Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:31 AM UTC

PDB ID	:	8JW0 / pdb_00008jw0
EMDB ID	:	EMD-36678
Title	:	PSI-AcpPCI supercomplex from Amphidinium carterae
Authors	:	Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on	:	2023-06-28
Resolution	:	2.90 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:

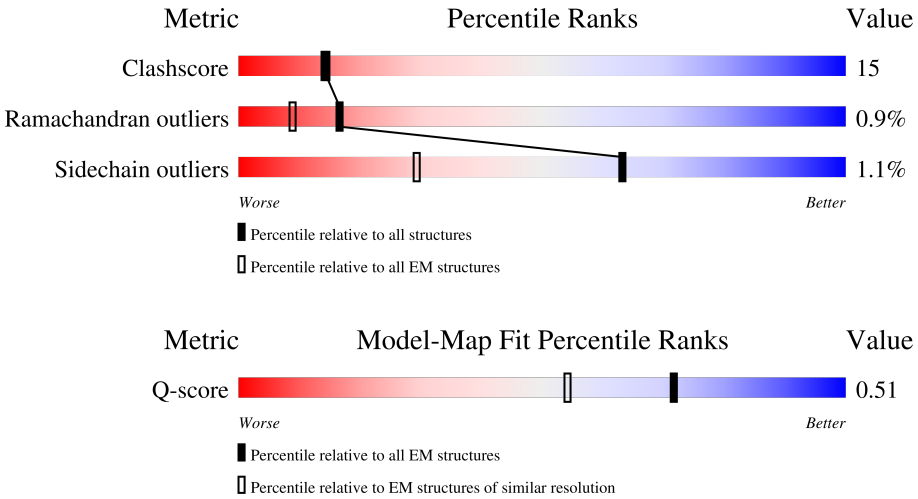
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.90 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.



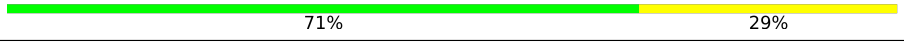
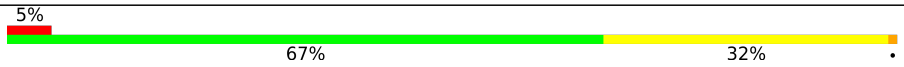
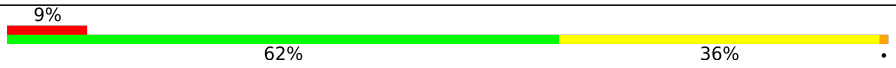
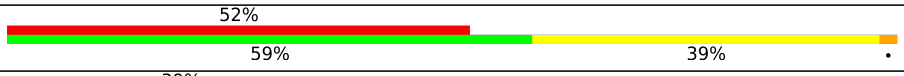
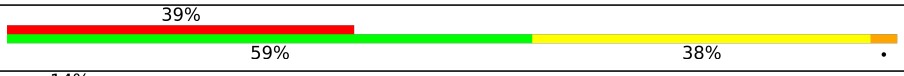
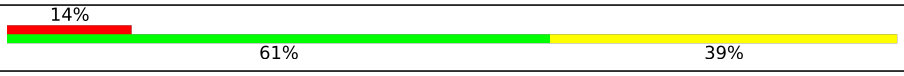
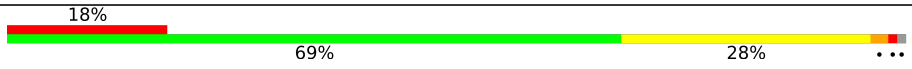
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	645	5% 74% 26%
2	b	617	70% 30%
3	c	86	76% 23%
4	d	257	75% 25%

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Mol	Chain	Length	Quality of chain
5	e	74	
6	f	185	
7	h	132	
8	i	126	
9	j	70	
10	l	253	
11	m	89	
12	A	180	
13	G	215	
14	I	194	
15	K	172	
16	F	176	
17	J	165	
18	M	168	
19	L	185	
20	D	160	
21	B	172	
22	H	160	
23	N	160	
24	O	161	
25	C	160	
25	T	160	
26	Q	162	
27	P	160	
28	E	142	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	206	X	-	-	-
29	CLA	A	207	X	-	-	-
29	CLA	A	208	X	-	-	-
29	CLA	A	209	X	-	-	-
29	CLA	A	210	X	-	-	-
29	CLA	A	211	X	-	-	-
29	CLA	A	212	X	-	-	-
29	CLA	A	214	X	-	-	-
29	CLA	A	215	X	-	-	-
29	CLA	A	216	X	-	-	-
29	CLA	A	217	X	-	-	-
29	CLA	A	218	X	-	-	-
29	CLA	B	306	X	-	-	-
29	CLA	B	307	X	-	-	-
29	CLA	B	308	X	-	-	-
29	CLA	B	309	X	-	-	-
29	CLA	B	310	X	-	-	-
29	CLA	B	311	X	-	-	-
29	CLA	B	312	X	-	-	-
29	CLA	B	314	X	-	-	-
29	CLA	B	315	X	-	-	-
29	CLA	B	316	X	-	-	-
29	CLA	C	308	X	-	-	-
29	CLA	C	309	X	-	-	-
29	CLA	C	311	X	-	-	-
29	CLA	C	313	X	-	-	-
29	CLA	C	314	X	-	-	-
29	CLA	C	316	X	-	-	-
29	CLA	D	308	X	-	-	-
29	CLA	D	309	X	-	-	-
29	CLA	D	311	X	-	-	-
29	CLA	D	312	X	-	-	-
29	CLA	D	313	X	-	-	-
29	CLA	D	314	X	-	-	-
29	CLA	D	316	X	-	-	-
29	CLA	E	305	X	-	-	-
29	CLA	E	306	X	-	-	-
29	CLA	E	308	X	-	-	-
29	CLA	E	309	X	-	-	-
29	CLA	E	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	E	311	X	-	-	-
29	CLA	E	313	X	-	-	-
29	CLA	E	315	X	-	-	-
29	CLA	F	307	X	-	-	-
29	CLA	F	308	X	-	-	-
29	CLA	F	310	X	-	-	-
29	CLA	F	311	X	-	-	-
29	CLA	F	312	X	-	-	-
29	CLA	F	313	X	-	-	-
29	CLA	F	315	X	-	-	-
29	CLA	F	316	X	-	-	-
29	CLA	G	301	X	-	-	-
29	CLA	G	302	X	-	-	-
29	CLA	G	304	X	-	-	-
29	CLA	G	311	X	-	-	-
29	CLA	G	312	X	-	-	-
29	CLA	G	313	X	-	-	-
29	CLA	G	314	X	-	-	-
29	CLA	G	316	X	-	-	-
29	CLA	G	317	X	-	-	-
29	CLA	G	319	X	-	-	-
29	CLA	H	307	X	-	-	-
29	CLA	H	308	X	-	-	-
29	CLA	H	310	X	-	-	-
29	CLA	H	312	X	-	-	-
29	CLA	H	313	X	-	-	-
29	CLA	H	315	X	-	-	-
29	CLA	I	201	X	-	-	-
29	CLA	I	207	X	-	-	-
29	CLA	I	208	X	-	-	-
29	CLA	I	209	X	-	-	-
29	CLA	I	210	X	-	-	-
29	CLA	I	211	X	-	-	-
29	CLA	I	212	X	-	-	-
29	CLA	I	213	X	-	-	-
29	CLA	I	214	X	-	-	-
29	CLA	I	216	X	-	-	-
29	CLA	I	217	X	-	-	-
29	CLA	J	305	X	-	-	-
29	CLA	J	306	X	-	-	-
29	CLA	J	307	X	-	-	-
29	CLA	J	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	J	309	X	-	-	-
29	CLA	J	310	X	-	-	-
29	CLA	J	311	X	-	-	-
29	CLA	J	313	X	-	-	-
29	CLA	K	207	X	-	-	-
29	CLA	K	208	X	-	-	-
29	CLA	K	209	X	-	-	-
29	CLA	K	210	X	-	-	-
29	CLA	K	211	X	-	-	-
29	CLA	K	212	X	-	-	-
29	CLA	K	213	X	-	-	-
29	CLA	K	214	X	-	-	-
29	CLA	K	216	X	-	-	-
29	CLA	K	217	X	-	-	-
29	CLA	K	218	X	-	-	-
29	CLA	L	307	X	-	-	-
29	CLA	L	308	X	-	-	-
29	CLA	L	309	X	-	-	-
29	CLA	L	310	X	-	-	-
29	CLA	L	311	X	-	-	-
29	CLA	L	312	X	-	-	-
29	CLA	L	313	X	-	-	-
29	CLA	L	315	X	-	-	-
29	CLA	L	316	X	-	-	-
29	CLA	L	317	X	-	-	-
29	CLA	M	306	X	-	-	-
29	CLA	M	307	X	-	-	-
29	CLA	M	308	X	-	-	-
29	CLA	M	309	X	-	-	-
29	CLA	M	310	X	-	-	-
29	CLA	M	311	X	-	-	-
29	CLA	M	313	X	-	-	-
29	CLA	M	314	X	-	-	-
29	CLA	M	315	X	-	-	-
29	CLA	N	308	X	-	-	-
29	CLA	N	309	X	-	-	-
29	CLA	N	311	X	-	-	-
29	CLA	N	313	X	-	-	-
29	CLA	N	314	X	-	-	-
29	CLA	N	316	X	-	-	-
29	CLA	O	308	X	-	-	-
29	CLA	O	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	O	313	X	-	-	-
29	CLA	O	316	X	-	-	-
29	CLA	P	209	X	-	-	-
29	CLA	P	210	X	-	-	-
29	CLA	P	212	X	-	-	-
29	CLA	P	214	X	-	-	-
29	CLA	P	215	X	-	-	-
29	CLA	P	217	X	-	-	-
29	CLA	Q	307	X	-	-	-
29	CLA	Q	308	X	-	-	-
29	CLA	Q	310	X	-	-	-
29	CLA	Q	312	X	-	-	-
29	CLA	Q	313	X	-	-	-
29	CLA	Q	315	X	-	-	-
29	CLA	T	308	X	-	-	-
29	CLA	T	309	X	-	-	-
29	CLA	T	311	X	-	-	-
29	CLA	T	313	X	-	-	-
29	CLA	T	314	X	-	-	-
29	CLA	T	316	X	-	-	-
29	CLA	a	801	X	-	-	-
29	CLA	a	802	X	-	-	-
29	CLA	a	803	X	-	-	-
29	CLA	a	804	X	-	-	-
29	CLA	a	805	X	-	-	-
29	CLA	a	806	X	-	-	-
29	CLA	a	807	X	-	-	-
29	CLA	a	808	X	-	-	-
29	CLA	a	809	X	-	-	-
29	CLA	a	810	X	-	-	-
29	CLA	a	811	X	-	-	-
29	CLA	a	812	X	-	-	-
29	CLA	a	813	X	-	-	-
29	CLA	a	814	X	-	-	-
29	CLA	a	815	X	-	-	-
29	CLA	a	816	X	-	-	-
29	CLA	a	817	X	-	-	-
29	CLA	a	818	X	-	-	-
29	CLA	a	819	X	-	-	-
29	CLA	a	820	X	-	-	-
29	CLA	a	821	X	-	-	-
29	CLA	a	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	a	823	X	-	-	-
29	CLA	a	824	X	-	-	-
29	CLA	a	825	X	-	-	-
29	CLA	a	826	X	-	-	-
29	CLA	a	827	X	-	-	-
29	CLA	a	828	X	-	-	-
29	CLA	a	829	X	-	-	-
29	CLA	a	830	X	-	-	-
29	CLA	a	831	X	-	-	-
29	CLA	a	837	X	-	-	-
29	CLA	b	701	X	-	-	-
29	CLA	b	702	X	-	-	-
29	CLA	b	703	X	-	-	-
29	CLA	b	704	X	-	-	-
29	CLA	b	705	X	-	-	-
29	CLA	b	706	X	-	-	-
29	CLA	b	707	X	-	-	-
29	CLA	b	708	X	-	-	-
29	CLA	b	709	X	-	-	-
29	CLA	b	710	X	-	-	-
29	CLA	b	711	X	-	-	-
29	CLA	b	712	X	-	-	-
29	CLA	b	713	X	-	-	-
29	CLA	b	714	X	-	-	-
29	CLA	b	715	X	-	-	-
29	CLA	b	716	X	-	-	-
29	CLA	b	717	X	-	-	-
29	CLA	b	718	X	-	-	-
29	CLA	b	719	X	-	-	-
29	CLA	b	720	X	-	-	-
29	CLA	b	721	X	-	-	-
29	CLA	b	722	X	-	-	-
29	CLA	b	723	X	-	-	-
29	CLA	b	724	X	-	-	-
29	CLA	b	725	X	-	-	-
29	CLA	b	726	X	-	-	-
29	CLA	b	731	X	-	-	-
29	CLA	b	736	X	-	-	-
29	CLA	f	802	X	-	-	-
29	CLA	f	803	X	-	-	-
29	CLA	f	805	X	-	-	-
29	CLA	h	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	i	201	X	-	-	-
29	CLA	i	202	X	-	-	-
29	CLA	i	203	X	-	-	-
29	CLA	j	104	X	-	-	-
29	CLA	l	501	X	-	-	-
29	CLA	l	502	X	-	-	-
29	CLA	l	503	X	-	-	-
29	CLA	l	504	X	-	-	-
29	CLA	l	505	X	-	-	-
29	CLA	l	508	X	-	-	-
29	CLA	l	509	X	-	-	-
29	CLA	l	510	X	-	-	-
33	SF4	a	836	-	-	X	-
33	SF4	c	102	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 63119 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	645	Total	C	N	O	S	0	0
			4980	3267	825	874	14		

- Molecule 2 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	617	Total	C	N	O	S	0	0
			4813	3185	765	848	15		

- Molecule 3 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	86	Total	C	N	O	S	0	0
			647	401	109	128	9		

- Molecule 4 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	257	Total	C	N	O	S	0	0
			1985	1259	340	375	11		

- Molecule 5 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	74	Total	C	N	O	0	0
			607	392	102	113		

- Molecule 6 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	185	Total	C	N	O	S	0	0
			1455	926	257	263	9		

- Molecule 7 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	132	Total	C	N	O	S	0	0
			1056	693	167	191	5		

- Molecule 8 is a protein called Photosystem I PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	126	Total	C	N	O	S	0	0
			1001	651	164	183	3		

- Molecule 9 is a protein called Photosystem I PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	70	Total	C	N	O	S	0	0
			549	362	86	100	1		

- Molecule 10 is a protein called Photosystem I PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	253	Total	C	N	O	S	0	0
			1961	1274	321	355	11		

- Molecule 11 is a protein called Photosystem I PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	89	Total	C	N	O	S	0	0
			679	438	109	131	1		

- Molecule 12 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	180	Total	C	N	O	S	0	0
			1358	882	221	245	10		

- Molecule 13 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	215	Total	C	N	O	S	0	0
			1675	1086	278	299	12		

- Molecule 14 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	194	Total	C	N	O	S	0	0
			1455	946	244	253	12		

- Molecule 15 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	172	Total	C	N	O	S	0	0
			1325	857	222	234	12		

- Molecule 16 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	176	Total	C	N	O	S	0	0
			1356	869	226	249	12		

- Molecule 17 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	165	Total	C	N	O	S	0	0
			1282	828	207	239	8		

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	168	Total	C	N	O	S	0	0
			1346	885	224	232	5		

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	185	Total	C	N	O	S	0	0
			1453	942	242	263	6		

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	160	Total	C	N	O	S	0	0
			1198	761	200	230	7		

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	172	Total	C	N	O	S	0	0
			1371	888	226	245	12		

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	160	Total	C	N	O	S	0	0
			1202	769	198	228	7		

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	160	Total	C	N	O	S	0	0
			1203	767	200	229	7		

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	161	Total	C	N	O	S	0	0
			1226	789	204	226	7		

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	159	Total	C	N	O	S	0	0
			1189	756	199	226	8		
25	C	160	Total	C	N	O	S	0	0
			1200	765	200	227	8		

- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	162	Total	C	N	O	S	0	0
			1219	787	204	219	9		

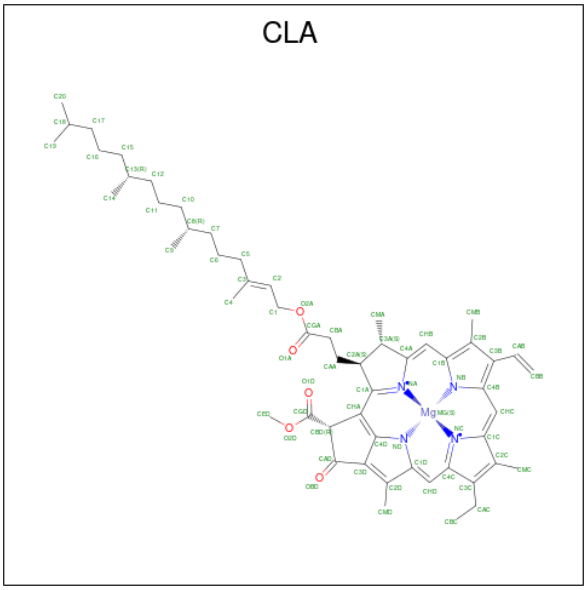
- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	160	Total	C	N	O	S	0	0
			1218	778	204	228	8		

- Molecule 28 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	142	Total	C	N	O	S	0	0
			1071	684	178	201	8		

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	M	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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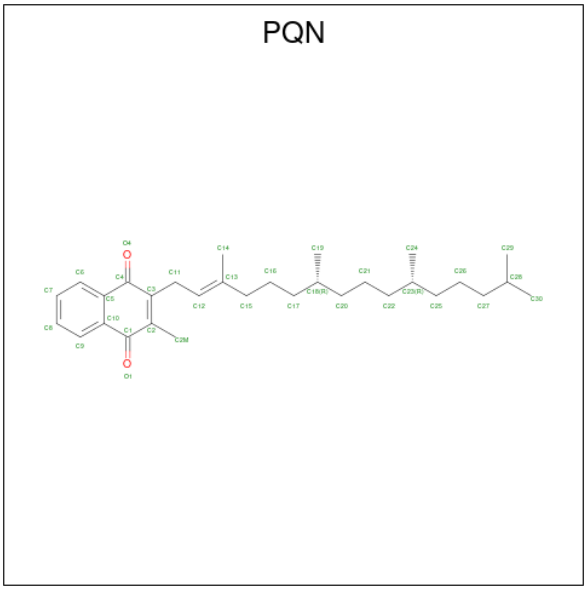
Mol	Chain	Residues	Atoms					AltConf
29	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	E	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	E	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



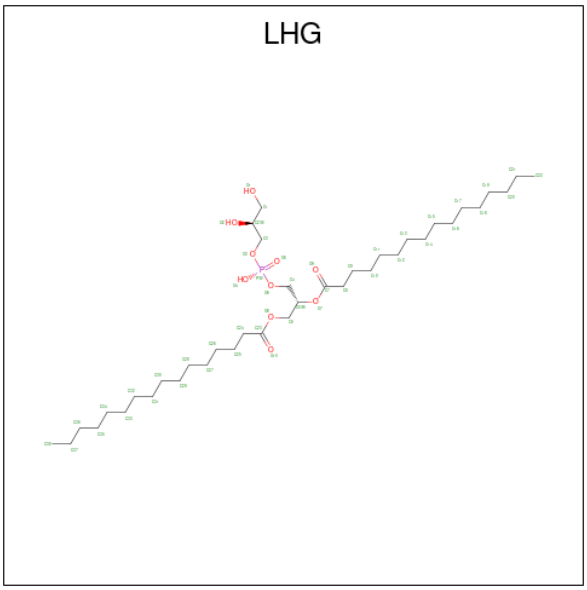
Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			33	31	2	

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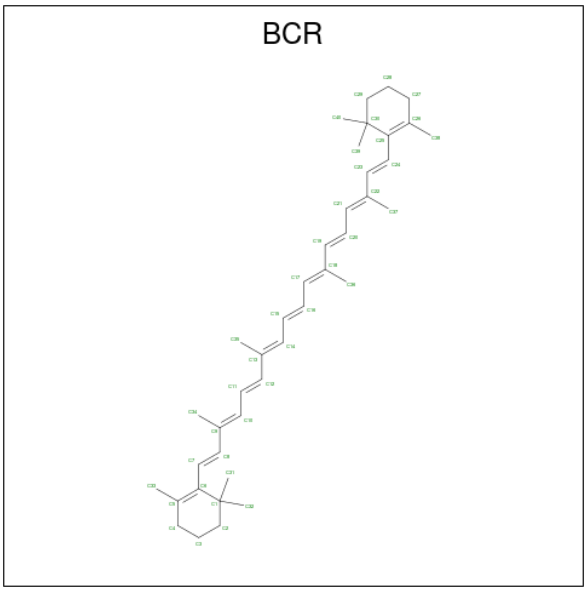
Mol	Chain	Residues	Atoms			AltConf
30	b	1	Total	C	O	0
			33	31	2	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



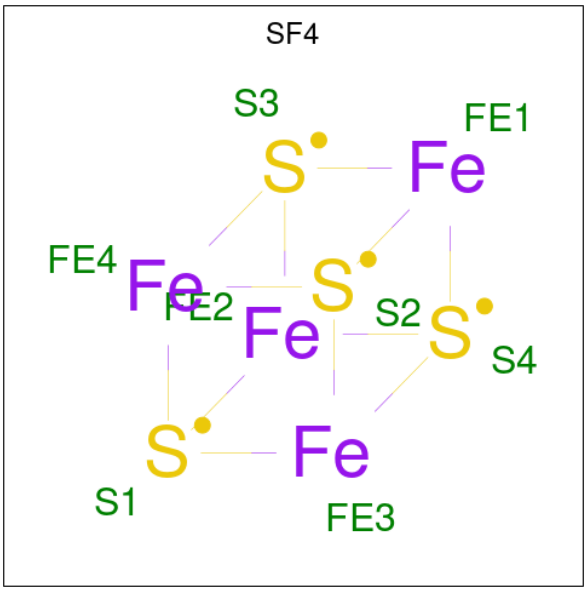
Mol	Chain	Residues	Atoms				AltConf
31	a	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



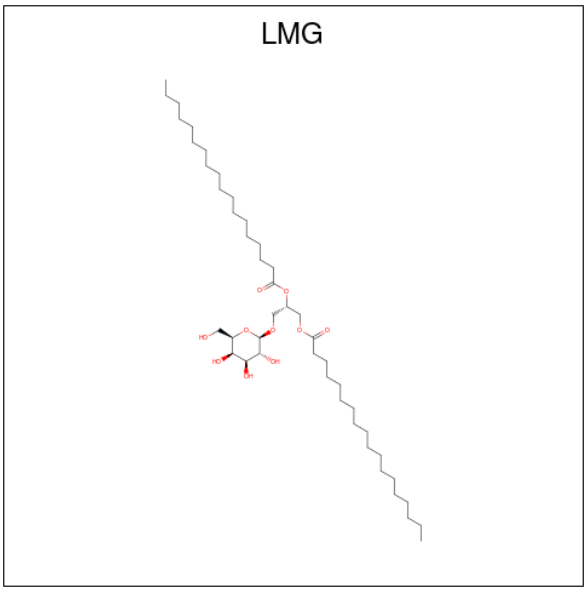
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C 40 40	0

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



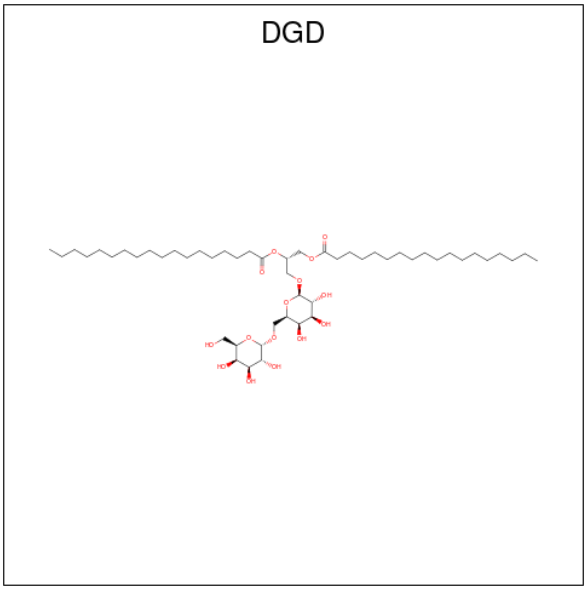
Mol	Chain	Residues	Atoms	AltConf
33	a	1	Total Fe S 8 4 4	0
33	c	1	Total Fe S 8 4 4	0
33	c	1	Total Fe S 8 4 4	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



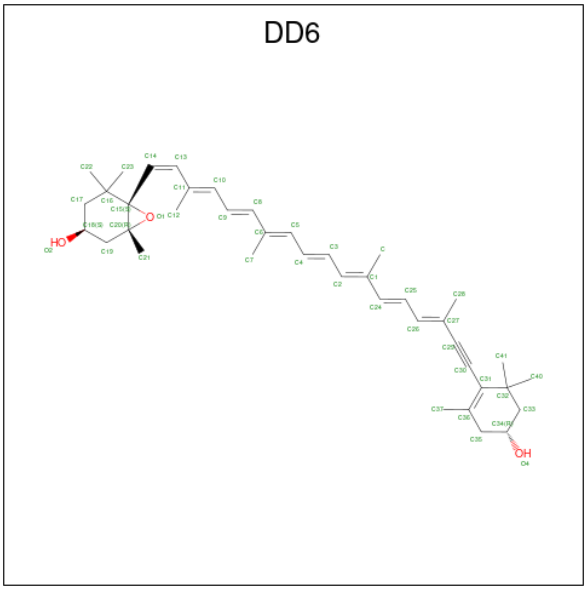
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			44	34	10	
34	b	1	Total	C	O	0
			40	30	10	
34	h	1	Total	C	O	0
			28	18	10	
34	j	1	Total	C	O	0
			43	33	10	
34	A	1	Total	C	O	0
			37	27	10	
34	K	1	Total	C	O	0
			43	33	10	
34	K	1	Total	C	O	0
			35	25	10	
34	K	1	Total	C	O	0
			36	26	10	
34	P	1	Total	C	O	0
			27	17	10	
34	E	1	Total	C	O	0
			32	22	10	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
35	b	1	Total C O 57 42 15	0
35	h	1	Total C O 54 39 15	0
35	j	1	Total C O 43 28 15	0
35	j	1	Total C O 41 26 15	0
35	j	1	Total C O 49 34 15	0
35	m	1	Total C O 66 51 15	0
35	G	1	Total C O 45 30 15	0
35	B	1	Total C O 45 30 15	0

- Molecule 36 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
36	h	1	Total C O 43 40 3	0
36	m	1	Total C O 43 40 3	0
36	A	1	Total C O 43 40 3	0

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Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			43	40	3	
36	A	1	Total	C	O	0
			43	40	3	
36	G	1	Total	C	O	0
			43	40	3	
36	G	1	Total	C	O	0
			43	40	3	
36	G	1	Total	C	O	0
			43	40	3	
36	G	1	Total	C	O	0
			43	40	3	
36	I	1	Total	C	O	0
			43	40	3	
36	I	1	Total	C	O	0
			43	40	3	
36	I	1	Total	C	O	0
			43	40	3	
36	I	1	Total	C	O	0
			43	40	3	
36	I	1	Total	C	O	0
			43	40	3	
36	K	1	Total	C	O	0
			43	40	3	
36	K	1	Total	C	O	0
			43	40	3	
36	K	1	Total	C	O	0
			43	40	3	
36	K	1	Total	C	O	0
			43	40	3	
36	K	1	Total	C	O	0
			43	40	3	
36	K	1	Total	C	O	0
			43	40	3	
36	F	1	Total	C	O	0
			43	40	3	
36	F	1	Total	C	O	0
			43	40	3	
36	J	1	Total	C	O	0
			43	40	3	
36	J	1	Total	C	O	0
			43	40	3	

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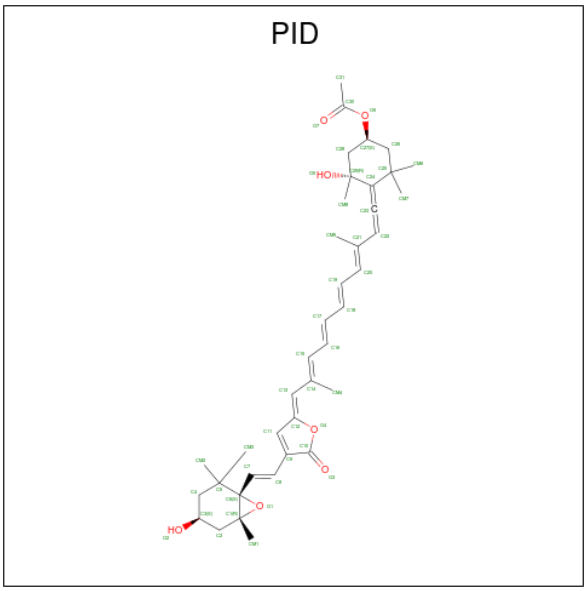
Mol	Chain	Residues	Atoms			AltConf
36	J	1	Total	C	O	0
			43	40	3	
36	M	1	Total	C	O	0
			43	40	3	
36	M	1	Total	C	O	0
			43	40	3	
36	M	1	Total	C	O	0
			43	40	3	
36	M	1	Total	C	O	0
			43	40	3	
36	L	1	Total	C	O	0
			43	40	3	
36	L	1	Total	C	O	0
			43	40	3	
36	L	1	Total	C	O	0
			43	40	3	
36	L	1	Total	C	O	0
			43	40	3	
36	D	1	Total	C	O	0
			43	40	3	
36	D	1	Total	C	O	0
			43	40	3	
36	B	1	Total	C	O	0
			42	39	3	
36	B	1	Total	C	O	0
			43	40	3	
36	B	1	Total	C	O	0
			43	40	3	
36	B	1	Total	C	O	0
			43	40	3	
36	B	1	Total	C	O	0
			43	40	3	
36	H	1	Total	C	O	0
			43	40	3	
36	N	1	Total	C	O	0
			43	40	3	
36	O	1	Total	C	O	0
			43	40	3	
36	T	1	Total	C	O	0
			43	40	3	
36	Q	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms	AltConf
36	C	1	Total C O 43 40 3	0
36	P	1	Total C O 43 40 3	0
36	E	1	Total C O 43 40 3	0
36	E	1	Total C O 43 40 3	0

- Molecule 37 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
37	h	1	Total C O 46 39 7	0
37	j	1	Total C O 46 39 7	0
37	G	1	Total C O 46 39 7	0
37	G	1	Total C O 46 39 7	0
37	G	1	Total C O 46 39 7	0
37	F	1	Total C O 46 39 7	0
37	F	1	Total C O 46 39 7	0

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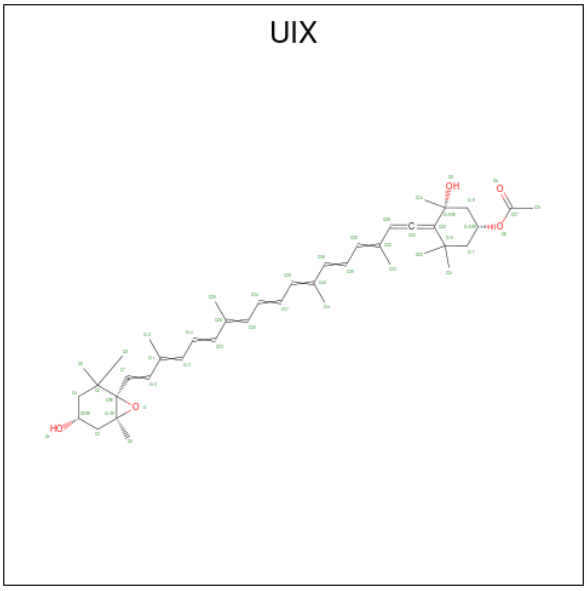
Mol	Chain	Residues	Atoms			AltConf
37	F	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	

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Mol	Chain	Residues	Atoms			AltConf
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	C	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	P	1	Total	C	O	0
			46	39	7	
37	E	1	Total	C	O	0
			46	39	7	

- Molecule 38 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: $C_{42}H_{58}O_5$) (labeled as "Ligand of Interest" by depositor).



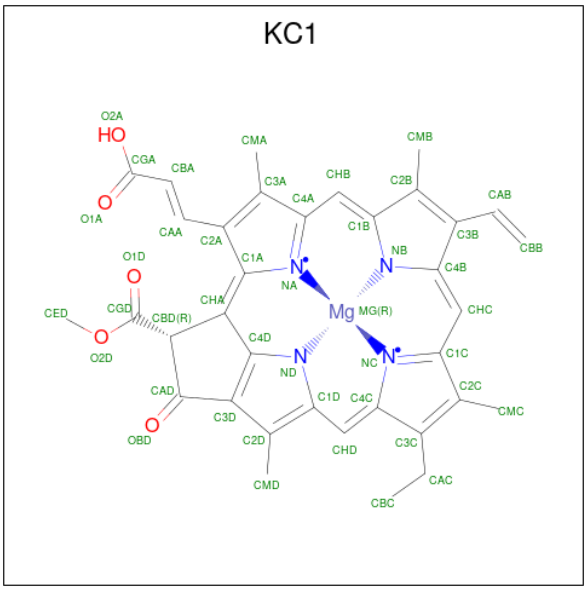
Mol	Chain	Residues	Atoms	AltConf
38	A	1	Total C O 47 42 5	0
38	F	1	Total C O 47 42 5	0
38	J	1	Total C O 47 42 5	0
38	L	1	Total C O 47 42 5	0
38	B	1	Total C O 47 42 5	0
38	N	1	Total C O 47 42 5	0
38	O	1	Total C O 47 42 5	0
38	T	1	Total C O 47 42 5	0
38	Q	1	Total C O 47 42 5	0
38	C	1	Total C O 47 42 5	0
38	P	1	Total C O 47 42 5	0

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Mol	Chain	Residues	Atoms			AltConf
38	E	1	Total	C	O	0
			47	42	5	

- Molecule 39 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
39	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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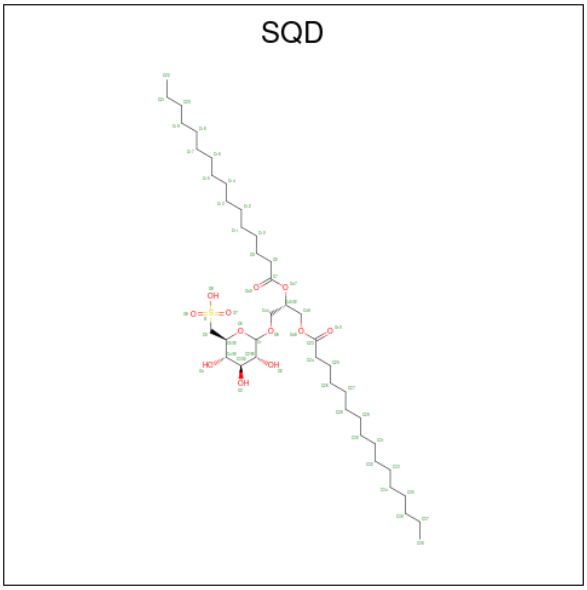
Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



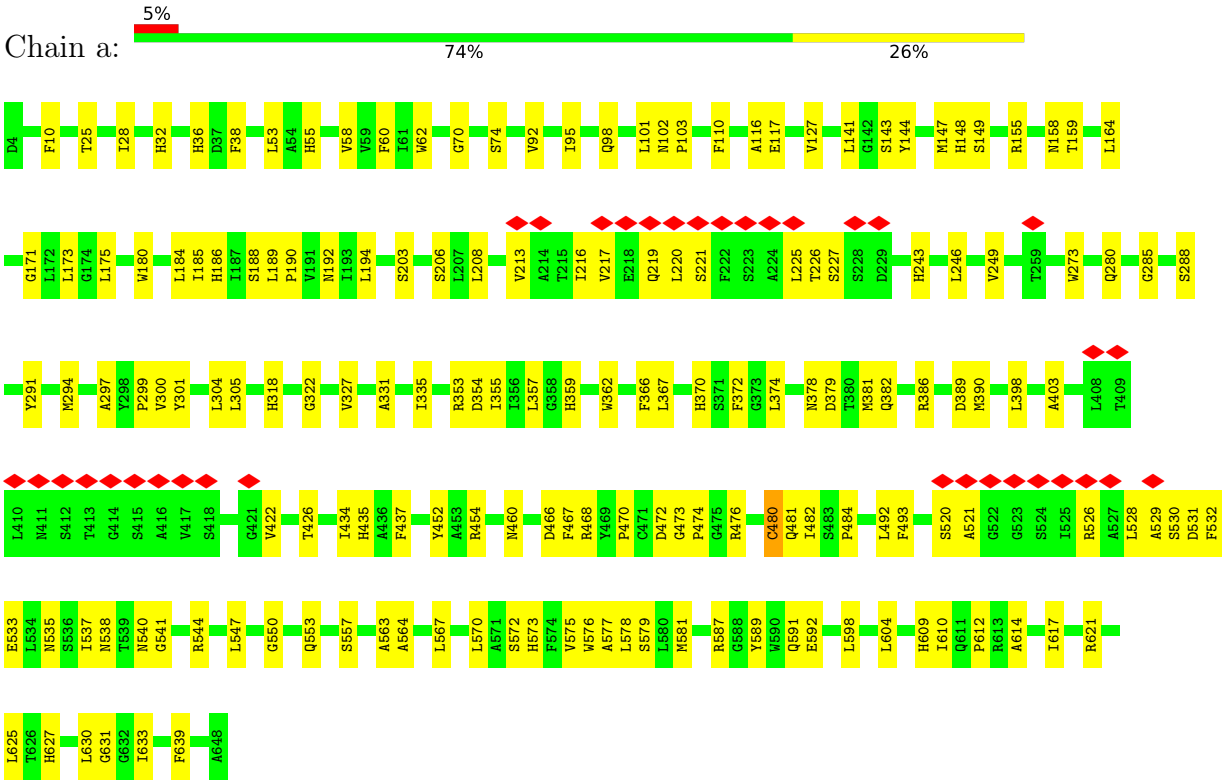
Mol	Chain	Residues	Atoms				AltConf
40	J	1	Total	C	O	S	0
			45	32	12	1	
40	B	1	Total	C	O	S	0
			42	29	12	1	

3 Residue-property plots (i)

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

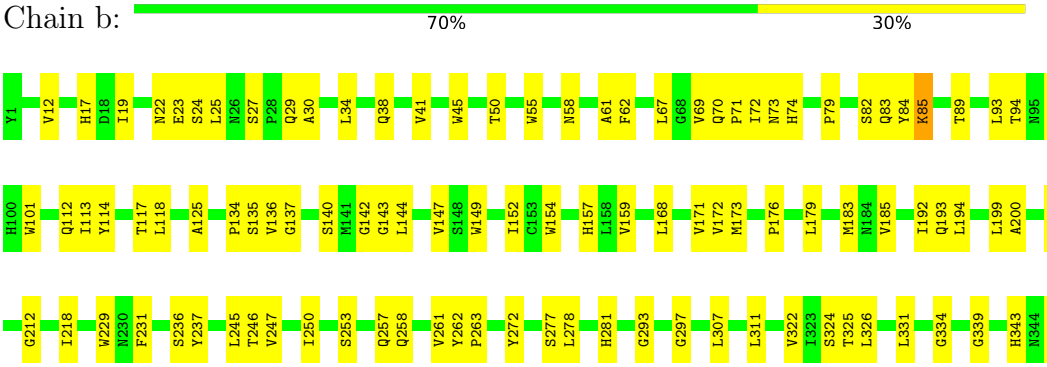
• Molecule 1: Photosystem I PsaA

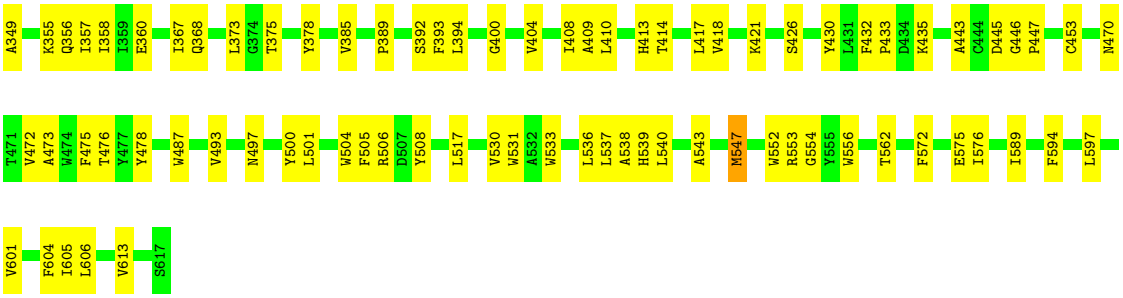
Chain a:



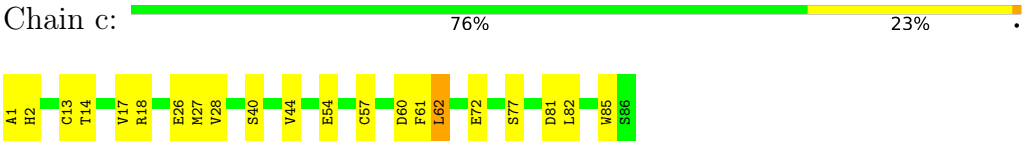
• Molecule 2: Photosystem I PsaB

Chain b:

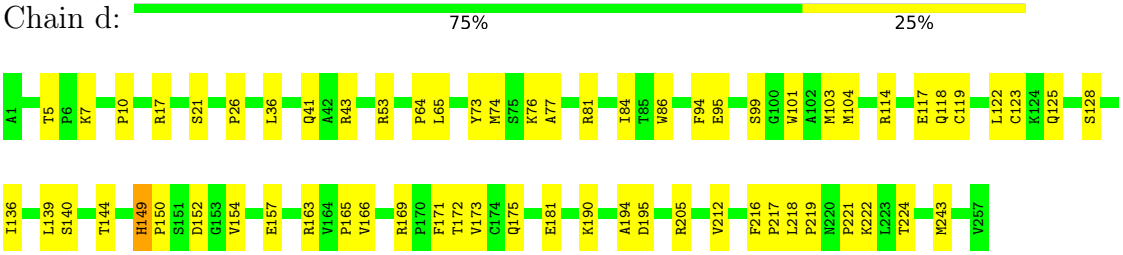




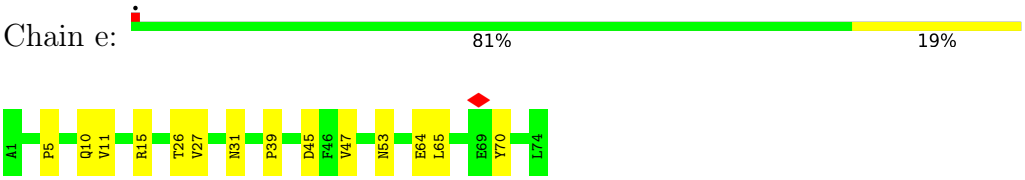
• Molecule 3: Photosystem I PsaC



• Molecule 4: Photosystem I PsaD

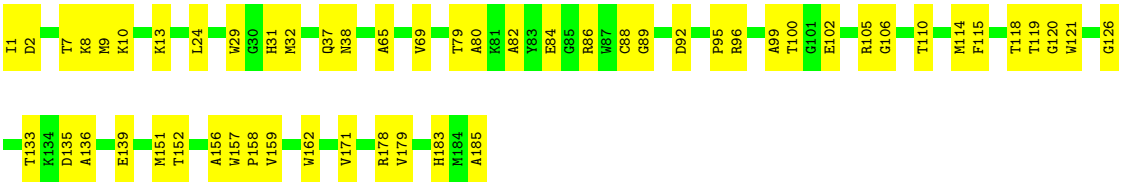


• Molecule 5: Photosystem I PsaE

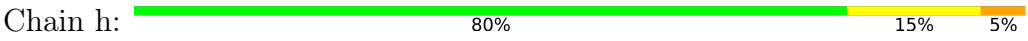


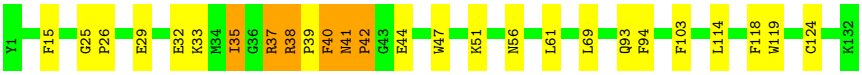
• Molecule 6: Photosystem I PsaF





• Molecule 7: Photosystem I PsaR

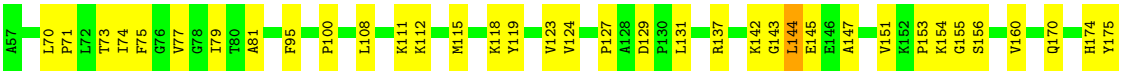


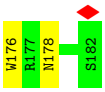


• Molecule 8: Photosystem I PsaI

Chain i:



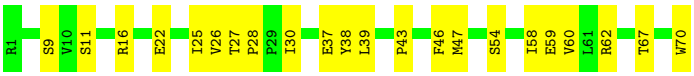




• Molecule 9: Photosystem I PsaJ

Chain j:

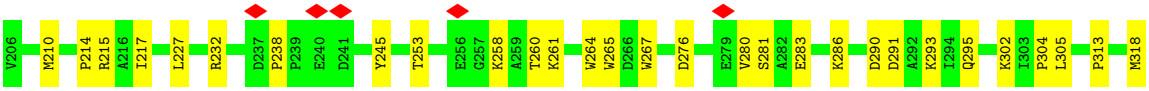




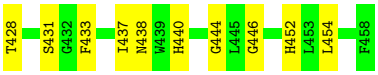
• Molecule 10: Photosystem I PsaL

Chain l:





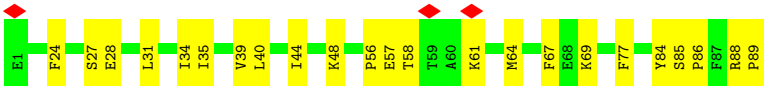




• Molecule 11: Photosystem I PsaM

Chain m:

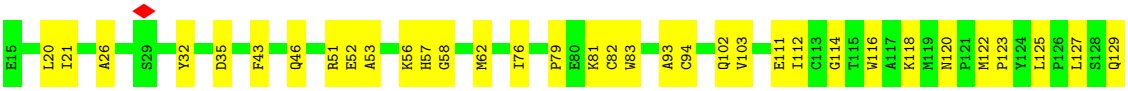




• Molecule 12: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

Chain A:



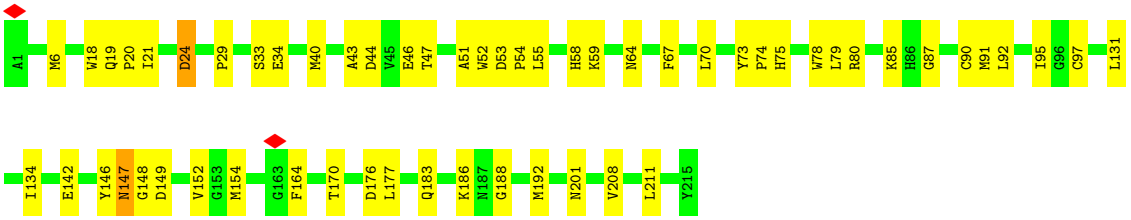




• Molecule 13: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8

Chain G:

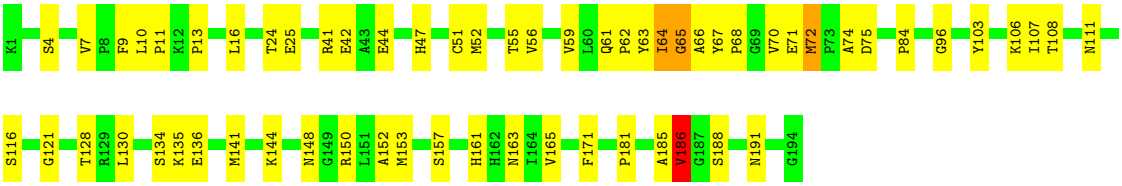




• Molecule 14: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7

Chain I:

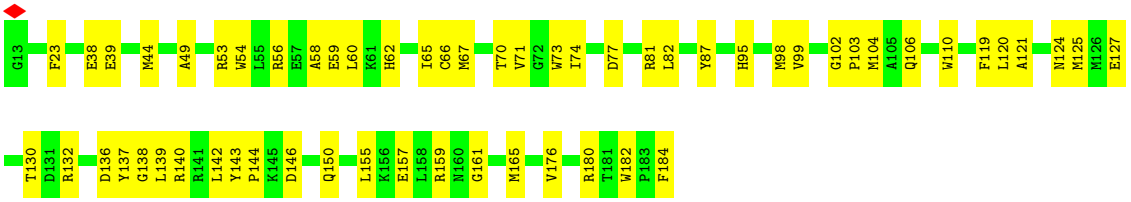




• Molecule 15: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6

Chain K:

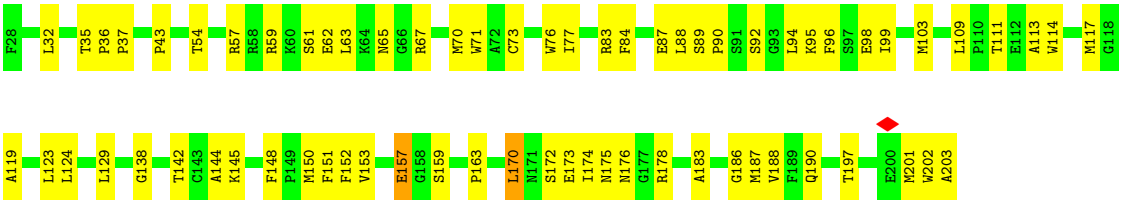




• Molecule 16: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2

Chain F:

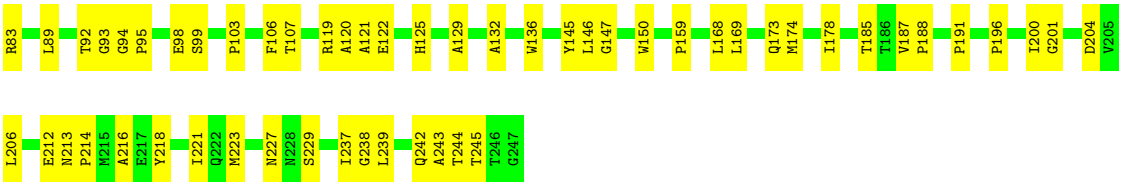




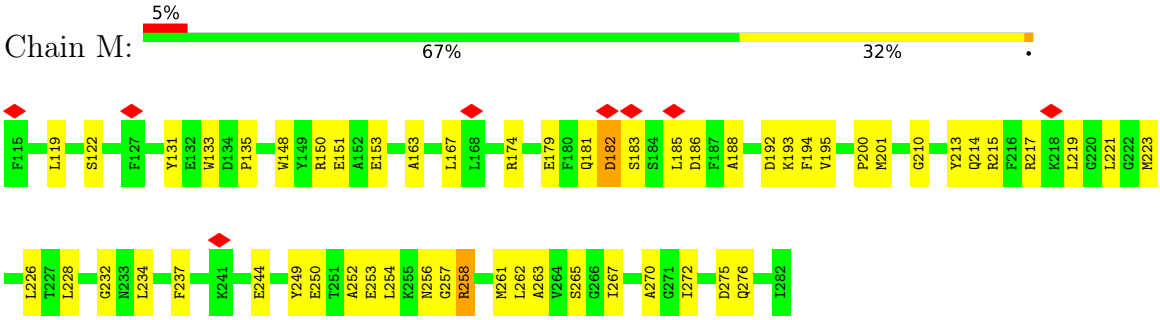
• Molecule 17: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3

Chain J:

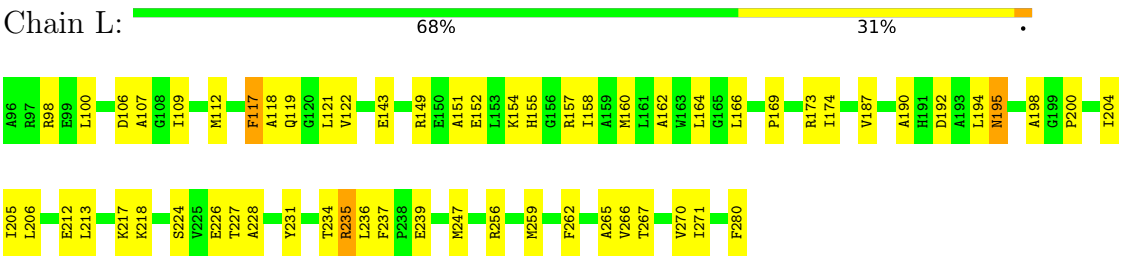




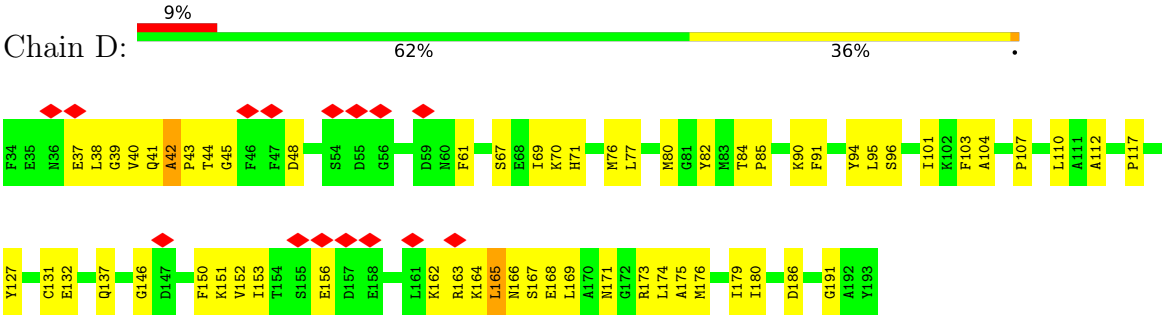
• Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4



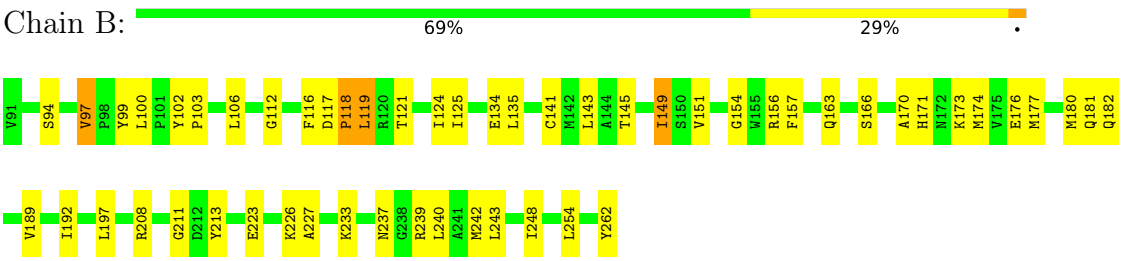
• Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



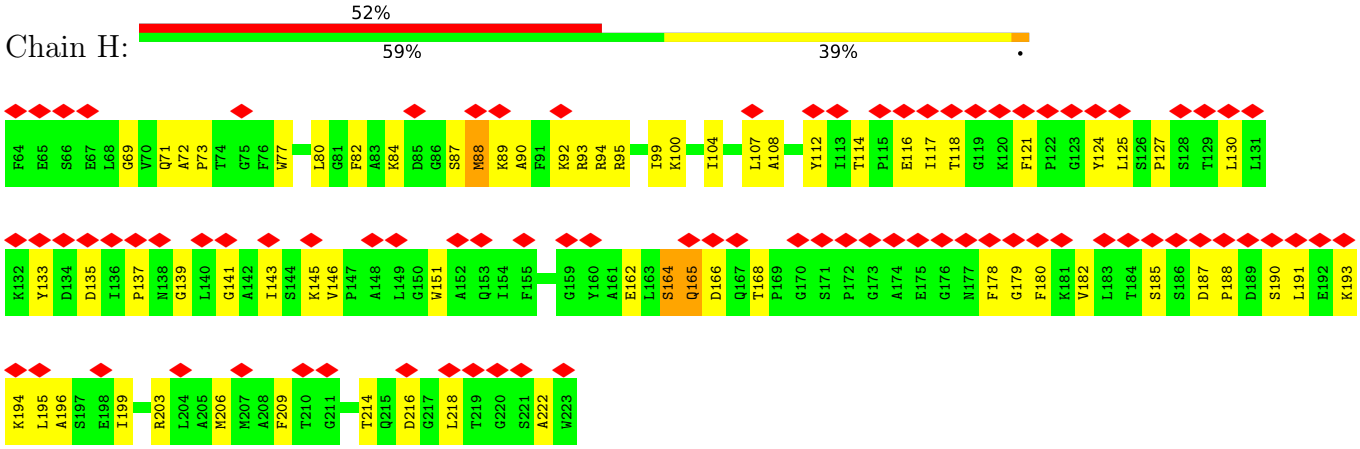
• Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9



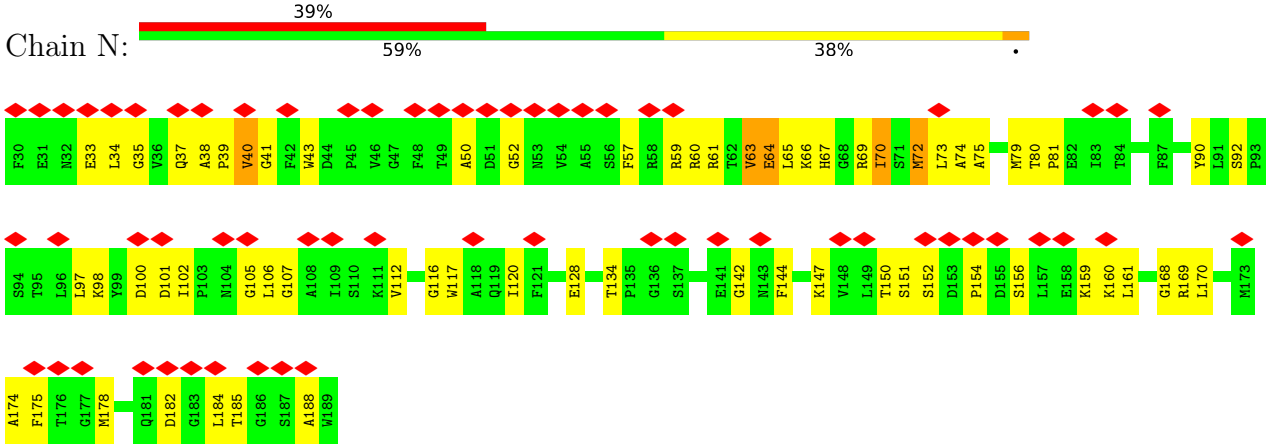
• Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11



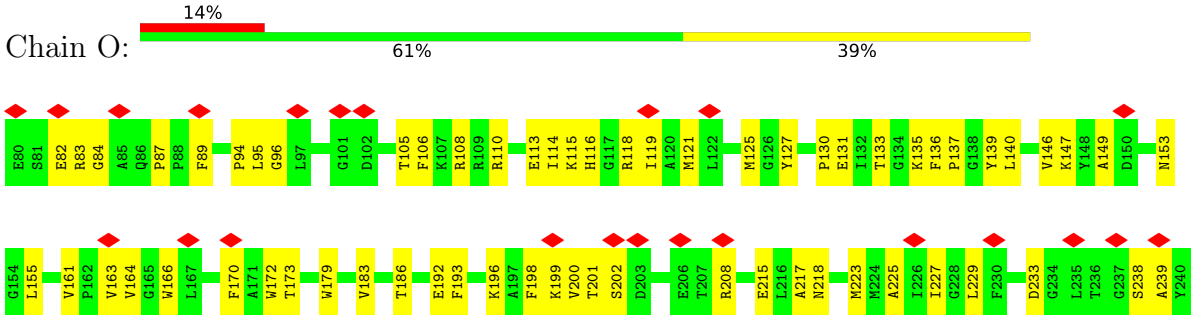
• Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



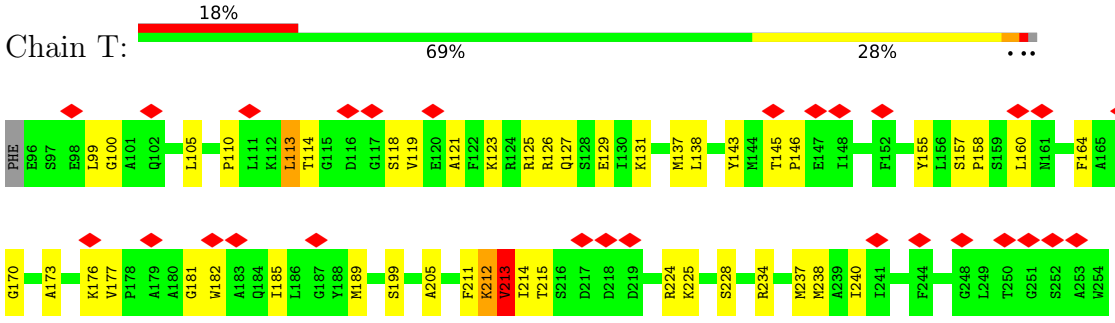
• Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13



• Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15

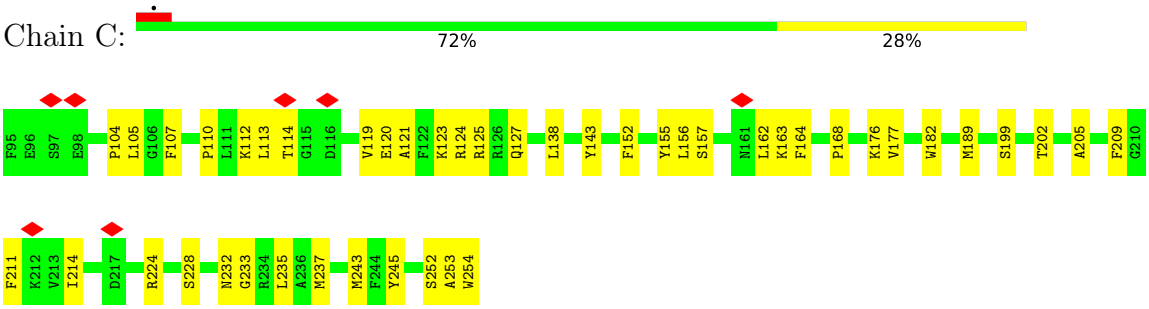


• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16



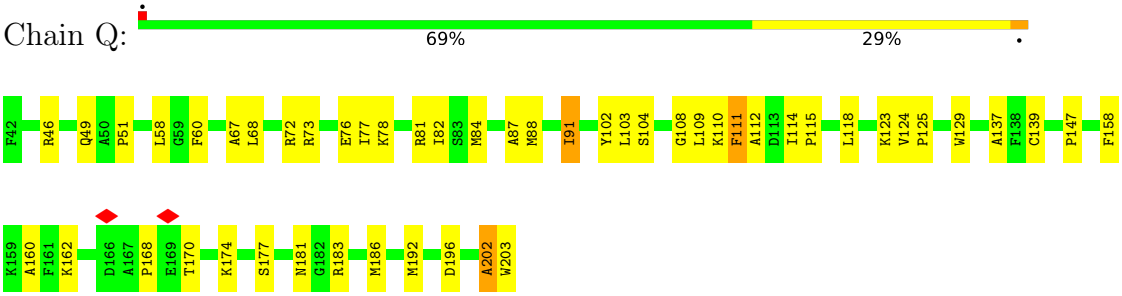
• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16

Chain C:



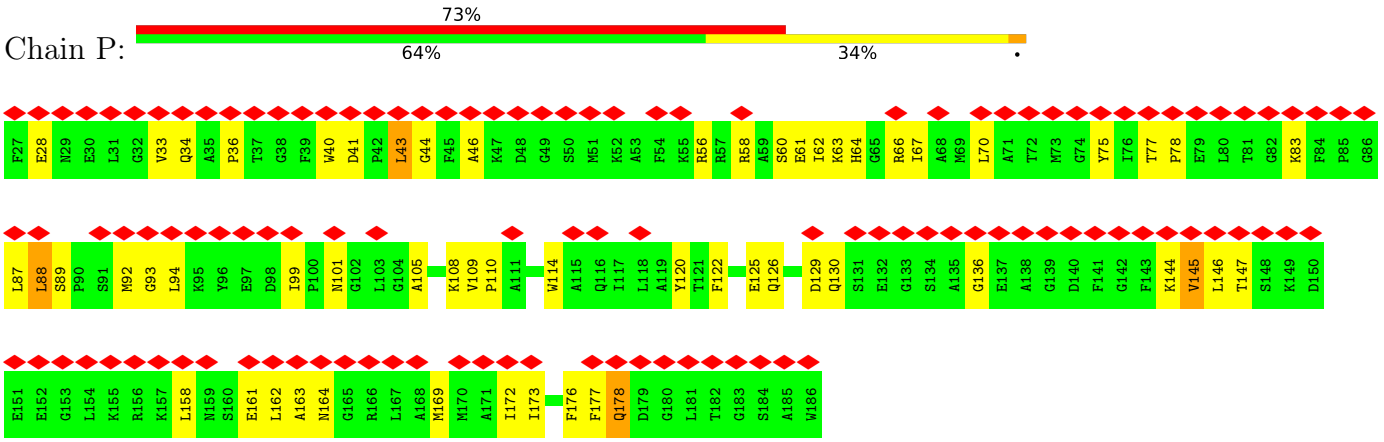
• Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17

Chain Q:



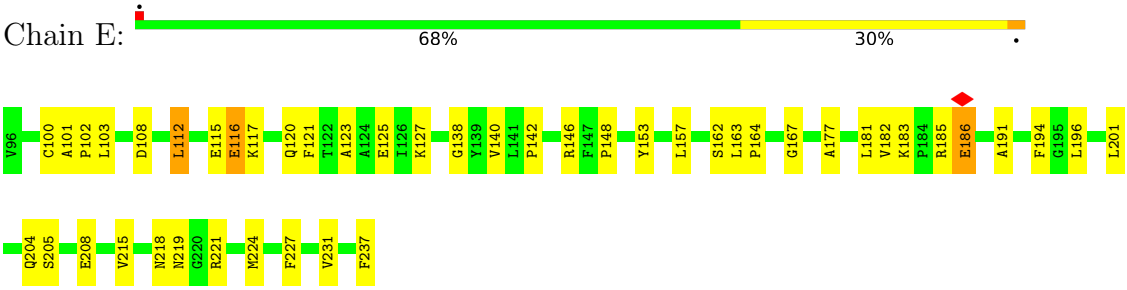
• Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14

Chain P:



• Molecule 28: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	356838	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.883	Depositor
Minimum map value	-0.563	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	665.6, 665.6, 665.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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: CLA, DD6, PQN, KC1, UIX, SF4, DGD, LHG, PID, LMG, SQD, BCR

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	0.30	1/5133 (0.0%)	0.36	0/7019
2	b	0.31	0/4968	0.39	0/6804
3	c	0.20	0/657	0.28	0/897
4	d	0.20	0/2034	0.34	0/2766
5	e	0.16	0/624	0.23	0/851
6	f	0.16	0/1484	0.26	0/1998
7	h	0.28	0/1089	0.43	0/1479
8	i	0.26	0/1030	0.45	0/1394
9	j	0.42	0/566	0.51	0/774
10	l	0.16	0/2014	0.29	0/2737
11	m	0.26	0/694	0.43	0/939
12	A	0.18	0/1395	0.31	0/1892
13	G	0.19	0/1730	0.32	0/2348
14	I	0.28	0/1499	0.42	0/2037
15	K	0.19	0/1358	0.30	0/1838
16	F	0.21	0/1395	0.45	0/1886
17	J	0.18	0/1317	0.38	0/1795
18	M	0.16	0/1395	0.45	0/1888
19	L	0.18	0/1490	0.42	0/2021
20	D	0.19	0/1223	0.46	2/1650 (0.1%)
21	B	0.28	0/1404	0.42	2/1891 (0.1%)
22	H	0.18	0/1232	0.39	0/1665
23	N	0.19	0/1233	0.45	0/1671
24	O	0.20	0/1260	0.45	0/1709
25	C	0.14	0/1226	0.33	0/1653
25	T	0.15	0/1214	0.37	0/1637
26	Q	0.18	0/1251	0.41	0/1690
27	P	0.17	0/1245	0.39	0/1673
28	E	0.19	0/1093	0.44	0/1473
All	All	0.23	1/44253 (0.0%)	0.38	4/60075 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	589	TYR	N-CA	-5.09	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	119	LEU	N-CA-C	-7.66	100.82	111.39
20	D	42	ALA	CA-C-N	-6.56	114.14	120.83
20	D	42	ALA	C-N-CA	-6.56	114.14	120.83
21	B	118	PRO	N-CA-C	-5.14	101.88	112.47

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	4980	0	4912	140	0
2	b	4813	0	4698	164	0
3	c	647	0	628	22	0
4	d	1985	0	1951	54	0
5	e	607	0	582	8	0
6	f	1455	0	1492	43	0
7	h	1056	0	1035	38	0
8	i	1001	0	999	33	0
9	j	549	0	546	20	0
10	l	1961	0	1942	68	0
11	m	679	0	685	28	0
12	A	1358	0	1328	37	0
13	G	1675	0	1614	49	0
14	I	1455	0	1392	45	0
15	K	1325	0	1317	54	0
16	F	1356	0	1315	66	0
17	J	1282	0	1255	45	0
18	M	1346	0	1263	43	0
19	L	1453	0	1423	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	1198	0	1176	52	0
21	B	1371	0	1372	45	0
22	H	1202	0	1182	58	0
23	N	1203	0	1172	56	0
24	O	1226	0	1200	65	0
25	C	1200	0	1185	43	0
25	T	1189	0	1176	43	0
26	Q	1219	0	1210	49	0
27	P	1218	0	1202	51	0
28	E	1071	0	1050	41	0
29	A	616	0	527	19	0
29	B	527	0	473	17	0
29	C	297	0	245	17	0
29	D	318	0	231	20	0
29	E	494	0	461	28	0
29	F	358	0	256	22	0
29	G	565	0	536	30	0
29	H	297	0	245	16	0
29	I	602	0	547	28	0
29	J	400	0	331	18	0
29	K	541	0	431	28	0
29	L	506	0	414	22	0
29	M	435	0	337	16	0
29	N	297	0	245	16	0
29	O	297	0	245	20	0
29	P	297	0	245	20	0
29	Q	311	0	276	19	0
29	T	273	0	198	18	0
29	a	1841	0	1790	120	0
29	b	1676	0	1696	119	0
29	f	152	0	125	8	0
29	h	60	0	59	7	0
29	i	185	0	193	19	0
29	j	52	0	43	0	0
29	l	447	0	438	35	0
30	a	33	0	46	6	0
30	b	33	0	46	3	0
31	a	48	0	69	5	0
32	a	120	0	168	16	0
32	b	120	0	168	19	0
32	f	80	0	112	13	0
32	i	40	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	l	80	0	112	8	0
32	m	40	0	56	8	0
33	a	8	0	0	2	0
33	c	16	0	0	3	0
34	A	37	0	44	2	0
34	E	32	0	34	6	0
34	K	114	0	138	7	0
34	P	27	0	24	1	0
34	b	130	0	170	13	0
34	h	28	0	26	2	0
34	j	43	0	56	3	0
35	B	45	0	48	0	0
35	G	45	0	48	2	0
35	b	57	0	72	2	0
35	h	54	0	69	9	0
35	j	133	0	140	9	0
35	m	66	0	96	5	0
36	A	129	0	0	2	0
36	B	214	0	0	8	0
36	C	43	0	0	1	0
36	D	86	0	0	3	0
36	E	86	0	0	0	0
36	F	86	0	0	2	0
36	G	172	0	0	4	0
36	H	43	0	0	0	0
36	I	215	0	0	4	0
36	J	129	0	0	5	0
36	K	258	0	0	4	0
36	L	172	0	0	2	0
36	M	172	0	0	6	0
36	N	43	0	0	1	0
36	O	43	0	0	2	0
36	P	43	0	0	1	0
36	Q	43	0	0	0	0
36	T	43	0	0	1	0
36	h	43	0	0	0	0
36	m	43	0	0	0	0
37	C	230	0	250	21	0
37	D	230	0	250	20	0
37	E	46	0	50	7	0
37	F	138	0	150	19	0
37	G	138	0	150	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	H	230	0	250	23	0
37	N	230	0	250	21	0
37	O	230	0	250	24	0
37	P	230	0	250	22	0
37	Q	184	0	200	17	0
37	T	276	0	300	20	0
37	h	46	0	50	1	0
37	j	46	0	50	5	0
38	A	47	0	0	0	0
38	B	47	0	0	1	0
38	C	47	0	0	0	0
38	E	47	0	0	1	0
38	F	47	0	0	2	0
38	J	47	0	0	1	0
38	L	47	0	0	0	0
38	N	47	0	0	0	0
38	O	47	0	0	0	0
38	P	47	0	0	0	0
38	Q	47	0	0	0	0
38	T	47	0	0	0	0
39	A	90	0	0	0	0
39	B	45	0	0	0	0
39	C	135	0	0	1	0
39	D	90	0	0	2	0
39	E	90	0	0	2	0
39	F	90	0	0	0	0
39	G	90	0	0	2	0
39	H	135	0	0	2	0
39	I	45	0	0	1	0
39	J	45	0	0	0	0
39	K	45	0	0	0	0
39	L	90	0	0	0	0
39	M	90	0	0	0	0
39	N	135	0	0	5	0
39	O	135	0	0	0	0
39	P	135	0	0	2	0
39	Q	135	0	0	2	0
39	T	135	0	0	0	0
40	B	42	0	48	3	0
40	J	45	0	54	7	0
All	All	63119	0	57239	1854	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 15.

