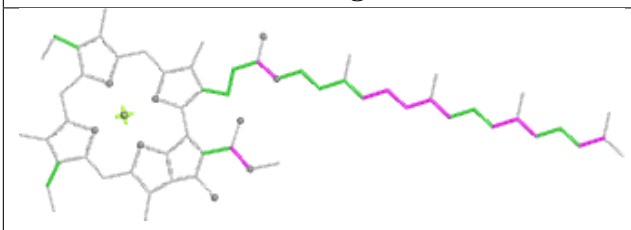
Ligand CLA A 840



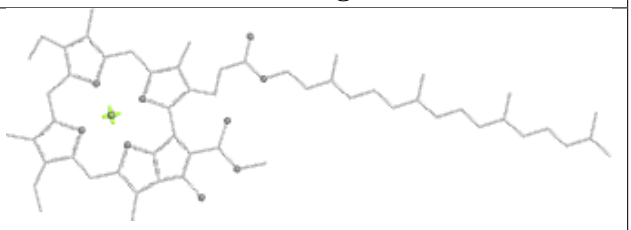
Bond lengths



Bond angles

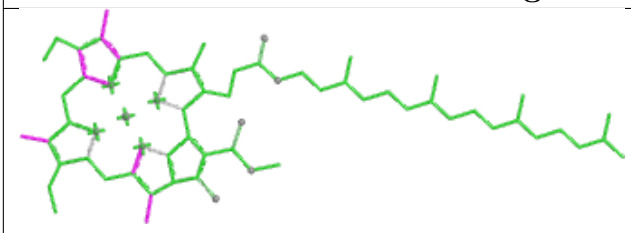


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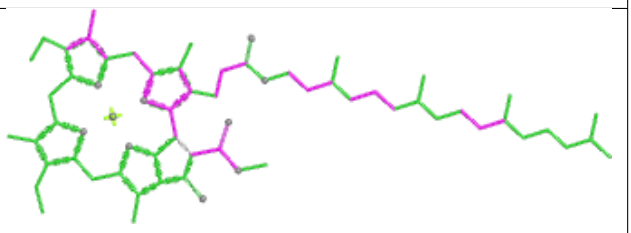


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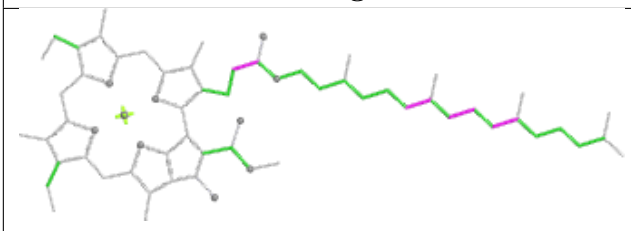
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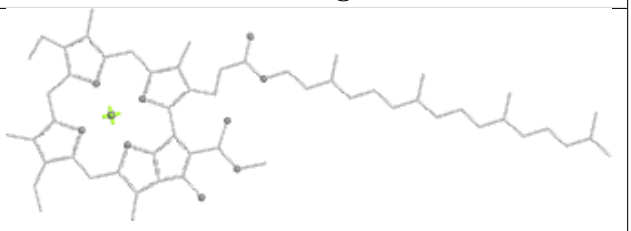
Bond lengths



Bond angles

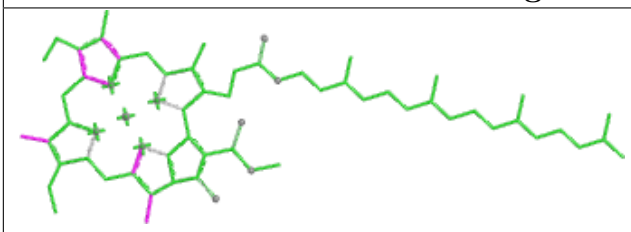


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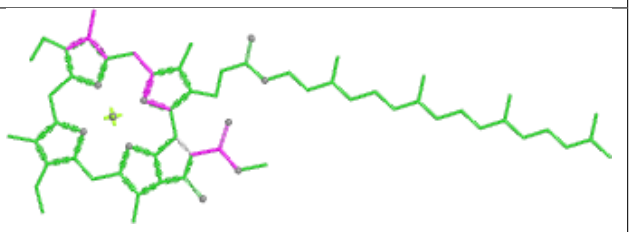


Rings

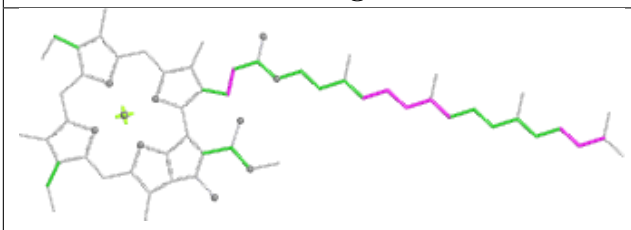
Ligand CLA B 805



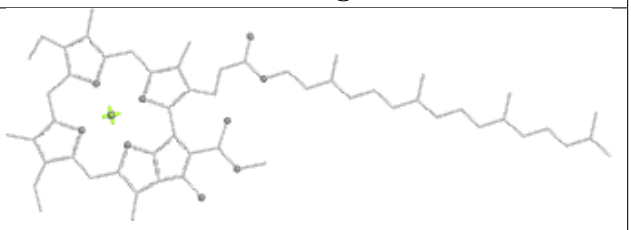
Bond lengths



Bond angles

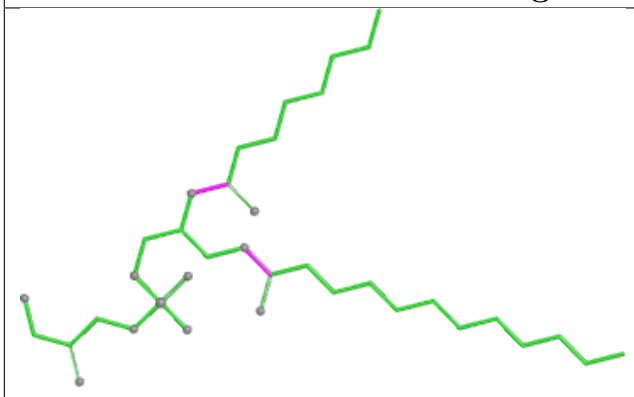


Torsions

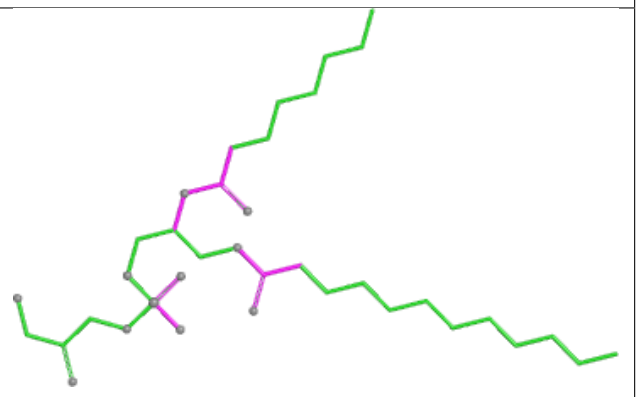


Rings

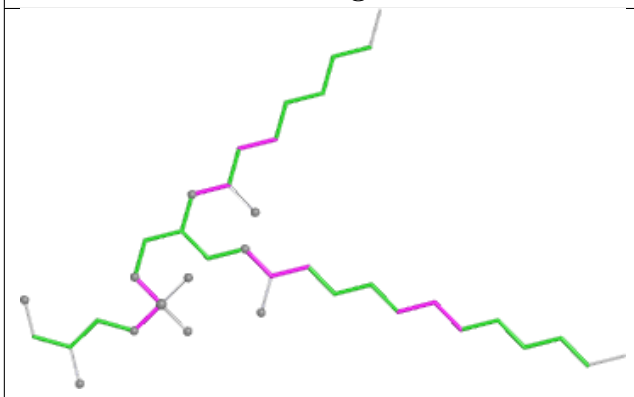
Ligand LHG i 316



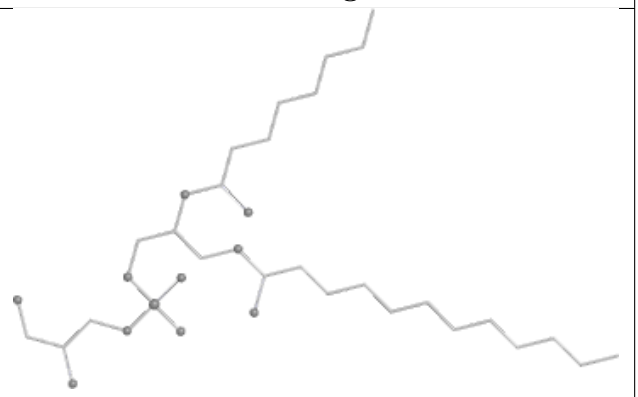
Bond lengths



Bond angles

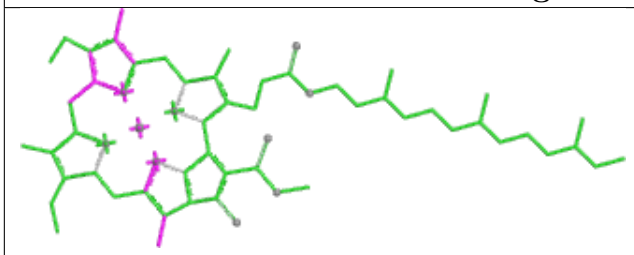


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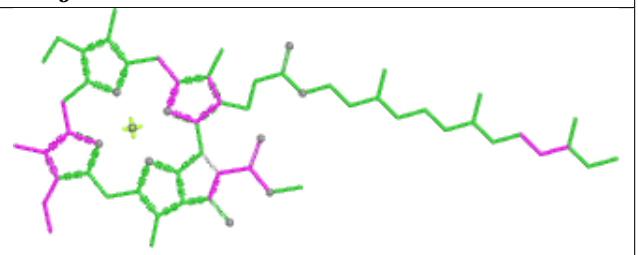


Rings

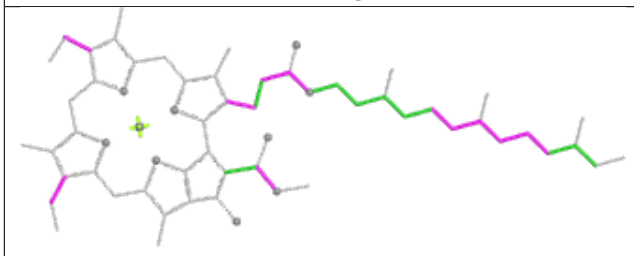
Ligand CLA j 609



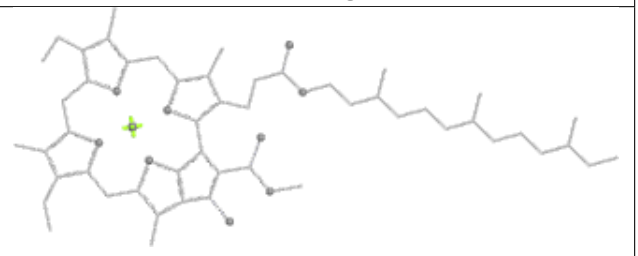
Bond lengths



Bond angles

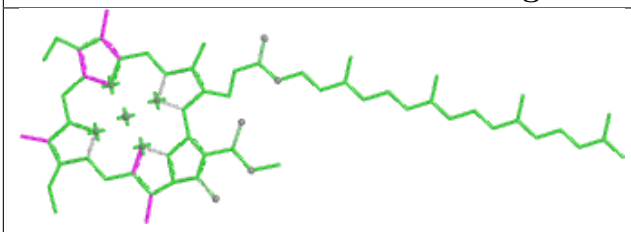


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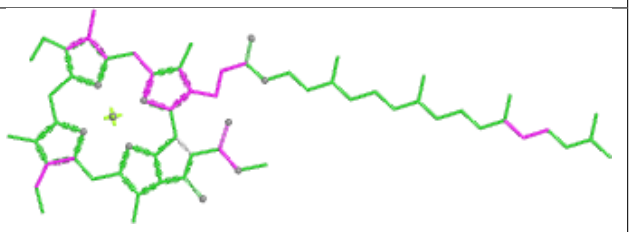


Rings

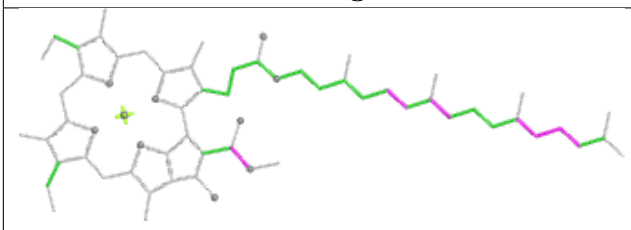
Ligand CLA m 603



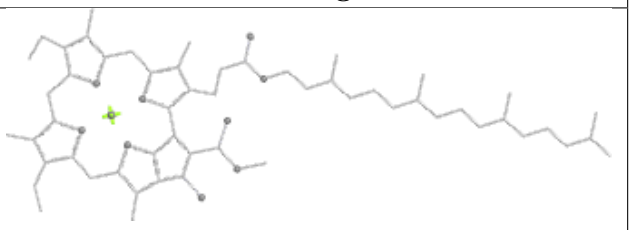
Bond lengths



Bond angles

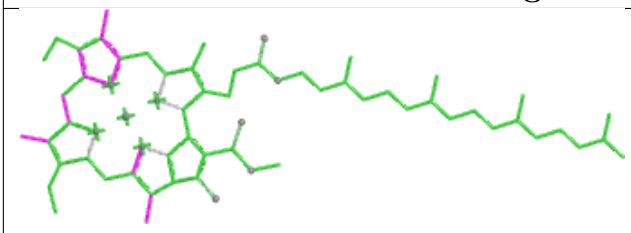


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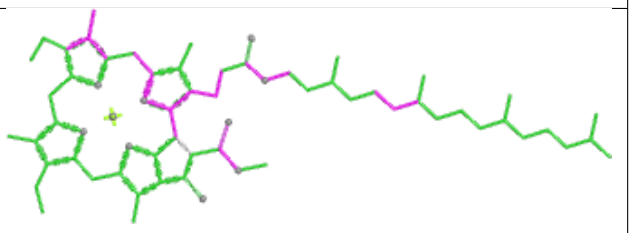


Rings

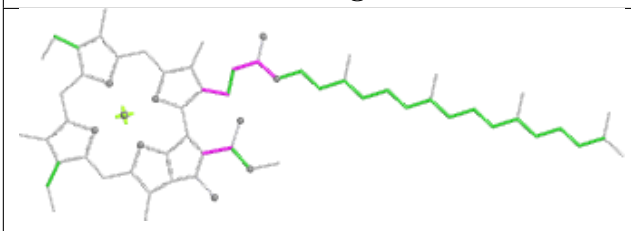
Ligand CLA A 804



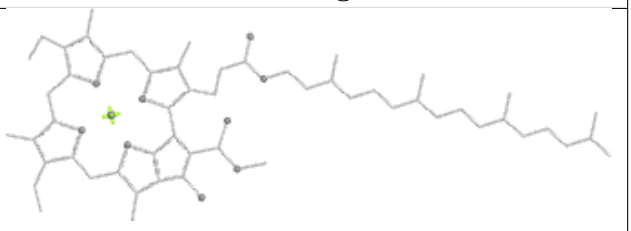
Bond lengths



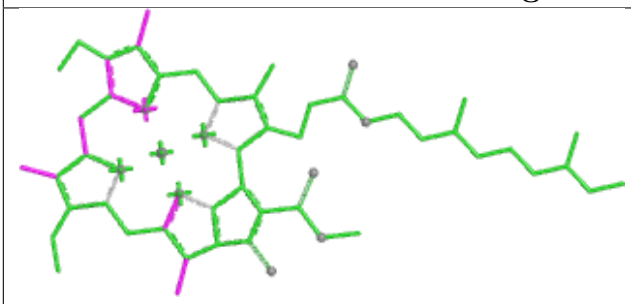
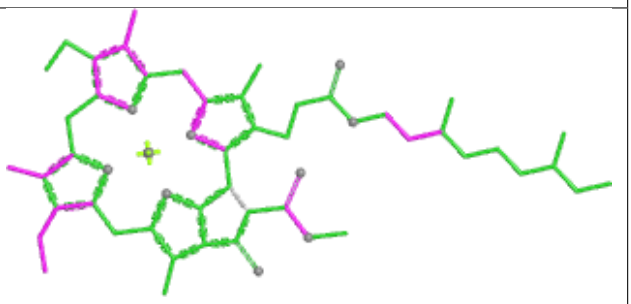
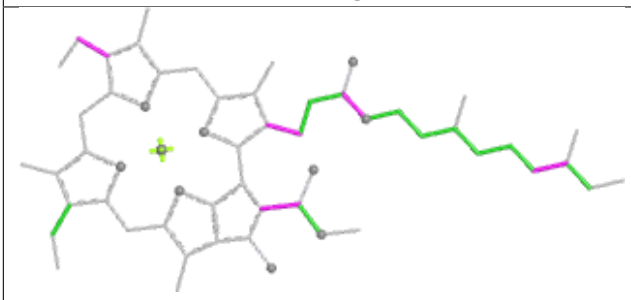
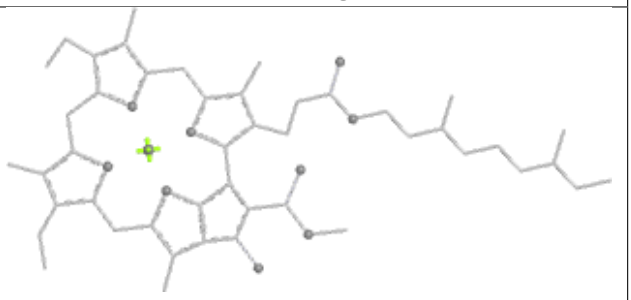
Bond angles

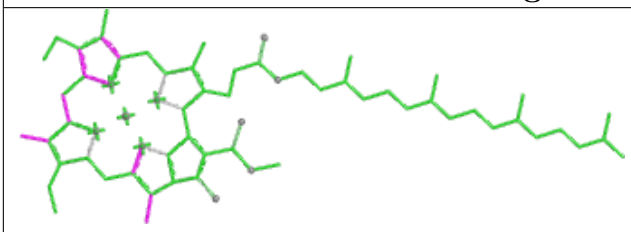
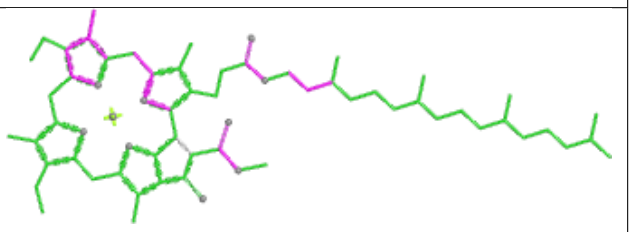
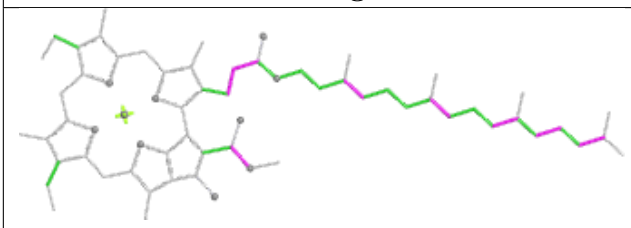
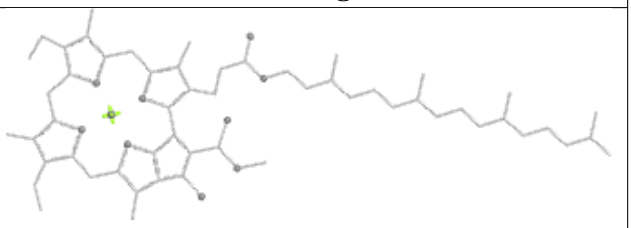


Torsions

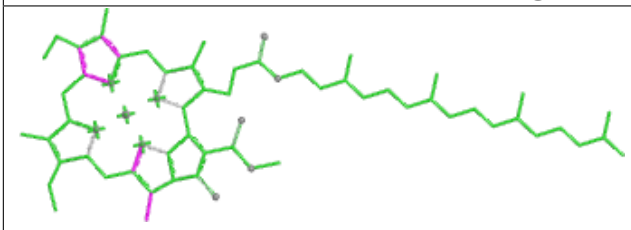


Rings

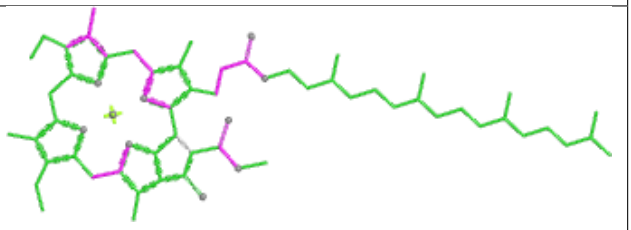
Ligand CLA m 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

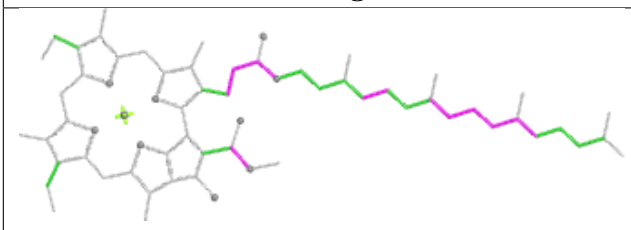
Ligand CLA c 612



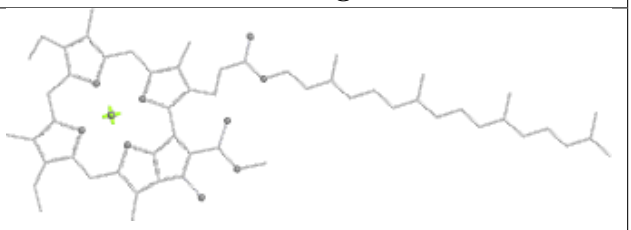
Bond lengths



Bond angles

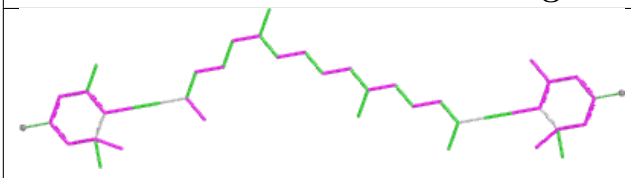


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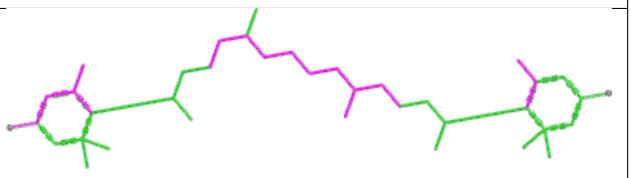


Rings

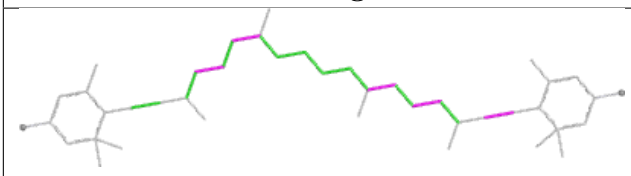
Ligand II0 J 104



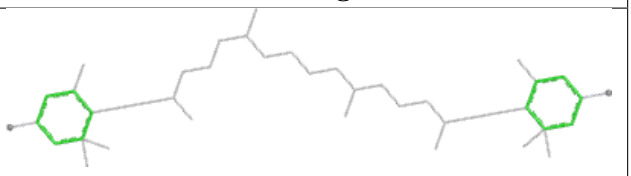
Bond lengths



Bond angles

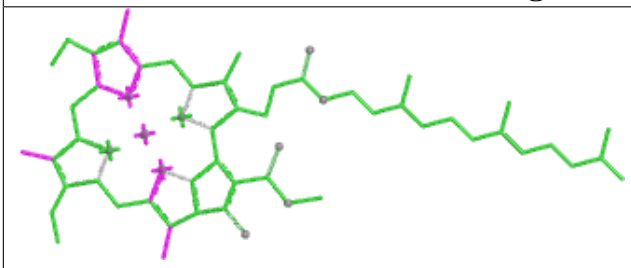


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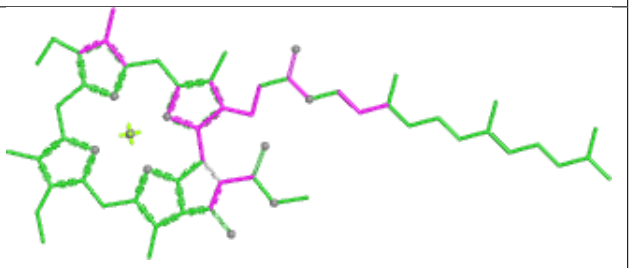