All (1854) 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)
37:F:304:PID:HM11	37:F:304:PID:H8	1.33	1.09
37:H:306:PID:HM11	37:H:306:PID:H8	1.45	0.96
7:h:38:ARG:H	7:h:39:PRO:HD2	1.31	0.95
16:F:183:ALA:HB1	37:F:304:PID:H8	1.52	0.91
37:Q:304:PID:H20	29:Q:313:CLA:HAB	1.55	0.87
29:a:810:CLA:HBB1	32:a:838:BCR:H23C	1.55	0.86
29:a:826:CLA:H41	29:b:702:CLA:HBC2	1.61	0.82
13:G:192:MET:HE1	29:G:312:CLA:HAB	1.63	0.80
16:F:190:GLN:HB3	16:F:201:MET:HG2	1.63	0.80
1:a:403:ALA:HA	29:a:828:CLA:HBA1	1.63	0.79
34:b:730:LMG:H361	29:i:202:CLA:HMA1	1.65	0.79
25:T:167:VAL:HG12	25:T:176:LYS:HB3	1.65	0.79
25:T:125:ARG:HB3	29:T:309:CLA:HHB	1.66	0.78
16:F:144:ALA:HB3	16:F:148:PHE:HB3	1.65	0.78
16:F:123:LEU:HD22	29:J:310:CLA:HBB2	1.66	0.77
29:b:713:CLA:HBC1	35:h:203:DGD:HA31	1.67	0.76
10:l:319:THR:HG21	17:J:213:ASN:HD21	1.49	0.76
29:a:819:CLA:HAB	29:a:824:CLA:H151	1.68	0.76
37:H:304:PID:HM71	37:H:306:PID:H15	1.68	0.76
24:O:83:ARG:HE	24:O:84:GLY:H	1.32	0.76
27:P:146:LEU:HG	37:P:206:PID:H281	1.69	0.75
2:b:192:ILE:HD11	2:b:263:PRO:HD2	1.69	0.75
27:P:125:GLU:HG2	27:P:130:GLN:HE22	1.52	0.75
37:O:305:PID:HM52	29:O:314:CLA:HAB	1.69	0.74
12:A:112:ILE:O	12:A:116:TRP:HB3	1.86	0.74
24:O:218:ASN:HD22	29:O:314:CLA:HBB2	1.52	0.74
35:j:106:DGD:HB32	15:K:120:LEU:HD21	1.69	0.73
37:P:206:PID:HM52	29:P:215:CLA:HAB	1.68	0.73
29:L:316:CLA:HHC	29:L:316:CLA:HBB1	1.70	0.73
25:C:107:PHE:HZ	25:C:113:LEU:HD23	1.51	0.73
29:P:209:CLA:HED3	29:P:209:CLA:H2A	1.71	0.73
29:H:310:CLA:HED2	29:H:310:CLA:H2A	1.71	0.73
2:b:142:GLY:O	11:m:88:ARG:NH1	2.20	0.73
37:C:304:PID:H18	37:C:305:PID:HM62	1.71	0.72
1:a:62:TRP:HA	29:a:808:CLA:HBB2	1.70	0.72
10:l:318:MET:HE3	17:J:206:LEU:HD21	1.71	0.72
20:D:151:LYS:O	20:D:153:ILE:N	2.22	0.72
1:a:480:CYS:HB3	33:a:836:SF4:S4	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:101:LEU:HD22	1:a:564:ALA:HB2	1.71	0.72
7:h:51:LYS:O	13:G:19:GLN:NE2	2.22	0.72
24:O:172:TRP:HD1	37:O:302:PID:H13	1.55	0.72
10:l:335:ARG:NH2	17:J:204:ASP:O	2.23	0.72
21:B:151:VAL:O	21:B:156:ARG:NH1	2.22	0.72
29:b:705:CLA:H3A	29:b:705:CLA:CGA	2.18	0.72
16:F:183:ALA:CB	37:F:304:PID:H8	2.20	0.71
22:H:135:ASP:O	22:H:145:LYS:NZ	2.23	0.71
23:N:144:PHE:HB3	37:N:304:PID:HM23	1.72	0.71
1:a:367:LEU:HB3	1:a:437:PHE:HB2	1.73	0.71
37:F:304:PID:HM11	37:F:304:PID:C8	2.13	0.71
37:O:305:PID:H20	29:O:314:CLA:HMC3	1.70	0.71
24:O:119:ILE:HD11	37:O:302:PID:HM22	1.73	0.70
11:m:88:ARG:HB2	11:m:89:PRO:HD3	1.73	0.70
16:F:175:ASN:ND2	29:F:307:CLA:O1D	2.22	0.70
26:Q:102:TYR:HA	26:Q:110:LYS:HA	1.72	0.70
3:c:14:THR:HA	3:c:27:MET:HE3	1.72	0.70
4:d:221:PRO:HG2	8:i:123:VAL:HG12	1.71	0.69
21:B:94:SER:HB3	21:B:102:TYR:HA	1.73	0.69
25:T:118:SER:HB2	25:T:121:ALA:HB3	1.74	0.69
24:O:125:MET:HE1	37:O:305:PID:H22	1.75	0.69
29:a:810:CLA:HAB	29:b:721:CLA:HMD2	1.74	0.69
29:b:707:CLA:H93	34:b:732:LMG:H372	1.73	0.69
24:O:201:THR:HG21	25:T:121:ALA:HB2	1.72	0.69
11:m:64:MET:O	11:m:69:LYS:NZ	2.26	0.69
11:m:77:PHE:HD1	11:m:88:ARG:HH21	1.39	0.69
19:L:121:LEU:HB3	19:L:149:ARG:HH21	1.58	0.69
27:P:87:LEU:O	27:P:89:SER:N	2.26	0.69
8:i:131:LEU:HD22	8:i:137:ARG:HH21	1.59	0.68
19:L:117:PHE:O	19:L:119:GLN:N	2.26	0.68
29:b:723:CLA:H152	32:f:804:BCR:H23C	1.75	0.68
7:h:51:LYS:HB3	35:h:203:DGD:HE4	1.75	0.68
19:L:122:VAL:O	19:L:149:ARG:NH2	2.27	0.68
10:l:281:SER:O	10:l:286:LYS:NZ	2.27	0.68
2:b:245:LEU:HD21	29:b:718:CLA:HAB	1.76	0.68
1:a:171:GLY:O	1:a:175:LEU:HB2	1.92	0.68
3:c:40:SER:HB2	4:d:166:VAL:H	1.58	0.68
7:h:38:ARG:N	7:h:39:PRO:HD2	2.04	0.68
28:E:120:GLN:NE2	39:E:307:KC1:O2A	2.26	0.68
1:a:184:LEU:HA	1:a:188:SER:HB3	1.74	0.67
4:d:84:ILE:HD11	4:d:119:CYS:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:208:CLA:HAC1	29:A:215:CLA:HAB	1.76	0.67
29:b:726:CLA:H191	32:b:735:BCR:H10C	1.75	0.67
7:h:40:PHE:HZ	7:h:47:TRP:CD2	2.12	0.67
20:D:174:LEU:HD22	29:D:308:CLA:HBC1	1.75	0.67
22:H:71:GLN:HE22	22:H:196:ALA:HB1	1.59	0.67
6:f:13:LYS:HD3	29:f:805:CLA:HBB1	1.75	0.67
4:d:53:ARG:NH1	4:d:140:SER:O	2.27	0.67
20:D:67:SER:O	20:D:71:HIS:ND1	2.28	0.67
37:H:304:PID:H18	37:H:305:PID:HM62	1.75	0.67
14:I:75:ASP:OD1	14:I:163:ASN:ND2	2.27	0.67
2:b:17:HIS:ND1	29:b:707:CLA:O1A	2.27	0.67
4:d:86:TRP:HE1	4:d:104:MET:HE3	1.59	0.67
1:a:563:ALA:HB1	2:b:349:ALA:HB1	1.76	0.67
20:D:48:ASP:HA	36:D:304:DD6:O2	1.94	0.67
14:I:59:VAL:HG13	14:I:171:PHE:HZ	1.59	0.66
16:F:71:TRP:CD1	29:F:310:CLA:HAB	2.30	0.66
29:H:313:CLA:HBA2	29:H:313:CLA:HED2	1.76	0.66
10:l:370:ALA:HB1	29:l:504:CLA:HMA3	1.78	0.66
26:Q:110:LYS:O	26:Q:112:ALA:N	2.28	0.66
18:M:249:TYR:CD2	29:M:311:CLA:H3A	2.31	0.66
22:H:93:ARG:NH1	39:H:309:KC1:O2A	2.28	0.66
19:L:169:PRO:O	19:L:173:ARG:NH1	2.29	0.66
11:m:34:ILE:HD11	32:m:103:BCR:H281	1.77	0.66
14:I:128:THR:HB	26:Q:67:ALA:HB1	1.76	0.66
37:P:205:PID:H18	37:P:206:PID:HM62	1.77	0.66
2:b:62:PHE:HA	2:b:69:VAL:HG11	1.77	0.66
16:F:32:LEU:HD11	16:F:163:PRO:HB3	1.78	0.66
2:b:360:GLU:OE1	6:f:96:ARG:NH1	2.27	0.65
29:b:718:CLA:H91	34:b:732:LMG:H371	1.77	0.65
6:f:38:ASN:ND2	6:f:88:CYS:O	2.29	0.65
19:L:154:LYS:NZ	19:L:212:GLU:OE2	2.23	0.65
10:l:320:LEU:HD23	29:l:501:CLA:HED1	1.77	0.65
1:a:540:ASN:HB2	2:b:536:LEU:HD11	1.77	0.65
24:O:139:TYR:HA	24:O:147:LYS:HA	1.77	0.65
27:P:64:HIS:HB3	27:P:169:MET:SD	2.37	0.65
2:b:118:LEU:HD22	11:m:35:ILE:HD12	1.78	0.65
2:b:258:GLN:HA	2:b:261:VAL:HG12	1.79	0.65
4:d:74:MET:HB3	4:d:77:ALA:HB3	1.77	0.65
29:b:719:CLA:H2	29:G:302:CLA:H61	1.78	0.65
7:h:103:PHE:HB2	29:h:201:CLA:H12	1.79	0.65
1:a:538:ASN:HB2	1:a:541:GLY:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:702:CLA:HBC1	30:b:727:PQN:H193	1.78	0.65
37:P:202:PID:HM22	29:P:210:CLA:HAC2	1.79	0.65
36:M:302:DD6:C24	29:M:307:CLA:HAB	2.27	0.64
25:T:238:MET:HE1	29:T:309:CLA:HAC1	1.79	0.64
2:b:218:ILE:HD11	29:b:731:CLA:HMA3	1.78	0.64
10:l:438:ASN:ND2	29:l:510:CLA:O1D	2.30	0.64
26:Q:115:PRO:HD2	26:Q:123:LYS:HG3	1.78	0.64
8:i:145:GLU:HA	8:i:160:VAL:HG21	1.78	0.64
10:l:385:LEU:HD12	10:l:394:VAL:HG21	1.80	0.64
22:H:124:TYR:HD2	22:H:127:PRO:HA	1.60	0.64
25:T:224:ARG:NH1	25:T:228:SER:OG	2.30	0.64
37:P:208:PID:HM51	37:P:208:PID:HM83	1.79	0.64
9:j:39:LEU:HD12	35:j:106:DGD:HA41	1.78	0.64
10:l:215:ARG:NH2	19:L:143:GLU:OE1	2.29	0.64
16:F:87:GLU:HA	16:F:95:LYS:HA	1.80	0.64
14:I:144:LYS:O	14:I:148:ASN:ND2	2.29	0.64
10:l:305:LEU:HD13	10:l:318:MET:HE2	1.78	0.64
11:m:27:SER:HB3	36:B:319:DD6:O2	1.98	0.64
12:A:127:LEU:HB2	29:A:217:CLA:HED3	1.79	0.64
20:D:37:GLU:HG3	20:D:61:PHE:HZ	1.63	0.64
13:G:201:ASN:ND2	13:G:211:LEU:O	2.31	0.64
17:J:174:MET:HA	29:J:309:CLA:HBC3	1.80	0.64
37:N:305:PID:H20	29:N:314:CLA:HMC3	1.80	0.64
29:b:702:CLA:H152	32:l:506:BCR:H17C	1.81	0.63
7:h:15:PHE:HD1	8:i:144:LEU:HD21	1.63	0.63
16:F:71:TRP:HD1	29:F:310:CLA:HAB	1.60	0.63
1:a:225:LEU:HG	1:a:226:THR:HG23	1.80	0.63
2:b:142:GLY:C	11:m:88:ARG:NH1	2.57	0.63
38:J:304:UIX:C35	29:J:311:CLA:HAB	2.28	0.63
1:a:299:PRO:HB3	1:a:305:LEU:HD11	1.78	0.63
21:B:106:LEU:HD11	21:B:117:ASP:HB2	1.81	0.63
23:N:105:GLY:O	23:N:107:GLY:N	2.32	0.63
24:O:218:ASN:HD21	37:O:305:PID:H17	1.64	0.63
10:l:355:ARG:NH2	10:l:366:GLU:OE1	2.32	0.63
12:A:123:PRO:HB2	21:B:119:LEU:HA	1.80	0.63
14:I:130:LEU:HD11	29:I:214:CLA:HMA2	1.81	0.63
21:B:174:MET:HG2	29:B:310:CLA:HAA2	1.80	0.63
22:H:94:ARG:HD2	29:H:308:CLA:H12	1.80	0.63
14:I:63:TYR:O	14:I:64:ILE:C	2.41	0.63
28:E:115:GLU:O	28:E:117:LYS:N	2.32	0.63
1:a:382:GLN:OE1	1:a:538:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:97:PRO:HG3	2:b:278:LEU:HD11	1.80	0.63
29:b:707:CLA:H101	29:b:716:CLA:HBC1	1.81	0.63
9:j:54:SER:O	9:j:58:ILE:HG12	1.98	0.63
10:l:365:LEU:HG	10:l:369:MET:HE2	1.81	0.63
24:O:147:LYS:HG3	24:O:149:ALA:H	1.63	0.63
37:E:301:PID:HM53	29:E:313:CLA:HBC2	1.79	0.63
22:H:104:ILE:HD11	37:H:302:PID:HM22	1.81	0.62
1:a:577:ALA:HB3	29:a:802:CLA:HBB2	1.81	0.62
1:a:530:SER:O	1:a:533:GLU:N	2.33	0.62
10:l:276:ASP:H	10:l:280:VAL:HG11	1.64	0.62
29:l:503:CLA:HAA1	29:F:312:CLA:H3A	1.81	0.62
16:F:152:PHE:HE2	37:F:306:PID:H8	1.65	0.62
26:Q:72:ARG:HD3	29:Q:308:CLA:H12	1.80	0.62
15:K:98:MET:HG3	29:K:211:CLA:HAA2	1.80	0.62
21:B:157:PHE:O	21:B:163:GLN:NE2	2.32	0.62
13:G:20:PRO:HB2	37:G:310:PID:H27	1.82	0.62
36:J:302:DD6:C3	29:J:309:CLA:HAC2	2.30	0.62
26:Q:88:MET:HE1	37:Q:304:PID:HM52	1.81	0.62
37:P:205:PID:H19	29:P:212:CLA:HAC1	1.80	0.62
32:a:834:BCR:H362	32:a:835:BCR:H21C	1.80	0.62
14:I:134:SER:O	14:I:136:GLU:N	2.33	0.62
22:H:80:LEU:HB2	22:H:82:PHE:CE1	2.34	0.62
24:O:105:THR:HG22	24:O:108:ARG:HH12	1.65	0.62
26:Q:177:SER:O	26:Q:181:ASN:ND2	2.30	0.62
29:b:714:CLA:HMA1	32:b:728:BCR:H17C	1.81	0.62
29:h:201:CLA:HBC1	34:h:205:LMG:HC71	1.81	0.62
26:Q:49:GLN:NE2	29:Q:307:CLA:O1D	2.32	0.62
2:b:575:GLU:OE2	4:d:7:LYS:N	2.32	0.62
21:B:121:THR:HG21	29:B:308:CLA:H2	1.80	0.62
11:m:85:SER:O	11:m:88:ARG:HG3	2.00	0.61
19:L:149:ARG:NH1	19:L:152:GLU:OE1	2.32	0.61
27:P:75:TYR:O	27:P:101:ASN:ND2	2.32	0.61
1:a:492:LEU:HD21	29:a:825:CLA:HBC1	1.82	0.61
2:b:547:MET:HB2	29:b:705:CLA:C1C	2.31	0.61
20:D:37:GLU:HG3	20:D:61:PHE:CZ	2.35	0.61
21:B:233:LYS:O	21:B:237:ASN:ND2	2.30	0.61
24:O:114:ILE:HG12	24:O:118:ARG:HE	1.65	0.61
29:a:804:CLA:HED2	29:a:837:CLA:HBA1	1.83	0.61
6:f:24:LEU:HG	29:f:803:CLA:HBC3	1.82	0.61
17:J:213:ASN:HB3	17:J:216:ALA:HB2	1.81	0.61
1:a:171:GLY:HA2	1:a:175:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:188:SER:O	1:a:192:ASN:ND2	2.30	0.61
3:c:13:CYS:N	33:c:102:SF4:S1	2.73	0.61
4:d:218:LEU:HD11	7:h:29:GLU:HG3	1.82	0.61
23:N:182:ASP:HB3	23:N:188:ALA:HA	1.81	0.61
29:b:719:CLA:HHC	29:b:724:CLA:HBB2	1.82	0.61
13:G:183:GLN:NE2	39:G:318:KC1:O2A	2.32	0.61
17:J:83:ARG:HH12	23:N:134:THR:HG21	1.64	0.61
5:e:11:VAL:HG12	5:e:64:GLU:HA	1.81	0.61
10:l:352:ALA:H	29:l:504:CLA:HED1	1.65	0.61
22:H:162:GLU:HG3	37:H:302:PID:HM32	1.82	0.61
36:O:303:DD6:C10	29:O:309:CLA:HAB	2.30	0.61
29:b:720:CLA:HBB2	32:f:801:BCR:HC41	1.83	0.61
12:A:21:ILE:O	12:A:51:ARG:NH1	2.28	0.61
13:G:44:ASP:OD2	13:G:186:LYS:NZ	2.34	0.61
37:C:301:PID:HM22	29:C:309:CLA:HAC2	1.82	0.61
4:d:65:LEU:HB3	4:d:103:MET:HB3	1.83	0.61
37:Q:304:PID:C20	29:Q:313:CLA:HAB	2.30	0.61
28:E:177:ALA:O	28:E:181:LEU:HB2	2.00	0.61
8:i:74:ILE:HG13	29:i:203:CLA:HBB2	1.83	0.61
18:M:252:ALA:O	18:M:256:ASN:ND2	2.30	0.61
24:O:200:VAL:HG23	29:O:314:CLA:HBA1	1.83	0.61
1:a:531:ASP:OD1	1:a:535:ASN:ND2	2.34	0.60
4:d:190:LYS:HE2	8:i:176:TRP:HE1	1.65	0.60
9:j:16:ARG:NH1	9:j:22:GLU:OE2	2.33	0.60
29:F:311:CLA:HMA3	17:J:168:LEU:HD11	1.84	0.60
2:b:38:GLN:HG3	29:b:706:CLA:HHB	1.83	0.60
25:C:143:TYR:HD2	25:C:243:MET:HE2	1.67	0.60
32:b:729:BCR:H312	34:b:730:LMG:H311	1.83	0.60
20:D:167:SER:O	20:D:171:ASN:ND2	2.34	0.60
21:B:124:ILE:HG23	21:B:125:ILE:HG12	1.82	0.60
1:a:357:LEU:HB3	2:b:562:THR:HG21	1.84	0.60
7:h:118:PHE:CZ	29:G:304:CLA:HBB1	2.36	0.60
29:l:505:CLA:HBC2	29:J:309:CLA:HBB2	1.82	0.60
37:T:307:PID:HM83	37:T:307:PID:HM51	1.83	0.60
28:E:215:VAL:O	28:E:219:ASN:ND2	2.32	0.60
29:a:807:CLA:H71	31:a:833:LHG:H321	1.84	0.60
29:b:731:CLA:OBD	7:h:119:TRP:NE1	2.33	0.60
10:l:367:ILE:HG21	32:l:506:BCR:H282	1.83	0.60
15:K:125:MET:SD	15:K:132:ARG:NH1	2.75	0.60
23:N:38:ALA:HB3	23:N:39:PRO:HD3	1.84	0.60
25:T:129:GLU:OE2	25:T:234:ARG:NE	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:213:VAL:HA	1:a:216:ILE:HB	1.84	0.60
13:G:33:SER:OG	13:G:58:HIS:O	2.20	0.60
1:a:389:ASP:OD1	10:l:386:ARG:NH2	2.34	0.60
35:b:733:DGD:HE2	4:d:212:VAL:HG11	1.84	0.60
10:l:411:LEU:HB3	34:E:316:LMG:H111	1.83	0.60
15:K:58:ALA:HB2	29:K:213:CLA:HED2	1.83	0.60
29:a:806:CLA:H51	32:a:835:BCR:HC8	1.83	0.59
29:a:823:CLA:HBC3	31:a:833:LHG:H382	1.84	0.59
35:j:103:DGD:O4D	35:j:103:DGD:O5D	2.17	0.59
16:F:159:SER:HB2	22:H:84:LYS:HD3	1.83	0.59
25:C:245:TYR:CD2	29:C:316:CLA:HAC2	2.37	0.59
2:b:71:PRO:HG2	2:b:94:THR:HB	1.85	0.59
2:b:443:ALA:HB1	2:b:589:ILE:HD12	1.85	0.59
27:P:28:GLU:HG3	27:P:33:VAL:HG11	1.85	0.59
15:K:119:PHE:HB2	29:K:213:CLA:HMA1	1.82	0.59
26:Q:162:LYS:HD3	25:C:124:ARG:HD2	1.82	0.59
1:a:280:GLN:HE22	29:a:821:CLA:HAA1	1.68	0.59
29:a:802:CLA:H3A	29:a:802:CLA:CGA	2.32	0.59
4:d:84:ILE:HD12	4:d:122:LEU:HD23	1.84	0.59
28:E:116:GLU:OE2	28:E:117:LYS:NZ	2.32	0.59
27:P:158:LEU:HD13	27:P:161:GLU:HG3	1.84	0.59
2:b:85:LYS:O	2:b:89:THR:HG22	2.02	0.59
6:f:162:TRP:NE1	13:G:55:LEU:O	2.36	0.59
7:h:33:LYS:O	7:h:39:PRO:HG3	2.02	0.59
29:i:202:CLA:H71	32:i:204:BCR:HC32	1.84	0.59
14:I:41:ARG:NH1	14:I:44:GLU:OE1	2.35	0.59
16:F:145:LYS:HG3	29:F:313:CLA:HAA1	1.84	0.59
23:N:61:ARG:NH2	29:N:309:CLA:O1D	2.35	0.59
37:N:301:PID:H7	29:N:309:CLA:HBC1	1.83	0.59
23:N:72:MET:SD	23:N:168:GLY:HA2	2.42	0.59
24:O:200:VAL:HG11	24:O:208:ARG:HA	1.84	0.59
25:T:126:ARG:NH1	25:T:129:GLU:OE1	2.35	0.59
27:P:77:THR:HG21	29:P:212:CLA:HAC2	1.85	0.59
4:d:222:LYS:NZ	4:d:224:THR:O	2.35	0.59
29:i:202:CLA:H151	32:i:204:BCR:H313	1.83	0.59
21:B:239:ARG:HA	21:B:242:MET:HE3	1.84	0.59
22:H:180:PHE:HE2	37:H:305:PID:H282	1.67	0.59
23:N:63:VAL:HG23	23:N:67:HIS:CE1	2.38	0.59
36:N:303:DD6:C10	29:N:309:CLA:HAB	2.32	0.59
25:C:245:TYR:HD2	29:C:316:CLA:HAC2	1.67	0.59
2:b:355:LYS:HE2	6:f:79:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:64:ASN:HD21	13:G:73:TYR:H	1.50	0.58
15:K:95:HIS:ND1	15:K:95:HIS:O	2.36	0.58
3:c:60:ASP:OD2	5:e:15:ARG:NH1	2.36	0.58
4:d:17:ARG:NH2	4:d:77:ALA:O	2.33	0.58
1:a:553:GLN:O	1:a:557:SER:OG	2.20	0.58
13:G:79:LEU:HD13	29:G:312:CLA:H11	1.84	0.58
21:B:118:PRO:O	21:B:119:LEU:C	2.44	0.58
29:a:804:CLA:H51	30:a:832:PQN:H211	1.85	0.58
16:F:88:LEU:HD11	29:F:310:CLA:HBA2	1.85	0.58
3:c:60:ASP:OD1	3:c:61:PHE:N	2.36	0.58
7:h:37:ARG:HH11	7:h:37:ARG:HG3	1.68	0.58
29:i:201:CLA:H18	32:m:103:BCR:H362	1.84	0.58
29:l:503:CLA:H121	32:l:507:BCR:H363	1.83	0.58
23:N:59:ARG:O	23:N:63:VAL:HG12	2.02	0.58
2:b:311:LEU:HD23	35:h:203:DGD:HBS1	1.86	0.58
13:G:70:LEU:HD22	29:G:302:CLA:H43	1.84	0.58
37:D:303:PID:HM61	29:D:312:CLA:HAA1	1.85	0.58
22:H:188:PRO:HD2	22:H:190:SER:HB3	1.85	0.58
29:b:716:CLA:H11	34:b:730:LMG:H142	1.86	0.58
16:F:148:PHE:HA	37:F:304:PID:H281	1.85	0.58
18:M:257:GLY:O	18:M:261:MET:HG3	2.04	0.58
37:T:304:PID:H15	37:T:305:PID:HM72	1.86	0.58
26:Q:46:ARG:O	26:Q:73:ARG:NH2	2.36	0.58
28:E:103:LEU:HD11	29:E:306:CLA:HMD1	1.84	0.58
1:a:92:VAL:HB	1:a:102:ASN:HA	1.85	0.58
2:b:206:HIS:HB3	29:b:711:CLA:HMB2	1.85	0.58
13:G:53:ASP:OD2	13:G:58:HIS:ND1	2.27	0.58
28:E:102:PRO:HG3	29:E:305:CLA:C4B	2.34	0.58
2:b:193:GLN:HG3	2:b:200:ALA:HB2	1.85	0.58
10:l:350:ASN:O	10:l:355:ARG:NH1	2.33	0.57
15:K:103:PRO:HD3	29:K:212:CLA:HED2	1.86	0.57
15:K:127:GLU:OE1	15:K:127:GLU:N	2.36	0.57
19:L:158:ILE:HD12	29:L:312:CLA:HMD3	1.86	0.57
37:N:307:PID:HM83	37:N:307:PID:HM51	1.85	0.57
37:O:304:PID:H18	37:O:305:PID:HM62	1.86	0.57
27:P:88:LEU:HB3	27:P:94:LEU:HB3	1.85	0.57
2:b:430:TYR:OH	6:f:179:VAL:O	2.23	0.57
10:l:415:ALA:HA	34:E:316:LMG:HC2	1.86	0.57
29:l:503:CLA:H62	29:l:503:CLA:HBB1	1.85	0.57
12:A:53:ALA:O	12:A:57:HIS:ND1	2.32	0.57
29:a:826:CLA:HBB1	29:a:827:CLA:H2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:56:ARG:NH1	15:K:59:GLU:OE1	2.36	0.57
16:F:35:THR:HG22	16:F:37:PRO:HD2	1.86	0.57
18:M:148:TRP:HZ3	18:M:223:MET:HG3	1.68	0.57
23:N:169:ARG:HB3	29:N:309:CLA:HAC2	1.85	0.57
1:a:127:VAL:HG11	29:a:817:CLA:H3A	1.86	0.57
24:O:127:TYR:OH	24:O:239:ALA:O	2.22	0.57
27:P:34:GLN:HG3	27:P:36:PRO:HD2	1.85	0.57
27:P:63:LYS:O	27:P:67:ILE:HG12	2.03	0.57
1:a:217:VAL:HG22	1:a:219:GLN:H	1.69	0.57
1:a:354:ASP:OD1	1:a:452:TYR:OH	2.22	0.57
1:a:386:ARG:HG2	2:b:82:SER:HB3	1.87	0.57
2:b:311:LEU:HD21	35:h:203:DGD:HBE2	1.85	0.57
24:O:130:PRO:HB3	24:O:136:PHE:HZ	1.70	0.57
2:b:137:GLY:HA2	11:m:67:PHE:HE2	1.69	0.57
32:f:804:BCR:H353	29:G:301:CLA:H11	1.85	0.57
17:J:169:LEU:HD22	40:J:314:SQD:H462	1.87	0.57
18:M:182:ASP:OD1	18:M:183:SER:N	2.31	0.57
20:D:76:MET:HE1	29:D:314:CLA:HAB	1.87	0.57
21:B:174:MET:HE3	29:B:310:CLA:H2A	1.85	0.57
37:T:301:PID:H13	29:T:316:CLA:HAB	1.86	0.57
1:a:474:PRO:HD3	2:b:446:GLY:HA2	1.84	0.57
2:b:540:LEU:HG	29:b:726:CLA:HAB	1.87	0.57
12:A:52:GLU:HG3	12:A:136:LEU:HD13	1.86	0.57
14:I:141:MET:SD	39:I:215:KC1:O2A	2.63	0.57
26:Q:168:PRO:C	26:Q:170:THR:H	2.12	0.57
25:C:199:SER:O	25:C:202:THR:OG1	2.22	0.57
23:N:70:ILE:HD11	37:N:302:PID:HM22	1.87	0.57
1:a:476:ARG:NH2	4:d:117:GLU:OE2	2.38	0.57
6:f:88:CYS:HB3	6:f:95:PRO:HA	1.86	0.57
29:l:505:CLA:H91	40:J:314:SQD:H302	1.86	0.57
24:O:161:VAL:HB	24:O:166:TRP:NE1	2.20	0.57
25:C:104:PRO:HD3	29:C:308:CLA:C1B	2.35	0.57
28:E:157:LEU:HD11	28:E:231:VAL:HG23	1.85	0.57
14:I:150:ARG:HA	14:I:153:MET:HE3	1.87	0.56
27:P:158:LEU:O	27:P:161:GLU:HB2	2.05	0.56
12:A:164:LYS:O	12:A:168:ASN:ND2	2.30	0.56
16:F:183:ALA:HB1	37:F:304:PID:HM11	1.86	0.56
1:a:294:MET:HA	1:a:297:ALA:HB3	1.87	0.56
2:b:72:ILE:O	2:b:99:TYR:OH	2.22	0.56
2:b:144:LEU:H	11:m:89:PRO:HD2	1.70	0.56
29:b:705:CLA:HBC2	29:b:705:CLA:HHD	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:166:LEU:HA	19:L:187:VAL:HG21	1.87	0.56
23:N:69:ARG:HB3	29:N:314:CLA:HAC2	1.86	0.56
37:E:301:PID:HM83	37:E:301:PID:H20	1.87	0.56
29:a:820:CLA:H52	29:l:504:CLA:H93	1.87	0.56
38:B:304:UIX:C38	29:B:312:CLA:HAB	2.35	0.56
25:C:112:LYS:HZ3	25:C:125:ARG:HD3	1.70	0.56
22:H:166:ASP:HB2	22:H:168:THR:HG23	1.87	0.56
27:P:40:TRP:HB3	29:P:210:CLA:HMD3	1.87	0.56
2:b:125:ALA:HB2	11:m:39:VAL:HG22	1.88	0.56
20:D:151:LYS:HD3	29:D:314:CLA:HBA1	1.86	0.56
24:O:110:ARG:NH1	24:O:113:GLU:OE1	2.38	0.56
16:F:84:PHE:HB2	16:F:96:PHE:CG	2.41	0.56
19:L:121:LEU:HD21	19:L:149:ARG:HB2	1.87	0.56
24:O:115:LYS:HZ2	37:O:302:PID:H42	1.71	0.56
7:h:44:GLU:HB3	7:h:56:ASN:HB3	1.87	0.56
26:Q:139:CYS:SG	37:Q:303:PID:H8	2.46	0.56
10:l:428:THR:OG1	10:l:431:SER:OG	2.21	0.56
14:I:66:ALA:HB2	14:I:72:MET:HE3	1.88	0.56
19:L:236:LEU:HD23	19:L:236:LEU:H	1.71	0.56
29:b:707:CLA:H51	34:b:732:LMG:H312	1.86	0.56
29:b:719:CLA:HAB	29:b:724:CLA:HBB2	1.87	0.56
7:h:15:PHE:CD1	8:i:144:LEU:HD21	2.41	0.56
36:I:205:DD6:C24	29:I:214:CLA:HAB	2.35	0.56
22:H:179:GLY:N	29:H:313:CLA:OBD	2.38	0.56
26:Q:87:ALA:HA	26:Q:192:MET:HE1	1.87	0.56
25:C:228:SER:O	25:C:232:ASN:ND2	2.36	0.56
28:E:100:CYS:SG	28:E:218:ASN:ND2	2.79	0.56
27:P:125:GLU:HG3	37:P:203:PID:HM32	1.88	0.55
1:a:378:ASN:HD22	1:a:537:ILE:HB	1.71	0.55
34:j:102:LMG:H131	34:K:201:LMG:H342	1.87	0.55
14:I:70:VAL:HG11	14:I:84:PRO:HD3	1.87	0.55
20:D:95:LEU:HD12	37:D:303:PID:H22	1.88	0.55
37:Q:301:PID:C16	29:Q:310:CLA:H2	2.36	0.55
27:P:145:VAL:HG13	27:P:146:LEU:H	1.71	0.55
32:m:103:BCR:H292	28:E:140:VAL:HG11	1.86	0.55
29:D:314:CLA:HBA2	29:D:314:CLA:HED2	1.88	0.55
28:E:146:ARG:NH1	28:E:153:TYR:O	2.38	0.55
1:a:155:ARG:HB3	1:a:159:THR:HB	1.88	0.55
26:Q:81:ARG:HB3	29:Q:313:CLA:HAC2	1.89	0.55
29:b:717:CLA:H102	29:b:717:CLA:HBC2	1.88	0.55
37:j:101:PID:HM51	37:j:101:PID:HM83	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:147:GLY:HA2	17:J:150:TRP:HB2	1.89	0.55
20:D:127:TYR:CD2	37:D:303:PID:H11	2.42	0.55
37:N:307:PID:HM21	37:N:307:PID:H8	1.88	0.55
10:l:323:LYS:HE2	10:l:328:LEU:HD13	1.89	0.55
37:F:304:PID:HM81	37:F:306:PID:HM13	1.89	0.55
23:N:147:LYS:HB3	23:N:150:THR:HA	1.88	0.55
1:a:621:ARG:NH2	33:a:836:SF4:S4	2.80	0.55
29:a:808:CLA:HBA1	29:a:810:CLA:H12	1.89	0.55
12:A:111:GLU:HG2	29:A:211:CLA:NB	2.21	0.55
15:K:82:LEU:HD21	29:K:211:CLA:H42	1.89	0.55
15:K:155:LEU:HD21	15:K:159:ARG:HH21	1.72	0.55
20:D:95:LEU:HB2	20:D:103:PHE:CZ	2.41	0.55
29:b:719:CLA:HAB	29:b:724:CLA:CBB	2.37	0.55
4:d:219:PRO:HA	7:h:35:ILE:HD11	1.89	0.55
18:M:249:TYR:CE2	29:M:311:CLA:H3A	2.41	0.55
25:C:155:TYR:HA	25:C:163:LYS:HA	1.89	0.55
2:b:112:GLN:NE2	29:b:709:CLA:O1D	2.37	0.55
8:i:153:PRO:O	8:i:156:SER:OG	2.22	0.55
16:F:150:MET:HG2	22:H:82:PHE:HE2	1.71	0.55
28:E:196:LEU:HD22	29:E:315:CLA:HBD	1.89	0.55
1:a:291:TYR:OH	29:a:824:CLA:O1D	2.23	0.54
2:b:231:PHE:HZ	7:h:40:PHE:CD1	2.24	0.54
7:h:61:LEU:HD23	7:h:61:LEU:H	1.72	0.54
22:H:73:PRO:HG2	37:H:301:PID:H22A	1.89	0.54
26:Q:174:LYS:NZ	39:Q:314:KC1:O1A	2.32	0.54
29:b:717:CLA:HBC3	29:b:717:CLA:H161	1.90	0.54
29:b:725:CLA:HMC2	32:b:729:BCR:H271	1.89	0.54
9:j:28:PRO:HD2	35:j:105:DGD:HB31	1.89	0.54
23:N:154:PRO:HG2	23:N:156:SER:HB3	1.89	0.54
24:O:136:PHE:O	24:O:147:LYS:NZ	2.40	0.54
29:a:803:CLA:HBD	2:b:539:HIS:HB3	1.90	0.54
2:b:192:ILE:HG12	2:b:392:SER:HA	1.88	0.54
7:h:40:PHE:HZ	7:h:47:TRP:CE2	2.25	0.54
16:F:124:LEU:HB3	16:F:129:LEU:HD12	1.88	0.54
21:B:97:VAL:HG21	21:B:100:LEU:HD12	1.90	0.54
25:T:100:GLY:HA3	25:T:234:ARG:HH22	1.72	0.54
37:T:304:PID:H17	37:T:305:PID:O5	2.07	0.54
27:P:70:LEU:HD11	29:P:215:CLA:HBC1	1.90	0.54
24:O:163:VAL:HG23	24:O:164:VAL:H	1.72	0.54
2:b:154:TRP:HD1	2:b:208:HIS:CD2	2.26	0.54
12:A:184:THR:HG21	29:A:216:CLA:H2A	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:95:ILE:HB	29:G:314:CLA:HMC2	1.89	0.54
16:F:117:MET:HE3	37:F:302:PID:H16	1.88	0.54
19:L:174:ILE:HD11	29:L:310:CLA:H42	1.90	0.54
22:H:104:ILE:HD12	29:H:312:CLA:HMD3	1.88	0.54
23:N:151:SER:OG	29:N:314:CLA:O1A	2.26	0.54
24:O:192:GLU:OE2	24:O:196:LYS:NZ	2.38	0.54
1:a:573:HIS:HB3	29:b:703:CLA:HBD	1.89	0.54
2:b:143:GLY:N	11:m:86:PRO:O	2.41	0.54
29:f:805:CLA:HHB	7:h:94:PHE:CE2	2.42	0.54
7:h:38:ARG:H	7:h:39:PRO:CD	2.14	0.54
20:D:90:LYS:HE3	20:D:104:ALA:HA	1.90	0.54
20:D:150:PHE:CZ	37:D:305:PID:H11	2.42	0.54
23:N:35:GLY:HA2	23:N:169:ARG:HH12	1.70	0.54
25:C:110:PRO:HD2	36:C:303:DD6:C17	2.38	0.54
14:I:165:VAL:HG13	29:I:217:CLA:HED2	1.89	0.54
16:F:73:CYS:HB2	37:F:304:PID:HM43	1.90	0.54
17:J:120:ALA:HB2	17:J:196:PRO:HG2	1.89	0.54
23:N:60:ARG:HD3	29:N:309:CLA:H12	1.90	0.54
1:a:32:HIS:HB3	31:a:833:LHG:H111	1.89	0.54
1:a:587:ARG:NH1	1:a:591:GLN:HB2	2.24	0.54
2:b:307:LEU:HD23	13:G:6:MET:SD	2.48	0.54
2:b:472:VAL:HA	2:b:475:PHE:CE2	2.43	0.54
17:J:238:GLY:O	17:J:242:GLN:HB3	2.08	0.54
19:L:198:ALA:O	19:L:200:PRO:HD3	2.07	0.54
6:f:115:PHE:CZ	6:f:119:THR:HG21	2.42	0.53
28:E:120:GLN:HE22	39:E:307:KC1:CGA	2.21	0.53
1:a:226:THR:OG1	1:a:227:SER:N	2.41	0.53
29:b:726:CLA:H121	32:i:204:BCR:H19C	1.90	0.53
14:I:72:MET:HE1	29:I:211:CLA:CAD	2.38	0.53
19:L:262:PHE:O	19:L:266:VAL:HG22	2.07	0.53
21:B:223:GLU:O	21:B:227:ALA:N	2.31	0.53
37:O:305:PID:H20	29:O:314:CLA:CMC	2.38	0.53
27:P:147:THR:HG22	29:P:215:CLA:HAA1	1.90	0.53
3:c:61:PHE:HD2	4:d:173:VAL:HG21	1.73	0.53
10:l:210:MET:SD	10:l:227:LEU:HD21	2.48	0.53
14:I:51:CYS:SG	14:I:153:MET:HG2	2.49	0.53
29:K:218:CLA:HBB2	19:L:206:LEU:HD11	1.90	0.53
17:J:169:LEU:HD13	40:J:314:SQD:H441	1.91	0.53
18:M:174:ARG:HH11	18:M:185:LEU:HD23	1.73	0.53
1:a:575:VAL:HG11	1:a:630:LEU:HD23	1.90	0.53
2:b:414:THR:O	2:b:418:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:N:156:SER:O	23:N:160:LYS:HG2	2.09	0.53
1:a:398:LEU:HB2	1:a:426:THR:HG23	1.91	0.53
1:a:454:ARG:NH2	4:d:95:GLU:OE2	2.40	0.53
29:b:702:CLA:H191	8:i:79:ILE:HG23	1.89	0.53
17:J:185:THR:O	17:J:191:PRO:HD3	2.09	0.53
18:M:194:PHE:HD2	18:M:200:PRO:HG2	1.74	0.53
20:D:164:LYS:NZ	39:D:315:KC1:O2A	2.41	0.53
37:E:301:PID:HM22	29:E:306:CLA:HAC2	1.90	0.53
4:d:217:PRO:HG2	7:h:42:PRO:HA	1.91	0.53
14:I:157:SER:HB3	29:I:216:CLA:HBC2	1.90	0.53
1:a:370:HIS:O	1:a:374:LEU:HG	2.08	0.53
2:b:113:ILE:O	2:b:117:THR:HG23	2.09	0.53
5:e:10:GLN:NE2	5:e:26:THR:OG1	2.41	0.53
29:i:202:CLA:H111	29:i:202:CLA:HAB	1.91	0.53
10:l:428:THR:HG1	10:l:431:SER:HG	1.54	0.53
29:l:503:CLA:H122	29:F:312:CLA:HBB1	1.91	0.53
34:A:219:LMG:HC1	29:B:307:CLA:HBB1	1.91	0.53
37:E:301:PID:H15	29:E:313:CLA:HMC1	1.90	0.53
1:a:544:ARG:HA	2:b:517:LEU:HD13	1.90	0.53
1:a:587:ARG:NH1	1:a:614:ALA:HB3	2.24	0.53
3:c:81:ASP:HA	4:d:114:ARG:HD2	1.91	0.53
19:L:239:GLU:OE1	19:L:239:GLU:N	2.33	0.53
37:O:307:PID:HM51	37:O:307:PID:HM83	1.90	0.53
25:T:212:LYS:O	25:T:214:ILE:N	2.42	0.53
25:T:213:VAL:HG13	25:T:214:ILE:H	1.73	0.53
28:E:185:ARG:HG3	28:E:186:GLU:H	1.73	0.53
6:f:82:ALA:O	6:f:105:ARG:NH2	2.42	0.53
35:j:106:DGD:HA72	35:j:106:DGD:HB21	1.90	0.53
15:K:142:LEU:HD21	29:O:313:CLA:HHB	1.90	0.53
37:H:301:PID:HM22	29:H:308:CLA:HAC2	1.90	0.53
1:a:117:GLU:HG2	1:a:180:TRP:HH2	1.74	0.52
32:a:838:BCR:H292	32:f:801:BCR:H332	1.91	0.52
2:b:55:TRP:CD1	11:m:24:PHE:HB2	2.44	0.52
29:l:510:CLA:HMB1	28:E:103:LEU:HD21	1.91	0.52
12:A:102:GLN:HE21	36:B:301:DD6:C13	2.22	0.52
15:K:44:MET:HE2	19:L:213:LEU:HB3	1.90	0.52
17:J:227:ASN:ND2	29:J:305:CLA:O1D	2.42	0.52
23:N:80:THR:N	23:N:81:PRO:HD2	2.25	0.52
2:b:373:LEU:O	6:f:10:LYS:NZ	2.34	0.52
34:b:730:LMG:H422	29:i:202:CLA:HMB2	1.89	0.52
15:K:120:LEU:O	15:K:124:ASN:ND2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:342:ARG:HB3	17:J:201:GLY:HA3	1.91	0.52
21:B:103:PRO:HG2	21:B:117:ASP:HB3	1.91	0.52
24:O:183:VAL:O	24:O:186:THR:OG1	2.27	0.52
35:h:203:DGD:HD61	29:G:302:CLA:HMD2	1.91	0.52
9:j:28:PRO:HD3	34:K:201:LMG:H192	1.90	0.52
14:I:106:LYS:HD2	14:I:111:ASN:HB3	1.92	0.52
15:K:81:ARG:O	24:O:163:VAL:HG21	2.08	0.52
15:K:103:PRO:HB3	29:K:212:CLA:CAD	2.40	0.52
22:H:112:TYR:HE1	22:H:139:GLY:HA2	1.74	0.52
27:P:144:LYS:O	27:P:146:LEU:N	2.42	0.52
1:a:612:PRO:HG2	29:a:837:CLA:HBC3	1.90	0.52
29:a:806:CLA:H121	32:a:834:BCR:HC41	1.91	0.52
13:G:188:GLY:O	13:G:192:MET:HG3	2.09	0.52
15:K:39:GLU:OE2	15:K:159:ARG:NH1	2.42	0.52
17:J:94:GLY:HA3	17:J:99:SER:HB2	1.91	0.52
21:B:182:GLN:OE1	28:E:148:PRO:HD3	2.10	0.52
21:B:223:GLU:HB3	21:B:226:LYS:HB2	1.92	0.52
22:H:117:ILE:HG13	22:H:118:THR:H	1.75	0.52
25:T:105:LEU:HD13	37:T:301:PID:HM12	1.91	0.52
26:Q:68:LEU:HD21	26:Q:72:ARG:HH21	1.74	0.52
29:a:824:CLA:C2	32:a:835:BCR:HC7	2.40	0.52
12:A:81:LYS:HG2	12:A:93:ALA:HB1	1.92	0.52
12:A:114:GLY:HA2	21:B:99:TYR:CE2	2.45	0.52
12:A:120:ASN:ND2	12:A:122:MET:O	2.43	0.52
6:f:32:MET:HG2	6:f:89:GLY:HA2	1.92	0.52
13:G:29:PRO:HB3	13:G:152:VAL:HB	1.90	0.52
35:G:320:DGD:O2D	29:I:212:CLA:OBD	2.26	0.52
14:I:107:ILE:HB	29:I:213:CLA:HMA1	1.92	0.52
16:F:90:PRO:HD2	29:F:311:CLA:HBA2	1.90	0.52
19:L:224:SER:H	19:L:227:THR:HG1	1.55	0.52
23:N:73:LEU:HD11	29:N:314:CLA:HBC1	1.90	0.52
5:e:31:ASN:HB3	5:e:39:PRO:HB3	1.92	0.52
13:G:146:TYR:CZ	13:G:148:GLY:HA3	2.44	0.52
24:O:233:ASP:HA	24:O:238:SER:O	2.09	0.52
29:a:821:CLA:HED2	29:a:821:CLA:H2A	1.92	0.52
37:G:303:PID:C18	29:G:304:CLA:HBB2	2.40	0.52
14:I:4:SER:OG	14:I:7:VAL:O	2.28	0.52
4:d:216:PHE:CD2	7:h:26:PRO:HB3	2.45	0.52
14:I:188:SER:H	14:I:191:ASN:HB3	1.75	0.52
23:N:33:GLU:O	23:N:35:GLY:N	2.41	0.52
24:O:115:LYS:HG3	37:O:302:PID:H41	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:130:PRO:HB3	24:O:136:PHE:CZ	2.45	0.52
27:P:120:TYR:CD2	37:P:203:PID:H11	2.45	0.52
28:E:201:LEU:HA	28:E:204:GLN:HG3	1.90	0.52
34:E:316:LMG:O1	34:E:316:LMG:O3	2.20	0.52
2:b:493:VAL:HG13	2:b:497:ASN:HD22	1.74	0.51
15:K:180:ARG:NH1	15:K:184:PHE:O	2.43	0.51
18:M:151:GLU:OE1	18:M:232:GLY:N	2.43	0.51
23:N:63:VAL:HG23	23:N:67:HIS:ND1	2.25	0.51
25:T:177:VAL:HB	25:T:182:TRP:CE2	2.45	0.51
37:T:301:PID:HM22	29:T:309:CLA:HAC2	1.92	0.51
17:J:237:ILE:HD11	29:J:307:CLA:HAB	1.91	0.51
36:D:304:DD6:C9	29:D:309:CLA:HMC1	2.40	0.51
26:Q:51:PRO:HG3	29:Q:307:CLA:C4B	2.40	0.51
37:C:305:PID:C8	37:C:305:PID:HM11	2.40	0.51
29:b:701:CLA:H172	6:f:126:GLY:HA2	1.93	0.51
8:i:153:PRO:O	8:i:154:LYS:HG3	2.09	0.51
1:a:95:ILE:HB	37:j:101:PID:HM32	1.93	0.51
1:a:203:SER:O	1:a:206:SER:OG	2.29	0.51
3:c:44:VAL:HB	8:i:174:HIS:CG	2.45	0.51
5:e:47:VAL:HG12	5:e:53:ASN:HB3	1.92	0.51
16:F:43:PRO:HD2	36:F:303:DD6:C17	2.40	0.51
37:F:306:PID:HM83	37:F:306:PID:HM51	1.92	0.51
20:D:132:GLU:HG2	37:D:303:PID:HM32	1.92	0.51
1:a:175:LEU:HD12	32:a:834:BCR:H361	1.92	0.51
10:l:238:PRO:HB2	10:l:245:TYR:HB2	1.91	0.51
11:m:48:LYS:HG2	35:m:102:DGD:HG32	1.93	0.51
24:O:172:TRP:CD1	37:O:302:PID:H13	2.41	0.51
27:P:120:TYR:HD2	37:P:203:PID:H11	1.76	0.51
1:a:185:ILE:HA	1:a:189:LEU:HD12	1.93	0.51
19:L:157:ARG:HA	19:L:160:MET:HE3	1.92	0.51
20:D:42:ALA:HB3	20:D:43:PRO:HD3	1.91	0.51
20:D:176:MET:O	20:D:180:ILE:HG22	2.11	0.51
29:a:803:CLA:H71	2:b:537:LEU:HD13	1.93	0.51
2:b:144:LEU:HA	2:b:147:VAL:HG12	1.93	0.51
2:b:400:GLY:O	2:b:404:VAL:HG23	2.11	0.51
15:K:106:GLN:HE22	15:K:110:TRP:HE1	1.57	0.51
23:N:64:GLU:OE1	23:N:64:GLU:HA	2.11	0.51
23:N:116:GLY:O	23:N:120:ILE:HG12	2.11	0.51
25:C:143:TYR:CE2	25:C:243:MET:HB3	2.46	0.51
27:P:88:LEU:HD23	27:P:94:LEU:HD23	1.93	0.51
1:a:149:SER:HA	9:j:11:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:66:ALA:HB1	14:I:70:VAL:HG23	1.93	0.51
19:L:194:LEU:HD13	19:L:200:PRO:HG2	1.93	0.51
19:L:212:GLU:HG2	29:L:312:CLA:NB	2.26	0.51
23:N:184:LEU:HD12	23:N:185:THR:HG23	1.92	0.51
24:O:200:VAL:HG11	24:O:208:ARG:CA	2.41	0.51
6:f:92:ASP:OD2	6:f:96:ARG:NH2	2.44	0.51
35:m:102:DGD:HAE2	29:E:305:CLA:H92	1.91	0.51
22:H:107:LEU:HD13	29:H:313:CLA:HAC1	1.92	0.51
22:H:191:LEU:HA	22:H:194:LYS:HZ2	1.75	0.51
26:Q:73:ARG:NH1	26:Q:76:GLU:OE1	2.43	0.51
2:b:247:VAL:HG11	29:b:712:CLA:H192	1.93	0.51
18:M:254:LEU:O	18:M:258:ARG:HG3	2.11	0.51
19:L:237:PHE:CD1	29:L:313:CLA:HAA2	2.46	0.50
20:D:94:TYR:O	20:D:95:LEU:HB3	2.11	0.50
21:B:145:THR:O	21:B:149:ILE:HD12	2.10	0.50
25:C:224:ARG:NH1	29:C:308:CLA:O2D	2.43	0.50
1:a:581:MET:HB2	29:a:802:CLA:CHC	2.41	0.50
2:b:41:VAL:HG13	29:i:202:CLA:H141	1.92	0.50
4:d:81:ARG:HB2	4:d:139:LEU:HB2	1.93	0.50
16:F:32:LEU:HD13	16:F:170:LEU:HG	1.93	0.50
18:M:250:GLU:HG2	29:M:311:CLA:HMA2	1.92	0.50
22:H:116:GLU:HG2	37:H:306:PID:H42	1.93	0.50
23:N:39:PRO:HG3	29:N:308:CLA:HBB1	1.93	0.50
12:A:143:ASP:OD2	12:A:145:ARG:NH2	2.43	0.50
15:K:70:THR:O	15:K:74:ILE:HG12	2.11	0.50
15:K:87:TYR:OH	29:K:212:CLA:OBD	2.28	0.50
17:J:107:THR:HG22	29:J:306:CLA:HBA1	1.94	0.50
21:B:181:GLN:OE1	21:B:181:GLN:N	2.43	0.50
24:O:121:MET:HE1	24:O:215:GLU:OE1	2.11	0.50
1:a:570:LEU:HD12	29:b:703:CLA:H42	1.93	0.50
2:b:152:ILE:HG13	2:b:212:GLY:HA3	1.93	0.50
18:M:223:MET:HB3	18:M:226:LEU:HD12	1.94	0.50
23:N:174:ALA:HB1	37:N:305:PID:C10	2.42	0.50
2:b:23:GLU:O	8:i:112:LYS:NZ	2.44	0.50
29:b:718:CLA:H93	29:b:726:CLA:HED3	1.93	0.50
29:b:736:CLA:HED2	29:b:736:CLA:H2A	1.93	0.50
4:d:140:SER:OG	4:d:144:THR:OG1	2.28	0.50
12:A:114:GLY:HA2	21:B:99:TYR:HE2	1.75	0.50
15:K:144:PRO:HA	24:O:183:VAL:HG21	1.93	0.50
21:B:102:TYR:OH	21:B:112:GLY:O	2.26	0.50
22:H:100:LYS:HD2	29:H:312:CLA:C3D	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:110:PRO:O	36:T:303:DD6:O2	2.29	0.50
25:C:157:SER:HB3	25:C:162:LEU:HB2	1.93	0.50
25:C:168:PRO:HD2	25:C:176:LYS:HG3	1.93	0.50
2:b:375:THR:HG22	2:b:385:VAL:HG23	1.92	0.50
4:d:95:GLU:HG2	4:d:101:TRP:NE1	2.27	0.50
9:j:47:MET:HG2	37:j:101:PID:HM62	1.92	0.50
20:D:169:LEU:HD21	20:D:173:ARG:CZ	2.41	0.50
27:P:58:ARG:NH1	27:P:61:GLU:OE1	2.45	0.50
20:D:40:VAL:HG13	20:D:45:GLY:HA2	1.94	0.50
20:D:70:LYS:HG3	37:D:303:PID:H41	1.93	0.50
21:B:171:HIS:CD2	21:B:180:MET:HE2	2.47	0.50
36:B:319:DD6:C2	29:E:308:CLA:H13	2.42	0.50
22:H:124:TYR:CD2	22:H:127:PRO:HA	2.44	0.50
29:b:711:CLA:HBB2	29:h:201:CLA:C1D	2.41	0.50
21:B:189:VAL:HG21	36:B:319:DD6:C4	2.41	0.50
29:b:726:CLA:HAC2	32:b:729:BCR:H21C	1.93	0.50
16:F:197:THR:O	16:F:202:TRP:NE1	2.40	0.50
20:D:80:MET:HE2	37:D:305:PID:H20	1.93	0.50
37:H:306:PID:HM11	37:H:306:PID:C8	2.27	0.50
26:Q:103:LEU:HB2	26:Q:111:PHE:CE1	2.46	0.50
27:P:177:PHE:HZ	29:P:210:CLA:H203	1.77	0.50
1:a:530:SER:O	1:a:532:PHE:N	2.45	0.49
29:a:827:CLA:HAA2	10:l:382:LEU:O	2.11	0.49
2:b:82:SER:O	2:b:83:GLN:C	2.55	0.49
2:b:576:ILE:HG22	10:l:413:PHE:CE1	2.47	0.49
14:I:161:HIS:HB3	29:I:217:CLA:HED1	1.94	0.49
29:K:210:CLA:HAB	29:K:218:CLA:HBC2	1.94	0.49
25:C:254:TRP:CZ3	37:C:305:PID:H3	2.47	0.49
28:E:164:PRO:O	28:E:167:GLY:N	2.44	0.49
1:a:288:SER:OG	1:a:318:HIS:O	2.28	0.49
2:b:505:PHE:CE1	29:b:703:CLA:HED3	2.47	0.49
15:K:146:ASP:O	15:K:150:GLN:HG3	2.12	0.49
25:C:211:PHE:HE2	37:C:305:PID:HM81	1.78	0.49
27:P:130:GLN:HA	27:P:136:GLY:HA3	1.94	0.49
28:E:237:PHE:CZ	37:E:301:PID:H313	2.47	0.49
7:h:25:GLY:O	7:h:33:LYS:NZ	2.45	0.49
14:I:181:PRO:HD2	29:K:212:CLA:HED1	1.94	0.49
25:C:119:VAL:O	25:C:123:LYS:HG2	2.13	0.49
1:a:366:PHE:CE2	29:a:829:CLA:HAB	2.48	0.49
4:d:169:ARG:NH2	4:d:194:ALA:O	2.35	0.49
22:H:216:ASP:OD1	22:H:222:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:155:TYR:HE1	25:T:158:PRO:HA	1.78	0.49
26:Q:46:ARG:HH22	26:Q:77:ILE:HD11	1.77	0.49
1:a:147:MET:HG2	29:a:812:CLA:C3D	2.42	0.49
2:b:394:LEU:HB3	6:f:7:THR:HG21	1.95	0.49
2:b:601:VAL:HG13	34:b:732:LMG:H381	1.94	0.49
13:G:18:TRP:CZ2	13:G:20:PRO:HG3	2.47	0.49
17:J:129:ALA:O	17:J:132:ALA:N	2.46	0.49
29:a:804:CLA:O2D	29:a:804:CLA:H2A	2.13	0.49
29:a:810:CLA:HMA1	9:j:58:ILE:HD12	1.95	0.49
29:b:714:CLA:H3A	29:b:724:CLA:O1A	2.12	0.49
15:K:65:ILE:HD12	29:K:213:CLA:HMD3	1.93	0.49
18:M:201:MET:HE3	29:M:309:CLA:H3A	1.95	0.49
24:O:94:PRO:O	24:O:96:GLY:N	2.45	0.49
27:P:78:PRO:HB3	27:P:83:LYS:HD3	1.94	0.49
27:P:92:MET:HE1	27:P:110:PRO:HB3	1.95	0.49
27:P:169:MET:HA	27:P:172:ILE:HG22	1.94	0.49
7:h:93:GLN:HB3	7:h:103:PHE:CD1	2.48	0.49
7:h:118:PHE:HZ	29:G:304:CLA:HBB1	1.76	0.49
10:l:325:GLU:HG3	10:l:335:ARG:HD2	1.95	0.49
12:A:35:ASP:OD1	36:A:202:DD6:O2	2.31	0.49
15:K:161:GLY:O	15:K:165:MET:HG3	2.12	0.49
2:b:199:LEU:HD11	2:b:262:TYR:HB3	1.95	0.49
2:b:229:TRP:HH2	35:h:203:DGD:HE1	1.78	0.49
18:M:192:ASP:HA	18:M:195:VAL:HG12	1.93	0.49
27:P:67:ILE:HD11	37:P:203:PID:HM22	1.94	0.49
29:a:804:CLA:H93	29:a:837:CLA:H61	1.94	0.49
29:a:819:CLA:H71	29:a:824:CLA:H143	1.95	0.49
13:G:46:GLU:OE2	13:G:186:LYS:NZ	2.38	0.49
28:E:123:ALA:HB2	28:E:191:ALA:HB3	1.95	0.49
1:a:60:PHE:HE1	29:a:806:CLA:H122	1.77	0.49
2:b:114:TYR:CZ	11:m:28:GLU:HB3	2.48	0.49
2:b:253:SER:O	2:b:257:GLN:HG2	2.12	0.49
2:b:433:PRO:HD2	3:c:61:PHE:CZ	2.47	0.49
25:C:152:PHE:HE2	29:C:311:CLA:H42	1.78	0.49
28:E:102:PRO:O	34:E:316:LMG:HC92	2.13	0.49
1:a:592:GLU:OE2	2:b:435:LYS:NZ	2.41	0.48
8:i:143:GLY:O	8:i:144:LEU:C	2.56	0.48
10:l:253:THR:H	10:l:258:LYS:HD2	1.78	0.48
18:M:186:ASP:C	18:M:188:ALA:H	2.20	0.48
29:M:308:CLA:HMC3	29:M:314:CLA:HBB2	1.95	0.48
29:L:311:CLA:H3A	29:L:311:CLA:HBA1	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:164:SER:O	22:H:165:GLN:C	2.55	0.48
24:O:127:TYR:CE2	24:O:229:LEU:HD22	2.48	0.48
25:C:254:TRP:HZ3	37:C:305:PID:HM33	1.78	0.48
4:d:36:LEU:HD13	4:d:41:GLN:HB3	1.95	0.48
16:F:63:LEU:HD13	16:F:138:GLY:HA3	1.94	0.48
16:F:150:MET:HG2	22:H:82:PHE:CE2	2.48	0.48
17:J:89:LEU:HD13	29:J:306:CLA:H2A	1.96	0.48
17:J:173:GLN:NE2	40:J:314:SQD:O10	2.46	0.48
18:M:237:PHE:HB2	29:M:311:CLA:HBA2	1.95	0.48
2:b:367:ILE:HD11	29:b:722:CLA:H2	1.95	0.48
8:i:73:THR:O	8:i:77:VAL:HB	2.13	0.48
12:A:103:VAL:HG12	29:A:215:CLA:HBC1	1.95	0.48
24:O:179:TRP:CG	37:O:304:PID:HO2	2.32	0.48
29:a:820:CLA:H122	29:l:504:CLA:H171	1.95	0.48
36:M:303:DD6:C24	29:M:311:CLA:HAB	2.43	0.48
1:a:460:ASN:CG	4:d:118:GLN:HG2	2.39	0.48
2:b:409:ALA:O	2:b:413:HIS:ND1	2.36	0.48
16:F:37:PRO:HB3	29:F:307:CLA:C4B	2.44	0.48
17:J:212:GLU:O	17:J:214:PRO:HD3	2.13	0.48
22:H:112:TYR:HE2	22:H:209:PHE:CE2	2.30	0.48
24:O:218:ASN:HD22	29:O:314:CLA:CBB	2.25	0.48
29:O:313:CLA:HBB1	29:O:313:CLA:HMB1	1.95	0.48
25:C:138:LEU:HD11	29:C:314:CLA:HBC1	1.95	0.48
1:a:70:GLY:O	1:a:74:SER:OG	2.27	0.48
29:a:824:CLA:H141	29:a:824:CLA:H162	1.63	0.48
29:a:828:CLA:H3A	29:a:829:CLA:HAA2	1.96	0.48
2:b:334:GLY:HA2	2:b:410:LEU:HD22	1.96	0.48
13:G:90:CYS:SG	36:G:307:DD6:C6	3.02	0.48
15:K:102:GLY:N	15:K:103:PRO:HD2	2.28	0.48
29:J:306:CLA:H62	29:J:306:CLA:H41	1.56	0.48
37:D:303:PID:H15	29:D:312:CLA:HBC1	1.96	0.48
26:Q:109:LEU:HD13	26:Q:125:PRO:HD3	1.96	0.48
2:b:24:SER:HA	8:i:108:LEU:HD21	1.96	0.48
2:b:601:VAL:HG11	34:b:732:LMG:H362	1.95	0.48
13:G:21:ILE:HG23	29:G:304:CLA:H3A	1.94	0.48
16:F:88:LEU:N	16:F:94:LEU:O	2.46	0.48
37:D:303:PID:H17	29:D:312:CLA:HBC2	1.95	0.48
25:T:237:MET:O	25:T:240:ILE:HG22	2.14	0.48
28:E:194:PHE:CG	29:E:315:CLA:HED1	2.48	0.48
2:b:237:TYR:HB3	29:b:706:CLA:HAC1	1.94	0.48
11:m:31:LEU:HD13	40:B:317:SQD:H241	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:G:312:CLA:C2B	29:G:312:CLA:H42	2.44	0.48
16:F:175:ASN:HA	16:F:178:ARG:HD2	1.95	0.48
18:M:195:VAL:HA	18:M:201:MET:HB2	1.96	0.48
22:H:87:SER:O	22:H:89:LYS:N	2.47	0.48
37:H:305:PID:H7	29:H:315:CLA:HMB1	1.96	0.48
29:N:309:CLA:H41	29:N:309:CLA:H61	1.50	0.48
25:T:123:LYS:O	25:T:127:GLN:HG3	2.13	0.48
27:P:173:ILE:O	27:P:177:PHE:HD1	1.97	0.48
2:b:572:PHE:HZ	10:l:351:THR:HG21	1.78	0.48
29:i:201:CLA:H91	11:m:44:ILE:HD13	1.96	0.48
35:j:105:DGD:O5E	15:K:53:ARG:NH1	2.47	0.48
10:l:454:LEU:HD13	29:l:505:CLA:H93	1.95	0.48
40:B:317:SQD:H2	40:B:317:SQD:H441	1.64	0.48
22:H:124:TYR:CZ	22:H:130:LEU:HA	2.48	0.48
28:E:125:GLU:HB2	29:E:306:CLA:C1B	2.43	0.48
29:E:305:CLA:H42	29:E:311:CLA:H191	1.96	0.48
29:a:804:CLA:C2C	37:j:101:PID:H313	2.44	0.48
29:b:711:CLA:HBC1	34:h:205:LMG:H132	1.96	0.48
32:f:804:BCR:H11C	32:f:804:BCR:H341	1.73	0.48
32:m:103:BCR:H11C	32:m:103:BCR:H341	1.67	0.48
18:M:150:ARG:NH1	18:M:153:GLU:OE1	2.47	0.48
22:H:178:PHE:HB3	37:H:304:PID:HM23	1.95	0.48
24:O:125:MET:HE1	37:O:305:PID:C22	2.43	0.48
25:T:143:TYR:HE1	25:T:170:GLY:HA2	1.79	0.48
26:Q:82:ILE:HD13	29:Q:312:CLA:HBC3	1.95	0.48
29:P:209:CLA:H2A	29:P:209:CLA:CED	2.41	0.48
1:a:614:ALA:HB1	30:a:832:PQN:O4	2.14	0.47
29:a:827:CLA:O2D	29:a:827:CLA:H2A	2.14	0.47
29:b:706:CLA:HBB1	29:i:201:CLA:HMB2	1.96	0.47
29:h:201:CLA:H3A	29:h:201:CLA:HBA2	1.47	0.47
8:i:154:LYS:HD2	8:i:155:GLY:N	2.29	0.47
34:A:219:LMG:O10	36:B:305:DD6:O2	2.32	0.47
29:I:211:CLA:HBB1	29:I:211:CLA:HMB1	1.95	0.47
16:F:103:MET:HE1	38:F:305:UIX:C25	2.44	0.47
17:J:121:ALA:O	17:J:125:HIS:ND1	2.37	0.47
22:H:121:PHE:CE2	29:H:310:CLA:H11	2.49	0.47
23:N:37:GLN:NE2	23:N:39:PRO:HD2	2.29	0.47
23:N:97:LEU:HG	23:N:102:ILE:HD11	1.96	0.47
34:P:201:LMG:O5	34:P:201:LMG:O4	2.29	0.47
36:P:204:DD6:C8	29:P:210:CLA:HAB	2.44	0.47
29:E:306:CLA:H12	29:E:306:CLA:CHB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:295:GLN:OE1	17:J:214:PRO:HD2	2.14	0.47
13:G:87:GLY:O	13:G:91:MET:HG3	2.14	0.47
37:D:305:PID:H15	37:D:306:PID:O6	2.14	0.47
24:O:172:TRP:CD1	37:O:302:PID:H11	2.48	0.47
29:Q:308:CLA:H3A	29:Q:308:CLA:HBA2	1.40	0.47
37:C:305:PID:H17	37:C:305:PID:HM41	1.97	0.47
13:G:34:GLU:HG2	13:G:59:LYS:HG2	1.96	0.47
34:K:201:LMG:H122	29:K:210:CLA:H43	1.96	0.47
16:F:111:THR:HG21	40:J:314:SQD:H61	1.95	0.47
16:F:157:GLU:OE2	22:H:93:ARG:NH2	2.44	0.47
23:N:69:ARG:HA	23:N:72:MET:HE2	1.96	0.47
37:T:317:PID:HM52	29:Q:315:CLA:C3D	2.44	0.47
3:c:85:TRP:O	4:d:21:SER:OG	2.29	0.47
10:l:336:SER:O	10:l:340:ASP:N	2.46	0.47
10:l:374:PHE:CZ	29:l:504:CLA:HBB1	2.49	0.47
14:I:66:ALA:HB2	14:I:72:MET:HB2	1.96	0.47
15:K:136:ASP:CG	15:K:140:ARG:HH22	2.21	0.47
16:F:36:PRO:N	16:F:37:PRO:HD2	2.28	0.47
19:L:198:ALA:C	19:L:200:PRO:HD3	2.40	0.47
26:Q:81:ARG:HA	26:Q:84:MET:HE3	1.95	0.47
26:Q:162:LYS:HE2	29:C:313:CLA:HED3	1.96	0.47
25:C:252:SER:OG	25:C:253:ALA:N	2.47	0.47
29:E:306:CLA:H143	29:E:306:CLA:H162	1.73	0.47
1:a:604:LEU:HD13	32:f:804:BCR:H321	1.97	0.47
29:b:718:CLA:H62	29:b:718:CLA:H41	1.55	0.47
35:b:733:DGD:HG11	35:h:203:DGD:HD62	1.96	0.47
8:i:111:LYS:HE2	8:i:115:MET:HE3	1.95	0.47
16:F:172:SER:O	16:F:176:ASN:ND2	2.47	0.47
26:Q:58:LEU:HD12	26:Q:60:PHE:HE2	1.79	0.47
28:E:112:LEU:HD22	29:E:306:CLA:H2	1.96	0.47
28:E:138:GLY:O	28:E:142:PRO:HD2	2.13	0.47
1:a:434:ILE:HG21	29:a:801:CLA:H161	1.97	0.47
1:a:470:PRO:HB3	1:a:617:ILE:HB	1.96	0.47
4:d:149:HIS:HB3	4:d:150:PRO:CD	2.45	0.47
4:d:169:ARG:HH21	4:d:171:PHE:HZ	1.63	0.47
9:j:59:GLU:OE1	9:j:62:ARG:NH2	2.34	0.47
29:A:214:CLA:HBC1	29:A:216:CLA:HAB	1.96	0.47
29:G:302:CLA:HBA2	29:G:302:CLA:HBD	1.97	0.47
18:M:253:GLU:HB2	29:M:311:CLA:CHB	2.44	0.47
26:Q:104:SER:O	26:Q:108:GLY:N	2.42	0.47
25:C:112:LYS:HG2	29:C:309:CLA:H11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:43:LEU:HA	27:P:46:ALA:HB2	1.97	0.47
27:P:122:PHE:CE1	27:P:126:GLN:HG3	2.50	0.47
1:a:300:VAL:HG22	29:a:819:CLA:HED3	1.95	0.47
31:a:833:LHG:O4	31:a:833:LHG:O2	2.32	0.47
29:b:702:CLA:H161	32:l:506:BCR:H15C	1.97	0.47
29:b:702:CLA:H192	29:b:726:CLA:H141	1.96	0.47
30:b:727:PQN:H292	32:l:506:BCR:H10C	1.96	0.47
6:f:133:THR:O	6:f:135:ASP:N	2.48	0.47
34:j:102:LMG:HC5	10:l:265:TRP:CD2	2.50	0.47
10:l:291:ASP:O	10:l:295:GLN:HG2	2.15	0.47
10:l:446:GLY:HA3	32:l:507:BCR:H272	1.97	0.47
12:A:62:MET:SD	29:A:212:CLA:HAB	2.54	0.47
15:K:176:VAL:HG11	29:K:218:CLA:H2A	1.96	0.47
16:F:151:PHE:C	16:F:153:VAL:H	2.23	0.47
37:F:306:PID:H16	37:F:306:PID:HM41	1.78	0.47
29:F:311:CLA:HMA3	17:J:168:LEU:HD21	1.96	0.47
17:J:122:GLU:HB2	29:J:306:CLA:C1B	2.44	0.47
19:L:151:ALA:HB2	29:L:312:CLA:HED2	1.95	0.47
19:L:256:ARG:HA	19:L:259:MET:HE3	1.96	0.47
22:H:88:MET:O	22:H:92:LYS:HG2	2.14	0.47
25:T:131:LYS:HG3	37:T:302:PID:H41	1.95	0.47
37:T:317:PID:HM41	37:T:317:PID:H16	1.54	0.47
26:Q:87:ALA:O	26:Q:91:ILE:HD12	2.15	0.47
27:P:60:SER:O	27:P:64:HIS:ND1	2.42	0.47
27:P:164:ASN:OD1	37:P:206:PID:H16	2.15	0.47
29:a:803:CLA:H151	29:i:203:CLA:HBC3	1.96	0.47
2:b:231:PHE:HZ	7:h:40:PHE:HD1	1.63	0.47
29:b:724:CLA:HMC2	29:G:302:CLA:H192	1.96	0.47
8:i:74:ILE:HG21	29:i:203:CLA:HAB	1.97	0.47
15:K:104:MET:HE2	29:K:211:CLA:H3A	1.97	0.47
18:M:151:GLU:OE1	18:M:215:ARG:NH2	2.48	0.47
20:D:76:MET:CE	29:D:314:CLA:HAB	2.44	0.47
22:H:69:GLY:HA3	22:H:203:ARG:HH22	1.80	0.47
37:H:301:PID:HM41	37:H:301:PID:H16	1.68	0.47
37:H:305:PID:HM41	37:H:305:PID:H16	1.67	0.47
24:O:115:LYS:NZ	37:O:302:PID:H42	2.30	0.47
25:T:143:TYR:CD2	25:T:240:ILE:HD11	2.50	0.47
29:E:305:CLA:H41	29:E:305:CLA:H61	1.49	0.47
1:a:110:PHE:HE1	29:a:824:CLA:HAA2	1.80	0.47
2:b:22:ASN:OD1	2:b:24:SER:OG	2.27	0.47
3:c:1:ALA:N	3:c:72:GLU:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:18:ARG:HG2	4:d:157:GLU:HG2	1.96	0.47
3:c:28:VAL:HG21	4:d:165:PRO:HB3	1.97	0.47
4:d:154:VAL:O	4:d:163:ARG:NH2	2.48	0.47
8:i:70:LEU:HD13	29:i:202:CLA:HAA2	1.97	0.47
14:I:185:ALA:O	14:I:186:VAL:HG22	2.14	0.47
15:K:67:MET:HE1	29:K:214:CLA:CAB	2.44	0.47
20:D:82:TYR:HE1	36:D:304:DD6:C34	2.27	0.47
25:T:212:LYS:HD3	29:T:314:CLA:HBA1	1.97	0.47
1:a:381:MET:HE1	1:a:386:ARG:HH21	1.80	0.47
1:a:581:MET:HB2	29:a:802:CLA:C1C	2.45	0.47
29:a:809:CLA:H143	29:a:809:CLA:H111	1.76	0.47
2:b:94:THR:HG23	2:b:96:HIS:CE1	2.50	0.47
2:b:343:HIS:CD2	2:b:357:ILE:HG13	2.50	0.47
3:c:54:GLU:O	3:c:62:LEU:HD11	2.14	0.47
10:l:260:THR:HB	19:L:112:MET:HG2	1.96	0.47
29:l:505:CLA:H93	29:l:505:CLA:H61	1.75	0.47
36:K:204:DD6:C24	29:K:209:CLA:HAB	2.45	0.47
37:F:304:PID:HM81	37:F:306:PID:CM1	2.45	0.47
18:M:219:LEU:HD22	18:M:226:LEU:H	1.80	0.47
20:D:38:LEU:CD2	20:D:162:LYS:HD3	2.45	0.47
21:B:166:SER:O	21:B:170:ALA:HB2	2.15	0.47
25:T:119:VAL:HG22	25:T:123:LYS:NZ	2.30	0.47
25:C:177:VAL:HB	25:C:182:TRP:NE1	2.29	0.47
29:a:807:CLA:H161	29:a:807:CLA:H121	1.73	0.46
4:d:26:PRO:HG2	8:i:100:PRO:O	2.15	0.46
4:d:172:THR:HB	4:d:175:GLN:HG3	1.96	0.46
19:L:200:PRO:O	19:L:204:ILE:HG13	2.14	0.46
37:D:307:PID:H13	39:D:315:KC1:CBB	2.45	0.46
21:B:248:ILE:HG23	21:B:262:TYR:HE2	1.79	0.46
37:N:301:PID:HM41	37:N:301:PID:H16	1.68	0.46
29:a:811:CLA:H3A	29:a:811:CLA:HBA1	1.60	0.46
2:b:470:ASN:HB2	29:b:703:CLA:HBC2	1.96	0.46
2:b:530:VAL:HA	29:b:708:CLA:HAC1	1.96	0.46
10:l:383:GLY:H	10:l:386:ARG:HG3	1.79	0.46
32:m:103:BCR:H373	29:E:305:CLA:H151	1.97	0.46
14:I:108:THR:HG22	14:I:111:ASN:HB2	1.98	0.46
16:F:203:ALA:HB2	29:F:315:CLA:HED1	1.97	0.46
17:J:145:TYR:O	17:J:146:LEU:C	2.57	0.46
19:L:192:ASP:HA	19:L:195:ASN:OD1	2.15	0.46
22:H:146:VAL:HB	22:H:151:TRP:NE1	2.30	0.46
25:T:114:THR:HG21	29:T:309:CLA:HAA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:T:305:PID:H20	29:T:314:CLA:CAB	2.45	0.46
26:Q:124:VAL:HB	26:Q:129:TRP:NE1	2.31	0.46
37:C:302:PID:HM51	37:C:302:PID:HM82	1.97	0.46
29:a:809:CLA:CHC	29:a:810:CLA:HMD2	2.46	0.46
29:a:825:CLA:H61	29:a:825:CLA:H41	1.56	0.46
32:f:801:BCR:H15C	32:f:801:BCR:H351	1.68	0.46
13:G:95:ILE:HG22	29:G:314:CLA:HAC1	1.97	0.46
14:I:42:GLU:OE1	14:I:121:GLY:N	2.40	0.46
14:I:62:PRO:HB3	14:I:74:ALA:HA	1.96	0.46
22:H:195:LEU:O	22:H:199:ILE:HG12	2.16	0.46
37:T:304:PID:H16	37:T:304:PID:HM41	1.75	0.46
37:C:307:PID:HM83	37:C:307:PID:HM51	1.96	0.46
2:b:25:LEU:HD23	2:b:25:LEU:H	1.80	0.46
2:b:168:LEU:HD22	2:b:185:VAL:HG11	1.97	0.46
35:j:105:DGD:HA42	29:K:210:CLA:HED1	1.98	0.46
10:l:290:ASP:HA	10:l:293:LYS:HE3	1.97	0.46
29:K:209:CLA:H62	29:K:209:CLA:H41	1.58	0.46
23:N:65:LEU:HD12	23:N:142:GLY:HA3	1.97	0.46
24:O:198:PHE:HB2	29:O:314:CLA:HAA1	1.96	0.46
24:O:227:ILE:HG13	29:O:316:CLA:HMC2	1.96	0.46
27:P:144:LYS:HA	29:P:215:CLA:HAA2	1.97	0.46
37:P:206:PID:H17	39:P:216:KC1:C3B	2.46	0.46
37:P:206:PID:H20	29:P:215:CLA:HMC1	1.97	0.46
1:a:116:ALA:O	1:a:188:SER:OG	2.22	0.46
1:a:592:GLU:HB2	2:b:421:LYS:NZ	2.31	0.46
32:a:834:BCR:H15C	32:a:834:BCR:H351	1.73	0.46
2:b:140:SER:HB3	11:m:67:PHE:HZ	1.80	0.46
2:b:311:LEU:HD12	29:b:719:CLA:CMD	2.46	0.46
10:l:264:TRP:HD1	19:L:109:ILE:HD11	1.81	0.46
29:K:210:CLA:HAC2	29:K:217:CLA:HBB1	1.96	0.46
36:K:221:DD6:O4	19:L:217:LYS:HE3	2.16	0.46
19:L:205:ILE:HG12	29:L:316:CLA:HBC2	1.98	0.46
24:O:135:LYS:C	24:O:137:PRO:HD3	2.40	0.46
29:a:801:CLA:HED2	29:a:801:CLA:HBD	1.58	0.46
10:l:283:GLU:HA	10:l:286:LYS:HE2	1.97	0.46
16:F:117:MET:HE1	29:F:310:CLA:CHB	2.45	0.46
29:L:308:CLA:H62	29:L:308:CLA:H41	1.63	0.46
20:D:127:TYR:CE2	37:D:303:PID:H11	2.50	0.46
22:H:182:VAL:HG11	37:H:305:PID:H282	1.98	0.46
24:O:82:GLU:OE1	24:O:82:GLU:N	2.48	0.46
37:T:302:PID:H8	37:T:304:PID:O3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:51:PRO:HG3	29:Q:307:CLA:NB	2.31	0.46
27:P:109:VAL:HB	27:P:114:TRP:NE1	2.31	0.46
29:a:823:CLA:HBB1	29:a:823:CLA:HMB3	1.98	0.46
2:b:409:ALA:HB2	29:b:723:CLA:HMA3	1.97	0.46
2:b:543:ALA:HB3	29:b:705:CLA:HBB2	1.97	0.46
7:h:33:LYS:HA	7:h:39:PRO:HD3	1.97	0.46
14:I:13:PRO:HG2	14:I:16:LEU:HD12	1.98	0.46
20:D:162:LYS:O	20:D:166:ASN:ND2	2.49	0.46
23:N:70:ILE:HD11	37:N:302:PID:H41	1.97	0.46
37:C:304:PID:H16	37:C:304:PID:HM41	1.70	0.46
1:a:148:HIS:O	9:j:9:SER:OG	2.33	0.46
1:a:633:ILE:HD13	29:a:823:CLA:HMC2	1.97	0.46
2:b:12:VAL:HG11	8:i:95:PHE:CG	2.51	0.46
4:d:123:CYS:HG	4:d:149:HIS:CD2	2.26	0.46
14:I:16:LEU:HD22	29:I:209:CLA:HED3	1.96	0.46
19:L:155:HIS:HB3	19:L:259:MET:SD	2.56	0.46
22:H:185:SER:O	22:H:187:ASP:N	2.49	0.46
23:N:37:GLN:CD	23:N:39:PRO:HD2	2.40	0.46
25:C:124:ARG:HH22	25:C:125:ARG:NH2	2.14	0.46
37:C:302:PID:H16	37:C:302:PID:HM41	1.80	0.46
27:P:62:ILE:O	27:P:66:ARG:HG3	2.16	0.46
1:a:62:TRP:HA	29:a:808:CLA:CBB	2.44	0.46
29:a:801:CLA:H102	29:a:801:CLA:H62	1.52	0.46
29:a:806:CLA:H151	32:a:834:BCR:H323	1.98	0.46
2:b:272:TYR:OH	6:f:2:ASP:O	2.21	0.46
29:b:703:CLA:HMA1	29:b:704:CLA:H161	1.98	0.46
7:h:38:ARG:N	7:h:39:PRO:CD	2.76	0.46
12:A:120:ASN:ND2	12:A:125:LEU:O	2.48	0.46
16:F:113:ALA:O	16:F:117:MET:HG3	2.15	0.46
29:T:311:CLA:H3A	29:T:311:CLA:HBA2	1.73	0.46
1:a:482:ILE:HG23	2:b:554:GLY:HA3	1.98	0.46
1:a:604:LEU:HD12	29:b:701:CLA:HMA3	1.98	0.46
29:b:723:CLA:H3A	29:b:724:CLA:OBD	2.16	0.46
32:m:103:BCR:H351	32:m:103:BCR:H15C	1.63	0.46
13:G:164:PHE:HB3	29:G:317:CLA:HMD3	1.97	0.46
15:K:136:ASP:OD1	15:K:138:GLY:N	2.49	0.46
22:H:143:ILE:HA	22:H:151:TRP:CZ2	2.51	0.46
23:N:90:TYR:C	23:N:92:SER:H	2.24	0.46
23:N:156:SER:O	23:N:159:LYS:HG3	2.15	0.46
24:O:127:TYR:CD2	24:O:229:LEU:HD13	2.51	0.46
34:E:316:LMG:HC1	34:E:316:LMG:HC8	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:173:LEU:HD13	29:a:824:CLA:H193	1.99	0.45
2:b:114:TYR:HB2	11:m:24:PHE:CE1	2.51	0.45
29:b:718:CLA:H92	29:b:718:CLA:H61	1.72	0.45
13:G:58:HIS:HE1	35:G:320:DGD:HE61	1.81	0.45
13:G:131:LEU:HD23	13:G:134:ILE:HD12	1.97	0.45
29:I:209:CLA:H62	29:I:209:CLA:H41	1.67	0.45
15:K:66:CYS:SG	15:K:165:MET:HG2	2.56	0.45
37:N:304:PID:HM41	37:N:304:PID:H16	1.68	0.45
25:T:157:SER:HB2	25:T:160:LEU:HB3	1.98	0.45
27:P:105:ALA:HA	27:P:108:LYS:HB2	1.96	0.45
1:a:530:SER:OG	1:a:533:GLU:HB3	2.16	0.45
32:a:835:BCR:H351	32:a:835:BCR:H15C	1.73	0.45
2:b:183:MET:HE1	29:h:201:CLA:HED3	1.98	0.45
2:b:538:ALA:HB2	2:b:606:LEU:HB3	1.97	0.45
29:b:705:CLA:H3A	29:b:705:CLA:O2A	2.17	0.45
4:d:73:TYR:HB3	4:d:114:ARG:HB2	1.98	0.45
29:I:207:CLA:HMB3	15:K:139:LEU:HD23	1.97	0.45
18:M:135:PRO:HD2	36:M:302:DD6:C33	2.46	0.45
25:T:181:GLY:O	25:T:185:ILE:HG12	2.16	0.45
28:E:227:PHE:O	28:E:231:VAL:HG12	2.15	0.45
10:l:261:LYS:HE2	19:L:106:ASP:HB3	1.98	0.45
13:G:33:SER:H	13:G:75:HIS:HE2	1.64	0.45
18:M:131:TYR:CE1	18:M:133:TRP:HB2	2.50	0.45
18:M:174:ARG:NH2	18:M:181:GLN:H	2.15	0.45
21:B:254:LEU:HG	29:B:316:CLA:HMA1	1.98	0.45
22:H:187:ASP:N	22:H:188:PRO:HD3	2.32	0.45
24:O:116:HIS:HB3	24:O:223:MET:CE	2.47	0.45
24:O:192:GLU:CD	29:O:314:CLA:HED1	2.42	0.45
25:T:155:TYR:O	37:T:302:PID:HM62	2.16	0.45
28:E:108:ASP:OD1	29:E:306:CLA:HBA2	2.16	0.45
1:a:25:THR:HA	1:a:28:ILE:HD12	1.97	0.45
2:b:404:VAL:HG11	2:b:478:TYR:CG	2.51	0.45
29:b:719:CLA:HAA2	13:G:70:LEU:HD13	1.99	0.45
29:b:721:CLA:H42	9:j:60:VAL:HG11	1.98	0.45
6:f:120:GLY:HA3	6:f:157:TRP:CE2	2.51	0.45
10:l:335:ARG:NE	10:l:340:ASP:OD2	2.48	0.45
29:I:211:CLA:H121	29:I:211:CLA:H162	1.81	0.45
16:F:84:PHE:HB2	16:F:96:PHE:CD2	2.51	0.45
17:J:92:THR:HG23	17:J:119:ARG:HH22	1.81	0.45
21:B:143:LEU:HB3	29:B:310:CLA:HAB	1.99	0.45
37:N:307:PID:HM11	37:N:307:PID:H7	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:189:LEU:HB2	1:a:190:PRO:HD3	1.98	0.45
29:b:712:CLA:H93	29:b:712:CLA:H111	1.79	0.45
30:b:727:PQN:H171	30:b:727:PQN:H212	1.73	0.45
3:c:62:LEU:O	4:d:173:VAL:HG11	2.16	0.45
4:d:5:THR:HG21	10:l:333:GLN:HG2	1.99	0.45
4:d:217:PRO:HA	7:h:39:PRO:CB	2.45	0.45
29:l:502:CLA:H93	29:l:502:CLA:H112	1.81	0.45
16:F:83:ARG:NH1	16:F:99:ILE:O	2.50	0.45
17:J:92:THR:OG1	17:J:119:ARG:NH1	2.40	0.45
19:L:98:ARG:HD3	19:L:226:GLU:OE1	2.17	0.45
37:N:305:PID:HM83	29:N:314:CLA:C1C	2.47	0.45
26:Q:114:ILE:HG23	26:Q:123:LYS:HB2	1.98	0.45
29:Q:308:CLA:H41	29:Q:308:CLA:H61	1.34	0.45
25:C:152:PHE:O	25:C:164:PHE:HB2	2.17	0.45
2:b:394:LEU:HD12	29:b:715:CLA:HAC1	1.99	0.45
29:b:709:CLA:HMB1	34:b:734:LMG:H211	1.98	0.45
13:G:40:MET:CE	13:G:80:ARG:HB2	2.47	0.45
29:I:213:CLA:H142	29:I:213:CLA:H111	1.75	0.45
16:F:32:LEU:O	16:F:59:ARG:NH2	2.49	0.45
19:L:164:LEU:HB3	29:L:310:CLA:HMC2	1.98	0.45
20:D:165:LEU:HD13	29:D:314:CLA:HMA3	1.98	0.45
23:N:128:GLU:HG2	37:N:302:PID:HM32	1.98	0.45
23:N:160:LYS:NZ	39:N:315:KC1:O1A	2.40	0.45
24:O:200:VAL:O	24:O:200:VAL:HG12	2.16	0.45
37:O:307:PID:HM11	37:O:307:PID:H7	1.73	0.45
37:P:202:PID:H22	29:P:217:CLA:HMD2	1.99	0.45
38:E:304:UIX:C38	29:E:311:CLA:HAB	2.46	0.45
29:a:810:CLA:HAB	29:b:721:CLA:CMD	2.45	0.45
29:b:720:CLA:H62	29:b:720:CLA:H2	1.79	0.45
25:C:156:LEU:HA	37:C:302:PID:HM62	1.98	0.45
2:b:159:VAL:HG23	2:b:205:ALA:HB1	1.99	0.45
2:b:408:ILE:HG12	2:b:475:PHE:HB3	1.99	0.45
29:b:725:CLA:H162	29:b:725:CLA:H202	1.69	0.45
18:M:263:ALA:O	18:M:267:ILE:HD12	2.17	0.45
25:T:137:MET:CE	29:T:314:CLA:HAB	2.47	0.45
25:T:138:LEU:HG	29:T:314:CLA:HAC1	1.98	0.45
25:T:168:PRO:O	25:T:173:ALA:HB2	2.16	0.45
26:Q:158:PHE:CE2	26:Q:160:ALA:HB3	2.52	0.45
25:C:112:LYS:HD2	25:C:112:LYS:HA	1.77	0.45
28:E:102:PRO:HB2	37:E:301:PID:H22A	1.99	0.45
1:a:95:ILE:HG22	1:a:98:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:832:PQN:H161	32:f:801:BCR:H382	1.99	0.45
6:f:29:TRP:HH2	6:f:100:THR:HG21	1.82	0.45
29:f:805:CLA:H93	29:f:805:CLA:H61	1.82	0.45
29:l:501:CLA:H71	29:l:504:CLA:H203	1.99	0.45
12:A:32:TYR:OH	36:A:204:DD6:O2	2.30	0.45
14:I:47:HIS:HB3	14:I:153:MET:SD	2.57	0.45
14:I:96:GLY:HA2	29:I:213:CLA:HAB	1.99	0.45
36:I:205:DD6:C26	29:I:214:CLA:H72	2.46	0.45
16:F:183:ALA:CB	37:F:304:PID:HM11	2.47	0.45
17:J:98:GLU:OE1	17:J:98:GLU:N	2.48	0.45
18:M:210:GLY:O	18:M:214:GLN:HG2	2.17	0.45
20:D:69:ILE:HD13	20:D:146:GLY:HA3	1.98	0.45
24:O:155:LEU:HD23	24:O:233:ASP:HB3	1.99	0.45
1:a:220:LEU:HD23	1:a:220:LEU:H	1.82	0.45
1:a:366:PHE:HE2	29:a:829:CLA:HAB	1.82	0.45
2:b:29:GLN:HB3	2:b:134:PRO:HB2	1.99	0.45
29:b:714:CLA:H3A	29:b:714:CLA:HBA2	1.63	0.45
29:b:715:CLA:H3A	29:b:715:CLA:HBA2	1.55	0.45
29:b:736:CLA:C4A	29:b:736:CLA:HBA2	2.46	0.45
4:d:195:ASP:OD1	8:i:170:GLN:NE2	2.49	0.45
6:f:102:GLU:HB2	29:f:803:CLA:HMD2	1.99	0.45
9:j:28:PRO:HB2	9:j:30:ILE:HG23	1.99	0.45
12:A:129:GLN:HG3	29:A:218:CLA:O1D	2.17	0.45
14:I:9:PHE:CD1	15:K:121:ALA:HB2	2.52	0.45
29:I:217:CLA:H92	29:I:217:CLA:H61	1.74	0.45
15:K:67:MET:HE1	29:K:214:CLA:HHC	1.98	0.45
18:M:262:LEU:HD13	36:M:301:DD6:C26	2.47	0.45
20:D:110:LEU:HD13	20:D:186:ASP:HB2	1.99	0.45
21:B:181:GLN:HE21	40:B:317:SQD:H61	1.82	0.45
23:N:59:ARG:NE	39:N:310:KC1:O2A	2.49	0.45
37:N:307:PID:H16	37:N:307:PID:HM41	1.86	0.45
37:O:307:PID:H8	37:O:307:PID:HM21	1.99	0.45
25:C:233:GLY:O	25:C:237:MET:HG3	2.17	0.45
27:P:56:ARG:NH1	39:P:211:KC1:O1A	2.50	0.45
28:E:117:LYS:HB3	28:E:121:PHE:CE2	2.52	0.45
1:a:550:GLY:C	1:a:639:PHE:HE1	2.25	0.44
29:a:811:CLA:H42	29:a:813:CLA:H2	1.99	0.44
10:l:379:PHE:HB3	10:l:395:GLY:HA2	1.99	0.44
13:G:54:PRO:O	36:G:307:DD6:O4	2.34	0.44
14:I:61:GLN:HG2	14:I:72:MET:SD	2.57	0.44
14:I:130:LEU:HG	29:I:214:CLA:HAA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:234:THR:OG1	19:L:235:ARG:N	2.50	0.44
23:N:59:ARG:HE	39:N:310:KC1:CGA	2.30	0.44
23:N:169:ARG:HB3	29:N:309:CLA:CAC	2.47	0.44
25:C:113:LEU:HD12	25:C:113:LEU:HA	1.80	0.44
25:C:254:TRP:HZ3	37:C:305:PID:H3	1.81	0.44
1:a:355:ILE:HG23	1:a:359:HIS:CE1	2.52	0.44
1:a:473:GLY:HA2	2:b:447:PRO:HD3	1.98	0.44
29:b:723:CLA:HMD3	6:f:99:ALA:HB3	2.00	0.44
9:j:26:VAL:HG12	15:K:49:ALA:HB1	1.99	0.44
12:A:118:LYS:NZ	12:A:140:ASN:O	2.33	0.44
15:K:142:LEU:HD23	29:K:214:CLA:H42	1.99	0.44
15:K:157:GLU:HB2	29:K:214:CLA:CHB	2.48	0.44
29:L:313:CLA:O1A	29:L:313:CLA:H3A	2.18	0.44
22:H:121:PHE:HB2	22:H:133:TYR:CD2	2.52	0.44
24:O:106:PHE:CZ	29:O:309:CLA:HED1	2.52	0.44
25:T:155:TYR:CE1	25:T:158:PRO:HA	2.52	0.44
37:P:203:PID:HM51	37:P:203:PID:HM82	1.98	0.44
28:E:221:ARG:HA	28:E:224:MET:HE3	1.98	0.44
29:a:819:CLA:HBA2	29:a:819:CLA:H3A	1.53	0.44
29:a:822:CLA:H101	29:a:822:CLA:H62	1.79	0.44
30:a:832:PQN:H192	30:a:832:PQN:H162	1.69	0.44
2:b:368:GLN:HG2	2:b:373:LEU:HG	2.00	0.44
2:b:472:VAL:O	2:b:476:THR:OG1	2.24	0.44
29:l:504:CLA:H192	29:l:504:CLA:H162	1.80	0.44
29:A:209:CLA:H111	29:A:209:CLA:H171	1.98	0.44
39:G:315:KC1:CMC	29:D:313:CLA:HHC	2.47	0.44
14:I:55:THR:HG21	36:I:205:DD6:C8	2.48	0.44
19:L:160:MET:SD	29:L:313:CLA:HAB	2.58	0.44
25:T:145:THR:OG1	25:T:146:PRO:HD3	2.18	0.44
27:P:63:LYS:HD2	29:P:214:CLA:C3D	2.48	0.44
1:a:372:PHE:CE1	29:a:803:CLA:HHB	2.52	0.44
29:a:803:CLA:O2A	2:b:536:LEU:HB3	2.17	0.44
29:a:815:CLA:HBA2	32:a:834:BCR:H342	1.99	0.44
29:a:831:CLA:H202	37:j:101:PID:H18	1.99	0.44
2:b:171:VAL:HG13	2:b:176:PRO:HA	1.99	0.44
29:b:705:CLA:O1D	32:b:729:BCR:H391	2.17	0.44
29:h:201:CLA:H41	29:h:201:CLA:H61	1.74	0.44
11:m:57:GLU:HG2	11:m:58:THR:N	2.32	0.44
12:A:167:LYS:HD2	29:A:206:CLA:O1D	2.17	0.44
19:L:270:VAL:HG11	29:L:317:CLA:H2A	1.99	0.44
25:T:215:THR:OG1	29:T:314:CLA:O2A	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:301:PID:H16	37:C:301:PID:HM41	1.63	0.44
1:a:36:HIS:HD1	29:a:807:CLA:CGA	2.28	0.44
29:a:809:CLA:H3A	29:a:809:CLA:HBA2	1.32	0.44
29:a:816:CLA:H2A	29:a:816:CLA:HED3	1.98	0.44
29:a:820:CLA:HBB2	32:b:735:BCR:H373	1.99	0.44
2:b:404:VAL:HG11	2:b:478:TYR:HB2	1.99	0.44
29:b:702:CLA:H191	8:i:79:ILE:HD12	1.99	0.44
29:b:721:CLA:HBA1	29:b:721:CLA:H3A	1.74	0.44
32:f:801:BCR:H11C	32:f:801:BCR:H341	1.83	0.44
7:h:118:PHE:CE1	29:G:304:CLA:HBB1	2.52	0.44
37:G:309:PID:HM41	37:G:309:PID:H16	1.70	0.44
14:I:11:PRO:HG3	15:K:130:THR:HG23	1.99	0.44
17:J:150:TRP:HZ2	36:J:302:DD6:C10	2.30	0.44
21:B:173:LYS:O	21:B:176:GLU:HG2	2.17	0.44
25:T:113:LEU:O	25:T:114:THR:OG1	2.30	0.44
29:E:305:CLA:H3A	29:E:305:CLA:HBA1	1.71	0.44
2:b:93:LEU:HB2	34:b:730:LMG:HC1	1.99	0.44
29:b:703:CLA:H112	29:b:703:CLA:H142	1.74	0.44
3:c:82:LEU:HD22	4:d:74:MET:HG2	1.99	0.44
4:d:152:ASP:OD2	4:d:163:ARG:NE	2.51	0.44
6:f:13:LYS:HG2	29:f:805:CLA:C2B	2.48	0.44
32:i:204:BCR:H351	32:i:204:BCR:H15C	1.81	0.44
10:l:368:GLY:O	10:l:444:GLY:HA2	2.18	0.44
10:l:433:PHE:O	10:l:437:ILE:HG12	2.18	0.44
29:l:505:CLA:H171	29:l:505:CLA:H13	1.86	0.44
37:F:304:PID:H22	29:F:313:CLA:C1C	2.47	0.44
22:H:185:SER:HG	22:H:194:LYS:HZ1	1.54	0.44
25:C:155:TYR:C	25:C:157:SER:H	2.26	0.44
29:P:210:CLA:H61	29:P:210:CLA:H92	1.76	0.44
1:a:58:VAL:HG13	32:a:838:BCR:HC31	1.99	0.44
29:a:829:CLA:H143	29:a:829:CLA:H161	1.79	0.44
29:a:831:CLA:H92	29:a:831:CLA:H61	1.78	0.44
32:a:834:BCR:H11C	32:a:834:BCR:H341	1.77	0.44
2:b:311:LEU:HD12	29:b:719:CLA:HMD3	1.99	0.44
2:b:325:THR:HG21	29:b:719:CLA:HMB1	2.00	0.44
29:b:714:CLA:CGD	29:b:715:CLA:HAB	2.46	0.44
11:m:88:ARG:HB2	11:m:89:PRO:CD	2.46	0.44
13:G:92:LEU:HB3	29:G:314:CLA:HAB	2.00	0.44
18:M:131:TYR:CZ	18:M:133:TRP:HB2	2.52	0.44
19:L:192:ASP:OD1	36:L:305:DD6:O4	2.35	0.44
21:B:243:LEU:HD11	29:B:308:CLA:HAC1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:N:170:LEU:HG	37:N:305:PID:H13	1.99	0.44
26:Q:174:LYS:O	29:Q:313:CLA:HMB2	2.17	0.44
25:C:235:LEU:HG	37:C:305:PID:H13	1.99	0.44
1:a:10:PHE:CZ	9:j:37:GLU:HG2	2.53	0.44
2:b:473:ALA:HB2	2:b:604:PHE:CZ	2.53	0.44
29:b:720:CLA:HBB1	32:f:801:BCR:H323	1.99	0.44
4:d:5:THR:HB	4:d:76:LYS:HD2	1.99	0.44
4:d:41:GLN:O	4:d:43:ARG:N	2.46	0.44
32:l:507:BCR:H351	32:l:507:BCR:H15C	1.61	0.44
13:G:97:CYS:SG	36:G:307:DD6:C23	3.05	0.44
14:I:52:MET:O	14:I:56:VAL:HG22	2.17	0.44
15:K:62:HIS:HB3	15:K:165:MET:HE3	1.99	0.44
18:M:244:GLU:HB2	23:N:152:SER:OG	2.18	0.44
19:L:218:LYS:HG2	19:L:231:TYR:CE1	2.53	0.44
20:D:80:MET:HE2	37:D:305:PID:C20	2.48	0.44
23:N:112:VAL:HB	23:N:117:TRP:NE1	2.33	0.44
26:Q:168:PRO:C	26:Q:170:THR:N	2.76	0.44
27:P:99:ILE:HG22	27:P:108:LYS:HB3	2.00	0.44
29:a:803:CLA:HBB2	29:b:705:CLA:HBA1	2.00	0.44
13:G:85:LYS:NZ	13:G:142:GLU:OE2	2.37	0.44
20:D:107:PRO:O	20:D:112:ALA:HB2	2.18	0.44
20:D:186:ASP:HA	20:D:191:GLY:O	2.18	0.44
37:H:305:PID:HM52	29:H:313:CLA:HAB	2.00	0.44
37:H:306:PID:HM41	37:H:306:PID:H16	1.77	0.44
23:N:80:THR:OG1	29:N:311:CLA:HAC2	2.18	0.44
24:O:106:PHE:HZ	29:O:309:CLA:HED1	1.82	0.44
25:T:164:PHE:CZ	37:T:302:PID:H22	2.52	0.44
37:T:307:PID:H16	37:T:307:PID:HM41	1.86	0.44
1:a:381:MET:HB2	1:a:390:MET:HG2	2.00	0.43
2:b:137:GLY:HA2	11:m:67:PHE:CE2	2.52	0.43
2:b:179:LEU:HD11	29:h:201:CLA:HAA2	1.99	0.43
2:b:250:ILE:HD11	32:b:728:BCR:H15C	2.00	0.43
7:h:114:LEU:HB3	37:h:204:PID:H8	2.00	0.43
8:i:111:LYS:HB3	11:m:56:PRO:HG3	1.99	0.43
10:l:355:ARG:HH22	10:l:366:GLU:CD	2.23	0.43
37:F:304:PID:H19	29:F:313:CLA:HAB	2.00	0.43
20:D:77:LEU:HD11	29:D:314:CLA:HBC1	1.99	0.43
20:D:84:THR:HB	20:D:85:PRO:HD3	2.00	0.43
20:D:156:GLU:OE1	20:D:156:GLU:N	2.51	0.43
21:B:197:LEU:HB3	21:B:208:ARG:HD3	2.00	0.43
36:O:303:DD6:O1	29:O:309:CLA:H52	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:O:307:PID:HM41	37:O:307:PID:H16	1.79	0.43
25:T:238:MET:HE2	25:T:238:MET:HB2	1.88	0.43
26:Q:139:CYS:HB2	37:Q:301:PID:HM13	2.00	0.43
25:C:214:ILE:O	29:C:314:CLA:H3A	2.18	0.43
1:a:219:GLN:NE2	1:a:221:SER:HB2	2.32	0.43
29:a:807:CLA:C14	29:a:824:CLA:HBB2	2.48	0.43
29:a:813:CLA:HBA2	29:a:813:CLA:H3A	1.32	0.43
29:a:831:CLA:H62	29:a:831:CLA:H41	1.69	0.43
32:f:801:BCR:H361	32:f:801:BCR:H20C	1.70	0.43
7:h:32:GLU:OE2	7:h:37:ARG:NH2	2.51	0.43
29:l:504:CLA:H201	17:J:200:ILE:HG23	2.01	0.43
14:I:63:TYR:O	14:I:65:GLY:N	2.51	0.43
29:J:306:CLA:H2A	29:J:306:CLA:O1D	2.18	0.43
19:L:154:LYS:HB2	19:L:154:LYS:HE3	1.82	0.43
19:L:190:ALA:HB2	29:L:310:CLA:HED3	2.01	0.43
21:B:176:GLU:HG3	21:B:177:MET:HE2	1.99	0.43
22:H:185:SER:H	22:H:194:LYS:HE2	1.82	0.43
29:H:310:CLA:HBA2	29:H:310:CLA:H3A	1.62	0.43
24:O:87:PRO:HG2	24:O:217:ALA:HB2	1.99	0.43
24:O:136:PHE:HD2	24:O:149:ALA:HA	1.83	0.43
37:Q:304:PID:HM22	29:Q:315:CLA:HMB2	2.00	0.43
29:E:306:CLA:C1B	29:E:306:CLA:H42	2.48	0.43
29:b:702:CLA:H51	29:b:725:CLA:H102	1.99	0.43
29:b:707:CLA:HBA1	29:b:707:CLA:H11	1.78	0.43
3:c:62:LEU:HA	3:c:62:LEU:HD13	1.70	0.43
4:d:140:SER:HG	4:d:144:THR:HG1	1.63	0.43
10:l:346:ASN:HB3	17:J:188:PRO:O	2.19	0.43
11:m:57:GLU:O	11:m:61:LYS:N	2.34	0.43
29:G:316:CLA:H52	29:G:316:CLA:H12	1.70	0.43
15:K:95:HIS:O	15:K:95:HIS:CG	2.72	0.43
15:K:99:VAL:HA	15:K:104:MET:HB2	1.99	0.43
16:F:67:ARG:HA	16:F:70:MET:HE3	2.01	0.43
20:D:38:LEU:HD22	20:D:165:LEU:HB3	2.01	0.43
21:B:182:GLN:HE22	28:E:148:PRO:CD	2.31	0.43
24:O:225:ALA:O	24:O:229:LEU:HG	2.18	0.43
27:P:162:LEU:HD13	27:P:162:LEU:HA	1.83	0.43
1:a:190:PRO:O	1:a:194:LEU:HG	2.19	0.43
29:a:823:CLA:O1D	29:a:824:CLA:HHB	2.18	0.43
2:b:347:MET:SD	2:b:355:LYS:HB2	2.58	0.43
29:b:712:CLA:H3A	29:b:712:CLA:HBA2	1.56	0.43
29:i:203:CLA:HBA1	29:i:203:CLA:H3A	1.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:67:THR:HG22	9:j:70:TRP:HB2	2.00	0.43
10:l:313:PRO:HB3	29:l:501:CLA:HMD2	1.99	0.43
12:A:169:GLY:O	12:A:173:MET:HG3	2.19	0.43
16:F:54:THR:HG23	16:F:57:ARG:HH21	1.83	0.43
18:M:270:ALA:HB1	29:M:313:CLA:HED1	1.99	0.43
20:D:131:CYS:SG	37:D:303:PID:HM33	2.58	0.43
20:D:162:LYS:HB2	20:D:162:LYS:HE3	1.78	0.43
28:E:182:VAL:HG13	28:E:183:LYS:N	2.34	0.43
1:a:578:LEU:HD23	1:a:627:HIS:CD2	2.53	0.43
29:a:805:CLA:H12	29:a:805:CLA:H52	1.72	0.43
8:i:127:PRO:HB2	8:i:129:ASP:O	2.18	0.43
18:M:249:TYR:CE1	29:M:311:CLA:HMB1	2.54	0.43
21:B:189:VAL:HG11	36:B:319:DD6:C6	2.48	0.43
21:B:192:ILE:HG22	29:E:311:CLA:H91	2.00	0.43
23:N:34:LEU:HD21	23:N:161:LEU:HD23	1.99	0.43
29:N:313:CLA:H3A	29:N:313:CLA:HBA2	1.42	0.43
37:P:202:PID:H16	37:P:202:PID:HM41	1.85	0.43
1:a:53:LEU:HB3	1:a:143:SER:HB2	2.00	0.43
29:a:827:CLA:H161	29:a:827:CLA:H141	1.79	0.43
2:b:93:LEU:O	34:b:730:LMG:HC72	2.19	0.43
2:b:246:THR:HG23	2:b:293:GLY:HA3	2.00	0.43
29:b:736:CLA:H11	29:A:217:CLA:HBD	2.00	0.43
4:d:125:GLN:O	4:d:128:SER:OG	2.31	0.43
4:d:181:GLU:O	4:d:205:ARG:NH2	2.52	0.43
29:i:202:CLA:H191	35:m:102:DGD:HBF1	2.00	0.43
35:j:103:DGD:HB21	35:j:106:DGD:HA82	2.00	0.43
12:A:43:PHE:HB3	12:A:46:GLN:HB2	2.00	0.43
29:G:302:CLA:H41	29:G:302:CLA:H62	1.47	0.43
36:G:305:DD6:C24	29:G:312:CLA:H191	2.48	0.43
17:J:187:VAL:HB	17:J:188:PRO:HD3	2.01	0.43
17:J:243:ALA:C	17:J:245:THR:H	2.26	0.43
20:D:168:GLU:HB2	29:D:314:CLA:C1B	2.48	0.43
23:N:90:TYR:CE1	23:N:98:LYS:HE3	2.53	0.43
26:Q:202:ALA:HB1	26:Q:203:TRP:HD1	1.83	0.43
29:P:210:CLA:CGA	29:P:210:CLA:H3A	2.49	0.43
28:E:204:GLN:O	28:E:205:SER:HB3	2.18	0.43
1:a:246:LEU:HA	1:a:249:VAL:HG22	2.00	0.43
29:a:806:CLA:H192	29:a:806:CLA:H162	1.83	0.43
2:b:277:SER:HB3	29:b:716:CLA:HMA1	2.01	0.43
29:b:701:CLA:H101	29:b:720:CLA:H43	2.01	0.43
29:b:720:CLA:H193	29:b:723:CLA:H111	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:76:ILE:HB	12:A:83:TRP:CD1	2.53	0.43
12:A:174:LEU:HD11	29:A:207:CLA:HAC1	1.99	0.43
29:G:317:CLA:H11	29:G:317:CLA:H51	1.82	0.43
16:F:59:ARG:NH1	16:F:62:GLU:OE1	2.52	0.43
18:M:193:LYS:HE2	18:M:193:LYS:HB2	1.86	0.43
22:H:190:SER:OG	22:H:193:LYS:HE3	2.19	0.43
22:H:214:THR:O	22:H:218:LEU:HB3	2.19	0.43
37:N:305:PID:H15	39:N:315:KC1:CHC	2.49	0.43
24:O:119:ILE:CD1	37:O:302:PID:H7	2.48	0.43
37:O:301:PID:H16	37:O:301:PID:HM41	1.71	0.43
26:Q:78:LYS:HE3	29:Q:312:CLA:C3D	2.49	0.43
1:a:164:LEU:HB2	29:a:814:CLA:HBC2	1.99	0.43
1:a:578:LEU:O	1:a:581:MET:HB3	2.18	0.43
29:a:807:CLA:H93	29:a:807:CLA:H112	1.74	0.43
29:b:708:CLA:HBA2	29:b:708:CLA:H3A	1.83	0.43
32:b:728:BCR:H15C	32:b:728:BCR:H351	1.83	0.43
6:f:110:THR:HG22	6:f:114:MET:HE2	2.00	0.43
8:i:147:ALA:O	8:i:151:VAL:HG22	2.19	0.43
34:j:102:LMG:H211	10:l:264:TRP:HZ2	1.83	0.43
29:I:208:CLA:HBA2	29:I:208:CLA:H3A	1.46	0.43
36:J:302:DD6:C4	29:J:309:CLA:HAC2	2.49	0.43
18:M:119:LEU:HD13	18:M:150:ARG:HB2	2.01	0.43
29:L:316:CLA:O2D	29:L:316:CLA:H2A	2.18	0.43
23:N:57:PHE:HE1	29:N:309:CLA:H2A	1.83	0.43
24:O:193:PHE:HB2	29:O:314:CLA:OBD	2.19	0.43
1:a:587:ARG:H	2:b:453:CYS:HB2	1.84	0.43
29:a:826:CLA:CAD	32:b:735:BCR:H21C	2.48	0.43
2:b:74:HIS:NE2	29:b:708:CLA:OBD	2.51	0.43
29:b:722:CLA:H62	29:b:722:CLA:H41	1.67	0.43
32:b:735:BCR:H15C	32:b:735:BCR:H351	1.84	0.43
4:d:10:PRO:HG3	4:d:76:LYS:HA	2.01	0.43
7:h:29:GLU:HG2	8:i:124:VAL:HG11	2.01	0.43
7:h:69:LEU:HD23	7:h:69:LEU:HA	1.91	0.43
29:A:208:CLA:HMB1	29:A:208:CLA:HBB1	2.00	0.43
13:G:85:LYS:HB2	13:G:85:LYS:HE3	1.80	0.43
13:G:147:ASN:O	13:G:149:ASP:N	2.44	0.43
19:L:267:THR:O	19:L:271:ILE:HG12	2.18	0.43
20:D:96:SER:HB3	20:D:101:ILE:HB	2.00	0.43
22:H:182:VAL:HG21	37:H:305:PID:H27	1.99	0.43
23:N:100:ASP:OD1	23:N:101:ASP:N	2.51	0.43
25:C:138:LEU:HG	29:C:314:CLA:HAC1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:36:HIS:HB3	29:a:806:CLA:HAB	1.99	0.43
2:b:345:ASP:OD1	2:b:500:TYR:HB2	2.19	0.43
29:b:704:CLA:H112	29:b:704:CLA:H152	1.79	0.43
29:b:717:CLA:H161	29:b:717:CLA:H122	1.80	0.43
32:f:804:BCR:H362	29:G:301:CLA:HBC3	2.01	0.43
10:l:322:TRP:CH2	10:l:334:ILE:HD12	2.54	0.43
29:I:207:CLA:HAB	15:K:137:TYR:O	2.19	0.43
29:I:216:CLA:H2A	29:I:216:CLA:O1D	2.18	0.43
15:K:67:MET:O	15:K:71:VAL:HG22	2.19	0.43
15:K:132:ARG:NE	15:K:136:ASP:O	2.51	0.43
16:F:65:ASN:ND2	29:F:312:CLA:OBD	2.51	0.43
20:D:101:ILE:HD12	20:D:117:PRO:HD3	2.00	0.43
24:O:136:PHE:CD2	24:O:149:ALA:HA	2.53	0.43
37:O:301:PID:HM22	29:O:309:CLA:HAC2	2.01	0.43
26:Q:137:ALA:CB	29:Q:312:CLA:HAB	2.49	0.43
37:Q:306:PID:H22	39:Q:314:KC1:C3A	2.49	0.43
29:C:314:CLA:O2D	29:C:314:CLA:HBA2	2.19	0.43
28:E:204:GLN:O	28:E:208:GLU:HB3	2.18	0.43
1:a:180:TRP:HD1	1:a:243:HIS:CD2	2.36	0.42
1:a:437:PHE:CE1	29:b:705:CLA:HBA2	2.54	0.42
12:A:56:LYS:HE3	12:A:56:LYS:HB2	1.79	0.42
29:F:311:CLA:H2A	17:J:168:LEU:HD11	1.99	0.42
17:J:93:GLY:HA2	17:J:223:MET:HE1	2.00	0.42
19:L:280:PHE:HD2	29:L:315:CLA:HED3	1.84	0.42
20:D:67:SER:C	20:D:71:HIS:HD1	2.23	0.42
26:Q:111:PHE:HZ	37:Q:301:PID:H22	1.84	0.42
27:P:169:MET:O	27:P:172:ILE:HG22	2.19	0.42
28:E:102:PRO:HG2	37:E:301:PID:H22A	2.00	0.42
29:E:315:CLA:H61	29:E:315:CLA:H93	1.79	0.42
1:a:280:GLN:NE2	29:a:821:CLA:HAA1	2.33	0.42
1:a:609:HIS:H	6:f:139:GLU:CD	2.27	0.42
29:a:807:CLA:HBD	29:a:807:CLA:HBA2	2.01	0.42
29:a:825:CLA:H202	29:a:825:CLA:H161	1.92	0.42
32:a:838:BCR:H351	32:a:838:BCR:H15C	1.76	0.42
2:b:79:PRO:HG2	29:i:203:CLA:HMB2	2.01	0.42
2:b:261:VAL:O	2:b:392:SER:OG	2.33	0.42
2:b:531:TRP:CE2	2:b:613:VAL:HG11	2.53	0.42
29:l:501:CLA:HBA1	29:l:501:CLA:H3A	1.76	0.42
12:A:183:ALA:HB2	12:A:192:TRP:CD1	2.54	0.42
29:A:212:CLA:H41	29:A:212:CLA:H61	1.67	0.42
17:J:136:TRP:CG	17:J:159:PRO:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:J:310:CLA:H3A	29:J:310:CLA:HBA1	1.62	0.42
22:H:206:MET:HE3	29:H:308:CLA:HMC3	2.01	0.42
37:H:306:PID:HM83	37:H:306:PID:HM51	2.01	0.42
25:C:112:LYS:C	25:C:114:THR:H	2.26	0.42
37:P:205:PID:HM41	37:P:205:PID:H16	1.67	0.42
1:a:186:HIS:HB3	1:a:208:LEU:HD21	1.99	0.42
1:a:327:VAL:HG11	1:a:492:LEU:HG	2.00	0.42
1:a:362:TRP:HB2	29:b:702:CLA:HED2	2.01	0.42
1:a:547:LEU:HD11	29:a:801:CLA:H72	2.02	0.42
1:a:572:SER:HB3	1:a:631:GLY:O	2.19	0.42
2:b:157:HIS:HB2	29:b:709:CLA:C1C	2.48	0.42
2:b:172:VAL:HG23	2:b:173:MET:HG2	2.01	0.42
2:b:339:GLY:HA3	29:b:721:CLA:HAB	2.00	0.42
29:l:503:CLA:HBA2	29:l:503:CLA:C4A	2.49	0.42
14:I:7:VAL:HG11	14:I:10:LEU:HD12	2.00	0.42
14:I:128:THR:CG2	26:Q:147:PRO:HG3	2.49	0.42
16:F:88:LEU:HG	16:F:109:LEU:HD11	2.01	0.42
21:B:240:LEU:HD13	29:B:307:CLA:HBC1	2.02	0.42
26:Q:91:ILE:CG2	37:Q:306:PID:H11	2.49	0.42
1:a:144:TYR:CE1	9:j:28:PRO:HG3	2.54	0.42
1:a:435:HIS:HB3	29:a:828:CLA:HAB	2.01	0.42
1:a:578:LEU:HD23	1:a:627:HIS:HD2	1.83	0.42
29:a:805:CLA:HBA1	29:a:805:CLA:H3A	1.80	0.42
29:a:809:CLA:HAA2	29:a:823:CLA:HED2	2.00	0.42
2:b:101:TRP:CD2	29:b:717:CLA:H11	2.55	0.42
3:c:17:VAL:HG21	3:c:27:MET:HG2	2.02	0.42
5:e:65:LEU:HD13	5:e:70:TYR:HB3	2.02	0.42
6:f:65:ALA:O	6:f:69:VAL:HG23	2.19	0.42
6:f:156:ALA:HA	29:I:212:CLA:HBC1	2.01	0.42
29:i:201:CLA:H61	29:i:201:CLA:H41	1.44	0.42
12:A:79:PRO:HD2	12:A:83:TRP:CE3	2.55	0.42
15:K:73:TRP:NE1	15:K:77:ASP:OD2	2.52	0.42
29:J:313:CLA:H2A	29:J:313:CLA:HED3	2.02	0.42
23:N:66:LYS:O	23:N:70:ILE:HD12	2.18	0.42
37:N:302:PID:H16	37:N:302:PID:HM41	1.89	0.42
27:P:78:PRO:HA	27:P:83:LYS:HG2	2.01	0.42
27:P:94:LEU:HD12	27:P:94:LEU:HA	1.80	0.42
29:E:308:CLA:H141	29:E:315:CLA:H43	2.01	0.42
1:a:422:VAL:HG21	29:a:828:CLA:HMD1	2.02	0.42
29:a:812:CLA:H41	29:a:812:CLA:H61	1.69	0.42
29:a:812:CLA:HBB1	29:a:812:CLA:HMB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:281:HIS:HB2	29:b:716:CLA:C1B	2.49	0.42
2:b:500:TYR:OH	2:b:506:ARG:NH2	2.50	0.42
2:b:504:TRP:O	2:b:508:TYR:HB3	2.19	0.42
29:b:702:CLA:H3A	32:b:735:BCR:H391	2.00	0.42
29:b:719:CLA:H3A	29:b:719:CLA:HBA2	1.54	0.42
35:h:203:DGD:HE62	13:G:19:GLN:NE2	2.35	0.42
10:l:214:PRO:HD2	10:l:217:ILE:HD13	2.01	0.42
11:m:84:TYR:CD2	11:m:86:PRO:HD3	2.54	0.42
29:K:214:CLA:CHB	29:K:214:CLA:H11	2.48	0.42
16:F:61:SER:O	16:F:65:ASN:ND2	2.32	0.42
16:F:95:LYS:O	16:F:98:GLU:HG2	2.20	0.42
17:J:106:PHE:HD2	36:J:303:DD6:O4	2.02	0.42
29:J:307:CLA:OBD	29:J:310:CLA:H12	2.20	0.42
29:M:309:CLA:H3A	29:M:309:CLA:HBA2	1.72	0.42
29:B:308:CLA:H52	29:B:309:CLA:HMA2	2.01	0.42
22:H:95:ARG:O	22:H:99:ILE:HG13	2.19	0.42
24:O:115:LYS:HD2	29:O:313:CLA:C3D	2.49	0.42
25:T:240:ILE:HD12	25:T:240:ILE:HA	1.79	0.42
26:Q:73:ARG:NH2	29:Q:308:CLA:HED3	2.34	0.42
28:E:115:GLU:C	28:E:116:GLU:HG3	2.43	0.42
1:a:141:LEU:HD22	34:K:201:LMG:H171	2.02	0.42
29:a:809:CLA:H162	29:a:809:CLA:H192	1.78	0.42
2:b:67:LEU:HB3	6:f:1:ILE:HG21	2.01	0.42
2:b:345:ASP:OD1	2:b:501:LEU:N	2.52	0.42
2:b:576:ILE:HD11	10:l:353:PHE:HZ	1.84	0.42
10:l:286:LYS:HE2	10:l:286:LYS:HB2	1.83	0.42
29:l:501:CLA:H111	29:l:501:CLA:H91	1.77	0.42
37:G:310:PID:H16	37:G:310:PID:HM41	1.85	0.42
29:I:212:CLA:HBA1	29:I:212:CLA:H3A	1.69	0.42
15:K:66:CYS:SG	36:K:204:DD6:C6	3.08	0.42
16:F:142:THR:HB	16:F:151:PHE:HB3	2.02	0.42
18:M:119:LEU:HD21	18:M:228:LEU:HD22	2.01	0.42
18:M:215:ARG:NH2	18:M:232:GLY:H	2.17	0.42
1:a:273:TRP:HB3	29:a:806:CLA:HAC1	2.00	0.42
29:a:803:CLA:H142	2:b:533:TRP:HH2	1.84	0.42
32:a:838:BCR:H20C	32:a:838:BCR:H361	1.79	0.42
2:b:41:VAL:HG22	32:m:103:BCR:HC8	2.01	0.42
7:h:61:LEU:HD12	7:h:69:LEU:HD21	2.01	0.42
11:m:57:GLU:HB2	11:m:61:LYS:HG2	2.02	0.42
13:G:147:ASN:CG	13:G:148:GLY:H	2.27	0.42
13:G:176:ASP:N	13:G:176:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:183:ALA:HB1	37:F:304:PID:C8	2.36	0.42
29:L:307:CLA:H3A	29:L:307:CLA:HBA2	1.26	0.42
37:D:306:PID:H312	37:D:306:PID:H27	1.84	0.42
23:N:174:ALA:HA	37:N:305:PID:HM11	2.02	0.42
24:O:127:TYR:HE2	24:O:229:LEU:HD22	1.85	0.42
37:T:305:PID:HM13	29:T:316:CLA:C3B	2.50	0.42
29:P:214:CLA:H3A	29:P:214:CLA:HBA2	1.43	0.42
29:E:308:CLA:H141	29:E:308:CLA:H162	1.71	0.42
1:a:110:PHE:CE1	29:a:824:CLA:HAA2	2.54	0.42
29:a:804:CLA:C1D	9:j:43:PRO:HG3	2.49	0.42
2:b:73:ASN:OD1	2:b:74:HIS:ND1	2.42	0.42
6:f:86:ARG:HD2	6:f:105:ARG:HG3	2.01	0.42
8:i:81:ALA:HB1	35:m:102:DGD:HBE2	2.00	0.42
8:i:175:TYR:O	8:i:178:ASN:HB2	2.19	0.42
10:l:396:LEU:HD21	29:l:509:CLA:CHD	2.50	0.42
13:G:90:CYS:SG	13:G:192:MET:HG2	2.60	0.42
29:G:302:CLA:CBB	37:G:303:PID:H18	2.50	0.42
14:I:52:MET:HG3	14:I:152:ALA:HB3	2.02	0.42
36:I:206:DD6:C4	29:I:210:CLA:HBB2	2.50	0.42
16:F:117:MET:HE1	29:F:310:CLA:HHB	2.02	0.42
18:M:262:LEU:O	18:M:265:SER:OG	2.31	0.42
20:D:39:GLY:HA3	29:D:309:CLA:HED3	2.01	0.42
29:D:311:CLA:H3A	29:D:311:CLA:HBA2	1.67	0.42
21:B:118:PRO:O	36:B:303:DD6:O4	2.37	0.42
21:B:135:LEU:HD13	21:B:211:GLY:HA3	2.01	0.42
23:N:79:MET:HE1	37:N:307:PID:HM31	2.01	0.42
24:O:153:ASN:O	24:O:239:ALA:HB2	2.19	0.42
1:a:55:HIS:ND1	29:a:806:CLA:O1A	2.49	0.42
1:a:466:ASP:CG	1:a:467:PHE:H	2.27	0.42
1:a:481:GLN:HG3	2:b:552:TRP:HB2	2.02	0.42
1:a:598:LEU:HD23	6:f:178:ARG:HH22	1.84	0.42
1:a:612:PRO:HB3	29:a:837:CLA:C2C	2.50	0.42
29:a:812:CLA:H42	9:j:38:TYR:OH	2.20	0.42
29:a:822:CLA:H171	29:l:501:CLA:H13	2.01	0.42
2:b:58:ASN:O	2:b:62:PHE:N	2.53	0.42
32:i:204:BCR:H361	32:i:204:BCR:H20C	1.79	0.42
13:G:74:PRO:HB3	13:G:78:TRP:CD1	2.55	0.42
29:G:302:CLA:HBB2	37:G:303:PID:H18	2.01	0.42
29:I:209:CLA:H52	29:I:210:CLA:H3A	2.01	0.42
29:K:214:CLA:H12	29:K:214:CLA:H52	1.89	0.42
16:F:186:GLY:O	16:F:190:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:136:TRP:CD2	17:J:159:PRO:HG2	2.54	0.42
18:M:213:TYR:OH	18:M:217:ARG:NH2	2.52	0.42
18:M:265:SER:HB2	36:M:304:DD6:C3	2.50	0.42
29:B:310:CLA:H3A	29:B:310:CLA:HBA2	1.54	0.42
24:O:199:LYS:O	24:O:201:THR:HG23	2.20	0.42
25:T:225:LYS:HB3	29:T:314:CLA:HMA3	2.01	0.42
26:Q:183:ARG:HA	26:Q:186:MET:HE3	2.01	0.42
37:Q:301:PID:H16	37:Q:301:PID:HM41	1.78	0.42
1:a:301:TYR:HB2	1:a:304:LEU:HD22	2.01	0.42
29:a:806:CLA:H141	29:a:806:CLA:H161	1.73	0.42
32:b:735:BCR:H321	32:i:204:BCR:H372	2.01	0.42
3:c:26:GLU:N	3:c:40:SER:O	2.50	0.42
32:f:801:BCR:H371	32:f:801:BCR:H24C	1.76	0.42
29:l:509:CLA:HHB	38:F:305:UIX:C24	2.50	0.42
29:I:217:CLA:H62	29:I:217:CLA:H41	1.79	0.42
18:M:163:ALA:O	18:M:167:LEU:HG	2.20	0.42
29:B:308:CLA:H61	29:B:308:CLA:H41	1.77	0.42
29:T:314:CLA:HED2	29:T:314:CLA:HBD	1.81	0.42
37:C:305:PID:H20	29:C:314:CLA:CAB	2.49	0.42
1:a:331:ALA:O	1:a:335:ILE:HG13	2.20	0.41
1:a:493:PHE:CE2	1:a:625:LEU:HD13	2.55	0.41
2:b:246:THR:HG21	32:b:728:BCR:H341	2.02	0.41
2:b:389:PRO:HB2	6:f:8:LYS:HB3	2.01	0.41
29:b:707:CLA:H171	29:b:707:CLA:H8	2.01	0.41
3:c:2:HIS:CD2	3:c:77:SER:HB2	2.55	0.41
13:G:19:GLN:NE2	13:G:24:ASP:O	2.53	0.41
13:G:20:PRO:HG2	13:G:21:ILE:HG12	2.01	0.41
13:G:152:VAL:HG23	13:G:154:MET:HG2	2.02	0.41
16:F:89:SER:OG	16:F:92:SER:HB2	2.19	0.41
36:F:303:DD6:C9	29:F:308:CLA:HMC1	2.50	0.41
17:J:243:ALA:O	17:J:244:THR:OG1	2.29	0.41
37:N:307:PID:HM62	39:N:315:KC1:CAA	2.49	0.41
37:T:307:PID:HM83	37:T:307:PID:CM5	2.49	0.41
29:a:830:CLA:HAB	29:l:501:CLA:HAB	2.01	0.41
29:b:712:CLA:H92	29:b:717:CLA:HMD3	2.02	0.41
6:f:9:MET:HB3	29:f:805:CLA:HAC1	2.02	0.41
7:h:69:LEU:HB3	7:h:124:CYS:HB2	2.01	0.41
10:l:348:ILE:O	10:l:351:THR:OG1	2.37	0.41
16:F:174:ILE:O	16:F:178:ARG:HG3	2.20	0.41
17:J:136:TRP:NE1	17:J:239:LEU:HD22	2.35	0.41
19:L:218:LYS:NZ	19:L:228:ALA:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:243:LEU:HD13	36:B:301:DD6:C26	2.50	0.41
22:H:87:SER:HB3	22:H:90:ALA:HB3	2.02	0.41
22:H:146:VAL:HB	22:H:151:TRP:CE2	2.55	0.41
37:T:301:PID:H17	29:T:316:CLA:C1C	2.50	0.41
26:Q:88:MET:HE3	37:Q:304:PID:H17	2.02	0.41
26:Q:170:THR:O	26:Q:174:LYS:HG2	2.20	0.41
37:C:305:PID:HM22	29:C:316:CLA:HMB2	2.02	0.41
29:C:314:CLA:HED2	29:C:314:CLA:HBD	1.86	0.41
27:P:89:SER:O	27:P:93:GLY:N	2.53	0.41
1:a:155:ARG:HH21	1:a:158:ASN:HD21	1.68	0.41
1:a:610:ILE:HD13	6:f:136:ALA:HB1	2.02	0.41
29:a:818:CLA:HBA2	29:a:818:CLA:H3A	1.41	0.41
29:a:826:CLA:H43	32:b:729:BCR:H24C	2.03	0.41
30:a:832:PQN:H28	30:a:832:PQN:H252	1.82	0.41
2:b:50:THR:OG1	2:b:117:THR:HG22	2.21	0.41
29:b:702:CLA:H3A	32:b:735:BCR:C39	2.51	0.41
3:c:57:CYS:HA	33:c:102:SF4:S4	2.61	0.41
8:i:176:TRP:C	8:i:178:ASN:H	2.29	0.41
10:l:232:ARG:O	10:l:232:ARG:NH1	2.42	0.41
12:A:52:GLU:OE2	12:A:136:LEU:HD22	2.20	0.41
15:K:38:GLU:N	15:K:38:GLU:OE1	2.53	0.41
18:M:249:TYR:HE2	29:M:311:CLA:CGA	2.33	0.41
18:M:261:MET:HE3	36:M:302:DD6:C1	2.50	0.41
21:B:141:CYS:SG	21:B:242:MET:HG2	2.60	0.41
21:B:197:LEU:HD12	21:B:213:TYR:CD1	2.56	0.41
22:H:114:THR:HG22	37:H:304:PID:HM83	2.01	0.41
23:N:74:ALA:HB1	23:N:175:PHE:CE1	2.55	0.41
37:N:305:PID:HM62	37:N:305:PID:HM51	2.01	0.41
37:Q:301:PID:H16	29:Q:310:CLA:H2	2.01	0.41
25:C:209:PHE:HB2	37:C:304:PID:HM23	2.02	0.41
1:a:102:ASN:HB3	1:a:103:PRO:HD3	2.01	0.41
1:a:147:MET:HE2	29:a:812:CLA:CGD	2.51	0.41
29:a:806:CLA:H91	29:a:806:CLA:H112	1.74	0.41
29:a:807:CLA:H143	29:a:807:CLA:H111	1.66	0.41
29:a:837:CLA:HAA2	9:j:46:PHE:CE2	2.55	0.41
2:b:322:VAL:HG22	29:b:719:CLA:C4B	2.50	0.41
4:d:64:PRO:HD2	10:l:329:PHE:HZ	1.86	0.41
4:d:243:MET:HE3	7:h:26:PRO:HG2	2.02	0.41
5:e:5:PRO:HB2	5:e:27:VAL:HG21	2.01	0.41
14:I:63:TYR:N	14:I:63:TYR:CD1	2.87	0.41
20:D:168:GLU:HB2	29:D:314:CLA:C2B	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:180:ILE:HG23	29:D:316:CLA:HMC1	2.01	0.41
29:B:310:CLA:H51	29:E:314:CLA:HBC1	2.02	0.41
24:O:118:ARG:HH12	29:O:314:CLA:C4D	2.33	0.41
25:T:211:PHE:HE2	37:T:305:PID:HM71	1.85	0.41
37:P:208:PID:H16	37:P:208:PID:HM41	1.59	0.41
29:a:803:CLA:HBB1	29:a:803:CLA:HMB3	2.02	0.41
2:b:326:LEU:HD13	2:b:417:LEU:HA	2.03	0.41
2:b:392:SER:OG	2:b:393:PHE:N	2.54	0.41
29:b:723:CLA:H122	29:b:723:CLA:H8	1.87	0.41
29:b:736:CLA:H43	29:A:211:CLA:H3A	2.03	0.41
12:A:62:MET:SD	29:A:212:CLA:HHC	2.61	0.41
12:A:82:CYS:HB2	12:A:94:CYS:HA	2.02	0.41
13:G:92:LEU:HD13	29:G:314:CLA:H91	2.02	0.41
14:I:24:THR:C	14:I:25:GLU:HG2	2.45	0.41
18:M:270:ALA:C	18:M:272:ILE:H	2.27	0.41
19:L:234:THR:O	19:L:236:LEU:N	2.54	0.41
29:L:316:CLA:H41	29:L:316:CLA:H61	1.86	0.41
37:D:303:PID:CM6	29:D:312:CLA:HAA1	2.49	0.41
23:N:50:ALA:C	23:N:52:GLY:H	2.28	0.41
26:Q:91:ILE:HG21	37:Q:306:PID:H11	2.02	0.41
27:P:164:ASN:CG	37:P:206:PID:H16	2.46	0.41
28:E:162:SER:OG	28:E:163:LEU:N	2.53	0.41
1:a:38:PHE:CD2	29:a:806:CLA:HMC2	2.56	0.41
1:a:529:ALA:O	1:a:530:SER:C	2.64	0.41
2:b:25:LEU:HB2	2:b:30:ALA:CB	2.51	0.41
2:b:297:GLY:CA	32:b:728:BCR:H311	2.51	0.41
2:b:378:TYR:HA	6:f:31:HIS:HB3	2.01	0.41
29:b:707:CLA:H141	29:b:707:CLA:H161	1.93	0.41
29:b:711:CLA:O1D	29:b:712:CLA:HHB	2.20	0.41
29:b:724:CLA:H11	32:b:728:BCR:H20C	2.03	0.41
6:f:171:VAL:HG21	13:G:67:PHE:CD1	2.56	0.41
29:i:201:CLA:H111	29:i:201:CLA:H142	1.82	0.41
29:l:505:CLA:H91	29:l:505:CLA:H112	1.66	0.41
13:G:43:ALA:HB2	13:G:51:ALA:HA	2.03	0.41
19:L:162:ALA:O	19:L:166:LEU:HG	2.20	0.41
36:L:301:DD6:C	29:L:315:CLA:HBB1	2.51	0.41
37:D:302:PID:H16	37:D:302:PID:HM41	1.91	0.41
29:B:312:CLA:H12	29:B:312:CLA:H52	1.93	0.41
24:O:140:LEU:N	24:O:146:VAL:O	2.53	0.41
26:Q:158:PHE:CD1	37:Q:303:PID:H7	2.55	0.41
28:E:103:LEU:HD11	29:E:306:CLA:CMD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:182:VAL:HG11	29:E:315:CLA:HED2	2.02	0.41
1:a:379:ASP:OD1	1:a:538:ASN:HB3	2.21	0.41
29:a:826:CLA:H12	29:a:826:CLA:H51	1.85	0.41
2:b:149:TRP:HB3	29:A:218:CLA:H71	2.03	0.41
2:b:594:PHE:CE1	34:b:732:LMG:H292	2.56	0.41
2:b:601:VAL:O	2:b:605:ILE:HG12	2.21	0.41
10:l:374:PHE:CE2	29:l:504:CLA:HBB1	2.55	0.41
10:l:396:LEU:HD22	10:l:452:HIS:CG	2.55	0.41
15:K:23:PHE:HA	19:L:100:LEU:HD23	2.02	0.41
15:K:54:TRP:CE2	29:K:213:CLA:HED1	2.55	0.41
16:F:109:LEU:HB3	16:F:114:TRP:NE1	2.36	0.41
16:F:183:ALA:O	16:F:187:MET:HG3	2.20	0.41
25:T:143:TYR:CE2	25:T:240:ILE:HD11	2.54	0.41
28:E:163:LEU:O	28:E:164:PRO:C	2.64	0.41
1:a:285:GLY:HA2	1:a:322:GLY:HA2	2.03	0.41
29:a:820:CLA:H192	29:a:820:CLA:H162	1.91	0.41
29:a:825:CLA:H61	29:a:825:CLA:H92	1.82	0.41
2:b:311:LEU:HD21	35:h:203:DGD:HB91	2.03	0.41
29:b:705:CLA:H142	32:i:204:BCR:H382	2.02	0.41
6:f:183:HIS:CE1	6:f:185:ALA:HB2	2.55	0.41
10:l:364:GLY:O	10:l:440:HIS:HA	2.21	0.41
29:G:302:CLA:HMA2	29:G:302:CLA:H51	2.03	0.41
29:G:304:CLA:H62	29:G:304:CLA:H41	1.85	0.41
17:J:95:PRO:HD2	17:J:99:SER:HB3	2.03	0.41
18:M:261:MET:HE1	29:M:307:CLA:HHC	2.03	0.41
29:M:315:CLA:H3A	29:M:315:CLA:HBA1	1.45	0.41
19:L:247:MET:CE	29:L:313:CLA:H2	2.51	0.41
20:D:91:PHE:HB2	20:D:103:PHE:CG	2.56	0.41
21:B:134:GLU:HB2	29:B:308:CLA:CHB	2.51	0.41
29:B:315:CLA:HBB1	29:B:315:CLA:HMB3	2.02	0.41
22:H:100:LYS:HG3	37:H:302:PID:H41	2.03	0.41
23:N:40:VAL:HG11	23:N:43:TRP:HB2	2.02	0.41
24:O:115:LYS:HE2	24:O:115:LYS:HB2	1.83	0.41
25:T:138:LEU:HD11	29:T:314:CLA:HBC1	2.03	0.41
26:Q:118:LEU:HB2	26:Q:196:ASP:OD1	2.21	0.41
25:C:120:GLU:H	25:C:120:GLU:CD	2.28	0.41
37:P:202:PID:H7	29:P:210:CLA:HBC1	2.03	0.41
28:E:127:LYS:HD2	29:E:310:CLA:C3D	2.51	0.41
29:a:809:CLA:H172	29:a:809:CLA:H13	2.01	0.41
2:b:25:LEU:HB2	2:b:30:ALA:HB1	2.03	0.41
29:b:711:CLA:HBA2	29:b:715:CLA:HED2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:45:ASP:OD1	5:e:45:ASP:N	2.54	0.41
6:f:37:GLN:OE1	6:f:37:GLN:N	2.54	0.41
6:f:157:TRP:CD1	6:f:158:PRO:HD3	2.55	0.41
10:l:267:TRP:CD1	19:L:109:ILE:HG21	2.55	0.41
10:l:337:PRO:HB2	29:l:501:CLA:H11	2.02	0.41
10:l:351:THR:O	10:l:355:ARG:N	2.51	0.41
29:l:501:CLA:H101	29:l:504:CLA:H161	2.01	0.41
32:l:507:BCR:H11C	32:l:507:BCR:H341	1.90	0.41
29:l:510:CLA:HMA1	34:E:316:LMG:HC91	2.03	0.41
12:A:58:GLY:O	12:A:62:MET:HG3	2.20	0.41
15:K:54:TRP:CD2	29:K:213:CLA:HED1	2.56	0.41
15:K:143:TYR:HD1	29:K:214:CLA:HAA2	1.86	0.41
34:K:219:LMG:H112	34:K:219:LMG:H141	1.85	0.41
17:J:174:MET:O	17:J:178:ILE:HG12	2.21	0.41
20:D:163:ARG:HA	20:D:166:ASN:HD21	1.86	0.41
21:B:116:PHE:HE1	29:B:306:CLA:HBC3	1.86	0.41
22:H:108:ALA:HB1	22:H:209:PHE:HE2	1.85	0.41
22:H:141:GLY:O	22:H:145:LYS:HG2	2.21	0.41
37:H:306:PID:H7	37:H:306:PID:HM21	1.91	0.41
23:N:40:VAL:HG12	23:N:41:GLY:H	1.86	0.41
37:O:304:PID:H16	37:O:304:PID:HM41	1.65	0.41
25:T:185:ILE:O	25:T:189:MET:HG2	2.21	0.41
25:C:125:ARG:NH1	39:C:310:KC1:O1A	2.54	0.41
25:C:127:GLN:HB2	25:C:205:ALA:O	2.21	0.41
27:P:34:GLN:OE1	27:P:163:ALA:HB2	2.21	0.41
27:P:41:ASP:OD1	27:P:41:ASP:N	2.54	0.41
27:P:75:TYR:OH	27:P:176:PHE:HE1	2.03	0.41
27:P:177:PHE:O	27:P:178:GLN:C	2.64	0.41
2:b:426:SER:HA	2:b:435:LYS:HD2	2.03	0.41
4:d:94:PHE:CD1	4:d:104:MET:HG3	2.56	0.41
8:i:145:GLU:HG2	8:i:160:VAL:HB	2.02	0.41
13:G:170:THR:HG23	13:G:177:LEU:HD22	2.03	0.41
29:G:304:CLA:HBD	29:G:304:CLA:HBA1	2.03	0.41
29:G:313:CLA:H51	29:G:313:CLA:H12	1.83	0.41
29:I:209:CLA:H91	29:I:209:CLA:H111	1.75	0.41
36:K:221:DD6:C24	29:L:312:CLA:HHB	2.51	0.41
16:F:103:MET:SD	16:F:188:VAL:HG13	2.61	0.41
29:M:306:CLA:H61	29:M:306:CLA:H41	1.80	0.41
29:L:308:CLA:CHB	29:L:308:CLA:H12	2.51	0.41
20:D:176:MET:O	20:D:179:ILE:HG22	2.21	0.41
37:D:306:PID:HM53	29:D:314:CLA:HMC1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:T:313:CLA:HED2	29:T:313:CLA:HBD	1.83	0.41
1:a:468:ARG:HD2	31:a:833:LHG:HC42	2.03	0.40
29:a:831:CLA:C1C	30:a:832:PQN:H251	2.50	0.40
2:b:19:ILE:HG13	2:b:34:LEU:HD11	2.02	0.40
2:b:27:SER:HB2	2:b:29:GLN:OE1	2.21	0.40
2:b:553:ARG:O	2:b:556:TRP:N	2.54	0.40
6:f:118:THR:HG23	29:f:802:CLA:HAA1	2.03	0.40
10:l:302:LYS:HE2	10:l:302:LYS:HB2	1.93	0.40
10:l:304:PRO:HA	10:l:319:THR:HG22	2.03	0.40
12:A:175:ALA:HA	29:A:214:CLA:HBB1	2.03	0.40
29:K:213:CLA:HBB2	34:K:220:LMG:H151	2.02	0.40
16:F:73:CYS:HB2	37:F:304:PID:CM4	2.51	0.40
16:F:173:GLU:HB2	29:F:313:CLA:C1B	2.51	0.40
16:F:175:ASN:HD21	29:F:307:CLA:CGD	2.21	0.40
37:F:304:PID:HM21	37:F:304:PID:H7	1.78	0.40
36:J:302:DD6:O1	29:J:309:CLA:HAA1	2.21	0.40
40:J:314:SQD:O7	40:J:314:SQD:O4	2.30	0.40
37:D:307:PID:O5	37:D:307:PID:HM51	2.21	0.40
22:H:137:PRO:HD2	22:H:145:LYS:HG3	2.03	0.40
22:H:193:LYS:NZ	39:H:314:KC1:O2A	2.44	0.40
37:H:301:PID:H20	29:H:315:CLA:HBC2	2.03	0.40
24:O:170:PHE:O	24:O:173:THR:OG1	2.31	0.40
24:O:200:VAL:O	24:O:201:THR:OG1	2.28	0.40
29:O:309:CLA:H141	29:O:309:CLA:H161	1.89	0.40
26:Q:88:MET:HB2	29:Q:310:CLA:HMC1	2.03	0.40
29:C:309:CLA:H61	29:C:309:CLA:H41	1.66	0.40
1:a:467:PHE:CD1	1:a:484:PRO:HB2	2.56	0.40
1:a:472:ASP:OD2	1:a:476:ARG:NH1	2.50	0.40
2:b:45:TRP:NE1	29:b:716:CLA:OBD	2.44	0.40
2:b:258:GLN:HG3	29:b:711:CLA:OBD	2.21	0.40
2:b:356:GLN:HB2	2:b:358:ILE:HD11	2.03	0.40
2:b:432:PHE:HE2	2:b:445:ASP:HB2	1.87	0.40
11:m:40:LEU:O	11:m:44:ILE:HG12	2.22	0.40
12:A:26:ALA:HB1	29:A:206:CLA:CHB	2.51	0.40
13:G:47:THR:OG1	13:G:52:TRP:HB2	2.21	0.40
15:K:60:LEU:HD23	15:K:60:LEU:HA	1.94	0.40
16:F:111:THR:HG21	40:J:314:SQD:C6	2.51	0.40
19:L:107:ALA:HA	19:L:224:SER:HB3	2.02	0.40
37:D:305:PID:HM41	37:D:305:PID:H16	1.78	0.40
23:N:75:ALA:HA	23:N:178:MET:HE1	2.02	0.40
37:T:317:PID:H41	26:Q:51:PRO:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:129:ASP:O	27:P:136:GLY:HA3	2.22	0.40
2:b:58:ASN:HB2	2:b:61:ALA:HB3	2.03	0.40
2:b:272:TYR:HB3	2:b:487:TRP:CZ3	2.55	0.40
2:b:392:SER:HB3	6:f:9:MET:HE2	2.04	0.40
2:b:597:LEU:O	2:b:601:VAL:HG12	2.21	0.40
29:i:201:CLA:H62	35:m:102:DGD:HBT2	2.04	0.40
29:J:311:CLA:H62	29:J:311:CLA:H41	1.51	0.40
20:D:175:ALA:O	20:D:176:MET:C	2.64	0.40
25:C:121:ALA:O	25:C:125:ARG:HG3	2.20	0.40
25:C:189:MET:HE2	37:C:302:PID:C10	2.51	0.40
1:a:576:TRP:HZ3	29:b:703:CLA:HMD3	1.87	0.40
29:a:829:CLA:H3A	29:a:829:CLA:HBA2	1.78	0.40
2:b:192:ILE:HG22	2:b:194:LEU:H	1.86	0.40
2:b:324:SER:HB3	29:b:701:CLA:HED2	2.03	0.40
32:b:735:BCR:H371	32:b:735:BCR:H24C	1.84	0.40
6:f:80:ALA:O	6:f:84:GLU:HG3	2.21	0.40
6:f:152:THR:HG21	29:I:210:CLA:H52	2.04	0.40
35:j:105:DGD:O2G	34:K:219:LMG:HC92	2.20	0.40
37:G:309:PID:HM22	37:G:310:PID:H7	2.02	0.40
16:F:76:TRP:CB	16:F:187:MET:HE1	2.51	0.40
16:F:119:ALA:O	16:F:123:LEU:HG	2.21	0.40
20:D:137:GLN:HE21	29:D:313:CLA:HMA2	1.87	0.40
21:B:154:GLY:HA2	21:B:156:ARG:NH1	2.35	0.40
29:H:308:CLA:H61	29:H:308:CLA:H41	1.61	0.40
25:T:131:LYS:HD2	29:T:313:CLA:C3D	2.51	0.40
37:Q:306:PID:H16	37:Q:306:PID:HM41	1.77	0.40
25:C:182:TRP:CH2	29:C:311:CLA:HMA3	2.56	0.40
37:C:307:PID:HM41	37:C:307:PID:H16	1.84	0.40
37:P:206:PID:H21	29:P:217:CLA:C1B	2.52	0.40
1:a:353:ARG:NH1	4:d:99:SER:OG	2.54	0.40
1:a:567:LEU:HD12	29:a:810:CLA:HAC1	2.03	0.40
32:a:834:BCR:H24C	32:a:834:BCR:H371	1.90	0.40
2:b:331:LEU:HD11	29:b:701:CLA:HMD3	2.03	0.40
3:c:27:MET:HE1	33:c:102:SF4:S1	2.61	0.40
4:d:119:CYS:HB3	4:d:136:ILE:HD13	2.02	0.40
6:f:106:GLY:N	9:j:70:TRP:O	2.45	0.40
6:f:121:TRP:NE1	6:f:151:MET:O	2.40	0.40
7:h:40:PHE:CZ	7:h:47:TRP:CD2	3.01	0.40
8:i:71:PRO:O	8:i:75:PHE:HB2	2.22	0.40
8:i:118:LYS:HE3	8:i:119:TYR:CE2	2.56	0.40
29:l:503:CLA:O1A	29:F:312:CLA:HHB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:m:103:BCR:H20C	32:m:103:BCR:H361	1.78	0.40
12:A:20:LEU:HD23	12:A:20:LEU:HA	1.98	0.40
14:I:103:TYR:HB2	14:I:107:ILE:HG22	2.03	0.40
17:J:218:TYR:HA	17:J:221:ILE:HG12	2.03	0.40
22:H:69:GLY:CA	22:H:203:ARG:HH22	2.35	0.40
22:H:77:TRP:HB3	29:H:308:CLA:HMD3	2.02	0.40
24:O:116:HIS:HB3	24:O:223:MET:SD	2.62	0.40
24:O:131:GLU:HB2	37:O:307:PID:HM32	2.04	0.40
25:T:199:SER:O	25:T:205:ALA:HB2	2.21	0.40
37:Q:306:PID:H8	37:Q:306:PID:HM31	2.04	0.40
37:C:304:PID:H261	37:C:307:PID:H13	2.03	0.40
37:P:206:PID:HM32	37:P:208:PID:HM12	2.04	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	643/645 (100%)	594 (92%)	47 (7%)	2 (0%)	36 65
2	b	615/617 (100%)	581 (94%)	34 (6%)	0	100 100
3	c	84/86 (98%)	81 (96%)	3 (4%)	0	100 100
4	d	255/257 (99%)	239 (94%)	15 (6%)	1 (0%)	30 59
5	e	72/74 (97%)	68 (94%)	4 (6%)	0	100 100
6	f	183/185 (99%)	177 (97%)	6 (3%)	0	100 100
7	h	130/132 (98%)	121 (93%)	6 (5%)	3 (2%)	5 19
8	i	124/126 (98%)	116 (94%)	8 (6%)	0	100 100
9	j	68/70 (97%)	60 (88%)	8 (12%)	0	100 100
10	l	251/253 (99%)	231 (92%)	20 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	m	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
12	A	178/180 (99%)	163 (92%)	15 (8%)	0	100	100
13	G	213/215 (99%)	189 (89%)	23 (11%)	1 (0%)	24	54
14	I	192/194 (99%)	165 (86%)	21 (11%)	6 (3%)	3	14
15	K	170/172 (99%)	153 (90%)	16 (9%)	1 (1%)	21	51
16	F	174/176 (99%)	154 (88%)	19 (11%)	1 (1%)	21	51
17	J	163/165 (99%)	144 (88%)	18 (11%)	1 (1%)	21	51
18	M	166/168 (99%)	134 (81%)	26 (16%)	6 (4%)	2	11
19	L	183/185 (99%)	152 (83%)	26 (14%)	5 (3%)	4	16
20	D	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	21	51
21	B	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
22	H	158/160 (99%)	135 (85%)	19 (12%)	4 (2%)	4	17
23	N	158/160 (99%)	126 (80%)	31 (20%)	1 (1%)	21	51
24	O	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	6	23
25	C	158/160 (99%)	146 (92%)	11 (7%)	1 (1%)	21	51
25	T	157/160 (98%)	142 (90%)	11 (7%)	4 (2%)	4	17
26	Q	160/162 (99%)	138 (86%)	20 (12%)	2 (1%)	9	32
27	P	158/160 (99%)	139 (88%)	16 (10%)	3 (2%)	6	23
28	E	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	5	21
All	All	5527/5586 (99%)	4986 (90%)	492 (9%)	49 (1%)	16	41