Rings

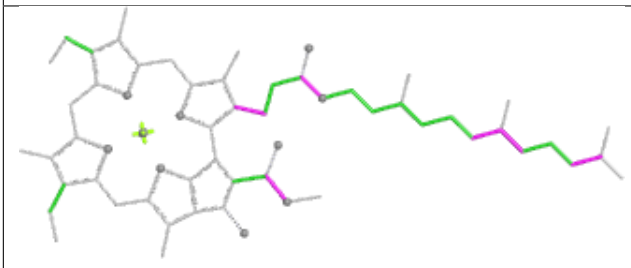
Ligand CLA n 604



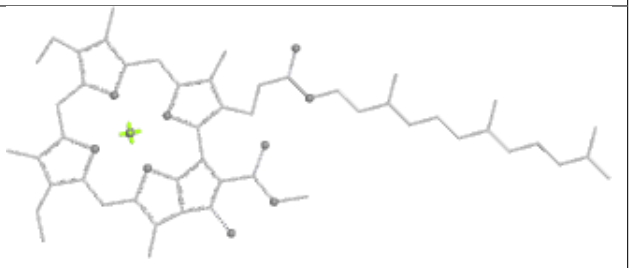
Bond lengths



Bond angles

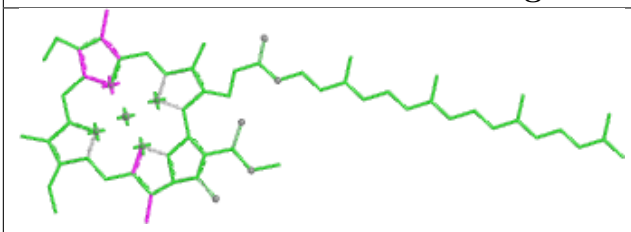


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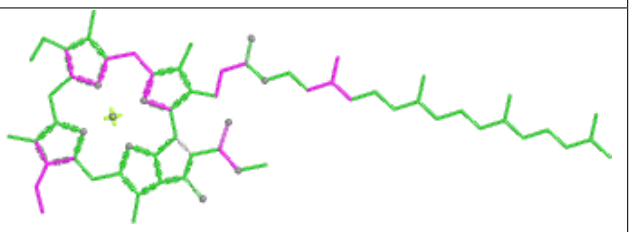


Rings

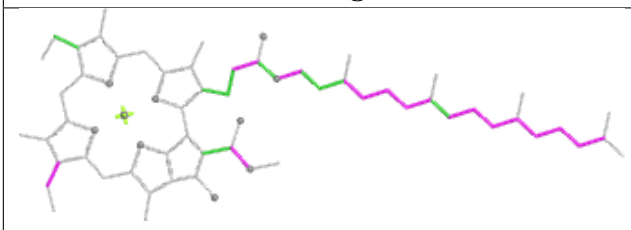
Ligand CLA B 835



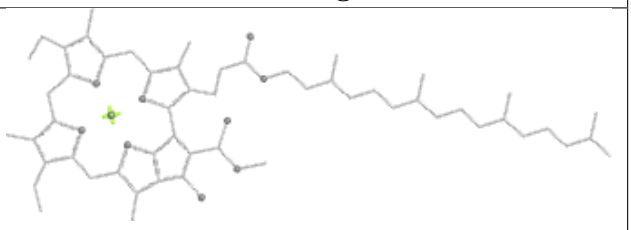
Bond lengths



Bond angles

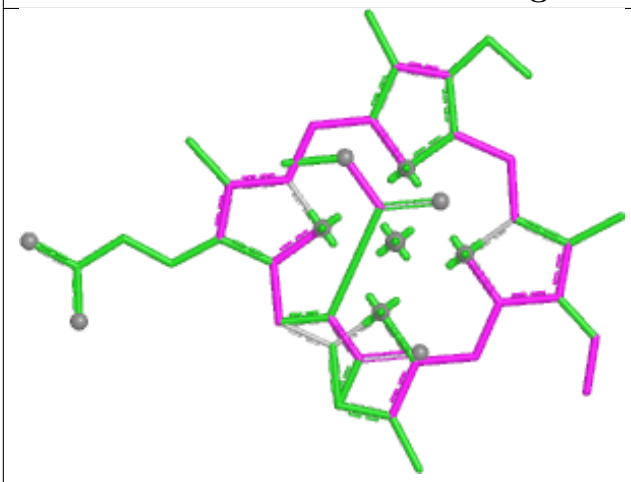


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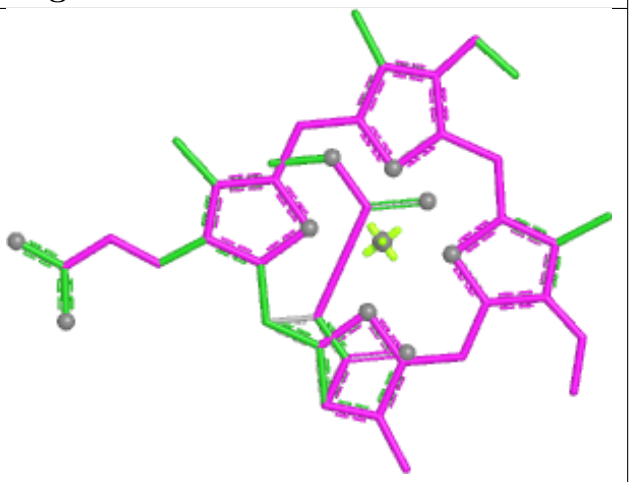


Rings

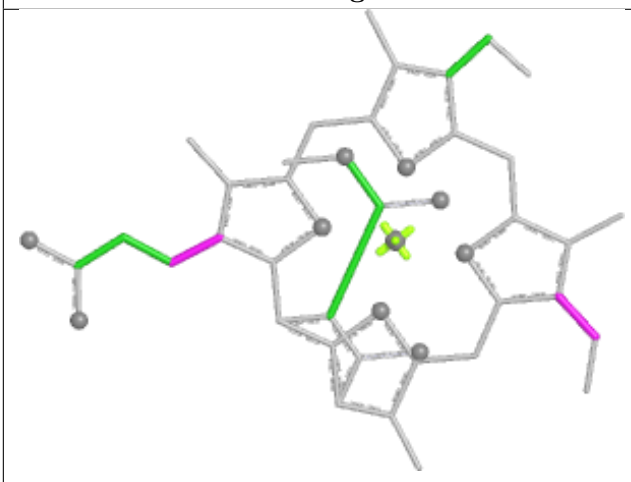
Ligand KC2 g 313



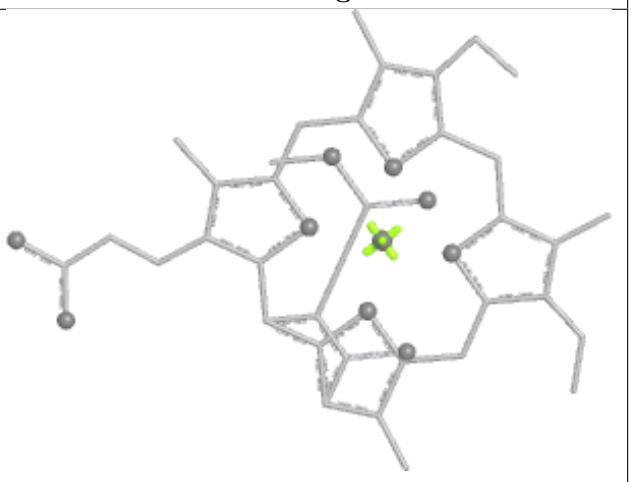
Bond lengths



Bond angles

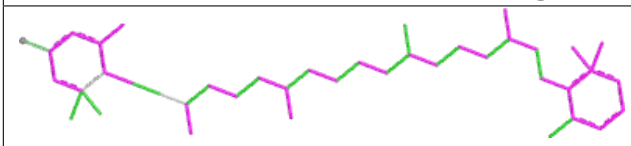


Torsions

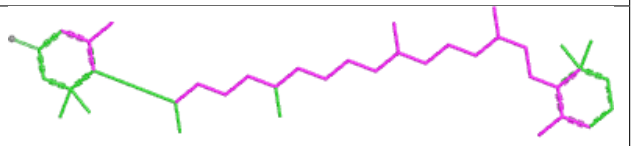


Rings

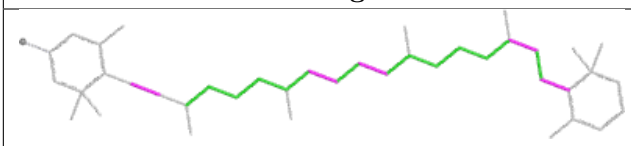
Ligand IHT k 317



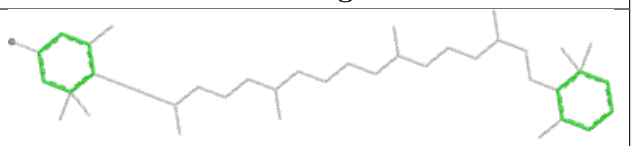
Bond lengths



Bond angles

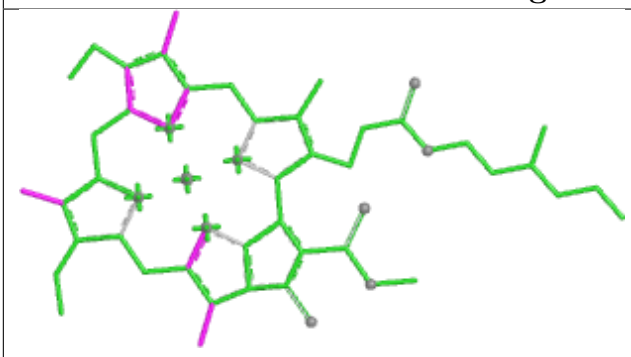


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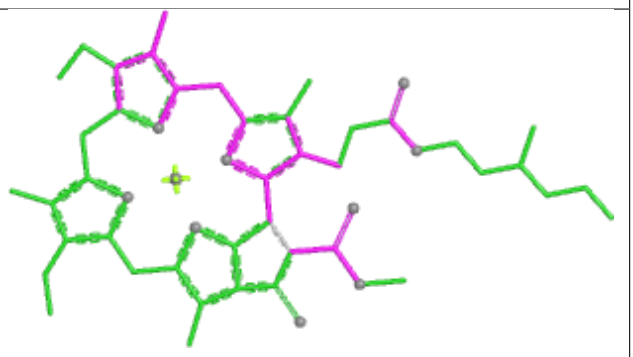


Rings

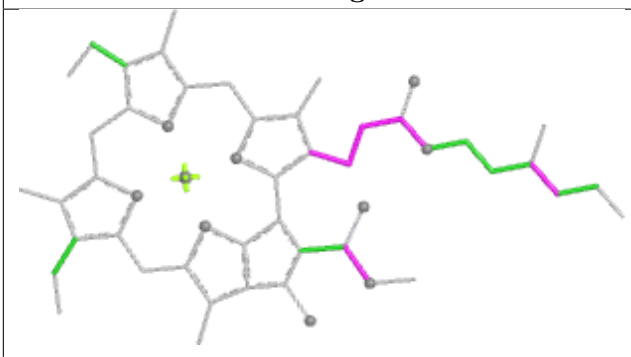
Ligand CLA c 606



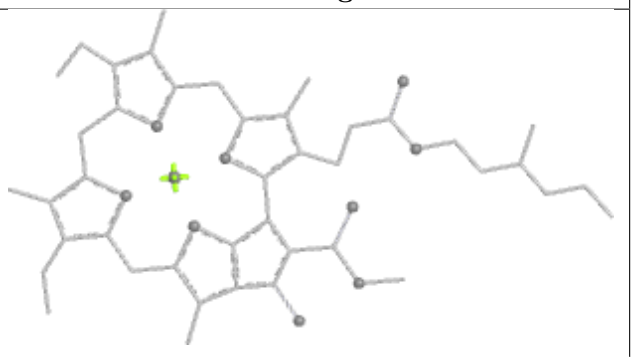
Bond lengths



Bond angles

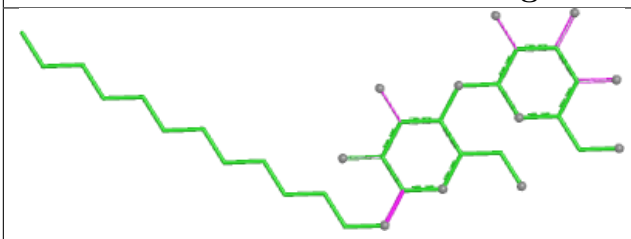


Torsions

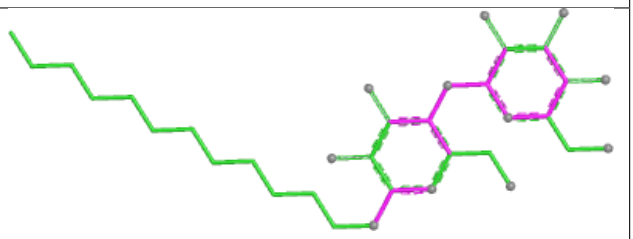


Rings

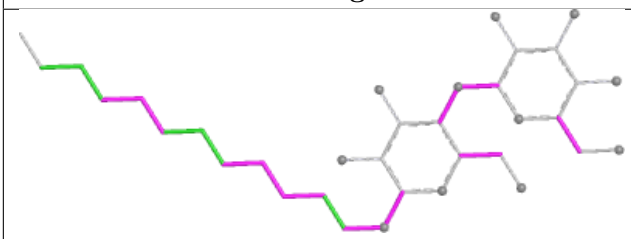
Ligand LMT A 851



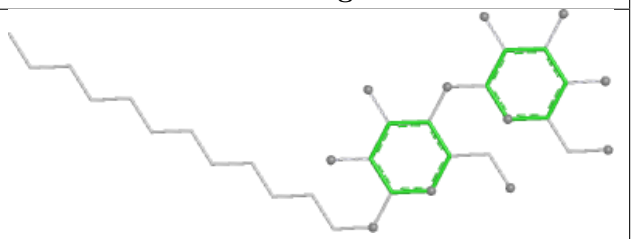
Bond lengths



Bond angles

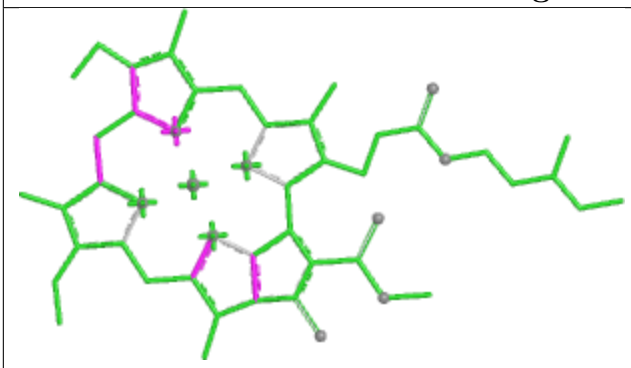


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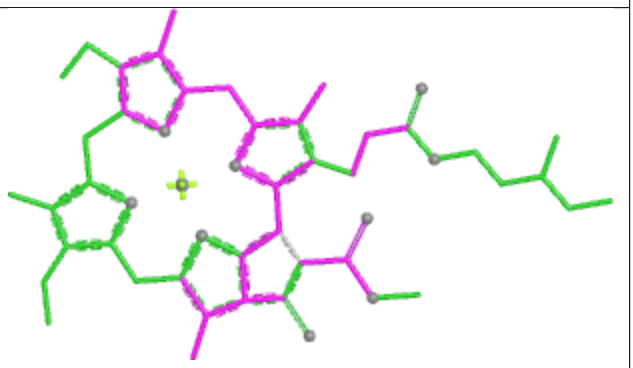


Rings

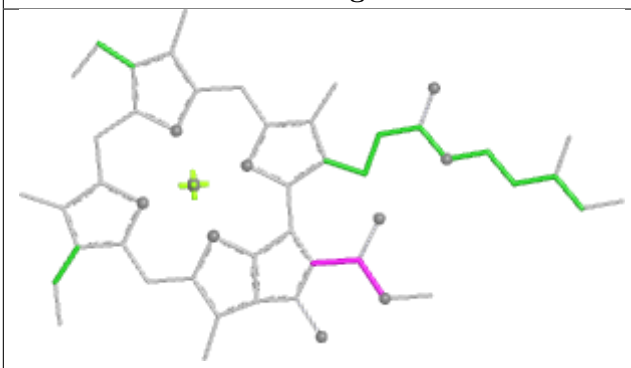
Ligand CLA i 308



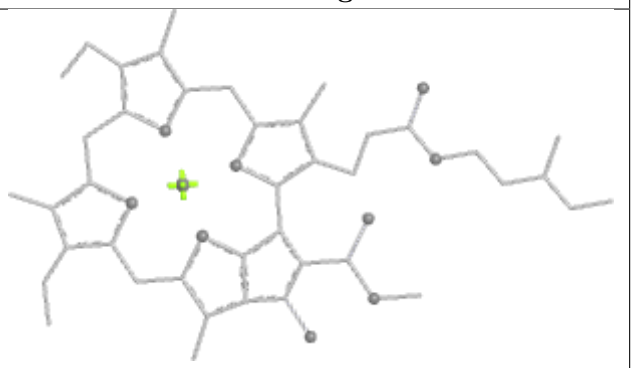
Bond lengths



Bond angles

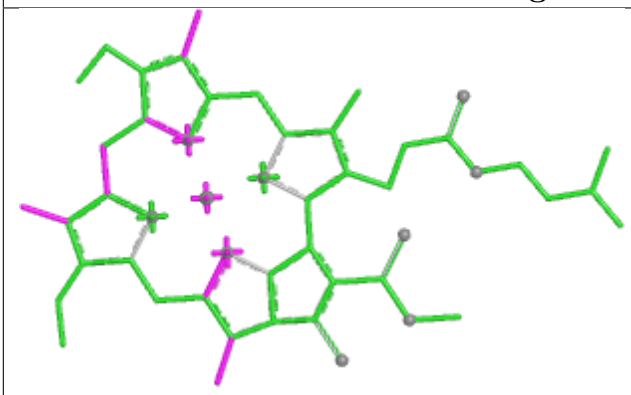


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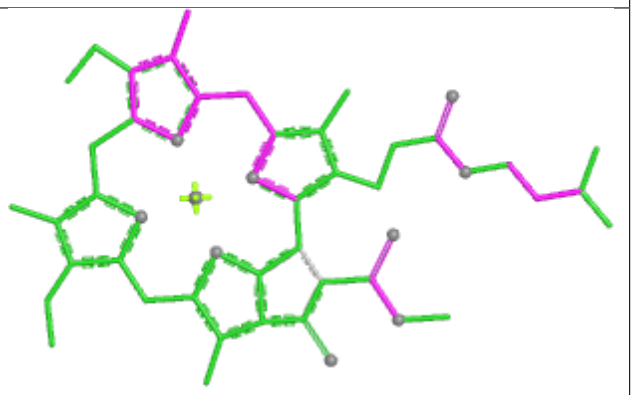


Rings

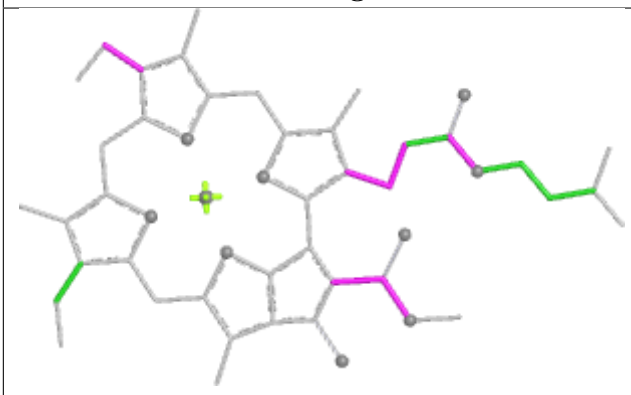
Ligand CLA e 602



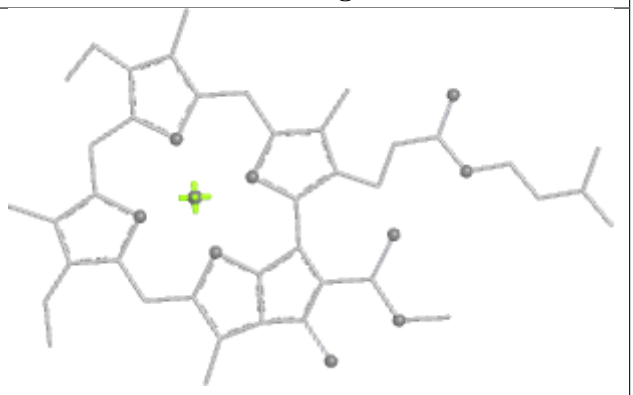
Bond lengths



Bond angles

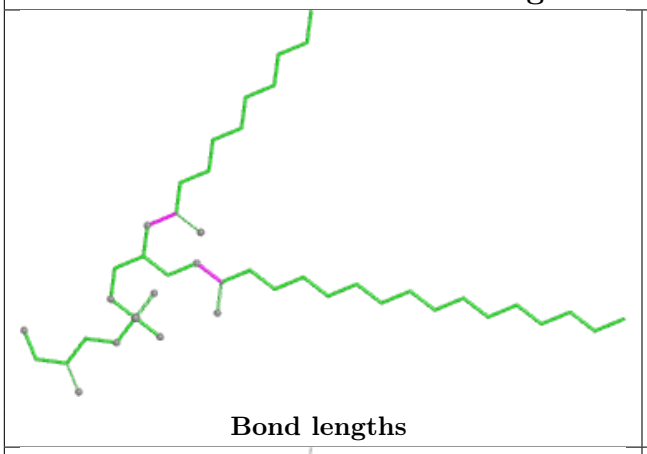


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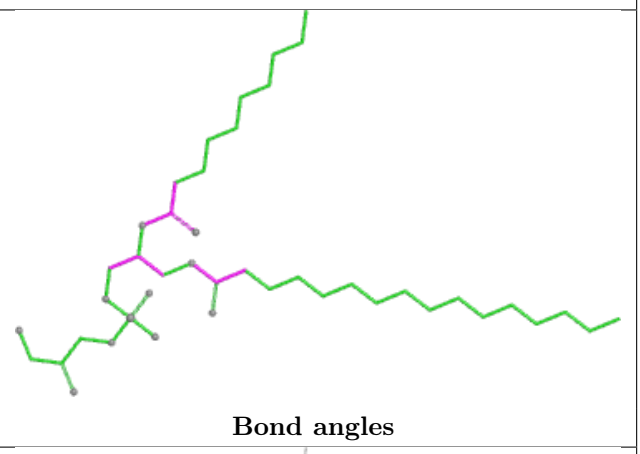


Rings

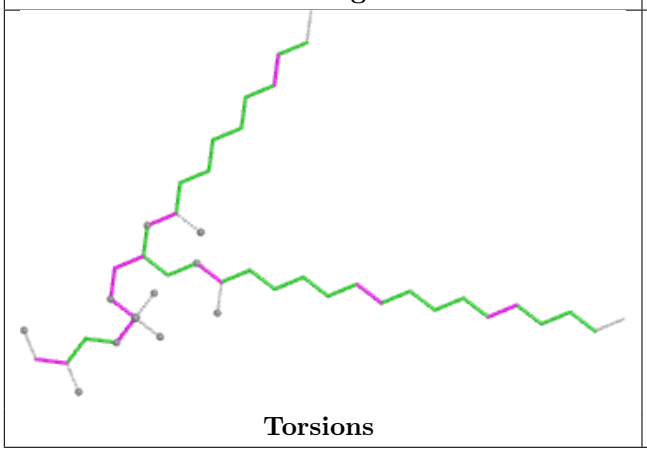
Ligand LHG n 619



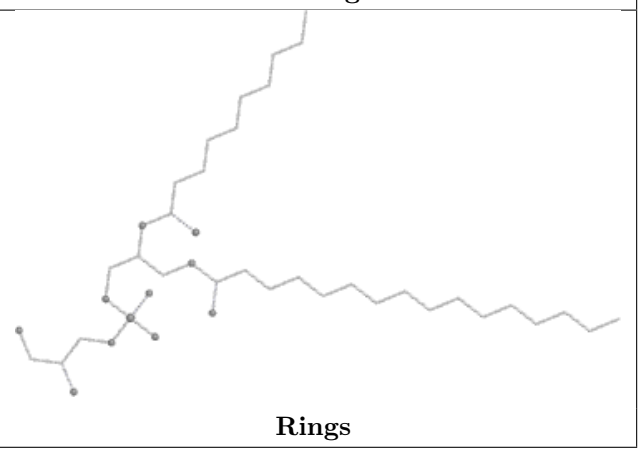
Bond lengths



Bond angles

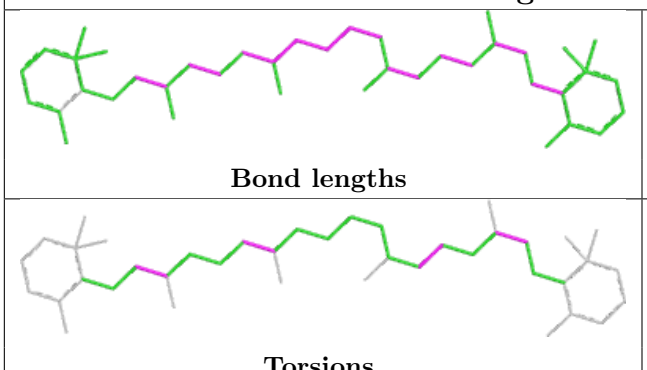


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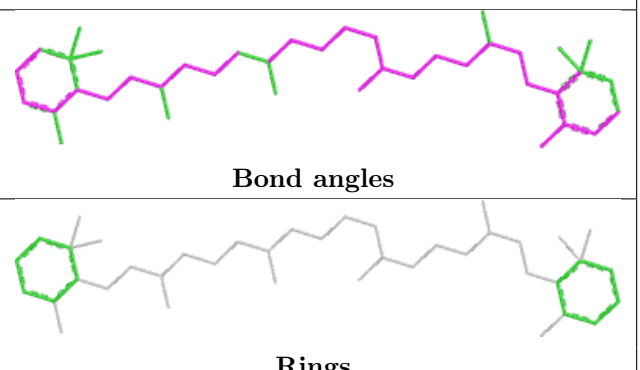


Rings

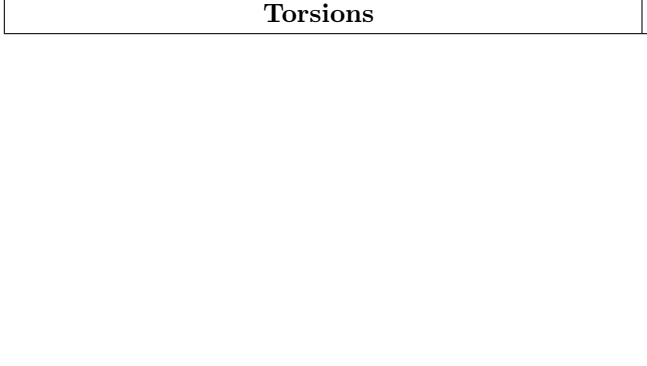
Ligand WVN B 848



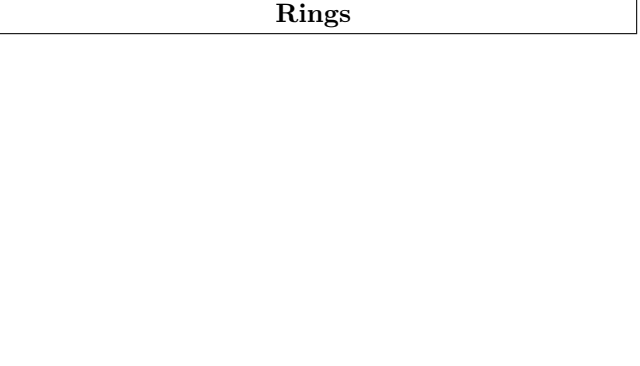
Bond lengths



Bond angles

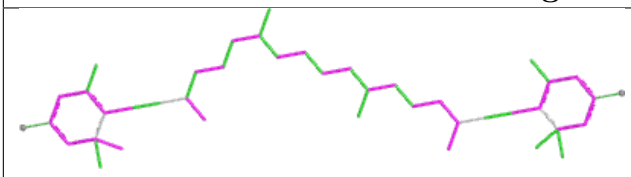


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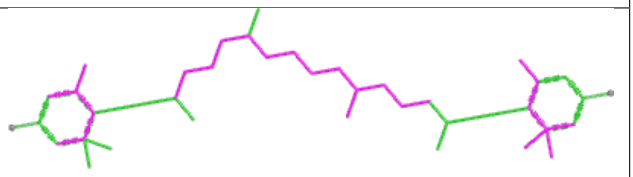


Rings

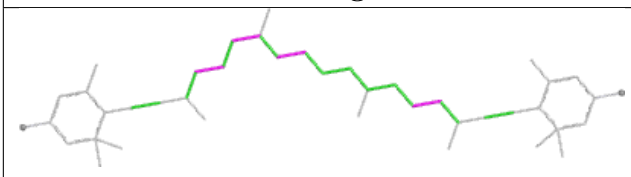
Ligand II0 h 312



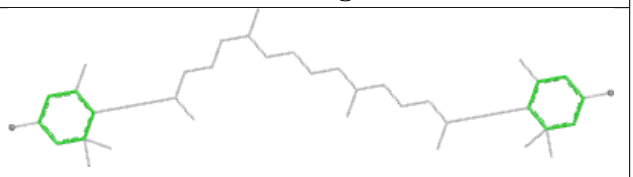
Bond lengths



Bond angles

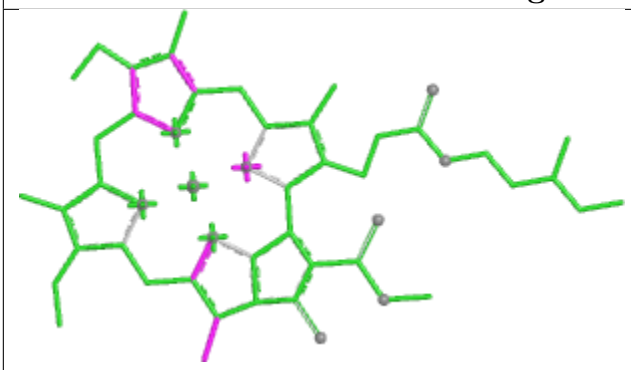


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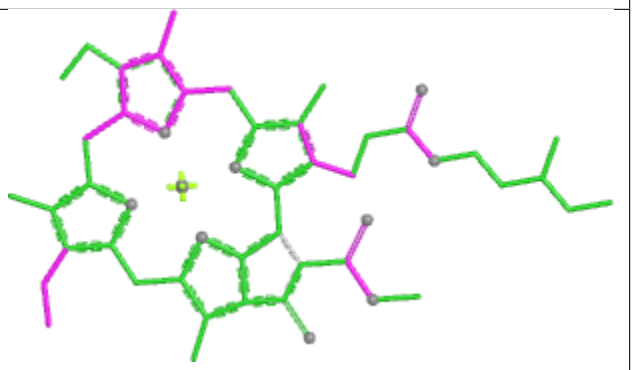


Rings

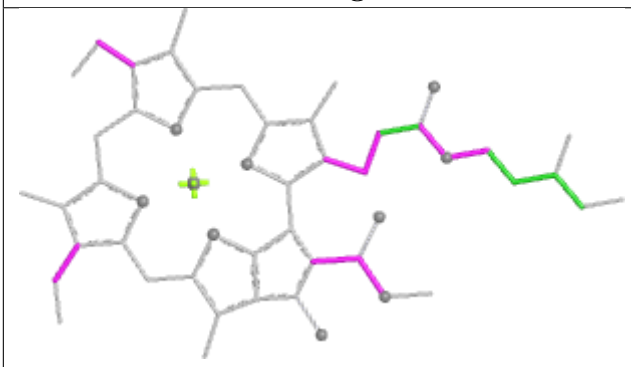
Ligand CLA k 313



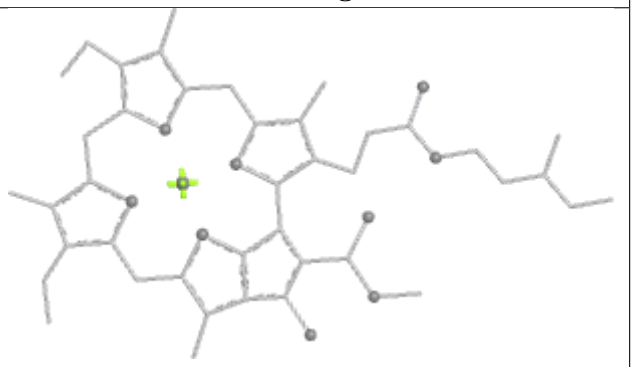
Bond lengths



Bond angles

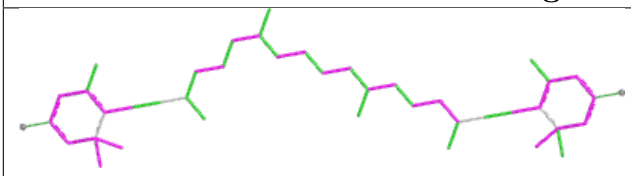


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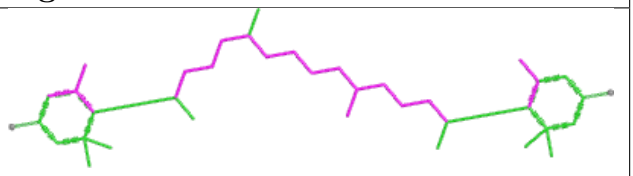


Rings

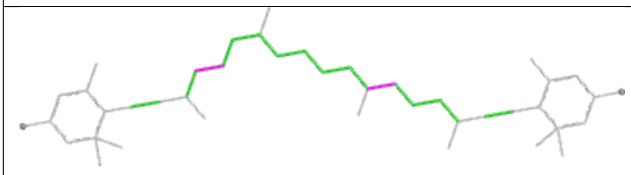
Ligand II0 g 317



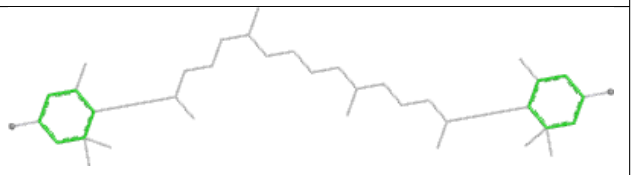
Bond lengths



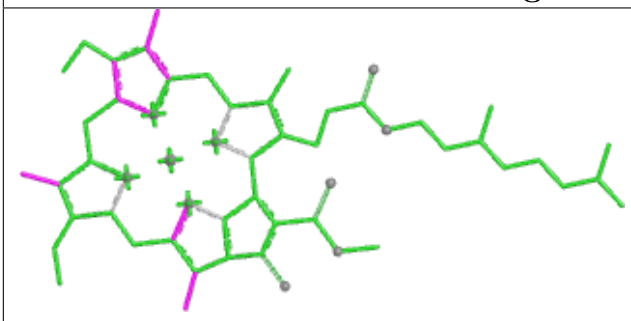
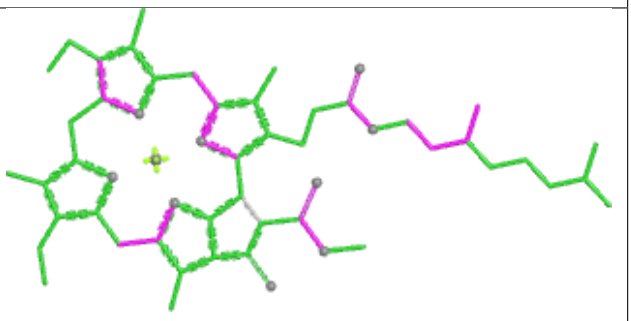
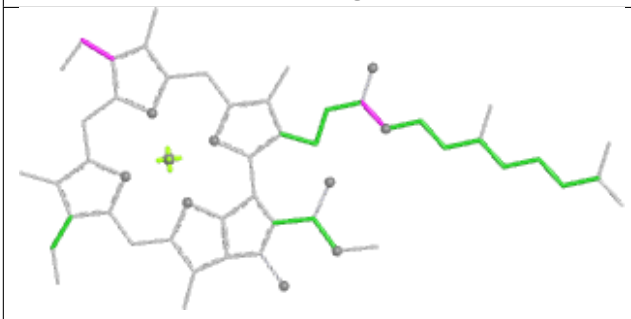
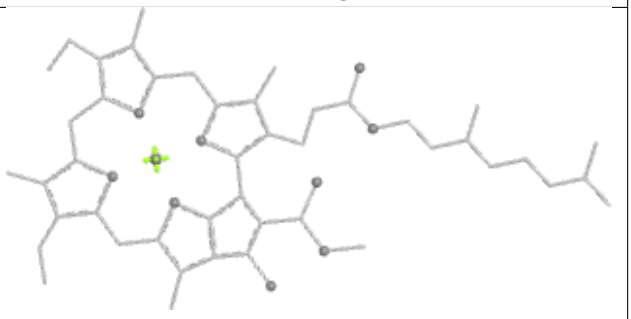
Bond angles

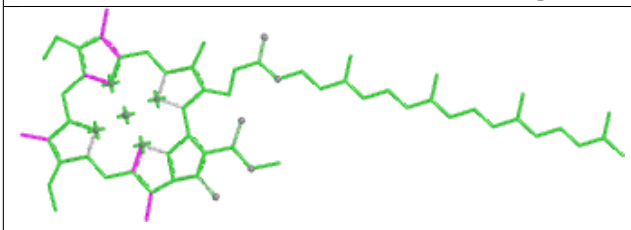
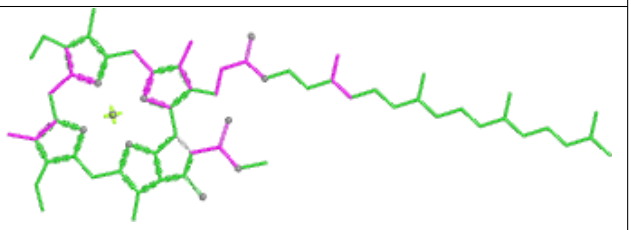
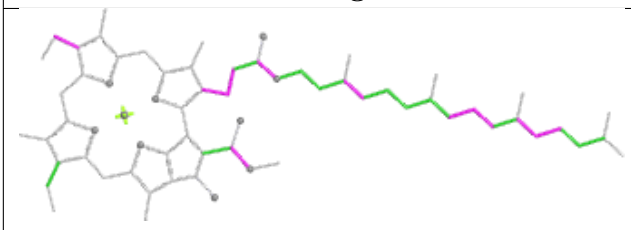
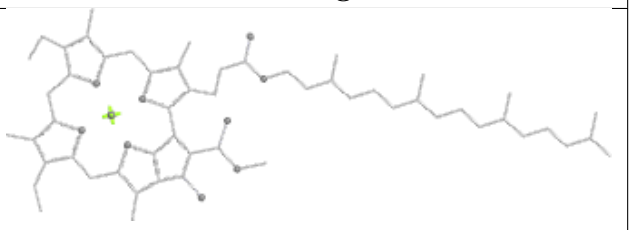


Torsions

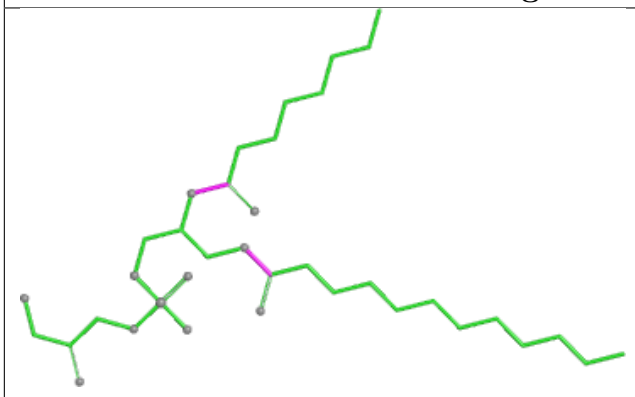


Rings

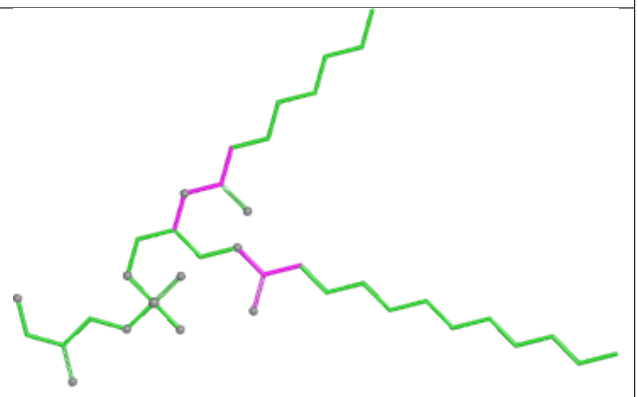
Ligand CLA A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

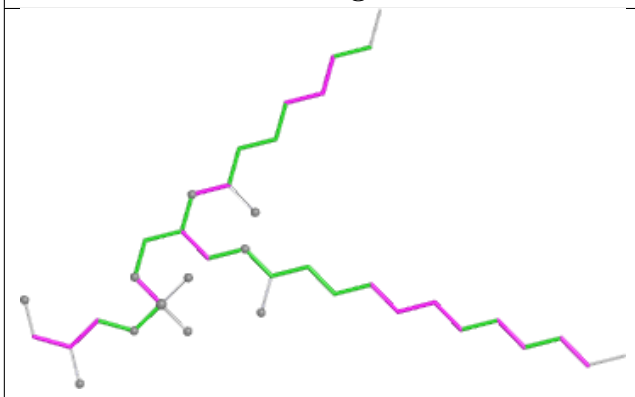
Ligand LHG m 617



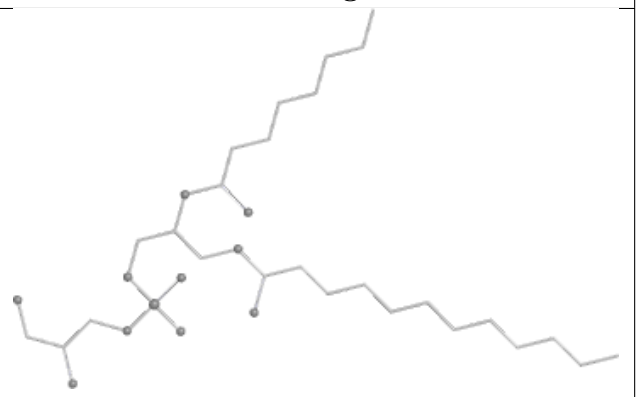
Bond lengths



Bond angles

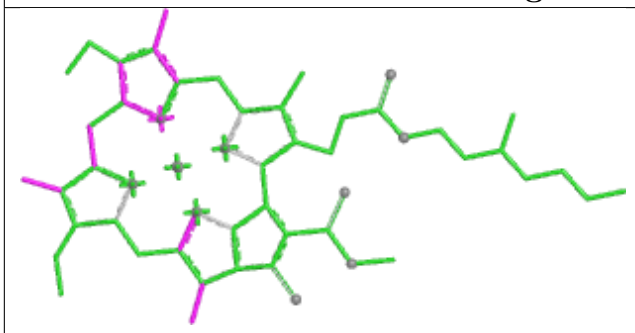


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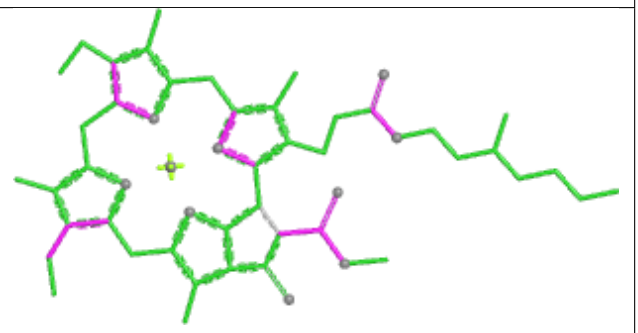


Rings

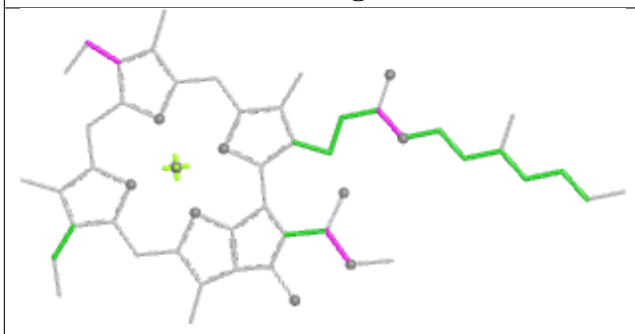
Ligand CLA B 819



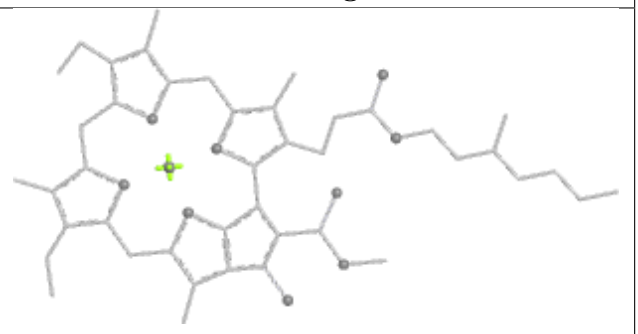
Bond lengths



Bond angles

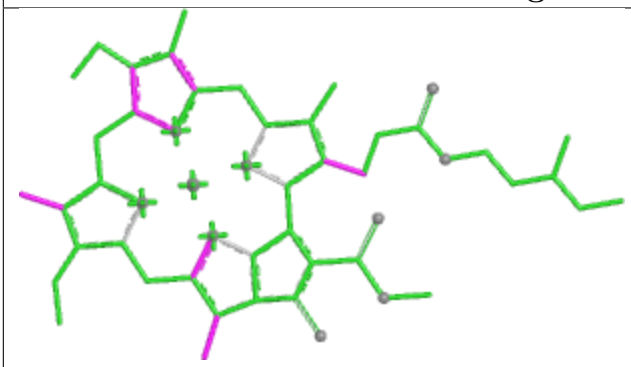


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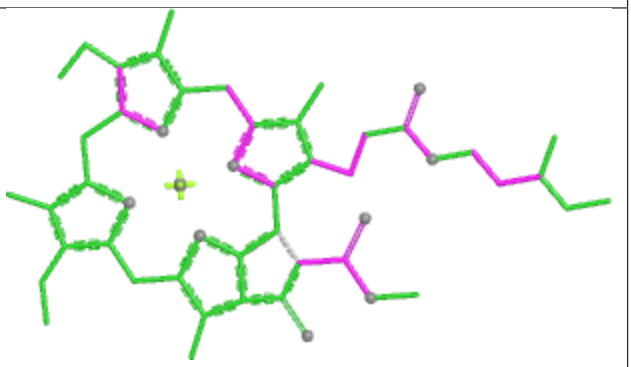