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	520	SER
4	d	149	HIS
14	I	116	SER
14	I	135	LYS
14	I	186	VAL
15	K	182	TRP
18	M	179	GLU
18	M	182	ASP
19	L	195	ASN
20	D	152	VAL
22	H	72	ALA

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Mol	Chain	Res	Type
23	N	106	LEU
24	O	95	LEU
25	T	213	VAL
26	Q	202	ALA
27	P	88	LEU
27	P	145	VAL
28	E	101	ALA
28	E	116	GLU
28	E	186	GLU
1	a	521	ALA
7	h	42	PRO
14	I	64	ILE
14	I	65	GLY
18	M	122	SER
19	L	235	ARG
19	L	265	ALA
22	H	88	MET
22	H	125	LEU
26	Q	111	PHE
18	M	276	GLN
25	T	99	LEU
25	T	212	LYS
25	C	105	LEU
27	P	44	GLY
13	G	147	ASN
16	F	157	GLU
19	L	117	PHE
7	h	38	ARG
19	L	118	ALA
22	H	164	SER
24	O	202	SER
25	T	113	LEU
7	h	41	ASN
18	M	221	LEU
18	M	275	ASP
24	O	89	PHE
14	I	68	PRO
17	J	103	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	531/535 (99%)	527 (99%)	4 (1%)	73 90
2	b	502/504 (100%)	495 (99%)	7 (1%)	59 85
3	c	73/74 (99%)	72 (99%)	1 (1%)	59 85
4	d	213/222 (96%)	213 (100%)	0	100 100
5	e	65/66 (98%)	65 (100%)	0	100 100
6	f	151/151 (100%)	150 (99%)	1 (1%)	76 92
7	h	109/109 (100%)	105 (96%)	4 (4%)	30 64
8	i	106/106 (100%)	104 (98%)	2 (2%)	50 79
9	j	60/60 (100%)	58 (97%)	2 (3%)	33 67
10	l	200/203 (98%)	200 (100%)	0	100 100
11	m	72/72 (100%)	72 (100%)	0	100 100
12	A	136/141 (96%)	136 (100%)	0	100 100
13	G	171/171 (100%)	169 (99%)	2 (1%)	63 86
14	I	141/156 (90%)	137 (97%)	4 (3%)	38 72
15	K	133/138 (96%)	133 (100%)	0	100 100
16	F	140/140 (100%)	138 (99%)	2 (1%)	59 85
17	J	136/136 (100%)	135 (99%)	1 (1%)	76 92
18	M	128/128 (100%)	126 (98%)	2 (2%)	55 83
19	L	145/145 (100%)	145 (100%)	0	100 100
20	D	123/123 (100%)	120 (98%)	3 (2%)	43 75
21	B	146/146 (100%)	144 (99%)	2 (1%)	59 85
22	H	123/123 (100%)	122 (99%)	1 (1%)	73 90
23	N	124/124 (100%)	119 (96%)	5 (4%)	28 62
24	O	124/124 (100%)	123 (99%)	1 (1%)	73 90
25	C	121/121 (100%)	121 (100%)	0	100 100
25	T	120/121 (99%)	118 (98%)	2 (2%)	53 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	Q	120/120 (100%)	119 (99%)	1 (1%)	73 90
27	P	123/123 (100%)	121 (98%)	2 (2%)	55 83
28	E	108/108 (100%)	107 (99%)	1 (1%)	70 90
All	All	4444/4490 (99%)	4394 (99%)	50 (1%)	63 88

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	480	CYS
1	a	526	ARG
1	a	528	LEU
1	a	579	SER
2	b	70	GLN
2	b	84	TYR
2	b	85	LYS
2	b	135	SER
2	b	136	VAL
2	b	236	SER
2	b	547	MET
3	c	62	LEU
6	f	159	VAL
7	h	35	ILE
7	h	37	ARG
7	h	40	PHE
7	h	41	ASN
8	i	142	LYS
8	i	144	LEU
9	j	25	ILE
9	j	27	THR
13	G	24	ASP
13	G	208	VAL
14	I	67	TYR
14	I	71	GLU
14	I	72	MET
14	I	186	VAL
16	F	77	ILE
16	F	170	LEU
17	J	229	SER
18	M	234	LEU
18	M	258	ARG
20	D	41	GLN

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Mol	Chain	Res	Type
20	D	44	THR
20	D	165	LEU
21	B	97	VAL
21	B	149	ILE
22	H	165	GLN
23	N	40	VAL
23	N	63	VAL
23	N	64	GLU
23	N	70	ILE
23	N	72	MET
24	O	133	THR
25	T	167	VAL
25	T	213	VAL
26	Q	91	ILE
27	P	43	LEU
27	P	178	GLN
28	E	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	15	ASN
2	b	52	HIS
2	b	160	ASN
2	b	436	GLN
2	b	512	ASN
6	f	38	ASN
12	A	24	GLN
12	A	33	ASN
12	A	182	GLN
13	G	64	ASN
13	G	104	HIS
13	G	187	ASN
17	J	227	ASN
18	M	191	HIS
18	M	276	GLN
19	L	114	ASN
21	B	251	GLN
22	H	71	GLN
23	N	133	GLN
24	O	218	ASN
26	Q	65	ASN

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Mol	Chain	Res	Type
26	Q	116	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

411 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	$\#\|Z\| > 2$
39	KC1	D	315	-	49,53,53	1.36	5 (10%)	61,89,89	1.73	11 (18%)
29	CLA	C	311	-	55,59,73	1.30	9 (16%)	64,96,113	1.40	5 (7%)
38	UIX	T	306	-	43,49,49	1.41	5 (11%)	53,74,74	2.80	22 (41%)
36	DD6	L	304	-	40,45,45	1.56	2 (5%)	51,67,67	1.97	16 (31%)
29	CLA	N	311	-	55,59,73	1.30	7 (12%)	64,96,113	1.38	5 (7%)
36	DD6	J	303	-	40,45,45	1.65	2 (5%)	51,67,67	2.10	17 (33%)
29	CLA	M	314	-	56,60,73	1.29	9 (16%)	65,97,113	1.32	5 (7%)
37	PID	N	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.43	5 (9%)
38	UIX	P	207	-	43,49,49	1.41	4 (9%)	53,74,74	2.59	19 (35%)
37	PID	O	307	-	43,49,49	1.25	3 (6%)	52,76,76	1.40	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PID	Q	303	-	43,49,49	1.27	3 (6%)	52,76,76	1.42	7 (13%)
29	CLA	G	311	13	55,59,73	1.29	8 (14%)	64,96,113	1.38	4 (6%)
36	DD6	B	301	-	39,44,45	1.57	2 (5%)	49,65,67	1.98	16 (32%)
29	CLA	D	312	20	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
36	DD6	G	307	-	40,45,45	2.35	8 (20%)	51,67,67	2.49	19 (37%)
36	DD6	I	205	-	40,45,45	2.09	4 (10%)	51,67,67	2.30	17 (33%)
29	CLA	a	804	-	59,63,73	1.26	9 (15%)	70,101,113	1.42	7 (10%)
37	PID	T	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	5 (9%)
29	CLA	a	828	-	50,54,73	1.36	9 (18%)	59,90,113	1.41	4 (6%)
39	KC1	P	211	-	49,53,53	1.34	6 (12%)	61,89,89	1.72	13 (21%)
36	DD6	Q	302	-	40,45,45	1.54	2 (5%)	51,67,67	1.84	13 (25%)
29	CLA	a	837	-	59,63,73	1.25	9 (15%)	70,101,113	1.29	6 (8%)
32	BCR	m	103	-	41,41,41	0.79	2 (4%)	56,56,56	2.37	17 (30%)
29	CLA	A	206	39	49,53,73	1.38	8 (16%)	58,89,113	1.48	5 (8%)
34	LMG	K	219	-	35,35,55	0.92	1 (2%)	43,43,63	1.20	4 (9%)
36	DD6	I	206	-	40,45,45	1.55	2 (5%)	51,67,67	1.88	16 (31%)
39	KC1	E	312	28	49,53,53	1.38	7 (14%)	61,89,89	1.71	14 (22%)
37	PID	O	305	-	43,49,49	1.25	3 (6%)	52,76,76	1.79	8 (15%)
29	CLA	Q	313	-	51,55,73	1.34	9 (17%)	60,91,113	1.41	5 (8%)
29	CLA	J	307	-	50,54,73	1.34	9 (18%)	59,90,113	1.38	4 (6%)
29	CLA	L	313	-	57,61,73	1.26	9 (15%)	67,98,113	1.37	5 (7%)
36	DD6	G	305	-	40,45,45	1.80	4 (10%)	51,67,67	2.97	16 (31%)
29	CLA	b	726	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
35	DGD	j	103	-	44,44,67	1.00	2 (4%)	58,58,81	1.33	8 (13%)
36	DD6	O	303	-	40,45,45	1.68	3 (7%)	51,67,67	2.15	16 (31%)
33	SF4	c	101	3	0,12,12	-	-	-		
29	CLA	I	209	-	64,68,73	1.20	9 (14%)	76,107,113	5.01	8 (10%)
34	LMG	b	732	-	44,44,55	0.80	1 (2%)	52,52,63	1.33	6 (11%)
29	CLA	O	309	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
37	PID	P	205	-	43,49,49	1.24	3 (6%)	52,76,76	1.48	7 (13%)
29	CLA	a	801	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
39	KC1	O	310	-	49,53,53	1.36	7 (14%)	61,89,89	1.73	12 (19%)
39	KC1	F	314	-	49,53,53	1.36	7 (14%)	61,89,89	1.74	13 (21%)
29	CLA	b	713	-	57,61,73	1.29	8 (14%)	67,98,113	1.34	6 (8%)
38	UIX	C	306	-	43,49,49	1.40	5 (11%)	53,74,74	2.54	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	B	311	21	55,59,73	1.30	9 (16%)	64,96,113	1.38	5 (7%)
29	CLA	K	208	-	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
29	CLA	M	310	18	52,56,73	1.33	9 (17%)	61,92,113	1.38	6 (9%)
36	DD6	P	204	-	40,45,45	1.53	2 (5%)	51,67,67	2.18	14 (27%)
29	CLA	H	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.45	5 (9%)
38	UIX	B	304	-	43,49,49	1.40	4 (9%)	53,74,74	2.41	18 (33%)
29	CLA	K	207	15	53,57,73	1.32	9 (16%)	61,93,113	1.40	5 (8%)
36	DD6	I	203	-	40,45,45	1.83	4 (10%)	51,67,67	2.33	17 (33%)
29	CLA	a	825	-	69,73,73	1.17	8 (11%)	82,113,113	1.36	8 (9%)
39	KC1	P	216	-	49,53,53	1.35	5 (10%)	61,89,89	1.72	12 (19%)
29	CLA	H	308	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
36	DD6	L	305	-	40,45,45	1.58	2 (5%)	51,67,67	1.98	16 (31%)
29	CLA	L	309	-	59,63,73	1.25	9 (15%)	70,101,113	1.33	6 (8%)
36	DD6	N	303	-	40,45,45	1.52	2 (5%)	51,67,67	1.73	13 (25%)
35	DGD	m	102	-	67,67,67	0.83	2 (2%)	81,81,81	0.92	4 (4%)
29	CLA	M	315	-	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
36	DD6	L	303	-	40,45,45	1.62	2 (5%)	51,67,67	1.76	15 (29%)
29	CLA	I	217	-	59,63,73	1.25	8 (13%)	70,101,113	1.32	6 (8%)
29	CLA	G	301	-	53,57,73	1.31	9 (16%)	61,93,113	1.38	6 (9%)
29	CLA	J	306	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
37	PID	h	204	-	43,49,49	1.27	3 (6%)	52,76,76	1.36	7 (13%)
29	CLA	a	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	5 (8%)
29	CLA	a	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	9 (10%)
37	PID	P	208	-	43,49,49	1.23	4 (9%)	52,76,76	2.33	7 (13%)
29	CLA	A	207	-	59,63,73	1.26	9 (15%)	70,101,113	1.33	5 (7%)
29	CLA	G	312	13	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
36	DD6	K	204	-	40,45,45	1.65	2 (5%)	51,67,67	1.98	17 (33%)
29	CLA	a	817	-	49,53,73	1.39	9 (18%)	58,89,113	1.40	4 (6%)
39	KC1	O	315	-	49,53,53	1.36	5 (10%)	61,89,89	1.74	14 (22%)
29	CLA	I	208	-	50,54,73	1.35	9 (18%)	59,90,113	5.66	6 (10%)
29	CLA	i	202	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	6 (7%)
29	CLA	N	314	-	51,55,73	1.34	9 (17%)	60,91,113	1.43	7 (11%)
37	PID	P	206	-	43,49,49	1.24	4 (9%)	52,76,76	1.76	10 (19%)
29	CLA	Q	308	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
29	CLA	K	211	-	59,63,73	1.24	9 (15%)	70,101,113	1.37	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PID	P	203	-	43,49,49	1.27	3 (6%)	52,76,76	1.42	9 (17%)
39	KC1	H	309	-	49,53,53	1.35	6 (12%)	61,89,89	1.74	13 (21%)
29	CLA	B	307	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
37	PID	H	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.56	5 (9%)
39	KC1	E	307	-	49,53,53	1.37	7 (14%)	61,89,89	1.76	13 (21%)
36	DD6	K	221	-	40,45,45	1.67	3 (7%)	51,67,67	2.17	16 (31%)
29	CLA	b	704	-	69,73,73	1.16	9 (13%)	82,113,113	3.89	7 (8%)
29	CLA	E	305	-	65,69,73	1.22	8 (12%)	77,108,113	1.34	5 (6%)
35	DGD	j	106	-	50,50,67	0.97	2 (4%)	64,64,81	1.05	4 (6%)
29	CLA	L	310	-	59,63,73	1.26	9 (15%)	70,101,113	1.35	6 (8%)
35	DGD	b	733	-	58,58,67	0.95	4 (6%)	72,72,81	1.26	7 (9%)
36	DD6	E	302	-	40,45,45	1.65	2 (5%)	51,67,67	2.27	16 (31%)
34	LMG	j	102	-	43,43,55	0.77	1 (2%)	51,51,63	1.30	5 (9%)
29	CLA	J	313	-	45,49,73	1.41	9 (20%)	54,84,113	1.49	5 (9%)
29	CLA	F	307	-	50,54,73	1.35	8 (16%)	59,90,113	1.41	5 (8%)
29	CLA	T	311	-	50,54,73	1.36	7 (14%)	59,90,113	1.40	4 (6%)
29	CLA	M	309	-	50,54,73	1.38	9 (18%)	59,90,113	1.36	5 (8%)
38	UIX	O	306	-	43,49,49	1.38	4 (9%)	53,74,74	2.69	19 (35%)
29	CLA	E	313	-	45,49,73	1.42	7 (15%)	54,84,113	1.46	5 (9%)
35	DGD	j	105	-	42,42,67	1.04	2 (4%)	56,56,81	1.08	5 (8%)
29	CLA	a	826	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
36	DD6	M	303	-	40,45,45	1.65	3 (7%)	51,67,67	2.10	12 (23%)
39	KC1	F	309	-	49,53,53	1.37	6 (12%)	61,89,89	1.77	13 (21%)
29	CLA	a	823	-	62,66,73	1.21	9 (14%)	73,104,113	1.30	7 (9%)
32	BCR	b	729	-	41,41,41	0.73	1 (2%)	56,56,56	1.90	20 (35%)
29	CLA	K	217	-	50,54,73	1.36	9 (18%)	59,90,113	1.41	4 (6%)
34	LMG	P	201	-	27,27,55	0.98	0	35,35,63	1.29	6 (17%)
32	BCR	l	507	-	41,41,41	0.71	0	56,56,56	1.99	17 (30%)
29	CLA	A	210	12	50,54,73	1.36	9 (18%)	59,90,113	1.33	4 (6%)
32	BCR	a	838	-	41,41,41	0.70	0	56,56,56	2.14	19 (33%)
29	CLA	I	214	-	59,63,73	1.24	9 (15%)	70,101,113	1.33	5 (7%)
29	CLA	a	811	-	60,64,73	1.26	9 (15%)	71,102,113	1.31	5 (7%)
29	CLA	N	308	-	51,55,73	1.36	8 (15%)	60,91,113	1.39	5 (8%)
29	CLA	b	725	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
37	PID	Q	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.52	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	B	309	-	59,63,73	1.25	8 (13%)	70,101,113	1.34	6 (8%)
29	CLA	H	312	22	50,54,73	1.35	6 (12%)	59,90,113	1.40	6 (10%)
29	CLA	a	819	-	61,65,73	1.23	9 (14%)	72,103,113	1.30	6 (8%)
36	DD6	B	303	-	40,45,45	1.58	2 (5%)	51,67,67	1.77	13 (25%)
29	CLA	b	702	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
29	CLA	A	217	-	55,59,73	1.30	9 (16%)	64,96,113	1.38	7 (10%)
39	KC1	T	315	25	49,53,53	1.36	5 (10%)	61,89,89	1.72	13 (21%)
29	CLA	M	308	-	52,56,73	1.33	9 (17%)	61,92,113	1.38	4 (6%)
29	CLA	b	701	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
36	DD6	H	303	-	40,45,45	1.50	2 (5%)	51,67,67	1.94	13 (25%)
29	CLA	a	827	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
29	CLA	b	736	-	69,73,73	1.16	9 (13%)	82,113,113	6.00	10 (12%)
29	CLA	G	304	-	63,67,73	1.21	9 (14%)	74,105,113	1.40	5 (6%)
29	CLA	a	820	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	5 (6%)
29	CLA	L	315	-	45,49,73	1.42	9 (20%)	54,84,113	1.48	5 (9%)
29	CLA	h	201	-	64,68,73	1.20	9 (14%)	76,107,113	1.31	7 (9%)
29	CLA	C	308	-	51,55,73	1.34	9 (17%)	60,91,113	1.38	5 (8%)
29	CLA	a	806	1	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
36	DD6	K	206	-	40,45,45	1.57	2 (5%)	51,67,67	2.01	15 (29%)
37	PID	O	302	-	43,49,49	1.27	3 (6%)	52,76,76	1.38	8 (15%)
29	CLA	F	308	-	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
36	DD6	B	302	-	40,45,45	1.57	2 (5%)	51,67,67	1.92	15 (29%)
29	CLA	f	802	-	50,54,73	1.34	9 (18%)	59,90,113	1.38	4 (6%)
37	PID	j	101	-	43,49,49	1.27	3 (6%)	52,76,76	1.50	12 (23%)
29	CLA	I	212	-	59,63,73	1.26	9 (15%)	70,101,113	6.47	10 (14%)
29	CLA	Q	312	-	50,54,73	1.35	9 (18%)	59,90,113	1.40	5 (8%)
37	PID	E	301	-	43,49,49	1.25	4 (9%)	52,76,76	1.90	11 (21%)
37	PID	H	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.94	10 (19%)
37	PID	C	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.39	7 (13%)
29	CLA	I	210	-	59,63,73	1.25	9 (15%)	70,101,113	1.33	5 (7%)
29	CLA	b	731	-	60,64,73	1.24	9 (15%)	71,102,113	1.34	6 (8%)
29	CLA	J	308	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	7 (9%)
37	PID	N	302	-	43,49,49	1.28	3 (6%)	52,76,76	1.39	7 (13%)
29	CLA	E	314	28	52,56,73	1.34	9 (17%)	61,92,113	1.36	5 (8%)
36	DD6	A	202	-	40,45,45	1.53	2 (5%)	51,67,67	1.79	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	a	810	1	59,63,73	1.26	9 (15%)	70,101,113	1.36	6 (8%)
29	CLA	H	313	-	51,55,73	1.34	9 (17%)	60,91,113	1.48	5 (8%)
29	CLA	D	308	-	51,55,73	1.35	7 (13%)	60,91,113	1.40	5 (8%)
29	CLA	F	315	-	45,49,73	1.42	8 (17%)	54,84,113	1.53	6 (11%)
38	UIX	F	305	-	43,49,49	1.38	4 (9%)	53,74,74	2.75	19 (35%)
29	CLA	O	313	24	50,54,73	1.35	8 (16%)	59,90,113	1.40	6 (10%)
29	CLA	a	813	-	55,59,73	1.32	9 (16%)	64,96,113	1.37	6 (9%)
29	CLA	E	310	28	50,54,73	1.35	7 (14%)	59,90,113	1.39	5 (8%)
29	CLA	b	714	-	68,72,73	1.16	9 (13%)	80,111,113	1.28	7 (8%)
29	CLA	b	724	-	51,55,73	1.33	9 (17%)	60,91,113	1.40	6 (10%)
39	KC1	N	315	-	49,53,53	1.35	5 (10%)	61,89,89	1.71	13 (21%)
36	DD6	D	304	-	40,45,45	1.65	3 (7%)	51,67,67	2.11	13 (25%)
36	DD6	M	301	-	40,45,45	1.56	2 (5%)	51,67,67	1.84	16 (31%)
37	PID	T	302	-	43,49,49	1.26	4 (9%)	52,76,76	1.51	9 (17%)
29	CLA	j	104	29	56,60,73	1.28	9 (16%)	65,97,113	1.42	5 (7%)
29	CLA	F	313	16	50,54,73	1.36	9 (18%)	59,90,113	1.43	4 (6%)
29	CLA	Q	315	-	45,49,73	1.42	9 (20%)	54,84,113	1.51	5 (9%)
29	CLA	A	216	-	45,49,73	1.41	9 (20%)	54,84,113	1.48	5 (9%)
29	CLA	K	218	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
29	CLA	b	703	-	69,73,73	1.16	9 (13%)	82,113,113	1.18	5 (6%)
29	CLA	i	201	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
29	CLA	N	309	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	5 (6%)
29	CLA	a	805	-	59,63,73	1.25	9 (15%)	70,101,113	1.36	5 (7%)
29	CLA	G	317	-	57,61,73	1.28	9 (15%)	67,98,113	1.33	6 (8%)
32	BCR	b	728	-	41,41,41	0.77	1 (2%)	56,56,56	2.05	14 (25%)
29	CLA	T	316	-	45,49,73	1.43	7 (15%)	54,84,113	1.49	5 (9%)
29	CLA	f	803	6	50,54,73	1.35	9 (18%)	59,90,113	1.40	4 (6%)
32	BCR	f	804	-	41,41,41	0.71	0	56,56,56	1.98	15 (26%)
29	CLA	F	311	-	50,54,73	1.34	9 (18%)	59,90,113	1.44	4 (6%)
39	KC1	C	315	25	49,53,53	1.38	5 (10%)	61,89,89	1.73	13 (21%)
37	PID	D	305	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	8 (15%)
34	LMG	K	220	-	36,36,55	0.86	1 (2%)	44,44,63	1.24	4 (9%)
29	CLA	a	822	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
38	UIX	Q	305	-	43,49,49	1.38	5 (11%)	53,74,74	2.79	20 (37%)
33	SF4	c	102	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b	712	-	69,73,73	1.16	9 (13%)	82,113,113	3.75	8 (9%)
29	CLA	i	203	-	59,63,73	1.24	9 (15%)	70,101,113	1.37	7 (10%)
29	CLA	b	707	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
29	CLA	A	215	-	51,55,73	1.35	9 (17%)	60,91,113	1.41	5 (8%)
29	CLA	P	210	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
36	DD6	L	301	-	40,45,45	1.54	2 (5%)	51,67,67	1.93	13 (25%)
39	KC1	G	315	-	49,53,53	1.45	7 (14%)	61,89,89	1.85	13 (21%)
39	KC1	Q	309	-	49,53,53	1.36	5 (10%)	61,89,89	1.75	13 (21%)
29	CLA	b	715	-	50,54,73	1.35	9 (18%)	59,90,113	1.39	5 (8%)
29	CLA	N	316	-	45,49,73	1.43	8 (17%)	54,84,113	1.48	5 (9%)
29	CLA	G	316	-	69,73,73	1.18	9 (13%)	82,113,113	4.82	8 (9%)
33	SF4	a	836	2,1	0,12,12	-	-	-		
37	PID	H	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	6 (11%)
29	CLA	a	814	-	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
40	SQD	J	314	-	43,45,54	0.43	1 (2%)	53,56,65	0.59	1 (1%)
29	CLA	T	308	-	51,55,73	1.35	8 (15%)	60,91,113	1.38	5 (8%)
39	KC1	M	305	-	49,53,53	1.37	6 (12%)	61,89,89	1.77	15 (24%)
39	KC1	P	213	27	49,53,53	1.39	5 (10%)	61,89,89	1.72	13 (21%)
29	CLA	B	312	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
29	CLA	b	716	-	57,61,73	1.26	9 (15%)	67,98,113	1.33	8 (11%)
29	CLA	b	722	-	62,66,73	1.22	9 (14%)	73,104,113	1.35	6 (8%)
29	CLA	H	310	-	55,59,73	1.32	8 (14%)	64,96,113	1.39	6 (9%)
29	CLA	D	309	-	50,54,73	1.36	8 (16%)	59,90,113	1.40	4 (6%)
29	CLA	C	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.54	5 (9%)
29	CLA	a	812	-	64,68,73	1.19	9 (14%)	76,107,113	1.34	7 (9%)
29	CLA	b	717	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	6 (7%)
37	PID	Q	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.40	6 (11%)
37	PID	C	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.39	6 (11%)
29	CLA	G	319	13	45,49,73	1.41	8 (17%)	54,84,113	1.49	5 (9%)
36	DD6	I	202	-	40,45,45	1.56	2 (5%)	51,67,67	1.93	15 (29%)
37	PID	T	305	-	43,49,49	1.24	3 (6%)	52,76,76	1.47	7 (13%)
39	KC1	L	306	29	49,53,53	1.35	6 (12%)	61,89,89	1.74	15 (24%)
29	CLA	M	313	-	45,49,73	1.42	9 (20%)	54,84,113	1.51	5 (9%)
36	DD6	G	306	-	40,45,45	1.66	3 (7%)	51,67,67	2.21	15 (29%)
29	CLA	N	313	23	50,54,73	1.35	7 (14%)	59,90,113	4.61	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	T	314	-	51,55,73	1.34	8 (15%)	60,91,113	1.46	9 (15%)
29	CLA	I	211	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	8 (9%)
35	DGD	h	203	-	55,55,67	0.91	2 (3%)	69,69,81	0.99	5 (7%)
29	CLA	D	311	-	50,54,73	1.35	9 (18%)	59,90,113	1.41	4 (6%)
29	CLA	H	307	-	51,55,73	1.35	8 (15%)	60,91,113	1.38	5 (8%)
29	CLA	D	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.52	5 (9%)
36	DD6	J	302	-	40,45,45	1.62	2 (5%)	51,67,67	2.22	17 (33%)
37	PID	F	302	-	43,49,49	1.25	3 (6%)	52,76,76	1.61	6 (11%)
39	KC1	D	310	-	49,53,53	1.36	6 (12%)	61,89,89	1.74	13 (21%)
29	CLA	a	830	-	60,64,73	1.24	8 (13%)	71,102,113	5.17	9 (12%)
29	CLA	l	505	-	69,73,73	1.18	9 (13%)	82,113,113	1.25	4 (4%)
39	KC1	L	314	-	49,53,53	1.36	7 (14%)	61,89,89	1.72	14 (22%)
36	DD6	F	301	-	40,45,45	1.66	4 (10%)	51,67,67	2.00	16 (31%)
34	LMG	h	205	-	28,28,55	1.02	1 (3%)	36,36,63	1.28	4 (11%)
29	CLA	C	313	25	50,54,73	1.35	9 (18%)	59,90,113	1.39	4 (6%)
29	CLA	E	311	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
32	BCR	a	835	-	41,41,41	0.75	0	56,56,56	2.12	16 (28%)
40	SQD	B	317	-	40,42,54	0.45	1 (2%)	50,53,65	0.49	0
29	CLA	C	309	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	4 (4%)
37	PID	H	302	-	43,49,49	1.27	3 (6%)	52,76,76	1.39	8 (15%)
36	DD6	A	204	-	40,45,45	1.56	2 (5%)	51,67,67	1.89	16 (31%)
37	PID	O	301	-	43,49,49	1.22	3 (6%)	52,76,76	1.55	6 (11%)
29	CLA	l	510	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	5 (8%)
29	CLA	B	316	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
34	LMG	b	734	-	40,40,55	0.81	1 (2%)	48,48,63	1.29	6 (12%)
37	PID	T	307	-	43,49,49	1.24	3 (6%)	52,76,76	1.55	9 (17%)
29	CLA	K	209	-	58,62,73	1.27	9 (15%)	68,99,113	1.35	6 (8%)
34	LMG	A	219	-	37,37,55	0.84	1 (2%)	45,45,63	1.31	6 (13%)
29	CLA	A	209	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
29	CLA	C	314	-	51,55,73	1.34	8 (15%)	60,91,113	1.46	6 (10%)
36	DD6	M	302	-	40,45,45	1.65	3 (7%)	51,67,67	2.07	15 (29%)
39	KC1	H	311	-	49,53,53	1.36	6 (12%)	61,89,89	1.70	13 (21%)
37	PID	G	309	-	43,49,49	1.25	3 (6%)	52,76,76	1.38	6 (11%)
29	CLA	L	316	-	56,60,73	1.31	9 (16%)	65,97,113	1.35	6 (9%)
29	CLA	P	214	27	50,54,73	1.37	8 (16%)	59,90,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PID	C	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.90	10 (19%)
29	CLA	a	816	-	50,54,73	1.35	9 (18%)	59,90,113	1.40	4 (6%)
36	DD6	D	301	-	40,45,45	1.62	2 (5%)	51,67,67	2.11	15 (29%)
29	CLA	l	509	-	45,49,73	1.40	9 (20%)	54,84,113	1.45	7 (12%)
37	PID	N	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.29	5 (9%)
29	CLA	K	216	-	45,49,73	1.41	9 (20%)	54,84,113	1.54	5 (9%)
29	CLA	b	708	2	56,60,73	1.30	9 (16%)	65,97,113	1.39	6 (9%)
39	KC1	C	310	-	49,53,53	1.38	6 (12%)	61,89,89	1.77	13 (21%)
37	PID	D	306	-	43,49,49	1.27	3 (6%)	52,76,76	1.41	9 (17%)
37	PID	F	304	-	43,49,49	1.59	4 (9%)	52,76,76	1.47	8 (15%)
39	KC1	Q	314	26	49,53,53	1.37	6 (12%)	61,89,89	1.76	12 (19%)
36	DD6	F	303	-	40,45,45	1.66	2 (5%)	51,67,67	2.04	12 (23%)
29	CLA	L	312	-	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
36	DD6	C	303	-	40,45,45	1.63	2 (5%)	51,67,67	2.04	14 (27%)
29	CLA	b	718	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
29	CLA	I	207	14	53,57,73	1.31	9 (16%)	61,93,113	1.43	5 (8%)
29	CLA	I	216	-	56,60,73	1.29	9 (16%)	65,97,113	1.44	7 (10%)
29	CLA	Q	310	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
37	PID	C	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.53	6 (11%)
29	CLA	a	821	-	51,55,73	1.35	8 (15%)	60,91,113	1.38	5 (8%)
29	CLA	B	314	21	45,49,73	1.40	9 (20%)	54,84,113	1.53	5 (9%)
29	CLA	K	210	-	54,58,73	1.30	7 (12%)	64,95,113	1.41	7 (10%)
29	CLA	f	805	-	64,68,73	1.21	8 (12%)	76,107,113	1.27	5 (6%)
29	CLA	G	313	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	5 (7%)
37	PID	O	304	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	7 (13%)
34	LMG	K	201	-	43,43,55	0.79	1 (2%)	51,51,63	1.33	6 (11%)
29	CLA	B	310	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
37	PID	Q	306	-	43,49,49	1.24	3 (6%)	52,76,76	1.46	6 (11%)
29	CLA	a	808	-	55,59,73	1.31	9 (16%)	64,96,113	1.40	5 (7%)
29	CLA	E	308	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
29	CLA	A	208	-	59,63,73	1.24	9 (15%)	70,101,113	1.34	7 (10%)
34	LMG	b	730	-	46,46,55	0.81	2 (4%)	54,54,63	1.32	5 (9%)
37	PID	G	310	-	43,49,49	1.26	3 (6%)	52,76,76	1.39	7 (13%)
29	CLA	J	311	-	57,61,73	1.27	9 (15%)	67,98,113	1.36	5 (7%)
36	DD6	K	205	-	40,45,45	1.59	2 (5%)	51,67,67	1.87	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b	723	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	7 (8%)
39	KC1	A	205	29	49,53,53	1.36	6 (12%)	61,89,89	1.74	15 (24%)
29	CLA	B	315	-	50,54,73	1.36	9 (18%)	59,90,113	1.42	5 (8%)
36	DD6	G	308	-	40,45,45	1.56	1 (2%)	51,67,67	2.07	14 (27%)
39	KC1	C	312	-	49,53,53	1.38	6 (12%)	61,89,89	1.77	14 (22%)
39	KC1	G	318	-	49,53,53	1.36	6 (12%)	61,89,89	1.69	12 (19%)
37	PID	C	307	-	43,49,49	1.24	3 (6%)	52,76,76	1.49	7 (13%)
29	CLA	M	307	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	5 (7%)
36	DD6	K	203	-	40,45,45	1.64	3 (7%)	51,67,67	1.89	14 (27%)
36	DD6	h	202	-	40,45,45	1.76	4 (10%)	51,67,67	2.25	18 (35%)
32	BCR	i	204	-	41,41,41	0.70	0	56,56,56	2.37	14 (25%)
39	KC1	J	312	17	49,53,53	1.36	6 (12%)	61,89,89	1.74	13 (21%)
29	CLA	b	706	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	5 (6%)
29	CLA	K	214	-	59,63,73	1.26	9 (15%)	70,101,113	1.33	6 (8%)
37	PID	N	307	-	43,49,49	1.25	4 (9%)	52,76,76	1.59	10 (19%)
36	DD6	B	319	-	40,45,45	1.62	2 (5%)	51,67,67	2.24	17 (33%)
29	CLA	P	212	-	55,59,73	1.31	7 (12%)	64,96,113	1.38	5 (7%)
32	BCR	b	735	-	41,41,41	0.73	0	56,56,56	2.05	19 (33%)
29	CLA	a	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
29	CLA	b	720	-	69,73,73	1.18	9 (13%)	82,113,113	1.25	4 (4%)
36	DD6	I	204	-	40,45,45	1.78	4 (10%)	51,67,67	2.11	15 (29%)
35	DGD	B	318	-	46,46,67	1.01	2 (4%)	60,60,81	1.33	10 (16%)
29	CLA	O	308	-	51,55,73	1.37	8 (15%)	60,91,113	1.40	5 (8%)
39	KC1	M	312	-	49,53,53	1.36	6 (12%)	61,89,89	1.76	13 (21%)
29	CLA	A	218	12	64,68,73	1.20	9 (14%)	76,107,113	1.32	7 (9%)
29	CLA	J	310	-	51,55,73	1.34	9 (17%)	60,91,113	1.41	7 (11%)
37	PID	P	202	-	43,49,49	1.22	3 (6%)	52,76,76	1.32	8 (15%)
29	CLA	D	313	20	49,53,73	1.38	9 (18%)	58,89,113	1.41	4 (6%)
29	CLA	A	214	12	45,49,73	1.41	9 (20%)	54,84,113	1.47	5 (9%)
29	CLA	O	311	-	55,59,73	1.31	9 (16%)	64,96,113	1.37	4 (6%)
39	KC1	H	314	-	49,53,53	1.35	5 (10%)	61,89,89	1.73	13 (21%)
29	CLA	L	308	-	57,61,73	1.28	9 (15%)	67,98,113	5.33	7 (10%)
29	CLA	b	721	-	62,66,73	1.23	9 (14%)	73,104,113	1.37	7 (9%)
29	CLA	a	809	1	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
29	CLA	l	508	-	45,49,73	1.40	9 (20%)	54,84,113	1.46	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PID	T	304	-	43,49,49	1.22	3 (6%)	52,76,76	1.39	5 (9%)
29	CLA	l	502	10	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
30	PQN	b	727	-	34,34,34	1.57	2 (5%)	43,45,45	1.25	4 (9%)
39	KC1	N	310	-	49,53,53	1.36	6 (12%)	61,89,89	1.73	12 (19%)
38	UIX	E	304	-	43,49,49	1.42	5 (11%)	53,74,74	2.41	19 (35%)
29	CLA	F	310	-	50,54,73	1.34	9 (18%)	59,90,113	1.47	5 (8%)
29	CLA	I	201	29	49,53,73	1.38	9 (18%)	58,89,113	1.45	4 (6%)
29	CLA	a	824	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
38	UIX	J	304	-	43,49,49	1.40	4 (9%)	53,74,74	2.29	14 (26%)
38	UIX	A	203	-	43,49,49	1.40	5 (11%)	53,74,74	2.35	21 (39%)
29	CLA	T	309	25	50,54,73	1.34	9 (18%)	59,90,113	1.41	5 (8%)
29	CLA	O	314	-	51,55,73	1.37	9 (17%)	60,91,113	1.43	8 (13%)
36	DD6	J	301	-	40,45,45	1.60	2 (5%)	51,67,67	2.26	16 (31%)
36	DD6	T	303	-	40,45,45	1.53	2 (5%)	51,67,67	1.97	14 (27%)
29	CLA	I	213	14	69,73,73	1.17	9 (13%)	82,113,113	3.76	9 (10%)
29	CLA	P	217	-	45,49,73	1.43	7 (15%)	54,84,113	1.55	5 (9%)
38	UIX	N	306	-	43,49,49	1.40	5 (11%)	53,74,74	2.57	16 (30%)
29	CLA	P	209	-	51,55,73	1.36	8 (15%)	60,91,113	1.38	5 (8%)
29	CLA	F	316	16	45,49,73	1.41	9 (20%)	54,84,113	1.50	5 (9%)
29	CLA	b	711	-	62,66,73	1.22	9 (14%)	73,104,113	1.33	5 (6%)
29	CLA	l	501	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	6 (7%)
37	PID	F	306	-	43,49,49	1.27	3 (6%)	52,76,76	1.43	7 (13%)
29	CLA	L	311	19	50,54,73	1.36	8 (16%)	59,90,113	1.34	4 (6%)
29	CLA	a	803	-	69,73,73	1.17	9 (13%)	82,113,113	1.20	5 (6%)
39	KC1	Q	311	-	49,53,53	1.42	7 (14%)	61,89,89	1.82	15 (24%)
32	BCR	l	506	-	41,41,41	0.68	0	56,56,56	1.94	15 (26%)
29	CLA	E	306	28	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
29	CLA	A	212	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	5 (7%)
29	CLA	b	710	-	50,54,73	1.34	9 (18%)	59,90,113	1.36	4 (6%)
29	CLA	L	317	-	50,54,73	1.35	9 (18%)	59,90,113	1.41	4 (6%)
29	CLA	F	312	16	50,54,73	1.35	8 (16%)	59,90,113	1.38	4 (6%)
37	PID	G	303	-	43,49,49	1.28	3 (6%)	52,76,76	1.31	7 (13%)
29	CLA	a	818	-	51,55,73	1.34	9 (17%)	60,91,113	1.38	5 (8%)
37	PID	N	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.46	7 (13%)
29	CLA	K	212	-	56,60,73	1.31	9 (16%)	65,97,113	1.35	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DD6	M	304	-	40,45,45	1.59	2 (5%)	51,67,67	1.74	14 (27%)
39	KC1	T	310	-	49,53,53	1.38	5 (10%)	61,89,89	1.71	13 (21%)
32	BCR	a	834	-	41,41,41	0.70	0	56,56,56	2.05	14 (25%)
29	CLA	a	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
37	PID	T	317	-	43,49,49	1.26	3 (6%)	52,76,76	1.62	9 (17%)
29	CLA	G	302	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
37	PID	D	303	-	43,49,49	1.29	3 (6%)	52,76,76	1.54	11 (21%)
39	KC1	O	312	-	49,53,53	1.40	6 (12%)	61,89,89	1.90	14 (22%)
30	PQN	a	832	-	34,34,34	1.55	2 (5%)	43,45,45	1.30	6 (13%)
29	CLA	D	314	-	51,55,73	1.35	9 (17%)	60,91,113	1.46	6 (10%)
29	CLA	b	719	-	54,58,73	1.31	9 (16%)	64,95,113	1.40	8 (12%)
31	LHG	a	833	-	47,47,48	0.28	0	50,53,54	0.31	0
29	CLA	L	307	39	54,58,73	1.31	9 (16%)	64,95,113	5.47	8 (12%)
32	BCR	f	801	-	41,41,41	0.71	0	56,56,56	2.02	15 (26%)
39	KC1	N	312	23	49,53,53	1.36	5 (10%)	61,89,89	1.72	14 (22%)
29	CLA	J	305	-	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
29	CLA	Q	307	-	51,55,73	1.35	9 (17%)	60,91,113	1.38	5 (8%)
39	KC1	T	312	-	49,53,53	1.36	6 (12%)	61,89,89	1.77	12 (19%)
29	CLA	b	705	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	5 (6%)
29	CLA	J	309	17	50,54,73	1.35	8 (16%)	59,90,113	1.45	4 (6%)
39	KC1	A	213	-	49,53,53	1.36	6 (12%)	61,89,89	1.72	13 (21%)
29	CLA	B	308	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	7 (8%)
29	CLA	B	306	21	53,57,73	1.32	9 (16%)	61,93,113	1.40	5 (8%)
29	CLA	O	316	-	45,49,73	1.43	8 (17%)	54,84,113	1.48	5 (9%)
29	CLA	T	313	-	50,54,73	1.37	8 (16%)	59,90,113	1.39	4 (6%)
29	CLA	E	309	-	50,54,73	1.36	8 (16%)	59,90,113	1.42	4 (6%)
36	DD6	m	101	-	40,45,45	1.57	2 (5%)	51,67,67	2.03	16 (31%)
38	UIX	L	302	-	43,49,49	1.37	4 (9%)	53,74,74	2.38	18 (33%)
36	DD6	B	305	-	40,45,45	1.56	2 (5%)	51,67,67	1.91	16 (31%)
36	DD6	E	303	-	40,45,45	1.58	2 (5%)	51,67,67	1.78	12 (23%)
36	DD6	K	202	-	40,45,45	1.67	2 (5%)	51,67,67	2.99	15 (29%)
36	DD6	A	201	-	40,45,45	1.56	2 (5%)	51,67,67	2.04	16 (31%)
34	LMG	E	316	-	32,32,55	0.99	2 (6%)	40,40,63	1.28	2 (5%)
29	CLA	l	503	10	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
37	PID	D	307	-	43,49,49	1.23	3 (6%)	52,76,76	1.53	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	P	215	-	51,55,73	1.36	8 (15%)	60,91,113	1.54	7 (11%)
29	CLA	A	211	-	59,63,73	1.24	9 (15%)	70,101,113	1.30	7 (10%)
29	CLA	M	306	-	57,61,73	1.28	8 (14%)	67,98,113	1.37	6 (8%)
29	CLA	K	213	-	52,56,73	1.33	9 (17%)	61,92,113	1.36	5 (8%)
29	CLA	a	831	-	69,73,73	1.16	9 (13%)	82,113,113	4.83	9 (10%)
37	PID	H	306	-	43,49,49	1.27	4 (9%)	52,76,76	1.37	5 (9%)
35	DGD	G	320	-	46,46,67	1.02	2 (4%)	60,60,81	0.98	3 (5%)
37	PID	D	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.39	5 (9%)
29	CLA	b	709	-	64,68,73	1.20	9 (14%)	76,107,113	1.31	6 (7%)
29	CLA	l	504	-	69,73,73	1.16	9 (13%)	82,113,113	3.77	10 (12%)
29	CLA	M	311	-	50,54,73	1.36	9 (18%)	59,90,113	1.38	5 (8%)
29	CLA	G	314	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	6 (7%)
39	KC1	K	215	-	49,53,53	1.39	7 (14%)	61,89,89	1.77	14 (22%)
39	KC1	B	313	21	49,53,53	1.36	7 (14%)	61,89,89	1.73	13 (21%)
29	CLA	E	315	-	61,65,73	1.24	8 (13%)	72,103,113	1.33	6 (8%)
39	KC1	I	215	14	49,53,53	1.36	7 (14%)	61,89,89	1.74	14 (22%)