Rings

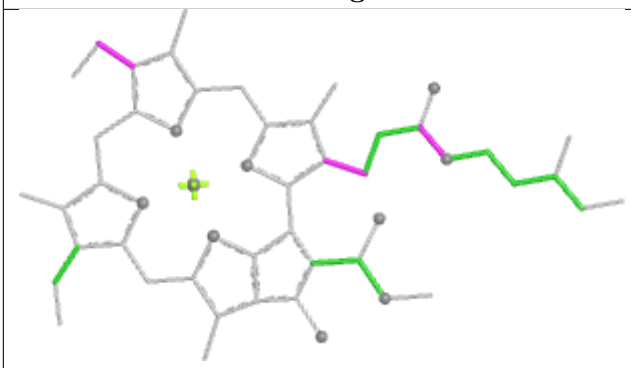
Ligand CLA n 606



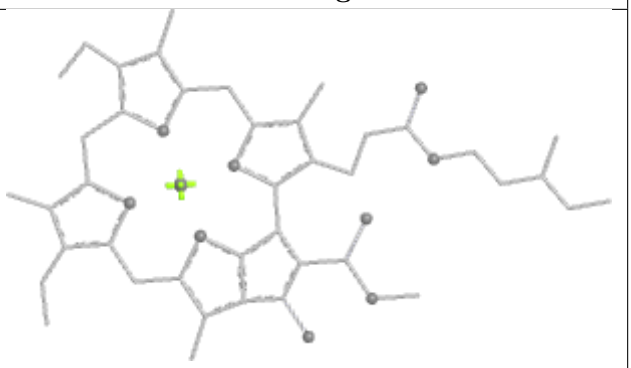
Bond lengths



Bond angles

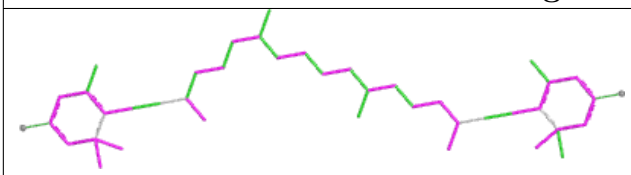


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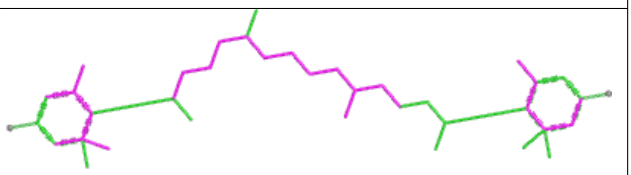


Rings

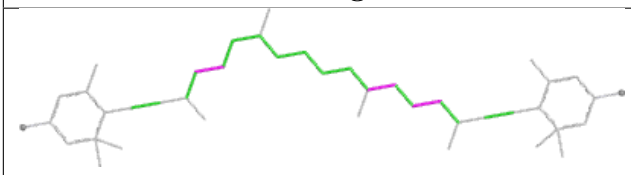
Ligand II0 a 315



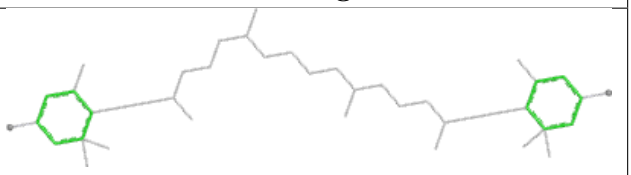
Bond lengths



Bond angles

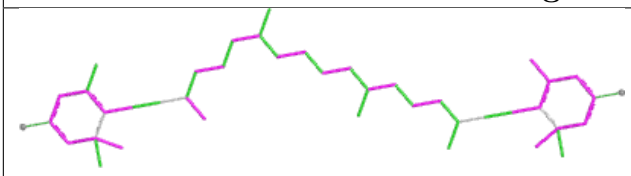


Torsions

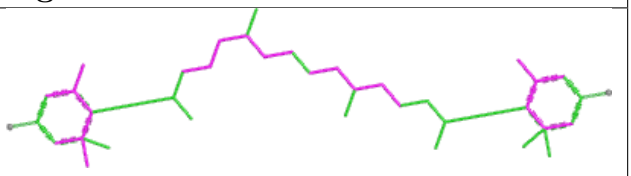


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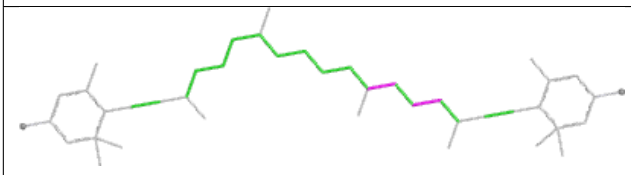
Ligand II0 g 320



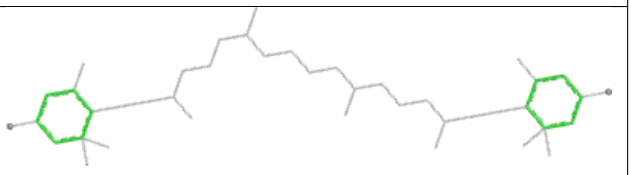
Bond lengths



Bond angles

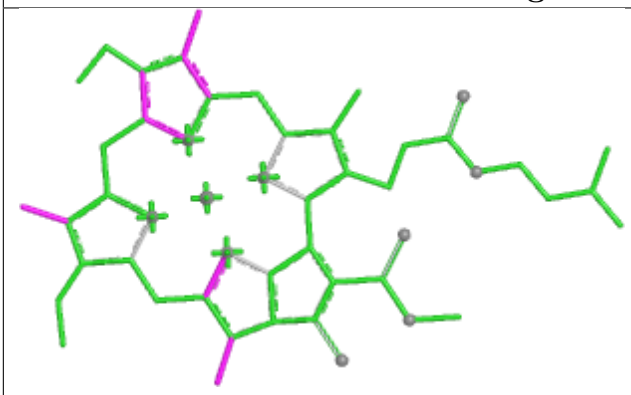


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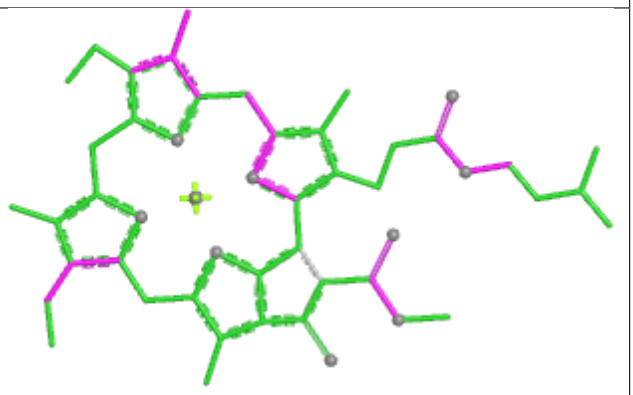


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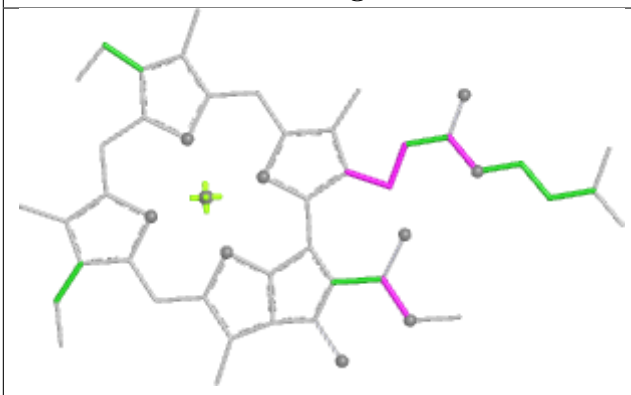
Ligand CLA h 302



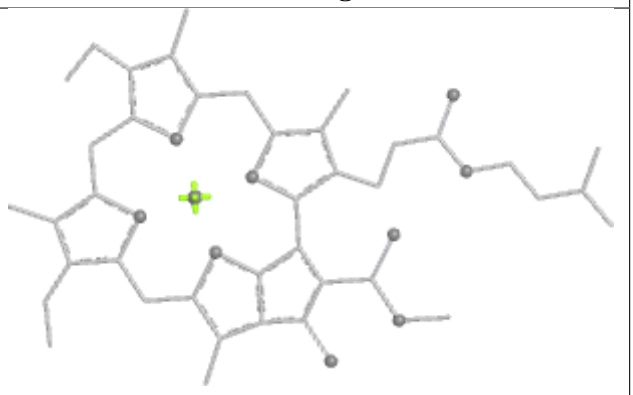
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Bond angles

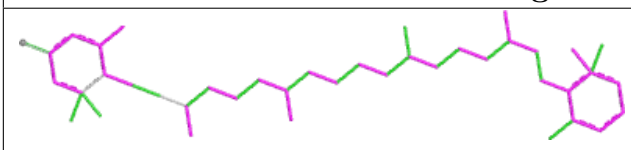


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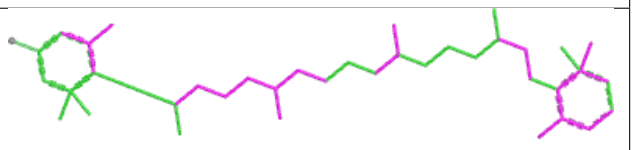


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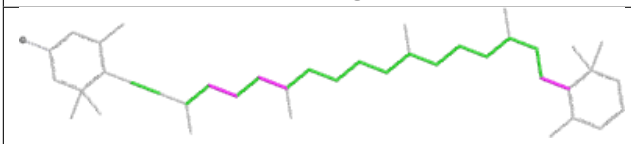
Ligand IHT b 614



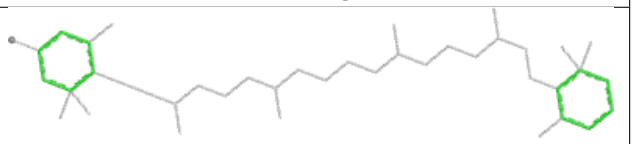
Bond lengths



Bond angles

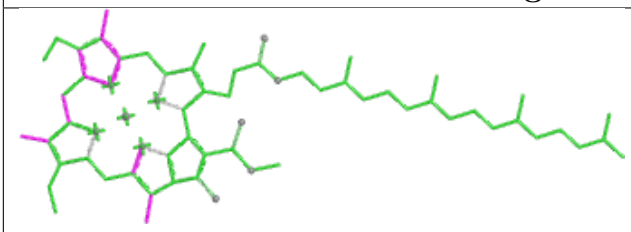


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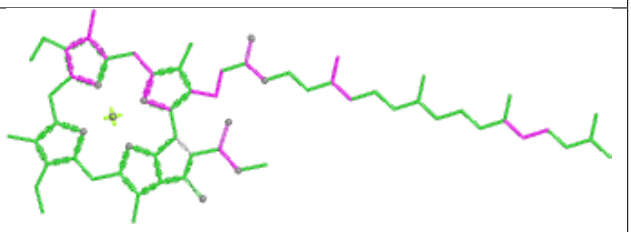


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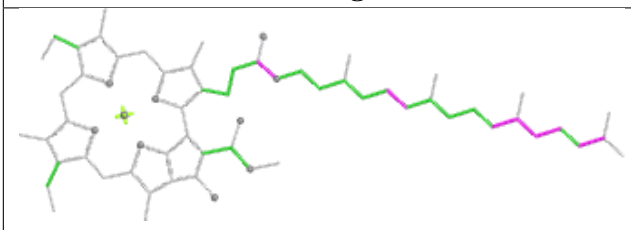
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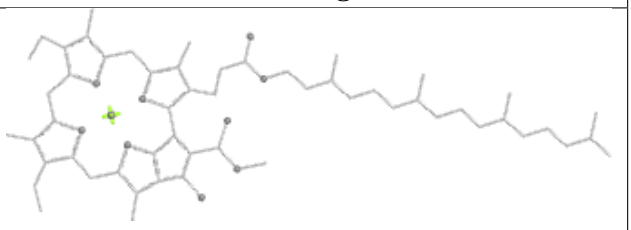
Bond lengths



Bond angles

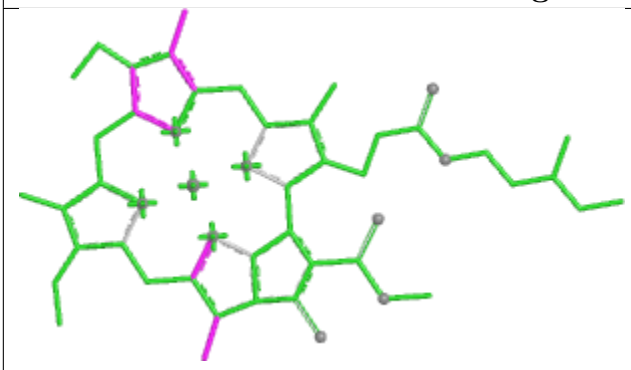


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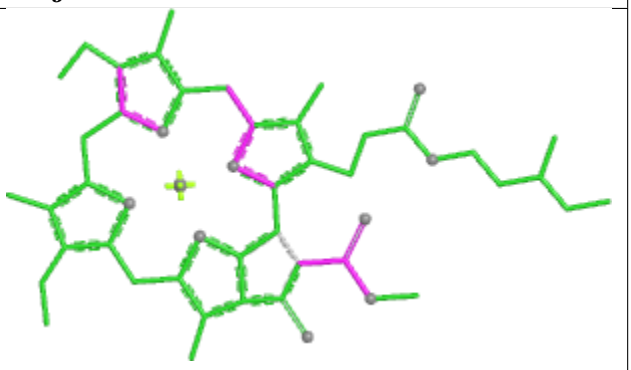


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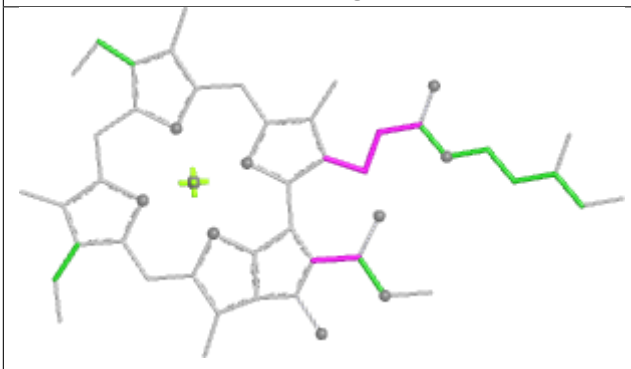
Ligand CLA j 601



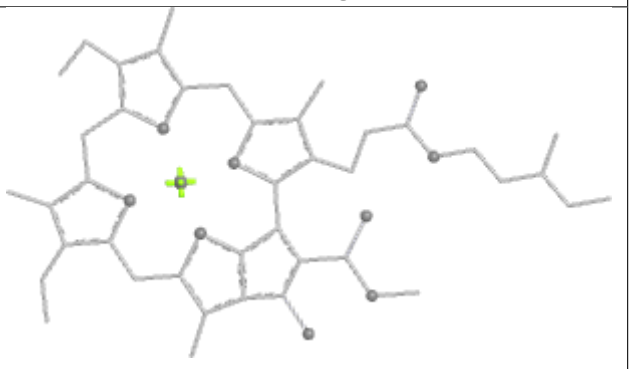
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Bond angles

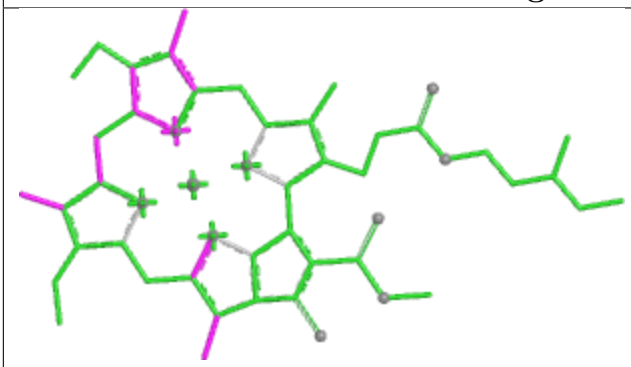


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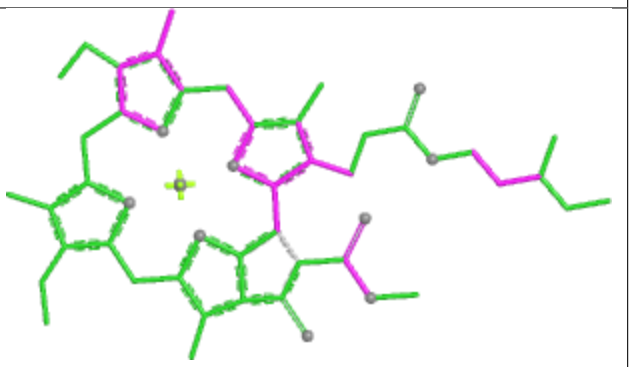


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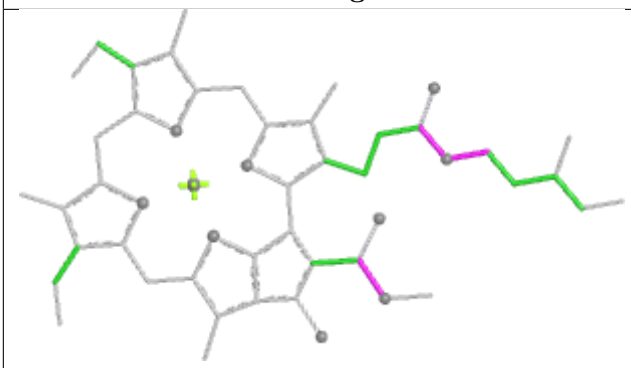
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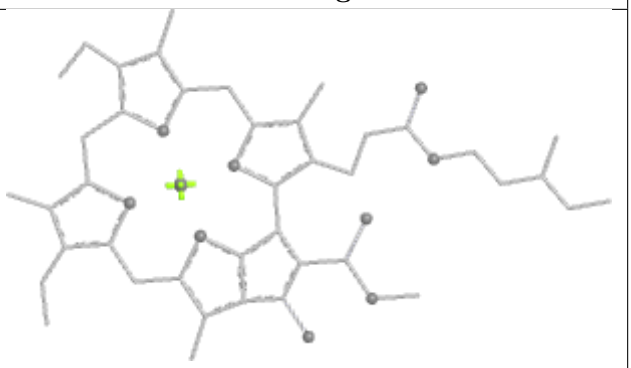
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Bond angles

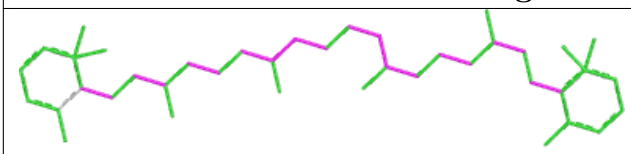


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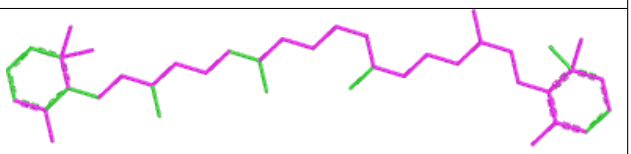


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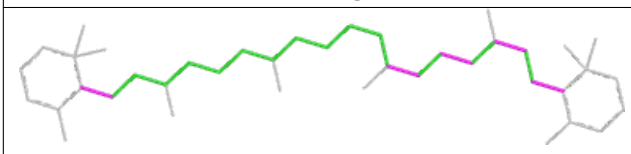
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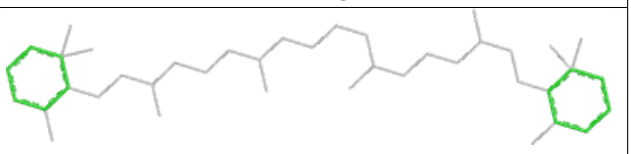
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Bond angles

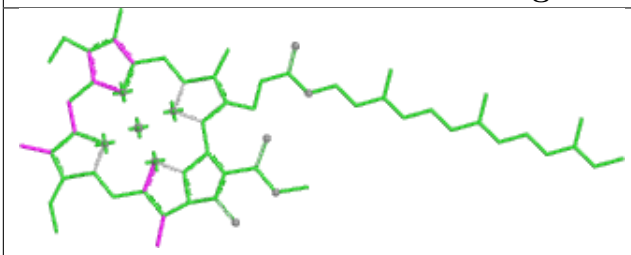


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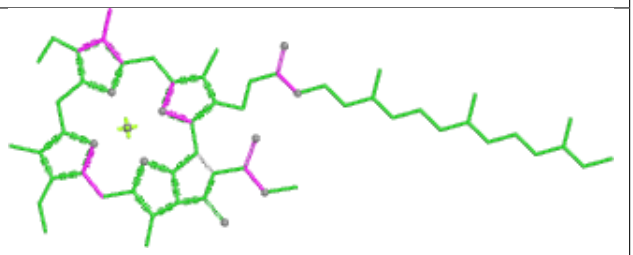


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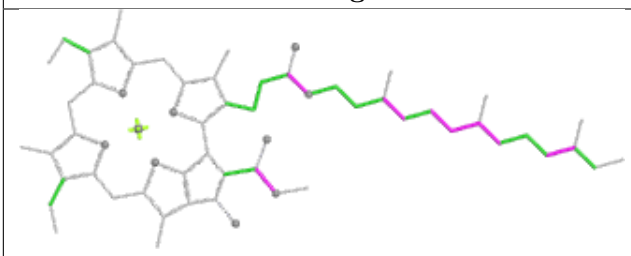
Ligand CLA i 307



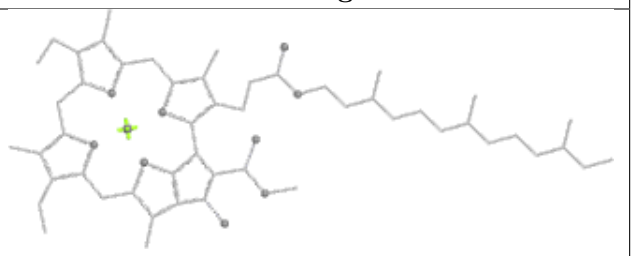
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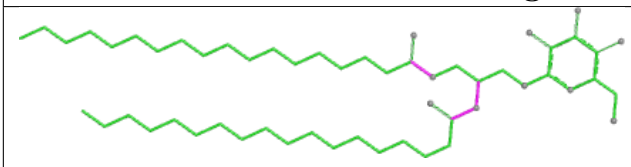


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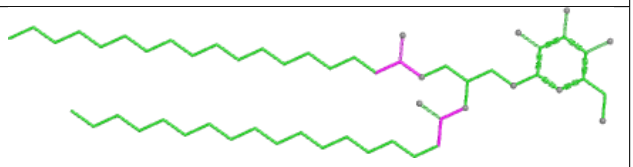


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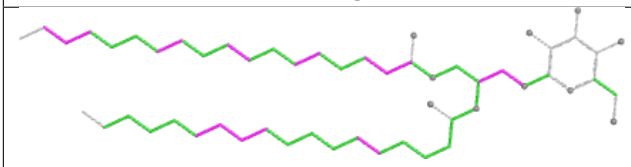
Ligand LMG J 106



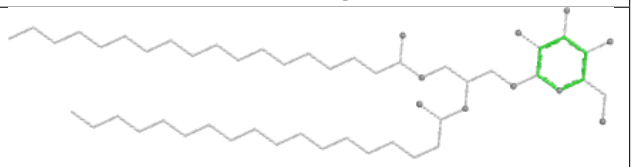
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Bond angles