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
39	KC1	D	315	-	-	6/15/71/71	-
29	CLA	C	311	-	1/1/12/20	5/23/99/115	-
38	UIX	T	306	-	-	4/31/87/87	0/3/3/3
36	DD6	L	304	-	-	2/26/80/80	0/3/3/3
29	CLA	N	311	-	1/1/12/20	4/23/99/115	-
36	DD6	J	303	-	-	2/26/80/80	0/3/3/3
29	CLA	M	314	-	1/1/12/20	7/24/100/115	-
37	PID	N	301	-	-	4/24/93/93	0/4/4/4
38	UIX	P	207	-	-	6/31/87/87	0/3/3/3
37	PID	O	307	-	-	4/24/93/93	0/4/4/4
37	PID	Q	303	-	-	0/24/93/93	0/4/4/4
29	CLA	G	311	13	1/1/12/20	9/23/99/115	-
36	DD6	B	301	-	-	4/24/78/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	D	312	20	1/1/11/20	7/17/93/115	-
36	DD6	G	307	-	-	2/26/80/80	0/3/3/3
36	DD6	I	205	-	-	6/26/80/80	0/3/3/3
29	CLA	a	804	-	1/1/13/20	1/27/103/115	-
37	PID	T	301	-	-	2/24/93/93	0/4/4/4
29	CLA	a	828	-	1/1/11/20	8/17/93/115	-
39	KC1	P	211	-	-	8/15/71/71	-
36	DD6	Q	302	-	-	1/26/80/80	0/3/3/3
29	CLA	a	837	-	1/1/13/20	11/27/103/115	-
32	BCR	m	103	-	-	5/29/63/63	0/2/2/2
29	CLA	A	206	39	1/1/11/20	4/15/91/115	-
34	LMG	K	219	-	-	17/30/50/70	0/1/1/1
36	DD6	I	206	-	-	2/26/80/80	0/3/3/3
39	KC1	E	312	28	-	6/15/71/71	-
37	PID	O	305	-	-	7/24/93/93	0/4/4/4
29	CLA	Q	313	-	1/1/11/20	6/18/94/115	-
29	CLA	J	307	-	1/1/11/20	3/17/93/115	-
29	CLA	L	313	-	1/1/12/20	6/25/101/115	-
36	DD6	G	305	-	-	7/26/80/80	0/3/3/3
29	CLA	b	726	-	1/1/15/20	7/39/115/115	-
35	DGD	j	103	-	-	10/32/72/95	0/2/2/2
36	DD6	O	303	-	-	4/26/80/80	0/3/3/3
33	SF4	c	101	3	-	-	0/6/5/5
29	CLA	I	209	-	1/1/14/20	13/33/109/115	-
34	LMG	b	732	-	-	20/39/59/70	0/1/1/1
29	CLA	O	309	-	-	8/39/115/115	-
37	PID	P	205	-	-	1/24/93/93	0/4/4/4
29	CLA	a	801	-	1/1/15/20	10/39/115/115	-
39	KC1	O	310	-	-	6/15/71/71	-
39	KC1	F	314	-	-	6/15/71/71	-
29	CLA	b	713	-	1/1/12/20	6/25/101/115	-
38	UIX	C	306	-	-	6/31/87/87	0/3/3/3
29	CLA	B	311	21	1/1/12/20	4/23/99/115	-
29	CLA	K	208	-	1/1/11/20	2/17/93/115	-
29	CLA	M	310	18	1/1/11/20	5/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DD6	P	204	-	-	2/26/80/80	0/3/3/3
29	CLA	H	315	-	1/1/10/20	4/10/86/115	-
38	UIX	B	304	-	-	2/31/87/87	0/3/3/3
29	CLA	K	207	15	1/1/11/20	6/20/96/115	-
36	DD6	I	203	-	-	7/26/80/80	0/3/3/3
29	CLA	a	825	-	1/1/15/20	13/39/115/115	-
39	KC1	P	216	-	-	6/15/71/71	-
29	CLA	H	308	-	1/1/15/20	9/39/115/115	-
36	DD6	L	305	-	-	4/26/80/80	0/3/3/3
29	CLA	L	309	-	1/1/13/20	2/27/103/115	-
36	DD6	N	303	-	-	1/26/80/80	0/3/3/3
35	DGD	m	102	-	-	7/55/95/95	0/2/2/2
29	CLA	M	315	-	1/1/11/20	5/17/93/115	-
36	DD6	L	303	-	-	0/26/80/80	0/3/3/3
29	CLA	I	217	-	1/1/13/20	10/27/103/115	-
29	CLA	G	301	-	1/1/11/20	5/20/96/115	-
29	CLA	J	306	-	1/1/15/20	16/39/115/115	-
37	PID	h	204	-	-	2/24/93/93	1/4/4/4
29	CLA	a	815	-	1/1/11/20	4/15/91/115	-
29	CLA	a	802	-	1/1/15/20	9/39/115/115	-
37	PID	P	208	-	-	5/24/93/93	0/4/4/4
29	CLA	A	207	-	1/1/13/20	5/27/103/115	-
29	CLA	G	312	13	1/1/15/20	16/39/115/115	-
36	DD6	K	204	-	-	5/26/80/80	0/3/3/3
29	CLA	a	817	-	1/1/11/20	6/15/91/115	-
39	KC1	O	315	-	-	9/15/71/71	-
29	CLA	I	208	-	1/1/11/20	9/17/93/115	-
29	CLA	i	202	-	1/1/15/20	12/39/115/115	-
29	CLA	N	314	-	1/1/11/20	7/18/94/115	-
37	PID	P	206	-	-	9/24/93/93	0/4/4/4
29	CLA	Q	308	-	1/1/15/20	17/39/115/115	-
29	CLA	K	211	-	1/1/13/20	5/27/103/115	-
37	PID	P	203	-	-	3/24/93/93	0/4/4/4
39	KC1	H	309	-	-	9/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	307	-	1/1/11/20	4/15/91/115	-
37	PID	H	304	-	-	0/24/93/93	0/4/4/4
39	KC1	E	307	-	-	6/15/71/71	-
36	DD6	K	221	-	-	5/26/80/80	0/3/3/3
29	CLA	b	704	-	1/1/15/20	12/39/115/115	-
29	CLA	E	305	-	1/1/14/20	11/35/111/115	-
35	DGD	j	106	-	-	15/38/78/95	0/2/2/2
29	CLA	L	310	-	1/1/13/20	5/27/103/115	-
35	DGD	b	733	-	-	24/46/86/95	0/2/2/2
36	DD6	E	302	-	-	2/26/80/80	0/3/3/3
34	LMG	j	102	-	-	23/38/58/70	0/1/1/1
29	CLA	J	313	-	1/1/10/20	2/10/86/115	-
29	CLA	F	307	-	1/1/11/20	3/17/93/115	-
29	CLA	T	311	-	1/1/11/20	7/17/93/115	-
29	CLA	M	309	-	1/1/11/20	6/17/93/115	-
38	UIX	O	306	-	-	7/31/87/87	0/3/3/3
29	CLA	E	313	-	1/1/10/20	0/10/86/115	-
35	DGD	j	105	-	-	1/30/70/95	0/2/2/2
29	CLA	a	826	-	1/1/15/20	11/39/115/115	-
36	DD6	M	303	-	-	6/26/80/80	0/3/3/3
39	KC1	F	309	-	-	7/15/71/71	-
29	CLA	a	823	-	1/1/13/20	9/31/107/115	-
32	BCR	b	729	-	-	5/29/63/63	0/2/2/2
29	CLA	K	217	-	1/1/11/20	6/17/93/115	-
34	LMG	P	201	-	-	6/22/42/70	0/1/1/1
32	BCR	l	507	-	-	5/29/63/63	0/2/2/2
29	CLA	A	210	12	1/1/11/20	6/17/93/115	-
32	BCR	a	838	-	-	6/29/63/63	0/2/2/2
29	CLA	I	214	-	1/1/13/20	4/27/103/115	-
29	CLA	a	811	-	1/1/13/20	9/29/105/115	-
29	CLA	N	308	-	1/1/11/20	6/18/94/115	-
29	CLA	b	725	-	1/1/15/20	9/39/115/115	-
37	PID	Q	304	-	-	2/24/93/93	0/4/4/4
29	CLA	B	309	-	1/1/13/20	6/27/103/115	-
29	CLA	H	312	22	1/1/11/20	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	a	819	-	1/1/13/20	6/30/106/115	-
36	DD6	B	303	-	-	0/26/80/80	0/3/3/3
29	CLA	b	702	-	1/1/15/20	14/39/115/115	-
29	CLA	A	217	-	1/1/12/20	6/23/99/115	-
39	KC1	T	315	25	-	6/15/71/71	-
29	CLA	M	308	-	1/1/11/20	7/19/95/115	-
29	CLA	b	701	-	1/1/15/20	11/39/115/115	-
36	DD6	H	303	-	-	1/26/80/80	0/3/3/3
29	CLA	a	827	-	1/1/15/20	10/39/115/115	-
29	CLA	b	736	-	1/1/15/20	18/39/115/115	-
29	CLA	G	304	-	1/1/13/20	12/32/108/115	-
29	CLA	a	820	-	1/1/15/20	12/39/115/115	-
29	CLA	L	315	-	1/1/10/20	4/10/86/115	-
29	CLA	h	201	-	1/1/14/20	6/33/109/115	-
29	CLA	C	308	-	1/1/11/20	6/18/94/115	-
29	CLA	a	806	1	1/1/15/20	15/39/115/115	-
36	DD6	K	206	-	-	1/26/80/80	0/3/3/3
37	PID	O	302	-	-	2/24/93/93	0/4/4/4
29	CLA	F	308	-	1/1/11/20	3/17/93/115	-
36	DD6	B	302	-	-	2/26/80/80	0/3/3/3
29	CLA	f	802	-	1/1/11/20	4/17/93/115	-
37	PID	j	101	-	-	2/24/93/93	0/4/4/4
29	CLA	I	212	-	1/1/13/20	13/27/103/115	-
29	CLA	Q	312	-	1/1/11/20	5/17/93/115	-
37	PID	E	301	-	-	5/24/93/93	0/4/4/4
37	PID	H	305	-	-	3/24/93/93	0/4/4/4
37	PID	C	302	-	-	2/24/93/93	0/4/4/4
29	CLA	I	210	-	1/1/13/20	6/27/103/115	-
29	CLA	b	731	-	1/1/13/20	3/29/105/115	-
29	CLA	J	308	-	1/1/13/20	9/29/105/115	-
37	PID	N	302	-	-	2/24/93/93	0/4/4/4
29	CLA	E	314	28	-	3/19/95/115	-
36	DD6	A	202	-	-	1/26/80/80	0/3/3/3
29	CLA	a	810	1	1/1/13/20	9/27/103/115	-
29	CLA	H	313	-	1/1/11/20	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	D	308	-	1/1/11/20	5/18/94/115	-
29	CLA	F	315	-	1/1/10/20	2/10/86/115	-
38	UIX	F	305	-	-	12/31/87/87	0/3/3/3
29	CLA	O	313	24	1/1/11/20	4/17/93/115	-
29	CLA	a	813	-	1/1/12/20	12/23/99/115	-
29	CLA	E	310	28	1/1/11/20	4/17/93/115	-
29	CLA	b	714	-	1/1/14/20	6/38/114/115	-
29	CLA	b	724	-	1/1/11/20	2/18/94/115	-
39	KC1	N	315	-	-	9/15/71/71	-
36	DD6	D	304	-	-	6/26/80/80	0/3/3/3
36	DD6	M	301	-	-	2/26/80/80	0/3/3/3
37	PID	T	302	-	-	2/24/93/93	0/4/4/4
29	CLA	j	104	29	1/1/12/20	4/24/100/115	-
29	CLA	F	313	16	1/1/11/20	8/17/93/115	-
29	CLA	Q	315	-	1/1/10/20	4/10/86/115	-
29	CLA	A	216	-	1/1/10/20	2/10/86/115	-
29	CLA	K	218	-	1/1/11/20	8/15/91/115	-
29	CLA	b	703	-	1/1/15/20	12/39/115/115	-
29	CLA	i	201	-	1/1/15/20	12/39/115/115	-
29	CLA	N	309	-	1/1/15/20	14/39/115/115	-
29	CLA	a	805	-	1/1/13/20	6/27/103/115	-
29	CLA	G	317	-	1/1/12/20	8/25/101/115	-
32	BCR	b	728	-	-	5/29/63/63	0/2/2/2
29	CLA	T	316	-	1/1/10/20	4/10/86/115	-
29	CLA	f	803	6	1/1/11/20	6/17/93/115	-
32	BCR	f	804	-	-	2/29/63/63	0/2/2/2
29	CLA	F	311	-	1/1/11/20	4/17/93/115	-
39	KC1	C	315	25	-	8/15/71/71	-
37	PID	D	305	-	-	5/24/93/93	0/4/4/4
34	LMG	K	220	-	-	13/31/51/70	0/1/1/1
29	CLA	a	822	-	1/1/15/20	7/39/115/115	-
38	UIX	Q	305	-	-	4/31/87/87	0/3/3/3
33	SF4	c	102	3	-	-	0/6/5/5
29	CLA	b	712	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	i	203	-	1/1/13/20	13/27/103/115	-
29	CLA	b	707	-	1/1/15/20	13/39/115/115	-
29	CLA	A	215	-	1/1/11/20	5/18/94/115	-
29	CLA	P	210	-	1/1/15/20	9/39/115/115	-
36	DD6	L	301	-	-	4/26/80/80	0/3/3/3
39	KC1	G	315	-	-	5/15/71/71	-
39	KC1	Q	309	-	-	5/15/71/71	-
29	CLA	b	715	-	1/1/11/20	8/17/93/115	-
29	CLA	N	316	-	1/1/10/20	4/10/86/115	-
29	CLA	G	316	-	1/1/15/20	10/39/115/115	-
33	SF4	a	836	2,1	-	-	0/6/5/5
37	PID	H	301	-	-	2/24/93/93	0/4/4/4
29	CLA	a	814	-	1/1/11/20	4/17/93/115	-
40	SQD	J	314	-	-	10/40/60/69	0/1/1/1
29	CLA	T	308	-	1/1/11/20	4/18/94/115	-
39	KC1	M	305	-	-	4/15/71/71	-
39	KC1	P	213	27	-	6/15/71/71	-
29	CLA	B	312	-	1/1/15/20	10/39/115/115	-
29	CLA	b	716	-	1/1/12/20	7/25/101/115	-
29	CLA	b	722	-	1/1/13/20	8/31/107/115	-
29	CLA	H	310	-	1/1/12/20	9/23/99/115	-
29	CLA	D	309	-	1/1/11/20	2/17/93/115	-
29	CLA	C	316	-	1/1/10/20	4/10/86/115	-
29	CLA	a	812	-	1/1/14/20	15/33/109/115	-
29	CLA	b	717	-	1/1/15/20	15/39/115/115	-
37	PID	Q	301	-	-	2/24/93/93	0/4/4/4
37	PID	C	304	-	-	3/24/93/93	0/4/4/4
29	CLA	G	319	13	1/1/10/20	2/10/86/115	-
36	DD6	I	202	-	-	4/26/80/80	0/3/3/3
37	PID	T	305	-	-	0/24/93/93	0/4/4/4
39	KC1	L	306	29	-	5/15/71/71	-
29	CLA	M	313	-	1/1/10/20	4/10/86/115	-
36	DD6	G	306	-	-	1/26/80/80	0/3/3/3
29	CLA	N	313	23	1/1/11/20	8/17/93/115	-
29	CLA	T	314	-	1/1/11/20	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	I	211	-	1/1/15/20	8/39/115/115	-
35	DGD	h	203	-	-	8/43/83/95	0/2/2/2
29	CLA	D	311	-	1/1/11/20	11/17/93/115	-
29	CLA	H	307	-	1/1/11/20	5/18/94/115	-
29	CLA	D	316	-	1/1/10/20	4/10/86/115	-
36	DD6	J	302	-	-	2/26/80/80	0/3/3/3
37	PID	F	302	-	-	3/24/93/93	0/4/4/4
39	KC1	D	310	-	-	5/15/71/71	-
29	CLA	a	830	-	1/1/13/20	6/29/105/115	-
29	CLA	l	505	-	1/1/15/20	11/39/115/115	-
39	KC1	L	314	-	-	6/15/71/71	-
36	DD6	F	301	-	-	8/26/80/80	0/3/3/3
34	LMG	h	205	-	-	4/23/43/70	0/1/1/1
29	CLA	C	313	25	1/1/11/20	7/17/93/115	-
29	CLA	E	311	-	1/1/15/20	11/39/115/115	-
32	BCR	a	835	-	-	2/29/63/63	0/2/2/2
40	SQD	B	317	-	-	4/37/57/69	0/1/1/1
29	CLA	C	309	-	1/1/15/20	6/39/115/115	-
37	PID	H	302	-	-	2/24/93/93	0/4/4/4
36	DD6	A	204	-	-	2/26/80/80	0/3/3/3
37	PID	O	301	-	-	3/24/93/93	0/4/4/4
29	CLA	l	510	-	1/1/11/20	7/15/91/115	-
29	CLA	B	316	-	1/1/11/20	6/15/91/115	-
34	LMG	b	734	-	-	10/35/55/70	0/1/1/1
37	PID	T	307	-	-	4/24/93/93	0/4/4/4
29	CLA	K	209	-	1/1/12/20	8/26/102/115	-
34	LMG	A	219	-	-	17/32/52/70	0/1/1/1
29	CLA	A	209	-	1/1/15/20	18/39/115/115	-
29	CLA	C	314	-	1/1/11/20	7/18/94/115	-
36	DD6	M	302	-	-	1/26/80/80	0/3/3/3
39	KC1	H	311	-	-	6/15/71/71	-
37	PID	G	309	-	-	2/24/93/93	0/4/4/4
29	CLA	L	316	-	1/1/12/20	11/24/100/115	-
29	CLA	P	214	27	1/1/11/20	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	C	305	-	-	9/24/93/93	0/4/4/4
29	CLA	a	816	-	1/1/11/20	8/17/93/115	-
36	DD6	D	301	-	-	7/26/80/80	0/3/3/3
29	CLA	l	509	-	1/1/10/20	0/10/86/115	-
37	PID	N	305	-	-	19/24/93/93	0/4/4/4
29	CLA	K	216	-	1/1/10/20	4/10/86/115	-
29	CLA	b	708	2	1/1/12/20	4/24/100/115	-
39	KC1	C	310	-	-	7/15/71/71	-
37	PID	D	306	-	-	3/24/93/93	0/4/4/4
37	PID	F	304	-	-	14/24/93/93	1/4/4/4
39	KC1	Q	314	26	-	8/15/71/71	-
36	DD6	F	303	-	-	0/26/80/80	0/3/3/3
29	CLA	L	312	-	1/1/13/20	10/27/103/115	-
36	DD6	C	303	-	-	0/26/80/80	0/3/3/3
29	CLA	b	718	-	1/1/15/20	13/39/115/115	-
29	CLA	I	207	14	1/1/11/20	7/20/96/115	-
29	CLA	I	216	-	1/1/12/20	4/24/100/115	-
29	CLA	Q	310	-	1/1/15/20	14/39/115/115	-
37	PID	C	301	-	-	4/24/93/93	0/4/4/4
29	CLA	a	821	-	1/1/11/20	8/18/94/115	-
29	CLA	B	314	21	1/1/10/20	4/10/86/115	-
29	CLA	K	210	-	1/1/12/20	5/21/97/115	-
29	CLA	f	805	-	1/1/14/20	10/33/109/115	-
29	CLA	G	313	-	1/1/13/20	3/27/103/115	-
37	PID	O	304	-	-	3/24/93/93	0/4/4/4
34	LMG	K	201	-	-	17/38/58/70	0/1/1/1
29	CLA	B	310	-	1/1/15/20	14/39/115/115	-
37	PID	Q	306	-	-	4/24/93/93	0/4/4/4
29	CLA	a	808	-	1/1/12/20	5/23/99/115	-
29	CLA	E	308	-	1/1/15/20	10/39/115/115	-
29	CLA	A	208	-	1/1/13/20	3/27/103/115	-
34	LMG	b	730	-	-	19/41/61/70	0/1/1/1
37	PID	G	310	-	-	2/24/93/93	0/4/4/4
29	CLA	J	311	-	1/1/12/20	8/25/101/115	-
36	DD6	K	205	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	723	-	1/1/15/20	5/39/115/115	-
39	KC1	A	205	29	-	7/15/71/71	-
29	CLA	B	315	-	1/1/11/20	3/17/93/115	-
36	DD6	G	308	-	-	1/26/80/80	0/3/3/3
39	KC1	C	312	-	-	8/15/71/71	-
39	KC1	G	318	-	-	6/15/71/71	-
37	PID	C	307	-	-	2/24/93/93	0/4/4/4
29	CLA	M	307	-	1/1/13/20	5/27/103/115	-
36	DD6	K	203	-	-	6/26/80/80	0/3/3/3
36	DD6	h	202	-	-	2/26/80/80	0/3/3/3
32	BCR	i	204	-	-	4/29/63/63	0/2/2/2
39	KC1	J	312	17	-	5/15/71/71	-
29	CLA	b	706	-	1/1/15/20	11/39/115/115	-
29	CLA	K	214	-	1/1/13/20	7/27/103/115	-
37	PID	N	307	-	-	6/24/93/93	0/4/4/4
36	DD6	B	319	-	-	9/26/80/80	0/3/3/3
29	CLA	P	212	-	1/1/12/20	9/23/99/115	-
32	BCR	b	735	-	-	4/29/63/63	0/2/2/2
29	CLA	a	829	-	1/1/15/20	16/39/115/115	-
29	CLA	b	720	-	1/1/15/20	13/39/115/115	-
36	DD6	I	204	-	-	3/26/80/80	0/3/3/3
35	DGD	B	318	-	-	9/34/74/95	0/2/2/2
29	CLA	O	308	-	1/1/11/20	6/18/94/115	-
39	KC1	M	312	-	-	6/15/71/71	-
29	CLA	A	218	12	1/1/14/20	8/33/109/115	-
29	CLA	J	310	-	1/1/11/20	6/18/94/115	-
37	PID	P	202	-	-	4/24/93/93	0/4/4/4
29	CLA	D	313	20	1/1/11/20	3/15/91/115	-
29	CLA	A	214	12	1/1/10/20	4/10/86/115	-
29	CLA	O	311	-	1/1/12/20	4/23/99/115	-
39	KC1	H	314	-	-	6/15/71/71	-
29	CLA	L	308	-	1/1/12/20	8/25/101/115	-
29	CLA	b	721	-	1/1/13/20	10/31/107/115	-
29	CLA	a	809	1	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	l	508	-	1/1/10/20	0/10/86/115	-
37	PID	T	304	-	-	1/24/93/93	0/4/4/4
29	CLA	l	502	10	1/1/15/20	15/39/115/115	-
30	PQN	b	727	-	-	4/23/43/43	0/2/2/2
39	KC1	N	310	-	-	7/15/71/71	-
38	UIX	E	304	-	-	2/31/87/87	0/3/3/3
29	CLA	F	310	-	1/1/11/20	8/17/93/115	-
29	CLA	I	201	29	1/1/11/20	3/15/91/115	-
29	CLA	a	824	-	1/1/15/20	8/39/115/115	-
38	UIX	J	304	-	-	4/31/87/87	0/3/3/3
38	UIX	A	203	-	-	4/31/87/87	0/3/3/3
29	CLA	T	309	25	1/1/11/20	3/17/93/115	-
29	CLA	O	314	-	-	6/18/94/115	-
36	DD6	J	301	-	-	2/26/80/80	0/3/3/3
36	DD6	T	303	-	-	7/26/80/80	0/3/3/3
29	CLA	I	213	14	1/1/15/20	14/39/115/115	-
29	CLA	P	217	-	1/1/10/20	2/10/86/115	-
38	UIX	N	306	-	-	9/31/87/87	0/3/3/3
29	CLA	P	209	-	1/1/11/20	7/18/94/115	-
29	CLA	F	316	16	1/1/10/20	2/10/86/115	-
29	CLA	b	711	-	1/1/13/20	11/31/107/115	-
29	CLA	l	501	-	1/1/14/20	11/33/109/115	-
37	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	CLA	L	311	19	1/1/11/20	6/17/93/115	-
29	CLA	a	803	-	1/1/15/20	8/39/115/115	-
39	KC1	Q	311	-	-	5/15/71/71	-
32	BCR	l	506	-	-	9/29/63/63	0/2/2/2
29	CLA	E	306	28	1/1/15/20	16/39/115/115	-
29	CLA	A	212	-	1/1/13/20	10/27/103/115	-
29	CLA	b	710	-	1/1/11/20	8/17/93/115	-
29	CLA	L	317	-	1/1/11/20	7/17/93/115	-
29	CLA	F	312	16	1/1/11/20	5/17/93/115	-
37	PID	G	303	-	-	6/24/93/93	0/4/4/4
29	CLA	a	818	-	1/1/11/20	6/18/94/115	-
37	PID	N	304	-	-	1/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	K	212	-	1/1/12/20	7/24/100/115	-
36	DD6	M	304	-	-	3/26/80/80	0/3/3/3
39	KC1	T	310	-	-	6/15/71/71	-
32	BCR	a	834	-	-	0/29/63/63	0/2/2/2
29	CLA	a	807	-	1/1/15/20	14/39/115/115	-
37	PID	T	317	-	-	11/24/93/93	1/4/4/4
29	CLA	G	302	-	1/1/15/20	14/39/115/115	-
37	PID	D	303	-	-	1/24/93/93	0/4/4/4
39	KC1	O	312	-	-	3/15/71/71	-
30	PQN	a	832	-	-	6/23/43/43	0/2/2/2
29	CLA	D	314	-	1/1/11/20	6/18/94/115	-
29	CLA	b	719	-	1/1/12/20	10/21/97/115	-
31	LHG	a	833	-	-	7/52/52/53	-
29	CLA	L	307	39	1/1/12/20	12/21/97/115	-
32	BCR	f	801	-	-	5/29/63/63	0/2/2/2
39	KC1	N	312	23	-	6/15/71/71	-
29	CLA	J	305	-	1/1/11/20	4/17/93/115	-
29	CLA	Q	307	-	1/1/11/20	2/18/94/115	-
39	KC1	T	312	-	-	4/15/71/71	-
29	CLA	b	705	-	1/1/15/20	11/39/115/115	-
29	CLA	J	309	17	1/1/11/20	5/17/93/115	-
39	KC1	A	213	-	-	5/15/71/71	-
29	CLA	B	308	-	1/1/15/20	12/39/115/115	-
29	CLA	B	306	21	1/1/11/20	5/20/96/115	-
29	CLA	O	316	-	1/1/10/20	4/10/86/115	-
29	CLA	T	313	-	1/1/11/20	5/17/93/115	-
29	CLA	E	309	-	1/1/11/20	8/17/93/115	-
36	DD6	m	101	-	-	0/26/80/80	0/3/3/3
38	UIX	L	302	-	-	2/31/87/87	0/3/3/3
36	DD6	B	305	-	-	2/26/80/80	0/3/3/3
36	DD6	E	303	-	-	1/26/80/80	0/3/3/3
36	DD6	K	202	-	-	8/26/80/80	0/3/3/3
36	DD6	A	201	-	-	3/26/80/80	0/3/3/3
34	LMG	E	316	-	-	10/27/47/70	0/1/1/1
29	CLA	l	503	10	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	D	307	-	-	4/24/93/93	0/4/4/4
29	CLA	P	215	-	1/1/11/20	8/18/94/115	-
29	CLA	A	211	-	1/1/13/20	5/27/103/115	-
29	CLA	M	306	-	1/1/12/20	5/25/101/115	-
29	CLA	K	213	-	1/1/11/20	7/19/95/115	-
29	CLA	a	831	-	1/1/15/20	11/39/115/115	-
37	PID	H	306	-	-	4/24/93/93	0/4/4/4
35	DGD	G	320	-	-	9/34/74/95	0/2/2/2
37	PID	D	302	-	-	1/24/93/93	0/4/4/4
29	CLA	b	709	-	1/1/14/20	16/33/109/115	-
29	CLA	l	504	-	1/1/15/20	10/39/115/115	-
29	CLA	M	311	-	1/1/11/20	6/17/93/115	-
29	CLA	G	314	-	1/1/14/20	9/33/109/115	-
39	KC1	K	215	-	-	7/15/71/71	-
39	KC1	B	313	21	-	7/15/71/71	-
29	CLA	E	315	-	1/1/13/20	7/30/106/115	-
39	KC1	I	215	14	-	11/15/71/71	-