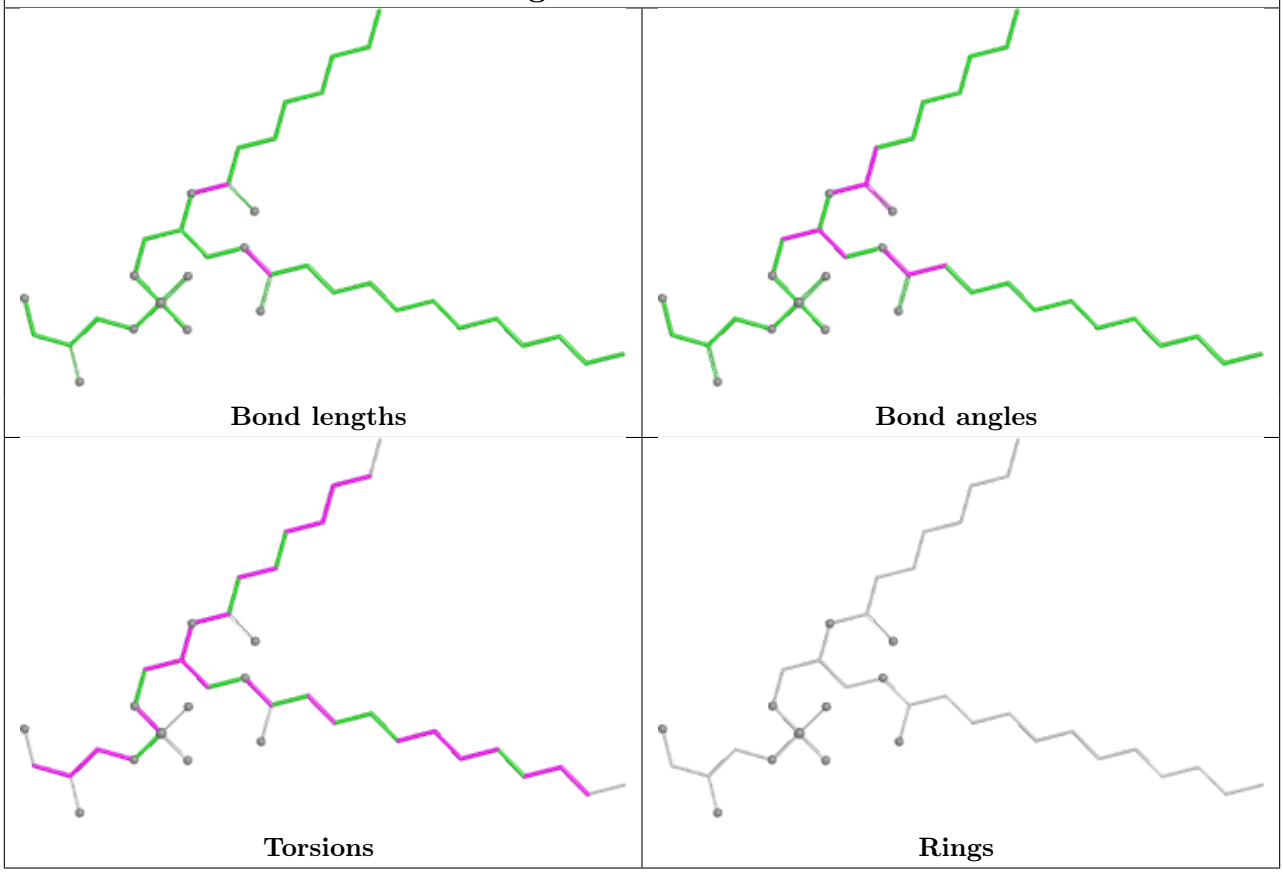


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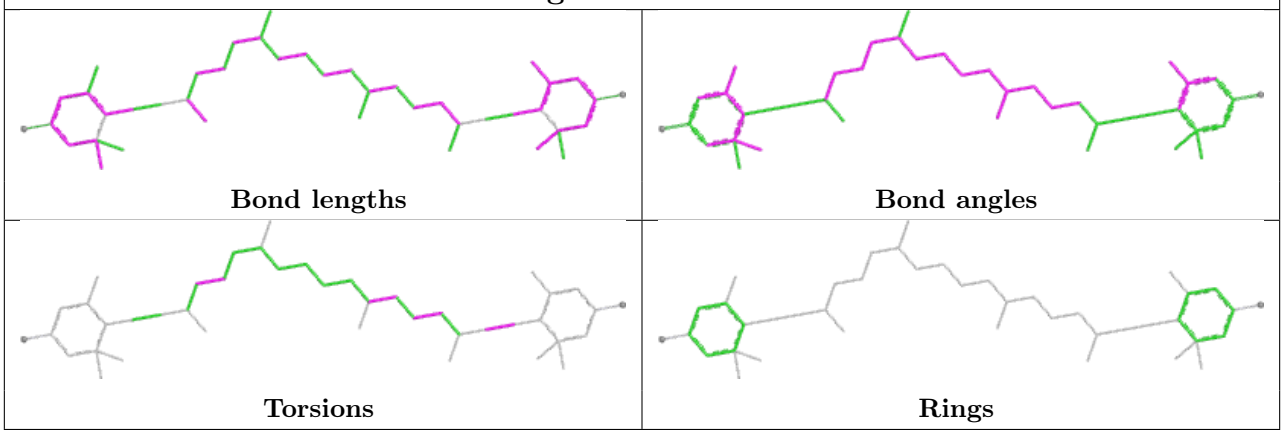


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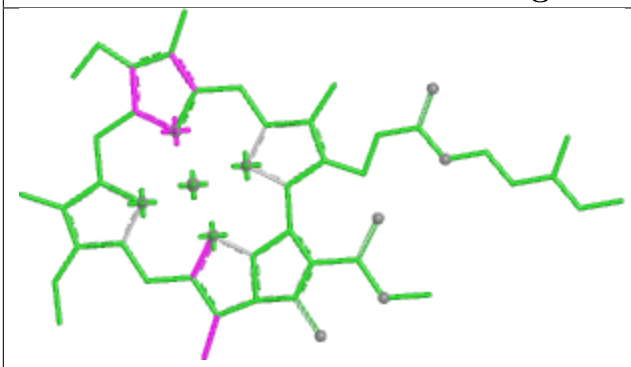
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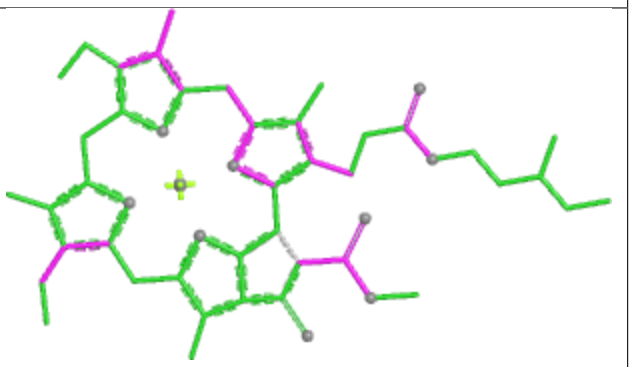
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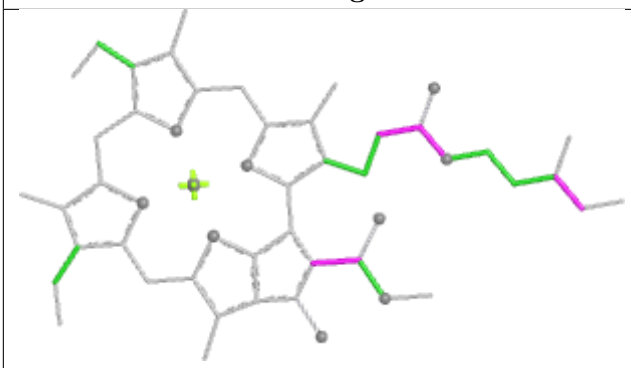
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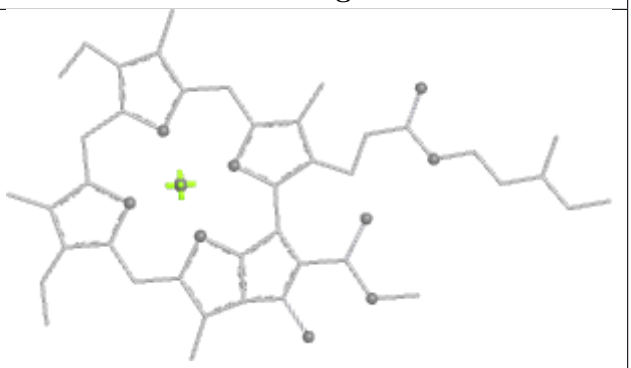
Bond lengths



Bond angles

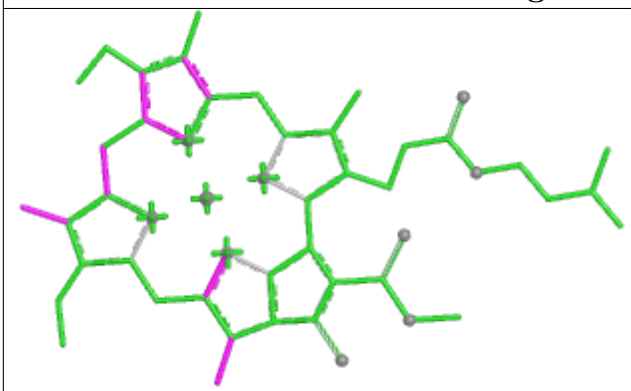


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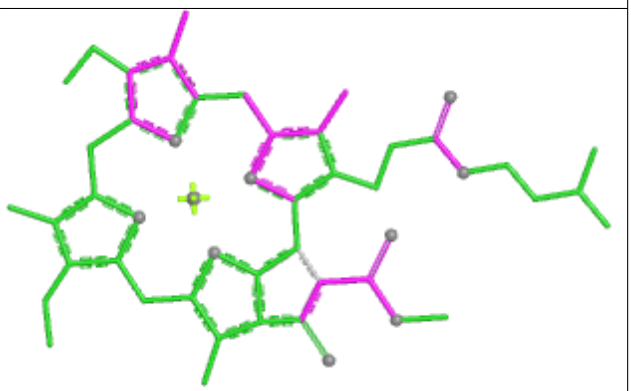


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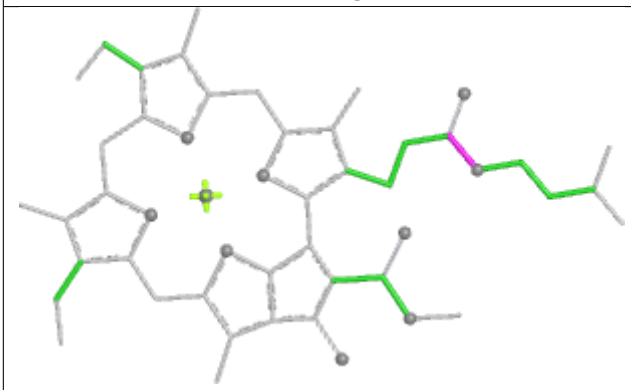
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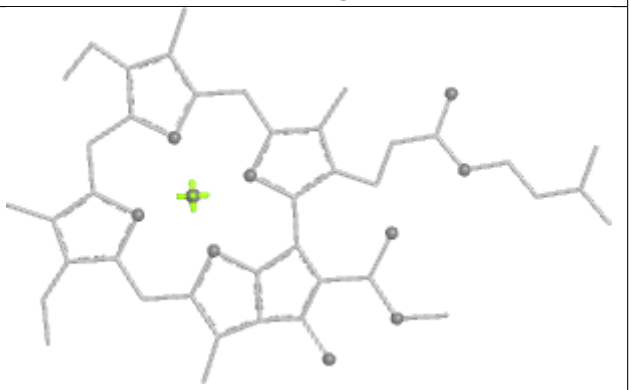
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Bond angles

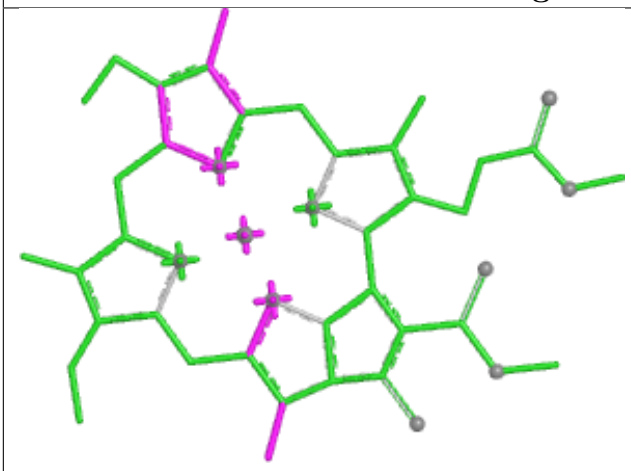


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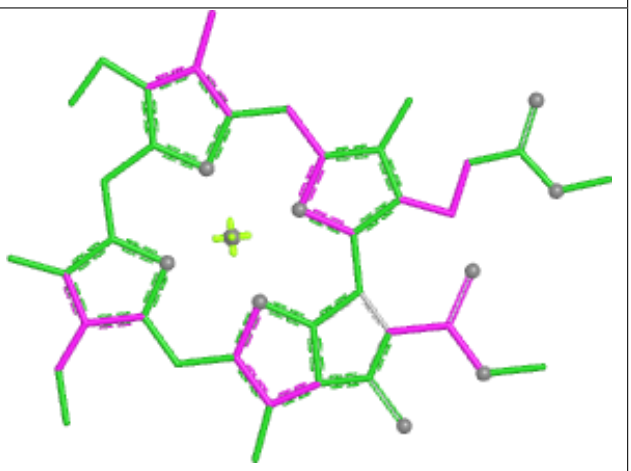


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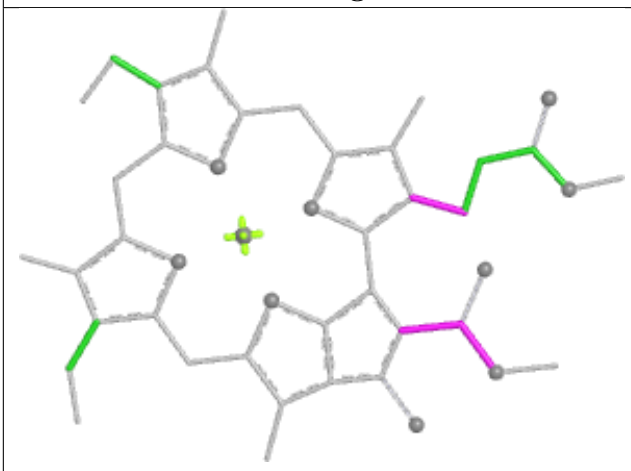
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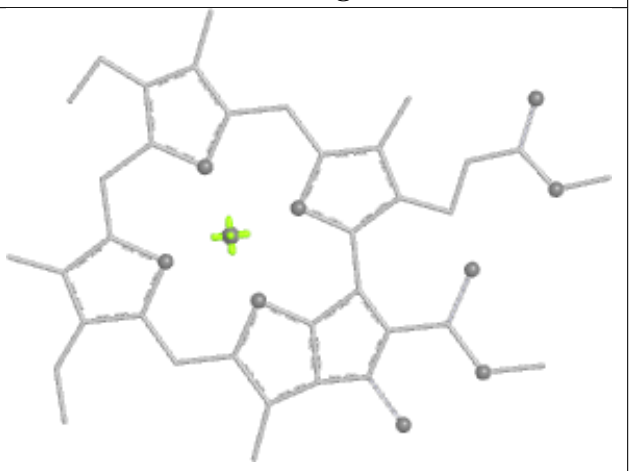
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Bond angles

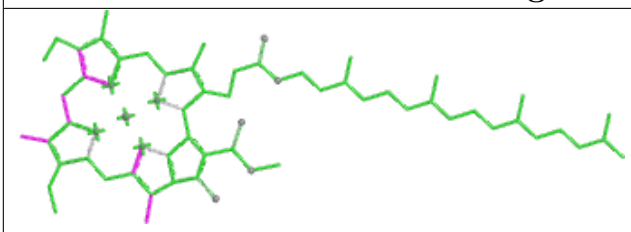


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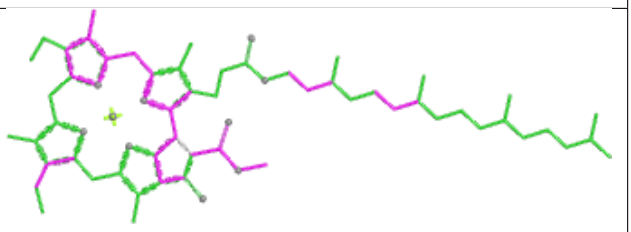


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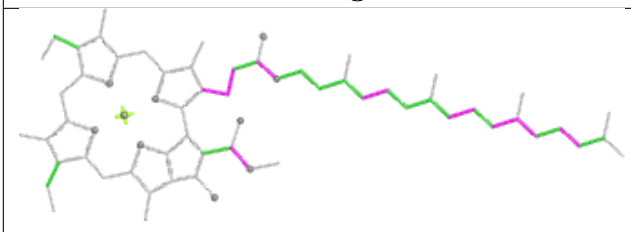
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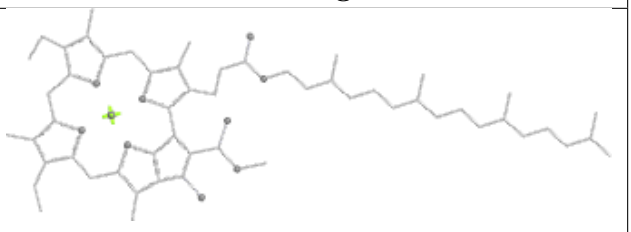
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Bond angles

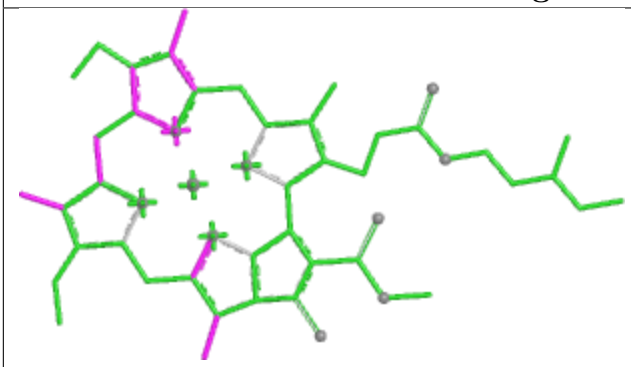


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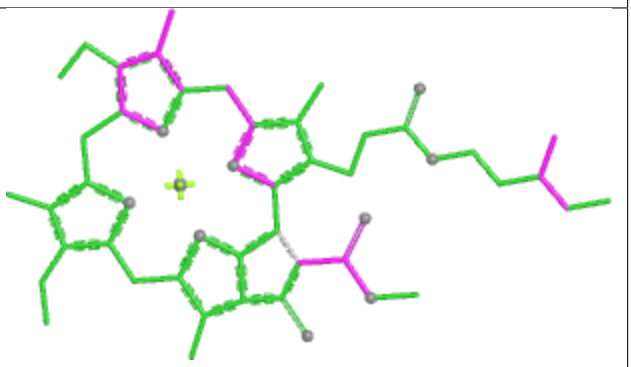


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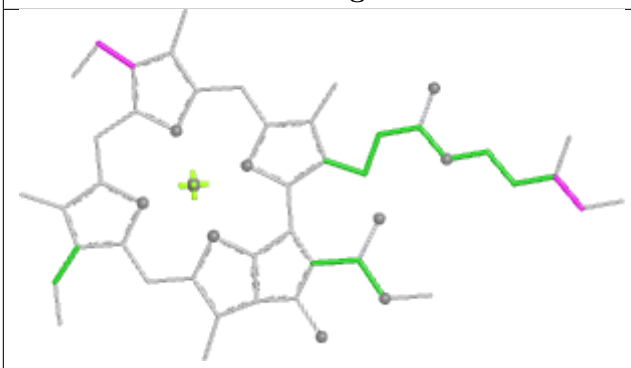
Ligand CLA l 305



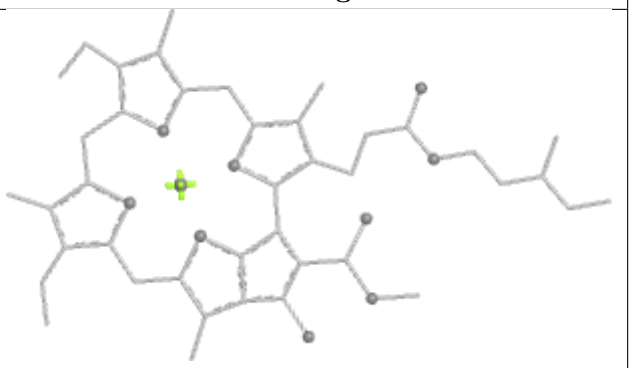
Bond lengths



Bond angles

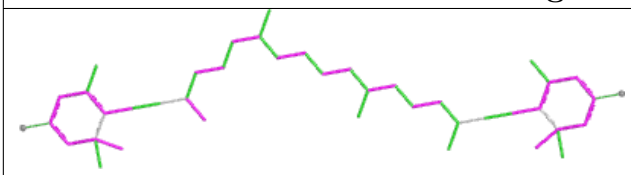


Torsions

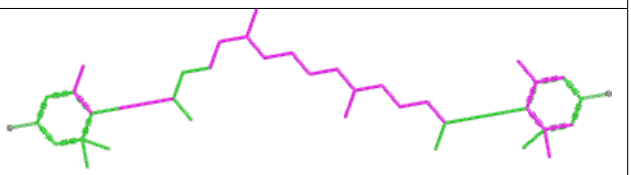


Rings

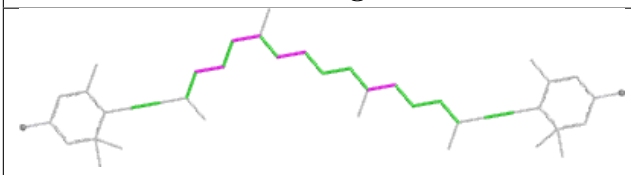
Ligand II0 l 302



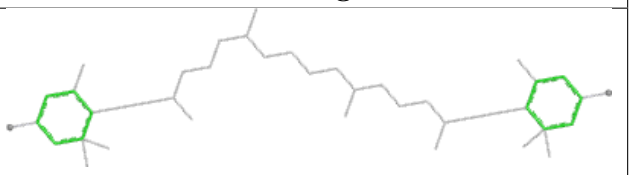
Bond lengths



Bond angles

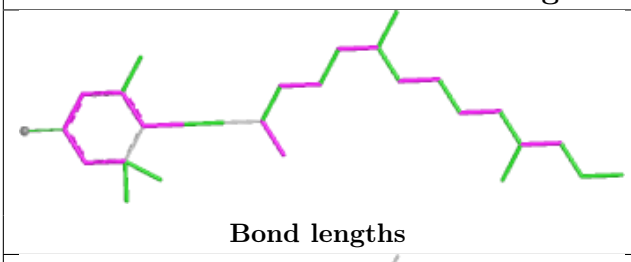


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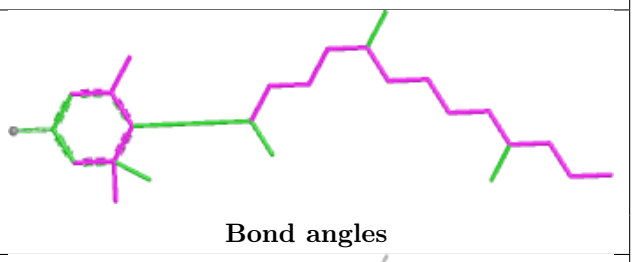