All (2538) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	307	DD6	C30-C31	-9.31	1.24	1.42
36	I	203	DD6	C30-C31	-9.07	1.24	1.42
36	G	305	DD6	C30-C31	-8.84	1.25	1.42
36	K	202	DD6	C30-C31	-8.83	1.25	1.42
36	J	303	DD6	C30-C31	-8.78	1.25	1.42
36	J	302	DD6	C30-C31	-8.76	1.25	1.42
36	E	302	DD6	C30-C31	-8.73	1.25	1.42
36	K	221	DD6	C30-C31	-8.71	1.25	1.42
36	h	202	DD6	C30-C31	-8.71	1.25	1.42
36	F	301	DD6	C30-C31	-8.71	1.25	1.42
36	I	204	DD6	C30-C31	-8.70	1.25	1.42
36	G	306	DD6	C30-C31	-8.67	1.25	1.42
36	M	302	DD6	C30-C31	-8.66	1.25	1.42
36	K	204	DD6	C30-C31	-8.65	1.25	1.42
36	M	303	DD6	C30-C31	-8.64	1.25	1.42
36	B	319	DD6	C30-C31	-8.64	1.25	1.42
36	L	303	DD6	C30-C31	-8.63	1.25	1.42
36	C	303	DD6	C30-C31	-8.62	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	303	DD6	C30-C31	-8.60	1.25	1.42
36	K	206	DD6	C30-C31	-8.60	1.25	1.42
36	L	305	DD6	C30-C31	-8.60	1.25	1.42
36	I	205	DD6	C30-C31	-8.57	1.25	1.42
36	K	205	DD6	C30-C31	-8.57	1.25	1.42
36	K	203	DD6	C30-C31	-8.55	1.25	1.42
36	m	101	DD6	C30-C31	-8.53	1.25	1.42
36	B	302	DD6	C30-C31	-8.53	1.25	1.42
36	D	304	DD6	C30-C31	-8.53	1.25	1.42
36	M	304	DD6	C30-C31	-8.51	1.25	1.42
36	B	303	DD6	C30-C31	-8.51	1.26	1.42
36	J	301	DD6	C30-C31	-8.50	1.26	1.42
36	G	308	DD6	C30-C31	-8.50	1.26	1.42
36	O	303	DD6	C30-C31	-8.48	1.26	1.42
36	B	305	DD6	C30-C31	-8.47	1.26	1.42
36	I	206	DD6	C30-C31	-8.45	1.26	1.42
36	A	204	DD6	C30-C31	-8.44	1.26	1.42
36	A	201	DD6	C30-C31	-8.44	1.26	1.42
36	D	301	DD6	C30-C31	-8.43	1.26	1.42
36	E	303	DD6	C30-C31	-8.42	1.26	1.42
36	L	301	DD6	C30-C31	-8.39	1.26	1.42
36	M	301	DD6	C30-C31	-8.38	1.26	1.42
36	B	301	DD6	C30-C31	-8.36	1.26	1.42
36	P	204	DD6	C30-C31	-8.34	1.26	1.42
36	I	202	DD6	C30-C31	-8.34	1.26	1.42
36	Q	302	DD6	C30-C31	-8.32	1.26	1.42
36	L	304	DD6	C30-C31	-8.30	1.26	1.42
36	T	303	DD6	C30-C31	-8.29	1.26	1.42
36	N	303	DD6	C30-C31	-8.21	1.26	1.42
36	A	202	DD6	C30-C31	-8.21	1.26	1.42
36	H	303	DD6	C30-C31	-8.13	1.26	1.42
30	b	727	PQN	C3-C2	7.47	1.48	1.35
30	a	832	PQN	C3-C2	7.41	1.48	1.35
36	I	205	DD6	C19-C20	6.91	1.61	1.52
37	F	304	PID	O1-C1	-6.39	1.37	1.46
37	D	303	PID	C13-C14	-6.05	1.34	1.45
37	N	302	PID	C13-C14	-5.94	1.34	1.45
37	G	303	PID	C13-C14	-5.94	1.34	1.45
37	P	203	PID	C13-C14	-5.94	1.34	1.45
37	H	305	PID	C13-C14	-5.92	1.34	1.45
37	D	306	PID	C13-C14	-5.89	1.34	1.45
37	F	304	PID	C13-C14	-5.89	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	O	302	PID	C13-C14	-5.89	1.34	1.45
37	h	204	PID	C13-C14	-5.87	1.34	1.45
37	G	310	PID	C13-C14	-5.86	1.34	1.45
37	H	302	PID	C13-C14	-5.84	1.34	1.45
37	T	317	PID	C13-C14	-5.82	1.34	1.45
37	N	305	PID	C13-C14	-5.80	1.34	1.45
37	F	306	PID	C13-C14	-5.79	1.34	1.45
37	Q	303	PID	C13-C14	-5.74	1.34	1.45
37	C	305	PID	C13-C14	-5.74	1.34	1.45
37	G	309	PID	C13-C14	-5.72	1.34	1.45
37	j	101	PID	C13-C14	-5.68	1.35	1.45
37	N	301	PID	C13-C14	-5.67	1.35	1.45
37	T	307	PID	C13-C14	-5.64	1.35	1.45
37	T	301	PID	C13-C14	-5.64	1.35	1.45
37	Q	301	PID	C13-C14	-5.64	1.35	1.45
37	T	302	PID	C13-C14	-5.64	1.35	1.45
37	C	304	PID	C13-C14	-5.63	1.35	1.45
37	F	302	PID	C13-C14	-5.63	1.35	1.45
37	D	302	PID	C13-C14	-5.63	1.35	1.45
37	T	305	PID	C13-C14	-5.62	1.35	1.45
37	O	307	PID	C13-C14	-5.62	1.35	1.45
37	E	301	PID	C13-C14	-5.61	1.35	1.45
37	C	301	PID	C13-C14	-5.60	1.35	1.45
37	Q	304	PID	C13-C14	-5.60	1.35	1.45
37	Q	306	PID	C13-C14	-5.59	1.35	1.45
37	O	304	PID	C13-C14	-5.59	1.35	1.45
37	D	305	PID	C13-C14	-5.58	1.35	1.45
37	N	304	PID	C13-C14	-5.55	1.35	1.45
37	H	301	PID	C13-C14	-5.54	1.35	1.45
37	C	307	PID	C13-C14	-5.53	1.35	1.45
37	O	305	PID	C13-C14	-5.51	1.35	1.45
37	D	307	PID	C13-C14	-5.51	1.35	1.45
37	C	302	PID	C13-C14	-5.51	1.35	1.45
37	N	307	PID	C13-C14	-5.49	1.35	1.45
37	P	205	PID	C13-C14	-5.46	1.35	1.45
37	P	202	PID	C13-C14	-5.45	1.35	1.45
37	O	301	PID	C13-C14	-5.42	1.35	1.45
37	H	304	PID	C13-C14	-5.40	1.35	1.45
36	G	307	DD6	C21-C20	-5.40	1.43	1.51
39	G	315	KC1	MG-ND	-5.39	1.95	2.05
37	T	304	PID	C13-C14	-5.39	1.35	1.45
37	P	206	PID	C13-C14	-5.35	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	H	306	PID	C13-C14	-5.31	1.35	1.45
37	P	208	PID	C13-C14	-5.28	1.35	1.45
36	G	307	DD6	C19-C20	5.23	1.59	1.52
39	Q	311	KC1	MG-ND	-5.22	1.95	2.05
39	O	312	KC1	MG-ND	-5.20	1.95	2.05
39	T	310	KC1	MG-ND	-5.15	1.95	2.05
39	P	213	KC1	MG-ND	-5.14	1.95	2.05
39	O	315	KC1	MG-ND	-5.13	1.95	2.05
39	C	315	KC1	MG-ND	-5.11	1.95	2.05
39	M	305	KC1	MG-ND	-5.10	1.95	2.05
39	E	307	KC1	MG-ND	-5.08	1.95	2.05
39	C	310	KC1	MG-ND	-5.08	1.95	2.05
39	T	315	KC1	MG-ND	-5.07	1.95	2.05
39	A	205	KC1	MG-ND	-5.06	1.95	2.05
39	D	315	KC1	MG-ND	-5.05	1.95	2.05
39	K	215	KC1	MG-ND	-5.05	1.95	2.05
39	F	309	KC1	MG-ND	-5.05	1.95	2.05
39	O	310	KC1	MG-ND	-5.05	1.95	2.05
39	J	312	KC1	MG-ND	-5.04	1.95	2.05
39	L	314	KC1	MG-ND	-5.04	1.95	2.05
39	N	310	KC1	MG-ND	-5.04	1.95	2.05
39	E	312	KC1	MG-ND	-5.03	1.95	2.05
39	N	315	KC1	MG-ND	-5.03	1.95	2.05
39	Q	314	KC1	MG-ND	-5.02	1.95	2.05
39	C	312	KC1	MG-ND	-5.02	1.95	2.05
39	D	310	KC1	MG-ND	-5.01	1.95	2.05
39	T	312	KC1	MG-ND	-5.01	1.95	2.05
39	L	306	KC1	MG-ND	-5.01	1.95	2.05
39	A	213	KC1	MG-ND	-5.01	1.95	2.05
39	H	314	KC1	MG-ND	-5.00	1.95	2.05
39	F	314	KC1	MG-ND	-5.00	1.95	2.05
39	M	312	KC1	MG-ND	-4.99	1.95	2.05
39	B	313	KC1	MG-ND	-4.98	1.95	2.05
39	N	312	KC1	MG-ND	-4.97	1.95	2.05
39	I	215	KC1	MG-ND	-4.97	1.95	2.05
39	H	311	KC1	MG-ND	-4.97	1.95	2.05
39	Q	309	KC1	MG-ND	-4.97	1.95	2.05
39	P	216	KC1	MG-ND	-4.97	1.95	2.05
39	H	309	KC1	MG-ND	-4.96	1.95	2.05
39	G	318	KC1	MG-ND	-4.95	1.96	2.05
39	G	315	KC1	MG-NB	-4.93	1.96	2.05
39	P	211	KC1	MG-ND	-4.93	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	B	304	UIX	O2-C27	4.92	1.46	1.35
38	T	306	UIX	O2-C27	4.88	1.46	1.35
39	Q	311	KC1	MG-NB	-4.86	1.96	2.05
38	N	306	UIX	O2-C27	4.84	1.45	1.35
38	C	306	UIX	O2-C27	4.84	1.45	1.35
38	P	207	UIX	O2-C27	4.84	1.45	1.35
38	Q	305	UIX	O2-C27	4.83	1.45	1.35
38	L	302	UIX	O2-C27	4.83	1.45	1.35
38	E	304	UIX	O2-C27	4.81	1.45	1.35
39	P	213	KC1	MG-NB	-4.80	1.96	2.05
39	C	312	KC1	MG-NB	-4.79	1.96	2.05
39	C	310	KC1	MG-NB	-4.79	1.96	2.05
30	b	727	PQN	C10-C5	4.79	1.48	1.40
38	O	306	UIX	O2-C27	4.79	1.45	1.35
39	T	310	KC1	MG-NB	-4.78	1.96	2.05
39	C	315	KC1	MG-NB	-4.78	1.96	2.05
39	O	312	KC1	MG-NB	-4.77	1.96	2.05
39	Q	314	KC1	MG-NB	-4.76	1.96	2.05
39	D	310	KC1	MG-NB	-4.76	1.96	2.05
39	K	215	KC1	MG-NB	-4.76	1.96	2.05
39	E	312	KC1	MG-NB	-4.73	1.96	2.05
38	A	203	UIX	O2-C27	4.72	1.45	1.35
38	F	305	UIX	O2-C27	4.72	1.45	1.35
39	D	315	KC1	MG-NB	-4.72	1.96	2.05
39	H	311	KC1	MG-NB	-4.72	1.96	2.05
39	Q	309	KC1	MG-NB	-4.72	1.96	2.05
39	M	312	KC1	MG-NB	-4.71	1.96	2.05
39	N	315	KC1	MG-NB	-4.70	1.96	2.05
39	G	318	KC1	MG-NB	-4.70	1.96	2.05
39	H	314	KC1	MG-NB	-4.70	1.96	2.05
39	O	315	KC1	MG-NB	-4.70	1.96	2.05
39	N	310	KC1	MG-NB	-4.70	1.96	2.05
39	E	307	KC1	MG-NB	-4.70	1.96	2.05
39	T	312	KC1	MG-NB	-4.69	1.96	2.05
39	M	305	KC1	MG-NB	-4.68	1.96	2.05
39	F	314	KC1	MG-NB	-4.68	1.96	2.05
30	a	832	PQN	C10-C5	4.67	1.48	1.40
39	J	312	KC1	MG-NB	-4.67	1.96	2.05
39	N	312	KC1	MG-NB	-4.66	1.96	2.05
39	O	310	KC1	MG-NB	-4.65	1.96	2.05
39	F	309	KC1	MG-NB	-4.65	1.96	2.05
39	H	309	KC1	MG-NB	-4.65	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	L	306	KC1	MG-NB	-4.65	1.96	2.05
39	I	215	KC1	MG-NB	-4.64	1.96	2.05
39	B	313	KC1	MG-NB	-4.64	1.96	2.05
39	A	213	KC1	MG-NB	-4.63	1.96	2.05
39	A	205	KC1	MG-NB	-4.62	1.96	2.05
39	T	315	KC1	MG-NB	-4.62	1.96	2.05
39	P	216	KC1	MG-NB	-4.62	1.96	2.05
39	P	211	KC1	MG-NB	-4.62	1.96	2.05
39	L	314	KC1	MG-NB	-4.58	1.96	2.05
36	I	203	DD6	C19-C20	4.56	1.58	1.52
38	J	304	UIX	O2-C27	4.45	1.45	1.35
38	A	203	UIX	C25-C20	-4.32	1.25	1.30
38	E	304	UIX	C25-C20	-4.30	1.25	1.30
38	J	304	UIX	C25-C20	-4.29	1.25	1.30
35	b	733	DGD	O2G-C1B	4.27	1.46	1.34
35	B	318	DGD	O1G-C1A	4.27	1.45	1.33
35	j	106	DGD	O1G-C1A	4.23	1.45	1.33
35	G	320	DGD	O1G-C1A	4.23	1.45	1.33
35	m	102	DGD	O1G-C1A	4.19	1.45	1.33
35	j	105	DGD	O1G-C1A	4.17	1.45	1.33
35	b	733	DGD	O1G-C1A	4.16	1.45	1.33
35	h	203	DGD	O1G-C1A	4.12	1.45	1.33
38	B	304	UIX	C25-C20	-4.10	1.25	1.30
35	G	320	DGD	O2G-C1B	4.10	1.45	1.34
35	j	106	DGD	O2G-C1B	4.08	1.45	1.34
38	P	207	UIX	C25-C20	-4.07	1.25	1.30
35	j	103	DGD	O1G-C1A	4.07	1.45	1.33
38	N	306	UIX	C25-C20	-4.06	1.25	1.30
35	j	105	DGD	O2G-C1B	4.03	1.45	1.34
35	h	203	DGD	O2G-C1B	4.02	1.45	1.34
38	F	305	UIX	C25-C20	-4.01	1.25	1.30
35	B	318	DGD	O2G-C1B	4.00	1.45	1.34
36	I	205	DD6	C21-C20	-3.99	1.45	1.51
38	Q	305	UIX	C25-C20	-3.95	1.26	1.30
38	C	306	UIX	C25-C20	-3.94	1.26	1.30
38	L	302	UIX	C25-C20	-3.91	1.26	1.30
35	m	102	DGD	O2G-C1B	3.90	1.45	1.34
35	j	103	DGD	O2G-C1B	3.88	1.45	1.34
38	O	306	UIX	C25-C20	-3.88	1.26	1.30
38	T	306	UIX	C25-C20	-3.87	1.26	1.30
38	A	203	UIX	C25-C28	-3.81	1.25	1.31
38	E	304	UIX	C25-C28	-3.77	1.25	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	J	304	UIX	C25-C28	-3.75	1.25	1.31
38	B	304	UIX	C25-C28	-3.72	1.25	1.31
29	P	217	CLA	C1D-ND	3.68	1.42	1.37
38	O	306	UIX	C25-C28	-3.68	1.25	1.31
38	F	305	UIX	C25-C28	-3.67	1.25	1.31
38	T	306	UIX	C25-C28	-3.63	1.26	1.31
29	O	314	CLA	C1D-ND	3.63	1.42	1.37
38	P	207	UIX	C25-C28	-3.63	1.26	1.31
29	P	209	CLA	C1D-ND	3.62	1.42	1.37
29	O	316	CLA	C1D-ND	3.61	1.42	1.37
29	F	315	CLA	C1D-ND	3.61	1.42	1.37
29	E	314	CLA	C1D-ND	3.60	1.42	1.37
38	L	302	UIX	C25-C28	-3.59	1.26	1.31
38	N	306	UIX	C25-C28	-3.59	1.26	1.31
29	T	316	CLA	C1D-ND	3.59	1.42	1.37
29	O	308	CLA	C1D-ND	3.58	1.42	1.37
29	O	311	CLA	C1D-ND	3.58	1.42	1.37
29	M	309	CLA	C1D-ND	3.58	1.42	1.37
36	G	307	DD6	C36-C31	-3.58	1.31	1.35
29	P	215	CLA	C1D-ND	3.58	1.42	1.37
29	D	316	CLA	C1D-ND	3.58	1.42	1.37
29	E	313	CLA	C1D-ND	3.57	1.42	1.37
29	N	316	CLA	C1D-ND	3.57	1.42	1.37
29	O	309	CLA	C1D-ND	3.57	1.42	1.37
29	H	315	CLA	C1D-ND	3.56	1.42	1.37
36	O	303	DD6	C19-C20	3.56	1.57	1.52
29	N	308	CLA	C1D-ND	3.56	1.42	1.37
29	P	212	CLA	C1D-ND	3.55	1.42	1.37
38	Q	305	UIX	C25-C28	-3.54	1.26	1.31
29	L	316	CLA	C1D-ND	3.53	1.42	1.37
29	T	313	CLA	C1D-ND	3.53	1.42	1.37
29	J	308	CLA	C1D-ND	3.53	1.42	1.37
29	G	319	CLA	C1D-ND	3.53	1.42	1.37
29	J	313	CLA	C1D-ND	3.53	1.42	1.37
29	a	817	CLA	C1D-ND	3.52	1.42	1.37
29	a	819	CLA	C1D-ND	3.52	1.42	1.37
29	A	210	CLA	C1D-ND	3.51	1.42	1.37
29	E	310	CLA	C1D-ND	3.51	1.42	1.37
29	a	813	CLA	C1D-ND	3.51	1.42	1.37
29	b	721	CLA	C1D-ND	3.51	1.42	1.37
29	H	307	CLA	C1D-ND	3.51	1.42	1.37
38	C	306	UIX	C25-C28	-3.50	1.26	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	312	CLA	C1D-ND	3.50	1.42	1.37
29	C	316	CLA	C1D-ND	3.50	1.42	1.37
29	P	214	CLA	C1D-ND	3.50	1.42	1.37
29	J	305	CLA	C1D-ND	3.50	1.42	1.37
29	M	314	CLA	C1D-ND	3.50	1.42	1.37
29	F	316	CLA	C1D-ND	3.50	1.42	1.37
29	M	313	CLA	C1D-ND	3.49	1.42	1.37
29	E	305	CLA	C1D-ND	3.49	1.42	1.37
29	A	206	CLA	C1D-ND	3.49	1.42	1.37
29	H	312	CLA	C1D-ND	3.49	1.42	1.37
29	b	715	CLA	C1D-ND	3.49	1.42	1.37
29	B	306	CLA	C1D-ND	3.48	1.42	1.37
29	T	308	CLA	C1D-ND	3.48	1.42	1.37
29	N	311	CLA	C1D-ND	3.47	1.42	1.37
29	E	309	CLA	C1D-ND	3.47	1.42	1.37
29	a	821	CLA	C1D-ND	3.47	1.42	1.37
29	G	317	CLA	C1D-ND	3.47	1.42	1.37
29	H	310	CLA	C1D-ND	3.47	1.42	1.37
29	l	502	CLA	C1D-ND	3.47	1.42	1.37
29	M	306	CLA	C1D-ND	3.46	1.42	1.37
29	L	311	CLA	C1D-ND	3.46	1.42	1.37
29	B	307	CLA	C1D-ND	3.46	1.42	1.37
29	b	713	CLA	C1D-ND	3.46	1.42	1.37
29	D	309	CLA	C1D-ND	3.46	1.42	1.37
29	L	315	CLA	C1D-ND	3.46	1.42	1.37
29	Q	307	CLA	C1D-ND	3.45	1.42	1.37
29	M	308	CLA	C1D-ND	3.45	1.42	1.37
29	a	804	CLA	C1D-ND	3.45	1.42	1.37
29	P	210	CLA	C1D-ND	3.44	1.42	1.37
29	T	311	CLA	C1D-ND	3.44	1.42	1.37
29	N	314	CLA	C1D-ND	3.44	1.42	1.37
29	B	312	CLA	C1D-ND	3.44	1.42	1.37
29	E	315	CLA	C1D-ND	3.44	1.42	1.37
36	I	205	DD6	O1-C20	-3.44	1.41	1.46
29	C	311	CLA	C1D-ND	3.44	1.42	1.37
29	F	312	CLA	C1D-ND	3.43	1.42	1.37
29	b	720	CLA	C1D-ND	3.43	1.42	1.37
29	Q	315	CLA	C1D-ND	3.43	1.42	1.37
29	M	311	CLA	C1D-ND	3.43	1.42	1.37
29	l	508	CLA	C1D-ND	3.43	1.42	1.37
29	K	207	CLA	C1D-ND	3.43	1.42	1.37
29	l	505	CLA	C1D-ND	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	212	CLA	C1D-ND	3.42	1.42	1.37
29	a	816	CLA	C1D-ND	3.42	1.42	1.37
29	C	309	CLA	C1D-ND	3.42	1.42	1.37
29	M	307	CLA	C1D-ND	3.42	1.42	1.37
29	L	308	CLA	C1D-ND	3.42	1.42	1.37
29	D	308	CLA	C1D-ND	3.42	1.42	1.37
29	a	811	CLA	C1D-ND	3.41	1.42	1.37
29	I	208	CLA	C1D-ND	3.41	1.42	1.37
29	L	310	CLA	C1D-ND	3.41	1.42	1.37
29	C	314	CLA	C1D-ND	3.41	1.42	1.37
29	h	201	CLA	C1D-ND	3.41	1.42	1.37
29	a	829	CLA	C1D-ND	3.41	1.42	1.37
29	C	308	CLA	C1D-ND	3.41	1.42	1.37
29	I	201	CLA	C1D-ND	3.41	1.42	1.37
29	D	314	CLA	C1D-ND	3.41	1.42	1.37
29	j	104	CLA	C1D-ND	3.41	1.42	1.37
29	T	309	CLA	C1D-ND	3.40	1.42	1.37
29	B	315	CLA	C1D-ND	3.40	1.42	1.37
29	F	308	CLA	C1D-ND	3.40	1.42	1.37
29	a	809	CLA	C1D-ND	3.40	1.42	1.37
29	M	315	CLA	C1D-ND	3.40	1.42	1.37
29	L	313	CLA	C1D-ND	3.40	1.42	1.37
29	M	310	CLA	C1D-ND	3.40	1.42	1.37
29	G	316	CLA	C1D-ND	3.40	1.42	1.37
29	K	216	CLA	C1D-ND	3.40	1.42	1.37
29	T	314	CLA	C1D-ND	3.39	1.42	1.37
29	F	313	CLA	C1D-ND	3.39	1.42	1.37
29	B	309	CLA	C1D-ND	3.39	1.42	1.37
29	D	311	CLA	C1D-ND	3.39	1.42	1.37
29	a	818	CLA	C1D-ND	3.39	1.42	1.37
29	Q	308	CLA	C1D-ND	3.39	1.42	1.37
29	a	803	CLA	C1D-ND	3.39	1.42	1.37
29	F	311	CLA	C1D-ND	3.39	1.42	1.37
29	J	310	CLA	C1D-ND	3.39	1.42	1.37
29	Q	313	CLA	C1D-ND	3.39	1.42	1.37
29	l	510	CLA	C1D-ND	3.38	1.42	1.37
29	J	309	CLA	C1D-ND	3.38	1.42	1.37
29	H	308	CLA	C1D-ND	3.38	1.42	1.37
29	I	216	CLA	C1D-ND	3.38	1.42	1.37
29	f	803	CLA	C1D-ND	3.38	1.42	1.37
29	K	210	CLA	C1D-ND	3.38	1.42	1.37
29	K	214	CLA	C1D-ND	3.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	217	CLA	C1D-ND	3.37	1.42	1.37
29	b	719	CLA	C1D-ND	3.37	1.42	1.37
29	a	822	CLA	C1D-ND	3.37	1.42	1.37
29	a	826	CLA	C1D-ND	3.37	1.42	1.37
29	F	307	CLA	C1D-ND	3.36	1.42	1.37
29	b	712	CLA	C1D-ND	3.36	1.42	1.37
29	L	309	CLA	C1D-ND	3.36	1.42	1.37
29	L	317	CLA	C1D-ND	3.36	1.42	1.37
29	Q	310	CLA	C1D-ND	3.36	1.42	1.37
29	b	706	CLA	C1D-ND	3.36	1.42	1.37
29	I	217	CLA	C1D-ND	3.36	1.42	1.37
29	N	309	CLA	C1D-ND	3.36	1.42	1.37
29	Q	312	CLA	C1D-ND	3.36	1.42	1.37
29	b	702	CLA	C1D-ND	3.35	1.42	1.37
29	I	209	CLA	C1D-ND	3.35	1.42	1.37
29	A	211	CLA	C1D-ND	3.35	1.42	1.37
29	A	209	CLA	C1D-ND	3.35	1.42	1.37
29	J	307	CLA	C1D-ND	3.35	1.42	1.37
29	K	213	CLA	C1D-ND	3.35	1.42	1.37
29	I	211	CLA	C1D-ND	3.35	1.42	1.37
29	a	815	CLA	C1D-ND	3.34	1.42	1.37
29	B	308	CLA	C1D-ND	3.34	1.42	1.37
29	A	207	CLA	C1D-ND	3.34	1.42	1.37
29	a	814	CLA	C1D-ND	3.34	1.42	1.37
29	a	823	CLA	C1D-ND	3.34	1.42	1.37
29	E	311	CLA	C1D-ND	3.34	1.42	1.37
29	l	501	CLA	C1D-ND	3.34	1.42	1.37
29	A	208	CLA	C1D-ND	3.34	1.42	1.37
29	b	724	CLA	C1D-ND	3.34	1.42	1.37
29	B	316	CLA	C1D-ND	3.34	1.42	1.37
29	G	301	CLA	C1D-ND	3.34	1.42	1.37
29	a	807	CLA	C1D-ND	3.33	1.42	1.37
29	b	716	CLA	C1D-ND	3.33	1.42	1.37
29	L	307	CLA	C1D-ND	3.33	1.42	1.37
29	a	830	CLA	C1D-ND	3.33	1.42	1.37
29	a	828	CLA	C1D-ND	3.33	1.42	1.37
29	A	216	CLA	C1D-ND	3.33	1.42	1.37
29	K	209	CLA	C1D-ND	3.33	1.42	1.37
29	b	722	CLA	C1D-ND	3.33	1.42	1.37
29	b	709	CLA	C1D-ND	3.33	1.42	1.37
29	B	311	CLA	C1D-ND	3.32	1.42	1.37
29	i	201	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	211	CLA	C1D-ND	3.32	1.42	1.37
29	A	215	CLA	C1D-ND	3.32	1.42	1.37
29	G	314	CLA	C1D-ND	3.32	1.42	1.37
29	a	831	CLA	C1D-ND	3.32	1.42	1.37
29	b	707	CLA	C1D-ND	3.32	1.42	1.37
29	i	202	CLA	C1D-ND	3.31	1.42	1.37
29	a	808	CLA	C1D-ND	3.31	1.42	1.37
29	a	827	CLA	C1D-ND	3.31	1.42	1.37
29	B	314	CLA	C1D-ND	3.30	1.42	1.37
29	G	312	CLA	C1D-ND	3.30	1.42	1.37
29	I	213	CLA	C1D-ND	3.30	1.42	1.37
29	G	311	CLA	C1D-ND	3.30	1.42	1.37
29	G	302	CLA	C1D-ND	3.30	1.42	1.37
29	b	736	CLA	C1D-ND	3.30	1.42	1.37
29	l	509	CLA	C1D-ND	3.29	1.42	1.37
29	I	207	CLA	C1D-ND	3.29	1.42	1.37
29	J	311	CLA	C1D-ND	3.29	1.42	1.37
29	I	212	CLA	C1D-ND	3.29	1.42	1.37
29	b	701	CLA	C1D-ND	3.29	1.42	1.37
29	H	313	CLA	C1D-ND	3.29	1.42	1.37
29	b	710	CLA	C1D-ND	3.29	1.42	1.37
29	f	802	CLA	C1D-ND	3.29	1.42	1.37
29	C	313	CLA	C1D-ND	3.29	1.42	1.37
29	b	708	CLA	C1D-ND	3.28	1.42	1.37
29	f	805	CLA	C1D-ND	3.28	1.42	1.37
29	a	825	CLA	C1D-ND	3.28	1.42	1.37
29	a	805	CLA	C1D-ND	3.27	1.42	1.37
29	a	820	CLA	C1D-ND	3.27	1.42	1.37
29	b	726	CLA	C1D-ND	3.27	1.42	1.37
29	E	308	CLA	C1D-ND	3.27	1.42	1.37
29	b	725	CLA	C1D-ND	3.27	1.42	1.37
29	i	203	CLA	C1D-ND	3.27	1.42	1.37
29	O	313	CLA	C1D-ND	3.26	1.42	1.37
29	L	312	CLA	C1D-ND	3.26	1.42	1.37
29	A	212	CLA	C1D-ND	3.26	1.42	1.37
29	K	208	CLA	C1D-ND	3.26	1.42	1.37
29	D	313	CLA	C1D-ND	3.26	1.42	1.37
29	G	313	CLA	C1D-ND	3.25	1.42	1.37
29	b	723	CLA	C1D-ND	3.25	1.42	1.37
29	b	731	CLA	C1D-ND	3.25	1.42	1.37
29	K	218	CLA	C1D-ND	3.25	1.42	1.37
29	a	810	CLA	C1D-ND	3.25	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	204	DD6	O1-C20	-3.24	1.42	1.46
29	a	812	CLA	C1D-ND	3.23	1.42	1.37
29	A	218	CLA	C1D-ND	3.23	1.42	1.37
29	I	210	CLA	C1D-ND	3.23	1.42	1.37
36	G	307	DD6	C28-C27	-3.22	1.48	1.50
29	b	703	CLA	C1D-ND	3.22	1.42	1.37
29	P	215	CLA	C4B-NB	3.22	1.42	1.37
29	a	837	CLA	C1D-ND	3.21	1.42	1.37
29	b	711	CLA	C1D-ND	3.21	1.42	1.37
29	a	802	CLA	C1D-ND	3.21	1.42	1.37
29	a	806	CLA	C1D-ND	3.21	1.42	1.37
29	G	304	CLA	C1D-ND	3.19	1.42	1.37
29	L	316	CLA	C4B-NB	3.18	1.42	1.37
29	I	214	CLA	C1D-ND	3.18	1.42	1.37
29	b	714	CLA	C1D-ND	3.18	1.42	1.37
38	T	306	UIX	O-C1	-3.17	1.42	1.46
29	l	503	CLA	C1D-ND	3.17	1.42	1.37
38	P	207	UIX	O-C1	-3.17	1.42	1.46
29	J	306	CLA	C1D-ND	3.17	1.42	1.37
29	B	310	CLA	C1D-ND	3.15	1.42	1.37
29	l	504	CLA	C1D-ND	3.15	1.42	1.37
29	L	315	CLA	C4B-NB	3.14	1.42	1.37
29	O	308	CLA	C4B-NB	3.14	1.42	1.37
29	a	804	CLA	C4B-NB	3.13	1.42	1.37
29	b	704	CLA	C1D-ND	3.13	1.42	1.37
29	H	313	CLA	C4B-NB	3.12	1.42	1.37
29	P	214	CLA	C4B-NB	3.12	1.42	1.37
29	A	217	CLA	C1D-ND	3.12	1.42	1.37
29	b	717	CLA	C1D-ND	3.12	1.42	1.37
29	b	718	CLA	C1D-ND	3.11	1.41	1.37
29	E	309	CLA	C4B-NB	3.11	1.41	1.37
29	a	824	CLA	C1D-ND	3.10	1.41	1.37
29	O	309	CLA	C4B-NB	3.10	1.41	1.37
29	l	510	CLA	C4B-NB	3.10	1.41	1.37
29	O	314	CLA	C4B-NB	3.10	1.41	1.37
29	C	314	CLA	C4B-NB	3.10	1.41	1.37
29	P	209	CLA	C4B-NB	3.10	1.41	1.37
29	O	316	CLA	C4B-NB	3.09	1.41	1.37
29	H	310	CLA	C4B-NB	3.09	1.41	1.37
29	F	310	CLA	C1D-ND	3.09	1.41	1.37
29	a	817	CLA	C4B-NB	3.08	1.41	1.37
29	N	308	CLA	C4B-NB	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	214	CLA	C1D-ND	3.08	1.41	1.37
29	T	308	CLA	C4B-NB	3.07	1.41	1.37
29	H	315	CLA	C4B-NB	3.06	1.41	1.37
29	N	309	CLA	C4B-NB	3.06	1.41	1.37
29	a	813	CLA	C4B-NB	3.06	1.41	1.37
29	a	801	CLA	C1D-ND	3.06	1.41	1.37
29	N	316	CLA	C4B-NB	3.06	1.41	1.37
29	E	306	CLA	C1D-ND	3.05	1.41	1.37
38	C	306	UIX	O-C1	-3.05	1.42	1.46
29	K	218	CLA	C4B-NB	3.05	1.41	1.37
29	a	811	CLA	C4B-NB	3.05	1.41	1.37
29	b	713	CLA	C4B-NB	3.05	1.41	1.37
29	E	315	CLA	C4B-NB	3.05	1.41	1.37
29	N	313	CLA	C1D-ND	3.04	1.41	1.37
29	a	818	CLA	C4B-NB	3.04	1.41	1.37
29	Q	307	CLA	C4B-NB	3.04	1.41	1.37
29	K	212	CLA	C4B-NB	3.04	1.41	1.37
29	T	316	CLA	C4B-NB	3.04	1.41	1.37
29	H	307	CLA	C4B-NB	3.04	1.41	1.37
29	D	308	CLA	C4B-NB	3.03	1.41	1.37
29	b	720	CLA	C4B-NB	3.03	1.41	1.37
29	b	705	CLA	C1D-ND	3.03	1.41	1.37
29	I	217	CLA	C4B-NB	3.03	1.41	1.37
29	T	313	CLA	C4B-NB	3.03	1.41	1.37
29	F	315	CLA	C4B-NB	3.03	1.41	1.37
29	E	313	CLA	C4B-NB	3.02	1.41	1.37
29	F	307	CLA	C4B-NB	3.02	1.41	1.37
29	K	208	CLA	C4B-NB	3.02	1.41	1.37
29	T	314	CLA	C4B-NB	3.02	1.41	1.37
29	P	212	CLA	C4B-NB	3.02	1.41	1.37
29	J	305	CLA	C4B-NB	3.01	1.41	1.37
29	D	316	CLA	C4B-NB	3.01	1.41	1.37
29	M	313	CLA	C4B-NB	3.01	1.41	1.37
29	K	217	CLA	C4B-NB	3.01	1.41	1.37
29	a	828	CLA	C4B-NB	3.01	1.41	1.37
29	Q	315	CLA	C4B-NB	3.01	1.41	1.37
29	C	308	CLA	C4B-NB	3.01	1.41	1.37
29	l	509	CLA	C4B-NB	3.00	1.41	1.37
29	L	311	CLA	C4B-NB	3.00	1.41	1.37
29	N	313	CLA	C4B-NB	3.00	1.41	1.37
29	O	311	CLA	C4B-NB	2.99	1.41	1.37
39	K	215	KC1	C4B-NB	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	708	CLA	C4B-NB	2.99	1.41	1.37
29	M	311	CLA	C4B-NB	2.99	1.41	1.37
29	A	214	CLA	C4B-NB	2.99	1.41	1.37
29	a	821	CLA	C4B-NB	2.98	1.41	1.37
29	B	307	CLA	C4B-NB	2.98	1.41	1.37
29	Q	308	CLA	C4B-NB	2.98	1.41	1.37
29	D	312	CLA	C4B-NB	2.98	1.41	1.37
29	T	309	CLA	C4B-NB	2.98	1.41	1.37
29	J	313	CLA	C4B-NB	2.98	1.41	1.37
29	G	316	CLA	C4B-NB	2.98	1.41	1.37
29	P	217	CLA	C4B-NB	2.98	1.41	1.37
29	N	314	CLA	C4B-NB	2.97	1.41	1.37
29	T	311	CLA	C4B-NB	2.97	1.41	1.37
29	L	307	CLA	C4B-NB	2.97	1.41	1.37
29	K	207	CLA	C4B-NB	2.97	1.41	1.37
29	G	301	CLA	C4B-NB	2.97	1.41	1.37
29	M	309	CLA	C4B-NB	2.96	1.41	1.37
29	b	710	CLA	C4B-NB	2.96	1.41	1.37
29	N	311	CLA	C4B-NB	2.96	1.41	1.37
29	F	316	CLA	C4B-NB	2.96	1.41	1.37
29	L	317	CLA	C4B-NB	2.96	1.41	1.37
29	B	316	CLA	C4B-NB	2.96	1.41	1.37
29	f	805	CLA	C4B-NB	2.95	1.41	1.37
29	M	310	CLA	C4B-NB	2.95	1.41	1.37
29	b	707	CLA	C4B-NB	2.95	1.41	1.37
29	A	210	CLA	C4B-NB	2.95	1.41	1.37
29	A	217	CLA	C4B-NB	2.95	1.41	1.37
29	I	207	CLA	C4B-NB	2.95	1.41	1.37
29	l	501	CLA	C4B-NB	2.94	1.41	1.37
29	E	305	CLA	C4B-NB	2.94	1.41	1.37
29	I	212	CLA	C4B-NB	2.94	1.41	1.37
29	b	703	CLA	C4B-NB	2.94	1.41	1.37
29	M	315	CLA	C4B-NB	2.94	1.41	1.37
29	a	807	CLA	C4B-NB	2.93	1.41	1.37
29	a	810	CLA	C4B-NB	2.93	1.41	1.37
29	B	306	CLA	C4B-NB	2.93	1.41	1.37
29	l	508	CLA	C4B-NB	2.93	1.41	1.37
29	a	825	CLA	C4B-NB	2.93	1.41	1.37
29	a	803	CLA	C4B-NB	2.93	1.41	1.37
29	G	304	CLA	C4B-NB	2.93	1.41	1.37
29	D	309	CLA	C4B-NB	2.93	1.41	1.37
29	a	837	CLA	C4B-NB	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	314	CLA	C4B-NB	2.93	1.41	1.37
29	E	308	CLA	C4B-NB	2.92	1.41	1.37
29	E	314	CLA	C4B-NB	2.92	1.41	1.37
29	A	216	CLA	C4B-NB	2.92	1.41	1.37
29	M	308	CLA	C4B-NB	2.92	1.41	1.37
29	b	706	CLA	C4B-NB	2.92	1.41	1.37
29	I	201	CLA	C4B-NB	2.92	1.41	1.37
29	O	313	CLA	C4B-NB	2.92	1.41	1.37
37	G	310	PID	C8-C9	-2.92	1.39	1.46
29	I	216	CLA	C4B-NB	2.92	1.41	1.37
39	Q	311	KC1	C4B-NB	-2.92	1.34	1.37
37	N	302	PID	C8-C9	-2.92	1.39	1.46
29	B	315	CLA	C4B-NB	2.92	1.41	1.37
36	h	202	DD6	O1-C20	-2.91	1.42	1.46
29	Q	310	CLA	C4B-NB	2.91	1.41	1.37
29	b	724	CLA	C4B-NB	2.91	1.41	1.37
29	A	206	CLA	C4B-NB	2.91	1.41	1.37
29	H	308	CLA	C4B-NB	2.91	1.41	1.37
29	j	104	CLA	C4B-NB	2.91	1.41	1.37
29	A	207	CLA	C4B-NB	2.91	1.41	1.37
29	I	213	CLA	C4B-NB	2.91	1.41	1.37
29	E	306	CLA	C4B-NB	2.91	1.41	1.37
29	H	312	CLA	C4B-NB	2.91	1.41	1.37
37	Q	303	PID	C8-C9	-2.90	1.39	1.46
29	b	736	CLA	C4B-NB	2.90	1.41	1.37
29	C	316	CLA	C4B-NB	2.90	1.41	1.37
29	b	719	CLA	C4B-NB	2.90	1.41	1.37
29	a	815	CLA	C4B-NB	2.90	1.41	1.37
29	a	816	CLA	C4B-NB	2.90	1.41	1.37
29	C	309	CLA	C4B-NB	2.90	1.41	1.37
29	Q	313	CLA	C4B-NB	2.90	1.41	1.37
29	A	215	CLA	C4B-NB	2.90	1.41	1.37
29	Q	312	CLA	C4B-NB	2.90	1.41	1.37
29	b	712	CLA	C4B-NB	2.89	1.41	1.37
29	K	213	CLA	C4B-NB	2.89	1.41	1.37
36	D	301	DD6	O1-C20	-2.89	1.42	1.46
29	a	814	CLA	C4B-NB	2.89	1.41	1.37
29	P	210	CLA	C4B-NB	2.89	1.41	1.37
29	f	802	CLA	C4B-NB	2.88	1.41	1.37
29	b	726	CLA	C4B-NB	2.88	1.41	1.37
29	F	311	CLA	C4B-NB	2.88	1.41	1.37
29	M	314	CLA	C4B-NB	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	308	CLA	C4B-NB	2.88	1.41	1.37
29	C	313	CLA	C4B-NB	2.88	1.41	1.37
29	a	819	CLA	C4B-NB	2.88	1.41	1.37
29	b	717	CLA	C4B-NB	2.88	1.41	1.37
29	l	505	CLA	C4B-NB	2.88	1.41	1.37
36	G	307	DD6	O1-C20	-2.88	1.42	1.46
29	l	503	CLA	C4B-NB	2.87	1.41	1.37
29	a	812	CLA	C4B-NB	2.87	1.41	1.37
29	L	310	CLA	C4B-NB	2.87	1.41	1.37
29	B	311	CLA	C4B-NB	2.87	1.41	1.37
29	b	709	CLA	C4B-NB	2.87	1.41	1.37
37	P	203	PID	C8-C9	-2.87	1.39	1.46
29	a	826	CLA	C4B-NB	2.87	1.41	1.37
29	L	309	CLA	C4B-NB	2.86	1.41	1.37
29	b	715	CLA	C4B-NB	2.86	1.41	1.37
29	E	310	CLA	C4B-NB	2.86	1.41	1.37
29	a	827	CLA	C4B-NB	2.86	1.41	1.37
29	I	208	CLA	C4B-NB	2.86	1.41	1.37
29	J	311	CLA	C4B-NB	2.85	1.41	1.37
38	Q	305	UIX	O-C1	-2.85	1.42	1.46
29	a	802	CLA	C4B-NB	2.85	1.41	1.37
29	a	805	CLA	C4B-NB	2.85	1.41	1.37
37	T	317	PID	C8-C9	-2.85	1.39	1.46
29	G	302	CLA	C4B-NB	2.85	1.41	1.37
29	M	307	CLA	C4B-NB	2.85	1.41	1.37
29	F	313	CLA	C4B-NB	2.85	1.41	1.37
37	F	306	PID	C8-C9	-2.85	1.39	1.46
38	L	302	UIX	O-C1	-2.85	1.42	1.46
37	Q	301	PID	C8-C9	-2.85	1.39	1.46
29	A	209	CLA	C4B-NB	2.84	1.41	1.37
37	G	309	PID	C8-C9	-2.84	1.39	1.46
37	N	304	PID	C8-C9	-2.84	1.39	1.46
29	K	216	CLA	C4B-NB	2.84	1.41	1.37
29	l	504	CLA	C4B-NB	2.84	1.41	1.37
34	E	316	LMG	C4-C5	2.84	1.59	1.53
29	B	314	CLA	C4B-NB	2.84	1.41	1.37
37	P	208	PID	C13-C12	2.84	1.44	1.36
37	D	306	PID	C8-C9	-2.84	1.39	1.46
29	B	310	CLA	C4B-NB	2.84	1.41	1.37
29	C	311	CLA	C4B-NB	2.84	1.41	1.37
38	F	305	UIX	O-C1	-2.83	1.42	1.46
29	A	218	CLA	C4B-NB	2.83	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	313	CLA	C4B-NB	2.83	1.41	1.37
29	f	803	CLA	C4B-NB	2.83	1.41	1.37
29	a	808	CLA	C4B-NB	2.83	1.41	1.37
29	B	308	CLA	C4B-NB	2.83	1.41	1.37
29	b	702	CLA	C4B-NB	2.83	1.41	1.37
29	a	831	CLA	C4B-NB	2.83	1.41	1.37
29	b	716	CLA	C4B-NB	2.83	1.41	1.37
39	G	315	KC1	C4B-NB	-2.83	1.34	1.37
37	D	303	PID	C8-C9	-2.83	1.39	1.46
29	C	316	CLA	C1B-C2B	2.83	1.49	1.43
37	T	307	PID	C8-C9	-2.83	1.39	1.46
29	K	214	CLA	C4B-NB	2.82	1.41	1.37
39	G	318	KC1	C4B-NB	-2.82	1.34	1.37
29	P	217	CLA	C1B-C2B	2.82	1.49	1.43
29	J	310	CLA	C4B-NB	2.82	1.41	1.37
37	O	304	PID	C8-C9	-2.82	1.39	1.46
37	T	301	PID	C8-C9	-2.82	1.39	1.46
29	M	306	CLA	C4B-NB	2.82	1.41	1.37
29	b	718	CLA	C4B-NB	2.82	1.41	1.37
29	a	829	CLA	C4B-NB	2.82	1.41	1.37
29	D	311	CLA	C4B-NB	2.82	1.41	1.37
29	b	704	CLA	C1B-C2B	2.82	1.49	1.43
29	K	209	CLA	C4B-NB	2.82	1.41	1.37
29	K	210	CLA	C4B-NB	2.81	1.41	1.37
37	C	302	PID	C8-C9	-2.81	1.39	1.46
29	a	824	CLA	C4B-NB	2.81	1.41	1.37
37	h	204	PID	C8-C9	-2.81	1.39	1.46
37	C	304	PID	C8-C9	-2.81	1.39	1.46
29	b	714	CLA	C4B-NB	2.81	1.41	1.37
29	G	317	CLA	C4B-NB	2.81	1.41	1.37
29	b	723	CLA	C4B-NB	2.81	1.41	1.37
29	l	502	CLA	C4B-NB	2.81	1.41	1.37
39	L	314	KC1	C4B-NB	-2.81	1.34	1.37
37	T	305	PID	C8-C9	-2.81	1.39	1.46
29	F	312	CLA	C4B-NB	2.81	1.41	1.37
29	a	810	CLA	C1B-C2B	2.81	1.49	1.43
29	b	721	CLA	C4B-NB	2.81	1.41	1.37
36	K	203	DD6	C28-C27	-2.80	1.49	1.50
36	I	204	DD6	C21-C20	-2.80	1.47	1.51
38	O	306	UIX	O-C1	-2.80	1.42	1.46
29	l	510	CLA	C1B-C2B	2.80	1.49	1.43
29	G	314	CLA	C4B-NB	2.80	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	706	CLA	C1B-C2B	2.80	1.49	1.43
29	a	820	CLA	C4B-NB	2.79	1.41	1.37
29	G	319	CLA	C4B-NB	2.79	1.41	1.37
29	J	309	CLA	C4B-NB	2.79	1.41	1.37
37	G	303	PID	C8-C9	-2.79	1.39	1.46
38	B	304	UIX	O-C1	-2.79	1.42	1.46
29	b	701	CLA	C4B-NB	2.79	1.41	1.37
29	A	208	CLA	C4B-NB	2.79	1.41	1.37
29	b	731	CLA	C4B-NB	2.79	1.41	1.37
29	J	307	CLA	C4B-NB	2.79	1.41	1.37
29	a	809	CLA	C4B-NB	2.79	1.41	1.37
29	L	312	CLA	C4B-NB	2.78	1.41	1.37
38	E	304	UIX	O-C1	-2.78	1.42	1.46
29	G	313	CLA	C4B-NB	2.78	1.41	1.37
29	G	312	CLA	C4B-NB	2.78	1.41	1.37
29	b	704	CLA	C4B-NB	2.78	1.41	1.37
29	N	313	CLA	C1B-C2B	2.78	1.49	1.43
29	I	211	CLA	C4B-NB	2.78	1.41	1.37
29	T	316	CLA	C1B-C2B	2.78	1.49	1.43
29	G	311	CLA	C4B-NB	2.78	1.41	1.37
39	C	312	KC1	C4B-NB	-2.78	1.34	1.37
29	N	316	CLA	C1B-C2B	2.77	1.49	1.43
37	F	302	PID	C8-C9	-2.77	1.39	1.46
29	B	309	CLA	C4B-NB	2.77	1.41	1.37
36	G	305	DD6	C36-C31	-2.77	1.31	1.35
29	N	308	CLA	C1B-C2B	2.77	1.49	1.43
29	F	310	CLA	C4B-NB	2.77	1.41	1.37
29	I	210	CLA	C4B-NB	2.77	1.41	1.37
37	O	307	PID	C8-C9	-2.77	1.39	1.46
29	h	201	CLA	C4B-NB	2.77	1.41	1.37
29	O	316	CLA	C1B-C2B	2.76	1.49	1.43
29	a	830	CLA	C4B-NB	2.76	1.41	1.37
29	b	711	CLA	C4B-NB	2.76	1.41	1.37
29	a	825	CLA	CMB-C2B	-2.76	1.45	1.50
29	J	306	CLA	C4B-NB	2.76	1.41	1.37
29	L	308	CLA	C4B-NB	2.76	1.41	1.37
29	E	311	CLA	C4B-NB	2.76	1.41	1.37
37	H	304	PID	C8-C9	-2.76	1.39	1.46
29	a	822	CLA	C4B-NB	2.76	1.41	1.37
29	a	823	CLA	C4B-NB	2.76	1.41	1.37
29	b	725	CLA	C4B-NB	2.76	1.41	1.37
39	T	312	KC1	C4B-NB	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	308	CLA	C1B-C2B	2.76	1.49	1.43
29	b	722	CLA	C4B-NB	2.76	1.41	1.37
29	T	313	CLA	C1B-C2B	2.75	1.49	1.43
39	C	315	KC1	C4B-NB	-2.75	1.34	1.37
29	Q	307	CLA	C1B-C2B	2.75	1.49	1.43
37	T	304	PID	C8-C9	-2.75	1.39	1.46
37	P	206	PID	C13-C12	2.75	1.44	1.36
29	M	308	CLA	C1B-C2B	2.75	1.49	1.43
39	O	312	KC1	C4B-NB	-2.75	1.34	1.37
29	F	315	CLA	C1B-C2B	2.75	1.49	1.43
29	a	806	CLA	C4B-NB	2.75	1.41	1.37
37	Q	306	PID	C8-C9	-2.75	1.39	1.46
39	C	310	KC1	C4B-NB	-2.75	1.34	1.37
29	P	212	CLA	C1B-C2B	2.75	1.49	1.43
29	Q	313	CLA	C1B-C2B	2.75	1.49	1.43
29	Q	315	CLA	C1B-C2B	2.74	1.49	1.43
29	L	313	CLA	C4B-NB	2.74	1.41	1.37
29	D	308	CLA	C1B-C2B	2.74	1.49	1.43
29	M	315	CLA	C1B-C2B	2.74	1.49	1.43
29	K	211	CLA	C4B-NB	2.74	1.41	1.37
29	D	316	CLA	C1B-C2B	2.74	1.49	1.43
36	D	304	DD6	C19-C20	2.74	1.56	1.52
39	P	213	KC1	C4B-NB	-2.74	1.34	1.37
29	T	308	CLA	C1B-C2B	2.74	1.49	1.43
37	H	301	PID	C8-C9	-2.73	1.39	1.46
29	P	209	CLA	C1B-C2B	2.73	1.49	1.43
37	H	302	PID	C8-C9	-2.73	1.39	1.46
39	E	312	KC1	C4B-NB	-2.73	1.34	1.37
37	C	305	PID	C8-C9	-2.73	1.39	1.46
29	B	314	CLA	C1B-C2B	2.73	1.49	1.43
29	E	310	CLA	C1B-C2B	2.73	1.49	1.43
37	O	305	PID	C13-C12	2.73	1.44	1.36
29	E	306	CLA	C1B-C2B	2.73	1.49	1.43
39	M	312	KC1	C4B-NB	-2.73	1.34	1.37
29	J	308	CLA	C4B-NB	2.73	1.41	1.37
37	H	304	PID	C13-C12	2.72	1.44	1.36
29	F	307	CLA	C1B-C2B	2.72	1.49	1.43
37	N	301	PID	C8-C9	-2.72	1.39	1.46
29	b	713	CLA	C1B-C2B	2.72	1.49	1.43
37	F	304	PID	C8-C9	-2.72	1.39	1.46
37	C	301	PID	C8-C9	-2.72	1.39	1.46
29	H	310	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	309	CLA	C1B-C2B	2.72	1.49	1.43
29	N	314	CLA	C1B-C2B	2.72	1.49	1.43
29	M	313	CLA	C1B-C2B	2.72	1.49	1.43
36	K	221	DD6	C19-C20	2.72	1.56	1.52
29	I	209	CLA	C4B-NB	2.72	1.41	1.37
39	M	305	KC1	C4B-NB	-2.71	1.34	1.37
37	O	302	PID	C8-C9	-2.71	1.39	1.46
29	b	721	CLA	C1B-C2B	2.71	1.49	1.43
29	E	309	CLA	C1B-C2B	2.71	1.49	1.43
29	E	313	CLA	C1B-C2B	2.71	1.49	1.43
29	M	310	CLA	C1B-C2B	2.71	1.49	1.43
37	H	306	PID	C13-C12	2.71	1.44	1.36
29	G	311	CLA	C1B-C2B	2.71	1.49	1.43
29	H	307	CLA	C1B-C2B	2.71	1.49	1.43
29	F	316	CLA	C1B-C2B	2.71	1.49	1.43
37	P	205	PID	C13-C12	2.71	1.44	1.36
37	D	302	PID	C8-C9	-2.71	1.40	1.46
29	a	821	CLA	C1B-C2B	2.71	1.49	1.43
29	M	306	CLA	C1B-C2B	2.71	1.49	1.43
39	B	313	KC1	C4B-NB	-2.70	1.34	1.37
29	a	814	CLA	C1B-C2B	2.70	1.49	1.43
39	E	307	KC1	C4B-NB	-2.70	1.34	1.37
29	T	311	CLA	C1B-C2B	2.70	1.49	1.43
29	A	211	CLA	C4B-NB	2.70	1.41	1.37
29	N	311	CLA	C1B-C2B	2.70	1.49	1.43
29	a	815	CLA	C1B-C2B	2.70	1.49	1.43
29	b	705	CLA	C4B-NB	2.70	1.41	1.37
29	I	214	CLA	C4B-NB	2.70	1.41	1.37
29	A	212	CLA	C4B-NB	2.70	1.41	1.37
39	T	310	KC1	C4B-NB	-2.70	1.34	1.37
29	f	803	CLA	C1B-C2B	2.70	1.49	1.43
29	C	308	CLA	C1B-C2B	2.70	1.49	1.43
39	Q	309	KC1	C4B-NB	-2.70	1.34	1.37
29	a	831	CLA	C1B-C2B	2.70	1.49	1.43
29	H	313	CLA	C1B-C2B	2.69	1.49	1.43
38	J	304	UIX	O-C1	-2.69	1.42	1.46
29	D	312	CLA	C1B-C2B	2.69	1.49	1.43
29	P	214	CLA	C1B-C2B	2.69	1.49	1.43
29	J	313	CLA	C1B-C2B	2.69	1.49	1.43
39	A	213	KC1	C4B-NB	-2.69	1.34	1.37
39	H	311	KC1	C4B-NB	-2.69	1.34	1.37
29	B	312	CLA	C4B-NB	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	313	CLA	C1B-C2B	2.69	1.49	1.43
29	N	309	CLA	C1B-C2B	2.69	1.49	1.43
29	Q	308	CLA	C1B-C2B	2.69	1.49	1.43
37	Q	304	PID	C8-C9	-2.69	1.40	1.46
29	H	308	CLA	C1B-C2B	2.69	1.49	1.43
39	F	309	KC1	C4B-NB	-2.68	1.34	1.37
29	H	315	CLA	C1B-C2B	2.68	1.49	1.43
29	B	311	CLA	C1B-C2B	2.68	1.49	1.43
29	a	817	CLA	C1B-C2B	2.68	1.49	1.43
29	A	206	CLA	C1B-C2B	2.68	1.49	1.43
29	O	311	CLA	C1B-C2B	2.68	1.49	1.43
29	G	319	CLA	C1B-C2B	2.68	1.49	1.43
39	H	309	KC1	C4B-NB	-2.68	1.34	1.37
39	G	315	KC1	CBA-CGA	-2.68	1.41	1.48
29	i	202	CLA	C4B-NB	2.68	1.41	1.37
39	F	314	KC1	C4B-NB	-2.68	1.34	1.37
37	N	305	PID	C8-C9	-2.68	1.40	1.46
29	D	309	CLA	C1B-C2B	2.68	1.49	1.43
37	D	305	PID	C8-C9	-2.68	1.40	1.46
39	I	215	KC1	C4B-NB	-2.67	1.34	1.37
39	H	309	KC1	CBA-CGA	-2.67	1.41	1.48
39	Q	314	KC1	C4B-NB	-2.67	1.34	1.37
29	b	722	CLA	C1B-C2B	2.67	1.49	1.43
37	O	301	PID	C13-C12	2.67	1.43	1.36
29	I	208	CLA	C1B-C2B	2.67	1.49	1.43
39	N	312	KC1	C4B-NB	-2.67	1.34	1.37
37	O	301	PID	C8-C9	-2.67	1.40	1.46
29	G	314	CLA	C1B-C2B	2.67	1.49	1.43
29	K	207	CLA	C1B-C2B	2.67	1.49	1.43
37	N	307	PID	C13-C12	2.67	1.43	1.36
29	Q	312	CLA	C1B-C2B	2.67	1.49	1.43
29	i	201	CLA	C1B-C2B	2.67	1.49	1.43
29	A	215	CLA	C1B-C2B	2.67	1.49	1.43
29	l	508	CLA	C1B-C2B	2.67	1.49	1.43
39	J	312	KC1	C4B-NB	-2.67	1.34	1.37
29	a	816	CLA	C1B-C2B	2.67	1.49	1.43
37	P	206	PID	C8-C9	-2.67	1.40	1.46
29	L	307	CLA	C1B-C2B	2.66	1.49	1.43
29	I	201	CLA	C1B-C2B	2.66	1.49	1.43
39	D	310	KC1	C4B-NB	-2.66	1.34	1.37
29	L	315	CLA	C1B-C2B	2.66	1.49	1.43
29	D	311	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L	317	CLA	C1B-C2B	2.66	1.49	1.43
29	J	305	CLA	C1B-C2B	2.66	1.49	1.43
29	i	203	CLA	C4B-NB	2.66	1.41	1.37
29	b	718	CLA	CMB-C2B	-2.66	1.45	1.50
29	K	216	CLA	C1B-C2B	2.66	1.49	1.43
29	P	210	CLA	C1B-C2B	2.66	1.49	1.43
36	G	306	DD6	C28-C27	-2.66	1.49	1.50
29	A	207	CLA	C1B-C2B	2.65	1.49	1.43
29	E	308	CLA	C1B-C2B	2.65	1.49	1.43
36	B	319	DD6	O1-C20	-2.65	1.42	1.46
29	a	813	CLA	C1B-C2B	2.65	1.49	1.43
29	T	309	CLA	C1B-C2B	2.65	1.49	1.43
29	P	215	CLA	C1B-C2B	2.65	1.49	1.43
29	K	212	CLA	C1B-C2B	2.65	1.49	1.43
29	F	311	CLA	C1B-C2B	2.65	1.49	1.43
36	O	303	DD6	O1-C20	-2.65	1.42	1.46
39	D	315	KC1	C4B-NB	-2.65	1.34	1.37
39	P	216	KC1	C4B-NB	-2.65	1.34	1.37
29	L	309	CLA	C1B-C2B	2.65	1.49	1.43
29	O	309	CLA	C1B-C2B	2.65	1.49	1.43
37	C	307	PID	C13-C12	2.65	1.43	1.36
37	P	202	PID	C8-C9	-2.65	1.40	1.46
29	E	305	CLA	C1B-C2B	2.64	1.49	1.43
29	M	307	CLA	C1B-C2B	2.64	1.49	1.43
29	f	802	CLA	C1B-C2B	2.64	1.49	1.43
29	M	311	CLA	C1B-C2B	2.64	1.49	1.43
39	T	310	KC1	CBA-CGA	-2.64	1.41	1.48
29	b	710	CLA	C1B-C2B	2.64	1.49	1.43
29	B	316	CLA	C1B-C2B	2.64	1.49	1.43
29	F	312	CLA	C1B-C2B	2.64	1.49	1.43
29	E	315	CLA	C1B-C2B	2.64	1.49	1.43
29	f	805	CLA	C1B-C2B	2.64	1.49	1.43
29	I	216	CLA	C1B-C2B	2.64	1.49	1.43
29	C	311	CLA	C1B-C2B	2.64	1.49	1.43
29	a	818	CLA	C1B-C2B	2.64	1.49	1.43
29	b	725	CLA	C1B-C2B	2.64	1.49	1.43
29	G	317	CLA	C1B-C2B	2.64	1.49	1.43
29	L	308	CLA	C1B-C2B	2.64	1.49	1.43
39	F	309	KC1	CBA-CGA	-2.64	1.41	1.48
39	N	315	KC1	C4B-NB	-2.63	1.34	1.37
37	T	302	PID	C13-C12	2.63	1.43	1.36
37	P	205	PID	C8-C9	-2.63	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	i	201	CLA	C4B-NB	2.63	1.41	1.37
38	N	306	UIX	O-C1	-2.63	1.42	1.46
29	A	218	CLA	C1B-C2B	2.63	1.49	1.43
39	A	205	KC1	C4B-NB	-2.63	1.34	1.37
36	M	303	DD6	O1-C20	-2.63	1.42	1.46
29	i	203	CLA	C1B-C2B	2.63	1.49	1.43
29	l	509	CLA	C1B-C2B	2.63	1.49	1.43
29	a	829	CLA	C1B-C2B	2.63	1.49	1.43
37	D	305	PID	C13-C12	2.63	1.43	1.36
29	I	207	CLA	C1B-C2B	2.63	1.49	1.43
37	E	301	PID	C8-C9	-2.62	1.40	1.46
37	D	307	PID	C13-C12	2.62	1.43	1.36
29	D	314	CLA	C1B-C2B	2.62	1.49	1.43
29	B	307	CLA	C1B-C2B	2.62	1.49	1.43
29	G	302	CLA	C1B-C2B	2.62	1.49	1.43
29	A	214	CLA	C1B-C2B	2.62	1.49	1.43
29	F	310	CLA	C1B-C2B	2.62	1.49	1.43
29	F	313	CLA	C1B-C2B	2.62	1.49	1.43
29	a	822	CLA	C1B-C2B	2.62	1.49	1.43
29	I	209	CLA	C1B-C2B	2.62	1.49	1.43
39	G	315	KC1	C1B-NB	-2.62	1.34	1.37
39	K	215	KC1	CBA-CGA	-2.62	1.41	1.48
36	C	303	DD6	O1-C20	-2.62	1.42	1.46
29	F	308	CLA	C1B-C2B	2.62	1.49	1.43
29	H	312	CLA	C1B-C2B	2.62	1.49	1.43
37	T	304	PID	C13-C12	2.62	1.43	1.36
37	Q	306	PID	C13-C12	2.61	1.43	1.36
29	b	712	CLA	C1B-C2B	2.61	1.49	1.43
39	C	312	KC1	CBA-CGA	-2.61	1.41	1.48
37	H	306	PID	C6-C7	2.61	1.55	1.50
29	J	308	CLA	C1B-C2B	2.61	1.49	1.43
29	C	314	CLA	C1B-C2B	2.61	1.49	1.43
29	G	304	CLA	C1B-C2B	2.61	1.49	1.43
39	E	307	KC1	CBA-CGA	-2.60	1.41	1.48
29	a	830	CLA	C1B-C2B	2.60	1.49	1.43
37	H	301	PID	C13-C12	2.60	1.43	1.36
29	l	504	CLA	C1B-C2B	2.60	1.49	1.43
37	D	302	PID	C13-C12	2.60	1.43	1.36
37	P	202	PID	C13-C12	2.60	1.43	1.36
29	A	208	CLA	C1B-C2B	2.60	1.49	1.43
39	T	315	KC1	CBA-CGA	-2.60	1.41	1.48
29	A	210	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	I	215	KC1	CBA-CGA	-2.60	1.41	1.48
39	O	315	KC1	C4B-NB	-2.60	1.34	1.37
29	B	310	CLA	C1B-C2B	2.60	1.49	1.43
39	T	315	KC1	C4B-NB	-2.60	1.34	1.37
29	a	801	CLA	C1B-C2B	2.60	1.49	1.43
29	G	301	CLA	C1B-C2B	2.60	1.49	1.43
29	O	314	CLA	CHC-C1C	2.60	1.43	1.38
37	j	101	PID	C13-C12	2.60	1.43	1.36
37	C	301	PID	C13-C12	2.60	1.43	1.36
29	l	505	CLA	C1B-C2B	2.60	1.49	1.43
39	L	306	KC1	C4B-NB	-2.60	1.34	1.37
39	G	318	KC1	CBA-CGA	-2.60	1.41	1.48
39	Q	309	KC1	CBA-CGA	-2.60	1.41	1.48
37	O	304	PID	C13-C12	2.60	1.43	1.36
29	a	824	CLA	C1B-C2B	2.59	1.49	1.43
29	M	309	CLA	C1B-C2B	2.59	1.49	1.43
29	B	315	CLA	C1B-C2B	2.59	1.49	1.43
37	T	302	PID	C8-C9	-2.59	1.40	1.46
29	b	702	CLA	C1B-C2B	2.59	1.49	1.43
29	Q	310	CLA	C1B-C2B	2.59	1.49	1.43
29	a	806	CLA	C1B-C2B	2.59	1.49	1.43
29	b	715	CLA	C1B-C2B	2.59	1.49	1.43
37	D	307	PID	C8-C9	-2.59	1.40	1.46
37	j	101	PID	C8-C9	-2.59	1.40	1.46
39	L	306	KC1	CBA-CGA	-2.59	1.42	1.48
39	N	315	KC1	CBA-CGA	-2.59	1.42	1.48
29	A	212	CLA	C1B-C2B	2.59	1.49	1.43
29	a	807	CLA	C1B-C2B	2.59	1.49	1.43
39	E	312	KC1	CBA-CGA	-2.59	1.42	1.48
37	F	302	PID	C13-C12	2.59	1.43	1.36
39	Q	314	KC1	CBA-CGA	-2.58	1.42	1.48
37	C	307	PID	C8-C9	-2.58	1.40	1.46
29	L	316	CLA	C1B-C2B	2.58	1.49	1.43
39	A	213	KC1	CBA-CGA	-2.58	1.42	1.48
39	Q	311	KC1	CBA-CGA	-2.58	1.42	1.48
39	P	211	KC1	CBA-CGA	-2.58	1.42	1.48
29	L	313	CLA	C1B-C2B	2.58	1.49	1.43
29	J	307	CLA	C1B-C2B	2.58	1.49	1.43
29	b	714	CLA	C1B-C2B	2.58	1.49	1.43
39	O	310	KC1	CBA-CGA	-2.58	1.42	1.48
29	L	310	CLA	C1B-C2B	2.58	1.49	1.43
37	C	302	PID	C13-C12	2.58	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	826	CLA	C1B-C2B	2.58	1.49	1.43
29	M	314	CLA	C1B-C2B	2.58	1.49	1.43
29	I	217	CLA	C1B-C2B	2.58	1.49	1.43
29	j	104	CLA	C1B-C2B	2.58	1.49	1.43
29	B	310	CLA	CMD-C2D	-2.58	1.45	1.50
29	B	312	CLA	C1B-C2B	2.58	1.49	1.43
29	a	804	CLA	C1B-C2B	2.58	1.49	1.43
29	b	723	CLA	C1B-C2B	2.58	1.49	1.43
39	N	310	KC1	C4B-NB	-2.58	1.34	1.37
29	B	308	CLA	C1B-C2B	2.57	1.49	1.43
29	L	311	CLA	C1B-C2B	2.57	1.49	1.43
29	a	805	CLA	C1B-C2B	2.57	1.49	1.43
39	D	315	KC1	CBA-CGA	-2.57	1.42	1.48
29	a	812	CLA	C1B-C2B	2.57	1.49	1.43
37	N	304	PID	C13-C12	2.57	1.43	1.36
29	B	309	CLA	C1B-C2B	2.57	1.49	1.43
29	K	209	CLA	C1B-C2B	2.57	1.49	1.43
29	b	716	CLA	C1B-C2B	2.57	1.49	1.43
29	i	202	CLA	C1B-C2B	2.57	1.49	1.43
29	J	306	CLA	C1B-C2B	2.56	1.49	1.43
39	P	216	KC1	CBA-CGA	-2.56	1.42	1.48
29	b	731	CLA	C1B-C2B	2.56	1.49	1.43
29	K	211	CLA	C1B-C2B	2.56	1.49	1.43
29	T	314	CLA	C1B-C2B	2.56	1.49	1.43
29	a	809	CLA	C1B-C2B	2.56	1.49	1.43
36	E	303	DD6	O1-C20	-2.56	1.42	1.46
29	K	208	CLA	C1B-C2B	2.56	1.49	1.43
39	N	310	KC1	CBA-CGA	-2.56	1.42	1.48
29	K	218	CLA	C1B-C2B	2.56	1.49	1.43
39	H	314	KC1	C4B-NB	-2.56	1.34	1.37
29	I	212	CLA	C1B-C2B	2.56	1.49	1.43
29	L	312	CLA	C1B-C2B	2.56	1.49	1.43
29	B	306	CLA	C1B-C2B	2.56	1.49	1.43
29	b	709	CLA	C1B-C2B	2.56	1.49	1.43
36	K	204	DD6	O1-C20	-2.56	1.42	1.46
29	I	213	CLA	C1B-C2B	2.55	1.49	1.43
39	F	314	KC1	CBA-CGA	-2.55	1.42	1.48
39	J	312	KC1	CBA-CGA	-2.55	1.42	1.48
29	a	837	CLA	C1B-C2B	2.55	1.49	1.43
39	A	205	KC1	CBA-CGA	-2.55	1.42	1.48
36	G	306	DD6	O1-C20	-2.55	1.42	1.46
39	B	313	KC1	CBA-CGA	-2.55	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	213	CLA	C1B-C2B	2.55	1.49	1.43
37	T	301	PID	C13-C12	2.55	1.43	1.36
29	b	720	CLA	C3B-C4B	2.55	1.50	1.42
39	O	315	KC1	CBA-CGA	-2.55	1.42	1.48
29	b	701	CLA	C1B-C2B	2.55	1.49	1.43
29	a	823	CLA	C1B-C2B	2.55	1.49	1.43
39	N	312	KC1	CBA-CGA	-2.55	1.42	1.48
29	D	313	CLA	C1B-C2B	2.55	1.49	1.43
29	A	209	CLA	C1B-C2B	2.54	1.49	1.43
29	a	819	CLA	C1B-C2B	2.54	1.49	1.43
36	M	303	DD6	C19-C20	2.54	1.55	1.52
38	A	203	UIX	O-C1	-2.54	1.42	1.46
29	J	311	CLA	C1B-C2B	2.54	1.49	1.43
37	N	301	PID	C13-C12	2.54	1.43	1.36
29	K	217	CLA	C1B-C2B	2.54	1.49	1.43
29	K	210	CLA	C1B-C2B	2.54	1.49	1.43
29	h	201	CLA	C1B-C2B	2.54	1.49	1.43
29	A	211	CLA	C1B-C2B	2.54	1.49	1.43
29	J	309	CLA	C1B-C2B	2.54	1.49	1.43
37	C	304	PID	C13-C12	2.53	1.43	1.36
29	G	313	CLA	C1B-C2B	2.53	1.49	1.43
37	F	306	PID	C13-C12	2.53	1.43	1.36
29	G	316	CLA	C1B-C2B	2.53	1.49	1.43
29	E	311	CLA	C1B-C2B	2.53	1.49	1.43
29	a	827	CLA	C1B-C2B	2.53	1.49	1.43
36	A	204	DD6	O1-C20	-2.53	1.42	1.46
29	A	216	CLA	C1B-C2B	2.53	1.49	1.43
36	B	303	DD6	O1-C20	-2.53	1.42	1.46
29	A	214	CLA	CMD-C2D	-2.53	1.45	1.50
29	b	718	CLA	CMD-C2D	-2.53	1.45	1.50
29	E	314	CLA	C1B-C2B	2.53	1.49	1.43
29	a	803	CLA	C1B-C2B	2.53	1.49	1.43
37	Q	304	PID	C13-C12	2.53	1.43	1.36
39	D	310	KC1	CBA-CGA	-2.52	1.42	1.48
39	P	213	KC1	CBA-CGA	-2.52	1.42	1.48
39	O	310	KC1	C4B-NB	-2.52	1.34	1.37
29	a	828	CLA	C1B-C2B	2.52	1.49	1.43
29	I	211	CLA	C1B-C2B	2.52	1.49	1.43
29	J	310	CLA	C1B-C2B	2.52	1.49	1.43
39	M	312	KC1	CBA-CGA	-2.52	1.42	1.48
36	J	303	DD6	O1-C20	-2.52	1.43	1.46
39	C	310	KC1	CBA-CGA	-2.52	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	O	307	PID	C13-C12	2.52	1.43	1.36
37	E	301	PID	C13-C12	2.52	1.43	1.36
39	L	314	KC1	CBA-CGA	-2.52	1.42	1.48
29	I	214	CLA	C1B-C2B	2.52	1.49	1.43
29	b	736	CLA	C1B-C2B	2.52	1.49	1.43
37	T	305	PID	C13-C12	2.52	1.43	1.36
29	K	214	CLA	C3B-C4B	2.51	1.50	1.42
36	B	301	DD6	O1-C20	-2.51	1.43	1.46
37	Q	301	PID	C13-C12	2.51	1.43	1.36
39	M	305	KC1	CBA-CGA	-2.51	1.42	1.48
29	G	312	CLA	C1B-C2B	2.51	1.49	1.43
39	H	314	KC1	CBA-CGA	-2.51	1.42	1.48
29	l	502	CLA	C1B-C2B	2.51	1.49	1.43
39	O	312	KC1	CBA-CGA	-2.51	1.42	1.48
37	N	305	PID	C13-C12	2.51	1.43	1.36
39	H	311	KC1	CBA-CGA	-2.51	1.42	1.48
29	b	707	CLA	C1B-C2B	2.51	1.49	1.43
39	C	315	KC1	CBA-CGA	-2.51	1.42	1.48
29	a	808	CLA	C1B-C2B	2.50	1.49	1.43
29	a	811	CLA	C1B-C2B	2.50	1.49	1.43
29	b	708	CLA	C1B-C2B	2.50	1.49	1.43
37	N	307	PID	C8-C9	-2.50	1.40	1.46
34	h	205	LMG	O7-C8	-2.50	1.40	1.46
36	H	303	DD6	O1-C20	-2.50	1.43	1.46
37	C	305	PID	C13-C12	2.49	1.43	1.36
29	b	719	CLA	CMD-C2D	-2.49	1.45	1.50
36	M	302	DD6	C19-C20	2.49	1.55	1.52
29	a	802	CLA	CHC-C1C	2.49	1.43	1.38
29	O	314	CLA	C1B-C2B	2.49	1.49	1.43
29	a	804	CLA	C3B-C4B	2.49	1.50	1.42
29	O	313	CLA	C1B-C2B	2.49	1.49	1.43
37	T	307	PID	C13-C12	2.49	1.43	1.36
36	N	303	DD6	O1-C20	-2.49	1.43	1.46
39	P	211	KC1	C4B-NB	-2.48	1.34	1.37
37	G	309	PID	C13-C12	2.48	1.43	1.36
37	Q	303	PID	C13-C12	2.48	1.43	1.36
39	C	310	KC1	C1B-NB	-2.48	1.34	1.37
36	m	101	DD6	O1-C20	-2.48	1.43	1.46
37	H	305	PID	C13-C12	2.48	1.43	1.36
29	L	316	CLA	C3B-C4B	2.48	1.50	1.42
36	E	302	DD6	O1-C20	-2.48	1.43	1.46
29	b	703	CLA	C1B-C2B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	H	302	PID	C13-C12	2.47	1.43	1.36
29	b	717	CLA	C1B-C2B	2.46	1.48	1.43
37	P	208	PID	C8-C9	-2.46	1.40	1.46
36	A	202	DD6	O1-C20	-2.46	1.43	1.46
29	b	726	CLA	C1B-C2B	2.45	1.48	1.43
36	P	204	DD6	O1-C20	-2.45	1.43	1.46
36	B	305	DD6	O1-C20	-2.45	1.43	1.46
29	b	705	CLA	C1B-C2B	2.45	1.48	1.43
29	A	217	CLA	C1B-C2B	2.45	1.48	1.43
29	I	210	CLA	C1B-C2B	2.45	1.48	1.43
36	K	203	DD6	O1-C20	-2.45	1.43	1.46
29	a	802	CLA	C3B-C4B	2.45	1.49	1.42
36	M	301	DD6	O1-C20	-2.45	1.43	1.46
36	L	303	DD6	O1-C20	-2.45	1.43	1.46
29	G	316	CLA	CMB-C2B	-2.44	1.45	1.50
29	N	309	CLA	C3B-C4B	2.44	1.49	1.42
36	L	305	DD6	O1-C20	-2.44	1.43	1.46
29	l	501	CLA	C1B-C2B	2.44	1.48	1.43
29	a	828	CLA	C3B-C4B	2.44	1.49	1.42
37	D	306	PID	C13-C12	2.44	1.43	1.36
34	K	219	LMG	O7-C8	-2.44	1.40	1.46
36	L	304	DD6	O1-C20	-2.43	1.43	1.46
29	D	313	CLA	CMD-C2D	-2.43	1.45	1.50
29	O	314	CLA	C3B-C4B	2.43	1.49	1.42
36	I	202	DD6	O1-C20	-2.43	1.43	1.46
36	K	205	DD6	O1-C20	-2.43	1.43	1.46
29	b	708	CLA	CMB-C2B	-2.43	1.45	1.50
39	Q	314	KC1	C1B-NB	-2.43	1.34	1.37
36	K	206	DD6	O1-C20	-2.43	1.43	1.46
29	b	704	CLA	CMD-C2D	-2.43	1.45	1.50
39	Q	311	KC1	C1B-NB	-2.43	1.34	1.37
37	T	317	PID	C13-C12	2.42	1.43	1.36
29	b	736	CLA	CMC-C2C	-2.42	1.45	1.50
29	I	217	CLA	C3B-C4B	2.42	1.49	1.42
39	O	312	KC1	C1B-NB	-2.42	1.34	1.37
37	O	302	PID	C13-C12	2.42	1.43	1.36
29	L	311	CLA	C3B-C4B	2.41	1.49	1.42
32	m	103	BCR	C30-C25	-2.41	1.50	1.53
29	l	505	CLA	CMD-C2D	-2.41	1.45	1.50
29	b	711	CLA	C1B-C2B	2.41	1.48	1.43
29	a	820	CLA	C1B-C2B	2.41	1.48	1.43
29	a	801	CLA	C4B-NB	2.41	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	724	CLA	C1B-C2B	2.41	1.48	1.43
29	b	707	CLA	C3B-C4B	2.41	1.49	1.42
37	h	204	PID	C13-C12	2.41	1.43	1.36
29	b	720	CLA	C1B-C2B	2.40	1.48	1.43
29	F	310	CLA	CMD-C2D	-2.40	1.45	1.50
36	Q	302	DD6	O1-C20	-2.40	1.43	1.46
37	E	301	PID	C20-C21	2.40	1.41	1.35
29	f	805	CLA	CMD-C2D	-2.40	1.45	1.50
39	T	312	KC1	CBA-CGA	-2.40	1.42	1.48
29	I	214	CLA	C3B-C4B	2.40	1.49	1.42
29	M	311	CLA	C3B-C4B	2.40	1.49	1.42
29	H	312	CLA	C3B-C4B	2.39	1.49	1.42
39	E	312	KC1	C1B-NB	-2.39	1.34	1.37
29	N	309	CLA	CHC-C1C	2.39	1.43	1.38
29	H	312	CLA	CHC-C1C	2.39	1.43	1.38
39	C	315	KC1	C1B-NB	-2.39	1.34	1.37
29	b	718	CLA	C1B-C2B	2.39	1.48	1.43
29	K	208	CLA	C3B-C4B	2.39	1.49	1.42
29	b	719	CLA	CHC-C1C	2.39	1.43	1.38
36	I	206	DD6	O1-C20	-2.39	1.43	1.46
39	K	215	KC1	C1B-NB	-2.39	1.34	1.37
39	C	312	KC1	C1B-NB	-2.39	1.34	1.37
39	F	309	KC1	C1B-NB	-2.38	1.34	1.37
29	L	315	CLA	C3B-C4B	2.38	1.49	1.42
29	K	214	CLA	C1B-C2B	2.38	1.48	1.43
29	l	503	CLA	C1B-C2B	2.38	1.48	1.43
37	N	302	PID	C13-C12	2.37	1.43	1.36
29	M	307	CLA	C3B-C4B	2.37	1.49	1.42
29	b	711	CLA	MG-NB	-2.37	2.01	2.05
36	T	303	DD6	O1-C20	-2.37	1.43	1.46
29	H	307	CLA	C3B-C4B	2.37	1.49	1.42
29	D	313	CLA	C3B-C4B	2.37	1.49	1.42
29	K	218	CLA	C3B-C4B	2.36	1.49	1.42
29	K	212	CLA	CMB-C2B	-2.36	1.45	1.50
37	G	310	PID	C13-C12	2.36	1.43	1.36
37	G	303	PID	C13-C12	2.36	1.43	1.36
37	F	304	PID	C13-C12	2.36	1.43	1.36
29	N	308	CLA	C3B-C4B	2.36	1.49	1.42
29	D	314	CLA	C3B-C4B	2.36	1.49	1.42
29	K	213	CLA	C3B-C4B	2.36	1.49	1.42
29	N	316	CLA	C3B-C4B	2.36	1.49	1.42
29	J	305	CLA	C3B-C4B	2.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	825	CLA	C1B-C2B	2.36	1.48	1.43
36	I	204	DD6	C19-C20	2.36	1.55	1.52
29	P	215	CLA	C3B-C4B	2.36	1.49	1.42
29	D	309	CLA	C3B-C4B	2.35	1.49	1.42
29	a	817	CLA	C3B-C4B	2.35	1.49	1.42
36	K	202	DD6	C21-C20	-2.35	1.48	1.51
29	F	308	CLA	C3B-C4B	2.35	1.49	1.42
29	K	209	CLA	C3B-C4B	2.35	1.49	1.42
37	P	203	PID	C13-C12	2.35	1.43	1.36
29	F	310	CLA	C3B-C4B	2.35	1.49	1.42
29	b	719	CLA	C3B-C4B	2.35	1.49	1.42
37	O	305	PID	C8-C9	-2.34	1.40	1.46
37	D	303	PID	C13-C12	2.34	1.43	1.36
39	M	312	KC1	C1B-NB	-2.34	1.34	1.37
39	T	315	KC1	C1B-NB	-2.34	1.34	1.37
29	E	309	CLA	C3B-C4B	2.34	1.49	1.42
29	a	813	CLA	C3B-C4B	2.34	1.49	1.42
29	a	818	CLA	C3B-C4B	2.34	1.49	1.42
29	K	207	CLA	C3B-C4B	2.34	1.49	1.42
29	D	311	CLA	C3B-C4B	2.34	1.49	1.42
29	b	719	CLA	C1B-C2B	2.34	1.48	1.43
34	b	732	LMG	O7-C8	-2.34	1.41	1.46
29	P	214	CLA	C3B-C4B	2.34	1.49	1.42
29	O	311	CLA	C3B-C4B	2.34	1.49	1.42
29	O	308	CLA	C3B-C4B	2.34	1.49	1.42
29	E	311	CLA	C3B-C4B	2.34	1.49	1.42
39	G	315	KC1	C4A-C3A	-2.34	1.39	1.44
29	G	302	CLA	C3B-C4B	2.34	1.49	1.42
36	M	302	DD6	O1-C20	-2.34	1.43	1.46
29	a	837	CLA	CMD-C2D	-2.33	1.46	1.50
29	G	302	CLA	CHC-C1C	2.33	1.43	1.38
29	a	811	CLA	C3B-C4B	2.33	1.49	1.42
29	P	209	CLA	C3B-C4B	2.33	1.49	1.42
29	J	310	CLA	C3B-C4B	2.33	1.49	1.42
39	P	211	KC1	C1B-NB	-2.33	1.34	1.37
29	T	314	CLA	C3B-C4B	2.33	1.49	1.42
29	a	821	CLA	C3B-C4B	2.33	1.49	1.42
29	G	316	CLA	C3B-C4B	2.33	1.49	1.42
29	T	316	CLA	C3B-C4B	2.33	1.49	1.42
29	b	723	CLA	C3B-C4B	2.33	1.49	1.42
29	P	212	CLA	C3B-C4B	2.33	1.49	1.42
39	I	215	KC1	C1B-NB	-2.33	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	217	CLA	CMD-C2D	-2.33	1.46	1.50
29	H	310	CLA	C3B-C4B	2.33	1.49	1.42
29	O	316	CLA	C3B-C4B	2.33	1.49	1.42
29	C	308	CLA	C3B-C4B	2.33	1.49	1.42
37	H	305	PID	C8-C9	-2.33	1.40	1.46
29	I	211	CLA	C3B-C4B	2.33	1.49	1.42
29	K	209	CLA	CHC-C1C	2.33	1.43	1.38
39	L	314	KC1	C1B-NB	-2.33	1.34	1.37
29	T	308	CLA	C3B-C4B	2.33	1.49	1.42
39	D	315	KC1	C1B-NB	-2.32	1.34	1.37
39	Q	309	KC1	C1B-NB	-2.32	1.34	1.37
29	B	307	CLA	C3B-C4B	2.32	1.49	1.42
39	O	310	KC1	C1B-NB	-2.32	1.34	1.37
29	a	805	CLA	C3B-C4B	2.32	1.49	1.42
29	M	315	CLA	C3B-C4B	2.32	1.49	1.42
29	Q	308	CLA	CHC-C1C	2.32	1.43	1.38
29	A	214	CLA	C3B-C4B	2.32	1.49	1.42
29	J	306	CLA	C3B-C4B	2.32	1.49	1.42
29	O	309	CLA	C3B-C4B	2.32	1.49	1.42
29	b	713	CLA	C3B-C4B	2.32	1.49	1.42
39	J	312	KC1	C1B-NB	-2.32	1.34	1.37
39	A	205	KC1	C1B-NB	-2.32	1.34	1.37
29	a	808	CLA	CHC-C1C	2.32	1.43	1.38
29	O	316	CLA	CHC-C1C	2.32	1.43	1.38
36	D	304	DD6	O1-C20	-2.32	1.43	1.46
36	B	302	DD6	O1-C20	-2.32	1.43	1.46
29	a	823	CLA	C3B-C4B	2.32	1.49	1.42
29	H	308	CLA	C3B-C4B	2.32	1.49	1.42
29	a	812	CLA	CMD-C2D	-2.32	1.46	1.50
29	l	503	CLA	CMB-C2B	-2.32	1.46	1.50
29	a	837	CLA	C3B-C4B	2.32	1.49	1.42
36	A	201	DD6	O1-C20	-2.32	1.43	1.46
29	H	315	CLA	C3B-C4B	2.32	1.49	1.42
29	a	801	CLA	MG-NB	-2.32	2.01	2.05
29	P	214	CLA	CHC-C1C	2.32	1.43	1.38
29	L	312	CLA	C3B-C4B	2.32	1.49	1.42
29	K	210	CLA	C3B-C4B	2.32	1.49	1.42
29	N	314	CLA	C3B-C4B	2.32	1.49	1.42
29	E	315	CLA	C3B-C4B	2.32	1.49	1.42