Rings

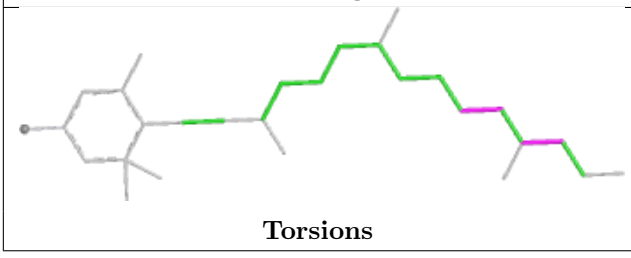
Ligand II0 h 310



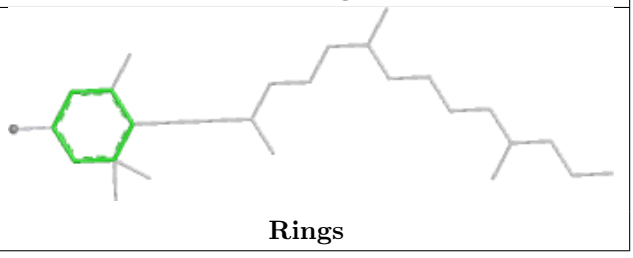
Bond lengths



Bond angles

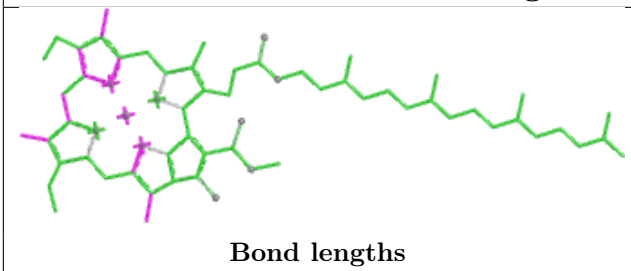


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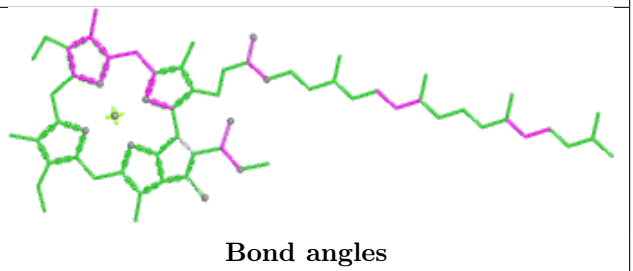


Rings

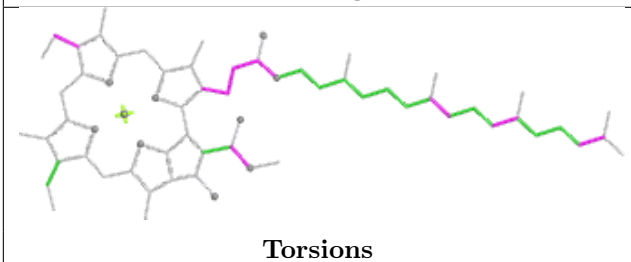
Ligand CLA A 817



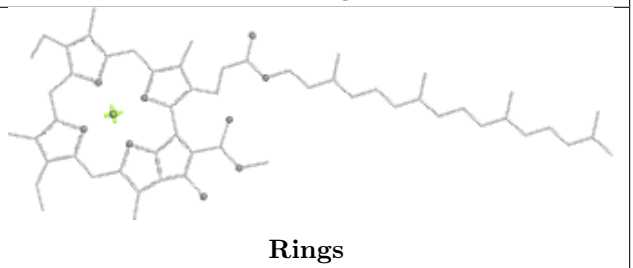
Bond lengths



Bond angles

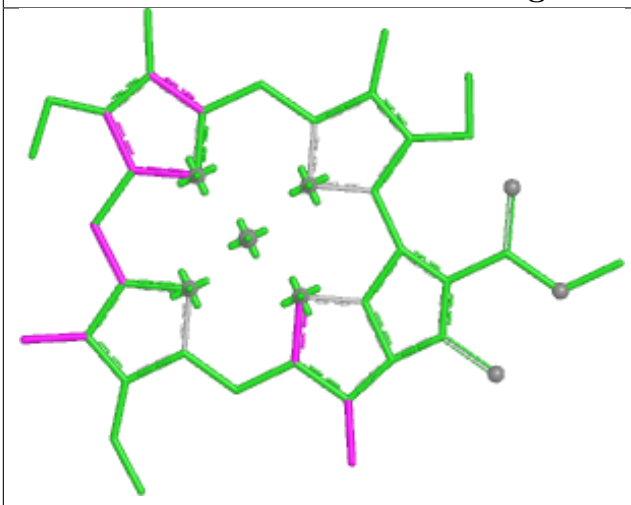


Torsions

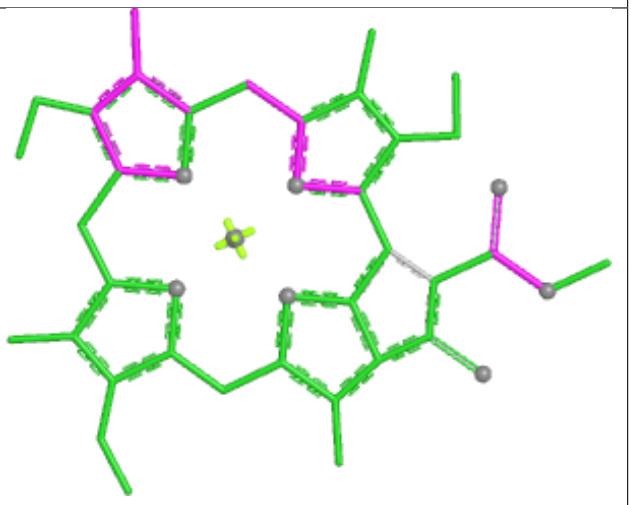


Rings

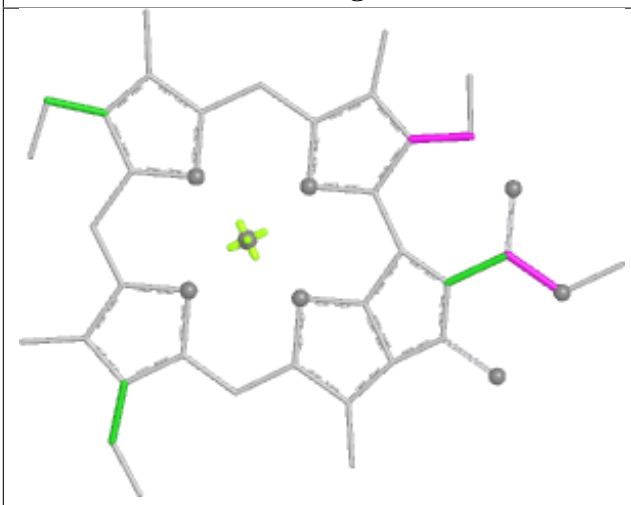
Ligand CLA J 103



Bond lengths



Bond angles

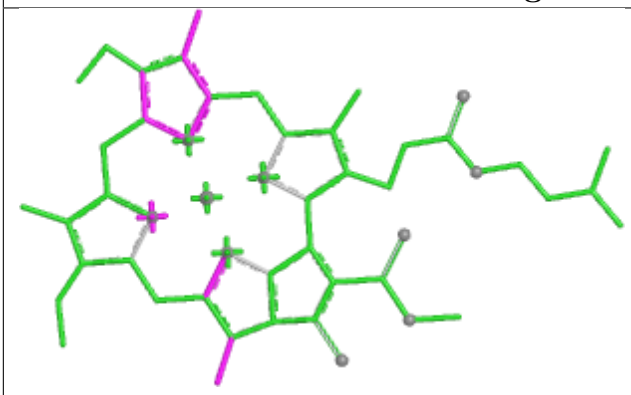


Torsions

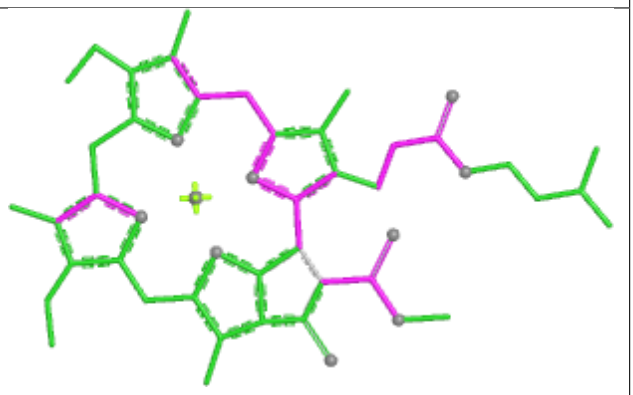


Rings

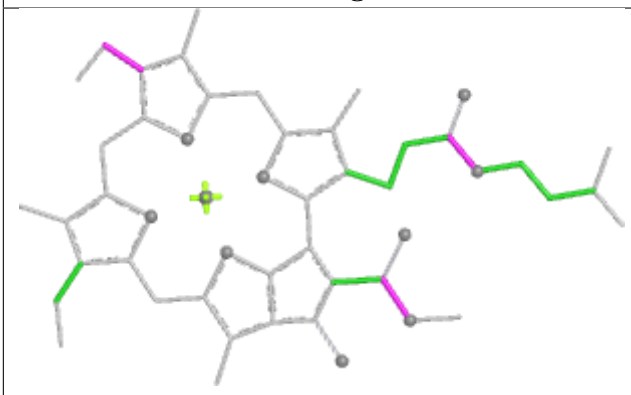
Ligand CLA B 828



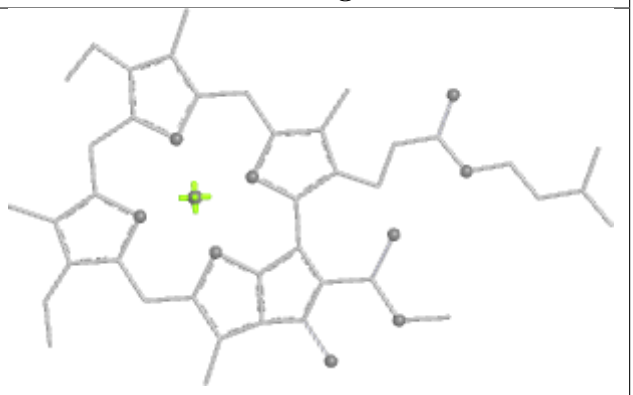
Bond lengths



Bond angles

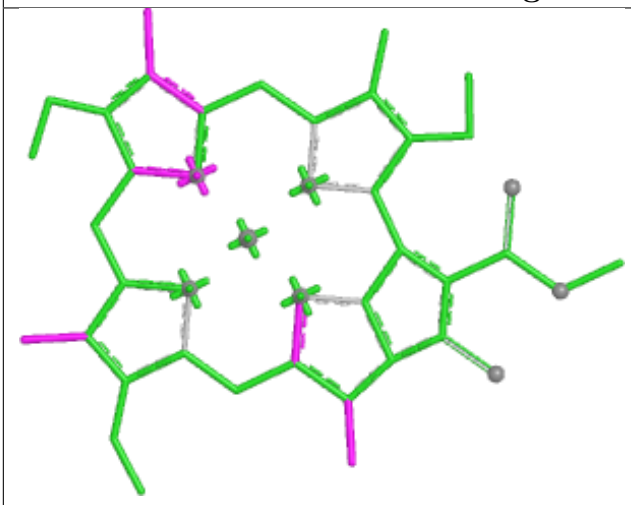


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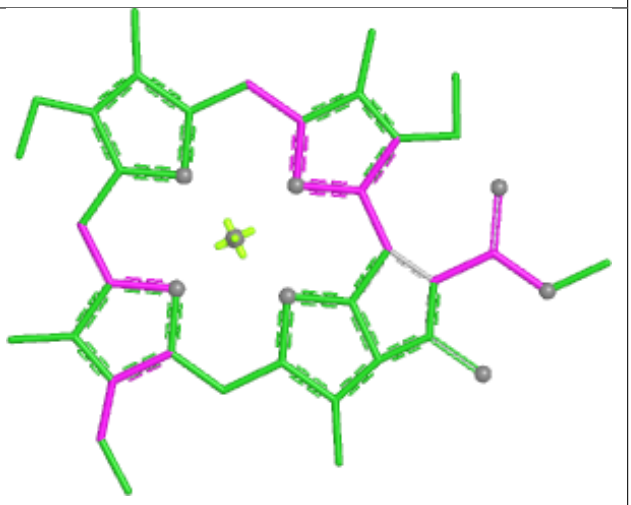


Rings

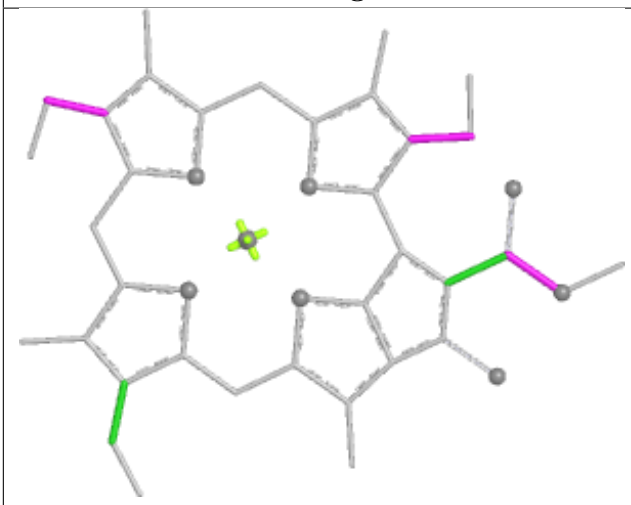
Ligand CLA K 102



Bond lengths



Bond angles

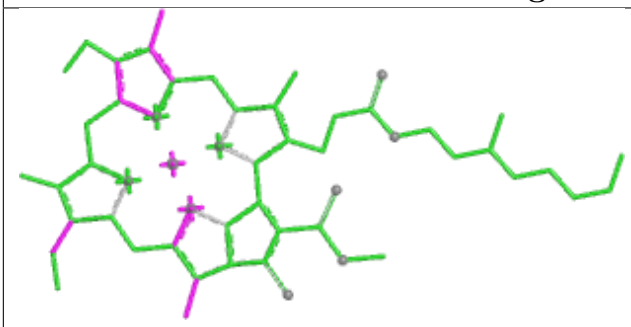


Torsions

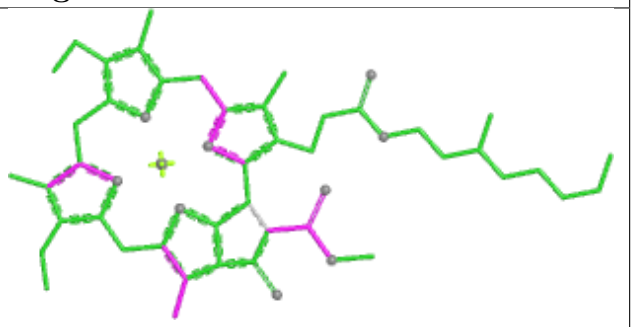


Rings

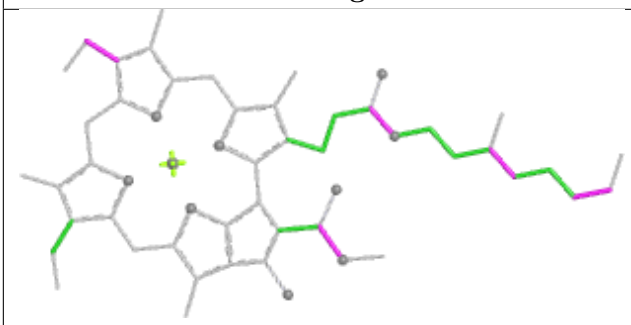
Ligand CLA g 311



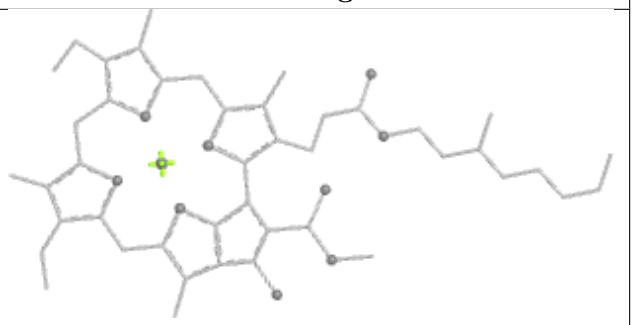
Bond lengths



Bond angles

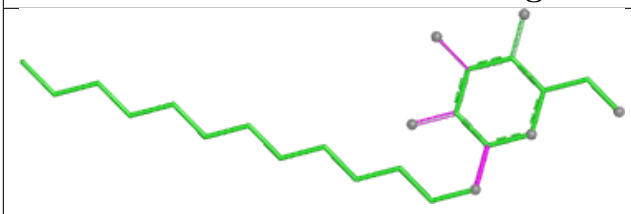


Torsions

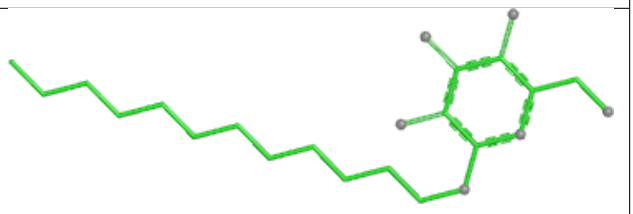


Rings

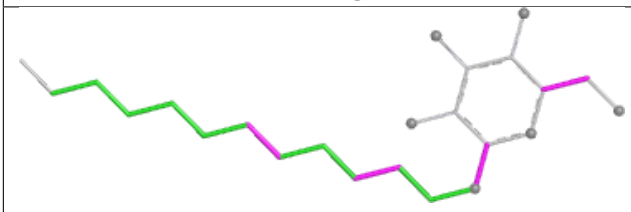
Ligand LMT a 302



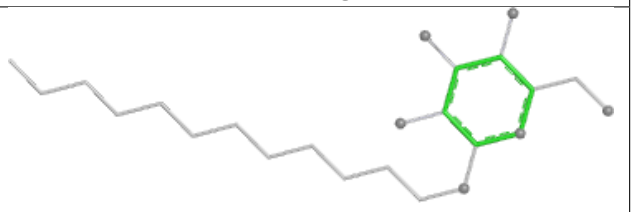
Bond lengths



Bond angles

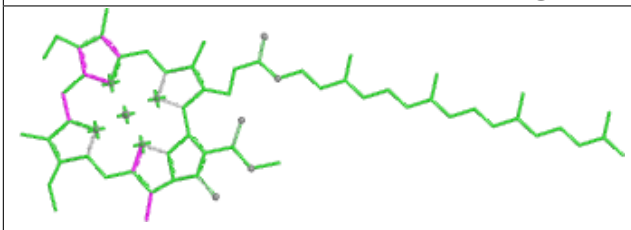


Torsions

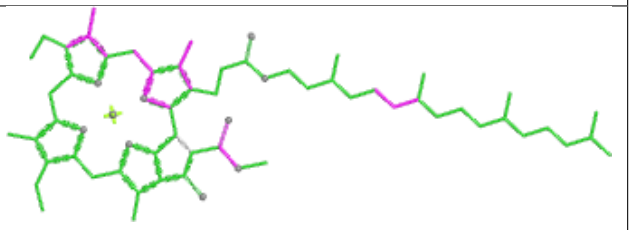


Rings

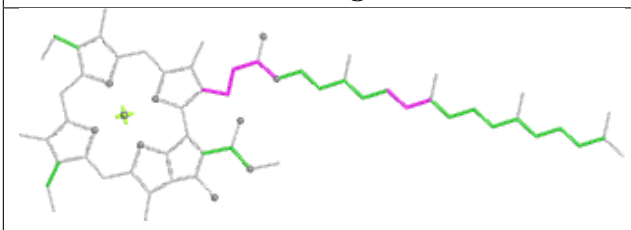
Ligand CLA l 308



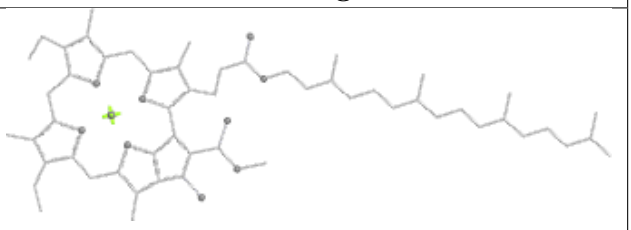
Bond lengths



Bond angles

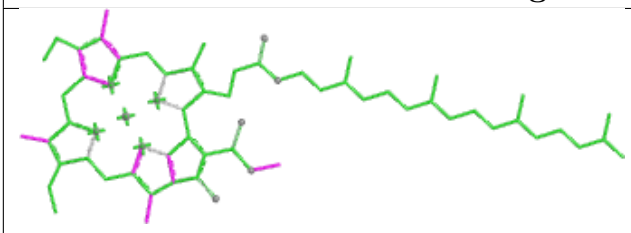


Torsions

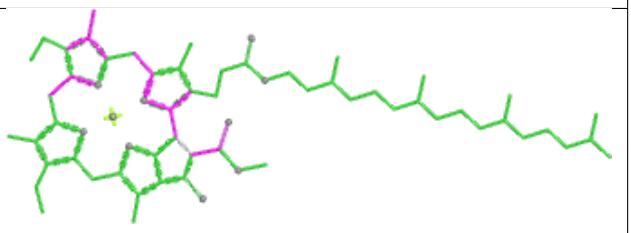


Rings

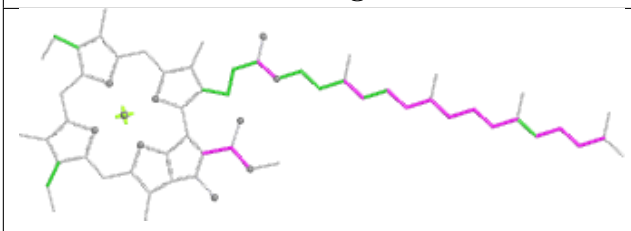
Ligand CLA e 606



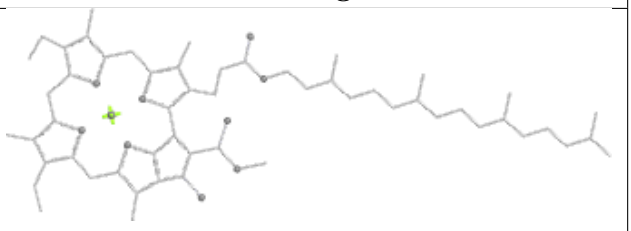
Bond lengths



Bond angles

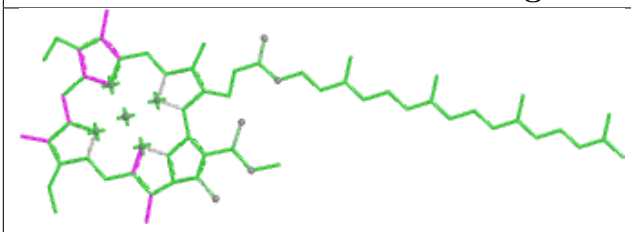


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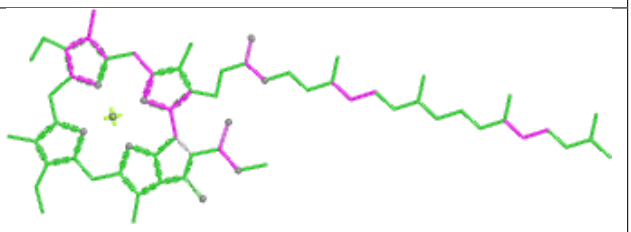