29	B	306	CLA	C3B-C4B	2.32	1.49	1.42
29	M	310	CLA	C3B-C4B	2.31	1.49	1.42
29	L	317	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	503	CLA	C3B-C4B	2.31	1.49	1.42
36	F	303	DD6	O1-C20	-2.31	1.43	1.46
29	i	202	CLA	C3B-C4B	2.31	1.49	1.42
29	A	215	CLA	CMD-C2D	-2.31	1.46	1.50
39	N	310	KC1	C1B-NB	-2.31	1.34	1.37
29	J	313	CLA	C3B-C4B	2.31	1.49	1.42
29	b	714	CLA	C3B-C4B	2.31	1.49	1.42
29	A	209	CLA	C3B-C4B	2.31	1.49	1.42
39	E	307	KC1	C1B-NB	-2.31	1.34	1.37
32	b	729	BCR	C30-C25	-2.31	1.50	1.53
29	b	726	CLA	C3B-C4B	2.31	1.49	1.42
29	M	309	CLA	C3B-C4B	2.31	1.49	1.42
29	M	311	CLA	CHC-C1C	2.31	1.43	1.38
29	h	201	CLA	C3B-C4B	2.31	1.49	1.42
29	b	736	CLA	C3B-C4B	2.31	1.49	1.42
29	a	820	CLA	CMD-C2D	-2.31	1.46	1.50
29	J	308	CLA	MG-NB	-2.31	2.01	2.05
29	M	313	CLA	CHC-C1C	2.31	1.43	1.38
29	P	215	CLA	CHC-C1C	2.31	1.43	1.38
29	A	217	CLA	C3B-C4B	2.31	1.49	1.42
29	A	217	CLA	MG-NB	-2.31	2.01	2.05
29	K	216	CLA	C3B-C4B	2.31	1.49	1.42
39	H	309	KC1	C1B-NB	-2.31	1.34	1.37
36	K	221	DD6	O1-C20	-2.31	1.43	1.46
29	J	310	CLA	CHC-C1C	2.31	1.43	1.38
29	I	212	CLA	C3B-C4B	2.31	1.49	1.42
29	B	312	CLA	C3B-C4B	2.30	1.49	1.42
29	H	313	CLA	C3B-C4B	2.30	1.49	1.42
29	P	210	CLA	C3B-C4B	2.30	1.49	1.42
29	a	811	CLA	CMB-C2B	-2.30	1.46	1.50
29	b	703	CLA	C3B-C4B	2.30	1.49	1.42
29	A	216	CLA	C3B-C4B	2.30	1.49	1.42
29	G	312	CLA	C3B-C4B	2.30	1.49	1.42
29	Q	308	CLA	C3B-C4B	2.30	1.49	1.42
29	h	201	CLA	CHC-C1C	2.30	1.43	1.38
29	a	819	CLA	C3B-C4B	2.30	1.49	1.42
29	M	307	CLA	CHC-C1C	2.30	1.43	1.38
29	P	212	CLA	CHC-C1C	2.30	1.43	1.38
29	b	714	CLA	CHC-C1C	2.30	1.43	1.38
29	T	313	CLA	CHC-C1C	2.30	1.43	1.38
29	I	213	CLA	C3B-C4B	2.30	1.49	1.42
29	a	823	CLA	CHC-C1C	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L	315	CLA	CHC-C1C	2.30	1.43	1.38
39	B	313	KC1	C1B-NB	-2.30	1.34	1.37
29	b	717	CLA	CMB-C2B	-2.30	1.46	1.50
29	b	703	CLA	CHC-C1C	2.30	1.43	1.38
29	K	210	CLA	CHC-C1C	2.30	1.43	1.38
29	G	313	CLA	C3B-C4B	2.30	1.49	1.42
29	A	217	CLA	CMB-C2B	-2.30	1.46	1.50
29	A	218	CLA	C3B-C4B	2.30	1.49	1.42
29	M	313	CLA	C3B-C4B	2.30	1.49	1.42
29	b	723	CLA	CHC-C1C	2.30	1.43	1.38
29	I	201	CLA	CHC-C1C	2.30	1.43	1.38
39	H	314	KC1	C1B-NB	-2.30	1.34	1.37
39	A	213	KC1	C1B-NB	-2.30	1.34	1.37
29	A	206	CLA	C3B-C4B	2.30	1.49	1.42
29	C	311	CLA	C3B-C4B	2.30	1.49	1.42
29	a	801	CLA	CMD-C2D	-2.29	1.46	1.50
29	T	311	CLA	C3B-C4B	2.29	1.49	1.42
29	A	207	CLA	C3B-C4B	2.29	1.49	1.42
39	M	305	KC1	C1B-NB	-2.29	1.34	1.37
29	Q	307	CLA	C3B-C4B	2.29	1.49	1.42
34	b	730	LMG	O7-C8	-2.29	1.41	1.46
29	F	316	CLA	C3B-C4B	2.29	1.49	1.42
29	b	705	CLA	CHC-C1C	2.29	1.43	1.38
39	T	310	KC1	C1B-NB	-2.29	1.34	1.37
29	a	815	CLA	C3B-C4B	2.29	1.49	1.42
39	O	312	KC1	C4A-C3A	-2.29	1.39	1.44
29	L	313	CLA	C3B-C4B	2.29	1.49	1.42
29	J	309	CLA	CMB-C2B	-2.29	1.46	1.50
29	B	310	CLA	C3B-C4B	2.29	1.49	1.42
29	N	313	CLA	C3B-C4B	2.29	1.49	1.42
29	I	208	CLA	C3B-C4B	2.29	1.49	1.42
29	b	718	CLA	MG-NB	-2.29	2.01	2.05
29	I	210	CLA	MG-NB	-2.29	2.01	2.05
29	O	313	CLA	MG-NB	-2.29	2.01	2.05
29	a	820	CLA	C3B-C4B	2.29	1.49	1.42
29	F	312	CLA	C3B-C4B	2.29	1.49	1.42
39	N	312	KC1	C1B-NB	-2.29	1.34	1.37
29	a	806	CLA	C3B-C4B	2.29	1.49	1.42
29	b	725	CLA	CMD-C2D	-2.29	1.46	1.50
29	b	731	CLA	C3B-C4B	2.29	1.49	1.42
29	A	212	CLA	C3B-C4B	2.29	1.49	1.42
29	I	210	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	311	CLA	CHC-C1C	2.29	1.43	1.38
29	A	218	CLA	CMC-C2C	-2.29	1.46	1.50
29	M	306	CLA	C3B-C4B	2.29	1.49	1.42
29	D	316	CLA	C3B-C4B	2.29	1.49	1.42
34	b	730	LMG	O8-C9	-2.28	1.40	1.45
29	P	217	CLA	C3B-C4B	2.28	1.49	1.42
29	B	316	CLA	C3B-C4B	2.28	1.49	1.42
29	E	305	CLA	CMB-C2B	-2.28	1.46	1.50
36	J	301	DD6	O1-C20	-2.28	1.43	1.46
39	P	213	KC1	C1B-NB	-2.28	1.34	1.37
29	L	308	CLA	C3B-C4B	2.28	1.49	1.42
29	b	724	CLA	CHC-C1C	2.28	1.43	1.38
29	E	313	CLA	CHC-C1C	2.28	1.43	1.38
29	f	805	CLA	C3B-C4B	2.28	1.49	1.42
29	C	314	CLA	C3B-C4B	2.28	1.49	1.42
29	K	213	CLA	CHC-C1C	2.28	1.43	1.38
29	a	802	CLA	MG-NB	-2.28	2.01	2.05
39	P	216	KC1	C1B-NB	-2.28	1.34	1.37
29	E	310	CLA	C3B-C4B	2.28	1.49	1.42
29	D	311	CLA	CHC-C1C	2.28	1.43	1.38
29	Q	315	CLA	C3B-C4B	2.28	1.49	1.42
29	D	313	CLA	MG-NB	-2.28	2.01	2.05
36	G	307	DD6	C-C1	-2.28	1.46	1.50
39	G	318	KC1	C1B-NB	-2.28	1.34	1.37
29	I	211	CLA	CHC-C1C	2.28	1.43	1.38
29	D	313	CLA	CHC-C1C	2.28	1.43	1.38
29	E	313	CLA	C3B-C4B	2.28	1.49	1.42
29	b	709	CLA	C3B-C4B	2.28	1.49	1.42
34	K	220	LMG	O7-C8	-2.28	1.41	1.46
29	E	308	CLA	C3B-C4B	2.28	1.49	1.42
29	E	306	CLA	CMD-C2D	-2.28	1.46	1.50
29	F	307	CLA	C3B-C4B	2.28	1.49	1.42
29	D	312	CLA	C3B-C4B	2.27	1.49	1.42
29	h	201	CLA	CMC-C2C	-2.27	1.46	1.50
39	O	315	KC1	C1B-NB	-2.27	1.34	1.37
29	T	313	CLA	C3B-C4B	2.27	1.49	1.42
29	b	726	CLA	MG-NB	-2.27	2.01	2.05
29	C	313	CLA	CMD-C2D	-2.27	1.46	1.50
29	b	724	CLA	C3B-C4B	2.27	1.49	1.42
29	b	706	CLA	CMB-C2B	-2.27	1.46	1.50
29	O	313	CLA	C3B-C4B	2.27	1.49	1.42
29	a	806	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	214	CLA	CHC-C1C	2.27	1.43	1.38
29	b	705	CLA	CMB-C2B	-2.27	1.46	1.50
29	a	827	CLA	C3B-C4B	2.27	1.49	1.42
29	I	213	CLA	CHC-C1C	2.27	1.43	1.38
29	Q	315	CLA	CHC-C1C	2.27	1.43	1.38
29	E	314	CLA	CHC-C1C	2.27	1.43	1.38
29	K	212	CLA	CMD-C2D	-2.27	1.46	1.50
29	I	214	CLA	CMD-C2D	-2.27	1.46	1.50
29	A	215	CLA	C3B-C4B	2.27	1.49	1.42
29	a	831	CLA	CMD-C2D	-2.27	1.46	1.50
29	B	310	CLA	MG-NB	-2.27	2.01	2.05
29	a	837	CLA	CHC-C1C	2.27	1.43	1.38
29	O	309	CLA	CHC-C1C	2.27	1.43	1.38
29	I	201	CLA	C3B-C4B	2.27	1.49	1.42
29	I	216	CLA	C3B-C4B	2.27	1.49	1.42
29	L	310	CLA	C3B-C4B	2.27	1.49	1.42
29	L	316	CLA	CMD-C2D	-2.27	1.46	1.50
29	G	317	CLA	C3B-C4B	2.26	1.49	1.42
29	a	810	CLA	CMB-C2B	-2.26	1.46	1.50
29	M	309	CLA	CHC-C1C	2.26	1.43	1.38
29	L	312	CLA	CHC-C1C	2.26	1.43	1.38
29	N	316	CLA	CHC-C1C	2.26	1.43	1.38
29	O	311	CLA	CHC-C1C	2.26	1.43	1.38
29	K	217	CLA	C3B-C4B	2.26	1.49	1.42
29	A	211	CLA	C3B-C4B	2.26	1.49	1.42
29	T	309	CLA	C3B-C4B	2.26	1.49	1.42
29	a	810	CLA	CMD-C2D	-2.26	1.46	1.50
29	b	708	CLA	MG-NB	-2.26	2.01	2.05
29	a	814	CLA	C3B-C4B	2.26	1.49	1.42
29	A	210	CLA	CMB-C2B	-2.26	1.46	1.50
29	G	319	CLA	C3B-C4B	2.26	1.49	1.42
29	F	315	CLA	C3B-C4B	2.26	1.49	1.42
29	a	802	CLA	CMD-C2D	-2.26	1.46	1.50
29	b	736	CLA	CHC-C1C	2.26	1.43	1.38
29	a	821	CLA	CHC-C1C	2.26	1.43	1.38
29	a	824	CLA	CHC-C1C	2.26	1.43	1.38
29	F	307	CLA	CHC-C1C	2.26	1.43	1.38
29	G	313	CLA	CMD-C2D	-2.26	1.46	1.50
38	E	304	UIX	C15-C20	-2.26	1.50	1.54
29	D	308	CLA	C3B-C4B	2.26	1.49	1.42
29	M	310	CLA	CHC-C1C	2.26	1.43	1.38
29	l	510	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	803	CLA	CMD-C2D	-2.26	1.46	1.50
29	C	309	CLA	C3B-C4B	2.26	1.49	1.42
29	F	310	CLA	CHC-C1C	2.26	1.43	1.38
29	a	812	CLA	C3B-C4B	2.26	1.49	1.42
29	I	209	CLA	C3B-C4B	2.26	1.49	1.42
29	B	309	CLA	C3B-C4B	2.26	1.49	1.42
29	a	818	CLA	CHC-C1C	2.26	1.43	1.38
39	D	310	KC1	C1B-NB	-2.26	1.34	1.37
29	F	311	CLA	C3B-C4B	2.26	1.49	1.42
29	l	504	CLA	CMD-C2D	-2.25	1.46	1.50
29	a	809	CLA	C3B-C4B	2.25	1.49	1.42
36	L	301	DD6	O1-C20	-2.25	1.43	1.46
29	l	502	CLA	CMB-C2B	-2.25	1.46	1.50
39	H	311	KC1	C1B-NB	-2.25	1.34	1.37
29	A	217	CLA	CHC-C1C	2.25	1.43	1.38
29	J	305	CLA	CHC-C1C	2.25	1.43	1.38
29	N	313	CLA	CMD-C2D	-2.25	1.46	1.50
29	b	711	CLA	CHC-C1C	2.25	1.43	1.38
29	l	504	CLA	CHC-C1C	2.25	1.43	1.38
29	G	317	CLA	CHC-C1C	2.25	1.43	1.38
29	E	308	CLA	CHC-C1C	2.25	1.43	1.38
29	H	315	CLA	CHC-C1C	2.25	1.43	1.38
29	O	308	CLA	CHC-C1C	2.25	1.43	1.38
29	a	806	CLA	CMD-C2D	-2.25	1.46	1.50
29	K	217	CLA	CMB-C2B	-2.25	1.46	1.50
29	B	308	CLA	C3B-C4B	2.25	1.49	1.42
29	L	317	CLA	CHC-C1C	2.25	1.43	1.38
29	F	310	CLA	CMC-C2C	-2.25	1.46	1.50
29	H	310	CLA	CHC-C1C	2.25	1.43	1.38
29	l	501	CLA	CMB-C2B	-2.25	1.46	1.50
29	L	313	CLA	CHC-C1C	2.25	1.43	1.38
29	l	509	CLA	C3B-C4B	2.25	1.49	1.42
37	H	306	PID	C8-C9	-2.25	1.41	1.46
29	N	313	CLA	MG-NB	-2.25	2.01	2.05
29	b	722	CLA	C3B-C4B	2.25	1.49	1.42
29	K	218	CLA	CMD-C2D	-2.25	1.46	1.50
29	Q	310	CLA	C3B-C4B	2.25	1.49	1.42
29	E	314	CLA	C3B-C4B	2.25	1.49	1.42
29	J	308	CLA	C3B-C4B	2.25	1.49	1.42
29	a	805	CLA	CHC-C1C	2.25	1.43	1.38
29	b	712	CLA	CMB-C2B	-2.25	1.46	1.50
39	T	312	KC1	C1B-NB	-2.25	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	218	CLA	CHC-C1C	2.25	1.43	1.38
29	I	210	CLA	C3B-C4B	2.25	1.49	1.42
29	G	301	CLA	CHC-C1C	2.25	1.43	1.38
29	D	309	CLA	CHC-C1C	2.24	1.43	1.38
29	b	709	CLA	CHC-C1C	2.24	1.43	1.38
29	A	211	CLA	CHC-C1C	2.24	1.43	1.38
29	Q	312	CLA	CHC-C1C	2.24	1.43	1.38
29	a	824	CLA	CMD-C2D	-2.24	1.46	1.50
29	I	207	CLA	C3B-C4B	2.24	1.49	1.42
29	J	311	CLA	C3B-C4B	2.24	1.49	1.42
39	L	306	KC1	C1B-NB	-2.24	1.34	1.37
29	a	816	CLA	C3B-C4B	2.24	1.49	1.42
29	E	306	CLA	C3B-C4B	2.24	1.49	1.42
29	A	208	CLA	CHC-C1C	2.24	1.43	1.38
29	C	311	CLA	CHC-C1C	2.24	1.43	1.38
29	b	725	CLA	C3B-C4B	2.24	1.49	1.42
29	B	310	CLA	CHC-C1C	2.24	1.43	1.38
29	i	203	CLA	CMD-C2D	-2.24	1.46	1.50
29	G	304	CLA	C3B-C4B	2.24	1.49	1.42
29	a	829	CLA	CMB-C2B	-2.24	1.46	1.50
29	G	301	CLA	C3B-C4B	2.24	1.49	1.42
29	G	312	CLA	CHC-C1C	2.24	1.43	1.38
29	b	705	CLA	C3B-C4B	2.24	1.49	1.42
29	J	306	CLA	CMD-C2D	-2.24	1.46	1.50
29	b	731	CLA	CHC-C1C	2.24	1.43	1.38
29	l	501	CLA	CHC-C1C	2.24	1.43	1.38
29	A	207	CLA	CHC-C1C	2.24	1.43	1.38
29	B	311	CLA	CHC-C1C	2.24	1.43	1.38
29	l	508	CLA	CHC-C1C	2.24	1.43	1.38
29	M	309	CLA	MG-NB	-2.24	2.01	2.05
29	K	211	CLA	C3B-C4B	2.24	1.49	1.42
29	b	705	CLA	CMC-C2C	-2.24	1.46	1.50
29	J	311	CLA	CMB-C2B	-2.24	1.46	1.50
36	M	304	DD6	O1-C20	-2.24	1.43	1.46
29	D	308	CLA	CHC-C1C	2.24	1.43	1.38
29	C	308	CLA	CHC-C1C	2.24	1.43	1.38
29	a	801	CLA	CMB-C2B	-2.24	1.46	1.50
29	A	209	CLA	CHC-C1C	2.24	1.43	1.38
29	K	213	CLA	CMD-C2D	-2.24	1.46	1.50
38	A	203	UIX	C15-C20	-2.24	1.50	1.54
29	l	503	CLA	CHC-C1C	2.24	1.43	1.38
29	A	218	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	309	CLA	CMB-C2B	-2.23	1.46	1.50
29	b	720	CLA	CHC-C1C	2.23	1.43	1.38
29	f	803	CLA	C3B-C4B	2.23	1.49	1.42
29	i	203	CLA	MG-NB	-2.23	2.01	2.05
36	G	305	DD6	C28-C27	-2.23	1.49	1.50
29	J	313	CLA	CHC-C1C	2.23	1.43	1.38
29	F	316	CLA	CHC-C1C	2.23	1.43	1.38
29	A	208	CLA	C3B-C4B	2.23	1.49	1.42
29	f	802	CLA	MG-NB	-2.23	2.01	2.05
29	a	822	CLA	C3B-C4B	2.23	1.49	1.42
29	N	311	CLA	C3B-C4B	2.23	1.49	1.42
29	a	808	CLA	CMD-C2D	-2.23	1.46	1.50
29	L	312	CLA	CMD-C2D	-2.23	1.46	1.50
29	F	315	CLA	CHC-C1C	2.23	1.43	1.38
29	i	201	CLA	C3B-C4B	2.23	1.49	1.42
29	Q	312	CLA	C3B-C4B	2.23	1.49	1.42
29	J	307	CLA	MG-NB	-2.23	2.01	2.05
29	G	302	CLA	CMD-C2D	-2.23	1.46	1.50
29	I	216	CLA	CHC-C1C	2.23	1.43	1.38
29	L	308	CLA	CHC-C1C	2.23	1.43	1.38
29	a	826	CLA	CMD-C2D	-2.23	1.46	1.50
29	H	313	CLA	CHC-C1C	2.23	1.43	1.38
29	a	831	CLA	C3B-C4B	2.23	1.49	1.42
29	a	813	CLA	CHC-C1C	2.23	1.43	1.38
29	b	710	CLA	CHC-C1C	2.23	1.43	1.38
29	E	310	CLA	CHC-C1C	2.23	1.43	1.38
29	L	309	CLA	MG-NB	-2.23	2.01	2.05
29	P	209	CLA	CHC-C1C	2.23	1.43	1.38
29	E	305	CLA	C3B-C4B	2.23	1.49	1.42
29	a	807	CLA	CHC-C1C	2.23	1.42	1.38
29	b	723	CLA	CMD-C2D	-2.23	1.46	1.50
29	O	313	CLA	CHC-C1C	2.23	1.42	1.38
29	T	311	CLA	CHC-C1C	2.23	1.42	1.38
29	B	314	CLA	C3B-C4B	2.23	1.49	1.42
29	b	707	CLA	CHC-C1C	2.23	1.42	1.38
29	b	725	CLA	CMB-C2B	-2.23	1.46	1.50
29	T	316	CLA	CHC-C1C	2.23	1.42	1.38
29	K	207	CLA	CHC-C1C	2.23	1.42	1.38
29	j	104	CLA	C3B-C4B	2.23	1.49	1.42
29	A	212	CLA	CHC-C1C	2.22	1.42	1.38
29	a	807	CLA	C3B-C4B	2.22	1.49	1.42
29	A	214	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	725	CLA	MG-NB	-2.22	2.01	2.05
29	b	703	CLA	CMD-C2D	-2.22	1.46	1.50
29	i	202	CLA	MG-NB	-2.22	2.01	2.05
29	b	702	CLA	MG-NB	-2.22	2.01	2.05
29	b	724	CLA	MG-NB	-2.22	2.01	2.05
29	a	817	CLA	CHC-C1C	2.22	1.42	1.38
29	T	309	CLA	CHC-C1C	2.22	1.42	1.38
29	a	830	CLA	C3B-C4B	2.22	1.49	1.42
29	l	508	CLA	C3B-C4B	2.22	1.49	1.42
29	M	315	CLA	CHC-C1C	2.22	1.42	1.38
29	N	313	CLA	CHC-C1C	2.22	1.42	1.38
29	C	309	CLA	CHC-C1C	2.22	1.42	1.38
29	C	313	CLA	CHC-C1C	2.22	1.42	1.38
29	l	502	CLA	C3B-C4B	2.22	1.49	1.42
29	L	310	CLA	CHC-C1C	2.22	1.42	1.38
29	H	308	CLA	CHC-C1C	2.22	1.42	1.38
29	G	317	CLA	MG-NB	-2.22	2.01	2.05
29	J	309	CLA	MG-NB	-2.22	2.01	2.05
29	H	307	CLA	CHC-C1C	2.22	1.42	1.38
29	N	308	CLA	CHC-C1C	2.22	1.42	1.38
29	L	309	CLA	C3B-C4B	2.22	1.49	1.42
29	C	309	CLA	MG-NB	-2.22	2.01	2.05
29	L	311	CLA	CHC-C1C	2.22	1.42	1.38
29	a	803	CLA	C3B-C4B	2.22	1.49	1.42
29	b	726	CLA	CMB-C2B	-2.22	1.46	1.50
29	A	214	CLA	MG-NB	-2.22	2.01	2.05
29	b	716	CLA	C3B-C4B	2.22	1.49	1.42
29	E	306	CLA	MG-NB	-2.22	2.01	2.05
29	a	805	CLA	CMD-C2D	-2.22	1.46	1.50
36	J	302	DD6	O1-C20	-2.22	1.43	1.46
29	b	714	CLA	CMD-C2D	-2.21	1.46	1.50
29	a	808	CLA	C3B-C4B	2.21	1.49	1.42
29	O	313	CLA	CMB-C2B	-2.21	1.46	1.50
29	G	311	CLA	CHC-C1C	2.21	1.42	1.38
29	K	216	CLA	CHC-C1C	2.21	1.42	1.38
29	b	702	CLA	CMB-C2B	-2.21	1.46	1.50
29	N	311	CLA	CHC-C1C	2.21	1.42	1.38
29	b	701	CLA	C3B-C4B	2.21	1.49	1.42
29	K	216	CLA	CMD-C2D	-2.21	1.46	1.50
29	l	504	CLA	C3B-C4B	2.21	1.49	1.42
29	Q	310	CLA	CHC-C1C	2.21	1.42	1.38
29	B	314	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	827	CLA	CHC-C1C	2.21	1.42	1.38
29	D	314	CLA	CHC-C1C	2.21	1.42	1.38
29	C	313	CLA	C3B-C4B	2.21	1.49	1.42
29	a	812	CLA	CHC-C1C	2.21	1.42	1.38
29	b	706	CLA	CMC-C2C	-2.21	1.46	1.50
29	K	211	CLA	CHC-C1C	2.21	1.42	1.38
29	a	826	CLA	C3B-C4B	2.21	1.49	1.42
29	B	308	CLA	CHC-C1C	2.21	1.42	1.38
29	N	314	CLA	CHC-C1C	2.21	1.42	1.38
29	b	705	CLA	CMD-C2D	-2.21	1.46	1.50
29	B	311	CLA	CMC-C2C	-2.21	1.46	1.50
29	a	826	CLA	CHC-C1C	2.21	1.42	1.38
29	Q	307	CLA	CHC-C1C	2.21	1.42	1.38
39	F	314	KC1	C1B-NB	-2.21	1.35	1.37
39	A	205	KC1	C4A-C3A	-2.21	1.40	1.44
29	b	701	CLA	CHC-C1C	2.21	1.42	1.38
29	a	809	CLA	CHC-C1C	2.21	1.42	1.38
29	l	502	CLA	CMC-C2C	-2.21	1.46	1.50
29	a	824	CLA	C3B-C4B	2.21	1.49	1.42
29	a	820	CLA	MG-NB	-2.20	2.01	2.05
29	B	312	CLA	CHC-C1C	2.20	1.42	1.38
29	K	212	CLA	C3B-C4B	2.20	1.49	1.42
29	b	720	CLA	MG-NB	-2.20	2.01	2.05
29	a	803	CLA	CMB-C2B	-2.20	1.46	1.50
29	A	216	CLA	CMB-C2B	-2.20	1.46	1.50
29	b	724	CLA	CMD-C2D	-2.20	1.46	1.50
29	b	715	CLA	CMD-C2D	-2.20	1.46	1.50
29	A	208	CLA	MG-NB	-2.20	2.01	2.05
29	J	307	CLA	CHC-C1C	2.20	1.42	1.38
29	Q	313	CLA	CHC-C1C	2.20	1.42	1.38
29	b	718	CLA	C3B-C4B	2.20	1.49	1.42
29	G	313	CLA	CHC-C1C	2.20	1.42	1.38
29	J	308	CLA	CHC-C1C	2.20	1.42	1.38
29	P	217	CLA	CMC-C2C	-2.20	1.46	1.50
29	a	831	CLA	CHC-C1C	2.20	1.42	1.38
29	I	214	CLA	CHC-C1C	2.20	1.42	1.38
29	F	308	CLA	CHC-C1C	2.20	1.42	1.38
29	b	717	CLA	CMD-C2D	-2.20	1.46	1.50
29	J	310	CLA	MG-NB	-2.20	2.01	2.05
29	T	308	CLA	CHC-C1C	2.20	1.42	1.38
29	a	830	CLA	MG-NB	-2.20	2.01	2.05
29	a	816	CLA	CHC-C1C	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	830	CLA	CHC-C1C	2.20	1.42	1.38
29	E	309	CLA	CHC-C1C	2.20	1.42	1.38
29	b	711	CLA	CMB-C2B	-2.20	1.46	1.50
29	Q	312	CLA	CMD-C2D	-2.20	1.46	1.50
29	a	820	CLA	CHC-C1C	2.20	1.42	1.38
29	b	710	CLA	CMD-C2D	-2.20	1.46	1.50
29	f	805	CLA	CHC-C1C	2.20	1.42	1.38
29	J	307	CLA	C3B-C4B	2.20	1.49	1.42
29	a	814	CLA	CMC-C2C	-2.20	1.46	1.50
29	M	315	CLA	MG-NB	-2.20	2.01	2.05
29	b	715	CLA	C3B-C4B	2.20	1.49	1.42
29	M	314	CLA	MG-NB	-2.20	2.01	2.05
29	I	212	CLA	CMB-C2B	-2.19	1.46	1.50
29	A	210	CLA	C3B-C4B	2.19	1.49	1.42
29	E	306	CLA	CHC-C1C	2.19	1.42	1.38
29	M	308	CLA	C3B-C4B	2.19	1.49	1.42
29	M	306	CLA	CHC-C1C	2.19	1.42	1.38
29	L	309	CLA	CHC-C1C	2.19	1.42	1.38
29	f	805	CLA	MG-NB	-2.19	2.01	2.05
29	B	311	CLA	C3B-C4B	2.19	1.49	1.42
29	a	828	CLA	CHC-C1C	2.19	1.42	1.38
29	a	824	CLA	MG-NB	-2.19	2.01	2.05
29	J	306	CLA	CHC-C1C	2.19	1.42	1.38
29	D	316	CLA	CHC-C1C	2.19	1.42	1.38
29	A	218	CLA	CMD-C2D	-2.19	1.46	1.50
29	E	315	CLA	CHC-C1C	2.19	1.42	1.38
29	I	212	CLA	MG-NB	-2.19	2.01	2.05
29	G	316	CLA	CMD-C2D	-2.19	1.46	1.50
29	O	313	CLA	CMD-C2D	-2.19	1.46	1.50
29	a	814	CLA	CHC-C1C	2.19	1.42	1.38
29	B	316	CLA	CHC-C1C	2.19	1.42	1.38
29	A	216	CLA	MG-NB	-2.19	2.01	2.05
29	B	309	CLA	CHC-C1C	2.19	1.42	1.38
29	a	829	CLA	C3B-C4B	2.19	1.49	1.42
29	b	717	CLA	C3B-C4B	2.19	1.49	1.42
29	b	721	CLA	CHC-C1C	2.19	1.42	1.38
29	a	808	CLA	MG-NB	-2.19	2.01	2.05
29	f	803	CLA	MG-NB	-2.19	2.01	2.05
29	G	312	CLA	CMD-C2D	-2.19	1.46	1.50
29	M	311	CLA	CMD-C2D	-2.19	1.46	1.50
29	D	316	CLA	CMC-C2C	-2.19	1.46	1.50
29	G	314	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	504	CLA	MG-NB	-2.19	2.01	2.05
29	B	309	CLA	MG-NB	-2.19	2.01	2.05
29	B	307	CLA	CHC-C1C	2.19	1.42	1.38
29	f	802	CLA	CMD-C2D	-2.19	1.46	1.50
29	M	315	CLA	CMD-C2D	-2.19	1.46	1.50
29	L	316	CLA	CMC-C2C	-2.19	1.46	1.50
29	B	311	CLA	CMD-C2D	-2.19	1.46	1.50
29	b	701	CLA	CMD-C2D	-2.19	1.46	1.50
29	A	211	CLA	CMD-C2D	-2.19	1.46	1.50
29	l	505	CLA	C3B-C4B	2.19	1.49	1.42
29	I	210	CLA	CMB-C2B	-2.19	1.46	1.50
29	E	315	CLA	CMB-C2B	-2.19	1.46	1.50
29	a	803	CLA	CMD-C2D	-2.19	1.46	1.50
29	a	807	CLA	CMD-C2D	-2.19	1.46	1.50
29	b	722	CLA	CMD-C2D	-2.19	1.46	1.50
29	L	307	CLA	C3B-C4B	2.19	1.49	1.42
29	a	827	CLA	MG-NB	-2.19	2.01	2.05
29	C	313	CLA	MG-NB	-2.19	2.01	2.05
29	b	726	CLA	CMD-C2D	-2.19	1.46	1.50
29	F	313	CLA	CMB-C2B	-2.19	1.46	1.50
39	N	315	KC1	C1B-NB	-2.18	1.35	1.37
29	b	717	CLA	CHC-C1C	2.18	1.42	1.38
29	A	216	CLA	CHC-C1C	2.18	1.42	1.38
29	P	210	CLA	CHC-C1C	2.18	1.42	1.38
29	a	823	CLA	CMC-C2C	-2.18	1.46	1.50
29	l	501	CLA	MG-NB	-2.18	2.01	2.05
29	K	210	CLA	MG-NB	-2.18	2.01	2.05
29	f	802	CLA	C3B-C4B	2.18	1.49	1.42
29	b	712	CLA	C3B-C4B	2.18	1.49	1.42
29	a	802	CLA	CMB-C2B	-2.18	1.46	1.50
29	B	315	CLA	C3B-C4B	2.18	1.49	1.42
29	B	306	CLA	CMB-C2B	-2.18	1.46	1.50
29	G	319	CLA	CHC-C1C	2.18	1.42	1.38
29	i	201	CLA	CMD-C2D	-2.18	1.46	1.50
37	P	208	PID	C20-C21	2.18	1.40	1.35
29	b	713	CLA	CHC-C1C	2.18	1.42	1.38
29	a	820	CLA	CMB-C2B	-2.18	1.46	1.50
29	b	720	CLA	CMB-C2B	-2.18	1.46	1.50
29	b	722	CLA	CMC-C2C	-2.18	1.46	1.50
29	I	208	CLA	CHC-C1C	2.18	1.42	1.38
39	K	215	KC1	C1D-ND	-2.18	1.35	1.37
29	B	315	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	304	CLA	CHC-C1C	2.18	1.42	1.38
29	K	209	CLA	CMD-C2D	-2.18	1.46	1.50
29	b	721	CLA	C3B-C4B	2.18	1.49	1.42
29	C	316	CLA	C3B-C4B	2.18	1.49	1.42
29	l	509	CLA	CHC-C1C	2.18	1.42	1.38
29	K	211	CLA	CMD-C2D	-2.18	1.46	1.50
29	J	309	CLA	C3B-C4B	2.18	1.49	1.42
36	F	301	DD6	C21-C20	2.18	1.55	1.51
29	a	810	CLA	MG-NB	-2.18	2.01	2.05
29	a	804	CLA	CMC-C2C	-2.18	1.46	1.50
29	D	308	CLA	CMD-C2D	-2.18	1.46	1.50
29	J	311	CLA	CMD-C2D	-2.18	1.46	1.50
29	l	505	CLA	CHC-C1C	2.18	1.42	1.38
29	J	311	CLA	MG-NB	-2.18	2.01	2.05
29	I	201	CLA	CMD-C2D	-2.18	1.46	1.50
29	B	315	CLA	CMB-C2B	-2.18	1.46	1.50
29	l	501	CLA	C3B-C4B	2.18	1.49	1.42
29	B	315	CLA	CHC-C1C	2.18	1.42	1.38
29	l	502	CLA	CHC-C1C	2.18	1.42	1.38
29	a	829	CLA	MG-NB	-2.18	2.01	2.05
29	G	316	CLA	MG-NB	-2.18	2.01	2.05
29	K	218	CLA	CMB-C2B	-2.18	1.46	1.50
29	a	815	CLA	CHC-C1C	2.18	1.42	1.38
29	a	822	CLA	CHC-C1C	2.18	1.42	1.38
29	a	811	CLA	CHC-C1C	2.18	1.42	1.38
29	G	314	CLA	CMD-C2D	-2.18	1.46	1.50
29	E	314	CLA	MG-NB	-2.18	2.01	2.05
29	F	311	CLA	CHC-C1C	2.17	1.42	1.38
29	I	207	CLA	CMD-C2D	-2.17	1.46	1.50
29	b	722	CLA	CHC-C1C	2.17	1.42	1.38
29	G	311	CLA	C3B-C4B	2.17	1.49	1.42
29	l	505	CLA	MG-NB	-2.17	2.01	2.05
29	b	724	CLA	CMB-C2B	-2.17	1.46	1.50
29	E	308	CLA	CMD-C2D	-2.17	1.46	1.50
29	B	308	CLA	MG-NB	-2.17	2.01	2.05
29	a	802	CLA	C1B-C2B	2.17	1.48	1.43
29	a	819	CLA	MG-NB	-2.17	2.01	2.05
29	I	207	CLA	MG-NB	-2.17	2.01	2.05
29	l	502	CLA	CMD-C2D	-2.17	1.46	1.50
29	G	314	CLA	CMC-C2C	-2.17	1.46	1.50
29	F	308	CLA	CMD-C2D	-2.17	1.46	1.50
29	B	316	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	207	CLA	MG-NB	-2.17	2.01	2.05
29	a	811	CLA	MG-NB	-2.17	2.01	2.05
29	a	831	CLA	MG-NB	-2.17	2.01	2.05
36	G	307	DD6	C19-C18	-2.17	1.49	1.52
29	K	208	CLA	CMB-C2B	-2.17	1.46	1.50
29	b	712	CLA	MG-NB	-2.17	2.01	2.05
29	K	209	CLA	MG-NB	-2.17	2.01	2.05
29	l	502	CLA	MG-NB	-2.17	2.01	2.05
29	a	808	CLA	CMB-C2B	-2.17	1.46	1.50
29	b	701	CLA	MG-NB	-2.17	2.01	2.05
29	b	710	CLA	C3B-C4B	2.17	1.49	1.42
29	a	823	CLA	CMD-C2D	-2.17	1.46	1.50
29	a	825	CLA	CMC-C2C	-2.17	1.46	1.50
29	Q	310	CLA	CMD-C2D	-2.17	1.46	1.50
29	a	809	CLA	MG-NB	-2.17	2.01	2.05
29	B	314	CLA	CHC-C1C	2.17	1.42	1.38
40	B	317	SQD	O8-S	2.17	1.55	1.47
29	G	311	CLA	CMD-C2D	-2.17	1.46	1.50
29	Q	315	CLA	MG-NB	-2.17	2.01	2.05
29	b	715	CLA	CMC-C2C	-2.17	1.46	1.50
29	A	208	CLA	CMD-C2D	-2.17	1.46	1.50
29	l	509	CLA	CMB-C2B	-2.17	1.46	1.50
29	K	208	CLA	CMD-C2D	-2.17	1.46	1.50
29	a	825	CLA	C3B-C4B	2.17	1.49	1.42
29	b	723	CLA	MG-NB	-2.17	2.01	2.05
29	E	311	CLA	MG-NB	-2.17	2.01	2.05
29	F	313	CLA	C3B-C4B	2.17	1.49	1.42
29	Q	313	CLA	CMB-C2B	-2.17	1.46	1.50
32	b	728	BCR	C1-C6	-2.17	1.51	1.53
29	I	209	CLA	CHC-C1C	2.17	1.42	1.38
29	i	202	CLA	CMD-C2D	-2.17	1.46	1.50
29	I	213	CLA	CMD-C2D	-2.17	1.46	1.50
29	J	310	CLA	CMD-C2D	-2.17	1.46	1.50
29	b	715	CLA	MG-NB	-2.17	2.01	2.05
29	b	703	CLA	CMC-C2C	-2.16	1.46	1.50
29	L	308	CLA	CMD-C2D	-2.16	1.46	1.50
29	b	708	CLA	C3B-C4B	2.16	1.49	1.42
29	K	208	CLA	MG-NB	-2.16	2.01	2.05
29	a	819	CLA	CHC-C1C	2.16	1.42	1.38
29	b	716	CLA	CMD-C2D	-2.16	1.46	1.50
29	K	217	CLA	CMD-C2D	-2.16	1.46	1.50
29	a	816	CLA	MG-NB	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	314	CLA	MG-NB	-2.16	2.01	2.05
29	b	715	CLA	CMB-C2B	-2.16	1.46	1.50
29	C	309	CLA	CMD-C2D	-2.16	1.46	1.50
29	F	312	CLA	CMD-C2D	-2.16	1.46	1.50
29	M	314	CLA	C3B-C4B	2.16	1.49	1.42
29	P	217	CLA	CHC-C1C	2.16	1.42	1.38
29	K	211	CLA	CMC-C2C	-2.16	1.46	1.50
29	L	309	CLA	CMD-C2D	-2.16	1.46	1.50
29	L	310	CLA	MG-NB	-2.16	2.01	2.05
29	Q	313	CLA	C3B-C4B	2.16	1.49	1.42
29	b	714	CLA	MG-NB	-2.16	2.01	2.05
29	A	206	CLA	CHC-C1C	2.16	1.42	1.38
29	M	307	CLA	CMD-C2D	-2.16	1.46	1.50
29	l	503	CLA	MG-NB	-2.16	2.01	2.05
29	A	207	CLA	CMD-C2D	-2.16	1.46	1.50
29	E	305	CLA	CMD-C2D	-2.16	1.46	1.50
29	H	313	CLA	MG-NB	-2.16	2.01	2.05
29	J	311	CLA	CHC-C1C	2.16	1.42	1.38
29	D	313	CLA	CMB-C2B	-2.16	1.46	1.50
29	I	212	CLA	CMD-C2D	-2.16	1.46	1.50
29	F	313	CLA	MG-NB	-2.16	2.01	2.05
29	l	510	CLA	CHC-C1C	2.16	1.42	1.38
29	a	824	CLA	CMB-C2B	-2.16	1.46	1.50
29	b	702	CLA	CMD-C2D	-2.16	1.46	1.50
29	a	822	CLA	MG-NB	-2.16	2.01	2.05
29	b	717	CLA	MG-NB	-2.16	2.01	2.05
29	b	707	CLA	CMB-C2B	-2.16	1.46	1.50
29	T	311	CLA	MG-NB	-2.16	2.01	2.05
29	b	706	CLA	CMD-C2D	-2.16	1.46	1.50
29	K	208	CLA	CHC-C1C	2.16	1.42	1.38
29	B	316	CLA	CMB-C2B	-2.16	1.46	1.50
29	D	314	CLA	CMB-C2B	-2.16	1.46	1.50
29	G	304	CLA	MG-NB	-2.16	2.01	2.05
29	I	217	CLA	CMB-C2B	-2.15	1.46	1.50
29	G	304	CLA	CMD-C2D	-2.15	1.46	1.50
39	E	312	KC1	C1D-ND	-2.15	1.35	1.37
29	b	711	CLA	CMD-C2D	-2.15	1.46	1.50
29	b	713	CLA	CMB-C2B	-2.15	1.46	1.50
29	F	307	CLA	CMD-C2D	-2.15	1.46	1.50
29	J	307	CLA	CMD-C2D	-2.15	1.46	1.50
29	b	711	CLA	C3B-C4B	2.15	1.49	1.42
29	b	724	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	315	CLA	CMD-C2D	-2.15	1.46	1.50
29	A	216	CLA	CMD-C2D	-2.15	1.46	1.50
29	B	306	CLA	CMD-C2D	-2.15	1.46	1.50
29	N	314	CLA	CMC-C2C	-2.15	1.46	1.50
29	K	211	CLA	MG-NB	-2.15	2.01	2.05
29	K	214	CLA	CMB-C2B	-2.15	1.46	1.50
29	E	314	CLA	CMB-C2B	-2.15	1.46	1.50
29	a	825	CLA	MG-NB	-2.15	2.01	2.05
29	G	313	CLA	MG-NB	-2.15	2.01	2.05
29	B	316	CLA	MG-NB	-2.15	2.01	2.05
29	b	708	CLA	CMC-C2C	-2.15	1.46	1.50
29	I	213	CLA	CMB-C2B	-2.15	1.46	1.50
29	K	218	CLA	MG-NB	-2.15	2.01	2.05
29	M	313	CLA	CMC-C2C	-2.15	1.46	1.50
29	a	806	CLA	CMC-C2C	-2.15	1.46	1.50
29	L	311	CLA	MG-NB	-2.15	2.01	2.05
29	l	509	CLA	MG-NB	-2.15	2.01	2.05
29	l	501	CLA	CMD-C2D	-2.15	1.46	1.50
29	l	505	CLA	CMB-C2B	-2.15	1.46	1.50
29	H	312	CLA	CMD-C2D	-2.15	1.46	1.50
29	G	301	CLA	CMD-C2D	-2.15	1.46	1.50
29	A	210	CLA	CHC-C1C	2.15	1.42	1.38
29	b	707	CLA	CMD-C2D	-2.15	1.46	1.50
29	D	312	CLA	CHC-C1C	2.15	1.42	1.38
39	B	313	KC1	C4A-C3A	-2.15	1.40	1.44
29	A	209	CLA	MG-NB	-2.15	2.01	2.05
29	a	826	CLA	CMB-C2B	-2.15	1.46	1.50
29	M	310	CLA	CMD-C2D	-2.15	1.46	1.50
29	A	212	CLA	MG-NB	-2.15	2.01	2.05
29	G	311	CLA	MG-NB	-2.15	2.01	2.05
29	G	312	CLA	MG-NB	-2.15	2.01	2.05
29	a	817	CLA	CMB-C2B	-2.15	1.46	1.50
29	b	719	CLA	CMB-C2B	-2.15	1.46	1.50
29	E	305	CLA	MG-NB	-2.14	2.01	2.05
29	b	716	CLA	CHC-C1C	2.14	1.42	1.38
29	F	316	CLA	CMD-C2D	-2.14	1.46	1.50
29	Q	313	CLA	MG-NB	-2.14	2.01	2.05
29	a	824	CLA	CMC-C2C	-2.14	1.46	1.50
29	M	307	CLA	MG-NB	-2.14	2.01	2.05
29	B	314	CLA	MG-NB	-2.14	2.01	2.05
29	a	830	CLA	CMD-C2D	-2.14	1.46	1.50
29	Q	310	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	308	CLA	MG-NB	-2.14	2.01	2.05
29	I	209	CLA	CMB-C2B	-2.14	1.46	1.50
29	L	312	CLA	CMB-C2B	-2.14	1.46	1.50
29	O	309	CLA	CMD-C2D	-2.14	1.46	1.50
36	G	305	DD6	O1-C20	-2.14	1.43	1.46
29	K	217	CLA	MG-NB	-2.14	2.01	2.05
29	I	214	CLA	CMB-C2B	-2.14	1.46	1.50
29	J	309	CLA	CHC-C1C	2.14	1.42	1.38
29	a	809	CLA	CMB-C2B	-2.14	1.46	1.50
29	a	829	CLA	CMD-C2D	-2.14	1.46	1.50
29	M	314	CLA	CMB-C2B	-2.14	1.46	1.50
29	B	309	CLA	CMD-C2D	-2.14	1.46	1.50
29	a	804	CLA	CHC-C1C	2.14	1.42	1.38
29	a	807	CLA	CMC-C2C	-2.14	1.46	1.50
29	K	210	CLA	CMD-C2D	-2.14	1.46	1.50
29	b	721	CLA	CMB-C2B	-2.14	1.46	1.50
29	a	826	CLA	MG-NB	-2.14	2.01	2.05
29	M	311	CLA	MG-NB	-2.14	2.01	2.05
29	K	207	CLA	CMD-C2D	-2.14	1.46	1.50
29	b	720	CLA	CMD-C2D	-2.14	1.46	1.50
39	F	309	KC1	C4A-C3A	-2.14	1.40	1.44
29	f	803	CLA	CHC-C1C	2.14	1.42	1.38
29	a	827	CLA	CMB-C2B	-2.14	1.46	1.50
29	b	718	CLA	CMC-C2C	-2.14	1.46	1.50
29	B	307	CLA	CMD-C2D	-2.14	1.46	1.50
29	b	736	CLA	CMB-C2B	-2.14	1.46	1.50
29	I	208	CLA	CMD-C2D	-2.14	1.46	1.50
29	L	310	CLA	CMB-C2B	-2.14	1.46	1.50
29	H	307	CLA	CMD-C2D	-2.14	1.46	1.50
29	G	314	CLA	MG-NB	-2.14	2.01	2.05
39	I	215	KC1	C1D-ND	-2.14	1.35	1.37
29	a	819	CLA	CMB-C2B	-2.14	1.46	1.50
29	b	714	CLA	CMB-C2B	-2.14	1.46	1.50
29	l	503	CLA	CMC-C2C	-2.14	1.46	1.50
29	G	302	CLA	MG-NB	-2.14	2.01	2.05
29	G	319	CLA	MG-NB	-2.14	2.01	2.05
29	G	317	CLA	CMD-C2D	-2.14	1.46	1.50
29	K	213	CLA	CMC-C2C	-2.14	1.46	1.50
29	L	315	CLA	CMC-C2C	-2.14	1.46	1.50
29	i	201	CLA	CHC-C1C	2.14	1.42	1.38
29	M	306	CLA	MG-NB	-2.14	2.01	2.05
29	a	818	CLA	CMB-C2B	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	309	CLA	CMC-C2C	-2.13	1.46	1.50
29	a	803	CLA	CHC-C1C	2.13	1.42	1.38
29	f	802	CLA	CHC-C1C	2.13	1.42	1.38
29	h	201	CLA	MG-NB	-2.13	2.01	2.05
29	I	209	CLA	CMD-C2D	-2.13	1.46	1.50
29	b	726	CLA	CHC-C1C	2.13	1.42	1.38
29	J	306	CLA	MG-NB	-2.13	2.01	2.05
29	E	310	CLA	MG-NB	-2.13	2.01	2.05
29	b	726	CLA	CMC-C2C	-2.13	1.46	1.50
29	l	509	CLA	CMD-C2D	-2.13	1.46	1.50
29	T	314	CLA	CMB-C2B	-2.13	1.46	1.50
29	b	704	CLA	CHC-C1C	2.13	1.42	1.38
29	b	712	CLA	CHC-C1C	2.13	1.42	1.38
29	i	203	CLA	CHC-C1C	2.13	1.42	1.38
29	L	307	CLA	CHC-C1C	2.13	1.42	1.38
29	A	215	CLA	MG-NB	-2.13	2.01	2.05
29	b	709	CLA	MG-NB	-2.13	2.01	2.05
29	B	314	CLA	CMC-C2C	-2.13	1.46	1.50
29	F	310	CLA	MG-NB	-2.13	2.01	2.05
29	a	827	CLA	CMD-C2D	-2.13	1.46	1.50
29	L	317	CLA	CMD-C2D	-2.13	1.46	1.50
29	Q	315	CLA	CMD-C2D	-2.13	1.46	1.50
29	I	212	CLA	CHC-C1C	2.13	1.42	1.38
39	O	310	KC1	C1D-ND	-2.13	1.35	1.37
29	L	308	CLA	MG-NB	-2.13	2.01	2.05
29	B	308	CLA	CMD-C2D	-2.13	1.46	1.50
29	Q	308	CLA	MG-NB	-2.13	2.01	2.05
29	b	736	CLA	CMD-C2D	-2.13	1.46	1.50
29	B	306	CLA	CHC-C1C	2.13	1.42	1.38
29	a	803	CLA	MG-NB	-2.13	2.01	2.05
29	l	510	CLA	CMB-C2B	-2.13	1.46	1.50
29	I	217	CLA	CMD-C2D	-2.13	1.46	1.50
29	M	311	CLA	CMB-C2B	-2.13	1.46	1.50
39	O	310	KC1	C4A-C3A	-2.13	1.40	1.44
29	a	822	CLA	CMD-C2D	-2.13	1.46	1.50
29	F	312	CLA	CMB-C2B	-2.13	1.46	1.50
29	i	201	CLA	CMB-C2B	-2.13	1.46	1.50
29	a	801	CLA	CMC-C2C	-2.13	1.46	1.50
29	F	312	CLA	CHC-C1C	2.13	1.42	1.38
39	B	313	KC1	C1D-ND	-2.13	1.35	1.37
29	a	837	CLA	MG-NB	-2.13	2.01	2.05
29	I	216	CLA	MG-NB	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	709	CLA	CMD-C2D	-2.13	1.46	1.50
29	h	201	CLA	CMD-C2D	-2.13	1.46	1.50
29	A	210	CLA	CMD-C2D	-2.13	1.46	1.50
29	l	510	CLA	CMD-C2D	-2.13	1.46	1.50
29	O	314	CLA	CMC-C2C	-2.13	1.46	1.50
39	E	307	KC1	C4A-C3A	-2.13	1.40	1.44
29	A	209	CLA	CMB-C2B	-2.13	1.46	1.50
29	G	312	CLA	CMB-C2B	-2.13	1.46	1.50
29	a	815	CLA	MG-NB	-2.13	2.01	2.05
29	I	213	CLA	MG-NB	-2.13	2.01	2.05
29	K	217	CLA	CHC-C1C	2.13	1.42	1.38
29	b	704	CLA	C3B-C4B	2.13	1.48	1.42
29	b	712	CLA	CMD-C2D	-2.13	1.46	1.50
29	F	308	CLA	MG-NB	-2.13	2.01	2.05
29	b	701	CLA	CMC-C2C	-2.13	1.46	1.50
29	F	313	CLA	CMD-C2D	-2.13	1.46	1.50
29	L	311	CLA	CMD-C2D	-2.13	1.46	1.50
29	I	210	CLA	CMD-C2D	-2.13	1.46	1.50
29	B	312	CLA	MG-NB	-2.13	2.01	2.05
29	A	209	CLA	CMD-C2D	-2.12	1.46	1.50
29	E	315	CLA	MG-NB	-2.12	2.01	2.05
29	A	215	CLA	CMB-C2B	-2.12	1.46	1.50
29	i	201	CLA	MG-NB	-2.12	2.01	2.05
40	J	314	SQD	O8-S	2.12	1.55	1.47
29	G	314	CLA	CHC-C1C	2.12	1.42	1.38
29	a	814	CLA	CMD-C2D	-2.12	1.46	1.50
29	b	710	CLA	CMB-C2B	-2.12	1.46	1.50
29	L	307	CLA	CMB-C2B	-2.12	1.46	1.50
29	a	806	CLA	MG-NB	-2.12	2.01	2.05
29	B	312	CLA	CMD-C2D	-2.12	1.46	1.50
29	b	705	CLA	MG-NB	-2.12	2.01	2.05
29	H	308	CLA	MG-NB	-2.12	2.01	2.05
29	b	725	CLA	CHC-C1C	2.12	1.42	1.38
29	j	104	CLA	CMD-C2D	-2.12	1.46	1.50
29	b	731	CLA	MG-NB	-2.12	2.01	2.05
29	L	307	CLA	CMD-C2D	-2.12	1.46	1.50
29	O	314	CLA	CMD-C2D	-2.12	1.46	1.50
29	P	214	CLA	CMD-C2D	-2.12	1.46	1.50
29	b	721	CLA	CMD-C2D	-2.12	1.46	1.50
29	A	212	CLA	CMD-C2D	-2.12	1.46	1.50
29	b	702	CLA	C3B-C4B	2.12	1.48	1.42
29	T	314	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Q	305	UIX	C15-C20	-2.12	1.51	1.54
29	a	812	CLA	CMC-C2C	-2.12	1.46	1.50
29	A	218	CLA	CMB-C2B	-2.12	1.46	1.50
29	L	315	CLA	CMD-C2D	-2.12	1.46	1.50
29	N	309	CLA	CMD-C2D	-2.12	1.46	1.50
29	a	818	CLA	CMD-C2D	-2.12	1.46	1.50
29	A	206	CLA	CMD-C2D	-2.12	1.46	1.50
29	J	308	CLA	CMD-C2D	-2.12	1.46	1.50
29	E	311	CLA	CMB-C2B	-2.12	1.46	1.50
29	L	317	CLA	MG-NB	-2.12	2.01	2.05
39	G	315	KC1	C1D-ND	-2.12	1.35	1.37
29	C	314	CLA	CHC-C1C	2.12	1.42	1.38
29	b	714	CLA	CMC-C2C	-2.12	1.46	1.50
29	b	702	CLA	CHC-C1C	2.12	1.42	1.38
29	F	312	CLA	MG-NB	-2.12	2.01	2.05
29	C	311	CLA	CMD-C2D	-2.12	1.46	1.50
29	K	213	CLA	MG-NB	-2.12	2.01	2.05
29	a	804	CLA	CMB-C2B	-2.12	1.46	1.50
29	b	716	CLA	CMB-C2B	-2.12	1.46	1.50
29	H	308	CLA	CMD-C2D	-2.12	1.46	1.50
29	i	203	CLA	C3B-C4B	2.12	1.48	1.42
29	D	308	CLA	MG-NB	-2.12	2.01	2.05
29	K	216	CLA	MG-NB	-2.12	2.01	2.05
39	Q	311	KC1	C4A-C3A	-2.12	1.40	1.44
29	b	706	CLA	C3B-C4B	2.12	1.48	1.42
29	F	307	CLA	MG-NB	-2.12	2.01	2.05
29	J	313	CLA	MG-NB	-2.12	2.01	2.05
29	G	319	CLA	CMD-C2D	-2.12	1.46	1.50
29	a	818	CLA	MG-NB	-2.12	2.01	2.05
37	T	302	PID	C20-C21	2.12	1.40	1.35
29	b	719	CLA	MG-NB	-2.12	2.01	2.05
29	I	211	CLA	CMD-C2D	-2.11	1.46	1.50
29	C	316	CLA	MG-NB	-2.11	2.01	2.05
29	a	815	CLA	CMC-C2C	-2.11	1.46	1.50
29	f	805	CLA	CMB-C2B	-2.11	1.46	1.50
29	L	311	CLA	CMB-C2B	-2.11	1.46	1.50
39	E	312	KC1	C4A-C3A	-2.11	1.40	1.44
29	a	812	CLA	MG-NB	-2.11	2.01	2.05
29	a	813	CLA	CMB-C2B	-2.11	1.46	1.50
29	b	704	CLA	CMC-C2C	-2.11	1.46	1.50
29	b	716	CLA	CMC-C2C	-2.11	1.46	1.50
29	J	305	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	216	CLA	CMD-C2D	-2.11	1.46	1.50
29	Q	313	CLA	CMD-C2D	-2.11	1.46	1.50
29	f	803	CLA	CMB-C2B	-2.11	1.46	1.50
29	G	301	CLA	CMB-C2B	-2.11	1.46	1.50
29	b	722	CLA	MG-NB	-2.11	2.01	2.05
29	I	214	CLA	MG-NB	-2.11	2.01	2.05
29	K	207	CLA	CMB-C2B	-2.11	1.46	1.50
29	J	307	CLA	CMB-C2B	-2.11	1.46	1.50
29	P	210	CLA	MG-NB	-2.11	2.01	2.05
29	M	307	CLA	CMC-C2C	-2.11	1.46	1.50
29	b	703	CLA	CMB-C2B	-2.11	1.46	1.50
29	I	208	CLA	CMB-C2B	-2.11	1.46	1.50
29	C	314	CLA	CMD-C2D	-2.11	1.46	1.50
29	j	104	CLA	CHC-C1C	2.11	1.42	1.38
29	a	811	CLA	CMD-C2D	-2.11	1.46	1.50
29	I	207	CLA	CMB-C2B	-2.11	1.46	1.50
29	E	311	CLA	CMD-C2D	-2.11	1.46	1.50
29	A	218	CLA	MG-NB	-2.11	2.01	2.05
29	a	827	CLA	CMC-C2C	-2.11	1.46	1.50
29	Q	307	CLA	CMD-C2D	-2.11	1.46	1.50
29	O	311	CLA	MG-NB	-2.11	2.01	2.05
29	A	211	CLA	CMB-C2B	-2.11	1.46	1.50
29	F	308	CLA	CMC-C2C	-2.11	1.46	1.50
29	b	706	CLA	MG-NB	-2.11	2.01	2.05
29	b	707	CLA	CMC-C2C	-2.11	1.46	1.50
29	Q	308	CLA	CMD-C2D	-2.11	1.46	1.50
29	F	316	CLA	MG-NB	-2.11	2.01	2.05
29	b	710	CLA	CMC-C2C	-2.11	1.46	1.50
29	b	703	CLA	MG-NB	-2.11	2.01	2.05
29	a	810	CLA	CHC-C1C	2.11	1.42	1.38
29	a	825	CLA	CMD-C2D	-2.11	1.46	1.50
29	C	316	CLA	CMD-C2D	-2.11	1.46	1.50
29	a	814	CLA	CMB-C2B	-2.11	1.46	1.50
29	a	812	CLA	CMB-C2B	-2.11	1.46	1.50
29	b	716	CLA	MG-NB	-2.11	2.01	2.05
29	M	308	CLA	CHC-C1C	2.11	1.42	1.38
29	D	314	CLA	CMC-C2C	-2.11	1.46	1.50
29	a	814	CLA	MG-NB	-2.11	2.01	2.05
29	a	809	CLA	CMD-C2D	-2.11	1.46	1.50
29	a	815	CLA	CMD-C2D	-2.11	1.46	1.50
29	F	308	CLA	CMB-C2B	-2.11	1.46	1.50
29	F	311	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J	309	CLA	CMD-C2D	-2.11	1.46	1.50
29	l	508	CLA	MG-NB	-2.11	2.01	2.05
29	a	805	CLA	CMC-C2C	-2.10	1.46	1.50
29	L	316	CLA	CHC-C1C	2.10	1.42	1.38
29	b	725	CLA	CMC-C2C	-2.10	1.46	1.50
29	b	731	CLA	CMD-C2D	-2.10	1.46	1.50
29	F	311	CLA	CMB-C2B	-2.10	1.46	1.50
29	B	309	CLA	CMB-C2B	-2.10	1.46	1.50
29	E	306	CLA	CMC-C2C	-2.10	1.46	1.50
29	L	313	CLA	MG-NB	-2.10	2.01	2.05
29	a	829	CLA	CHC-C1C	2.10	1.42	1.38
29	b	709	CLA	CMC-C2C	-2.10	1.46	1.50
29	i	202	CLA	CMC-C2C	-2.10	1.46	1.50
29	K	216	CLA	CMC-C2C	-2.10	1.46	1.50
29	A	210	CLA	MG-NB	-2.10	2.01	2.05
29	a	816	CLA	CMB-C2B	-2.10	1.46	1.50
29	M	307	CLA	CMB-C2B	-2.10	1.46	1.50
29	D	312	CLA	CMD-C2D	-2.10	1.46	1.50
29	E	309	CLA	CMD-C2D	-2.10	1.46	1.50
29	L	310	CLA	CMD-C2D	-2.10	1.46	1.50
29	B	306	CLA	MG-NB	-2.10	2.01	2.05
29	b	731	CLA	CMB-C2B	-2.10	1.46	1.50
29	a	821	CLA	CMD-C2D	-2.10	1.46	1.50
39	C	310	KC1	C4A-C3A	-2.10	1.40	1.44
29	K	212	CLA	MG-NB	-2.10	2.01	2.05
29	a	804	CLA	CMD-C2D	-2.10	1.46	1.50
39	N	310	KC1	C4A-C3A	-2.10	1.40	1.44
29	f	802	CLA	CMC-C2C	-2.10	1.46	1.50
29	L	313	CLA	CMB-C2B	-2.10	1.46	1.50
29	E	314	CLA	CMD-C2D	-2.10	1.46	1.50
29	f	802	CLA	CMB-C2B	-2.10	1.46	1.50
29	I	211	CLA	CMC-C2C	-2.10	1.46	1.50
29	K	213	CLA	CMB-C2B	-2.10	1.46	1.50
29	D	311	CLA	CMD-C2D	-2.10	1.46	1.50
29	D	314	CLA	CMD-C2D	-2.10	1.46	1.50
29	B	307	CLA	MG-NB	-2.10	2.01	2.05
29	a	806	CLA	CMB-C2B	-2.10	1.46	1.50
29	l	508	CLA	CMB-C2B	-2.10	1.46	1.50
29	Q	310	CLA	CMB-C2B	-2.10	1.46	1.50
29	E	313	CLA	CMD-C2D	-2.10	1.46	1.50
29	B	308	CLA	CMC-C2C	-2.10	1.46	1.50
29	I	209	CLA	MG-NB	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	312	CLA	MG-NB	-2.10	2.01	2.05
39	M	312	KC1	C4A-C3A	-2.10	1.40	1.44
29	a	813	CLA	CMD-C2D	-2.09	1.46	1.50
29	O	311	CLA	CMC-C2C	-2.09	1.46	1.50
29	E	305	CLA	CHC-C1C	2.09	1.42	1.38
29	M	313	CLA	MG-NB	-2.09	2.01	2.05
29	a	813	CLA	MG-NB	-2.09	2.01	2.05
29	b	709	CLA	CMB-C2B	-2.09	1.46	1.50
29	T	316	CLA	CMD-C2D	-2.09	1.46	1.50
29	A	211	CLA	MG-NB	-2.09	2.01	2.05
29	T	313	CLA	MG-NB	-2.09	2.01	2.05
29	l	504	CLA	CMB-C2B	-2.09	1.46	1.50
29	M	306	CLA	CMD-C2D	-2.09	1.46	1.50
29	Q	315	CLA	CMC-C2C	-2.09	1.46	1.50
29	M	314	CLA	CHC-C1C	2.09	1.42	1.38
39	I	215	KC1	C4A-C3A	-2.09	1.40	1.44
29	C	314	CLA	MG-NB	-2.09	2.01	2.05
29	P	214	CLA	MG-NB	-2.09	2.01	2.05
29	a	810	CLA	C3B-C4B	2.09	1.48	1.42
29	J	305	CLA	CMB-C2B	-2.09	1.46	1.50
34	E	316	LMG	O7-C8	-2.09	1.41	1.46
38	C	306	UIX	C15-C20	-2.09	1.51	1.54
29	J	306	CLA	CMC-C2C	-2.09	1.46	1.50
29	a	805	CLA	CMB-C2B	-2.09	1.46	1.50
29	a	816	CLA	CMC-C2C	-2.09	1.46	1.50
29	D	309	CLA	MG-NB	-2.09	2.01	2.05
29	a	822	CLA	CMB-C2B	-2.09	1.46	1.50
29	i	202	CLA	CHC-C1C	2.09	1.42	1.38
29	K	212	CLA	CHC-C1C	2.09	1.42	1.38
35	b	733	DGD	O3G-C1D	2.09	1.43	1.40
29	a	828	CLA	MG-NB	-2.09	2.01	2.05
29	D	314	CLA	MG-NB	-2.09	2.01	2.05
29	a	816	CLA	CMD-C2D	-2.09	1.46	1.50
29	A	208	CLA	CMC-C2C	-2.09	1.46	1.50
29	G	304	CLA	CMC-C2C	-2.09	1.46	1.50
29	a	828	CLA	CMB-C2B	-2.09	1.46	1.50
29	C	308	CLA	MG-NB	-2.09	2.01	2.05
34	K	201	LMG	O7-C8	-2.09	1.41	1.46
29	a	819	CLA	CMD-C2D	-2.09	1.46	1.50
29	l	503	CLA	CMD-C2D	-2.09	1.46	1.50
29	A	206	CLA	CMB-C2B	-2.09	1.46	1.50
29	M	308	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	308	CLA	MG-NB	-2.09	2.01	2.05
29	A	206	CLA	MG-NB	-2.09	2.01	2.05
29	L	316	CLA	CMB-C2B	-2.09	1.46	1.50
29	O	308	CLA	CMD-C2D	-2.09	1.46	1.50
29	K	214	CLA	MG-NB	-2.09	2.01	2.05
29	T	314	CLA	MG-NB	-2.09	2.01	2.05
29	G	317	CLA	CMC-C2C	-2.09	1.46	1.50
29	K	208	CLA	CMC-C2C	-2.09	1.46	1.50
29	M	313	CLA	CMD-C2D	-2.09	1.46	1.50
29	H	313	CLA	CMB-C2B	-2.09	1.46	1.50
29	i	203	CLA	CMB-C2B	-2.09	1.46	1.50
29	A	207	CLA	CMC-C2C	-2.09	1.46	1.50
29	G	304	CLA	CMB-C2B	-2.09	1.46	1.50
29	K	211	CLA	CMB-C2B	-2.09	1.46	1.50
29	L	315	CLA	CMB-C2B	-2.09	1.46	1.50
29	Q	312	CLA	CMB-C2B	-2.09	1.46	1.50
29	Q	312	CLA	MG-NB	-2.09	2.01	2.05
29	K	214	CLA	CMD-C2D	-2.09	1.46	1.50
29	C	313	CLA	CMB-C2B	-2.09	1.46	1.50
29	E	306	CLA	CMB-C2B	-2.09	1.46	1.50
36	F	301	DD6	C19-C20	2.08	1.55	1.52
39	A	213	KC1	C4A-C3A	-2.08	1.40	1.44
29	G	312	CLA	CMC-C2C	-2.08	1.46	1.50
29	G	317	CLA	CMB-C2B	-2.08	1.46	1.50
29	B	307	CLA	CMB-C2B	-2.08	1.46	1.50
29	H	315	CLA	CMD-C2D	-2.08	1.46	1.50
29	L	307	CLA	MG-NB	-2.08	2.01	2.05
29	M	308	CLA	CMD-C2D	-2.08	1.46	1.50
29	E	309	CLA	MG-NB	-2.08	2.01	2.05
29	E	313	CLA	MG-NB	-2.08	2.01	2.05
29	L	309	CLA	CMB-C2B	-2.08	1.46	1.50
29	C	311	CLA	MG-NB	-2.08	2.01	2.05
29	a	817	CLA	MG-NB	-2.08	2.01	2.05
29	a	830	CLA	CMB-C2B	-2.08	1.46	1.50
29	L	313	CLA	CMC-C2C	-2.08	1.46	1.50
29	H	313	CLA	CMC-C2C	-2.08	1.46	1.50
39	T	312	KC1	C4A-C3A	-2.08	1.40	1.44
39	C	312	KC1	C4A-C3A	-2.08	1.40	1.44
29	L	317	CLA	CMB-C2B	-2.08	1.46	1.50
29	b	721	CLA	MG-NB	-2.08	2.01	2.05
29	I	211	CLA	CMB-C2B	-2.08	1.46	1.50
29	C	314	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	211	CLA	MG-NB	-2.08	2.01	2.05
29	a	817	CLA	CMD-C2D	-2.08	1.46	1.50
29	T	308	CLA	MG-NB	-2.08	2.01	2.05
29	T	316	CLA	MG-NB	-2.08	2.01	2.05
39	Q	314	KC1	C4A-C3A	-2.08	1.40	1.44
29	b	721	CLA	CMC-C2C	-2.08	1.46	1.50
29	E	315	CLA	CMD-C2D	-2.08	1.46	1.50
29	A	212	CLA	CMB-C2B	-2.08	1.46	1.50
29	A	215	CLA	CMC-C2C	-2.08	1.46	1.50
29	Q	308	CLA	CMB-C2B	-2.08	1.46	1.50
29	I	216	CLA	CMB-C2B	-2.08	1.46	1.50
29	M	308	CLA	CMB-C2B	-2.08	1.46	1.50
29	M	309	CLA	CMD-C2D	-2.08	1.46	1.50
29	L	308	CLA	CMB-C2B	-2.08	1.46	1.50
29	b	710	CLA	MG-NB	-2.08	2.01	2.05
34	j	102	LMG	O7-C8	-2.08	1.41	1.46
29	a	813	CLA	CMC-C2C	-2.08	1.46	1.50
29	b	708	CLA	CMD-C2D	-2.08	1.46	1.50
29	A	207	CLA	CMB-C2B	-2.08	1.46	1.50
29	a	828	CLA	CMD-C2D	-2.07	1.46	1.50
29	O	316	CLA	CMC-C2C	-2.07	1.46	1.50
36	I	203	DD6	O1-C20	-2.07	1.43	1.46
29	l	508	CLA	CMC-C2C	-2.07	1.46	1.50
29	K	214	CLA	CMC-C2C	-2.07	1.46	1.50
29	b	707	CLA	MG-NB	-2.07	2.01	2.05
32	m	103	BCR	C1-C6	-2.07	1.51	1.53
29	I	207	CLA	CMC-C2C	-2.07	1.46	1.50
29	F	310	CLA	CMB-C2B	-2.07	1.46	1.50
29	E	310	CLA	CMD-C2D	-2.07	1.46	1.50
29	I	201	CLA	MG-NB	-2.07	2.01	2.05
29	I	214	CLA	CMC-C2C	-2.07	1.46	1.50
29	T	309	CLA	MG-NB	-2.07	2.01	2.05
29	a	828	CLA	CMC-C2C	-2.07	1.46	1.50
29	l	508	CLA	CMD-C2D	-2.07	1.46	1.50
29	G	319	CLA	CMB-C2B	-2.07	1.46	1.50
29	h	201	CLA	CMB-C2B	-2.07	1.46	1.50
29	j	104	CLA	CMC-C2C	-2.07	1.46	1.50
29	E	311	CLA	CMC-C2C	-2.07	1.46	1.50
39	L	314	KC1	C4A-C3A	-2.07	1.40	1.44
29	l	509	CLA	CMC-C2C	-2.07	1.46	1.50
29	a	807	CLA	CMB-C2B	-2.07	1.46	1.50
29	J	308	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	805	CLA	MG-NB	-2.07	2.01	2.05
29	a	837	CLA	CMB-C2B	-2.07	1.46	1.50
29	B	311	CLA	MG-NB	-2.07	2.01	2.05
29	E	314	CLA	CMC-C2C	-2.07	1.46	1.50
29	a	820	CLA	CMC-C2C	-2.07	1.46	1.50
29	F	316	CLA	CMB-C2B	-2.07	1.46	1.50
29	P	210	CLA	CMD-C2D	-2.07	1.46	1.50
29	N	311	CLA	MG-NB	-2.07	2.01	2.05
29	J	311	CLA	CMC-C2C	-2.07	1.46	1.50
29	T	308	CLA	CMB-C2B	-2.07	1.46	1.50
39	K	215	KC1	C4A-C3A	-2.07	1.40	1.44
29	G	301	CLA	MG-NB	-2.07	2.01	2.05
29	I	209	CLA	CMC-C2C	-2.07	1.46	1.50
29	N	314	CLA	CMD-C2D	-2.07	1.46	1.50
37	P	206	PID	C20-C21	2.07	1.40	1.35
29	b	736	CLA	MG-NB	-2.07	2.01	2.05
29	B	312	CLA	CMC-C2C	-2.07	1.46	1.50
34	A	219	LMG	O7-C8	-2.07	1.41	1.46
29	b	704	CLA	CMB-C2B	-2.07	1.46	1.50
29	B	308	CLA	CMB-C2B	-2.07	1.46	1.50
29	b	723	CLA	CMC-C2C	-2.07	1.46	1.50
29	K	209	CLA	CMC-C2C	-2.07	1.46	1.50
29	F	311	CLA	MG-NB	-2.07	2.01	2.05
29	A	214	CLA	CMB-C2B	-2.07	1.46	1.50
29	b	720	CLA	CMC-C2C	-2.07	1.46	1.50
29	J	313	CLA	CMD-C2D	-2.07	1.46	1.50
29	I	217	CLA	CHC-C1C	2.07	1.42	1.38
29	K	217	CLA	CMC-C2C	-2.07	1.46	1.50
29	N	308	CLA	CMD-C2D	-2.07	1.46	1.50
29	K	216	CLA	CMB-C2B	-2.06	1.46	1.50
29	L	316	CLA	MG-NB	-2.06	2.01	2.05
29	P	217	CLA	MG-NB	-2.06	2.01	2.05
29	a	831	CLA	CMC-C2C	-2.06	1.46	1.50
29	H	307	CLA	MG-NB	-2.06	2.01	2.05
29	J	310	CLA	CMB-C2B	-2.06	1.46	1.50
29	D	309	CLA	CMD-C2D	-2.06	1.46	1.50
29	C	316	CLA	CMB-C2B	-2.06	1.46	1.50
29	T	313	CLA	CMD-C2D	-2.06	1.46	1.50
29	L	312	CLA	MG-NB	-2.06	2.01	2.05
29	O	309	CLA	MG-NB	-2.06	2.01	2.05
29	a	803	CLA	CMC-C2C	-2.06	1.46	1.50
29	b	722	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	310	CLA	MG-NB	-2.06	2.01	2.05
29	P	209	CLA	MG-NB	-2.06	2.01	2.05
29	A	212	CLA	CMC-C2C	-2.06	1.46	1.50
29	I	216	CLA	CMC-C2C	-2.06	1.46	1.50
29	C	308	CLA	CMD-C2D	-2.06	1.46	1.50
29	D	311	CLA	MG-NB	-2.06	2.01	2.05
29	Q	307	CLA	MG-NB	-2.06	2.01	2.05
29	A	216	CLA	CMC-C2C	-2.06	1.46	1.50
29	G	311	CLA	CMB-C2B	-2.06	1.46	1.50
29	G	313	CLA	CMB-C2B	-2.06	1.46	1.50
29	B	311	CLA	CMB-C2B	-2.06	1.46	1.50
29	Q	308	CLA	CMC-C2C	-2.06	1.46	1.50
29	b	723	CLA	CMB-C2B	-2.06	1.46	1.50
29	a	821	CLA	MG-NB	-2.06	2.01	2.05
29	a	815	CLA	CMB-C2B	-2.06	1.46	1.50
29	j	104	CLA	CMB-C2B	-2.06	1.46	1.50
29	a	807	CLA	MG-NB	-2.06	2.01	2.05
29	T	309	CLA	CMD-C2D	-2.06	1.46	1.50
29	P	212	CLA	CMD-C2D	-2.06	1.46	1.50
29	a	809	CLA	CMC-C2C	-2.06	1.46	1.50
29	L	307	CLA	CMC-C2C	-2.06	1.46	1.50
29	H	310	CLA	CMD-C2D	-2.06	1.46	1.50
39	M	305	KC1	C4A-C3A	-2.06	1.40	1.44
29	a	819	CLA	CMC-C2C	-2.06	1.46	1.50
29	a	829	CLA	CMC-C2C	-2.06	1.46	1.50
29	b	712	CLA	CMC-C2C	-2.06	1.46	1.50
29	G	301	CLA	CMC-C2C	-2.06	1.46	1.50
29	N	316	CLA	CMD-C2D	-2.06	1.46	1.50
39	J	312	KC1	C4A-C3A	-2.06	1.40	1.44
29	B	310	CLA	CMC-C2C	-2.06	1.46	1.50
29	T	308	CLA	CMD-C2D	-2.06	1.46	1.50
29	Q	307	CLA	CMB-C2B	-2.06	1.46	1.50
29	J	305	CLA	MG-NB	-2.06	2.01	2.05
29	N	316	CLA	MG-NB	-2.06	2.01	2.05
29	G	316	CLA	CMC-C2C	-2.06	1.46	1.50
29	O	316	CLA	MG-NB	-2.06	2.01	2.05
29	H	308	CLA	CMB-C2B	-2.05	1.46	1.50
29	L	315	CLA	MG-NB	-2.05	2.01	2.05
29	a	810	CLA	CMC-C2C	-2.05	1.46	1.50
29	b	711	CLA	CMC-C2C	-2.05	1.46	1.50
29	b	713	CLA	MG-NB	-2.05	2.01	2.05
29	b	713	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	311	CLA	CMD-C2D	-2.05	1.46	1.50
29	G	316	CLA	CHC-C1C	2.05	1.42	1.38
29	b	704	CLA	MG-NB	-2.05	2.01	2.05
29	I	208	CLA	MG-NB	-2.05	2.01	2.05
29	L	313	CLA	CMD-C2D	-2.05	1.46	1.50
29	O	308	CLA	MG-NB	-2.05	2.01	2.05
29	C	316	CLA	CHC-C1C	2.05	1.42	1.38
29	A	210	CLA	CMC-C2C	-2.05	1.46	1.50
29	A	214	CLA	CMC-C2C	-2.05	1.46	1.50
29	F	316	CLA	CMC-C2C	-2.05	1.46	1.50
29	D	316	CLA	CMD-C2D	-2.05	1.46	1.50
29	O	309	CLA	CMB-C2B	-2.05	1.46	1.50
29	I	207	CLA	CHC-C1C	2.05	1.42	1.38
29	f	803	CLA	CMC-C2C	-2.05	1.46	1.50
29	F	315	CLA	CMD-C2D	-2.05	1.46	1.50
29	L	309	CLA	CMC-C2C	-2.05	1.46	1.50
39	L	306	KC1	C4A-C3A	-2.05	1.40	1.44
29	G	314	CLA	CMB-C2B	-2.05	1.46	1.50
29	I	201	CLA	CMB-C2B	-2.05	1.46	1.50
29	M	311	CLA	CMC-C2C	-2.05	1.46	1.50
29	a	802	CLA	CMC-C2C	-2.05	1.46	1.50
29	K	209	CLA	CMB-C2B	-2.05	1.46	1.50
29	C	311	CLA	CMC-C2C	-2.05	1.46	1.50
29	b	702	CLA	CMC-C2C	-2.05	1.46	1.50
29	I	212	CLA	CMC-C2C	-2.05	1.46	1.50
29	T	309	CLA	CMB-C2B	-2.05	1.46	1.50
29	F	313	CLA	CMC-C2C	-2.05	1.46	1.50
29	C	313	CLA	CMC-C2C	-2.05	1.46	1.50
29	P	215	CLA	CMD-C2D	-2.05	1.46	1.50
39	L	314	KC1	C1D-ND	-2.05	1.35	1.37
29	H	313	CLA	CMD-C2D	-2.04	1.46	1.50
29	F	315	CLA	MG-NB	-2.04	2.01	2.05
29	C	309	CLA	CMC-C2C	-2.04	1.46	1.50
29	P	210	CLA	CMB-C2B	-2.04	1.46	1.50
29	a	826	CLA	CMC-C2C	-2.04	1.46	1.50
29	A	215	CLA	CHC-C1C	2.04	1.42	1.38
39	P	211	KC1	C4A-C3A	-2.04	1.40	1.44
29	b	701	CLA	CMB-C2B	-2.04	1.46	1.50
29	F	307	CLA	CMB-C2B	-2.04	1.46	1.50
29	l	504	CLA	CMC-C2C	-2.04	1.46	1.50
29	P	214	CLA	CMB-C2B	-2.04	1.46	1.50
29	A	211	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	308	CLA	CMB-C2B	-2.04	1.46	1.50
39	F	314	KC1	C4A-C3A	-2.04	1.40	1.44
29	b	731	CLA	CMC-C2C	-2.04	1.46	1.50
29	A	208	CLA	CMB-C2B	-2.04	1.46	1.50
29	O	314	CLA	CMB-C2B	-2.04	1.46	1.50
29	i	202	CLA	CMB-C2B	-2.04	1.46	1.50
29	G	302	CLA	CMC-C2C	-2.04	1.46	1.50
29	Q	310	CLA	CMC-C2C	-2.04	1.46	1.50
29	l	501	CLA	CMC-C2C	-2.04	1.46	1.50
29	a	822	CLA	CMC-C2C	-2.04	1.46	1.50
29	J	308	CLA	CMC-C2C	-2.04	1.46	1.50
29	J	306	CLA	CMB-C2B	-2.04	1.46	1.50
29	P	212	CLA	MG-NB	-2.04	2.01	2.05
29	A	209	CLA	CMC-C2C	-2.04	1.46	1.50
29	L	312	CLA	CMC-C2C	-2.04	1.46	1.50
29	I	217	CLA	CMC-C2C	-2.04	1.46	1.50
29	a	801	CLA	MG-ND	-2.04	2.01	2.05
29	a	804	CLA	MG-NB	-2.04	2.01	2.05
29	L	317	CLA	CMC-C2C	-2.03	1.46	1.50
36	I	203	DD6	C21-C20	-2.03	1.48	1.51
29	l	505	CLA	CMC-C2C	-2.03	1.46	1.50
29	L	308	CLA	CMC-C2C	-2.03	1.46	1.50
29	H	315	CLA	MG-NB	-2.03	2.01	2.05
29	O	311	CLA	CMD-C2D	-2.03	1.46	1.50
29	E	308	CLA	CMC-C2C	-2.03	1.46	1.50
39	E	307	KC1	C1D-ND	-2.03	1.35	1.37
29	a	821	CLA	CMB-C2B	-2.03	1.46	1.50
29	M	314	CLA	CMC-C2C	-2.03	1.46	1.50
34	b	734	LMG	O7-C8	-2.03	1.41	1.46
29	a	837	CLA	CMC-C2C	-2.03	1.46	1.50
29	a	831	CLA	CMB-C2B	-2.03	1.46	1.50
29	D	313	CLA	CMC-C2C	-2.03	1.46	1.50
29	O	308	CLA	CMB-C2B	-2.03	1.46	1.50
29	M	314	CLA	CMD-C2D	-2.03	1.46	1.50
29	B	312	CLA	CMB-C2B	-2.03	1.46	1.50
29	D	312	CLA	CMB-C2B	-2.03	1.46	1.50
29	C	308	CLA	CMB-C2B	-2.03	1.46	1.50
29	F	313	CLA	CHC-C1C	2.03	1.42	1.38
36	h	202	DD6	C-C1	-2.03	1.46	1.50
35	b	733	DGD	O5D-C1E	2.03	1.43	1.40
29	b	717	CLA	CMC-C2C	-2.03	1.46	1.50
29	H	307	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	306	CLA	CMB-C2B	-2.03	1.46	1.50
29	Q	312	CLA	CMC-C2C	-2.03	1.46	1.50
29	M	313	CLA	CMB-C2B	-2.03	1.46	1.50
39	Q	311	KC1	C1D-ND	-2.03	1.35	1.37
29	J	313	CLA	CMB-C2B	-2.03	1.46	1.50
29	B	316	CLA	CMC-C2C	-2.03	1.46	1.50
29	I	201	CLA	CMC-C2C	-2.03	1.46	1.50
29	F	311	CLA	CMC-C2C	-2.03	1.46	1.50
29	T	314	CLA	CMD-C2D	-2.03	1.46	1.50
29	Q	307	CLA	CMC-C2C	-2.03	1.46	1.50
29	O	311	CLA	CMB-C2B	-2.02	1.46	1.50
29	F	315	CLA	CMB-C2B	-2.02	1.46	1.50
29	K	207	CLA	CMC-C2C	-2.02	1.46	1.50
29	G	302	CLA	CMB-C2B	-2.02	1.46	1.50
29	C	311	CLA	CMB-C2B	-2.02	1.46	1.50
29	P	215	CLA	CMB-C2B	-2.02	1.46	1.50
29	j	104	CLA	MG-NB	-2.02	2.01	2.05
29	J	307	CLA	CMC-C2C	-2.02	1.46	1.50
29	O	316	CLA	CMD-C2D	-2.02	1.46	1.50
39	D	310	KC1	C4A-C3A	-2.02	1.40	1.44
29	M	310	CLA	CMB-C2B	-2.02	1.46	1.50
29	i	203	CLA	CMC-C2C	-2.02	1.46	1.50
29	P	209	CLA	CMD-C2D	-2.02	1.46	1.50
29	B	314	CLA	CMB-C2B	-2.02	1.46	1.50
29	b	715	CLA	CHC-C1C	2.02	1.42	1.38
29	N	309	CLA	CMB-C2B	-2.02	1.46	1.50
37	N	307	PID	C20-C21	2.02	1.40	1.35
36	F	301	DD6	O1-C20	-2.02	1.43	1.46
29	I	210	CLA	CMC-C2C	-2.02	1.46	1.50
29	D	311	CLA	CMB-C2B	-2.02	1.46	1.50
29	P	215	CLA	CMC-C2C	-2.02	1.46	1.50
29	l	510	CLA	MG-NB	-2.02	2.01	2.05
36	h	202	DD6	C28-C27	-2.02	1.49	1.50
29	N	314	CLA	MG-NB	-2.01	2.01	2.05
29	I	213	CLA	CMC-C2C	-2.01	1.46	1.50
39	F	314	KC1	C1D-ND	-2.01	1.35	1.37
29	N	308	CLA	MG-NB	-2.01	2.01	2.05
29	D	316	CLA	MG-NB	-2.01	2.01	2.05
29	A	217	CLA	CMC-C2C	-2.01	1.46	1.50
29	J	310	CLA	CMC-C2C	-2.01	1.46	1.50
29	B	310	CLA	CMB-C2B	-2.01	1.46	1.50
29	E	309	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	310	CLA	CMC-C2C	-2.01	1.46	1.50
29	P	210	CLA	CMC-C2C	-2.01	1.46	1.50
29	b	718	CLA	CHC-C1C	2.01	1.42	1.38
29	a	811	CLA	CMC-C2C	-2.01	1.46	1.50
29	Q	313	CLA	CMC-C2C	-2.01	1.46	1.50
29	P	209	CLA	CMB-C2B	-2.01	1.46	1.50
29	a	823	CLA	MG-NB	-2.01	2.01	2.05
29	a	823	CLA	CMB-C2B	-2.01	1.46	1.50
29	H	308	CLA	CMC-C2C	-2.01	1.46	1.50
29	K	207	CLA	MG-NB	-2.01	2.01	2.05
29	D	309	CLA	CMB-C2B	-2.01	1.46	1.50
29	C	309	CLA	CMB-C2B	-2.01	1.46	1.50
29	b	708	CLA	CHC-C1C	2.01	1.42	1.38
29	M	309	CLA	CMC-C2C	-2.01	1.46	1.50
29	B	315	CLA	CMC-C2C	-2.01	1.46	1.50
29	J	313	CLA	CMC-C2C	-2.01	1.46	1.50
29	D	311	CLA	CMC-C2C	-2.01	1.46	1.50
29	C	308	CLA	CMC-C2C	-2.01	1.46	1.50
29	M	310	CLA	MG-NB	-2.01	2.01	2.05
29	a	808	CLA	CMC-C2C	-2.01	1.46	1.50
29	a	817	CLA	CMC-C2C	-2.01	1.46	1.50
29	B	306	CLA	CMC-C2C	-2.01	1.46	1.50
29	N	314	CLA	CMB-C2B	-2.01	1.46	1.50
29	N	311	CLA	CMD-C2D	-2.01	1.46	1.50
29	a	818	CLA	CMC-C2C	-2.01	1.46	1.50
29	G	313	CLA	CMC-C2C	-2.01	1.46	1.50
29	L	310	CLA	CMC-C2C	-2.01	1.46	1.50
29	H	310	CLA	CMB-C2B	-2.01	1.46	1.50
29	N	308	CLA	CMB-C2B	-2.00	1.46	1.50
29	Q	315	CLA	CMB-C2B	-2.00	1.46	1.50
29	T	313	CLA	CMC-C2C	-2.00	1.46	1.50
29	I	208	CLA	CMC-C2C	-2.00	1.46	1.50
29	K	212	CLA	CMC-C2C	-2.00	1.46	1.50
39	G	318	KC1	C1D-ND	-2.00	1.35	1.37
39	H	311	KC1	C1D-ND	-2.00	1.35	1.37
29	M	315	CLA	CMC-C2C	-2.00	1.46	1.50
29	b	719	CLA	CMC-C2C	-2.00	1.46	1.50
39	H	309	KC1	C4A-C3A	-2.00	1.40	1.44
38	T	306	UIX	C15-C20	-2.00	1.51	1.54
29	N	316	CLA	CMB-C2B	-2.00	1.46	1.50
29	a	801	CLA	CHC-C1C	2.00	1.42	1.38
38	N	306	UIX	C15-C20	-2.00	1.51	1.54

All (3397) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	308	CLA	O2D-CGD-CBD	27.01	158.46	111.23
29	b	736	CLA	O2D-CGD-CBD	27.00	158.43	111.23
29	I	209	CLA	O2D-CGD-CBD	26.93	158.31	111.23
29	I	212	CLA	O2D-CGD-CBD	26.75	157.99	111.23
29	a	831	CLA	O2D-CGD-CBD	26.70	157.91	111.23
29	L	307	CLA	O2D-CGD-CBD	26.66	157.84	111.23
29	a	830	CLA	O2D-CGD-CBD	26.59	157.72	111.23
29	I	208	CLA	O2D-CGD-CBD	26.37	157.32	111.23
29	G	316	CLA	O2D-CGD-CBD	26.24	157.10	111.23
29	I	209	CLA	O2D-CGD-O1D	-25.74	73.74	123.85
29	L	308	CLA	O2D-CGD-O1D	-25.72	73.79	123.85
29	a	831	CLA	O2D-CGD-O1D	-25.64	73.93	123.85
29	I	208	CLA	O2D-CGD-O1D	-25.60	74.02	123.85
29	L	307	CLA	O2D-CGD-O1D	-25.56	74.09	123.85
29	I	212	CLA	O2D-CGD-O1D	-25.51	74.19	123.85
29	b	736	CLA	O2D-CGD-O1D	-25.51	74.20	123.85
29	a	830	CLA	O2D-CGD-O1D	-25.51	74.20	123.85
29	G	316	CLA	O2D-CGD-O1D	-25.10	75.00	123.85
29	b	712	CLA	C4-C3-C5	-21.90	77.21	115.23
29	b	736	CLA	C4-C3-C5	-21.89	77.23	115.23
29	I	213	CLA	C4-C3-C5	-21.72	77.52	115.23
29	l	504	CLA	C4-C3-C5	-21.69	77.57	115.23
29	I	212	CLA	C4-C3-C5	-21.67	77.62	115.23
29	G	316	CLA	O1D-CGD-CBD	-21.50	82.11	124.52
29	I	208	CLA	O1D-CGD-CBD	-20.89	83.31	124.52
29	a	830	CLA	O1D-CGD-CBD	-20.78	83.53	124.52
29	N	313	CLA	O2D-CGD-O1D	-20.69	83.57	123.85
29	L	307	CLA	O1D-CGD-CBD	-20.67	83.75	124.52
29	I	212	CLA	O1D-CGD-CBD	-20.64	83.80	124.52
29	b	704	CLA	O2D-CGD-O1D	-20.60	83.76	123.85
29	a	831	CLA	O1D-CGD-CBD	-20.55	83.98	124.52
29	b	736	CLA	O1D-CGD-CBD	-20.42	84.23	124.52
29	I	209	CLA	O1D-CGD-CBD	-20.25	84.58	124.52
29	L	308	CLA	O1D-CGD-CBD	-20.20	84.67	124.52
29	N	313	CLA	O1D-CGD-CBD	19.90	163.76	124.52
29	b	704	CLA	O1D-CGD-CBD	19.54	163.06	124.52
29	b	704	CLA	O2D-CGD-CBD	-18.17	79.46	111.23
29	N	313	CLA	O2D-CGD-CBD	-17.71	80.27	111.23
29	I	212	CLA	C5-C3-C2	17.42	160.26	121.17
29	I	213	CLA	C5-C3-C2	17.38	160.18	121.17
29	l	504	CLA	C5-C3-C2	17.30	159.99	121.17
29	b	736	CLA	C5-C3-C2	17.23	159.84	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	712	CLA	C5-C3-C2	17.21	159.81	121.17
29	l	504	CLA	C4-C3-C2	-16.04	82.42	123.63
29	b	712	CLA	C4-C3-C2	-15.98	82.59	123.63
29	b	736	CLA	C4-C3-C2	-15.97	82.62	123.63
29	I	212	CLA	C4-C3-C2	-15.96	82.65	123.63
29	I	213	CLA	C4-C3-C2	-15.95	82.67	123.63
36	K	202	DD6	C21-C20-C19	11.99	127.71	114.24
36	G	305	DD6	C21-C20-C19	10.53	126.07	114.24
37	P	208	PID	C18-C19-C20	10.13	144.25	123.52
36	K	202	DD6	C21-C20-C15	-9.88	106.05	122.30
38	F	305	UIX	O-C1-C3	8.52	121.47	113.49
37	C	305	PID	C17-C16-C15	7.86	139.60	123.52
37	E	301	PID	C17-C16-C15	7.81	139.49	123.52
36	G	305	DD6	C21-C20-C15	-7.71	109.62	122.30
38	J	304	UIX	O-C1-C3	7.59	120.61	113.49
36	G	305	DD6	C3-C2-C1	-7.48	116.78	127.28
29	P	215	CLA	C4A-NA-C1A	7.39	110.05	106.68
36	J	301	DD6	C3-C2-C1	-7.38	116.92	127.28
38	L	302	UIX	C6-C1-C	-7.28	110.33	122.30
29	b	706	CLA	C4A-NA-C1A	7.17	109.95	106.68
36	M	302	DD6	C3-C2-C1	-7.16	117.23	127.28
38	A	203	UIX	C6-C1-C	-7.16	110.51	122.30
38	Q	305	UIX	C14-C13-C11	-7.15	117.25	127.28
29	H	313	CLA	C4A-NA-C1A	7.14	109.94	106.68
38	B	304	UIX	C6-C1-C	-7.12	110.59	122.30
38	E	304	UIX	C6-C1-C	-7.10	110.61	122.30
29	a	801	CLA	C4A-NA-C1A	7.08	109.91	106.68
29	a	810	CLA	C4A-NA-C1A	7.07	109.91	106.68
29	j	104	CLA	C4A-NA-C1A	7.04	109.89	106.68
38	F	305	UIX	C34-C30-C26	-7.03	117.42	127.28
29	G	304	CLA	C4A-NA-C1A	6.98	109.86	106.68
36	F	301	DD6	C9-C10-C11	-6.97	117.50	127.28
29	i	201	CLA	C4A-NA-C1A	6.97	109.86	106.68
29	L	307	CLA	C4A-NA-C1A	6.96	109.85	106.68
29	P	217	CLA	C4A-NA-C1A	6.94	109.84	106.68
29	F	311	CLA	C4A-NA-C1A	6.93	109.84	106.68
29	F	310	CLA	C4A-NA-C1A	6.93	109.84	106.68
36	I	205	DD6	O1-C20-C21	6.92	122.78	115.05
37	P	208	PID	C17-C16-C15	6.92	137.68	123.52
29	N	313	CLA	C4A-NA-C1A	6.92	109.83	106.68
29	C	314	CLA	C4A-NA-C1A	6.92	109.83	106.68
29	b	736	CLA	C4A-NA-C1A	6.91	109.83	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	721	CLA	C4A-NA-C1A	6.91	109.83	106.68
29	I	207	CLA	C4A-NA-C1A	6.88	109.82	106.68
38	J	304	UIX	C6-C1-C	-6.87	111.00	122.30
36	h	202	DD6	C21-C20-C19	6.85	121.94	114.24
29	T	309	CLA	C4A-NA-C1A	6.85	109.81	106.68
38	Q	305	UIX	C6-C1-C	-6.83	111.05	122.30
36	G	307	DD6	C3-C2-C1	-6.83	117.69	127.28
38	T	306	UIX	C14-C13-C11	-6.81	117.72	127.28
29	C	316	CLA	C4A-NA-C1A	6.80	109.78	106.68
29	F	315	CLA	C4A-NA-C1A	6.79	109.78	106.68
29	G	314	CLA	C4A-NA-C1A	6.79	109.78	106.68
36	B	319	DD6	C3-C2-C1	-6.76	117.79	127.28
29	F	316	CLA	C4A-NA-C1A	6.76	109.76	106.68
29	D	316	CLA	C4A-NA-C1A	6.76	109.76	106.68
29	l	504	CLA	C4A-NA-C1A	6.73	109.75	106.68
29	a	825	CLA	C4A-NA-C1A	6.73	109.75	106.68
29	D	314	CLA	C4A-NA-C1A	6.73	109.75	106.68
29	a	804	CLA	C4A-NA-C1A	6.72	109.75	106.68
29	A	206	CLA	C4A-NA-C1A	6.72	109.75	106.68
29	B	311	CLA	C4A-NA-C1A	6.72	109.75	106.68
29	T	314	CLA	C4A-NA-C1A	6.72	109.74	106.68
29	a	812	CLA	C4A-NA-C1A	6.72	109.74	106.68
29	I	216	CLA	C4A-NA-C1A	6.71	109.74	106.68
29	E	309	CLA	C4A-NA-C1A	6.71	109.74	106.68
29	l	501	CLA	C4A-NA-C1A	6.70	109.74	106.68
29	I	208	CLA	C4A-NA-C1A	6.70	109.73	106.68
29	J	309	CLA	C4A-NA-C1A	6.69	109.73	106.68
29	P	214	CLA	C4A-NA-C1A	6.69	109.73	106.68
29	b	701	CLA	C4A-NA-C1A	6.69	109.73	106.68
29	b	702	CLA	C4A-NA-C1A	6.68	109.73	106.68
29	F	313	CLA	C4A-NA-C1A	6.68	109.73	106.68
29	Q	315	CLA	C4A-NA-C1A	6.68	109.73	106.68
29	B	314	CLA	C4A-NA-C1A	6.68	109.72	106.68
29	l	502	CLA	C4A-NA-C1A	6.67	109.72	106.68
29	I	201	CLA	C4A-NA-C1A	6.67	109.72	106.68
29	B	312	CLA	C4A-NA-C1A	6.67	109.72	106.68
29	Q	313	CLA	C4A-NA-C1A	6.67	109.72	106.68
29	L	310	CLA	C4A-NA-C1A	6.67	109.72	106.68
29	a	807	CLA	C4A-NA-C1A	6.66	109.72	106.68
29	B	307	CLA	C4A-NA-C1A	6.66	109.72	106.68
29	C	311	CLA	C4A-NA-C1A	6.66	109.72	106.68
32	i	204	BCR	C24-C23-C22	-6.65	116.40	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	313	CLA	C4A-NA-C1A	6.65	109.71	106.68
29	J	311	CLA	C4A-NA-C1A	6.64	109.71	106.68
29	a	815	CLA	C4A-NA-C1A	6.63	109.71	106.68
29	a	827	CLA	C4A-NA-C1A	6.63	109.71	106.68
29	L	313	CLA	C4A-NA-C1A	6.63	109.71	106.68
29	b	709	CLA	C4A-NA-C1A	6.63	109.70	106.68
29	E	308	CLA	C4A-NA-C1A	6.63	109.70	106.68
29	J	306	CLA	C4A-NA-C1A	6.63	109.70	106.68
29	M	313	CLA	C4A-NA-C1A	6.63	109.70	106.68
29	a	831	CLA	C4A-NA-C1A	6.62	109.70	106.68
29	a	828	CLA	C4A-NA-C1A	6.62	109.70	106.68
29	a	805	CLA	C4A-NA-C1A	6.61	109.69	106.68
29	D	308	CLA	C4A-NA-C1A	6.60	109.69	106.68
29	a	824	CLA	C4A-NA-C1A	6.59	109.69	106.68
29	b	722	CLA	C4A-NA-C1A	6.59	109.69	106.68
29	A	215	CLA	C4A-NA-C1A	6.59	109.69	106.68
29	A	214	CLA	C4A-NA-C1A	6.59	109.68	106.68
29	M	308	CLA	C4A-NA-C1A	6.59	109.68	106.68
29	K	216	CLA	C4A-NA-C1A	6.58	109.68	106.68
29	I	217	CLA	C4A-NA-C1A	6.58	109.68	106.68
29	Q	310	CLA	C4A-NA-C1A	6.58	109.68	106.68
29	D	311	CLA	C4A-NA-C1A	6.58	109.68	106.68
29	J	308	CLA	C4A-NA-C1A	6.57	109.67	106.68
29	N	311	CLA	C4A-NA-C1A	6.56	109.67	106.68
36	K	221	DD6	C9-C10-C11	-6.56	118.07	127.28
29	b	705	CLA	C4A-NA-C1A	6.56	109.67	106.68
29	a	806	CLA	C4A-NA-C1A	6.56	109.67	106.68
29	A	207	CLA	C4A-NA-C1A	6.56	109.67	106.68
29	H	310	CLA	C4A-NA-C1A	6.56	109.67	106.68
29	a	817	CLA	C4A-NA-C1A	6.56	109.67	106.68
29	a	816	CLA	C4A-NA-C1A	6.55	109.67	106.68
29	K	217	CLA	C4A-NA-C1A	6.55	109.67	106.68
29	L	317	CLA	C4A-NA-C1A	6.55	109.67	106.68
29	b	707	CLA	C4A-NA-C1A	6.54	109.66	106.68
29	A	208	CLA	C4A-NA-C1A	6.54	109.66	106.68
29	K	207	CLA	C4A-NA-C1A	6.54	109.66	106.68
29	L	309	CLA	C4A-NA-C1A	6.54	109.66	106.68
36	J	301	DD6	C9-C10-C11	-6.54	118.11	127.28
29	F	307	CLA	C4A-NA-C1A	6.53	109.66	106.68
32	m	103	BCR	C15-C14-C13	-6.52	118.13	127.28
29	I	211	CLA	C4A-NA-C1A	6.52	109.65	106.68
29	E	305	CLA	C4A-NA-C1A	6.51	109.65	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	308	DD6	C14-C13-C11	-6.51	115.43	125.53
29	a	809	CLA	C4A-NA-C1A	6.51	109.65	106.68
29	h	201	CLA	C4A-NA-C1A	6.51	109.65	106.68
29	f	802	CLA	C4A-NA-C1A	6.50	109.65	106.68
29	i	203	CLA	C4A-NA-C1A	6.50	109.65	106.68
29	N	308	CLA	C4A-NA-C1A	6.50	109.65	106.68
29	M	306	CLA	C4A-NA-C1A	6.50	109.64	106.68
29	N	314	CLA	C4A-NA-C1A	6.50	109.64	106.68
29	Q	307	CLA	C4A-NA-C1A	6.50	109.64	106.68
38	O	306	UIX	C14-C13-C11	-6.50	118.17	127.28
29	B	316	CLA	C4A-NA-C1A	6.50	109.64	106.68
29	O	311	CLA	C4A-NA-C1A	6.49	109.64	106.68
38	Q	305	UIX	O-C1-C6	6.49	122.31	115.05
29	I	214	CLA	C4A-NA-C1A	6.49	109.64	106.68
29	O	308	CLA	C4A-NA-C1A	6.49	109.64	106.68
29	b	713	CLA	C4A-NA-C1A	6.49	109.64	106.68
29	a	823	CLA	C4A-NA-C1A	6.48	109.64	106.68
29	P	212	CLA	C4A-NA-C1A	6.48	109.64	106.68
29	M	310	CLA	C4A-NA-C1A	6.48	109.64	106.68
29	G	316	CLA	C4A-NA-C1A	6.47	109.63	106.68
29	L	316	CLA	C4A-NA-C1A	6.47	109.63	106.68
38	O	306	UIX	C6-C1-C	-6.47	111.66	122.30
29	A	212	CLA	C4A-NA-C1A	6.47	109.63	106.68
29	C	309	CLA	C4A-NA-C1A	6.47	109.63	106.68
29	K	218	CLA	C4A-NA-C1A	6.46	109.63	106.68
29	G	301	CLA	C4A-NA-C1A	6.46	109.63	106.68
32	m	103	BCR	C7-C8-C9	-6.46	116.68	126.23
29	C	308	CLA	C4A-NA-C1A	6.46	109.63	106.68
29	G	311	CLA	C4A-NA-C1A	6.46	109.62	106.68
29	f	803	CLA	C4A-NA-C1A	6.45	109.62	106.68
29	a	829	CLA	C4A-NA-C1A	6.45	109.62	106.68
29	M	315	CLA	C4A-NA-C1A	6.45	109.62	106.68
29	H	307	CLA	C4A-NA-C1A	6.45	109.62	106.68
29	K	210	CLA	C4A-NA-C1A	6.44	109.62	106.68
29	E	306	CLA	C4A-NA-C1A	6.44	109.62	106.68
29	a	818	CLA	C4A-NA-C1A	6.44	109.62	106.68
29	l	503	CLA	C4A-NA-C1A	6.44	109.62	106.68
39	O	312	KC1	O2D-CGD-CBD	6.43	122.47	111.23
29	T	316	CLA	C4A-NA-C1A	6.43	109.61	106.68
29	a	813	CLA	C4A-NA-C1A	6.43	109.61	106.68
29	i	202	CLA	C4A-NA-C1A	6.42	109.61	106.68
29	b	710	CLA	C4A-NA-C1A	6.42	109.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	316	CLA	C4A-NA-C1A	6.42	109.61	106.68
29	D	309	CLA	C4A-NA-C1A	6.42	109.61	106.68
29	D	312	CLA	C4A-NA-C1A	6.41	109.61	106.68
29	O	316	CLA	C4A-NA-C1A	6.41	109.61	106.68
29	Q	312	CLA	C4A-NA-C1A	6.41	109.61	106.68
29	G	313	CLA	C4A-NA-C1A	6.41	109.60	106.68
29	A	218	CLA	C4A-NA-C1A	6.41	109.60	106.68
29	Q	308	CLA	C4A-NA-C1A	6.41	109.60	106.68
29	G	319	CLA	C4A-NA-C1A	6.40	109.60	106.68
29	H	308	CLA	C4A-NA-C1A	6.40	109.60	106.68
29	K	209	CLA	C4A-NA-C1A	6.40	109.60	106.68
29	l	508	CLA	C4A-NA-C1A	6.40	109.60	106.68
29	P	210	CLA	C4A-NA-C1A	6.39	109.60	106.68
29	A	216	CLA	C4A-NA-C1A	6.39	109.59	106.68
32	a	838	BCR	C16-C17-C18	-6.39	118.32	127.28
36	E	302	DD6	C14-C13-C11	-6.38	115.63	125.53
29	A	209	CLA	C4A-NA-C1A	6.38	109.59	106.68
29	T	308	CLA	C4A-NA-C1A	6.38	109.59	106.68
37	T	317	PID	C17-C16-C15	6.37	136.55	123.52
29	a	826	CLA	C4A-NA-C1A	6.36	109.58	106.68
29	F	312	CLA	C4A-NA-C1A	6.36	109.58	106.68
29	E	315	CLA	C4A-NA-C1A	6.36	109.58	106.68
29	J	313	CLA	C4A-NA-C1A	6.36	109.58	106.68
29	G	312	CLA	C4A-NA-C1A	6.36	109.58	106.68
38	F	305	UIX	C6-C1-C	-6.35	111.84	122.30
29	E	313	CLA	C4A-NA-C1A	6.35	109.58	106.68
29	b	725	CLA	C4A-NA-C1A	6.35	109.57	106.68
29	B	315	CLA	C4A-NA-C1A	6.35	109.57	106.68
29	T	311	CLA	C4A-NA-C1A	6.35	109.57	106.68
29	b	714	CLA	C4A-NA-C1A	6.34	109.57	106.68
29	a	821	CLA	C4A-NA-C1A	6.33	109.57	106.68
29	b	716	CLA	C4A-NA-C1A	6.33	109.56	106.68
29	L	308	CLA	C4A-NA-C1A	6.33	109.56	106.68
29	L	315	CLA	C4A-NA-C1A	6.32	109.56	106.68
29	b	708	CLA	C4A-NA-C1A	6.32	109.56	106.68
38	L	302	UIX	O-C1-C3	6.32	119.42	113.49
29	L	312	CLA	C4A-NA-C1A	6.32	109.56	106.68
29	l	509	CLA	C4A-NA-C1A	6.31	109.56	106.68
29	f	805	CLA	C4A-NA-C1A	6.31	109.56	106.68
29	b	712	CLA	C4A-NA-C1A	6.31	109.56	106.68
29	F	308	CLA	C4A-NA-C1A	6.31	109.56	106.68
29	B	309	CLA	C4A-NA-C1A	6.30	109.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	731	CLA	C4A-NA-C1A	6.30	109.55	106.68
29	B	306	CLA	C4A-NA-C1A	6.30	109.55	106.68
29	B	310	CLA	C4A-NA-C1A	6.30	109.55	106.68
29	T	313	CLA	C4A-NA-C1A	6.29	109.55	106.68
29	a	830	CLA	C4A-NA-C1A	6.29	109.55	106.68
29	b	720	CLA	C4A-NA-C1A	6.29	109.55	106.68
29	D	313	CLA	C4A-NA-C1A	6.29	109.55	106.68
32	l	507	BCR	C15-C14-C13	-6.28	118.46	127.28
29	b	715	CLA	C4A-NA-C1A	6.28	109.55	106.68
29	b	726	CLA	C4A-NA-C1A	6.28	109.55	106.68
29	K	208	CLA	C4A-NA-C1A	6.28	109.54	106.68
29	J	305	CLA	C4A-NA-C1A	6.28	109.54	106.68
29	B	308	CLA	C4A-NA-C1A	6.28	109.54	106.68
37	H	305	PID	C7-C8-C9	6.28	133.97	126.06
29	G	302	CLA	C4A-NA-C1A	6.27	109.54	106.68
29	b	718	CLA	C4A-NA-C1A	6.26	109.54	106.68
29	I	212	CLA	C4A-NA-C1A	6.24	109.53	106.68
29	P	209	CLA	C4A-NA-C1A	6.23	109.52	106.68
29	E	310	CLA	C4A-NA-C1A	6.23	109.52	106.68
29	E	311	CLA	C4A-NA-C1A	6.23	109.52	106.68
36	C	303	DD6	C4-C5-C6	-6.22	118.56	127.28
38	E	304	UIX	O-C1-C3	6.22	119.32	113.49
29	H	312	CLA	C4A-NA-C1A	6.21	109.51	106.68
29	a	822	CLA	C4A-NA-C1A	6.21	109.51	106.68
29	I	213	CLA	C4A-NA-C1A	6.21	109.51	106.68
29	a	814	CLA	C4A-NA-C1A	6.21	109.51	106.68
29	b	723	CLA	C4A-NA-C1A	6.20	109.51	106.68
36	E	302	DD6	C4-C5-C6	-6.20	118.58	127.28
29	K	211	CLA	C4A-NA-C1A	6.20	109.51	106.68
38	Q	305	UIX	C7-C10-C11	-6.20	115.92	125.53
29	l	510	CLA	C4A-NA-C1A	6.19	109.50	106.68
29	H	315	CLA	C4A-NA-C1A	6.19	109.50	106.68
38	C	306	UIX	C14-C13-C11	-6.18	118.61	127.28
29	I	209	CLA	C4A-NA-C1A	6.17	109.49	106.68
29	K	212	CLA	C4A-NA-C1A	6.17	109.49	106.68
29	a	811	CLA	C4A-NA-C1A	6.17	109.49	106.68
29	G	317	CLA	C4A-NA-C1A	6.16	109.49	106.68
29	K	213	CLA	C4A-NA-C1A	6.15	109.48	106.68
29	a	837	CLA	C4A-NA-C1A	6.14	109.48	106.68
29	a	808	CLA	C4A-NA-C1A	6.13	109.47	106.68
29	I	210	CLA	C4A-NA-C1A	6.13	109.47	106.68
38	T	306	UIX	C6-C1-C	-6.13	112.22	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	M	307	CLA	C4A-NA-C1A	6.13	109.47	106.68
29	O	309	CLA	C4A-NA-C1A	6.13	109.47	106.68
29	a	819	CLA	C4A-NA-C1A	6.09	109.46	106.68
29	A	211	CLA	C4A-NA-C1A	6.09	109.46	106.68
37	P	206	PID	C17-C16-C15	6.09	135.97	123.52
38	N	306	UIX	C6-C1-C	-6.08	112.29	122.30
38	B	304	UIX	O-C1-C3	6.07	119.18	113.49
36	G	308	DD6	C9-C10-C11	-6.07	118.76	127.28
29	b	717	CLA	C4A-NA-C1A	6.07	109.45	106.68
29	J	307	CLA	C4A-NA-C1A	6.06	109.44	106.68
29	A	217	CLA	C4A-NA-C1A	6.06	109.44	106.68
29	N	309	CLA	C4A-NA-C1A	6.06	109.44	106.68
29	a	820	CLA	C4A-NA-C1A	6.05	109.44	106.68
29	b	719	CLA	C4A-NA-C1A	6.05	109.44	106.68
38	C	306	UIX	C6-C1-C	-6.04	112.36	122.30
29	L	311	CLA	C4A-NA-C1A	6.04	109.43	106.68
29	O	313	CLA	C4A-NA-C1A	6.03	109.43	106.68
36	J	303	DD6	C9-C10-C11	-6.02	118.84	127.28
29	J	310	CLA	C4A-NA-C1A	6.02	109.42	106.68
36	P	204	DD6	C4-C5-C6	-6.02	118.84	127.28
29	M	314	CLA	C4A-NA-C1A	6.01	109.42	106.68
29	M	311	CLA	C4A-NA-C1A	5.99	109.41	106.68
32	i	204	BCR	C20-C21-C22	-5.98	118.89	127.28
36	D	301	DD6	C3-C2-C1	-5.98	118.89	127.28
37	O	305	PID	C7-C8-C9	5.97	133.58	126.06
29	b	724	CLA	C4A-NA-C1A	5.97	109.40	106.68
29	K	214	CLA	C4A-NA-C1A	5.96	109.40	106.68
29	E	314	CLA	C4A-NA-C1A	5.96	109.40	106.68
38	P	207	UIX	C14-C13-C11	-5.94	118.94	127.28
39	Q	311	KC1	C1D-ND-C4D	5.94	110.48	106.31
29	b	704	CLA	C4A-NA-C1A	5.91	109.38	106.68
39	O	312	KC1	C1D-ND-C4D	5.91	110.46	106.31
39	G	315	KC1	C1D-ND-C4D	5.89	110.44	106.31
32	m	103	BCR	C11-C10-C9	-5.88	119.03	127.28
32	b	728	BCR	C24-C23-C22	-5.87	117.55	126.23
38	T	306	UIX	C36-C35-C32	-5.87	119.05	127.28
37	F	302	PID	C18-C19-C20	5.86	135.52	123.52
36	I	203	DD6	O1-C20-C19	5.85	118.97	113.49
29	l	505	CLA	C4A-NA-C1A	5.85	109.35	106.68
36	O	303	DD6	C4-C5-C6	-5.84	119.09	127.28
36	G	306	DD6	C9-C10-C11	-5.83	119.10	127.28
29	A	210	CLA	C4A-NA-C1A	5.83	109.34	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	T	303	DD6	C9-C10-C11	-5.83	119.11	127.28
36	I	205	DD6	O1-C15-C14	-5.82	100.21	116.88
29	a	803	CLA	C4A-NA-C1A	5.81	109.33	106.68
37	H	304	PID	C17-C16-C15	5.80	135.38	123.52
29	a	802	CLA	C4A-NA-C1A	5.79	109.32	106.68
29	b	711	CLA	C4A-NA-C1A	5.79	109.32	106.68
36	A	201	DD6	C9-C10-C11	-5.78	119.17	127.28
29	b	703	CLA	C4A-NA-C1A	5.78	109.32	106.68
38	P	207	UIX	C6-C1-C	-5.77	112.80	122.30
32	i	204	BCR	C16-C17-C18	-5.76	119.19	127.28
38	O	306	UIX	O-C1-C6	5.76	121.49	115.05
36	J	303	DD6	C3-C2-C1	-5.74	119.22	127.28
38	N	306	UIX	C37-C39-C40	-5.70	119.29	127.28
36	K	202	DD6	O1-C20-C19	-5.70	108.15	113.49
38	O	306	UIX	C37-C39-C40	-5.70	119.29	127.28
29	M	309	CLA	C4A-NA-C1A	5.70	109.28	106.68
36	D	304	DD6	C4-C5-C6	-5.69	119.30	127.28
36	F	303	DD6	C4-C5-C6	-5.65	119.35	127.28
37	T	307	PID	C18-C19-C20	5.63	135.03	123.52
32	f	801	BCR	C20-C21-C22	-5.62	119.39	127.28
38	O	306	UIX	C7-C10-C11	-5.62	116.81	125.53
38	T	306	UIX	C7-C10-C11	-5.62	116.82	125.53
32	f	801	BCR	C15-C14-C13	-5.60	119.43	127.28
38	T	306	UIX	C37-C39-C40	-5.59	119.44	127.28
37	E	301	PID	C18-C19-C20	5.57	134.92	123.52
36	K	206	DD6	C3-C2-C1	-5.57	119.46	127.28
36	G	307	DD6	C9-C10-C11	-5.56	119.48	127.28
32	b	728	BCR	C20-C21-C22	-5.56	119.49	127.28
37	C	301	PID	C17-C16-C15	5.55	134.88	123.52
38	F	305	UIX	C14-C13-C11	-5.55	119.49	127.28
38	T	306	UIX	C34-C30-C26	-5.55	119.50	127.28
39	P	213	KC1	C1D-ND-C4D	5.54	110.20	106.31
36	I	204	DD6	C3-C2-C1	-5.53	119.52	127.28
37	O	301	PID	C17-C16-C15	5.53	134.83	123.52
37	P	208	PID	C17-C18-C19	5.53	137.50	124.72
36	D	304	DD6	C3-C2-C1	-5.53	119.53	127.28
32	f	804	BCR	C15-C14-C13	-5.52	119.53	127.28
39	T	312	KC1	C1D-ND-C4D	5.52	110.19	106.31
36	G	307	DD6	C4-C5-C6	-5.52	119.53	127.28
29	O	314	CLA	C4A-NA-C1A	5.51	109.19	106.68
38	Q	305	UIX	C34-C30-C26	-5.51	119.55	127.28
36	M	303	DD6	C9-C10-C11	-5.49	119.57	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	H	305	PID	C17-C16-C15	5.49	134.75	123.52
36	K	202	DD6	C3-C2-C1	-5.47	119.61	127.28
39	G	315	KC1	O2D-CGD-CBD	5.45	120.76	111.23
38	T	306	UIX	O-C1-C6	5.44	121.13	115.05
36	G	306	DD6	C3-C2-C1	-5.43	119.67	127.28
36	I	203	DD6	C3-C2-C1	-5.42	119.67	127.28
38	C	306	UIX	C7-C10-C11	-5.40	117.15	125.53
32	i	204	BCR	C7-C8-C9	-5.40	118.24	126.23
36	K	203	DD6	C9-C10-C11	-5.36	119.75	127.28
38	N	306	UIX	C34-C30-C26	-5.35	119.77	127.28
36	I	205	DD6	C4-C5-C6	-5.34	119.78	127.28
36	m	101	DD6	C3-C2-C1	-5.34	119.79	127.28
39	F	309	KC1	O2D-CGD-CBD	5.33	120.55	111.23
36	B	319	DD6	C21-C20-C19	5.32	120.21	114.24
36	J	302	DD6	C21-C20-C15	-5.30	113.59	122.30
36	B	305	DD6	C3-C2-C1	-5.29	119.86	127.28
39	T	310	KC1	C1D-ND-C4D	5.29	110.03	106.31
39	C	312	KC1	C1D-ND-C4D	5.29	110.02	106.31
38	P	207	UIX	O-C1-C6	5.28	120.95	115.05
39	Q	311	KC1	O2D-CGD-CBD	5.28	120.46	111.23
36	L	305	DD6	C21-C20-C19	5.28	120.17	114.24
38	T	306	UIX	O-C-C7	-5.27	101.78	116.88
36	G	307	DD6	C-C1-C2	-5.27	114.28	122.82
36	I	205	DD6	C3-C2-C1	-5.25	119.92	127.28
39	C	315	KC1	C1D-ND-C4D	5.25	110.00	106.31
32	a	834	BCR	C16-C17-C18	-5.24	119.92	127.28
36	G	305	DD6	C4-C5-C6	-5.24	119.93	127.28
36	P	204	DD6	C21-C20-C19	5.24	120.12	114.24
37	P	205	PID	C17-C16-C15	5.23	134.23	123.52
36	L	304	DD6	C3-C2-C1	-5.23	119.95	127.28
38	N	306	UIX	C14-C13-C11	-5.22	119.96	127.28
38	A	203	UIX	O-C1-C3	5.21	118.38	113.49
39	C	310	KC1	O2D-CGD-CBD	5.21	120.34	111.23
36	M	301	DD6	C3-C2-C1	-5.19	120.00	127.28
36	M	303	DD6	C4-C5-C6	-5.19	120.01	127.28
36	M	303	DD6	C3-C2-C1	-5.18	120.02	127.28
38	N	306	UIX	O-C1-C6	5.17	120.83	115.05
36	A	204	DD6	C21-C20-C19	5.16	120.04	114.24
38	C	306	UIX	O-C1-C6	5.16	120.81	115.05
32	a	834	BCR	C15-C14-C13	-5.15	120.05	127.28
39	D	310	KC1	C1D-ND-C4D	5.15	109.92	106.31
39	E	307	KC1	C1D-ND-C4D	5.14	109.92	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	T	303	DD6	C4-C5-C6	-5.14	120.07	127.28
39	D	315	KC1	C1D-ND-C4D	5.14	109.92	106.31
36	A	201	DD6	C3-C2-C1	-5.14	120.08	127.28
38	B	304	UIX	O2-C27-C31	5.12	120.22	111.09
36	I	205	DD6	C9-C10-C11	-5.11	120.11	127.28
32	a	835	BCR	C15-C14-C13	-5.11	120.11	127.28
39	M	305	KC1	C1D-ND-C4D	5.11	109.89	106.31
38	E	304	UIX	O2-C27-C31	5.09	120.17	111.09
39	J	312	KC1	C1D-ND-C4D	5.09	109.88	106.31
36	O	303	DD6	O1-C20-C19	5.08	118.25	113.49
38	F	305	UIX	C36-C35-C32	-5.08	120.15	127.28
39	C	310	KC1	C1D-ND-C4D	5.08	109.87	106.31
32	b	735	BCR	C24-C23-C22	-5.07	118.73	126.23
36	D	304	DD6	C21-C20-C19	5.07	119.94	114.24
36	K	221	DD6	C4-C5-C6	-5.07	120.17	127.28
36	K	221	DD6	O1-C20-C19	5.06	118.24	113.49
36	m	101	DD6	C21-C20-C19	5.06	119.93	114.24
36	K	221	DD6	C3-C2-C1	-5.06	120.18	127.28
39	Q	314	KC1	C1D-ND-C4D	5.06	109.86	106.31
39	D	315	KC1	O2D-CGD-CBD	5.06	120.08	111.23
38	Q	305	UIX	C6-C1-C3	5.06	119.92	114.24
36	I	204	DD6	O1-C15-C14	-5.05	102.40	116.88
38	P	207	UIX	C34-C30-C26	-5.05	120.19	127.28
36	K	206	DD6	C21-C20-C19	5.05	119.91	114.24
36	h	202	DD6	C4-C5-C6	-5.04	120.21	127.28
36	I	202	DD6	C3-C2-C1	-5.03	120.22	127.28
36	J	302	DD6	C21-C20-C19	5.03	119.89	114.24
36	B	302	DD6	C21-C20-C19	5.03	119.89	114.24
39	L	314	KC1	O2D-CGD-CBD	5.03	120.02	111.23
36	A	201	DD6	C21-C20-C19	5.02	119.88	114.24
36	J	302	DD6	C3-C2-C1	-5.02	120.24	127.28
36	I	204	DD6	C9-C10-C11	-5.02	120.24	127.28
39	C	312	KC1	O2D-CGD-CBD	5.02	120.00	111.23
39	K	215	KC1	O2D-CGD-CBD	5.01	120.00	111.23
36	E	302	DD6	C9-C10-C11	-5.01	120.25	127.28
36	B	301	DD6	C21-C20-C19	5.01	119.87	114.24
32	i	204	BCR	C11-C10-C9	-5.00	120.26	127.28
36	H	303	DD6	C4-C5-C6	-5.00	120.26	127.28
39	J	312	KC1	O2D-CGD-CBD	5.00	119.97	111.23
39	M	305	KC1	O2D-CGD-CBD	5.00	119.97	111.23
38	P	207	UIX	O-C-C7	-5.00	102.56	116.88
39	T	315	KC1	C1D-ND-C4D	5.00	109.82	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Q	314	KC1	O2D-CGD-CBD	5.00	119.96	111.23
39	N	312	KC1	C1D-ND-C4D	4.99	109.82	106.31
39	I	215	KC1	O2D-CGD-CBD	4.99	119.96	111.23
39	D	310	KC1	O2D-CGD-CBD	4.99	119.95	111.23
39	P	216	KC1	O2D-CGD-CBD	4.99	119.95	111.23
38	A	203	UIX	O-C1-C6	4.98	120.62	115.05
39	N	315	KC1	C1D-ND-C4D	4.98	109.81	106.31
39	P	211	KC1	O2D-CGD-CBD	4.98	119.93	111.23
38	C	306	UIX	C37-C39-C40	-4.98	120.30	127.28
39	H	311	KC1	C1D-ND-C4D	4.97	109.80	106.31
39	F	314	KC1	C1D-ND-C4D	4.97	109.80	106.31
36	I	202	DD6	C21-C20-C19	4.97	119.82	114.24
36	G	305	DD6	C9-C10-C11	-4.97	120.31	127.28
32	a	835	BCR	C20-C21-C22	-4.97	120.31	127.28
39	T	312	KC1	O2D-CGD-CBD	4.97	119.91	111.23
39	F	309	KC1	C1D-ND-C4D	4.96	109.79	106.31
36	O	303	DD6	O1-C20-C21	4.96	120.59	115.05
39	O	310	KC1	O2D-CGD-CBD	4.96	119.89	111.23
37	O	304	PID	C17-C16-C15	4.95	133.65	123.52
37	Q	304	PID	C18-C19-C20	4.95	133.64	123.52
39	K	215	KC1	C1D-ND-C4D	4.95	109.78	106.31
39	O	315	KC1	C1D-ND-C4D	4.94	109.78	106.31
36	A	202	DD6	C21-C20-C19	4.94	119.79	114.24
32	a	835	BCR	C16-C17-C18	-4.94	120.35	127.28
39	P	216	KC1	C1D-ND-C4D	4.94	109.78	106.31
37	T	305	PID	C18-C19-C20	4.94	133.62	123.52
39	M	312	KC1	O2D-CGD-CBD	4.94	119.86	111.23
36	L	305	DD6	C4-C5-C6	-4.94	120.36	127.28
36	K	202	DD6	C4-C5-C6	-4.94	120.36	127.28
36	B	305	DD6	C21-C20-C19	4.92	119.77	114.24
36	L	301	DD6	C21-C20-C19	4.92	119.77	114.24
39	E	312	KC1	C1D-ND-C4D	4.91	109.76	106.31
39	H	314	KC1	O2D-CGD-CBD	4.91	119.81	111.23
36	T	303	DD6	C21-C20-C19	4.90	119.74	114.24
36	P	204	DD6	O1-C20-C19	-4.90	108.90	113.49
36	D	301	DD6	O1-C20-C21	-4.88	109.59	115.05
36	K	205	DD6	C21-C20-C19	4.88	119.72	114.24
39	A	205	KC1	C1D-ND-C4D	4.88	109.73	106.31
39	Q	309	KC1	O2D-CGD-CBD	4.87	119.75	111.23
38	L	302	UIX	C34-C30-C26	-4.86	120.46	127.28
36	K	204	DD6	O1-C15-C14	-4.86	102.95	116.88
39	H	314	KC1	C1D-ND-C4D	4.86	109.72	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	F	305	UIX	C7-C10-C11	-4.85	118.00	125.53
36	K	204	DD6	C9-C10-C11	-4.85	120.48	127.28
39	N	310	KC1	C1D-ND-C4D	4.84	109.71	106.31
37	N	301	PID	C17-C16-C15	4.84	133.43	123.52
36	D	304	DD6	C9-C10-C11	-4.84	120.50	127.28
36	F	303	DD6	C3-C2-C1	-4.83	120.50	127.28
39	Q	309	KC1	C1D-ND-C4D	4.83	109.70	106.31
39	A	213	KC1	O2D-CGD-CBD	4.83	119.67	111.23
39	N	310	KC1	O2D-CGD-CBD	4.83	119.67	111.23
39	M	312	KC1	C1D-ND-C4D	4.82	109.69	106.31
36	J	302	DD6	C4-C5-C6	-4.82	120.52	127.28
36	K	203	DD6	C21-C20-C19	4.82	119.65	114.24
39	N	312	KC1	O2D-CGD-CBD	4.82	119.65	111.23
36	G	306	DD6	C4-C5-C6	-4.81	120.53	127.28
36	L	301	DD6	C3-C2-C1	-4.81	120.53	127.28
38	N	306	UIX	C36-C35-C32	-4.81	120.53	127.28
39	L	314	KC1	C1D-ND-C4D	4.80	109.68	106.31
39	A	213	KC1	C1D-ND-C4D	4.80	109.68	106.31
32	b	728	BCR	C16-C17-C18	-4.80	120.55	127.28
36	B	301	DD6	C3-C2-C1	-4.79	120.56	127.28
38	F	305	UIX	C37-C39-C40	-4.79	120.56	127.28
38	P	207	UIX	C37-C39-C40	-4.79	120.56	127.28
39	H	309	KC1	C1D-ND-C4D	4.79	109.67	106.31
36	L	304	DD6	C9-C10-C11	-4.78	120.57	127.28
37	C	304	PID	C17-C16-C15	4.78	133.30	123.52
37	H	301	PID	C17-C16-C15	4.78	133.30	123.52
38	T	306	UIX	O2-C27-C31	4.78	119.61	111.09
39	G	318	KC1	O2D-CGD-CBD	4.77	119.57	111.23
39	B	313	KC1	O2D-CGD-CBD	4.77	119.57	111.23
32	a	838	BCR	C15-C14-C13	-4.77	120.59	127.28
36	I	203	DD6	C9-C10-C11	-4.77	120.59	127.28
39	T	315	KC1	O2D-CGD-CBD	4.77	119.57	111.23
39	N	315	KC1	O2D-CGD-CBD	4.77	119.57	111.23
38	P	207	UIX	O-C1-C3	4.77	117.96	113.49
38	Q	305	UIX	C37-C39-C40	-4.76	120.60	127.28
39	B	313	KC1	C1D-ND-C4D	4.75	109.65	106.31
36	I	203	DD6	C21-C20-C19	4.75	119.58	114.24
36	G	306	DD6	C21-C20-C19	4.75	119.58	114.24
36	B	303	DD6	C21-C20-C19	4.74	119.57	114.24
39	O	310	KC1	C1D-ND-C4D	4.73	109.63	106.31
37	Q	303	PID	C17-C16-C15	4.73	133.20	123.52
36	D	301	DD6	C14-C13-C11	4.73	132.87	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	l	506	BCR	C28-C27-C26	-4.72	105.63	114.06
36	I	206	DD6	C3-C2-C1	-4.72	120.65	127.28
38	O	306	UIX	O2-C27-C31	4.72	119.51	111.09
36	N	303	DD6	C21-C20-C19	4.72	119.54	114.24
36	G	305	DD6	C24-C1-C2	4.72	126.43	119.01
36	G	308	DD6	C3-C2-C1	-4.71	120.67	127.28
38	Q	305	UIX	C36-C35-C32	-4.71	120.67	127.28
36	M	303	DD6	O1-C15-C14	-4.71	103.38	116.88
32	b	728	BCR	C33-C5-C6	-4.71	119.35	124.48
36	I	206	DD6	C21-C20-C19	4.71	119.53	114.24
32	f	804	BCR	C11-C10-C9	-4.70	120.69	127.28
36	B	302	DD6	C4-C5-C6	-4.70	120.69	127.28
38	O	306	UIX	C34-C30-C26	-4.70	120.69	127.28
38	C	306	UIX	O2-C27-C31	4.69	119.46	111.09
38	C	306	UIX	O-C-C7	-4.69	103.44	116.88
39	L	306	KC1	O2D-CGD-CBD	4.69	119.42	111.23
39	E	307	KC1	O2D-CGD-CBD	4.68	119.41	111.23
37	E	301	PID	C16-C15-C14	4.68	133.84	127.28
32	b	729	BCR	C3-C4-C5	-4.68	105.72	114.06
36	B	319	DD6	O1-C15-C14	-4.68	103.48	116.88
36	Q	302	DD6	C4-C5-C6	-4.67	120.73	127.28
39	G	318	KC1	C1D-ND-C4D	4.67	109.59	106.31
38	Q	305	UIX	O-C-C7	-4.66	103.52	116.88
37	P	203	PID	C18-C19-C20	4.66	133.05	123.52
35	B	318	DGD	O2G-C1B-C2B	4.66	121.56	111.48
36	Q	302	DD6	C21-C20-C19	4.66	119.47	114.24
32	m	103	BCR	C16-C17-C18	-4.65	120.75	127.28
38	J	304	UIX	C14-C23-C26	-4.65	113.61	126.36
36	K	202	DD6	C15-C14-C13	-4.65	116.17	125.99
37	O	301	PID	CM4-C14-C15	-4.65	115.29	122.82
36	M	304	DD6	C3-C2-C1	-4.64	120.77	127.28
39	I	215	KC1	C1D-ND-C4D	4.64	109.57	106.31
38	N	306	UIX	O-C1-C3	4.64	117.84	113.49
35	b	733	DGD	O2G-C1B-C2B	4.63	121.50	111.48
36	I	203	DD6	C4-C5-C6	-4.63	120.78	127.28
39	C	315	KC1	O2D-CGD-CBD	4.63	119.32	111.23
39	L	306	KC1	C1D-ND-C4D	4.63	109.56	106.31
39	P	211	KC1	C1D-ND-C4D	4.62	109.56	106.31
37	P	208	PID	C12-O4-C10	4.62	109.92	107.68
38	A	203	UIX	O2-C27-C31	4.62	119.33	111.09
38	C	306	UIX	C34-C30-C26	-4.62	120.80	127.28
38	O	306	UIX	C6-C1-C3	4.61	119.42	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Q	305	UIX	O2-C27-C31	4.61	119.31	111.09
36	E	303	DD6	C21-C20-C19	4.61	119.42	114.24
39	F	314	KC1	O2D-CGD-CBD	4.61	119.29	111.23
39	T	310	KC1	O2D-CGD-CBD	4.61	119.29	111.23
37	D	307	PID	C17-C16-C15	4.61	132.95	123.52
38	P	207	UIX	C7-C10-C11	-4.60	118.39	125.53
37	N	304	PID	C17-C16-C15	4.60	132.93	123.52
38	C	306	UIX	O-C1-C3	4.59	117.80	113.49
39	A	205	KC1	O2D-CGD-CBD	4.59	119.25	111.23
37	T	317	PID	CM4-C14-C15	-4.59	115.38	122.82
37	G	303	PID	C17-C16-C15	4.59	132.91	123.52
37	D	307	PID	C18-C19-C20	4.59	132.90	123.52
36	h	202	DD6	C3-C2-C1	-4.58	120.86	127.28
38	J	304	UIX	C34-C30-C26	-4.58	120.86	127.28
37	H	304	PID	CM4-C14-C15	-4.56	115.42	122.82
38	E	304	UIX	C34-C30-C26	-4.56	120.88	127.28
39	H	309	KC1	O2D-CGD-CBD	4.56	119.20	111.23
32	f	801	BCR	C24-C23-C22	-4.56	119.49	126.23
38	P	207	UIX	O2-C27-C31	4.56	119.21	111.09
38	N	306	UIX	O2-C27-C31	4.55	119.21	111.09
36	A	201	DD6	C14-C13-C11	-4.55	118.48	125.53
36	O	303	DD6	C9-C10-C11	-4.54	120.90	127.28
38	E	304	UIX	O-C1-C6	4.54	120.12	115.05
37	T	301	PID	C18-C19-C20	4.54	132.81	123.52
37	G	310	PID	C18-C19-C20	4.53	132.78	123.52
36	C	303	DD6	C9-C10-C11	-4.52	120.94	127.28
37	O	305	PID	C6-C7-C8	4.52	135.54	125.99
37	H	305	PID	C6-C7-C8	4.52	135.54	125.99
36	H	303	DD6	C21-C20-C19	4.52	119.31	114.24
38	L	302	UIX	O2-C27-C31	4.50	119.11	111.09
38	B	304	UIX	O-C1-C6	4.48	120.05	115.05
37	P	208	PID	CM4-C14-C15	-4.48	115.56	122.82
36	J	303	DD6	C4-C5-C6	-4.47	121.02	127.28
32	a	835	BCR	C24-C23-C22	-4.46	119.63	126.23
37	C	305	PID	C16-C15-C14	4.46	133.54	127.28
32	b	735	BCR	C16-C17-C18	-4.46	121.02	127.28
37	Q	306	PID	C17-C16-C15	4.46	132.64	123.52
38	F	305	UIX	O2-C27-C31	4.46	119.03	111.09
38	N	306	UIX	C6-C1-C3	4.45	119.24	114.24
37	H	304	PID	C12-O4-C10	4.45	109.84	107.68
36	L	301	DD6	C4-C5-C6	-4.44	121.05	127.28
37	O	301	PID	C12-O4-C10	4.42	109.83	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	301	DD6	C21-C20-C19	4.41	119.20	114.24
36	K	204	DD6	C3-C2-C1	-4.41	121.09	127.28
38	O	306	UIX	O-C-C7	-4.41	104.24	116.88
37	O	304	PID	CM4-C14-C15	-4.41	115.67	122.82
37	C	301	PID	CM4-C14-C15	-4.41	115.67	122.82
37	D	302	PID	C18-C19-C20	4.41	132.53	123.52
36	L	305	DD6	C3-C2-C1	-4.41	121.10	127.28
37	F	304	PID	CM4-C14-C15	-4.40	115.68	122.82
36	I	204	DD6	C4-C5-C6	-4.40	121.10	127.28
37	N	302	PID	C18-C19-C20	4.40	132.53	123.52
37	C	302	PID	C18-C19-C20	4.40	132.52	123.52
36	L	303	DD6	C21-C20-C19	4.39	119.17	114.24
39	P	213	KC1	O2D-CGD-CBD	4.38	118.89	111.23
36	M	302	DD6	C9-C10-C11	-4.38	121.14	127.28
36	B	302	DD6	C3-C2-C1	-4.38	121.14	127.28
36	L	304	DD6	C21-C20-C19	4.37	119.15	114.24
37	P	208	PID	C19-C20-C21	4.37	133.40	127.28
32	m	103	BCR	C20-C21-C22	-4.37	121.16	127.28
37	C	301	PID	C12-O4-C10	4.36	109.79	107.68
37	G	309	PID	C17-C16-C15	4.35	132.41	123.52
39	O	315	KC1	O2D-CGD-CBD	4.34	118.82	111.23
35	j	105	DGD	O2G-C1B-C2B	4.33	120.85	111.48
36	P	204	DD6	C15-C14-C13	-4.33	116.85	125.99
36	J	301	DD6	C4-C5-C6	-4.32	121.22	127.28
37	O	302	PID	C18-C19-C20	4.31	132.35	123.52
36	L	304	DD6	C15-C14-C13	-4.31	116.87	125.99
36	L	301	DD6	C9-C10-C11	-4.31	121.23	127.28
37	T	301	PID	C17-C16-C15	4.31	132.34	123.52
39	E	312	KC1	O2D-CGD-CBD	4.30	118.74	111.23
36	H	303	DD6	C3-C2-C1	-4.29	121.26	127.28
37	H	306	PID	C18-C19-C20	4.29	132.30	123.52
32	l	506	BCR	C3-C4-C5	-4.29	106.41	114.06
36	A	204	DD6	C3-C2-C1	-4.29	121.26	127.28
36	P	204	DD6	C3-C2-C1	-4.26	121.30	127.28
38	T	306	UIX	O-C1-C3	4.26	117.49	113.49
36	J	302	DD6	O1-C20-C21	4.26	119.81	115.05
37	F	304	PID	O1-C1-CM1	4.26	119.81	115.05
38	O	306	UIX	C36-C35-C32	-4.26	121.31	127.28
38	A	203	UIX	C6-C1-C3	4.26	119.02	114.24
36	F	303	DD6	O1-C20-C19	4.26	117.48	113.49
37	N	304	PID	CM4-C14-C15	-4.25	115.93	122.82
36	B	303	DD6	C3-C2-C1	-4.25	121.32	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	P	205	PID	CM4-C14-C15	-4.25	115.93	122.82
32	i	204	BCR	C15-C14-C13	-4.25	121.32	127.28
32	a	834	BCR	C11-C10-C9	-4.24	121.33	127.28
35	j	106	DGD	O2G-C1B-C2B	4.24	120.66	111.48
36	B	319	DD6	C14-C13-C11	-4.24	118.95	125.53
36	M	304	DD6	C21-C20-C19	4.23	119.00	114.24
39	H	311	KC1	O2D-CGD-CBD	4.22	118.61	111.23
37	Q	301	PID	C18-C19-C20	4.22	132.15	123.52
37	T	302	PID	C18-C19-C20	4.20	132.11	123.52
38	L	302	UIX	O-C1-C6	4.20	119.74	115.05
37	H	301	PID	CM4-C14-C15	-4.20	116.02	122.82
36	I	204	DD6	O1-C20-C21	4.19	119.73	115.05
39	K	215	KC1	CHC-C4B-NB	4.19	130.70	124.80
32	l	507	BCR	C3-C4-C5	-4.19	106.59	114.06
37	N	301	PID	C12-O4-C10	4.18	109.71	107.68
32	l	506	BCR	C7-C8-C9	-4.18	120.05	126.23
36	G	307	DD6	O1-C20-C15	-4.18	55.61	58.93
36	C	303	DD6	C3-C2-C1	-4.18	121.42	127.28
38	N	306	UIX	C7-C10-C11	-4.17	119.06	125.53
36	E	302	DD6	C3-C2-C1	-4.17	121.44	127.28
37	T	304	PID	C17-C16-C15	4.16	132.04	123.52
37	T	304	PID	CM4-C14-C15	-4.16	116.08	122.82
37	H	302	PID	C18-C19-C20	4.15	132.02	123.52
37	P	205	PID	C12-O4-C10	4.15	109.69	107.68
37	Q	306	PID	C12-O4-C10	4.13	109.69	107.68
37	P	206	PID	C12-O4-C10	4.13	109.69	107.68
37	C	307	PID	C18-C19-C20	4.13	131.98	123.52
36	J	302	DD6	C15-C14-C13	-4.13	117.25	125.99
36	E	302	DD6	O1-C15-C14	-4.13	105.04	116.88
36	A	202	DD6	C3-C2-C1	-4.13	121.49	127.28
37	Q	303	PID	CM4-C14-C15	-4.12	116.14	122.82
35	h	203	DGD	O2G-C1B-C2B	4.12	120.39	111.48
37	F	302	PID	C12-O4-C10	4.11	109.68	107.68
37	N	301	PID	CM4-C14-C15	-4.11	116.16	122.82
37	D	307	PID	C12-O4-C10	4.11	109.67	107.68
38	P	207	UIX	C16-C20-C15	4.11	123.77	119.70
37	D	305	PID	C17-C16-C15	4.10	131.91	123.52
32	a	835	BCR	C11-C10-C9	-4.10	121.53	127.28
36	M	301	DD6	C21-C20-C19	4.10	118.84	114.24
32	f	804	BCR	C7-C8-C9	-4.10	120.17	126.23
37	H	301	PID	C12-O4-C10	4.09	109.66	107.68
36	B	319	DD6	C9-C10-C11	-4.09	121.55	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	P	206	PID	C18-C19-C20	4.09	131.88	123.52
39	P	211	KC1	CHB-C1B-NB	4.08	130.54	124.80
36	K	202	DD6	C9-C10-C11	-4.08	121.56	127.28
36	J	302	DD6	C9-C10-C11	-4.07	121.57	127.28
36	H	303	DD6	C9-C10-C11	-4.07	121.57	127.28
39	H	314	KC1	CHB-C1B-NB	4.06	130.52	124.80
37	C	304	PID	CM4-C14-C15	-4.06	116.24	122.82
36	P	204	DD6	C9-C10-C11	-4.05	121.59	127.28
35	m	102	DGD	O2G-C1B-C2B	4.05	120.25	111.48
37	P	202	PID	C12-O4-C10	4.05	109.64	107.68
36	Q	302	DD6	C9-C10-C11	-4.05	121.60	127.28
38	L	302	UIX	C-C7-C10	-4.04	117.45	125.99
36	K	221	DD6	C14-C13-C11	-4.03	119.27	125.53
36	D	304	DD6	C14-C13-C11	-4.03	119.27	125.53
38	B	304	UIX	C37-C39-C40	-4.03	121.62	127.28
36	K	206	DD6	C9-C10-C11	-4.03	121.63	127.28
37	Q	306	PID	CM4-C14-C15	-4.03	116.29	122.82
36	G	305	DD6	C9-C8-C6	-4.02	115.34	126.36
32	b	735	BCR	C28-C27-C26	-4.02	106.89	114.06
37	C	302	PID	C12-O4-C10	4.01	109.63	107.68
39	Q	314	KC1	CHB-C1B-NB	4.01	130.45	124.80
37	G	309	PID	CM4-C14-C15	-4.01	116.32	122.82
37	j	101	PID	C18-C19-C20	4.00	131.71	123.52
32	b	729	BCR	C16-C17-C18	-4.00	121.67	127.28
36	M	303	DD6	C14-C13-C11	-3.99	119.34	125.53
37	T	304	PID	C12-O4-C10	3.99	109.62	107.68
37	O	305	PID	C12-O4-C10	3.99	109.61	107.68
36	K	203	DD6	C14-C13-C11	-3.98	119.35	125.53
36	G	308	DD6	C21-C20-C19	3.98	118.71	114.24
37	C	305	PID	C17-C18-C19	3.98	133.92	124.72
39	N	312	KC1	CHC-C4B-NB	3.98	130.40	124.80
35	j	103	DGD	C2G-O2G-C1B	-3.97	108.29	117.80
36	M	302	DD6	C4-C5-C6	-3.97	121.71	127.28
32	b	735	BCR	C20-C21-C22	-3.97	121.71	127.28
32	l	507	BCR	C11-C10-C9	-3.97	121.71	127.28
32	f	801	BCR	C16-C17-C18	-3.96	121.72	127.28
37	N	304	PID	C12-O4-C10	3.96	109.60	107.68
37	C	304	PID	C12-O4-C10	3.96	109.60	107.68
32	a	835	BCR	C33-C5-C6	-3.96	120.17	124.48
39	N	310	KC1	CHB-C1B-NB	3.96	130.37	124.80
37	C	305	PID	C6-C7-C8	3.96	134.36	125.99
37	C	307	PID	C12-O4-C10	3.96	109.60	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	H	311	KC1	CHC-C4B-NB	3.95	130.37	124.80
37	N	305	PID	C17-C16-C15	3.95	131.61	123.52
36	I	203	DD6	C25-C26-C27	-3.95	115.56	126.61
37	Q	304	PID	C12-O4-C10	3.95	109.60	107.68
37	F	306	PID	C18-C19-C20	3.95	131.60	123.52
36	h	202	DD6	C32-C33-C34	-3.95	104.93	113.59
39	G	318	KC1	CHC-C4B-NB	3.95	130.36	124.80
39	M	312	KC1	CHB-C1B-NB	3.95	130.36	124.80
36	M	304	DD6	C15-C14-C13	-3.95	117.65	125.99
39	L	306	KC1	CHC-C4B-NB	3.95	130.36	124.80
39	A	213	KC1	CHB-C1B-NB	3.94	130.35	124.80
37	T	305	PID	C12-O4-C10	3.93	109.59	107.68
36	J	302	DD6	O1-C15-C14	-3.93	105.61	116.88
38	E	304	UIX	C-C7-C10	-3.93	117.68	125.99
37	T	301	PID	CM4-C14-C15	-3.93	116.45	122.82
39	E	312	KC1	CHB-C1B-NB	3.93	130.33	124.80
36	E	303	DD6	C3-C2-C1	-3.93	121.77	127.28
36	C	303	DD6	O1-C15-C14	-3.92	105.63	116.88
39	H	309	KC1	CHB-C1B-NB	3.92	130.32	124.80
36	L	303	DD6	C3-C2-C1	-3.92	121.78	127.28
39	O	315	KC1	CHB-C1B-NB	3.92	130.32	124.80
37	F	304	PID	C18-C19-C20	3.92	131.53	123.52
36	m	101	DD6	C15-C14-C13	-3.91	117.72	125.99
37	F	302	PID	CM4-C14-C15	-3.91	116.48	122.82
38	L	302	UIX	C6-C1-C3	3.91	118.64	114.24
38	C	306	UIX	C6-C1-C3	3.91	118.64	114.24
38	E	304	UIX	C37-C39-C40	-3.91	121.79	127.28
37	T	301	PID	C12-O4-C10	3.90	109.57	107.68
39	A	205	KC1	CHB-C1B-NB	3.90	130.30	124.80
32	i	204	BCR	C33-C5-C6	-3.90	120.23	124.48
39	H	309	KC1	CHC-C4B-NB	3.90	130.29	124.80
36	h	202	DD6	O1-C15-C14	-3.90	105.71	116.88
36	I	203	DD6	C14-C13-C11	-3.90	119.48	125.53
39	E	307	KC1	CHC-C4B-NB	3.90	130.29	124.80
37	O	305	PID	CM4-C14-C15	-3.89	116.51	122.82
39	C	310	KC1	CHB-C1B-NB	3.89	130.28	124.80
37	D	305	PID	C12-O4-C10	3.89	109.57	107.68
39	B	313	KC1	CHB-C1B-NB	3.89	130.27	124.80
35	G	320	DGD	O2G-C1B-C2B	3.89	119.89	111.48
39	G	315	KC1	CHD-C1D-ND	3.88	129.88	124.05
32	i	204	BCR	C3-C4-C5	-3.88	107.13	114.06
37	Q	303	PID	C12-O4-C10	3.88	109.56	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	T	312	KC1	CHC-C4B-NB	3.88	130.26	124.80
39	C	312	KC1	CHC-C4B-NB	3.87	130.25	124.80
36	G	307	DD6	C24-C1-C2	3.87	125.09	119.01
37	D	307	PID	CM4-C14-C15	-3.87	116.55	122.82
37	D	302	PID	C12-O4-C10	3.86	109.56	107.68
34	E	316	LMG	O6-C5-C4	3.86	116.65	109.70
39	F	309	KC1	CHC-C4B-NB	3.86	130.23	124.80
39	J	312	KC1	CHB-C1B-NB	3.86	130.23	124.80
37	H	306	PID	C17-C16-C15	3.86	131.41	123.52
37	O	307	PID	C17-C16-C15	3.86	131.41	123.52
39	Q	309	KC1	CHC-C4B-NB	3.86	130.23	124.80
37	C	302	PID	CM4-C14-C15	-3.85	116.58	122.82
36	K	204	DD6	C4-C5-C6	-3.85	121.88	127.28
39	I	215	KC1	CHB-C1B-NB	3.85	130.22	124.80
35	j	103	DGD	C1E-O6E-C5E	3.85	121.23	113.72
36	B	302	DD6	C9-C10-C11	-3.84	121.90	127.28
37	Q	301	PID	CM4-C14-C15	-3.84	116.60	122.82
39	L	314	KC1	CHB-C1B-NB	3.83	130.19	124.80
32	a	835	BCR	C7-C8-C9	-3.83	120.58	126.23
39	L	306	KC1	CHB-C1B-NB	3.82	130.19	124.80
39	N	312	KC1	CHB-C1B-NB	3.82	130.19	124.80
39	D	310	KC1	CHB-C1B-NB	3.82	130.19	124.80
37	G	309	PID	C12-O4-C10	3.82	109.53	107.68
36	B	301	DD6	C15-C14-C13	-3.82	117.91	125.99
39	Q	309	KC1	CHB-C1B-NB	3.82	130.18	124.80
39	D	315	KC1	CHB-C1B-NB	3.82	130.18	124.80
37	Q	301	PID	C12-O4-C10	3.82	109.53	107.68
37	H	305	PID	CM4-C14-C15	-3.82	116.63	122.82
38	J	304	UIX	C35-C36-C38	-3.81	112.15	123.20
36	L	304	DD6	C4-C5-C6	-3.81	121.93	127.28
39	C	315	KC1	CHB-C1B-NB	3.81	130.17	124.80
39	P	216	KC1	CHB-C1B-NB	3.81	130.17	124.80
36	J	303	DD6	O1-C15-C14	-3.81	105.96	116.88
39	Q	314	KC1	CHC-C4B-NB	3.81	130.17	124.80
36	N	303	DD6	C4-C5-C6	-3.81	121.94	127.28
32	m	103	BCR	C27-C26-C25	-3.81	117.56	122.70
39	F	309	KC1	CHB-C1B-NB	3.81	130.16	124.80
39	F	314	KC1	CHC-C4B-NB	3.81	130.16	124.80
39	P	216	KC1	CHC-C4B-NB	3.80	130.15	124.80
39	O	310	KC1	CHB-C1B-NB	3.80	130.15	124.80
36	D	301	DD6	C12-C11-C13	3.80	123.89	118.09
37	O	307	PID	C12-O4-C10	3.79	109.52	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	L	302	UIX	O-C-C7	-3.79	106.01	116.88
37	T	317	PID	C12-O4-C10	3.79	109.52	107.68
37	O	304	PID	C12-O4-C10	3.79	109.52	107.68
37	F	306	PID	CM4-C14-C15	-3.79	116.67	122.82
36	I	206	DD6	O1-C20-C19	-3.79	109.94	113.49
36	F	301	DD6	O1-C20-C21	3.79	119.28	115.05
39	N	310	KC1	CHC-C4B-NB	3.79	130.14	124.80
37	H	305	PID	C12-O4-C10	3.79	109.52	107.68
39	M	312	KC1	CHC-C4B-NB	3.79	130.13	124.80
39	B	313	KC1	CHC-C4B-NB	3.78	130.13	124.80
39	D	310	KC1	CHC-C4B-NB	3.78	130.13	124.80
35	j	103	DGD	O2G-C1B-C2B	3.78	119.66	111.48
32	l	506	BCR	C16-C17-C18	-3.78	121.98	127.28
39	A	205	KC1	CHC-C4B-NB	3.78	130.12	124.80
37	N	307	PID	C12-O4-C10	3.77	109.51	107.68
39	F	314	KC1	CHB-C1B-NB	3.77	130.11	124.80
38	J	304	UIX	O-C1-C6	3.77	119.26	115.05
36	P	204	DD6	O1-C15-C14	-3.77	106.09	116.88
32	a	838	BCR	C3-C4-C5	-3.77	107.34	114.06
39	H	314	KC1	CHC-C4B-NB	3.76	130.10	124.80
39	M	305	KC1	CHB-C1B-NB	3.76	130.10	124.80
39	T	315	KC1	CHB-C1B-NB	3.76	130.10	124.80
36	A	201	DD6	C4-C5-C6	-3.76	122.00	127.28
39	N	315	KC1	CHB-C1B-NB	3.76	130.09	124.80
38	B	304	UIX	C34-C30-C26	-3.76	122.01	127.28
39	C	310	KC1	CHC-C4B-NB	3.76	130.09	124.80
37	F	306	PID	C12-O4-C10	3.76	109.50	107.68
37	D	305	PID	CM4-C14-C15	-3.76	116.73	122.82
39	G	315	KC1	CHB-C1B-NB	3.75	130.09	124.80
36	L	303	DD6	C4-C5-C6	-3.75	122.02	127.28
39	G	318	KC1	CHB-C1B-NB	3.75	130.08	124.80
39	Q	311	KC1	CHC-C4B-NB	3.75	130.08	124.80
38	E	304	UIX	O-C-C7	-3.75	106.15	116.88
38	B	304	UIX	C6-C1-C3	3.75	118.45	114.24
36	J	301	DD6	C25-C24-C1	-3.74	116.10	126.36
37	h	204	PID	C12-O4-C10	3.74	109.50	107.68
39	O	315	KC1	CHC-C4B-NB	3.74	130.07	124.80
39	T	310	KC1	CHB-C1B-NB	3.74	130.07	124.80
38	P	207	UIX	C36-C35-C32	-3.74	122.03	127.28
39	T	315	KC1	CHC-C4B-NB	3.74	130.07	124.80
32	b	729	BCR	C15-C14-C13	-3.74	122.04	127.28
32	m	103	BCR	C24-C23-C22	-3.73	120.71	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	O	310	KC1	CHC-C4B-NB	3.73	130.06	124.80
39	A	213	KC1	CHC-C4B-NB	3.73	130.05	124.80
32	a	834	BCR	C38-C26-C25	-3.73	120.41	124.48
36	G	305	DD6	C-C1-C2	-3.73	116.77	122.82
39	E	307	KC1	CHB-C1B-NB	3.73	130.05	124.80
36	B	301	DD6	C9-C10-C11	-3.73	122.05	127.28
39	D	315	KC1	CHC-C4B-NB	3.73	130.05	124.80
32	a	838	BCR	C20-C21-C22	-3.72	122.05	127.28
37	F	306	PID	C17-C16-C15	3.72	131.14	123.52
32	b	735	BCR	C3-C4-C5	-3.72	107.42	114.06
37	P	202	PID	CM4-C14-C15	-3.72	116.78	122.82
37	O	307	PID	CM4-C14-C15	-3.72	116.79	122.82
32	a	838	BCR	C24-C23-C22	-3.72	120.73	126.23
39	M	305	KC1	CHC-C4B-NB	3.72	130.04	124.80
39	I	215	KC1	CHC-C4B-NB	3.72	130.04	124.80
37	F	302	PID	C17-C16-C15	3.72	131.13	123.52
37	C	305	PID	C12-O4-C10	3.72	109.48	107.68
39	H	311	KC1	CHB-C1B-NB	3.72	130.04	124.80
39	C	312	KC1	CHB-C1B-NB	3.72	130.03	124.80
38	T	306	UIX	C6-C1-C3	3.71	118.41	114.24
39	C	315	KC1	CHC-C4B-NB	3.71	130.03	124.80
36	I	202	DD6	C4-C5-C6	-3.71	122.07	127.28
37	H	306	PID	CM4-C14-C15	-3.71	116.81	122.82
37	P	206	PID	CM4-C14-C15	-3.70	116.82	122.82
36	G	306	DD6	C15-C14-C13	-3.70	118.17	125.99
39	P	213	KC1	CHC-C4B-NB	3.70	130.01	124.80
39	F	309	KC1	CHD-C1D-ND	3.70	129.59	124.05
32	a	838	BCR	C7-C8-C9	-3.69	120.77	126.23
32	a	838	BCR	C28-C27-C26	-3.69	107.47	114.06
36	B	301	DD6	O1-C20-C19	-3.69	110.03	113.49
36	F	303	DD6	C15-C14-C13	-3.69	118.18	125.99
39	T	312	KC1	CHB-C1B-NB	3.69	130.00	124.80
37	T	302	PID	C12-O4-C10	3.69	109.47	107.68
37	E	301	PID	C12-O4-C10	3.69	109.47	107.68
36	H	303	DD6	C15-C14-C13	-3.68	118.20	125.99
36	K	203	DD6	C4-C5-C6	-3.68	122.11	127.28
32	f	804	BCR	C16-C17-C18	-3.68	122.11	127.28
32	f	804	BCR	C20-C21-C22	-3.68	122.12	127.28
39	O	312	KC1	CHC-C4B-NB	3.67	129.97	124.80
36	B	319	DD6	C4-C5-C6	-3.67	122.13	127.28
38	L	302	UIX	C34-C37-C39	-3.66	116.02	123.52
36	G	305	DD6	C14-C13-C11	-3.66	119.85	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	735	BCR	C15-C14-C13	-3.66	122.14	127.28
36	K	205	DD6	C15-C14-C13	-3.66	118.25	125.99
39	L	314	KC1	CHC-C4B-NB	3.66	129.95	124.80
36	J	301	DD6	C21-C20-C19	3.66	118.35	114.24
37	N	305	PID	CM4-C14-C15	-3.65	116.90	122.82
37	C	307	PID	CM4-C14-C15	-3.65	116.90	122.82
36	E	302	DD6	O1-C20-C21	3.65	119.12	115.05
39	K	215	KC1	CHB-C1B-NB	3.65	129.94	124.80
36	K	205	DD6	C41-C32-C31	-3.64	103.99	110.52
37	T	307	PID	CM4-C14-C15	-3.64	116.91	122.82
37	T	305	PID	CM4-C14-C15	-3.64	116.91	122.82
30	b	727	PQN	C11-C12-C13	-3.64	120.56	126.83
39	N	315	KC1	CHC-C4B-NB	3.63	129.92	124.80
37	N	307	PID	C17-C16-C15	3.63	130.95	123.52
37	D	302	PID	CM4-C14-C15	-3.63	116.93	122.82
37	N	305	PID	C18-C19-C20	3.63	130.95	123.52
39	Q	314	KC1	CHD-C1D-ND	3.63	129.49	124.05
36	M	301	DD6	C4-C5-C6	-3.63	122.19	127.28
37	D	306	PID	C18-C19-C20	3.62	130.93	123.52
38	O	306	UIX	O-C1-C3	3.62	116.88	113.49
36	G	307	DD6	C21-C20-C19	3.62	118.30	114.24
39	K	215	KC1	CHD-C1D-ND	3.61	129.47	124.05
39	O	312	KC1	CHB-C1B-NB	3.61	129.89	124.80
36	G	305	DD6	C32-C33-C34	-3.61	105.67	113.59
38	F	305	UIX	C6-C1-C3	3.61	118.30	114.24
36	K	206	DD6	C15-C14-C13	-3.61	118.36	125.99
37	H	302	PID	C12-O4-C10	3.61	109.43	107.68
29	a	804	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
38	B	304	UIX	C14-C13-C11	-3.60	122.23	127.28
36	m	101	DD6	C9-C10-C11	-3.60	122.23	127.28
39	T	310	KC1	CHC-C4B-NB	3.59	129.86	124.80
37	Q	304	PID	CM4-C14-C15	-3.59	117.00	122.82
39	P	213	KC1	CHB-C1B-NB	3.59	129.85	124.80
36	G	306	DD6	O1-C15-C14	-3.59	106.60	116.88
36	B	303	DD6	C15-C14-C13	-3.59	118.41	125.99
36	C	303	DD6	C15-C14-C13	-3.58	118.42	125.99
32	a	834	BCR	C33-C5-C6	-3.58	120.57	124.48
36	J	301	DD6	O1-C20-C21	-3.58	111.05	115.05
36	Q	302	DD6	C3-C2-C1	-3.58	122.25	127.28
36	L	305	DD6	C15-C14-C13	-3.58	118.42	125.99
32	a	834	BCR	C7-C8-C9	-3.58	120.94	126.23
38	J	304	UIX	O2-C27-C31	3.58	117.47	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	M	302	DD6	C15-C14-C13	-3.58	118.43	125.99
37	G	310	PID	C12-O4-C10	3.57	109.41	107.68
38	B	304	UIX	O-C-C7	-3.57	106.64	116.88
37	Q	306	PID	C18-C19-C20	3.57	130.82	123.52
36	T	303	DD6	C15-C14-C13	-3.57	118.45	125.99
39	G	315	KC1	CHC-C4B-NB	3.57	129.82	124.80
38	E	304	UIX	C6-C1-C3	3.56	118.24	114.24
37	O	305	PID	C17-C16-C15	3.56	130.81	123.52
35	b	733	DGD	O1G-C1A-C2A	3.56	122.70	111.83
38	N	306	UIX	O-C-C7	-3.56	106.67	116.88
36	K	203	DD6	C3-C2-C1	-3.56	122.28	127.28
36	J	303	DD6	C25-C24-C1	-3.56	116.60	126.36
36	A	202	DD6	C4-C5-C6	-3.56	122.29	127.28
39	J	312	KC1	CHC-C4B-NB	3.56	129.81	124.80
36	I	203	DD6	O1-C20-C15	-3.56	56.11	58.93
36	h	202	DD6	C15-C14-C13	-3.55	118.48	125.99
37	N	307	PID	CM4-C14-C15	-3.55	117.06	122.82
32	f	804	BCR	C38-C26-C25	-3.55	120.61	124.48
39	M	312	KC1	CHD-C1D-ND	3.55	129.37	124.05
39	P	216	KC1	CHD-C1D-ND	3.54	129.37	124.05
36	G	308	DD6	C4-C5-C6	-3.54	122.31	127.28
39	E	312	KC1	CHC-C4B-NB	3.54	129.78	124.80
32	l	507	BCR	C24-C23-C22	-3.53	121.01	126.23
36	E	303	DD6	C4-C5-C6	-3.53	122.33	127.28
39	F	314	KC1	CHD-C1D-ND	3.53	129.34	124.05
36	O	303	DD6	O1-C15-C14	-3.53	106.77	116.88
36	K	204	DD6	O1-C20-C21	3.53	118.99	115.05
37	G	310	PID	CM4-C14-C15	-3.52	117.11	122.82
39	P	211	KC1	CHC-C4B-NB	3.52	129.76	124.80
36	K	204	DD6	C14-C13-C11	-3.52	120.07	125.53
36	O	303	DD6	C21-C20-C15	-3.52	116.51	122.30
39	A	213	KC1	CHD-C1D-ND	3.52	129.33	124.05
32	l	506	BCR	C38-C26-C25	-3.51	120.65	124.48
29	M	311	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
37	N	307	PID	C18-C19-C20	3.51	130.71	123.52
39	H	309	KC1	CHD-C1D-ND	3.51	129.32	124.05
32	b	728	BCR	C8-C7-C6	-3.51	117.62	127.00
39	H	314	KC1	CHD-C1D-ND	3.51	129.31	124.05
36	J	301	DD6	C25-C26-C27	-3.51	116.80	126.61
39	O	312	KC1	CHD-C1D-ND	3.51	129.31	124.05
36	F	303	DD6	O1-C20-C21	3.50	118.97	115.05
36	m	101	DD6	C4-C5-C6	-3.50	122.36	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	J	304	UIX	C6-C1-C3	3.50	118.18	114.24
37	N	307	PID	CM2-C5-C4	-3.50	102.82	108.97
39	Q	311	KC1	CHB-C1B-NB	3.50	129.73	124.80
32	a	838	BCR	C11-C10-C9	-3.50	122.38	127.28
39	I	215	KC1	CHD-C1D-ND	3.49	129.29	124.05
39	O	315	KC1	CHD-C1D-ND	3.49	129.28	124.05
39	E	307	KC1	CHD-C1D-ND	3.49	129.28	124.05
36	G	307	DD6	C19-C18-C17	-3.49	104.27	110.79
36	G	306	DD6	O1-C20-C19	-3.48	110.23	113.49
29	O	314	CLA	C3B-C4B-NB	-3.48	107.42	110.53
39	O	310	KC1	CHD-C1D-ND	3.48	129.27	124.05
36	A	204	DD6	C15-C14-C13	-3.47	118.65	125.99
37	D	306	PID	C12-O4-C10	3.47	109.36	107.68
39	T	315	KC1	CHD-C1D-ND	3.47	129.26	124.05
32	a	834	BCR	C20-C21-C22	-3.47	122.41	127.28
39	C	315	KC1	CHD-C1D-ND	3.47	129.26	124.05
37	O	302	PID	C12-O4-C10	3.47	109.36	107.68
36	I	203	DD6	C21-C20-C15	-3.46	116.60	122.30
37	C	307	PID	C17-C16-C15	3.46	130.60	123.52
39	N	312	KC1	CHD-C1D-ND	3.46	129.24	124.05
39	T	312	KC1	CHD-C1D-ND	3.45	129.23	124.05
36	G	307	DD6	C14-C13-C11	-3.45	120.17	125.53
29	A	206	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
36	m	101	DD6	O1-C15-C14	-3.45	106.99	116.88
39	N	310	KC1	CHD-C1D-ND	3.45	129.23	124.05
37	H	305	PID	C17-C18-C19	3.45	132.70	124.72
36	B	305	DD6	C15-C14-C13	-3.45	118.70	125.99
36	F	301	DD6	O1-C20-C19	3.45	116.72	113.49
37	T	307	PID	C12-O4-C10	3.45	109.35	107.68
37	j	101	PID	C12-O4-C10	3.44	109.35	107.68
37	Q	301	PID	C17-C16-C15	3.44	130.55	123.52
37	P	203	PID	C12-O4-C10	3.43	109.35	107.68
29	a	808	CLA	C3B-C4B-NB	-3.43	107.46	110.53
36	L	303	DD6	O1-C20-C21	-3.43	111.22	115.05
36	B	302	DD6	C15-C14-C13	-3.43	118.74	125.99
39	B	313	KC1	CHD-C1D-ND	3.43	129.19	124.05
36	m	101	DD6	O1-C20-C19	-3.43	110.28	113.49
36	D	301	DD6	C10-C9-C8	-3.42	113.29	123.20
36	A	202	DD6	C15-C14-C13	-3.42	118.76	125.99
39	D	310	KC1	CHD-C1D-ND	3.42	129.18	124.05
39	Q	311	KC1	CHD-C1D-ND	3.42	129.18	124.05
29	a	802	CLA	C3B-C4B-NB	-3.41	107.48	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	l	507	BCR	C38-C26-C25	-3.41	120.76	124.48
29	P	215	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
38	A	203	UIX	C34-C30-C26	-3.41	122.50	127.28
39	A	205	KC1	CHD-C1D-ND	3.41	129.16	124.05
37	H	305	PID	C8-C9-C10	3.41	130.27	123.60
37	N	302	PID	C12-O4-C10	3.40	109.33	107.68
37	T	302	PID	CM4-C14-C15	-3.40	117.31	122.82
36	D	301	DD6	O1-C15-C14	-3.40	107.14	116.88
39	K	215	KC1	CHC-C4B-C3B	-3.39	119.48	125.21
29	I	216	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
36	M	301	DD6	O1-C20-C21	-3.39	111.26	115.05
36	E	303	DD6	O1-C20-C21	-3.39	111.26	115.05
29	K	211	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
38	A	203	UIX	C37-C39-C40	-3.39	122.53	127.28
36	I	202	DD6	C15-C14-C13	-3.38	118.84	125.99
36	B	301	DD6	O1-C15-C14	-3.38	107.18	116.88
32	f	804	BCR	C24-C23-C22	-3.38	121.23	126.23
32	b	728	BCR	C15-C14-C13	-3.38	122.53	127.28
36	G	306	DD6	C14-C13-C11	-3.38	120.28	125.53
29	a	820	CLA	C3B-C4B-NB	-3.38	107.51	110.53
36	E	302	DD6	C21-C20-C19	3.38	118.03	114.24
37	h	204	PID	CM4-C14-C15	-3.38	117.35	122.82
32	f	801	BCR	C11-C10-C9	-3.38	122.54	127.28
39	J	312	KC1	CHD-C1D-ND	3.37	129.11	124.05
29	a	825	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
36	F	301	DD6	C3-C2-C1	-3.37	122.56	127.28
36	h	202	DD6	C9-C10-C11	-3.37	122.56	127.28
32	f	804	BCR	C33-C5-C6	-3.36	120.82	124.48
36	K	202	DD6	C3-C4-C5	-3.36	116.64	123.52
39	D	315	KC1	CHD-C1D-ND	3.36	129.09	124.05
36	N	303	DD6	C15-C14-C13	-3.36	118.89	125.99
36	G	305	DD6	C25-C24-C1	-3.36	117.16	126.36
37	D	303	PID	C6-C7-C8	-3.36	118.90	125.99
39	G	318	KC1	CHD-C1D-ND	3.35	129.08	124.05
39	L	306	KC1	CHD-C1D-ND	3.35	129.08	124.05
39	P	211	KC1	CHD-C1D-ND	3.35	129.08	124.05
36	B	303	DD6	C4-C5-C6	-3.35	122.58	127.28
29	i	203	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
29	O	314	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
29	J	306	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
39	C	312	KC1	CHD-C1D-ND	3.33	129.04	124.05
38	P	207	UIX	C6-C1-C3	3.33	117.98	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	N	315	KC1	CHD-C1D-ND	3.32	129.04	124.05
39	C	310	KC1	CHD-C1D-ND	3.32	129.03	124.05
32	l	507	BCR	C20-C21-C22	-3.32	122.63	127.28
36	h	202	DD6	C21-C20-C15	-3.32	116.84	122.30
35	B	318	DGD	O6E-C5E-C4E	3.31	115.67	109.70
29	b	711	CLA	C3B-C4B-NB	-3.31	107.57	110.53
29	A	214	CLA	C3B-C4B-NB	-3.31	107.57	110.53
29	l	501	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
29	E	315	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
39	L	314	KC1	CHD-C1D-ND	3.31	129.01	124.05
37	h	204	PID	C18-C19-C20	3.30	130.28	123.52
29	J	308	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
39	Q	309	KC1	CHD-C1D-ND	3.30	129.00	124.05
36	E	303	DD6	C15-C14-C13	-3.30	119.02	125.99
29	b	721	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
36	K	205	DD6	C3-C2-C1	-3.29	122.66	127.28
36	G	305	DD6	C28-C27-C26	-3.29	117.79	124.18
38	A	203	UIX	C-C7-C10	-3.29	119.04	125.99
30	a	832	PQN	C11-C3-C2	-3.29	119.25	124.89
36	E	302	DD6	C21-C20-C15	-3.29	116.89	122.30
37	D	302	PID	C17-C16-C15	3.28	130.24	123.52
32	f	801	BCR	C33-C5-C6	-3.28	120.90	124.48
39	M	305	KC1	CHD-C1D-ND	3.28	128.97	124.05
29	F	310	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
29	b	707	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
36	B	319	DD6	O1-C20-C19	-3.28	110.42	113.49
36	F	303	DD6	C21-C20-C15	-3.28	116.91	122.30
36	O	303	DD6	C3-C2-C1	-3.28	122.69	127.28
36	D	301	DD6	C4-C5-C6	-3.27	122.69	127.28
39	O	312	KC1	O1D-CGD-CBD	-3.27	118.07	124.52
36	H	303	DD6	O1-C15-C14	-3.27	107.51	116.88
36	H	303	DD6	O1-C20-C19	-3.27	110.43	113.49
32	m	103	BCR	C38-C26-C27	3.27	120.56	113.60
38	B	304	UIX	C-C7-C10	-3.26	119.09	125.99
37	G	303	PID	CM4-C14-C15	-3.26	117.53	122.82
36	M	304	DD6	C9-C10-C11	-3.26	122.71	127.28
39	E	312	KC1	CHD-C1D-ND	3.26	128.94	124.05
29	I	211	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
39	P	213	KC1	C2D-C1D-ND	-3.25	106.95	110.33
37	D	303	PID	C18-C19-C20	3.25	130.17	123.52
37	N	302	PID	CM4-C14-C15	-3.25	117.55	122.82
38	F	305	UIX	C18-O2-C27	-3.25	112.11	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	N	304	PID	C18-C19-C20	3.25	130.17	123.52
38	J	304	UIX	C34-C37-C39	-3.25	116.87	123.52
37	H	306	PID	C12-O4-C10	3.25	109.25	107.68
29	G	314	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
36	N	303	DD6	C9-C10-C11	-3.24	122.73	127.28
32	l	506	BCR	C20-C21-C22	-3.24	122.73	127.28
36	I	206	DD6	C4-C5-C6	-3.24	122.73	127.28
29	Q	308	CLA	C1-C2-C3	-3.24	120.89	126.20
32	l	506	BCR	C23-C24-C25	-3.24	118.35	127.00
32	l	507	BCR	C2-C1-C6	3.24	115.14	110.44
29	a	802	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
39	H	311	KC1	CHD-C1D-ND	3.23	128.89	124.05
29	B	314	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
29	b	716	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
36	O	303	DD6	C15-C14-C13	-3.22	119.18	125.99
39	P	213	KC1	CHD-C1D-ND	3.22	128.87	124.05
36	D	304	DD6	O1-C15-C14	-3.21	107.68	116.88
39	Q	311	KC1	C2D-C1D-ND	-3.21	107.00	110.33
36	L	303	DD6	C10-C9-C8	-3.21	113.91	123.20
29	K	214	CLA	C3B-C4B-NB	-3.20	107.67	110.53
37	C	307	PID	CM2-C5-C4	-3.20	103.34	108.97
30	a	832	PQN	C2M-C2-C3	-3.20	119.19	124.45
36	J	303	DD6	C14-C13-C11	-3.20	120.57	125.53
29	C	314	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
36	I	206	DD6	C15-C14-C13	-3.19	119.24	125.99
32	b	735	BCR	C33-C5-C6	-3.19	121.00	124.48
29	K	216	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
29	a	826	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
36	T	303	DD6	C3-C2-C1	-3.19	122.81	127.28
29	a	827	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
29	a	809	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
29	K	214	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
29	a	829	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
29	a	828	CLA	C3B-C4B-NB	-3.17	107.70	110.53
32	b	735	BCR	C29-C30-C25	3.17	115.04	110.44
29	D	314	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
37	D	306	PID	CM4-C14-C15	-3.17	117.69	122.82
29	A	217	CLA	C3B-C4B-NB	-3.17	107.70	110.53
36	N	303	DD6	C3-C2-C1	-3.17	122.84	127.28
36	I	203	DD6	C37-C36-C31	-3.17	118.24	124.16
36	G	305	DD6	O1-C15-C14	-3.17	107.81	116.88
29	F	307	CLA	O2D-CGD-O1D	-3.17	117.69	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	837	CLA	C3B-C4B-NB	-3.17	107.70	110.53
29	L	316	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
29	T	314	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
36	G	308	DD6	C21-C20-C15	-3.16	117.11	122.30
32	a	838	BCR	C33-C5-C6	-3.16	121.04	124.48
29	b	724	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
29	E	311	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
29	L	315	CLA	C3B-C4B-NB	-3.15	107.72	110.53
36	I	205	DD6	C25-C24-C1	-3.15	117.72	126.36
29	l	504	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
36	K	206	DD6	C4-C5-C6	-3.15	122.86	127.28
39	T	312	KC1	C2D-C1D-ND	-3.15	107.06	110.33
36	F	301	DD6	O1-C15-C14	-3.15	107.86	116.88
32	m	103	BCR	C30-C25-C26	-3.15	118.33	122.64
36	B	305	DD6	O1-C15-C14	-3.15	107.87	116.88
35	b	733	DGD	C1D-C2D-C3D	3.14	116.63	110.01
38	P	207	UIX	C18-O2-C27	-3.14	112.29	117.85
29	N	314	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
39	O	312	KC1	O2D-CGD-O1D	-3.14	117.73	123.85
29	D	313	CLA	C3B-C4B-NB	-3.14	107.73	110.53
36	F	303	DD6	O1-C15-C14	-3.14	107.88	116.88
29	l	509	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
37	H	302	PID	CM4-C14-C15	-3.14	117.73	122.82
36	m	101	DD6	C3-C4-C5	-3.13	117.11	123.52
37	T	307	PID	CM5-C21-C20	-3.13	117.74	122.82
38	P	207	UIX	C22-C15-C20	-3.13	107.67	110.47
32	m	103	BCR	C23-C24-C25	-3.13	118.65	127.00
36	I	206	DD6	C9-C10-C11	-3.12	122.90	127.28
36	G	305	DD6	C25-C26-C27	-3.12	117.88	126.61
39	T	310	KC1	CHD-C1D-ND	3.12	128.73	124.05
29	l	502	CLA	C3B-C4B-NB	-3.12	107.75	110.53
36	M	302	DD6	C21-C20-C19	3.12	117.74	114.24
37	C	305	PID	CM5-C21-C20	-3.11	117.77	122.82
39	T	310	KC1	C2D-C1D-ND	-3.11	107.10	110.33
39	C	312	KC1	C2D-C1D-ND	-3.11	107.10	110.33
29	C	311	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
29	E	305	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
29	b	714	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
29	F	311	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
37	D	303	PID	CM4-C14-C15	-3.11	117.78	122.82
29	I	213	CLA	C3B-C4B-NB	-3.11	107.75	110.53
29	b	718	CLA	O2D-CGD-O1D	-3.11	117.80	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	j	106	DGD	O1G-C1A-C2A	3.10	121.30	111.83
29	K	218	CLA	C3B-C4B-NB	-3.10	107.76	110.53
29	J	311	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
36	K	205	DD6	C37-C36-C31	-3.10	118.36	124.16
30	a	832	PQN	C11-C12-C13	-3.10	121.49	126.83
29	F	315	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
29	b	705	CLA	C3B-C4B-NB	-3.10	107.76	110.53
38	A	203	UIX	C18-O2-C27	-3.10	112.37	117.85
36	I	204	DD6	C24-C1-C2	3.10	123.88	119.01
29	K	208	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
36	A	204	DD6	C9-C10-C11	-3.09	122.94	127.28
29	b	711	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
36	Q	302	DD6	C15-C14-C13	-3.09	119.45	125.99
29	T	311	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
32	a	835	BCR	C38-C26-C25	-3.09	121.11	124.48
36	K	206	DD6	O1-C15-C14	-3.09	108.02	116.88
30	a	832	PQN	C14-C13-C15	3.09	120.59	115.23
36	h	202	DD6	C14-C13-C11	-3.09	120.74	125.53
29	l	502	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
37	D	303	PID	C12-O4-C10	3.09	109.18	107.68
29	a	811	CLA	C3B-C4B-NB	-3.09	107.78	110.53
29	J	307	CLA	C3B-C4B-NB	-3.09	107.78	110.53
29	G	304	CLA	C3B-C4B-NB	-3.09	107.78	110.53
29	I	210	CLA	C3B-C4B-NB	-3.08	107.78	110.53
29	a	806	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
29	l	503	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
38	O	306	UIX	C16-C20-C15	3.08	122.75	119.70
29	Q	312	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
32	a	834	BCR	C3-C4-C5	-3.08	108.57	114.06
36	L	305	DD6	C9-C8-C6	-3.08	117.93	126.36
38	F	305	UIX	O-C1-C6	3.07	118.48	115.05
29	b	724	CLA	C3B-C4B-NB	-3.07	107.79	110.53
29	B	310	CLA	C3B-C4B-NB	-3.07	107.79	110.53
29	b	715	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
29	G	313	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
37	F	304	PID	C17-C16-C15	3.07	129.80	123.52
37	C	301	PID	C18-C19-C20	3.07	129.80	123.52
29	E	306	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
29	a	815	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
36	L	303	DD6	C15-C14-C13	-3.07	119.51	125.99
37	O	305	PID	C8-C9-C10	3.07	129.61	123.60
36	J	303	DD6	C25-C26-C27	-3.07	118.03	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	719	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
38	A	203	UIX	O-C-C7	-3.07	108.09	116.88
29	I	201	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
36	E	303	DD6	C10-C9-C8	-3.06	114.32	123.20
29	L	312	CLA	C3B-C4B-NB	-3.06	107.80	110.53
29	b	708	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
29	a	824	CLA	C3B-C4B-NB	-3.06	107.80	110.53
29	K	213	CLA	C3B-C4B-NB	-3.06	107.80	110.53
29	M	306	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
29	b	726	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
32	l	507	BCR	C7-C8-C9	-3.06	121.71	126.23
39	Q	314	KC1	C2D-C1D-ND	-3.06	107.16	110.33
29	K	207	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
36	J	301	DD6	C37-C36-C35	3.05	120.04	114.42
29	b	702	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
29	b	725	CLA	C3B-C4B-NB	-3.05	107.81	110.53
38	Q	305	UIX	C14-C23-C26	-3.05	118.00	126.36
36	M	301	DD6	C9-C10-C11	-3.05	123.00	127.28
29	B	306	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
36	L	301	DD6	C14-C13-C11	-3.05	120.80	125.53
38	B	304	UIX	C18-O2-C27	-3.05	112.46	117.85
37	H	301	PID	C18-C19-C20	3.05	129.76	123.52
29	b	712	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
29	O	309	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
29	B	308	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
38	A	203	UIX	C35-C36-C38	-3.04	114.39	123.20
29	N	309	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
39	N	312	KC1	CHC-C4B-C3B	-3.04	120.08	125.21
29	J	313	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
29	f	803	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
32	a	834	BCR	C28-C27-C26	-3.04	108.64	114.06
37	N	307	PID	O1-C6-C7	-3.04	108.18	116.88
39	D	310	KC1	C2D-C1D-ND	-3.04	107.18	110.33
29	O	316	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
37	j	101	PID	CM4-C14-C15	-3.03	117.90	122.82
32	l	507	BCR	C15-C16-C17	-3.03	117.32	123.52
29	a	813	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
29	h	201	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
29	P	217	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
37	F	302	PID	CM5-C21-C20	-3.03	117.91	122.82
29	K	210	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
37	N	301	PID	C18-C19-C20	3.02	129.71	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	T	317	PID	C16-C15-C14	-3.02	123.04	127.28
36	M	303	DD6	C21-C20-C19	3.02	117.64	114.24
29	B	316	CLA	C3B-C4B-NB	-3.02	107.83	110.53
29	l	508	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
39	D	315	KC1	C2D-C1D-ND	-3.02	107.19	110.33
29	K	213	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
38	T	306	UIX	C16-C20-C15	3.02	122.69	119.70
36	h	202	DD6	C26-C25-C24	-3.02	114.45	123.20
29	f	802	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
29	H	315	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
29	G	312	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
29	b	723	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
29	b	731	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
29	b	703	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
29	P	214	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
36	I	202	DD6	C9-C10-C11	-3.01	123.05	127.28
29	P	212	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
29	a	805	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
29	E	308	CLA	C3B-C4B-NB	-3.01	107.85	110.53
39	G	318	KC1	CHC-C4B-C3B	-3.01	120.14	125.21
36	E	302	DD6	C4-C3-C2	-3.01	117.37	123.52
29	Q	315	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
29	N	309	CLA	C3B-C4B-NB	-3.00	107.85	110.53
37	P	206	PID	C26-C25-C24	3.00	112.13	109.21
36	A	204	DD6	O1-C15-C14	-3.00	108.28	116.88
29	a	819	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
29	A	207	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
29	Q	307	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
37	C	302	PID	C17-C16-C15	3.00	129.66	123.52
29	a	804	CLA	C3B-C4B-NB	-3.00	107.85	110.53
39	T	312	KC1	CHC-C4B-C3B	-3.00	120.15	125.21
39	C	315	KC1	C2D-C1D-ND	-3.00	107.22	110.33
32	b	729	BCR	C10-C11-C12	-3.00	114.51	123.20
37	G	303	PID	C12-O4-C10	3.00	109.13	107.68
36	G	307	DD6	O1-C20-C19	3.00	116.30	113.49
29	a	812	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
29	P	215	CLA	CHB-C4A-NA	3.00	128.72	124.40
37	P	203	PID	CM4-C14-C15	-3.00	117.96	122.82
39	C	310	KC1	C2D-C1D-ND	-3.00	107.22	110.33
29	G	301	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
32	f	801	BCR	C3-C4-C5	-2.99	108.72	114.06
32	i	204	BCR	C28-C27-C26	-2.99	108.72	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	L	305	DD6	C21-C20-C15	-2.99	117.38	122.30
29	G	304	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
35	B	318	DGD	C2G-O2G-C1B	-2.99	110.64	117.80
29	a	827	CLA	C3B-C4B-NB	-2.99	107.86	110.53
39	O	312	KC1	C2D-C1D-ND	-2.99	107.23	110.33
29	G	319	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
36	G	307	DD6	C15-C14-C13	-2.99	119.68	125.99
36	J	301	DD6	C14-C13-C11	-2.99	120.90	125.53
29	A	209	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
29	K	212	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
37	T	304	PID	C18-C19-C20	2.99	129.63	123.52
29	B	312	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
29	a	810	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
38	N	306	UIX	C22-C15-C20	-2.98	107.80	110.47
39	H	311	KC1	CHC-C4B-C3B	-2.98	120.18	125.21
29	I	212	CLA	C3B-C4B-NB	-2.98	107.87	110.53
29	L	311	CLA	C3B-C4B-NB	-2.98	107.87	110.53
29	A	208	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
29	L	315	CLA	CAA-C2A-C3A	-2.98	109.40	116.23
29	J	310	CLA	C3B-C4B-NB	-2.98	107.87	110.53
32	m	103	BCR	C28-C27-C26	-2.98	108.75	114.06
39	M	305	KC1	C2D-C1D-ND	-2.98	107.24	110.33
29	B	309	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
36	h	202	DD6	C10-C9-C8	-2.98	114.58	123.20
36	L	305	DD6	O1-C15-C14	-2.98	108.35	116.88
36	M	302	DD6	C-C1-C2	-2.97	118.00	122.82
36	B	305	DD6	C4-C5-C6	-2.97	123.11	127.28
36	K	204	DD6	C25-C24-C1	-2.97	118.21	126.36
39	C	312	KC1	CHC-C4B-C3B	-2.97	120.20	125.21
39	Q	309	KC1	C2D-C1D-ND	-2.97	107.24	110.33
29	a	818	CLA	C3B-C4B-NB	-2.97	107.88	110.53
29	K	208	CLA	C3B-C4B-NB	-2.97	107.88	110.53
36	F	301	DD6	C4-C5-C6	-2.97	123.11	127.28
29	G	302	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	Q	308	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	M	313	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	J	306	CLA	C1-C2-C3	-2.97	121.34	126.20
36	h	202	DD6	C37-C36-C31	-2.97	118.61	124.16
29	E	308	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
36	K	205	DD6	O1-C15-C14	-2.96	108.38	116.88
29	I	207	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
29	a	805	CLA	C3B-C4B-NB	-2.96	107.88	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	315	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
36	K	202	DD6	O1-C15-C14	-2.96	108.39	116.88
29	Q	312	CLA	C3B-C4B-NB	-2.96	107.89	110.53
29	J	310	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
29	G	311	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
29	I	217	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
36	L	305	DD6	C9-C10-C11	-2.96	123.13	127.28
29	G	317	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
36	F	301	DD6	C15-C14-C13	-2.96	119.74	125.99
36	B	319	DD6	C37-C36-C31	-2.96	118.63	124.16
39	Q	314	KC1	CHC-C4B-C3B	-2.96	120.22	125.21
29	B	310	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
37	O	302	PID	CM4-C14-C15	-2.96	118.03	122.82
29	a	818	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
29	Q	313	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
29	K	217	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
39	G	315	KC1	C2D-C1D-ND	-2.95	107.26	110.33
38	N	306	UIX	C16-C20-C15	2.95	122.63	119.70
35	j	106	DGD	C2G-O2G-C1B	-2.95	110.73	117.80
29	I	210	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
29	b	705	CLA	CAC-C3C-C4C	2.95	128.63	124.79
29	T	316	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
39	F	309	KC1	CHC-C4B-C3B	-2.95	120.23	125.21
29	P	214	CLA	C3B-C4B-NB	-2.95	107.89	110.53
36	K	202	DD6	C37-C36-C31	-2.95	118.64	124.16
39	J	312	KC1	C2D-C1D-ND	-2.95	107.27	110.33
29	P	217	CLA	CAA-C2A-C3A	-2.95	109.46	116.23
32	m	103	BCR	C11-C12-C13	-2.95	118.27	126.36
29	H	308	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
29	A	218	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
29	B	306	CLA	C3B-C4B-NB	-2.95	107.90	110.53
39	P	216	KC1	CHC-C4B-C3B	-2.95	120.24	125.21
29	b	714	CLA	C3B-C4B-NB	-2.95	107.90	110.53
29	K	209	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
29	A	209	CLA	C3B-C4B-NB	-2.94	107.90	110.53
29	K	211	CLA	C3B-C4B-NB	-2.94	107.90	110.53
32	i	204	BCR	C16-C15-C14	-2.94	117.50	123.52
39	H	314	KC1	CHC-C4B-C3B	-2.94	120.25	125.21
29	K	216	CLA	CAA-C2A-C3A	-2.94	109.48	116.23
39	P	211	KC1	CHB-C1B-C2B	-2.94	119.36	125.49
39	E	307	KC1	C2D-C1D-ND	-2.94	107.27	110.33
29	a	803	CLA	O2D-CGD-O1D	-2.94	118.12	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	804	CLA	O2D-CGD-CBD	2.94	116.37	111.23
36	A	204	DD6	C25-C26-C27	-2.94	118.39	126.61
29	a	824	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
29	b	720	CLA	C3B-C4B-NB	-2.94	107.91	110.53
38	B	304	UIX	C16-C20-C15	2.94	122.61	119.70
36	F	303	DD6	C9-C10-C11	-2.94	123.16	127.28
36	I	202	DD6	C25-C26-C27	-2.94	118.40	126.61
39	L	306	KC1	CHC-C4B-C3B	-2.94	120.26	125.21
29	L	313	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	A	204	DD6	C4-C5-C6	-2.93	123.16	127.28
29	D	311	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
29	D	312	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
38	N	306	UIX	C18-O2-C27	-2.93	112.67	117.85
29	C	316	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
32	l	507	BCR	C16-C17-C18	-2.93	123.17	127.28
29	D	316	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
29	F	312	CLA	C3B-C4B-NB	-2.93	107.92	110.53
29	Q	307	CLA	C3B-C4B-NB	-2.93	107.92	110.53
39	N	315	KC1	C2D-C1D-ND	-2.93	107.29	110.33
39	E	307	KC1	CHC-C4B-C3B	-2.93	120.27	125.21
39	K	215	KC1	C2D-C1D-ND	-2.93	107.29	110.33
29	b	707	CLA	C3B-C4B-NB	-2.92	107.92	110.53
29	J	313	CLA	C3B-C4B-NB	-2.92	107.92	110.53
32	f	804	BCR	C28-C27-C26	-2.92	108.84	114.06
29	L	310	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
29	H	313	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
29	Q	310	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
29	a	808	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	m	103	BCR	C15-C16-C17	-2.92	117.54	123.52
29	E	310	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
29	b	731	CLA	C3B-C4B-NB	-2.92	107.92	110.53
39	A	213	KC1	C2D-C1D-ND	-2.92	107.30	110.33
29	B	316	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
35	h	203	DGD	C2G-O2G-C1B	-2.92	110.81	117.80
29	J	308	CLA	C3B-C4B-NB	-2.92	107.92	110.53
29	P	212	CLA	C3B-C4B-NB	-2.92	107.92	110.53
39	F	309	KC1	C2D-C1D-ND	-2.92	107.30	110.33
39	H	309	KC1	C2D-C1D-ND	-2.92	107.30	110.33
34	j	102	LMG	O6-C1-O1	-2.92	103.15	110.04
29	b	713	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
36	K	203	DD6	C37-C36-C31	-2.92	118.71	124.16
29	b	717	CLA	O2D-CGD-O1D	-2.91	118.17	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	E	312	KC1	C2D-C1D-ND	-2.91	107.30	110.33
36	T	303	DD6	C9-C8-C6	-2.91	118.37	126.36
39	G	315	KC1	C1D-CHD-C4C	-2.91	119.39	126.25
36	A	202	DD6	C21-C20-C15	-2.91	117.51	122.30
35	B	318	DGD	C3D-C4D-C5D	2.91	115.51	110.23
29	b	726	CLA	C3B-C4B-NB	-2.91	107.93	110.53
29	A	216	CLA	C3B-C4B-NB	-2.91	107.93	110.53
39	G	318	KC1	C2D-C1D-ND	-2.91	107.31	110.33
29	A	212	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
29	L	315	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
29	Q	313	CLA	C3B-C4B-NB	-2.91	107.93	110.53
39	H	311	KC1	C2D-C1D-ND	-2.91	107.31	110.33
29	A	215	CLA	C3B-C4B-NB	-2.91	107.93	110.53
29	G	304	CLA	C1-C2-C3	-2.91	121.43	126.20
32	a	835	BCR	C3-C4-C5	-2.91	108.87	114.06
38	E	304	UIX	C36-C35-C32	-2.91	123.20	127.28
29	a	802	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
29	N	316	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
29	b	720	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
29	O	313	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
39	L	314	KC1	CHC-C4B-C3B	-2.91	120.31	125.21
29	i	203	CLA	C3B-C4B-NB	-2.90	107.94	110.53
36	I	202	DD6	C37-C36-C35	2.90	119.76	114.42
29	b	718	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
29	l	505	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
39	A	205	KC1	C2D-C1D-ND	-2.90	107.32	110.33
39	P	211	KC1	C2D-C1D-ND	-2.90	107.32	110.33
36	C	303	DD6	C21-C20-C19	2.90	117.50	114.24
29	a	806	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	E	309	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	b	709	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
29	E	313	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
39	N	310	KC1	C2D-C1D-ND	-2.90	107.32	110.33
29	l	510	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
29	E	309	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
29	K	217	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	L	308	CLA	C3B-C4B-NB	-2.90	107.94	110.53
36	h	202	DD6	C24-C1-C2	2.90	123.56	119.01
29	B	307	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
29	I	213	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
32	l	506	BCR	C11-C10-C9	-2.89	123.22	127.28
29	i	202	CLA	O2D-CGD-O1D	-2.89	118.22	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	H	309	KC1	CHC-C4B-C3B	-2.89	120.33	125.21
29	b	713	CLA	C3B-C4B-NB	-2.89	107.95	110.53
29	L	310	CLA	C3B-C4B-NB	-2.89	107.95	110.53
29	b	705	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
29	a	822	CLA	C3B-C4B-NB	-2.89	107.95	110.53
39	O	315	KC1	C2D-C1D-ND	-2.89	107.33	110.33
39	T	315	KC1	C2D-C1D-ND	-2.89	107.33	110.33
37	Q	304	PID	CM5-C21-C20	-2.89	118.14	122.82
29	C	308	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
35	j	103	DGD	O1G-C1A-C2A	2.88	120.63	111.83
29	b	709	CLA	C3B-C4B-NB	-2.88	107.95	110.53
29	F	308	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
29	J	309	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
32	f	801	BCR	C7-C8-C9	-2.88	121.97	126.23
37	C	305	PID	C19-C20-C21	2.88	131.32	127.28
29	B	307	CLA	C3B-C4B-NB	-2.88	107.96	110.53
39	H	314	KC1	C2D-C1D-ND	-2.88	107.34	110.33
29	a	807	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
29	N	308	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
37	T	305	PID	CM5-C21-C20	-2.88	118.15	122.82
29	a	817	CLA	C3B-C4B-NB	-2.88	107.96	110.53
29	a	837	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
38	F	305	UIX	C34-C37-C39	-2.88	117.62	123.52
39	B	313	KC1	C2D-C1D-ND	-2.88	107.34	110.33
29	M	315	CLA	C3B-C4B-NB	-2.88	107.96	110.53
29	L	317	CLA	C3B-C4B-NB	-2.88	107.96	110.53
37	H	304	PID	C17-C18-C19	2.88	131.38	124.72
32	a	834	BCR	C23-C24-C25	-2.88	119.31	127.00
38	T	306	UIX	C22-C15-C20	-2.88	107.90	110.47
39	N	312	KC1	C2D-C1D-ND	-2.88	107.34	110.33
37	O	304	PID	C18-C19-C20	2.88	129.41	123.52
32	b	729	BCR	C20-C21-C22	-2.88	123.24	127.28
39	M	312	KC1	CHC-C4B-C3B	-2.88	120.36	125.21
32	b	735	BCR	C8-C7-C6	-2.88	119.32	127.00
29	O	308	CLA	C3B-C4B-NB	-2.87	107.97	110.53
38	T	306	UIX	C14-C23-C26	-2.87	118.49	126.36
29	H	307	CLA	C3B-C4B-NB	-2.87	107.97	110.53
29	T	311	CLA	C3B-C4B-NB	-2.87	107.97	110.53
29	G	312	CLA	C3B-C4B-NB	-2.87	107.97	110.53
29	E	315	CLA	C3B-C4B-NB	-2.87	107.97	110.53
39	H	314	KC1	CHB-C1B-C2B	-2.87	119.52	125.49
29	A	215	CLA	O2D-CGD-O1D	-2.87	118.26	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	311	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
29	O	311	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
39	O	315	KC1	CHC-C4B-C3B	-2.87	120.37	125.21
29	P	209	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
29	P	210	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
29	N	308	CLA	C3B-C4B-NB	-2.87	107.97	110.53
39	E	312	KC1	O1D-CGD-CBD	-2.87	118.86	124.52
34	K	220	LMG	O6-C1-O1	-2.87	103.27	110.04
29	G	316	CLA	C3B-C4B-NB	-2.87	107.97	110.53
36	B	319	DD6	C32-C33-C34	-2.87	107.31	113.59