Rings

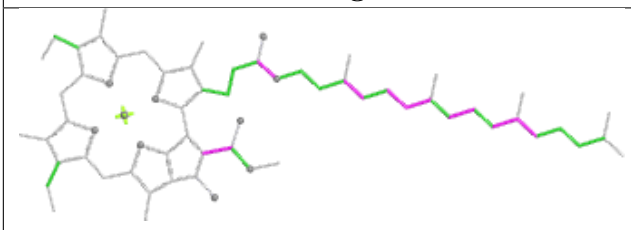
Ligand CLA B 820



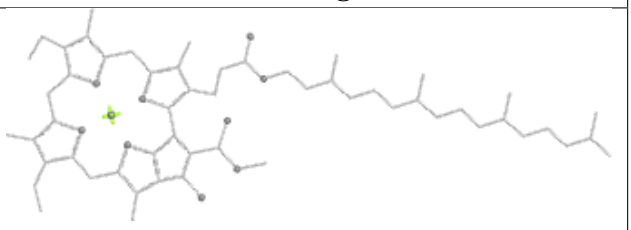
Bond lengths



Bond angles

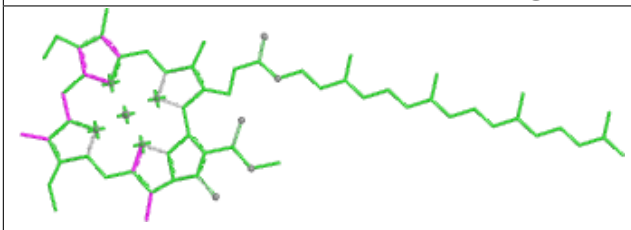


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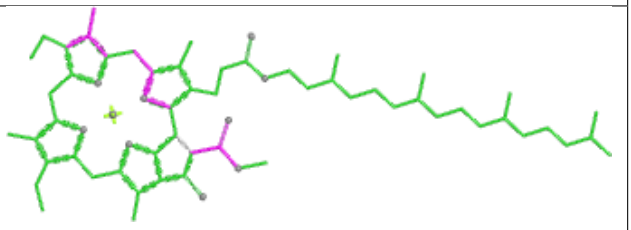


Rings

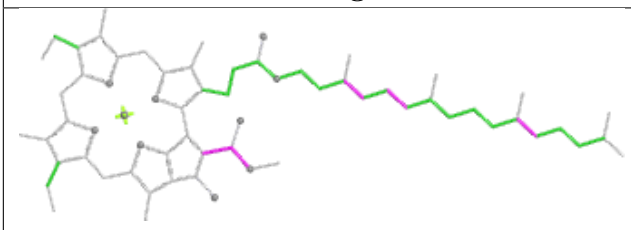
Ligand CLA h 313



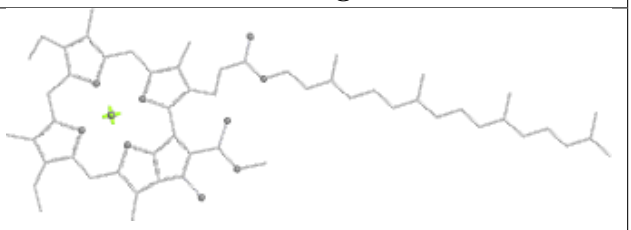
Bond lengths



Bond angles

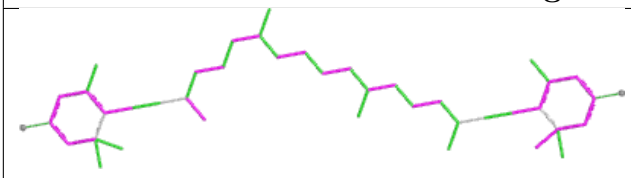


Torsions

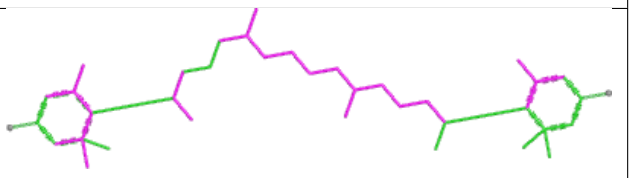


Rings

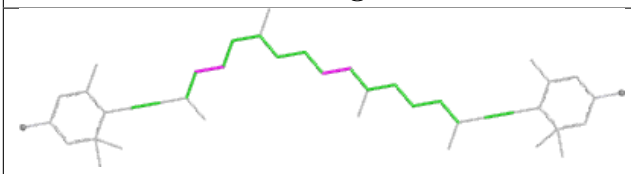
Ligand II0 c 615



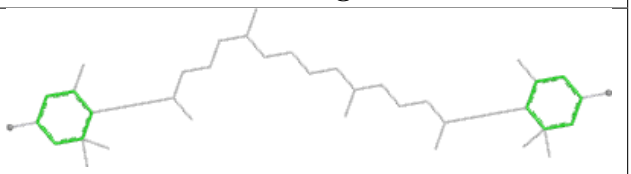
Bond lengths



Bond angles

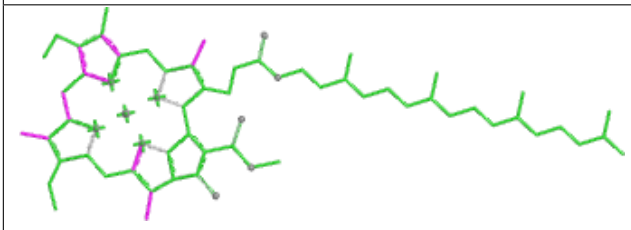


Torsions

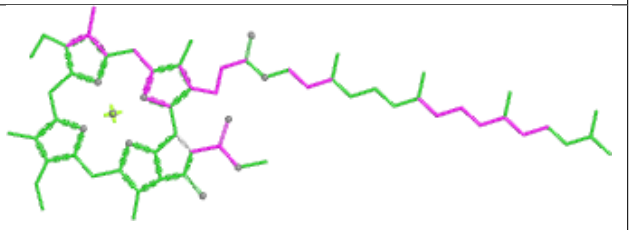


Rings

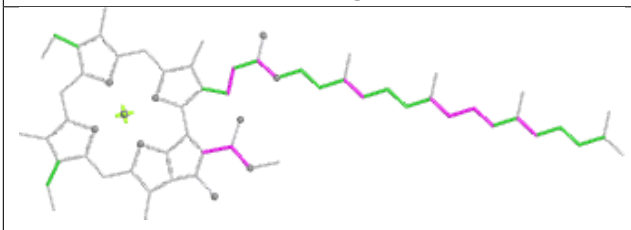
Ligand CLA l 306



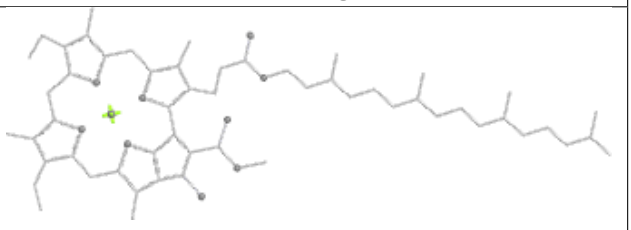
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

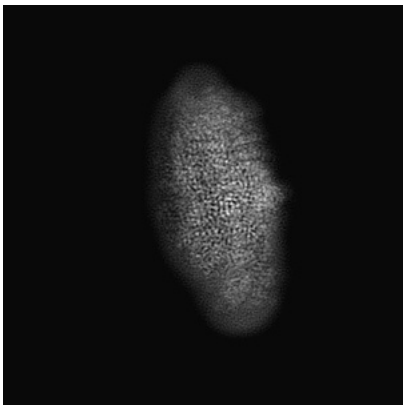
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37659. These allow visual inspection of the internal detail of the map and identification of artifacts.

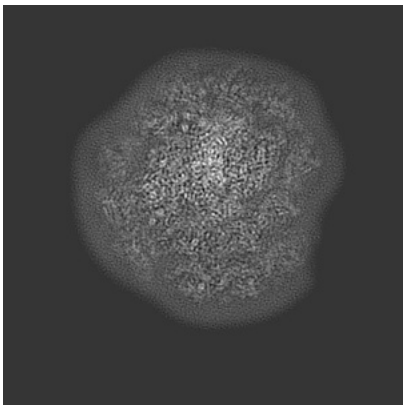
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

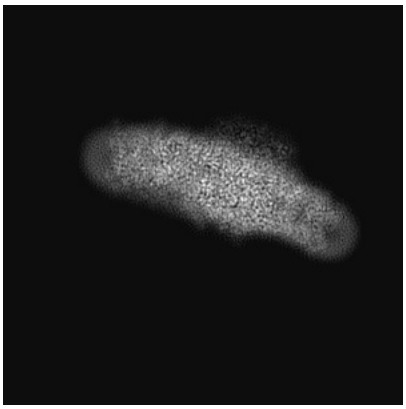
6.1.1 Primary map



X

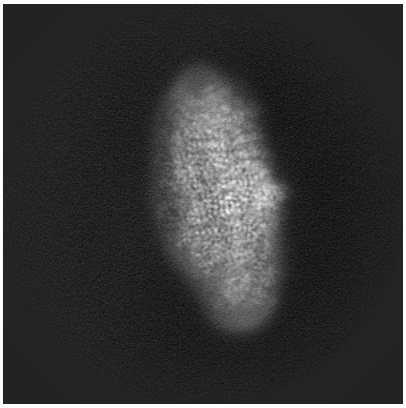


Y

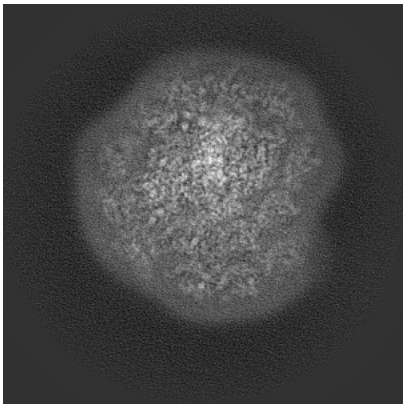


Z

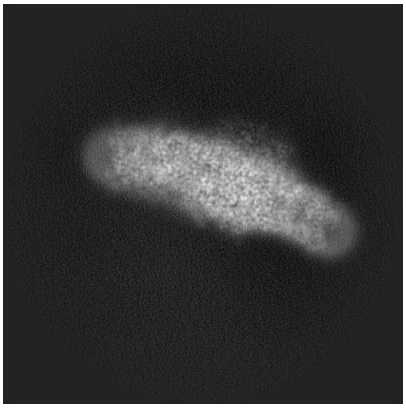
6.1.2 Raw map



X



Y

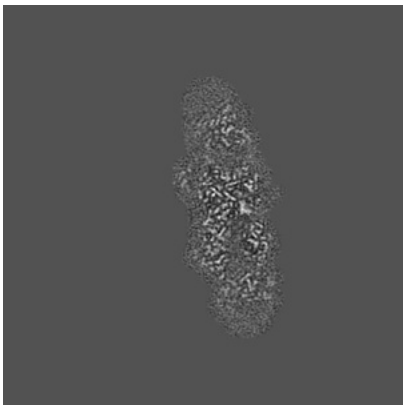


Z

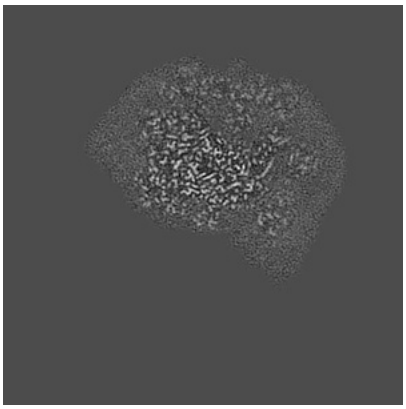
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

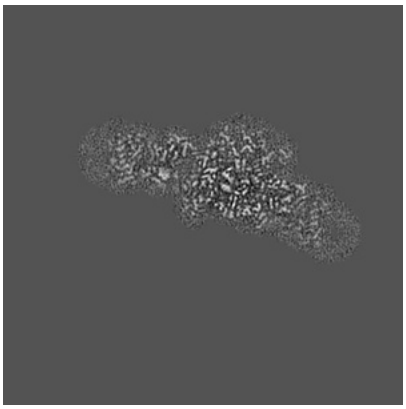
6.2.1 Primary map



X Index: 160

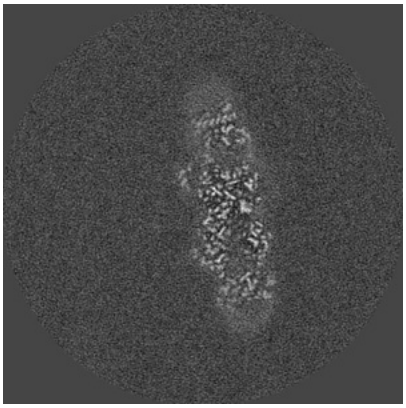


Y Index: 160

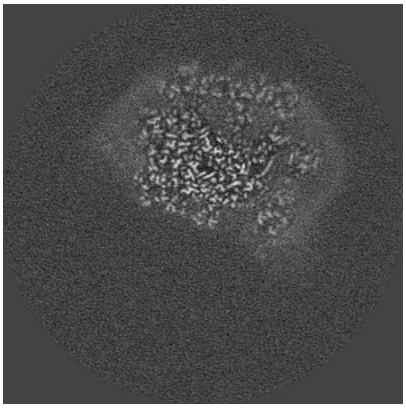


Z Index: 160

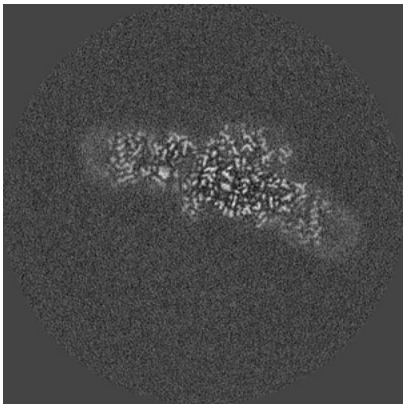
6.2.2 Raw map



X Index: 160



Y Index: 160

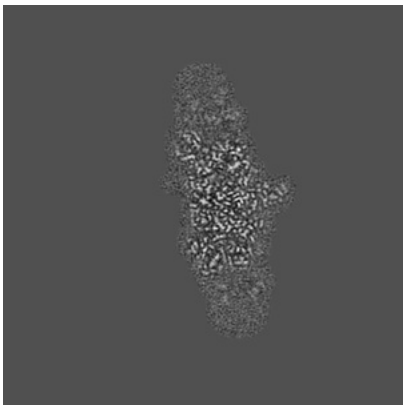


Z Index: 160

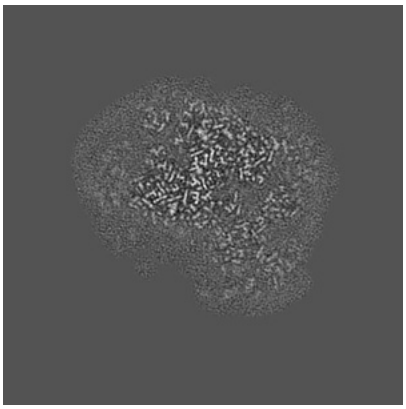
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

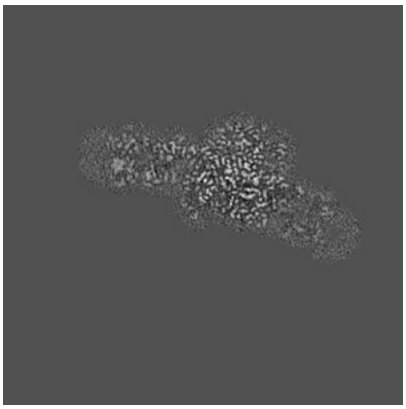
6.3.1 Primary map



X Index: 181

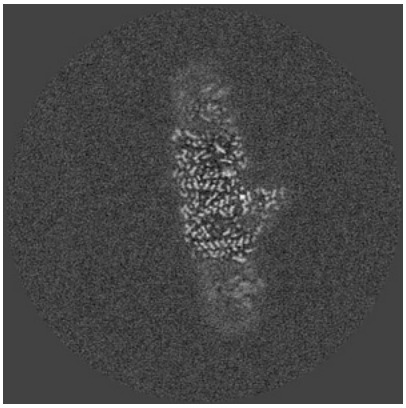


Y Index: 174

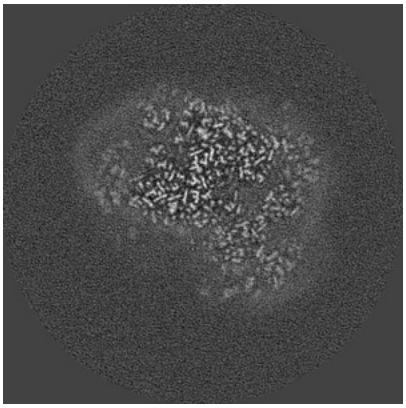


Z Index: 164

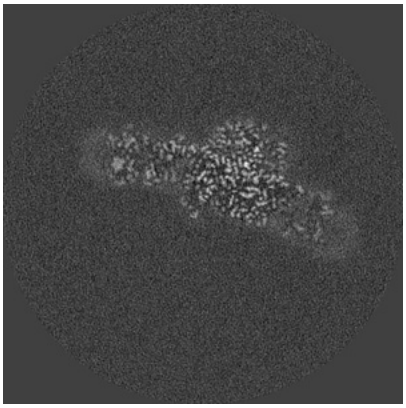
6.3.2 Raw map



X Index: 193



Y Index: 174

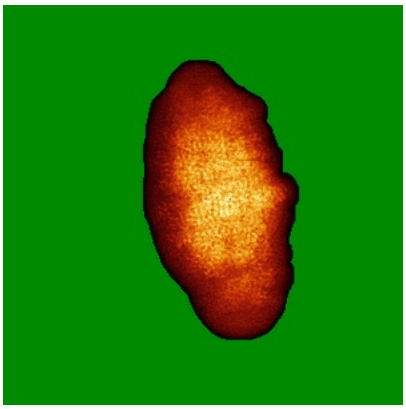


Z Index: 164

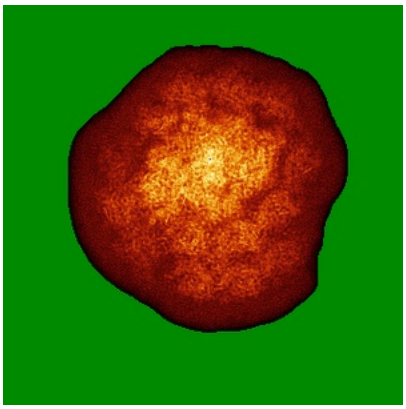
The images above show the largest variance slices of the map in three orthogonal directions.

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

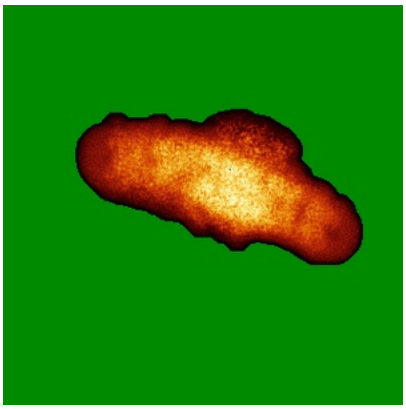
6.4.1 Primary map



X

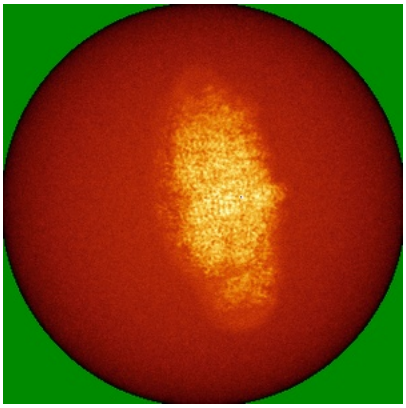


Y

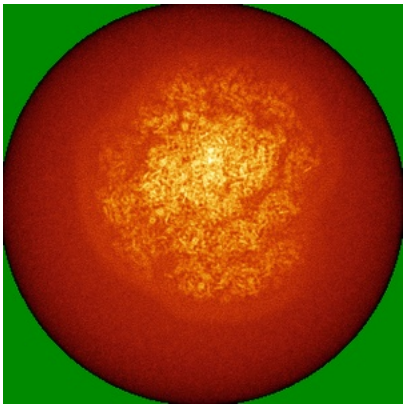


Z

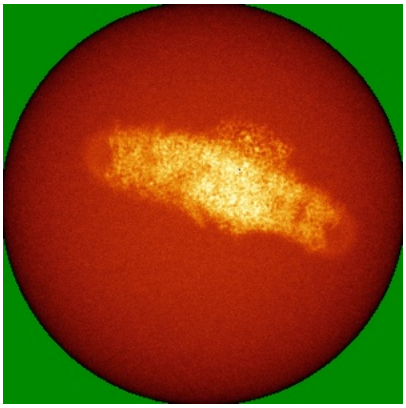
6.4.2 Raw map



X



Y

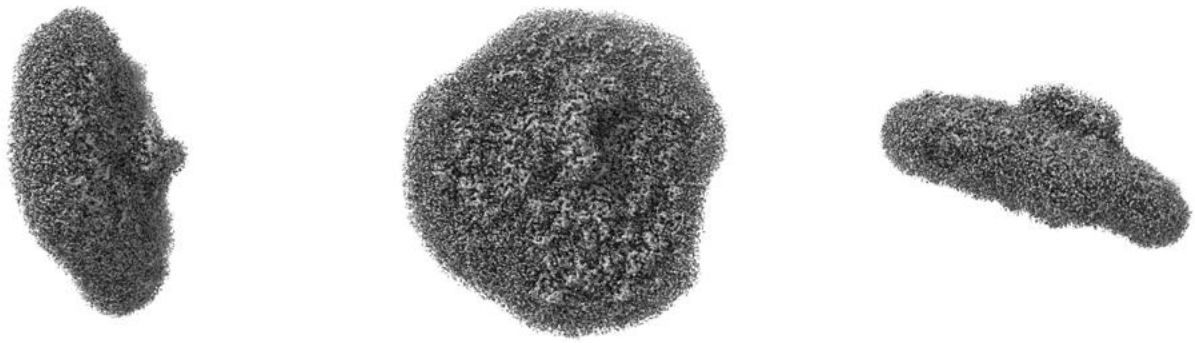


Z

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)

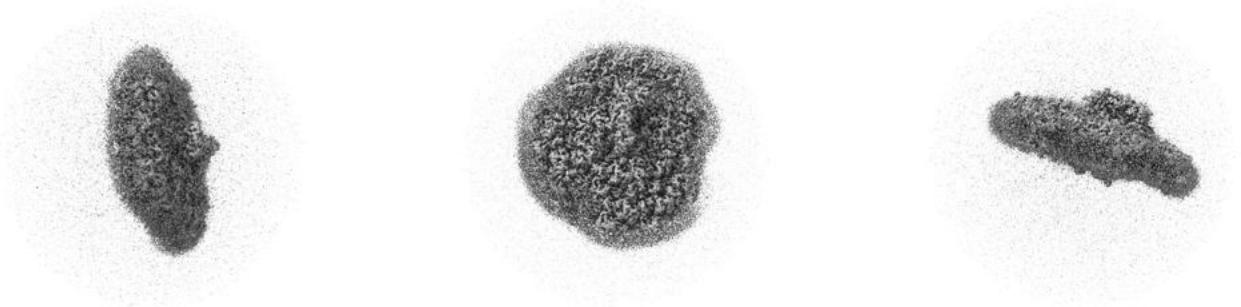
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

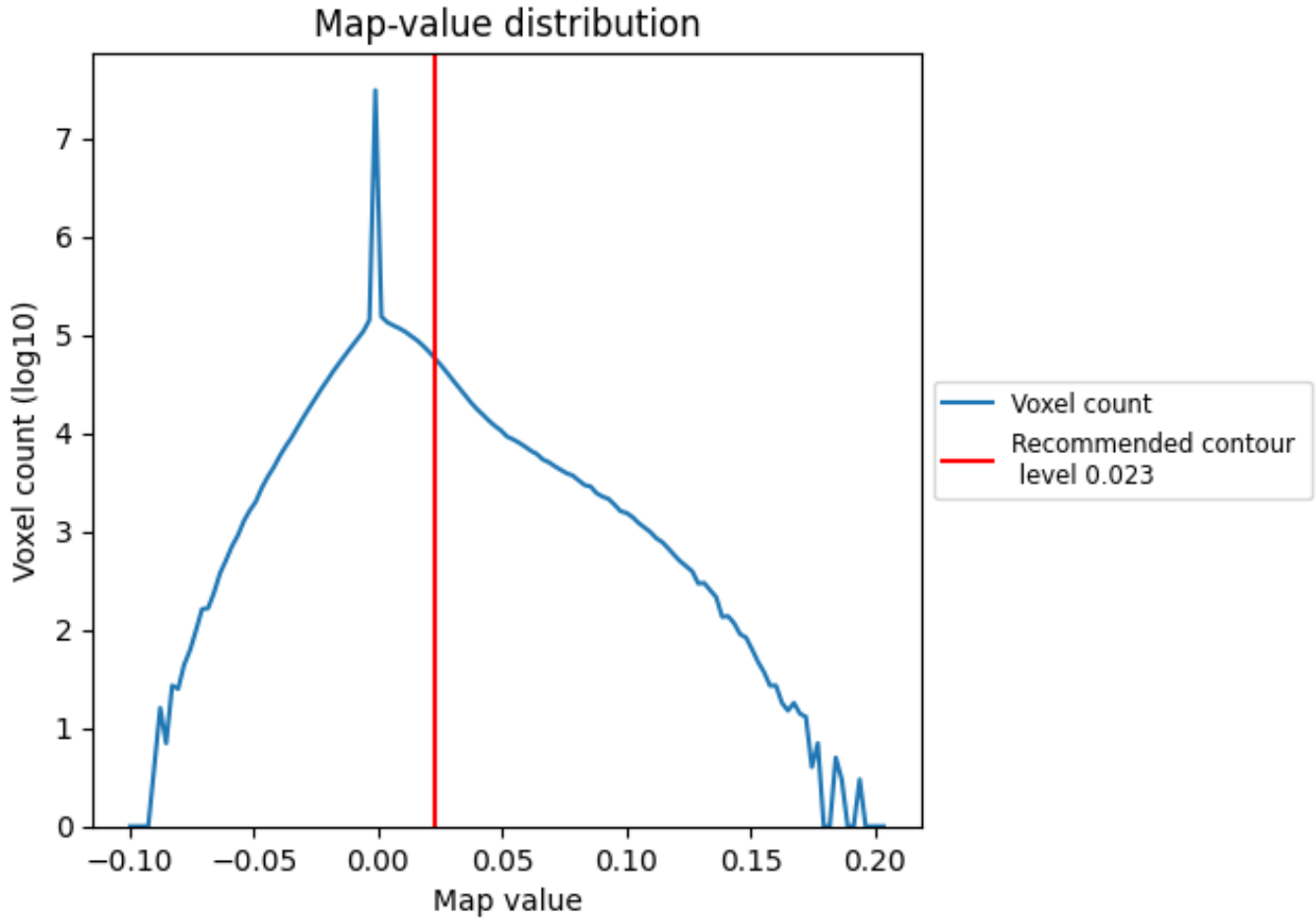
6.6 Mask visualisation (i)

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

7 Map analysis

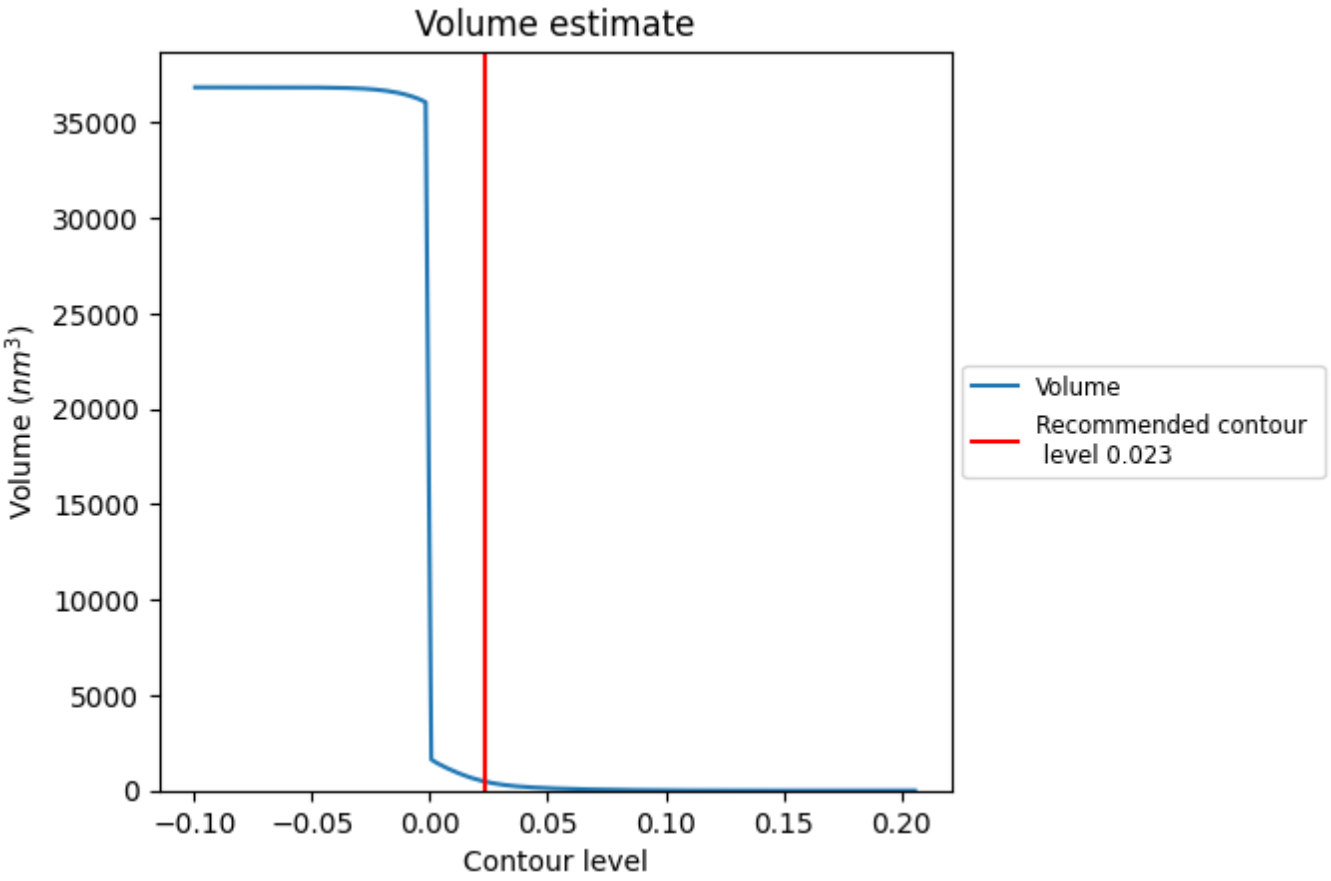
This section contains the results of statistical analysis of the map.

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.

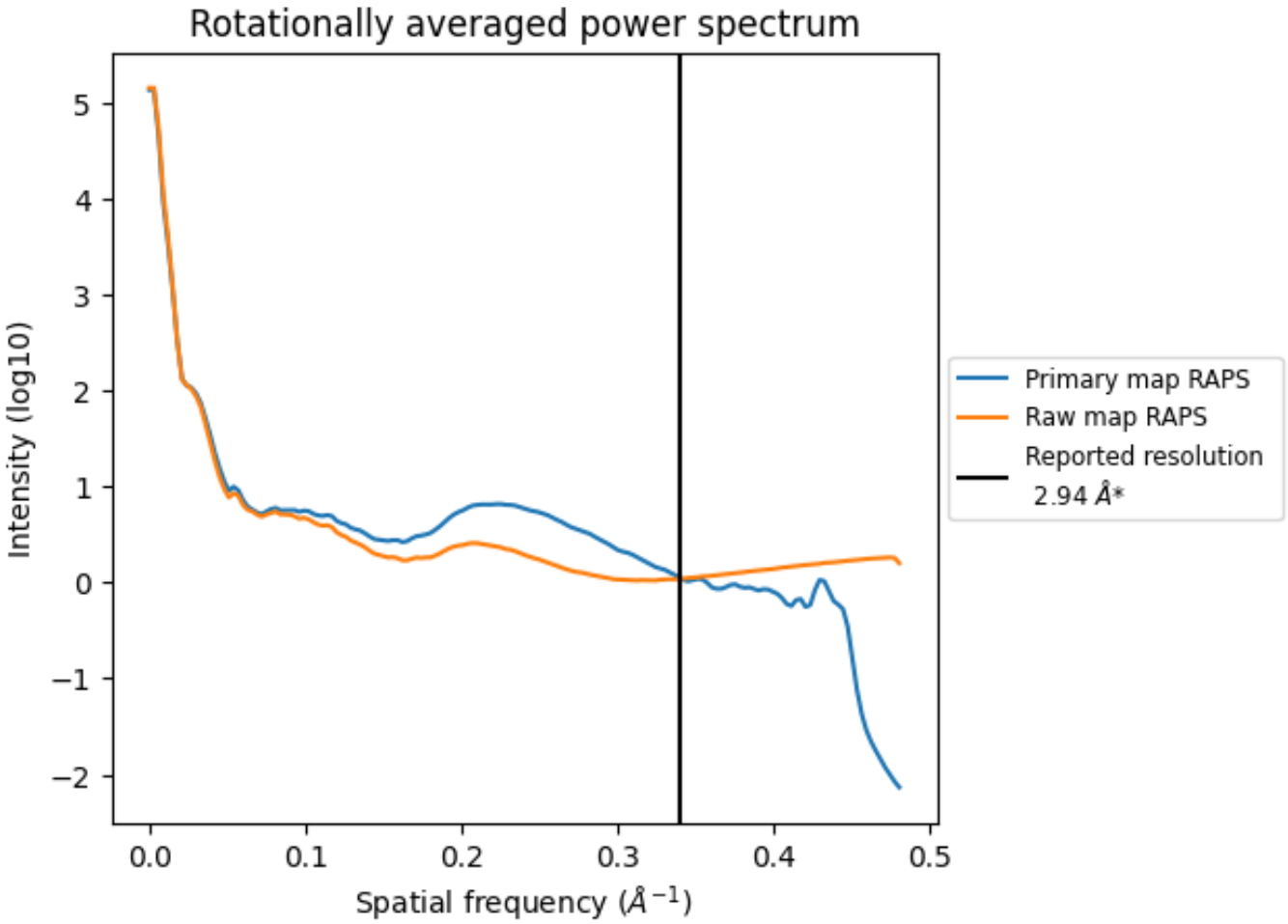
7.2 Volume estimate



The volume at the recommended contour level is 484 nm^3; this corresponds to an approximate mass of 437 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)

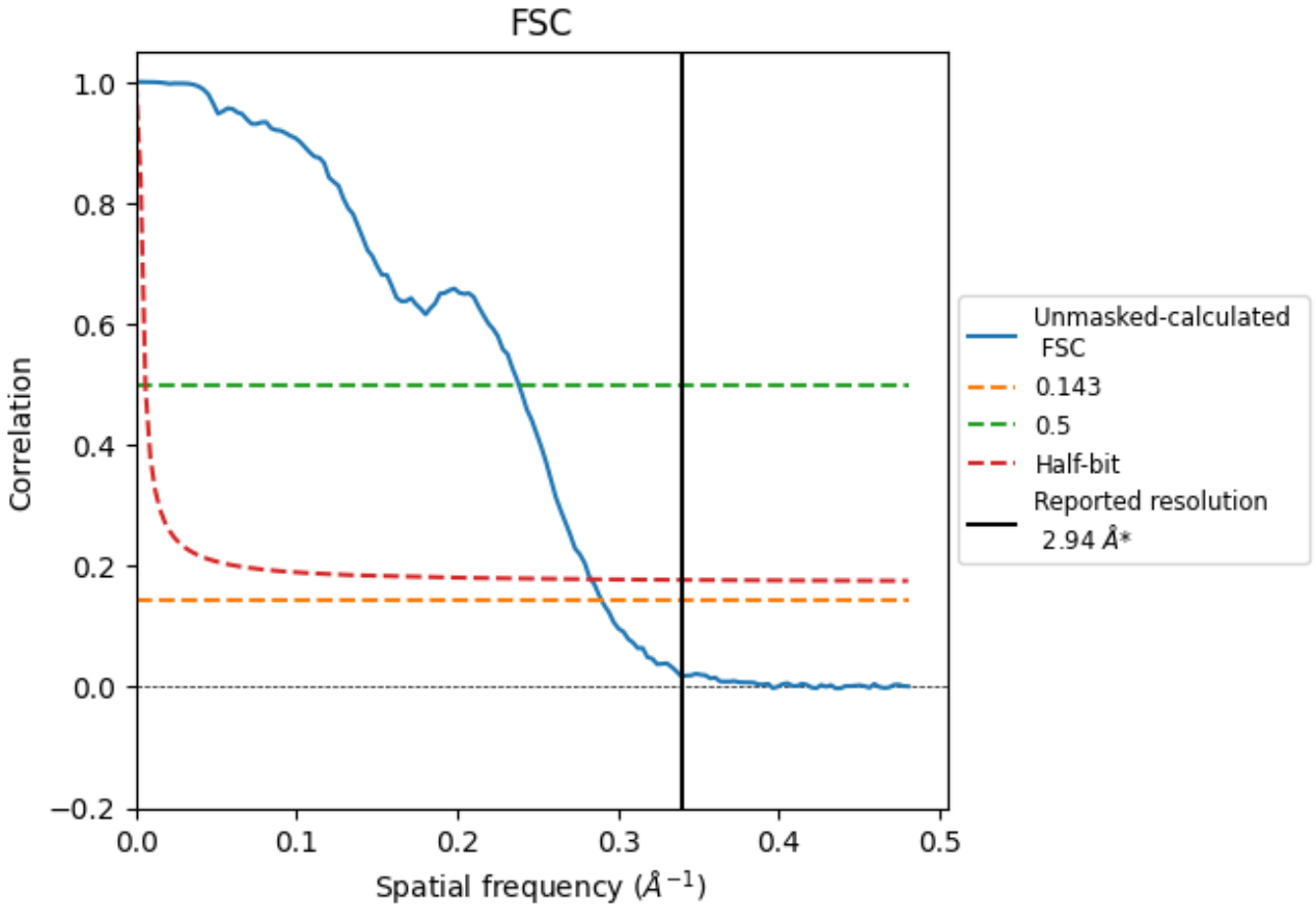


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

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 0.340 Å^{-1}

8.2 Resolution estimates (i)

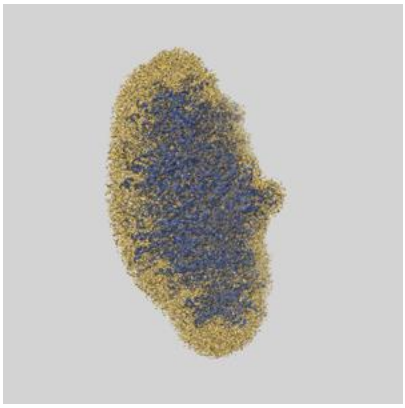
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	4.20	3.53

*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 3.45 differs from the reported value 2.94 by more than 10 %

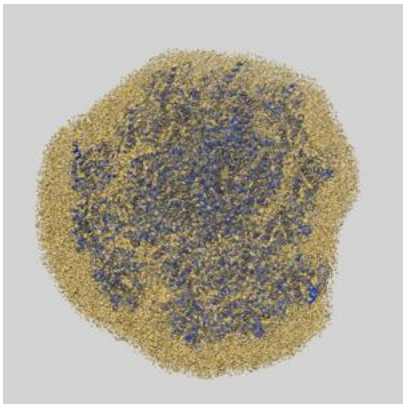
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37659 and PDB model 8WMV. Per-residue inclusion information can be found in section 3 on page 40.

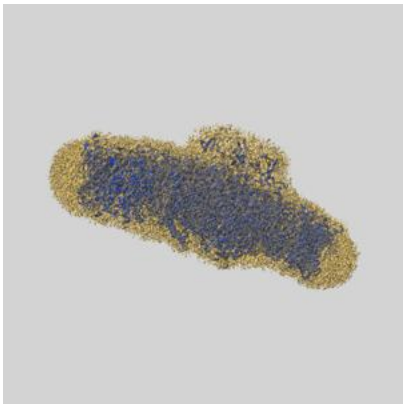
9.1 Map-model overlay



X



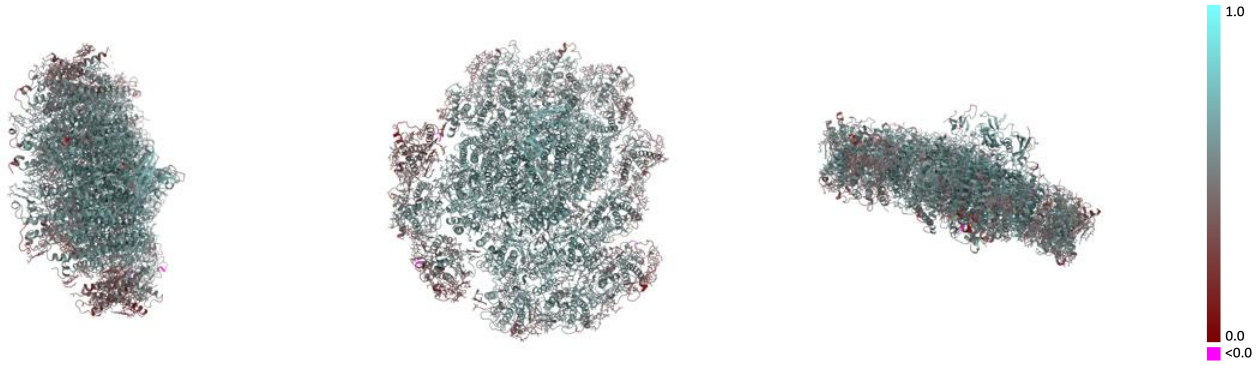
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

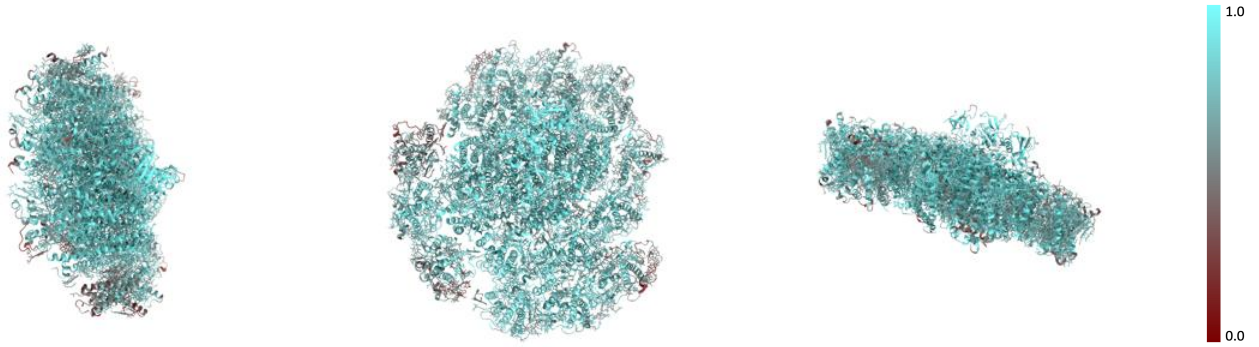
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

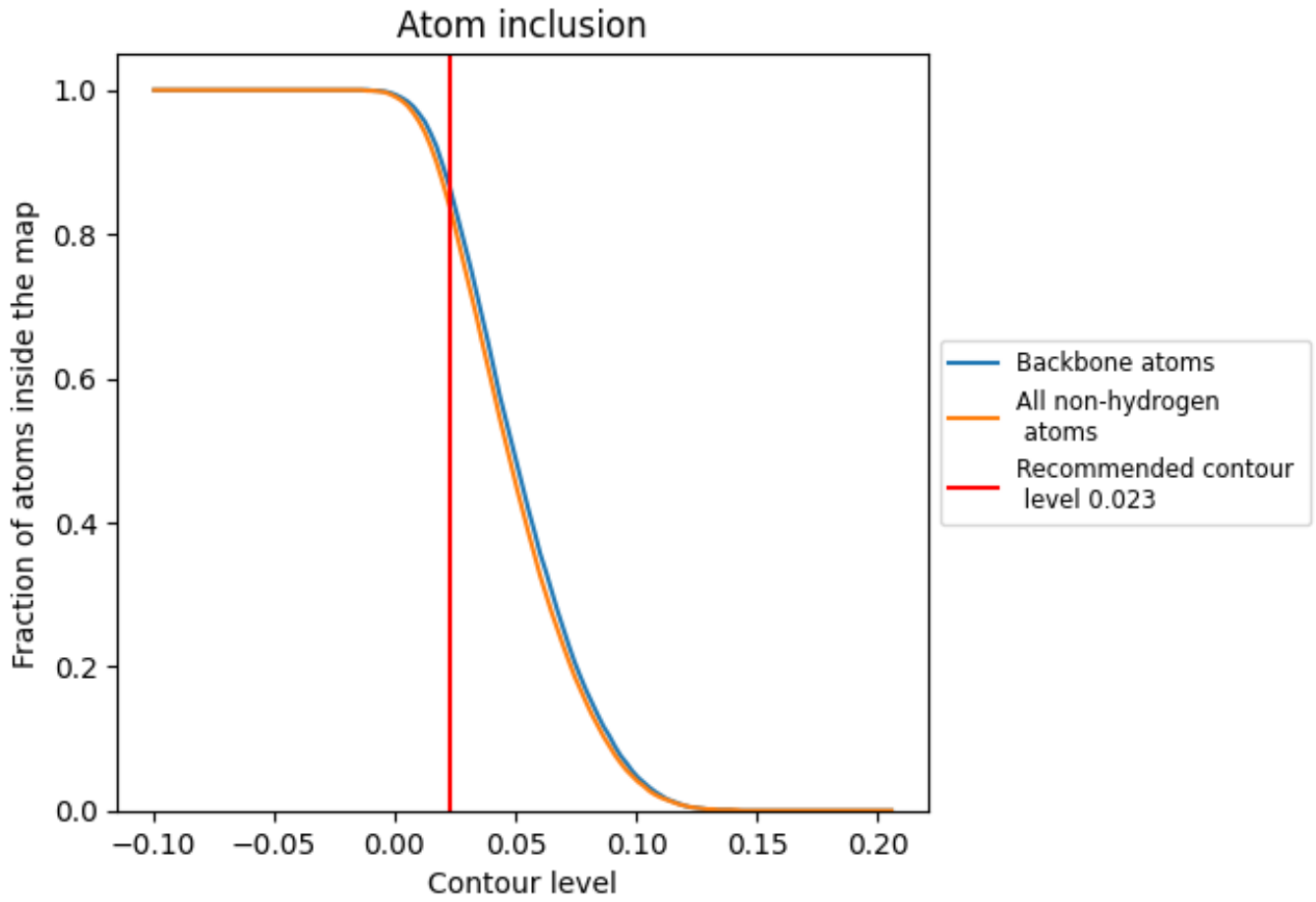
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 86% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.5550
A	0.9490	0.6430
B	0.9550	0.6440
C	0.9700	0.6420
D	0.8900	0.5820
E	0.8700	0.5730
F	0.9040	0.6050
I	0.9170	0.5980
J	0.9030	0.6120
K	0.8540	0.5580
L	0.8580	0.5780
M	0.8990	0.5790
O	0.8390	0.5640
R	0.9040	0.5990
a	0.9020	0.5930
b	0.8810	0.5900
c	0.8250	0.5370
d	0.6560	0.4160
e	0.6940	0.4670
f	0.7600	0.5150
g	0.6950	0.4750
h	0.8320	0.5430
i	0.5180	0.3390
j	0.7880	0.5030
k	0.6630	0.4110
l	0.8050	0.5130
m	0.8210	0.5450
n	0.6470	0.4390
s	0.8520	0.5650