29	a	816	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
30	b	727	PQN	C11-C3-C2	-2.86	119.98	124.89
29	b	722	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
29	L	312	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
29	f	805	CLA	C3B-C4B-NB	-2.86	107.97	110.53
37	N	304	PID	C7-C8-C9	-2.86	122.45	126.06
29	H	310	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
29	H	313	CLA	C3B-C4B-NB	-2.86	107.97	110.53
36	L	304	DD6	C37-C36-C31	-2.86	118.81	124.16
35	h	203	DGD	O1G-C1A-C2A	2.86	120.56	111.83
29	b	706	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
29	J	307	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
36	F	301	DD6	C25-C26-C27	-2.86	118.61	126.61
29	G	317	CLA	C3B-C4B-NB	-2.86	107.98	110.53
36	I	206	DD6	O1-C15-C14	-2.86	108.69	116.88
29	J	311	CLA	C3B-C4B-NB	-2.86	107.98	110.53
29	A	218	CLA	C3B-C4B-NB	-2.85	107.98	110.53
36	B	305	DD6	O1-C20-C19	-2.85	110.82	113.49
39	F	314	KC1	CHC-C4B-C3B	-2.85	120.40	125.21
39	P	213	KC1	O1D-CGD-CBD	-2.85	118.89	124.52
32	a	834	BCR	C24-C23-C22	-2.85	122.01	126.23
29	K	218	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
29	a	821	CLA	C3B-C4B-NB	-2.85	107.98	110.53
39	O	310	KC1	C2D-C1D-ND	-2.85	107.37	110.33
36	K	205	DD6	C3-C4-C5	-2.85	117.68	123.52
38	B	304	UIX	C36-C35-C32	-2.85	123.28	127.28
39	Q	311	KC1	C4B-CHC-C1C	-2.85	119.96	126.02
29	Q	315	CLA	C3B-C4B-NB	-2.85	107.98	110.53
29	O	314	CLA	O2D-CGD-CBD	2.85	116.21	111.23
36	M	302	DD6	O1-C15-C14	-2.85	108.71	116.88
29	F	316	CLA	C3B-C4B-NB	-2.85	107.99	110.53
37	G	309	PID	C18-C19-C20	2.85	129.35	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	N	303	DD6	C21-C20-C15	-2.85	117.61	122.30
29	M	308	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
29	G	302	CLA	C3B-C4B-NB	-2.85	107.99	110.53
29	H	312	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
36	L	303	DD6	C12-C11-C13	2.84	122.43	118.09
39	M	305	KC1	O1D-CGD-CBD	-2.84	118.91	124.52
29	F	308	CLA	C3B-C4B-NB	-2.84	107.99	110.53
29	J	305	CLA	C3B-C4B-NB	-2.84	107.99	110.53
29	P	209	CLA	C3B-C4B-NB	-2.84	107.99	110.53
29	L	309	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
39	L	314	KC1	C2D-C1D-ND	-2.84	107.38	110.33
36	h	202	DD6	O1-C20-C21	2.84	118.23	115.05
29	T	316	CLA	CAA-C2A-C3A	-2.84	109.71	116.23
29	I	214	CLA	C3B-C4B-NB	-2.84	107.99	110.53
37	T	301	PID	CM5-C21-C20	-2.84	118.21	122.82
29	L	317	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
29	D	313	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
29	h	201	CLA	C3B-C4B-NB	-2.84	108.00	110.53
37	G	310	PID	CM5-C21-C20	-2.84	118.22	122.82
29	b	725	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
29	M	309	CLA	C3B-C4B-NB	-2.84	108.00	110.53
39	B	313	KC1	CHC-C4B-C3B	-2.83	120.43	125.21
29	C	309	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
39	M	312	KC1	C2D-C1D-ND	-2.83	107.39	110.33
29	a	814	CLA	C3B-C4B-NB	-2.83	108.00	110.53
29	T	316	CLA	C3B-C4B-NB	-2.83	108.00	110.53
36	Q	302	DD6	O1-C15-C14	-2.83	108.76	116.88
29	H	307	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
29	P	215	CLA	C3B-C4B-NB	-2.83	108.00	110.53
29	M	315	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
37	Q	304	PID	C17-C16-C15	2.83	129.31	123.52
29	T	308	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
39	T	315	KC1	CHC-C4B-C3B	-2.83	120.44	125.21
29	l	504	CLA	C3B-C4B-NB	-2.83	108.00	110.53
29	I	201	CLA	C3B-C4B-NB	-2.83	108.00	110.53
29	C	308	CLA	C3B-C4B-NB	-2.83	108.00	110.53
29	T	313	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
36	K	206	DD6	C21-C20-C15	-2.83	117.65	122.30
39	L	314	KC1	CHB-C1B-C2B	-2.83	119.61	125.49
37	D	302	PID	CM5-C21-C20	-2.83	118.24	122.82
29	M	310	CLA	C3B-C4B-NB	-2.83	108.01	110.53
29	K	207	CLA	C3B-C4B-NB	-2.82	108.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	736	CLA	C3B-C4B-NB	-2.82	108.01	110.53
29	E	314	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
29	a	811	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
29	a	823	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
39	P	216	KC1	C2D-C1D-ND	-2.82	107.40	110.33
36	F	301	DD6	C37-C36-C35	2.82	119.60	114.42
29	K	209	CLA	C3B-C4B-NB	-2.82	108.02	110.53
36	A	202	DD6	C9-C10-C11	-2.82	123.33	127.28
29	M	307	CLA	C3B-C4B-NB	-2.82	108.02	110.53
29	C	311	CLA	C3B-C4B-NB	-2.82	108.02	110.53
36	G	306	DD6	C37-C36-C31	-2.82	118.89	124.16
29	O	308	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
36	O	303	DD6	C37-C36-C35	2.82	119.60	114.42
32	l	506	BCR	C33-C5-C6	-2.82	121.41	124.48
36	B	305	DD6	C9-C10-C11	-2.81	123.33	127.28
29	a	826	CLA	C3B-C4B-NB	-2.81	108.02	110.53
29	T	309	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
36	B	303	DD6	O1-C15-C14	-2.81	108.82	116.88
36	K	206	DD6	O1-C20-C19	-2.81	110.86	113.49
32	f	801	BCR	C28-C27-C26	-2.81	109.04	114.06
29	a	820	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	b	710	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	I	216	CLA	C3B-C4B-NB	-2.81	108.02	110.53
29	M	313	CLA	C3B-C4B-NB	-2.81	108.02	110.53
29	G	314	CLA	C1-C2-C3	-2.81	121.59	126.20
29	L	307	CLA	C3B-C4B-NB	-2.81	108.02	110.53
39	M	312	KC1	CHB-C1B-C2B	-2.81	119.64	125.49
32	l	507	BCR	C28-C27-C26	-2.81	109.05	114.06
39	G	315	KC1	C4B-CHC-C1C	-2.81	120.05	126.02
39	O	315	KC1	O1D-CGD-CBD	-2.81	118.98	124.52
32	f	801	BCR	C20-C19-C18	-2.81	118.67	126.36
29	I	208	CLA	C3B-C4B-NB	-2.81	108.02	110.53
29	T	308	CLA	C3B-C4B-NB	-2.81	108.03	110.53
39	A	213	KC1	CHC-C4B-C3B	-2.81	120.48	125.21
29	D	308	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
39	Q	309	KC1	CHC-C4B-C3B	-2.80	120.48	125.21
29	a	809	CLA	C3B-C4B-NB	-2.80	108.03	110.53
29	L	313	CLA	C3B-C4B-NB	-2.80	108.03	110.53
29	a	822	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
32	b	728	BCR	C28-C27-C26	-2.80	109.06	114.06
29	a	816	CLA	C3B-C4B-NB	-2.80	108.03	110.53
29	A	212	CLA	C3B-C4B-NB	-2.80	108.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	M	314	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
36	E	302	DD6	C9-C8-C6	-2.80	118.68	126.36
29	G	313	CLA	C3B-C4B-NB	-2.80	108.03	110.53
29	N	311	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
39	K	215	KC1	C1D-CHD-C4C	-2.80	119.67	126.25
29	F	310	CLA	C3B-C4B-NB	-2.80	108.03	110.53
39	A	213	KC1	CHB-C1B-C2B	-2.80	119.67	125.49
38	E	304	UIX	C22-C15-C20	-2.80	107.97	110.47
29	O	313	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	b	735	BCR	C38-C26-C25	-2.80	121.43	124.48
39	O	310	KC1	CHC-C4B-C3B	-2.80	120.50	125.21
39	Q	311	KC1	CHC-C4B-C3B	-2.80	120.50	125.21
29	a	813	CLA	C3B-C4B-NB	-2.79	108.03	110.53
39	F	314	KC1	C2D-C1D-ND	-2.79	107.43	110.33
37	P	202	PID	C17-C18-C19	2.79	131.18	124.72
29	L	309	CLA	C3B-C4B-NB	-2.79	108.04	110.53
29	b	701	CLA	C1-C2-C3	-2.79	121.62	126.20
39	L	306	KC1	C2D-C1D-ND	-2.79	107.43	110.33
36	I	204	DD6	C37-C36-C31	-2.79	118.94	124.16
39	N	310	KC1	CHC-C4B-C3B	-2.79	120.50	125.21
29	A	211	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
29	M	307	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
29	N	313	CLA	C3B-C4B-NB	-2.79	108.04	110.53
29	j	104	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
29	b	701	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
32	b	728	BCR	C33-C5-C4	2.78	119.53	113.60
35	j	105	DGD	C2G-O2G-C1B	-2.78	111.13	117.80
29	A	216	CLA	CAA-C2A-C3A	-2.78	109.85	116.23
39	I	215	KC1	C2D-C1D-ND	-2.78	107.44	110.33
37	O	301	PID	C18-C19-C20	2.78	129.21	123.52
29	C	313	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
34	b	730	LMG	O6-C1-O1	-2.78	103.47	110.04
29	J	313	CLA	CAA-C2A-C3A	-2.78	109.86	116.23
39	Q	309	KC1	O1D-CGD-CBD	-2.78	119.03	124.52
36	M	303	DD6	C37-C36-C31	-2.78	118.96	124.16
34	b	734	LMG	O6-C1-O1	-2.78	103.48	110.04
29	a	817	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
36	K	206	DD6	C25-C24-C1	-2.78	118.75	126.36
39	O	312	KC1	C4B-CHC-C1C	-2.78	120.12	126.02
29	l	503	CLA	C3B-C4B-NB	-2.78	108.05	110.53
29	D	309	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	a	838	BCR	C38-C26-C25	-2.78	121.45	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	H	308	CLA	C1-C2-C3	-2.78	121.65	126.20
39	C	310	KC1	CHC-C4B-C3B	-2.78	120.53	125.21
36	F	303	DD6	C37-C36-C31	-2.78	118.97	124.16
29	a	814	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
36	K	203	DD6	C21-C20-C15	-2.78	117.73	122.30
36	B	301	DD6	O1-C20-C21	-2.77	111.95	115.05
29	b	701	CLA	C3B-C4B-NB	-2.77	108.05	110.53
36	K	221	DD6	O1-C15-C14	-2.77	108.93	116.88
29	H	308	CLA	C3B-C4B-NB	-2.77	108.05	110.53
29	N	316	CLA	C3B-C4B-NB	-2.77	108.05	110.53
29	Q	310	CLA	C3B-C4B-NB	-2.77	108.05	110.53
32	f	801	BCR	C38-C26-C25	-2.77	121.46	124.48
36	L	303	DD6	C37-C36-C31	-2.77	118.98	124.16
36	K	205	DD6	C37-C36-C35	2.77	119.52	114.42
39	A	205	KC1	CHB-C1B-C2B	-2.77	119.72	125.49
29	b	705	CLA	CHB-C4A-NA	2.77	128.40	124.40
29	C	313	CLA	C3B-C4B-NB	-2.77	108.06	110.53
36	A	204	DD6	C21-C20-C15	-2.77	117.74	122.30
36	A	204	DD6	C28-C27-C26	-2.77	118.80	124.18
36	J	302	DD6	C37-C36-C31	-2.77	118.98	124.16
29	D	308	CLA	C3B-C4B-NB	-2.77	108.06	110.53
39	G	318	KC1	C1D-CHD-C4C	-2.77	119.74	126.25
29	J	305	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
36	J	302	DD6	C25-C24-C1	-2.77	118.78	126.36
29	F	312	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
29	M	311	CLA	C3B-C4B-NB	-2.77	108.06	110.53
29	E	305	CLA	C3B-C4B-NB	-2.77	108.06	110.53
36	J	301	DD6	C3-C4-C5	-2.77	117.86	123.52
29	D	311	CLA	C3B-C4B-NB	-2.76	108.06	110.53
29	E	306	CLA	C3B-C4B-NB	-2.76	108.06	110.53
38	J	304	UIX	C7-C10-C11	-2.76	121.24	125.53
29	a	828	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
32	b	729	BCR	C23-C24-C25	-2.76	119.62	127.00
38	O	306	UIX	C14-C23-C26	-2.76	118.79	126.36
29	B	312	CLA	C3B-C4B-NB	-2.76	108.06	110.53
29	T	313	CLA	C3B-C4B-NB	-2.76	108.06	110.53
36	I	202	DD6	C28-C27-C26	-2.76	118.82	124.18
36	O	303	DD6	C25-C24-C1	-2.76	118.80	126.36
37	O	305	PID	C19-C20-C21	2.76	131.15	127.28
29	J	309	CLA	C3B-C4B-NB	-2.76	108.07	110.53
39	Q	314	KC1	CHB-C1B-C2B	-2.76	119.75	125.49
32	l	506	BCR	C2-C1-C6	2.76	114.44	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	309	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
39	P	213	KC1	C4B-CHC-C1C	-2.75	120.17	126.02
37	T	317	PID	C15-C14-C13	2.75	123.88	116.80
29	F	313	CLA	CHB-C4A-NA	2.75	128.37	124.40
39	N	310	KC1	CHB-C1B-C2B	-2.75	119.77	125.49
38	Q	305	UIX	C18-O2-C27	-2.75	112.99	117.85
39	C	315	KC1	CHC-C4B-C3B	-2.75	120.58	125.21
29	F	315	CLA	CAA-C2A-C3A	-2.75	109.93	116.23
36	G	307	DD6	C23-C16-C22	2.75	111.36	107.37
29	G	304	CLA	CHB-C4A-NA	2.75	128.36	124.40
29	A	216	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
39	E	312	KC1	CHB-C1B-C2B	-2.74	119.78	125.49
36	L	305	DD6	C14-C13-C11	-2.74	121.28	125.53
29	B	311	CLA	C3B-C4B-NB	-2.74	108.08	110.53
34	K	201	LMG	O6-C1-O1	-2.74	103.57	110.04
39	D	310	KC1	CHC-C4B-C3B	-2.74	120.59	125.21
29	O	311	CLA	C3B-C4B-NB	-2.74	108.08	110.53
29	F	313	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
36	I	205	DD6	C24-C1-C2	2.74	123.32	119.01
29	F	311	CLA	C3B-C4B-NB	-2.74	108.08	110.53
29	A	217	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
39	I	215	KC1	CHC-C4B-C3B	-2.74	120.59	125.21
29	Q	315	CLA	CAA-C2A-C3A	-2.74	109.95	116.23
29	A	206	CLA	C3B-C4B-NB	-2.74	108.08	110.53
29	K	210	CLA	C3B-C4B-NB	-2.74	108.08	110.53
29	C	309	CLA	C3B-C4B-NB	-2.74	108.08	110.53
36	L	301	DD6	C15-C14-C13	-2.74	120.20	125.99
37	E	301	PID	CM4-C14-C15	-2.74	118.38	122.82
37	F	306	PID	CM5-C21-C20	-2.74	118.38	122.82
29	J	306	CLA	C3B-C4B-NB	-2.74	108.09	110.53
29	E	311	CLA	C3B-C4B-NB	-2.74	108.09	110.53
39	O	310	KC1	C1D-CHD-C4C	-2.74	119.81	126.25
29	B	311	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
36	J	303	DD6	C24-C1-C2	2.74	123.31	119.01
35	G	320	DGD	O1G-C1A-C2A	2.74	120.18	111.83
29	a	831	CLA	C3B-C4B-NB	-2.74	108.09	110.53
36	C	303	DD6	C37-C36-C31	-2.74	119.05	124.16
35	m	102	DGD	O1G-C1A-C2A	2.73	120.17	111.83
29	A	207	CLA	C3B-C4B-NB	-2.73	108.09	110.53
29	a	805	CLA	CHB-C4A-NA	2.73	128.35	124.40
29	C	316	CLA	CAA-C2A-C3A	-2.73	109.96	116.23
38	F	305	UIX	C36-C38-C40	-2.73	118.87	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	l	506	BCR	C10-C11-C12	-2.73	115.28	123.20
37	N	302	PID	CM5-C21-C20	-2.73	118.39	122.82
29	P	215	CLA	O2D-CGD-CBD	2.73	116.00	111.23
36	M	302	DD6	C37-C36-C31	-2.73	119.06	124.16
36	C	303	DD6	O1-C20-C21	2.73	118.10	115.05
39	O	312	KC1	CHC-C4B-C3B	-2.73	120.61	125.21
36	P	204	DD6	C37-C36-C35	2.73	119.44	114.42
36	G	305	DD6	C37-C36-C31	-2.73	119.06	124.16
30	b	727	PQN	C2M-C2-C3	-2.73	119.97	124.45
36	B	302	DD6	C37-C36-C31	-2.72	119.06	124.16
39	A	205	KC1	CHC-C4B-C3B	-2.72	120.62	125.21
38	P	207	UIX	C36-C38-C40	-2.72	118.90	126.36
39	I	215	KC1	O1D-CGD-CBD	-2.72	119.15	124.52
29	a	821	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
39	I	215	KC1	CHB-C1B-C2B	-2.72	119.83	125.49
29	A	210	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
39	T	310	KC1	C1D-CHD-C4C	-2.72	119.86	126.25
32	b	735	BCR	C10-C11-C12	-2.72	115.32	123.20
38	Q	305	UIX	C16-C20-C15	2.72	122.39	119.70
29	b	721	CLA	C3B-C4B-NB	-2.72	108.10	110.53
39	B	313	KC1	CHB-C1B-C2B	-2.72	119.83	125.49
36	I	205	DD6	C25-C26-C27	-2.72	119.01	126.61
37	H	306	PID	CM5-C21-C20	-2.72	118.42	122.82
36	G	306	DD6	C3-C4-C5	-2.72	117.96	123.52
32	i	204	BCR	C20-C19-C18	-2.71	118.92	126.36
29	G	311	CLA	C3B-C4B-NB	-2.71	108.11	110.53
29	I	214	CLA	CHB-C4A-NA	2.71	128.32	124.40
29	f	803	CLA	C3B-C4B-NB	-2.71	108.11	110.53
36	I	203	DD6	C15-C14-C13	-2.71	120.26	125.99
29	I	214	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
29	H	312	CLA	C3B-C4B-NB	-2.71	108.11	110.53
36	J	301	DD6	C9-C8-C6	-2.71	118.93	126.36
29	G	314	CLA	C3B-C4B-NB	-2.71	108.11	110.53
29	I	217	CLA	C3B-C4B-NB	-2.71	108.11	110.53
37	C	304	PID	C18-C19-C20	2.71	129.06	123.52
38	P	207	UIX	C14-C23-C26	-2.71	118.94	126.36
36	B	302	DD6	C14-C13-C11	-2.71	121.33	125.53
37	H	302	PID	CM5-C21-C20	-2.71	118.43	122.82
32	m	103	BCR	C3-C4-C5	-2.70	109.24	114.06
37	C	307	PID	CM5-C21-C20	-2.70	118.44	122.82
32	a	838	BCR	C20-C19-C18	-2.70	118.96	126.36
39	H	309	KC1	O1D-CGD-CBD	-2.70	119.19	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	T	306	UIX	C36-C38-C40	-2.70	118.96	126.36
29	B	314	CLA	CAA-C2A-C3A	-2.70	110.05	116.23
38	J	304	UIX	O-C-C7	-2.70	109.15	116.88
38	L	302	UIX	C14-C13-C11	-2.69	123.50	127.28
36	L	301	DD6	C21-C20-C15	-2.69	117.87	122.30
29	N	316	CLA	CAA-C2A-C3A	-2.69	110.06	116.23
39	P	216	KC1	CHB-C1B-C2B	-2.69	119.89	125.49
39	N	312	KC1	CHB-C1B-C2B	-2.69	119.89	125.49
29	a	830	CLA	C3B-C4B-NB	-2.69	108.13	110.53
29	a	810	CLA	C3B-C4B-NB	-2.69	108.13	110.53
37	Q	301	PID	CM5-C21-C20	-2.69	118.46	122.82
38	F	305	UIX	O-C-C7	-2.69	109.17	116.88
38	O	306	UIX	C22-C15-C20	-2.69	108.06	110.47
29	F	316	CLA	CAA-C2A-C3A	-2.69	110.06	116.23
29	O	313	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
29	I	211	CLA	C3B-C4B-NB	-2.69	108.13	110.53
36	H	303	DD6	C9-C8-C6	-2.69	118.99	126.36
29	D	316	CLA	CAA-C2A-C3A	-2.69	110.07	116.23
39	C	310	KC1	CHB-C1B-C2B	-2.69	119.90	125.49
39	C	312	KC1	C4B-CHC-C1C	-2.68	120.31	126.02
38	L	302	UIX	C36-C35-C32	-2.68	123.51	127.28
29	I	207	CLA	C3B-C4B-NB	-2.68	108.13	110.53
29	D	314	CLA	CHB-C4A-NA	2.68	128.27	124.40
29	K	216	CLA	C3B-C4B-NB	-2.68	108.14	110.53
29	i	201	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
29	M	309	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
36	K	205	DD6	O1-C20-C19	-2.68	110.98	113.49
29	a	802	CLA	C1-C2-C3	-2.68	121.80	126.20
37	D	303	PID	C8-C9-C10	2.68	128.85	123.60
39	F	309	KC1	CHB-C1B-C2B	-2.68	119.91	125.49
36	O	303	DD6	C14-C13-C11	-2.68	121.37	125.53
37	D	306	PID	C17-C16-C15	2.68	129.01	123.52
39	H	309	KC1	CHB-C1B-C2B	-2.68	119.91	125.49
36	L	305	DD6	C25-C26-C27	-2.68	119.11	126.61
37	T	302	PID	C18-C17-C16	2.68	130.92	124.72
39	O	310	KC1	CHB-C1B-C2B	-2.68	119.91	125.49
29	l	510	CLA	C3B-C4B-NB	-2.68	108.14	110.53
35	m	102	DGD	C2G-O2G-C1B	-2.68	111.39	117.80
36	B	303	DD6	C10-C9-C8	-2.68	115.44	123.20
29	A	211	CLA	C3B-C4B-NB	-2.68	108.14	110.53
36	F	303	DD6	C4-C3-C2	-2.68	118.04	123.52
29	a	806	CLA	CHB-C4A-NA	2.68	128.26	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	E	304	UIX	C35-C36-C38	-2.68	115.44	123.20
36	M	302	DD6	C3-C4-C5	-2.68	118.04	123.52
29	G	319	CLA	CAA-C2A-C3A	-2.68	110.09	116.23
36	B	319	DD6	C4-C3-C2	-2.68	118.04	123.52
36	K	206	DD6	C25-C26-C27	-2.68	119.13	126.61
38	L	302	UIX	C18-O2-C27	-2.67	113.12	117.85
38	O	306	UIX	C36-C38-C40	-2.67	119.03	126.36
39	M	305	KC1	C1D-CHD-C4C	-2.67	119.96	126.25
39	N	315	KC1	CHC-C4B-C3B	-2.67	120.70	125.21
29	F	315	CLA	C3B-C4B-NB	-2.67	108.14	110.53
37	Q	306	PID	CM5-C21-C20	-2.67	118.49	122.82
36	K	221	DD6	O1-C20-C21	2.67	118.03	115.05
39	J	312	KC1	CHB-C1B-C2B	-2.67	119.93	125.49
29	F	316	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
29	F	310	CLA	CHB-C4A-NA	2.67	128.25	124.40
29	I	209	CLA	C3B-C4B-NB	-2.67	108.15	110.53
39	C	315	KC1	C4B-CHC-C1C	-2.67	120.35	126.02
29	F	311	CLA	CHB-C4A-NA	2.67	128.25	124.40
36	C	303	DD6	C9-C8-C6	-2.67	119.05	126.36
39	L	306	KC1	CHB-C1B-C2B	-2.67	119.94	125.49
36	A	201	DD6	C21-C20-C15	-2.66	117.92	122.30
36	N	303	DD6	O1-C20-C21	-2.66	112.07	115.05
38	E	304	UIX	O2-C27-O4	-2.66	117.85	122.99
36	M	303	DD6	O1-C20-C21	2.66	118.03	115.05
39	Q	311	KC1	O1D-CGD-CBD	-2.66	119.26	124.52
36	B	301	DD6	C28-C27-C26	-2.66	119.01	124.18
38	O	306	UIX	C18-O2-C27	-2.66	113.14	117.85
29	A	214	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
39	E	307	KC1	C1D-CHD-C4C	-2.66	119.99	126.25
39	C	315	KC1	O1D-CGD-CBD	-2.66	119.28	124.52
29	K	214	CLA	CHB-C4A-NA	2.66	128.24	124.40
29	a	815	CLA	C3B-C4B-NB	-2.66	108.16	110.53
39	E	312	KC1	O2D-CGD-O1D	-2.66	118.68	123.85
29	K	211	CLA	C1-C2-C3	-2.66	121.84	126.20
36	I	203	DD6	C37-C36-C35	2.66	119.31	114.42
32	a	838	BCR	C23-C24-C25	-2.66	119.90	127.00
36	E	303	DD6	O1-C15-C14	-2.66	109.27	116.88
29	B	315	CLA	C3B-C4B-NB	-2.66	108.16	110.53
39	P	213	KC1	CHC-C4B-C3B	-2.66	120.73	125.21
39	D	315	KC1	CHC-C4B-C3B	-2.65	120.73	125.21
36	K	206	DD6	C14-C13-C11	-2.65	121.41	125.53
37	E	301	PID	C17-C18-C19	2.65	130.85	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	729	BCR	C39-C30-C25	-2.65	106.08	110.24
39	I	215	KC1	C1D-CHD-C4C	-2.65	120.01	126.25
29	C	314	CLA	CHB-C4A-NA	2.65	128.22	124.40
29	M	306	CLA	C3B-C4B-NB	-2.65	108.16	110.53
29	F	313	CLA	C3B-C4B-NB	-2.65	108.17	110.53
39	O	310	KC1	C2A-C3A-C4A	2.65	108.40	106.41
29	B	314	CLA	C3B-C4B-NB	-2.65	108.17	110.53
39	Q	314	KC1	C1D-CHD-C4C	-2.65	120.02	126.25
37	O	302	PID	CM5-C21-C20	-2.65	118.53	122.82
36	G	306	DD6	O1-C20-C21	-2.65	112.09	115.05
36	K	205	DD6	C4-C5-C6	-2.65	123.56	127.28
37	N	307	PID	CM5-C21-C20	-2.65	118.53	122.82
29	L	307	CLA	C1-C2-C3	-2.65	122.48	126.76
36	I	203	DD6	C25-C24-C1	-2.65	119.11	126.36
39	O	315	KC1	C4B-CHC-C1C	-2.65	120.40	126.02
29	I	211	CLA	O2D-CGD-CBD	2.65	115.86	111.23
39	H	311	KC1	O1D-CGD-CBD	-2.64	119.30	124.52
39	T	315	KC1	CHB-C1B-C2B	-2.64	119.99	125.49
29	b	707	CLA	CHB-C4A-NA	2.64	128.21	124.40
38	C	306	UIX	C22-C15-C20	-2.64	108.11	110.47
38	B	304	UIX	C7-C10-C11	-2.64	121.44	125.53
39	E	307	KC1	C2A-C3A-C4A	2.64	108.39	106.41
29	a	809	CLA	CHB-C4A-NA	2.64	128.21	124.40
36	B	302	DD6	C21-C20-C15	-2.64	117.96	122.30
38	A	203	UIX	C21-C15-C20	-2.64	108.11	110.47
36	L	305	DD6	C37-C36-C31	-2.64	119.23	124.16
37	C	302	PID	CM5-C21-C20	-2.63	118.55	122.82
38	Q	305	UIX	C22-C15-C20	-2.63	108.11	110.47
29	l	505	CLA	C3B-C4B-NB	-2.63	108.18	110.53
39	K	215	KC1	CHB-C1B-C2B	-2.63	120.01	125.49
37	O	307	PID	CM3-C5-C4	-2.63	104.34	108.97
37	P	203	PID	CM5-C21-C20	-2.63	118.55	122.82
36	F	301	DD6	C14-C13-C11	-2.63	121.45	125.53
29	M	310	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
29	D	309	CLA	CHB-C4A-NA	2.63	128.20	124.40
39	Q	309	KC1	C2A-C3A-C4A	2.63	108.39	106.41
39	L	306	KC1	O1D-CGD-CBD	-2.63	119.33	124.52
36	I	202	DD6	C37-C36-C31	-2.63	119.24	124.16
29	B	309	CLA	C3B-C4B-NB	-2.63	108.18	110.53
39	D	315	KC1	CHB-C1B-C2B	-2.63	120.02	125.49
35	j	105	DGD	O1G-C1A-C2A	2.63	119.85	111.83
29	a	801	CLA	C3B-C4B-NB	-2.63	108.18	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	H	309	KC1	C1D-CHD-C4C	-2.63	120.07	126.25
39	M	305	KC1	CHC-C4B-C3B	-2.63	120.78	125.21
39	G	318	KC1	CHB-C1B-C2B	-2.63	120.02	125.49
30	b	727	PQN	C14-C13-C15	2.62	119.78	115.23
29	G	302	CLA	CHB-C4A-NA	2.62	128.19	124.40
36	E	302	DD6	C37-C36-C35	2.62	119.24	114.42
36	I	202	DD6	O1-C15-C14	-2.62	109.36	116.88
29	b	715	CLA	C3B-C4B-NB	-2.62	108.19	110.53
29	D	316	CLA	C3B-C4B-NB	-2.62	108.19	110.53
39	M	312	KC1	C1D-CHD-C4C	-2.62	120.09	126.25
29	f	805	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
39	P	213	KC1	C1D-CHD-C4C	-2.62	120.09	126.25
39	C	312	KC1	O1D-CGD-CBD	-2.62	119.35	124.52
36	L	304	DD6	C21-C20-C15	-2.62	117.99	122.30
36	T	303	DD6	C21-C20-C15	-2.62	117.99	122.30
39	C	315	KC1	CHB-C1B-C2B	-2.62	120.05	125.49
37	j	101	PID	O1-C6-C7	-2.62	109.38	116.88
37	T	307	PID	CM2-C5-C4	-2.61	104.37	108.97
36	M	304	DD6	C21-C20-C15	-2.61	118.00	122.30
38	C	306	UIX	C18-O2-C27	-2.61	113.23	117.85
39	F	314	KC1	CHB-C1B-C2B	-2.61	120.06	125.49
39	T	312	KC1	C4B-CHC-C1C	-2.61	120.47	126.02
39	C	310	KC1	C1D-CHD-C4C	-2.61	120.11	126.25
29	b	723	CLA	C3B-C4B-NB	-2.61	108.20	110.53
29	a	820	CLA	CHB-C4A-NA	2.61	128.16	124.40
39	D	315	KC1	C1D-CHD-C4C	-2.61	120.11	126.25
36	F	301	DD6	C37-C36-C31	-2.61	119.28	124.16
39	H	311	KC1	C4B-CHC-C1C	-2.61	120.48	126.02
29	L	317	CLA	CHB-C4A-NA	2.61	128.16	124.40
29	M	308	CLA	C3B-C4B-NB	-2.61	108.20	110.53
37	P	206	PID	C29-C24-C25	2.61	122.28	119.70
39	Q	309	KC1	C1D-CHD-C4C	-2.61	120.12	126.25
36	J	301	DD6	C28-C27-C26	-2.61	119.12	124.18
32	f	804	BCR	C3-C4-C5	-2.60	109.41	114.06
36	L	305	DD6	O1-C20-C19	-2.60	111.05	113.49
39	N	315	KC1	C1D-CHD-C4C	-2.60	120.12	126.25
36	Q	302	DD6	C14-C13-C11	-2.60	121.49	125.53
39	M	312	KC1	C4B-CHC-C1C	-2.60	120.49	126.02
29	E	310	CLA	C3B-C4B-NB	-2.60	108.21	110.53
29	L	307	CLA	CHB-C4A-NA	2.60	128.15	124.40
32	a	835	BCR	C28-C27-C26	-2.60	109.42	114.06
39	L	306	KC1	C1D-CHD-C4C	-2.60	120.13	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	M	304	DD6	C25-C26-C27	-2.60	119.34	126.61
39	F	309	KC1	C1D-CHD-C4C	-2.60	120.14	126.25
32	b	729	BCR	C21-C20-C19	-2.60	115.67	123.20
39	T	310	KC1	O1D-CGD-CBD	-2.59	119.40	124.52
39	A	213	KC1	C1D-CHD-C4C	-2.59	120.15	126.25
39	O	315	KC1	CHB-C1B-C2B	-2.59	120.09	125.49
39	O	315	KC1	C1D-CHD-C4C	-2.59	120.15	126.25
35	B	318	DGD	O1G-C1A-C2A	2.59	119.74	111.83
29	L	316	CLA	C3B-C4B-NB	-2.59	108.22	110.53
39	T	312	KC1	CHB-C1B-C2B	-2.59	120.10	125.49
38	E	304	UIX	C14-C13-C11	-2.59	123.64	127.28
39	T	315	KC1	C1D-CHD-C4C	-2.59	120.15	126.25
39	O	312	KC1	CHB-C1B-C2B	-2.59	120.10	125.49
36	m	101	DD6	C37-C36-C35	2.59	119.18	114.42
39	D	310	KC1	CHB-C1B-C2B	-2.59	120.10	125.49
36	E	303	DD6	C37-C36-C31	-2.59	119.32	124.16
39	M	305	KC1	CHB-C1B-C2B	-2.59	120.10	125.49
39	P	211	KC1	CHC-C4B-C3B	-2.59	120.84	125.21
39	A	205	KC1	O1D-CGD-CBD	-2.59	119.41	124.52
29	b	736	CLA	CHB-C4A-NA	2.59	128.13	124.40
32	a	835	BCR	C33-C5-C4	2.59	119.11	113.60
39	D	310	KC1	C1D-CHD-C4C	-2.59	120.16	126.25
29	b	725	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
39	F	314	KC1	C4B-CHC-C1C	-2.59	120.52	126.02
39	D	315	KC1	C4B-CHC-C1C	-2.59	120.52	126.02
39	N	310	KC1	C1D-CHD-C4C	-2.59	120.17	126.25
36	M	301	DD6	O1-C15-C14	-2.59	109.47	116.88
39	F	309	KC1	C4B-CHC-C1C	-2.59	120.53	126.02
39	P	211	KC1	C1D-CHD-C4C	-2.58	120.17	126.25
36	I	202	DD6	C21-C20-C15	-2.58	118.05	122.30
37	C	305	PID	CM4-C14-C15	-2.58	118.63	122.82
32	b	729	BCR	C2-C1-C6	2.58	114.19	110.44
29	E	308	CLA	CHB-C4A-NA	2.58	128.13	124.40
36	B	319	DD6	C-C1-C2	-2.58	118.63	122.82
36	A	202	DD6	O1-C15-C14	-2.58	109.48	116.88
39	E	307	KC1	C4B-CHC-C1C	-2.58	120.53	126.02
36	M	301	DD6	C37-C36-C31	-2.58	119.33	124.16
39	T	312	KC1	C1D-CHD-C4C	-2.58	120.18	126.25
39	P	216	KC1	C1D-CHD-C4C	-2.58	120.18	126.25
39	H	314	KC1	C1D-CHD-C4C	-2.58	120.18	126.25
39	C	315	KC1	C1D-CHD-C4C	-2.58	120.18	126.25
39	J	312	KC1	C4B-CHC-C1C	-2.58	120.54	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	J	303	DD6	C37-C36-C31	-2.58	119.34	124.16
34	b	732	LMG	C1-C2-C3	-2.58	104.58	110.01
29	j	104	CLA	CHB-C4A-NA	2.58	128.12	124.40
36	I	204	DD6	C25-C24-C1	-2.58	119.29	126.36
34	h	205	LMG	O6-C1-O1	-2.58	103.95	110.04
39	B	313	KC1	O1D-CGD-CBD	-2.58	119.44	124.52
29	M	311	CLA	O2D-CGD-CBD	2.57	115.73	111.23
37	E	301	PID	C19-C20-C21	2.57	130.89	127.28
36	E	302	DD6	C37-C36-C31	-2.57	119.35	124.16
36	G	307	DD6	C37-C36-C35	2.57	119.15	114.42
36	M	303	DD6	C9-C8-C6	-2.57	119.31	126.36
35	j	103	DGD	O6E-C5E-C4E	2.57	114.33	109.70
37	D	306	PID	CM5-C21-C20	-2.57	118.65	122.82
36	M	302	DD6	C14-C13-C11	-2.57	121.54	125.53
39	T	315	KC1	C4B-CHC-C1C	-2.57	120.56	126.02
29	E	309	CLA	CHB-C4A-NA	2.57	128.11	124.40
29	G	319	CLA	C3B-C4B-NB	-2.57	108.24	110.53
29	O	316	CLA	C3B-C4B-NB	-2.57	108.24	110.53
29	P	210	CLA	C3B-C4B-NB	-2.57	108.24	110.53
39	T	312	KC1	O1D-CGD-CBD	-2.57	119.46	124.52
29	A	206	CLA	CHB-C4A-NA	2.57	128.10	124.40
29	b	719	CLA	C3B-C4B-NB	-2.57	108.24	110.53
29	F	307	CLA	C3B-C4B-NB	-2.57	108.24	110.53
36	L	305	DD6	C28-C27-C26	-2.56	119.20	124.18
29	T	309	CLA	C3B-C4B-NB	-2.56	108.24	110.53
36	A	201	DD6	C25-C26-C27	-2.56	119.44	126.61
39	H	311	KC1	CHB-C1B-C2B	-2.56	120.16	125.49
39	A	205	KC1	C2A-C3A-C4A	2.56	108.33	106.41
29	i	201	CLA	CHB-C4A-NA	2.56	128.09	124.40
36	J	303	DD6	C37-C36-C35	2.56	119.13	114.42
37	D	307	PID	CM5-C21-C20	-2.56	118.67	122.82
29	D	312	CLA	C3B-C4B-NB	-2.56	108.25	110.53
29	a	807	CLA	CHB-C4A-NA	2.56	128.09	124.40
39	N	315	KC1	CHB-C1B-C2B	-2.56	120.17	125.49
39	N	315	KC1	O1D-CGD-CBD	-2.56	119.48	124.52
29	E	313	CLA	CAA-C2A-C3A	-2.55	110.37	116.23
29	K	207	CLA	CHB-C4A-NA	2.55	128.09	124.40
38	B	304	UIX	O2-C27-O4	-2.55	118.06	122.99
37	T	305	PID	C17-C16-C15	2.55	128.75	123.52
39	L	314	KC1	C1D-CHD-C4C	-2.55	120.24	126.25
29	a	804	CLA	CHB-C4A-NA	2.55	128.08	124.40
39	N	312	KC1	C1D-CHD-C4C	-2.55	120.25	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Q	308	CLA	C3B-C4B-NB	-2.55	108.25	110.53
36	D	304	DD6	C-C1-C2	-2.55	118.68	122.82
32	b	729	BCR	C15-C16-C17	-2.55	118.30	123.52
39	A	205	KC1	C1D-CHD-C4C	-2.55	120.25	126.25
36	M	302	DD6	C32-C33-C34	-2.55	108.00	113.59
36	J	301	DD6	C37-C36-C31	-2.55	119.39	124.16
29	G	312	CLA	CHB-C4A-NA	2.55	128.08	124.40
29	M	306	CLA	CHB-C4A-NA	2.55	128.08	124.40
29	O	309	CLA	C3B-C4B-NB	-2.55	108.25	110.53
36	B	305	DD6	C21-C20-C15	-2.55	118.11	122.30
36	G	308	DD6	C37-C36-C31	-2.55	119.39	124.16
39	Q	309	KC1	CHB-C1B-C2B	-2.55	120.19	125.49
39	J	312	KC1	CHC-C4B-C3B	-2.55	120.91	125.21
29	F	316	CLA	CHB-C4A-NA	2.55	128.08	124.40
39	C	312	KC1	CHB-C1B-C2B	-2.55	120.19	125.49
29	b	702	CLA	C3B-C4B-NB	-2.55	108.26	110.53
36	L	305	DD6	C37-C36-C35	2.55	119.11	114.42
38	T	306	UIX	C18-O2-C27	-2.55	113.35	117.85
29	b	701	CLA	CHB-C4A-NA	2.55	128.07	124.40
39	H	311	KC1	C1D-CHD-C4C	-2.55	120.26	126.25
37	N	305	PID	CM5-C21-C20	-2.55	118.69	122.82
36	D	301	DD6	C-C1-C2	-2.54	118.69	122.82
32	a	834	BCR	C38-C26-C27	2.54	119.02	113.60
36	G	306	DD6	C25-C24-C1	-2.54	119.39	126.36
29	M	313	CLA	CAA-C2A-C3A	-2.54	110.41	116.23
39	B	313	KC1	C1D-CHD-C4C	-2.54	120.28	126.25
37	G	309	PID	CM5-C21-C20	-2.54	118.70	122.82
39	N	310	KC1	C4B-CHC-C1C	-2.54	120.63	126.02
36	I	203	DD6	C28-C27-C26	-2.54	119.25	124.18
32	i	204	BCR	C33-C5-C4	2.54	119.00	113.60
36	m	101	DD6	C25-C24-C1	-2.54	119.41	126.36
29	H	308	CLA	CHB-C4A-NA	2.53	128.06	124.40
36	K	221	DD6	C37-C36-C35	2.53	119.08	114.42
29	A	215	CLA	CHB-C4A-NA	2.53	128.06	124.40
29	l	508	CLA	CAA-C2A-C3A	-2.53	110.42	116.23
36	N	303	DD6	C14-C13-C11	-2.53	121.60	125.53
39	Q	309	KC1	C4B-CHC-C1C	-2.53	120.64	126.02
29	O	316	CLA	CAA-C2A-C3A	-2.53	110.42	116.23
36	L	304	DD6	O1-C15-C14	-2.53	109.62	116.88
29	D	311	CLA	CHB-C4A-NA	2.53	128.05	124.40
36	I	206	DD6	C21-C20-C15	-2.53	118.14	122.30
37	h	204	PID	C17-C16-C15	2.53	128.70	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	D	310	KC1	C4B-CHC-C1C	-2.53	120.64	126.02
36	M	304	DD6	C25-C24-C1	-2.53	119.43	126.36
29	G	314	CLA	CHB-C4A-NA	2.53	128.05	124.40
37	P	206	PID	C7-C8-C9	2.53	129.24	126.06
29	a	828	CLA	CHB-C4A-NA	2.53	128.05	124.40
37	P	203	PID	CM4-C14-C13	2.53	124.63	119.05
36	H	303	DD6	C14-C13-C11	-2.53	121.61	125.53
39	Q	309	KC1	O2D-CGD-O1D	-2.53	118.93	123.85
29	a	812	CLA	C3B-C4B-NB	-2.53	108.28	110.53
29	I	211	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
39	M	305	KC1	C4B-CHC-C1C	-2.53	120.65	126.02
37	P	205	PID	C17-C18-C19	2.53	130.56	124.72
29	T	314	CLA	CHB-C4A-NA	2.53	128.04	124.40
36	K	205	DD6	C21-C20-C15	-2.53	118.14	122.30
36	B	305	DD6	C25-C24-C1	-2.53	119.44	126.36
29	H	312	CLA	CHB-C4A-NA	2.53	128.04	124.40
29	H	313	CLA	CHB-C4A-NA	2.53	128.04	124.40
37	j	101	PID	C16-C15-C14	2.52	130.82	127.28
37	j	101	PID	C7-C8-C9	2.52	129.24	126.06
36	B	302	DD6	O1-C15-C14	-2.52	109.65	116.88
29	C	311	CLA	CHB-C4A-NA	2.52	128.04	124.40
39	F	314	KC1	O1D-CGD-CBD	-2.52	119.55	124.52
32	f	804	BCR	C15-C16-C17	-2.52	118.36	123.52
29	l	501	CLA	O2D-CGD-CBD	2.52	115.63	111.23
29	i	202	CLA	C1-C2-C3	-2.52	122.07	126.20
36	I	205	DD6	C37-C36-C35	2.52	119.05	114.42
36	F	301	DD6	C28-C27-C26	-2.52	119.30	124.18
39	G	315	KC1	CHB-C1B-C2B	-2.52	120.25	125.49
39	O	315	KC1	C2A-C3A-C4A	2.52	108.30	106.41
39	C	310	KC1	C2A-C3A-C4A	2.52	108.30	106.41
39	T	310	KC1	CHB-C1B-C2B	-2.52	120.25	125.49
29	a	812	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
29	K	212	CLA	C3B-C4B-NB	-2.51	108.28	110.53
29	a	825	CLA	O2D-CGD-CBD	2.51	115.63	111.23
29	I	207	CLA	CHB-C4A-NA	2.51	128.03	124.40
29	f	802	CLA	C3B-C4B-NB	-2.51	108.29	110.53
36	P	204	DD6	C21-C20-C15	-2.51	118.17	122.30
29	G	302	CLA	CAA-C2A-C3A	-2.51	106.21	113.00
29	K	218	CLA	CHB-C4A-NA	2.51	128.03	124.40
39	N	312	KC1	C4B-CHC-C1C	-2.51	120.68	126.02
29	B	308	CLA	C3B-C4B-NB	-2.51	108.29	110.53
39	H	314	KC1	C4B-CHC-C1C	-2.51	120.68	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	K	202	DD6	C37-C36-C35	2.51	119.04	114.42
36	C	303	DD6	C37-C36-C35	2.51	119.04	114.42
36	K	202	DD6	C10-C9-C8	-2.51	115.93	123.20
39	Q	311	KC1	C1D-CHD-C4C	-2.51	120.34	126.25
29	a	812	CLA	CHB-C4A-NA	2.51	128.02	124.40
29	b	722	CLA	CHB-C4A-NA	2.51	128.02	124.40
29	B	311	CLA	CHB-C4A-NA	2.51	128.02	124.40
29	b	721	CLA	CHB-C4A-NA	2.51	128.02	124.40
29	N	314	CLA	CHB-C4A-NA	2.51	128.02	124.40
39	C	310	KC1	C4B-CHC-C1C	-2.51	120.69	126.02
29	l	501	CLA	C3B-C4B-NB	-2.50	108.29	110.53
37	H	301	PID	CM5-C21-C20	-2.50	118.76	122.82
39	F	314	KC1	C1D-CHD-C4C	-2.50	120.36	126.25
37	C	301	PID	CM5-C21-C20	-2.50	118.76	122.82
39	T	315	KC1	O1D-CGD-CBD	-2.50	119.58	124.52
38	B	304	UIX	C22-C15-C20	-2.50	108.23	110.47
29	b	704	CLA	C3B-C4B-NB	-2.50	108.30	110.53
29	a	827	CLA	CHB-C4A-NA	2.50	128.01	124.40
39	H	309	KC1	O2D-CGD-O1D	-2.50	118.97	123.85
39	P	216	KC1	C4B-CHC-C1C	-2.50	120.70	126.02
39	L	314	KC1	CAC-C3C-C4C	2.50	128.05	124.79
39	L	306	KC1	C4B-CHC-C1C	-2.50	120.70	126.02
39	C	312	KC1	C1D-CHD-C4C	-2.50	120.36	126.25
39	M	312	KC1	O1D-CGD-CBD	-2.50	119.58	124.52
29	L	315	CLA	CHB-C4A-NA	2.50	128.01	124.40
29	Q	310	CLA	CHB-C4A-NA	2.50	128.01	124.40
32	a	835	BCR	C8-C7-C6	-2.50	120.32	127.00
29	O	311	CLA	CHB-C4A-NA	2.50	128.01	124.40
36	K	204	DD6	C24-C1-C2	2.50	122.94	119.01
29	A	214	CLA	CAA-C2A-C3A	-2.50	110.50	116.23
29	D	314	CLA	C3B-C4B-NB	-2.50	108.30	110.53
29	K	211	CLA	O2D-CGD-CBD	2.50	115.60	111.23
29	h	201	CLA	CHB-C4A-NA	2.50	128.00	124.40
29	T	311	CLA	CHB-C4A-NA	2.50	128.00	124.40
29	b	706	CLA	CHB-C4A-NA	2.50	128.00	124.40
39	G	315	KC1	O2D-CGD-O1D	-2.50	118.99	123.85
39	Q	311	KC1	O2D-CGD-O1D	-2.50	118.99	123.85
36	A	204	DD6	C37-C36-C31	-2.49	119.50	124.16
39	M	305	KC1	C2A-C3A-C4A	2.49	108.28	106.41
29	A	216	CLA	CHB-C4A-NA	2.49	128.00	124.40
29	G	313	CLA	CHB-C4A-NA	2.49	128.00	124.40
29	F	315	CLA	CHB-C4A-NA	2.49	128.00	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	O	305	PID	C17-C18-C19	2.49	130.48	124.72
29	a	815	CLA	CHB-C4A-NA	2.49	128.00	124.40
29	K	216	CLA	CHB-C4A-NA	2.49	128.00	124.40
29	P	217	CLA	CHB-C4A-NA	2.49	128.00	124.40
39	P	211	KC1	C2A-C3A-C4A	2.49	108.28	106.41
38	C	306	UIX	C16-C20-C15	2.49	122.17	119.70
32	b	729	BCR	C8-C7-C6	-2.49	120.34	127.00
36	D	301	DD6	C25-C24-C1	-2.49	119.53	126.36
29	M	310	CLA	CHB-C4A-NA	2.49	128.00	124.40
37	P	203	PID	C18-C17-C16	2.49	130.48	124.72
36	L	301	DD6	C37-C36-C31	-2.49	119.50	124.16
29	A	212	CLA	CHB-C4A-NA	2.49	127.99	124.40
37	N	301	PID	CM5-C21-C20	-2.49	118.78	122.82
36	I	204	DD6	O1-C20-C15	-2.49	56.96	58.93
39	A	205	KC1	C4B-CHC-C1C	-2.49	120.73	126.02
39	T	310	KC1	C4B-CHC-C1C	-2.49	120.73	126.02
36	D	301	DD6	C24-C1-C2	2.49	122.92	119.01
29	G	311	CLA	CHB-C4A-NA	2.49	127.99	124.40
36	K	221	DD6	C37-C36-C31	-2.49	119.51	124.16
36	T	303	DD6	O1-C15-C14	-2.49	109.76	116.88
29	l	509	CLA	CAA-C2A-C3A	-2.49	110.53	116.23
29	b	731	CLA	CHB-C4A-NA	2.49	127.99	124.40
37	h	204	PID	CM5-C21-C20	-2.49	118.79	122.82
37	D	303	PID	C26-C25-C24	2.48	111.63	109.21
37	j	101	PID	C8-C9-C10	2.48	128.47	123.60
39	F	314	KC1	C2A-C3A-C4A	2.48	108.28	106.41
29	E	305	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
35	j	103	DGD	O6E-C1E-C2E	2.48	115.47	110.37
29	T	313	CLA	CHB-C4A-NA	2.48	127.98	124.40
29	Q	313	CLA	CHB-C4A-NA	2.48	127.98	124.40
36	M	301	DD6	C15-C14-C13	-2.48	120.75	125.99
39	K	215	KC1	C4B-CHC-C1C	-2.48	120.75	126.02
29	J	311	CLA	CHB-C4A-NA	2.48	127.98	124.40
37	D	303	PID	C7-C8-C9	2.48	129.18	126.06
29	G	319	CLA	CHB-C4A-NA	2.48	127.98	124.40
36	P	204	DD6	C9-C8-C6	-2.48	119.56	126.36
36	G	307	DD6	O1-C15-C14	-2.48	109.77	116.88
39	T	310	KC1	CHC-C4B-C3B	-2.48	121.03	125.21
39	L	306	KC1	C2A-C3A-C4A	2.48	108.27	106.41
39	E	312	KC1	CHC-C4B-C3B	-2.48	121.03	125.21
39	A	213	KC1	C4B-CHC-C1C	-2.48	120.75	126.02
29	C	316	CLA	CHB-C4A-NA	2.48	127.97	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	208	CLA	C3B-C4B-NB	-2.48	108.32	110.53
39	E	307	KC1	CHB-C1B-C2B	-2.48	120.34	125.49
36	Q	302	DD6	O1-C20-C19	-2.48	111.17	113.49
39	H	309	KC1	C4B-CHC-C1C	-2.48	120.76	126.02
29	L	310	CLA	CHB-C4A-NA	2.48	127.97	124.40
36	M	304	DD6	C37-C36-C35	2.48	118.97	114.42
29	b	709	CLA	CHB-C4A-NA	2.47	127.97	124.40
29	J	306	CLA	CHB-C4A-NA	2.47	127.97	124.40
29	H	310	CLA	C3B-C4B-NB	-2.47	108.32	110.53
29	I	216	CLA	CHB-C4A-NA	2.47	127.97	124.40
36	B	301	DD6	C8-C6-C5	-2.47	119.00	124.72
36	B	319	DD6	C19-C18-C17	-2.47	106.17	110.79
29	C	309	CLA	CHB-C4A-NA	2.47	127.97	124.40
36	K	204	DD6	C19-C18-C17	-2.47	106.17	110.79
29	a	825	CLA	C3B-C4B-NB	-2.47	108.32	110.53
39	J	312	KC1	C1D-CHD-C4C	-2.47	120.44	126.25
29	I	216	CLA	C1-C2-C3	-2.47	122.15	126.20
29	l	502	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	B	312	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	F	315	CLA	O2D-CGD-CBD	2.47	115.55	111.23
29	N	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	l	501	CLA	CHB-C4A-NA	2.47	127.96	124.40
36	B	301	DD6	C8-C9-C10	-2.47	118.47	123.52
38	J	304	UIX	C37-C39-C40	-2.47	123.82	127.28
29	b	701	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
29	B	309	CLA	CHB-C4A-NA	2.47	127.96	124.40
34	P	201	LMG	O6-C1-O1	-2.47	104.21	110.04
29	a	801	CLA	C1-C2-C3	-2.47	122.16	126.20
29	l	503	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	T	316	CLA	CHB-C4A-NA	2.47	127.96	124.40
39	E	312	KC1	C2A-C3A-C4A	2.47	108.26	106.41
29	J	309	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	L	312	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	N	309	CLA	CHB-C4A-NA	2.47	127.96	124.40
29	L	313	CLA	CHB-C4A-NA	2.47	127.96	124.40
37	O	302	PID	CM4-C14-C13	2.47	124.49	119.05
36	L	304	DD6	C3-C4-C5	-2.46	118.48	123.52
36	K	204	DD6	C12-C11-C10	-2.46	118.82	122.82
36	A	202	DD6	C37-C36-C31	-2.46	119.55	124.16
29	l	504	CLA	CHB-C4A-NA	2.46	127.96	124.40
29	N	313	CLA	CHB-C4A-NA	2.46	127.96	124.40
29	I	213	CLA	C1-C2-C3	-2.46	122.16	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	E	304	UIX	C13-C14-C23	-2.46	116.06	123.20
38	O	306	UIX	C12-C11-C13	-2.46	118.83	122.82
29	T	309	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	E	314	CLA	C3B-C4B-NB	-2.46	108.33	110.53
29	G	314	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
29	a	818	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	I	208	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	B	316	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	B	307	CLA	CHB-C4A-NA	2.46	127.95	124.40
37	O	301	PID	CM5-C21-C20	-2.46	118.83	122.82
37	P	202	PID	C18-C17-C16	2.46	130.41	124.72
37	Q	304	PID	O1-C6-C7	-2.46	109.83	116.88
36	m	101	DD6	C21-C20-C15	-2.46	118.25	122.30
29	E	311	CLA	CHB-C4A-NA	2.46	127.95	124.40
39	M	305	KC1	O2D-CGD-O1D	-2.46	119.06	123.85
29	b	721	CLA	O2D-CGD-CBD	2.46	115.53	111.23
29	L	311	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	I	204	DD6	C12-C11-C10	-2.46	118.83	122.82
29	A	218	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	Q	315	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	G	308	DD6	O1-C20-C21	-2.46	112.30	115.05
29	I	209	CLA	C1-C2-C3	-2.46	122.17	126.20
29	a	813	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	B	303	DD6	C37-C36-C31	-2.46	119.57	124.16
29	b	702	CLA	CHB-C4A-NA	2.46	127.94	124.40
29	b	719	CLA	CHB-C4A-NA	2.46	127.94	124.40
29	B	306	CLA	CHB-C4A-NA	2.46	127.94	124.40
29	a	819	CLA	C1-C2-C3	-2.46	122.17	126.20
29	I	213	CLA	CHB-C4A-NA	2.46	127.94	124.40
29	P	214	CLA	CHB-C4A-NA	2.46	127.94	124.40
32	b	735	BCR	C38-C26-C27	2.45	118.83	113.60
29	I	201	CLA	CHB-C4A-NA	2.45	127.94	124.40
36	F	301	DD6	C9-C8-C6	-2.45	119.64	126.36
38	A	203	UIX	O2-C27-O4	-2.45	118.25	122.99
29	b	721	CLA	C1-C2-C3	-2.45	122.18	126.20
39	G	315	KC1	CHC-C4B-C3B	-2.45	121.07	125.21
36	B	302	DD6	C26-C25-C24	-2.45	116.09	123.20
39	N	315	KC1	C4B-CHC-C1C	-2.45	120.81	126.02
29	i	203	CLA	CHB-C4A-NA	2.45	127.94	124.40
37	Q	303	PID	CM2-C5-C4	-2.45	104.66	108.97
29	a	829	CLA	C3B-C4B-NB	-2.45	108.34	110.53
29	i	201	CLA	C3B-C4B-NB	-2.45	108.34	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	i	202	CLA	C3B-C4B-NB	-2.45	108.34	110.53
29	E	306	CLA	CHB-C4A-NA	2.45	127.94	124.40
37	P	206	PID	C6-C7-C8	-2.45	120.81	125.99
29	a	825	CLA	CHB-C4A-NA	2.45	127.94	124.40
36	B	319	DD6	C10-C9-C8	-2.45	116.10	123.20
29	B	314	CLA	CHB-C4A-NA	2.45	127.93	124.40
29	J	310	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
38	A	203	UIX	C37-C34-C30	-2.45	118.51	123.52
39	Q	314	KC1	C2A-C3A-C4A	2.45	108.25	106.41
34	K	219	LMG	O6-C1-O1	-2.44	104.27	110.04
29	M	313	CLA	CHB-C4A-NA	2.44	127.93	124.40
29	O	308	CLA	CHB-C4A-NA	2.44	127.93	124.40
39	B	313	KC1	C4B-CHC-C1C	-2.44	120.83	126.02
29	l	509	CLA	C3B-C4B-NB	-2.44	108.35	110.53
36	A	201	DD6	C37-C36-C31	-2.44	119.59	124.16
36	I	205	DD6	C7-C6-C5	-2.44	118.86	122.82
37	P	206	PID	CM5-C21-C20	-2.44	118.86	122.82
38	C	306	UIX	C14-C23-C26	-2.44	119.67	126.36
29	E	313	CLA	C3B-C4B-NB	-2.44	108.35	110.53
37	N	304	PID	CM5-C21-C20	-2.44	118.86	122.82
29	P	209	CLA	CHB-C4A-NA	2.44	127.92	124.40
29	b	712	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
29	F	307	CLA	CHB-C4A-NA	2.44	127.92	124.40
39	Q	314	KC1	C4B-CHC-C1C	-2.44	120.84	126.02
37	T	317	PID	CM5-C21-C20	-2.44	118.87	122.82
39	E	312	KC1	C4B-CHC-C1C	-2.44	120.84	126.02
29	H	310	CLA	CHB-C4A-NA	2.44	127.92	124.40
39	F	314	KC1	O2D-CGD-O1D	-2.44	119.11	123.85
36	M	304	DD6	C4-C5-C6	-2.44	123.86	127.28
36	F	301	DD6	C25-C24-C1	-2.43	119.69	126.36
29	N	314	CLA	O2D-CGD-CBD	2.43	115.48	111.23
29	a	826	CLA	CHB-C4A-NA	2.43	127.91	124.40
38	C	306	UIX	C36-C35-C32	-2.43	123.86	127.28
29	b	706	CLA	C3B-C4B-NB	-2.43	108.36	110.53
29	H	307	CLA	CHB-C4A-NA	2.43	127.91	124.40
29	a	817	CLA	CHB-C4A-NA	2.43	127.91	124.40
29	A	209	CLA	CHB-C4A-NA	2.43	127.91	124.40
37	O	302	PID	C16-C15-C14	2.43	130.69	127.28
32	f	801	BCR	C36-C18-C17	-2.43	118.88	122.82
29	a	810	CLA	C1-C2-C3	-2.43	122.21	126.20
36	M	304	DD6	C37-C36-C31	-2.43	119.61	124.16
39	C	310	KC1	O1D-CGD-CBD	-2.43	119.72	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	306	PID	C6-C7-C8	-2.43	120.86	125.99
36	B	301	DD6	C37-C36-C35	2.43	118.89	114.42
39	O	310	KC1	C4B-CHC-C1C	-2.43	120.86	126.02
35	B	318	DGD	O6D-C1D-C2D	-2.43	105.38	110.37
29	a	816	CLA	CHB-C4A-NA	2.43	127.91	124.40
29	P	217	CLA	C3B-C4B-NB	-2.43	108.36	110.53
39	J	312	KC1	O1D-CGD-CBD	-2.43	119.73	124.52
36	B	303	DD6	C21-C20-C15	-2.43	118.31	122.30
36	Q	302	DD6	C21-C20-C15	-2.43	118.31	122.30
29	b	710	CLA	C3B-C4B-NB	-2.43	108.36	110.53
39	I	215	KC1	O2D-CGD-O1D	-2.43	119.12	123.85
29	D	316	CLA	CHB-C4A-NA	2.43	127.90	124.40
39	G	318	KC1	C4B-CHC-C1C	-2.43	120.86	126.02
36	I	206	DD6	C37-C36-C31	-2.43	119.62	124.16
29	D	308	CLA	CHB-C4A-NA	2.43	127.90	124.40
29	E	315	CLA	CHB-C4A-NA	2.43	127.90	124.40
29	b	713	CLA	CHB-C4A-NA	2.42	127.90	124.40
29	b	714	CLA	CHB-C4A-NA	2.42	127.90	124.40
38	O	306	UIX	O2-C27-O4	-2.42	118.31	122.99
29	K	217	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	K	205	DD6	C9-C10-C11	-2.42	123.88	127.28
29	C	313	CLA	CHB-C4A-NA	2.42	127.89	124.40
29	T	308	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	C	303	DD6	C14-C13-C11	-2.42	121.78	125.53
38	A	203	UIX	C14-C13-C11	-2.42	123.89	127.28
29	J	313	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	I	204	DD6	C14-C13-C11	-2.42	121.78	125.53
32	b	728	BCR	C20-C19-C18	-2.42	119.73	126.36
32	m	103	BCR	C38-C26-C25	-2.42	121.84	124.48
29	K	210	CLA	CHB-C4A-NA	2.42	127.89	124.40
29	b	717	CLA	C3B-C4B-NB	-2.42	108.37	110.53
38	P	207	UIX	C3-C5-C4	-2.42	106.27	110.79
37	T	307	PID	C17-C16-C15	2.41	128.46	123.52
36	K	221	DD6	O1-C20-C15	-2.41	57.02	58.93
34	b	732	LMG	O6-C1-O1	-2.41	104.34	110.04
32	b	728	BCR	C11-C10-C9	-2.41	123.89	127.28
37	P	202	PID	C17-C16-C15	2.41	128.46	123.52
38	C	306	UIX	O2-C27-O4	-2.41	118.33	122.99
29	A	208	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
36	A	201	DD6	C9-C8-C6	-2.41	119.75	126.36
29	H	310	CLA	C1-C2-C3	-2.41	122.25	126.20
38	Q	305	UIX	O-C1-C3	2.41	115.75	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	G	310	PID	C28-C27-C26	2.41	114.22	109.89
36	I	205	DD6	C14-C13-C11	-2.41	121.79	125.53
29	b	718	CLA	C3B-C4B-NB	-2.41	108.38	110.53
36	K	204	DD6	C37-C36-C31	-2.41	119.65	124.16
39	F	309	KC1	O1D-CGD-CBD	-2.41	119.76	124.52
36	G	307	DD6	C9-C8-C6	-2.41	119.75	126.36
29	l	510	CLA	CAA-C2A-C3A	-2.41	106.49	113.00
29	J	307	CLA	CHB-C4A-NA	2.41	127.88	124.40
34	b	734	LMG	O1-C7-C8	-2.41	104.96	110.82
37	N	302	PID	CM4-C14-C13	2.41	124.36	119.05
37	F	302	PID	C17-C18-C19	2.41	130.29	124.72
29	J	310	CLA	CHB-C4A-NA	2.41	127.88	124.40
39	K	215	KC1	O1D-CGD-CBD	-2.41	119.77	124.52
38	T	306	UIX	O2-C27-O4	-2.41	118.34	122.99
29	Q	312	CLA	CHB-C4A-NA	2.41	127.87	124.40
39	I	215	KC1	C4B-CHC-C1C	-2.41	120.90	126.02
39	O	315	KC1	O2D-CGD-O1D	-2.41	119.16	123.85
29	D	312	CLA	CHB-C4A-NA	2.41	127.87	124.40
36	B	305	DD6	C25-C26-C27	-2.41	119.88	126.61
37	D	305	PID	CM5-C21-C20	-2.41	118.92	122.82
29	O	316	CLA	CHB-C4A-NA	2.41	127.87	124.40
34	b	730	LMG	C40-C39-C38	-2.41	102.21	114.37
29	a	819	CLA	C3B-C4B-NB	-2.41	108.38	110.53
37	O	307	PID	CM5-C21-C20	-2.40	118.92	122.82
38	Q	305	UIX	C12-C11-C13	-2.40	118.92	122.82
34	K	201	LMG	O1-C1-C2	-2.40	104.62	108.27
37	P	205	PID	C18-C19-C20	2.40	128.44	123.52
34	K	201	LMG	O2-C2-C1	-2.40	104.35	110.08
36	Q	302	DD6	C9-C8-C6	-2.40	119.77	126.36
29	f	803	CLA	CHB-C4A-NA	2.40	127.87	124.40
29	M	311	CLA	CHB-C4A-NA	2.40	127.87	124.40
34	P	201	LMG	O3-C3-C2	-2.40	104.71	110.38
39	O	310	KC1	O1D-CGD-CBD	-2.40	119.78	124.52
29	D	313	CLA	CHB-C4A-NA	2.40	127.86	124.40
29	N	311	CLA	CHB-C4A-NA	2.40	127.86	124.40
32	b	729	BCR	C33-C5-C6	-2.40	121.86	124.48
36	J	303	DD6	C28-C27-C26	-2.40	119.52	124.18
38	C	306	UIX	C12-C11-C13	-2.40	118.93	122.82
29	K	213	CLA	CHB-C4A-NA	2.40	127.86	124.40
39	M	312	KC1	C2A-C3A-C4A	2.40	108.21	106.41
36	G	306	DD6	C28-C27-C26	-2.40	119.52	124.18
29	l	510	CLA	CHB-C4A-NA	2.40	127.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	808	CLA	CHB-C4A-NA	2.40	127.86	124.40
29	M	315	CLA	CHB-C4A-NA	2.40	127.86	124.40
29	B	310	CLA	CHB-C4A-NA	2.40	127.86	124.40
32	b	729	BCR	C38-C26-C25	-2.39	121.87	124.48
37	T	304	PID	CM5-C21-C20	-2.39	118.94	122.82
29	l	508	CLA	C3B-C4B-NB	-2.39	108.39	110.53
39	E	307	KC1	O1D-CGD-CBD	-2.39	119.80	124.52
29	H	315	CLA	CAA-C2A-C3A	-2.39	110.75	116.23
39	G	315	KC1	O1D-CGD-CBD	-2.39	119.80	124.52
38	L	302	UIX	C13-C14-C23	-2.39	116.28	123.20
36	M	303	DD6	C32-C33-C34	-2.39	108.35	113.59
38	L	302	UIX	C41-C40-C38	2.39	121.74	118.09
29	b	711	CLA	CHB-C4A-NA	2.39	127.85	124.40
29	A	208	CLA	CHB-C4A-NA	2.39	127.85	124.40
36	B	303	DD6	O1-C20-C21	-2.39	112.38	115.05
38	F	305	UIX	C22-C15-C20	-2.39	108.33	110.47
37	D	305	PID	O1-C6-C7	-2.39	110.03	116.88
29	a	807	CLA	C3B-C4B-NB	-2.39	108.40	110.53
29	G	301	CLA	C3B-C4B-NB	-2.39	108.40	110.53
39	K	215	KC1	O2A-CGA-O1A	-2.39	117.84	122.70
29	N	311	CLA	C3B-C4B-NB	-2.39	108.40	110.53
35	b	733	DGD	O1G-C1A-O1A	-2.39	117.66	123.63
36	L	303	DD6	C37-C36-C35	2.39	118.81	114.42
36	D	304	DD6	C37-C36-C35	2.39	118.81	114.42
37	G	310	PID	CM4-C14-C13	2.38	124.31	119.05
36	L	301	DD6	O1-C20-C19	-2.38	111.26	113.49
37	C	301	PID	C15-C14-C13	2.38	122.93	116.80
36	I	202	DD6	O1-C20-C21	-2.38	112.38	115.05
29	a	822	CLA	CHB-C4A-NA	2.38	127.84	124.40
36	H	303	DD6	C21-C20-C15	-2.38	118.38	122.30
39	D	310	KC1	O1D-CGD-CBD	-2.38	119.82	124.52
29	Q	307	CLA	CHB-C4A-NA	2.38	127.84	124.40
29	F	308	CLA	CHB-C4A-NA	2.38	127.84	124.40
37	j	101	PID	CM5-C21-C20	-2.38	118.96	122.82
29	I	217	CLA	CHB-C4A-NA	2.38	127.83	124.40
29	H	315	CLA	C3B-C4B-NB	-2.38	108.41	110.53
36	D	304	DD6	O1-C20-C15	-2.38	57.04	58.93
36	K	203	DD6	C37-C36-C35	2.38	118.80	114.42
37	H	302	PID	C17-C16-C15	2.38	128.38	123.52
39	P	211	KC1	C4B-CHC-C1C	-2.38	120.97	126.02
36	O	303	DD6	C9-C8-C6	-2.38	119.84	126.36
29	a	802	CLA	CHB-C4A-NA	2.38	127.83	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	C	310	KC1	O2D-CGD-O1D	-2.38	119.22	123.85
36	B	319	DD6	O1-C20-C15	-2.38	57.05	58.93
36	E	303	DD6	C25-C26-C27	-2.38	119.97	126.61
36	I	204	DD6	C-C1-C2	-2.38	118.97	122.82
32	f	804	BCR	C23-C24-C25	-2.37	120.65	127.00
36	J	303	DD6	C13-C11-C10	2.37	122.74	119.01
39	A	213	KC1	O1D-CGD-CBD	-2.37	119.83	124.52
29	a	821	CLA	CHB-C4A-NA	2.37	127.83	124.40
34	A	219	LMG	O6-C1-O1	-2.37	104.43	110.04
39	B	313	KC1	O2D-CGD-O1D	-2.37	119.23	123.85
39	J	312	KC1	O2D-CGD-O1D	-2.37	119.23	123.85
36	P	204	DD6	C33-C32-C31	2.37	114.17	109.49
38	A	203	UIX	C16-C20-C15	2.37	122.05	119.70
29	a	811	CLA	CHB-C4A-NA	2.37	127.82	124.40
38	L	302	UIX	C35-C36-C38	-2.37	116.33	123.20
36	I	205	DD6	C28-C27-C26	-2.37	119.58	124.18
36	F	301	DD6	C21-C20-C15	-2.37	118.40	122.30
29	N	316	CLA	CHB-C4A-NA	2.37	127.82	124.40
29	K	214	CLA	O2D-CGD-CBD	2.37	115.37	111.23
37	N	307	PID	C8-C9-C10	2.37	128.24	123.60
38	A	203	UIX	C13-C14-C23	-2.37	116.34	123.20
29	P	212	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	b	735	BCR	C16-C15-C14	-2.37	118.67	123.52
29	B	308	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
29	b	712	CLA	C3B-C4B-NB	-2.37	108.42	110.53
39	P	216	KC1	C2A-C3A-C4A	2.37	108.19	106.41
29	b	723	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
32	a	838	BCR	C16-C15-C14	-2.37	118.67	123.52
29	M	308	CLA	CHB-C4A-NA	2.37	127.82	124.40
29	E	313	CLA	CHB-C4A-NA	2.37	127.82	124.40
39	L	314	KC1	C4B-CHC-C1C	-2.37	120.99	126.02
39	G	315	KC1	C2A-C3A-C4A	2.37	108.19	106.41
37	D	307	PID	C26-C25-C24	2.37	111.51	109.21
29	a	802	CLA	CMB-C2B-C3B	2.37	132.11	126.55
29	A	214	CLA	CHB-C4A-NA	2.36	127.81	124.40
37	O	307	PID	C18-C19-C20	2.36	128.36	123.52
29	J	305	CLA	CHB-C4A-NA	2.36	127.81	124.40
35	b	733	DGD	O2D-C2D-C3D	-2.36	104.81	110.38
37	D	306	PID	C8-C9-C10	2.36	128.23	123.60
36	Q	302	DD6	C37-C36-C31	-2.36	119.74	124.16
39	E	312	KC1	C1D-CHD-C4C	-2.36	120.69	126.25
29	K	211	CLA	CHB-C4A-NA	2.36	127.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	T	307	PID	O1-C6-C7	-2.36	110.12	116.88
39	N	310	KC1	O1D-CGD-CBD	-2.36	119.86	124.52
36	B	301	DD6	C37-C36-C31	-2.36	119.75	124.16
29	K	209	CLA	CHB-C4A-NA	2.36	127.80	124.40
38	N	306	UIX	C14-C23-C26	-2.36	119.90	126.36
39	N	310	KC1	C2A-C3A-C4A	2.36	108.18	106.41
34	A	219	LMG	O1-C7-C8	-2.36	105.08	110.82
38	L	302	UIX	C37-C39-C40	-2.36	123.97	127.28
39	O	312	KC1	C1D-CHD-C4C	-2.36	120.71	126.25
36	B	301	DD6	C21-C20-C15	-2.35	118.43	122.30
29	b	725	CLA	CHB-C4A-NA	2.35	127.80	124.40
29	E	310	CLA	CHB-C4A-NA	2.35	127.80	124.40
29	h	201	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
39	P	211	KC1	O1D-CGD-CBD	-2.35	119.88	124.52
36	K	203	DD6	O1-C20-C21	-2.35	112.42	115.05
38	Q	305	UIX	O2-C27-O4	-2.35	118.45	122.99
36	L	303	DD6	O1-C15-C14	-2.35	110.14	116.88
29	G	316	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	F	312	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	a	830	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	b	710	CLA	CHB-C4A-NA	2.35	127.79	124.40
37	C	307	PID	O1-C6-C7	-2.35	110.15	116.88
29	a	831	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	b	718	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	a	804	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
34	h	205	LMG	O2-C2-C1	-2.35	104.48	110.08
35	B	318	DGD	O2G-C1B-O1B	-2.35	118.22	123.70
29	C	308	CLA	CHB-C4A-NA	2.35	127.78	124.40
39	T	315	KC1	C2A-C3A-C4A	2.35	108.17	106.41
36	M	301	DD6	C41-C32-C31	-2.35	106.32	110.52
29	a	810	CLA	CHB-C4A-NA	2.34	127.78	124.40
29	L	308	CLA	CHB-C4A-NA	2.34	127.78	124.40
34	j	102	LMG	O3-C3-C2	-2.34	104.85	110.38
39	P	213	KC1	CHB-C1B-C2B	-2.34	120.61	125.49
36	M	303	DD6	C25-C24-C1	-2.34	119.94	126.36
36	J	303	DD6	C12-C11-C10	-2.34	119.02	122.82
37	T	302	PID	CM5-C21-C20	-2.34	119.02	122.82
39	D	315	KC1	O1D-CGD-CBD	-2.34	119.90	124.52
34	b	730	LMG	C38-C37-C36	-2.34	102.54	114.37
29	K	212	CLA	CHB-C4A-NA	2.34	127.78	124.40
36	A	204	DD6	C10-C9-C8	-2.34	116.42	123.20
37	D	303	PID	CM4-C14-C13	2.34	124.21	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	715	CLA	CHB-C4A-NA	2.34	127.78	124.40
37	D	303	PID	CM5-C21-C20	-2.34	119.03	122.82
37	D	303	PID	O1-C6-C7	-2.34	110.18	116.88
36	G	307	DD6	C23-C16-C15	-2.34	103.73	110.05
29	j	104	CLA	C3B-C4B-NB	-2.34	108.44	110.53
29	J	308	CLA	CHB-C4A-NA	2.34	127.78	124.40
39	P	216	KC1	O1D-CGD-CBD	-2.34	119.91	124.52
29	K	210	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
36	J	303	DD6	O1-C20-C21	2.34	117.66	115.05
32	b	728	BCR	C7-C8-C9	-2.34	122.78	126.23
29	O	313	CLA	CHB-C4A-NA	2.34	127.77	124.40
36	I	205	DD6	C37-C36-C31	-2.34	119.79	124.16
38	N	306	UIX	O2-C27-O4	-2.34	118.48	122.99
36	M	301	DD6	C3-C4-C5	-2.34	118.74	123.52
29	C	316	CLA	C3B-C4B-NB	-2.34	108.44	110.53
29	B	308	CLA	C1-C2-C3	-2.33	122.37	126.20
29	L	316	CLA	CHB-C4A-NA	2.33	127.77	124.40
29	a	804	CLA	C1-C2-C3	-2.33	122.37	126.20
29	A	207	CLA	CHB-C4A-NA	2.33	127.77	124.40
37	G	303	PID	C17-C18-C19	2.33	130.12	124.72
36	E	303	DD6	C28-C27-C26	-2.33	119.65	124.18
37	T	302	PID	C17-C16-C15	2.33	128.29	123.52
36	F	303	DD6	C-C1-C2	-2.33	119.04	122.82
29	a	814	CLA	CHB-C4A-NA	2.33	127.77	124.40
32	m	103	BCR	C20-C19-C18	-2.33	119.97	126.36
37	P	203	PID	C8-C9-C10	2.33	128.17	123.60
29	a	823	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
36	K	206	DD6	C37-C36-C31	-2.33	119.80	124.16
29	N	314	CLA	C3B-C4B-NB	-2.33	108.45	110.53
29	b	720	CLA	CHB-C4A-NA	2.33	127.77	124.40
29	A	206	CLA	O2D-CGD-CBD	2.33	115.31	111.23
29	J	308	CLA	O2D-CGD-CBD	2.33	115.31	111.23
32	b	729	BCR	C28-C27-C26	-2.33	109.90	114.06
29	L	309	CLA	CHB-C4A-NA	2.33	127.76	124.40
37	D	305	PID	C18-C19-C20	2.33	128.28	123.52
36	A	201	DD6	C15-C14-C13	-2.33	121.07	125.99
29	I	209	CLA	CHB-C4A-NA	2.33	127.76	124.40
36	I	202	DD6	C3-C4-C5	-2.33	118.76	123.52
29	l	505	CLA	CHB-C4A-NA	2.33	127.76	124.40
29	H	315	CLA	CHB-C4A-NA	2.33	127.76	124.40
36	m	101	DD6	C37-C36-C31	-2.33	119.81	124.16
29	B	315	CLA	CHB-C4A-NA	2.33	127.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	T	302	PID	C8-C9-C10	2.33	128.16	123.60
36	K	221	DD6	C24-C1-C2	2.33	122.67	119.01
37	O	304	PID	CM5-C21-C20	-2.33	119.05	122.82
39	H	314	KC1	O1D-CGD-CBD	-2.33	119.93	124.52
29	P	210	CLA	CHB-C4A-NA	2.33	127.76	124.40
36	M	304	DD6	C3-C4-C5	-2.33	118.76	123.52
38	A	203	UIX	C19-C18-C17	2.33	114.06	109.89
36	J	301	DD6	C-C1-C2	-2.32	119.05	122.82
36	G	308	DD6	C13-C11-C10	2.32	122.67	119.01
36	O	303	DD6	O1-C20-C15	-2.32	57.09	58.93
36	K	206	DD6	C3-C4-C5	-2.32	118.77	123.52
29	b	726	CLA	CHB-C4A-NA	2.32	127.75	124.40
39	C	312	KC1	O2D-CGD-O1D	-2.32	119.33	123.85
32	b	735	BCR	C33-C5-C4	2.32	118.55	113.60
36	A	201	DD6	O1-C20-C21	-2.32	112.45	115.05
38	P	207	UIX	O2-C27-O4	-2.32	118.51	122.99
29	l	504	CLA	C1-C2-C3	-2.32	122.40	126.20
29	b	719	CLA	C1-C2-C3	-2.32	123.01	126.76
39	D	310	KC1	C2A-C3A-C4A	2.32	108.15	106.41
29	I	210	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	I	211	CLA	CHB-C4A-NA	2.32	127.75	124.40
38	Q	305	UIX	C10-C11-C13	2.32	122.66	119.01
29	T	314	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
36	G	307	DD6	O1-C20-C21	2.32	117.64	115.05
34	A	219	LMG	C38-C37-C36	-2.32	102.66	114.37
36	I	205	DD6	C19-C18-C17	-2.32	106.46	110.79
32	f	801	BCR	C2-C1-C6	2.32	113.80	110.44
36	D	304	DD6	C9-C8-C6	-2.32	120.02	126.36
39	C	315	KC1	C2A-C3A-C4A	2.31	108.15	106.41
38	T	306	UIX	C3-C5-C4	-2.31	106.46	110.79
37	G	310	PID	C17-C16-C15	2.31	128.25	123.52
36	G	306	DD6	C25-C26-C27	-2.31	120.14	126.61
39	Q	311	KC1	CHB-C1B-C2B	-2.31	120.67	125.49
29	Q	312	CLA	O1D-CGD-CBD	2.31	129.08	124.52
32	i	204	BCR	C10-C11-C12	-2.31	116.50	123.20
29	a	810	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
29	a	809	CLA	C1-C2-C3	-2.31	122.41	126.20
37	P	203	PID	C16-C15-C14	2.31	130.52	127.28
39	Q	314	KC1	O1D-CGD-CBD	-2.31	119.96	124.52
29	K	208	CLA	CHB-C4A-NA	2.31	127.73	124.40
37	D	303	PID	O4-C12-C13	2.31	127.82	122.89
29	G	301	CLA	CHB-C4A-NA	2.31	127.73	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	T	306	UIX	C12-C11-C13	-2.31	119.08	122.82
36	J	302	DD6	C9-C8-C6	-2.31	120.03	126.36
37	D	306	PID	CM4-C14-C13	2.31	124.14	119.05
38	Q	305	UIX	C21-C15-C20	-2.31	108.41	110.47
29	a	825	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
37	P	205	PID	CM5-C21-C20	-2.31	119.08	122.82
29	b	722	CLA	C3B-C4B-NB	-2.31	108.47	110.53
39	B	313	KC1	C2A-C3A-C4A	2.31	108.14	106.41
38	F	305	UIX	O2-C27-O4	-2.30	118.54	122.99
29	D	314	CLA	O2D-CGD-CBD	2.30	115.26	111.23
29	l	508	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	Q	308	CLA	CHB-C4A-NA	2.30	127.72	124.40
37	P	208	PID	C15-C14-C13	2.30	122.72	116.80
36	K	205	DD6	C10-C9-C8	-2.30	116.53	123.20
39	C	315	KC1	O2D-CGD-O1D	-2.30	119.37	123.85
34	h	205	LMG	O7-C10-O9	-2.30	118.32	123.70
39	P	213	KC1	O2D-CGD-O1D	-2.30	119.37	123.85
29	a	824	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	b	723	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	a	823	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
37	D	305	PID	CM2-C5-C4	-2.30	104.92	108.97
29	l	502	CLA	C1-C2-C3	-2.30	122.43	126.20
29	a	837	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	L	301	DD6	C37-C36-C35	2.30	118.65	114.42
29	b	708	CLA	C3B-C4B-NB	-2.30	108.48	110.53
40	J	314	SQD	O6-C1-C2	2.30	111.76	108.27
39	L	314	KC1	C2A-C3A-C4A	2.30	108.14	106.41
29	a	807	CLA	C1-C2-C3	-2.30	122.43	126.20
36	T	303	DD6	C37-C36-C31	-2.30	119.86	124.16
39	L	306	KC1	O2D-CGD-O1D	-2.30	119.38	123.85
37	E	301	PID	CM5-C21-C20	-2.30	119.10	122.82
30	a	832	PQN	C11-C3-C4	2.30	121.00	118.58
29	b	731	CLA	C1-C2-C3	-2.29	122.44	126.20
36	L	305	DD6	C4-C3-C2	-2.29	118.82	123.52
36	M	304	DD6	C28-C27-C26	-2.29	119.73	124.18
29	G	317	CLA	CHB-C4A-NA	2.29	127.71	124.40
32	f	804	BCR	C11-C12-C13	-2.29	120.07	126.36
38	F	305	UIX	C16-C20-C15	2.29	121.97	119.70
34	b	730	LMG	O3-C3-C2	-2.29	104.97	110.38
39	A	205	KC1	C1A-C2A-C3A	-2.29	105.17	107.28
36	H	303	DD6	C37-C36-C31	-2.29	119.87	124.16
38	E	304	UIX	C34-C37-C39	-2.29	118.83	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	M	301	DD6	C25-C24-C1	-2.29	120.08	126.36
36	I	206	DD6	C37-C36-C35	2.29	118.64	114.42
29	I	212	CLA	CHB-C4A-NA	2.29	127.70	124.40
34	b	732	LMG	O2-C2-C1	-2.29	104.62	110.08
29	j	104	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
29	a	823	CLA	CHB-C4A-NA	2.29	127.70	124.40
29	O	309	CLA	CHB-C4A-NA	2.29	127.70	124.40
29	A	209	CLA	C1-C2-C3	-2.29	122.45	126.20
34	b	734	LMG	O3-C3-C2	-2.28	104.99	110.38
29	a	830	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
36	J	303	DD6	C-C1-C2	-2.28	119.12	122.82
37	C	304	PID	CM5-C21-C20	-2.28	119.12	122.82
39	K	215	KC1	C2A-C3A-C4A	2.28	108.12	106.41
36	M	304	DD6	O1-C20-C21	-2.28	112.50	115.05
34	b	732	LMG	O1-C7-C8	-2.28	105.27	110.82
37	H	305	PID	C19-C20-C21	2.28	130.48	127.28
36	M	301	DD6	C14-C13-C11	-2.28	121.99	125.53
37	F	304	PID	CM5-C21-C20	-2.28	119.12	122.82
36	E	302	DD6	C26-C25-C24	-2.28	116.59	123.20
34	K	220	LMG	O3-C3-C2	-2.28	105.00	110.38
36	J	302	DD6	C32-C33-C34	-2.28	108.59	113.59
34	K	201	LMG	O1-C7-C8	-2.28	105.28	110.82
29	P	215	CLA	CED-O2D-CGD	2.28	121.08	115.92
39	H	311	KC1	O2D-CGD-O1D	-2.28	119.41	123.85
37	T	317	PID	C18-C19-C20	2.28	128.18	123.52
35	B	318	DGD	C1E-O6E-C5E	2.28	118.17	113.72
36	J	303	DD6	C9-C8-C6	-2.28	120.12	126.36
37	T	305	PID	CM4-C14-C13	2.28	124.07	119.05
39	N	312	KC1	O1D-CGD-CBD	-2.28	120.03	124.52
29	a	822	CLA	C1-C2-C3	-2.28	122.47	126.20
36	I	206	DD6	C10-C9-C8	-2.28	116.61	123.20
39	T	312	KC1	C2A-C3A-C4A	2.27	108.12	106.41
36	L	301	DD6	O1-C15-C14	-2.27	110.36	116.88
38	O	306	UIX	C10-C11-C13	2.27	122.59	119.01
36	T	303	DD6	C28-C27-C26	-2.27	119.77	124.18
36	A	202	DD6	O1-C20-C19	-2.27	111.36	113.49
29	b	712	CLA	CHB-C4A-NA	2.27	127.68	124.40
36	A	201	DD6	C28-C27-C26	-2.27	119.77	124.18
29	b	708	CLA	CHB-C4A-NA	2.27	127.68	124.40
29	l	509	CLA	CHB-C4A-NA	2.27	127.68	124.40
36	L	304	DD6	C13-C11-C10	2.27	122.58	119.01
37	F	304	PID	O1-C1-C2	2.27	115.62	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	H	312	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
29	B	308	CLA	CHB-C4A-NA	2.27	127.68	124.40
36	T	303	DD6	C4-C3-C2	-2.27	118.87	123.52
32	a	838	BCR	C8-C7-C6	-2.27	120.93	127.00
29	E	305	CLA	CHB-C4A-NA	2.27	127.68	124.40
37	O	307	PID	C6-C7-C8	2.27	130.79	125.99
29	A	210	CLA	C3B-C4B-NB	-2.27	108.50	110.53
29	C	314	CLA	O2D-CGD-CBD	2.27	115.20	111.23
29	b	724	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
37	N	307	PID	CM1-C1-C6	-2.27	118.57	122.30
37	H	304	PID	CM5-C21-C20	-2.27	119.14	122.82
29	N	313	CLA	CMD-C2D-C1D	-2.27	120.74	124.73
39	N	315	KC1	C2A-C3A-C4A	2.27	108.11	106.41
29	f	805	CLA	CHB-C4A-NA	2.27	127.67	124.40
39	N	315	KC1	O2D-CGD-O1D	-2.27	119.44	123.85
29	a	801	CLA	CHB-C4A-NA	2.26	127.67	124.40
29	b	714	CLA	C1-C2-C3	-2.26	122.49	126.20
29	a	823	CLA	C3B-C4B-NB	-2.26	108.51	110.53
36	J	301	DD6	C24-C1-C2	2.26	122.57	119.01
36	D	304	DD6	C37-C36-C31	-2.26	119.93	124.16
39	L	314	KC1	O1D-CGD-CBD	-2.26	120.05	124.52
29	b	724	CLA	CHB-C4A-NA	2.26	127.67	124.40
32	i	204	BCR	C29-C30-C25	2.26	113.73	110.44
29	b	719	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
29	I	217	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
36	B	305	DD6	C10-C9-C8	-2.26	116.65	123.20
35	B	318	DGD	O6D-C5D-C4D	2.26	113.77	109.70
32	l	506	BCR	C38-C26-C27	2.26	118.41	113.60
36	C	303	DD6	C4-C3-C2	-2.26	118.90	123.52
37	H	302	PID	C8-C9-C10	2.26	128.02	123.60
36	h	202	DD6	C37-C36-C35	2.26	118.57	114.42
29	E	315	CLA	O2D-CGD-CBD	2.26	115.17	111.23
34	j	102	LMG	O1-C1-C2	-2.26	104.85	108.27
37	j	101	PID	C18-C17-C16	2.26	129.94	124.72
36	M	301	DD6	C37-C36-C35	2.26	118.57	114.42
36	I	202	DD6	C10-C9-C8	-2.25	116.67	123.20
32	b	728	BCR	C1-C6-C7	2.25	121.76	115.65
29	M	307	CLA	CHB-C4A-NA	2.25	127.65	124.40
29	A	217	CLA	CHB-C4A-NA	2.25	127.65	124.40
36	M	302	DD6	C37-C36-C35	2.25	118.56	114.42
37	T	317	PID	C28-C27-C26	2.25	113.93	109.89
36	K	202	DD6	C25-C24-C1	-2.25	120.19	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	101	PID	C6-C7-C8	-2.25	121.24	125.99
29	K	214	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
32	a	838	BCR	C38-C26-C27	2.25	118.39	113.60
29	A	211	CLA	CHB-C4A-NA	2.25	127.64	124.40
29	f	802	CLA	CHB-C4A-NA	2.25	127.64	124.40
29	G	316	CLA	C1-C2-C3	-2.25	122.51	126.20
36	B	302	DD6	C4-C3-C2	-2.25	118.92	123.52
29	E	311	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
29	b	716	CLA	O2D-CGD-CBD	2.25	115.16	111.23
32	b	728	BCR	C10-C11-C12	-2.24	116.70	123.20
39	A	205	KC1	O2A-CGA-O1A	-2.24	118.13	122.70
29	K	209	CLA	C1-C2-C3	-2.24	122.52	126.20
36	K	205	DD6	C14-C13-C11	-2.24	122.05	125.53
32	b	728	BCR	C16-C15-C14	-2.24	118.93	123.52
34	b	734	LMG	O1-C1-C2	-2.24	104.87	108.27
37	N	302	PID	C8-C9-C10	2.24	127.99	123.60
36	N	303	DD6	C37-C36-C31	-2.24	119.97	124.16
29	b	717	CLA	C1-C2-C3	-2.24	122.52	126.20
29	A	217	CLA	C1-C2-C3	-2.24	122.52	126.20
29	A	210	CLA	CHB-C4A-NA	2.24	127.64	124.40
34	b	730	LMG	O2-C2-C1	-2.24	104.74	110.08
36	M	301	DD6	C28-C27-C26	-2.24	119.83	124.18
37	T	307	PID	CM4-C14-C13	2.24	123.99	119.05
36	L	304	DD6	C25-C24-C1	-2.24	120.22	126.36
39	L	306	KC1	O2A-CGA-O1A	-2.24	118.14	122.70
29	a	829	CLA	CHB-C4A-NA	2.24	127.63	124.40
32	a	838	BCR	C10-C11-C12	-2.24	116.72	123.20
39	I	215	KC1	C2A-C3A-C4A	2.24	108.09	106.41
39	J	312	KC1	C2A-C3A-C4A	2.24	108.09	106.41
36	N	303	DD6	C37-C36-C35	2.24	118.53	114.42
29	i	202	CLA	CHB-C4A-NA	2.23	127.62	124.40
39	F	309	KC1	C2A-C3A-C4A	2.23	108.09	106.41
35	G	320	DGD	C2G-O2G-C1B	-2.23	112.45	117.80
29	E	314	CLA	CHB-C4A-NA	2.23	127.62	124.40
36	K	221	DD6	C12-C11-C10	-2.23	119.20	122.82
29	I	212	CLA	C1-C2-C3	-2.23	122.54	126.20
29	G	312	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
32	l	507	BCR	C35-C13-C14	-2.23	119.20	122.82
37	P	202	PID	CM5-C21-C20	-2.23	119.20	122.82
38	E	304	UIX	C18-O2-C27	-2.23	113.91	117.85
34	K	219	LMG	O3-C3-C2	-2.23	105.12	110.38
36	G	308	DD6	C3-C4-C5	-2.23	118.96	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	b	734	LMG	O2-C2-C1	-2.23	104.77	110.08
36	B	305	DD6	C37-C36-C31	-2.23	119.99	124.16
36	A	201	DD6	C25-C24-C1	-2.23	120.26	126.36
36	K	206	DD6	C37-C36-C35	2.23	118.52	114.42
36	B	301	DD6	C5-C4-C3	-2.23	119.57	124.72
32	a	838	BCR	C29-C30-C25	2.23	113.67	110.44
36	I	203	DD6	C32-C33-C34	-2.23	108.71	113.59
36	E	303	DD6	C37-C36-C35	2.23	118.51	114.42
32	b	729	BCR	C7-C8-C9	-2.23	122.94	126.23
32	b	729	BCR	C34-C9-C8	2.23	121.49	118.09
38	L	302	UIX	O2-C27-O4	-2.22	118.70	122.99
36	K	203	DD6	C9-C8-C6	-2.22	120.27	126.36
39	N	312	KC1	C2A-C3A-C4A	2.22	108.08	106.41
34	K	219	LMG	O2-C2-C1	-2.22	104.79	110.08
29	B	315	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
29	F	310	CLA	O2D-CGD-CBD	2.22	115.11	111.23
29	a	808	CLA	C1-C2-C3	-2.22	122.56	126.20
36	A	204	DD6	O1-C20-C19	-2.22	111.41	113.49
29	J	310	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
32	l	506	BCR	C35-C13-C12	2.22	121.47	118.09
37	h	204	PID	CM4-C14-C13	2.22	123.94	119.05
39	C	312	KC1	C2A-C3A-C4A	2.21	108.07	106.41
36	C	303	DD6	C28-C27-C26	-2.21	119.88	124.18
39	A	213	KC1	O2D-CGD-O1D	-2.21	119.54	123.85
37	T	317	PID	C17-C18-C19	2.21	129.83	124.72
35	b	733	DGD	O6D-C5D-C6D	2.21	111.08	106.69
37	P	202	PID	CM4-C14-C13	2.21	123.93	119.05
29	b	716	CLA	CHB-C4A-NA	2.21	127.59	124.40
38	F	305	UIX	C14-C23-C26	-2.21	120.30	126.36
37	j	101	PID	CM4-C14-C13	2.21	123.93	119.05
39	O	312	KC1	C2A-C3A-C4A	2.21	108.07	106.41
36	T	303	DD6	O1-C20-C21	-2.21	112.58	115.05
36	B	305	DD6	C3-C4-C5	-2.21	119.00	123.52
36	N	303	DD6	O1-C15-C14	-2.21	110.55	116.88
36	h	202	DD6	C-C1-C2	-2.21	119.24	122.82
36	L	304	DD6	C32-C33-C34	-2.21	108.75	113.59
29	a	825	CLA	C1-C2-C3	-2.21	122.58	126.20
39	H	314	KC1	C2A-C3A-C4A	2.21	108.07	106.41
32	b	735	BCR	C27-C26-C25	-2.21	119.72	122.70
36	M	302	DD6	O1-C20-C15	-2.21	57.18	58.93
29	I	213	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
36	A	202	DD6	C14-C13-C11	-2.20	122.11	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	O	302	PID	C18-C17-C16	2.20	129.81	124.72
36	D	301	DD6	C37-C36-C35	2.20	118.47	114.42
36	T	303	DD6	C37-C36-C35	2.20	118.47	114.42
29	P	212	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
34	K	220	LMG	O2-C2-C1	-2.20	104.83	110.08
36	D	301	DD6	C32-C33-C34	-2.20	108.76	113.59
32	a	835	BCR	C38-C26-C27	2.20	118.29	113.60
29	a	803	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
39	A	205	KC1	O2D-CGD-O1D	-2.20	119.56	123.85
32	a	835	BCR	C15-C16-C17	-2.20	119.02	123.52
34	K	201	LMG	O3-C3-C2	-2.20	105.19	110.38
36	B	305	DD6	C28-C27-C26	-2.20	119.91	124.18
29	G	301	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
34	A	219	LMG	O2-C2-C1	-2.20	104.84	110.08
36	I	203	DD6	C3-C4-C5	-2.20	119.02	123.52
37	H	302	PID	CM4-C14-C13	2.20	123.90	119.05
29	K	212	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
37	T	307	PID	C18-C17-C16	2.20	129.80	124.72
36	J	302	DD6	C3-C4-C5	-2.20	119.03	123.52
34	h	205	LMG	O3-C3-C2	-2.19	105.20	110.38
36	K	206	DD6	C28-C27-C26	-2.19	119.92	124.18
36	O	303	DD6	C4-C3-C2	-2.19	119.03	123.52
36	G	306	DD6	C10-C9-C8	-2.19	116.84	123.20
29	a	801	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
36	J	303	DD6	C19-C18-C17	-2.19	106.69	110.79
34	j	102	LMG	O2-C2-C1	-2.19	104.85	110.08
39	A	213	KC1	C2A-C3A-C4A	2.19	108.06	106.41
29	b	707	CLA	O1D-CGD-CBD	2.19	128.84	124.52
37	j	101	PID	C17-C16-C15	2.19	128.00	123.52
37	G	303	PID	CM5-C21-C20	-2.19	119.27	122.82
39	Q	311	KC1	C2A-C3A-C4A	2.19	108.06	106.41
29	b	736	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
29	b	707	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
29	L	316	CLA	O2D-CGD-CBD	2.19	115.06	111.23
36	L	304	DD6	C28-C27-C26	-2.19	119.93	124.18
37	Q	303	PID	CM5-C21-C20	-2.19	119.27	122.82
37	P	202	PID	C19-C20-C21	2.19	130.34	127.28
29	P	215	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
32	b	735	BCR	C34-C9-C8	2.19	121.43	118.09
29	b	723	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
38	A	203	UIX	C7-C10-C11	-2.18	122.14	125.53
37	G	303	PID	C15-C14-C13	2.18	122.42	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B	303	DD6	C3-C4-C5	-2.18	119.05	123.52
29	a	826	CLA	O2D-CGD-CBD	2.18	115.05	111.23
36	D	301	DD6	C15-C14-C13	2.18	130.61	125.99
29	J	308	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
37	H	301	PID	C7-C8-C9	-2.18	123.31	126.06
29	N	313	CLA	CMD-C2D-C3D	2.18	132.69	127.69
29	H	308	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
29	a	819	CLA	CHB-C4A-NA	2.18	127.55	124.40
35	j	103	DGD	O2G-C1B-O1B	-2.18	118.61	123.70
29	a	823	CLA	CMB-C2B-C3B	2.18	131.68	126.55
29	C	314	CLA	C3B-C4B-NB	-2.18	108.58	110.53
36	Q	302	DD6	O1-C20-C21	-2.18	112.61	115.05
36	T	303	DD6	C25-C24-C1	-2.18	120.39	126.36
29	I	210	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
36	N	303	DD6	C9-C8-C6	-2.18	120.39	126.36
29	Q	310	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
29	O	313	CLA	CMB-C2B-C3B	2.18	131.67	126.55
29	B	309	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
36	K	221	DD6	C21-C20-C19	2.18	116.69	114.24
39	L	306	KC1	C1A-C2A-C3A	-2.18	105.28	107.28
29	E	306	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
29	E	310	CLA	CMB-C2B-C1B	-2.18	122.11	125.42
29	J	310	CLA	CMB-C2B-C3B	2.18	131.67	126.55
34	A	219	LMG	O3-C3-C2	-2.17	105.25	110.38
36	A	204	DD6	O1-C20-C21	-2.17	112.62	115.05
29	a	818	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
29	M	309	CLA	CHB-C4A-NA	2.17	127.53	124.40
39	H	309	KC1	C2A-C3A-C4A	2.17	108.04	106.41
36	B	305	DD6	C37-C36-C35	2.17	118.42	114.42
36	L	304	DD6	C37-C36-C35	2.17	118.41	114.42
37	O	304	PID	CM2-C5-C4	-2.17	105.16	108.97
29	A	211	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
36	M	302	DD6	C28-C27-C26	-2.17	119.98	124.18
36	D	304	DD6	C15-C14-C13	-2.17	121.42	125.99
38	J	304	UIX	C-C7-C10	-2.17	121.42	125.99
29	a	827	CLA	O2D-CGD-CBD	2.17	115.02	111.23
29	L	309	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
34	P	201	LMG	O2-C2-C1	-2.16	104.92	110.08
29	M	309	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
34	P	201	LMG	O7-C10-O9	-2.16	118.65	123.70
29	a	809	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
29	L	313	CLA	O2A-CGA-O1A	-2.16	118.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	P	203	PID	O4-C12-C13	2.16	127.50	122.89
36	h	202	DD6	C4-C3-C2	-2.16	119.10	123.52
29	J	311	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
29	H	310	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
37	P	206	PID	O1-C6-C7	-2.16	110.69	116.88
32	m	103	BCR	C33-C5-C6	-2.16	122.13	124.48
36	J	301	DD6	C12-C11-C10	-2.16	119.32	122.82
37	Q	301	PID	CM4-C14-C13	2.16	123.81	119.05
36	B	319	DD6	C37-C36-C35	2.16	118.38	114.42
36	J	302	DD6	C37-C36-C35	2.15	118.38	114.42
29	a	822	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
36	I	205	DD6	O1-C20-C15	-2.15	57.22	58.93
36	O	303	DD6	C28-C27-C26	-2.15	120.00	124.18
29	a	821	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
37	H	305	PID	C26-C25-C24	2.15	111.30	109.21
29	O	314	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
36	M	301	DD6	C10-C9-C8	-2.15	116.97	123.20
39	P	213	KC1	C2A-C3A-C4A	2.15	108.03	106.41
29	M	314	CLA	C3B-C4B-NB	-2.15	108.61	110.53
29	b	714	CLA	O2D-CGD-CBD	2.15	114.99	111.23
36	L	304	DD6	C19-C18-C17	2.15	114.81	110.79
36	m	101	DD6	C7-C6-C8	2.15	121.37	118.09
36	B	301	DD6	C25-C26-C27	-2.15	120.60	126.61
34	K	219	LMG	O7-C10-O9	-2.15	118.68	123.70
29	b	722	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
37	H	302	PID	O1-C6-C7	-2.15	110.73	116.88
37	Q	304	PID	CM4-C14-C13	2.15	123.79	119.05
39	G	318	KC1	O1D-CGD-CBD	-2.15	120.28	124.52
36	G	308	DD6	C12-C11-C10	-2.15	119.34	122.82
39	F	309	KC1	O2D-CGD-O1D	-2.14	119.67	123.85
29	b	708	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
29	b	722	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
29	D	314	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
32	a	834	BCR	C8-C7-C6	-2.14	121.27	127.00
36	L	303	DD6	C25-C26-C27	-2.14	120.62	126.61
29	I	214	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
39	M	305	KC1	O2A-CGA-O1A	-2.14	118.34	122.70
29	i	201	CLA	C1-C2-C3	-2.14	122.69	126.20
29	a	812	CLA	CMB-C2B-C3B	2.14	131.59	126.55
29	l	503	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
29	A	209	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
37	C	304	PID	C17-C18-C19	2.14	129.66	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	310	CLA	C1-C2-C3	-2.14	122.69	126.20
29	A	208	CLA	CMB-C2B-C3B	2.14	131.58	126.55
29	I	211	CLA	CMB-C2B-C3B	2.14	131.57	126.55
36	A	202	DD6	C26-C25-C24	-2.14	117.01	123.20
29	Q	307	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
35	j	105	DGD	O2G-C1B-O1B	-2.14	118.71	123.70
29	B	310	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
39	T	310	KC1	C2A-C3A-C4A	2.13	108.01	106.41
36	K	205	DD6	C32-C33-C34	-2.13	108.92	113.59
29	i	202	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
36	K	204	DD6	C13-C11-C10	2.13	122.36	119.01
29	E	308	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
36	D	301	DD6	C37-C36-C31	-2.13	120.17	124.16
36	J	302	DD6	C19-C18-C17	-2.13	106.81	110.79
29	a	830	CLA	C1-C2-C3	-2.13	122.71	126.20
36	K	221	DD6	C3-C4-C5	-2.13	119.16	123.52
34	b	734	LMG	O7-C10-O9	-2.13	118.73	123.70
29	a	825	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
36	H	303	DD6	C28-C27-C26	-2.13	120.05	124.18
36	I	206	DD6	C14-C13-C11	-2.13	122.23	125.53
39	E	312	KC1	CAC-C3C-C4C	2.13	127.56	124.79
37	Q	303	PID	C17-C18-C19	2.13	129.64	124.72
37	T	302	PID	CM4-C14-C13	2.13	123.75	119.05
29	G	313	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
36	I	204	DD6	C37-C36-C35	2.13	118.33	114.42
29	b	717	CLA	CHB-C4A-NA	2.13	127.47	124.40
29	I	216	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
29	N	308	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
37	O	302	PID	C8-C9-C10	2.13	127.76	123.60
29	K	209	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
36	L	301	DD6	C28-C27-C26	-2.12	120.06	124.18
36	K	221	DD6	C26-C25-C24	-2.12	117.05	123.20
29	K	210	CLA	C1-C2-C3	-2.12	123.33	126.76
32	l	506	BCR	C29-C30-C25	2.12	113.52	110.44
37	C	302	PID	CM4-C14-C13	2.12	123.73	119.05
34	b	732	LMG	C38-C37-C36	-2.12	103.64	114.37
29	A	218	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
39	M	312	KC1	O2D-CGD-O1D	-2.12	119.72	123.85
29	b	706	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
29	a	831	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
32	l	507	BCR	C23-C24-C25	-2.12	121.33	127.00
29	b	711	CLA	O2D-CGD-CBD	2.12	114.94	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	l	507	BCR	C21-C20-C19	-2.12	117.06	123.20
36	K	202	DD6	C26-C25-C24	-2.12	117.06	123.20
36	K	203	DD6	C15-C14-C13	-2.12	121.51	125.99
29	b	719	CLA	CMB-C2B-C3B	2.12	131.54	126.55
29	Q	313	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
29	a	826	CLA	C1-C2-C3	-2.12	122.72	126.20
29	A	212	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
36	A	204	DD6	C25-C24-C1	-2.12	120.55	126.36
29	M	314	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
29	b	715	CLA	O2D-CGD-CBD	2.12	114.93	111.23
37	G	303	PID	C8-C9-C10	2.12	127.75	123.60
32	l	506	BCR	C33-C5-C4	2.12	118.11	113.60
36	F	303	DD6	C32-C33-C34	-2.12	108.95	113.59
36	Q	302	DD6	C28-C27-C26	-2.12	120.07	124.18
36	K	204	DD6	O1-C20-C15	-2.12	57.25	58.93
35	m	102	DGD	O2G-C1B-O1B	-2.12	118.76	123.70
29	M	314	CLA	CHB-C4A-NA	2.12	127.45	124.40
29	T	308	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
36	K	202	DD6	C32-C33-C34	-2.12	108.95	113.59
36	M	303	DD6	O1-C20-C15	-2.12	57.25	58.93
38	J	304	UIX	C41-C40-C38	2.12	121.32	118.09
36	P	204	DD6	C34-C35-C36	-2.11	106.92	112.18
37	C	305	PID	CM4-C14-C13	2.11	123.71	119.05
32	l	507	BCR	C4-C5-C6	-2.11	119.85	122.70
36	I	206	DD6	C28-C27-C26	-2.11	120.08	124.18
36	I	205	DD6	C-C1-C2	-2.11	119.39	122.82
38	P	207	UIX	C12-C11-C13	-2.11	119.39	122.82
29	a	819	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
36	A	201	DD6	O1-C15-C14	-2.11	110.83	116.88
29	A	217	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
29	b	702	CLA	C1-C2-C3	-2.11	122.74	126.20
39	H	314	KC1	O2D-CGD-O1D	-2.11	119.74	123.85
36	A	202	DD6	C28-C27-C26	-2.11	120.09	124.18
29	a	837	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
29	L	307	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
37	F	304	PID	C28-C27-C26	2.11	113.67	109.89
29	i	203	CLA	C1-C2-C3	-2.11	122.75	126.20
29	E	314	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
29	b	723	CLA	CMB-C2B-C3B	2.11	131.50	126.55
38	A	203	UIX	C29-C26-C23	2.11	121.31	118.09
29	C	311	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
29	a	820	CLA	O2A-CGA-O1A	-2.11	118.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	308	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
29	P	210	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
37	Q	303	PID	O1-C6-C7	-2.10	110.85	116.88
37	H	305	PID	CM5-C21-C20	-2.10	119.41	122.82
29	i	201	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
39	N	312	KC1	C1A-C2A-C3A	-2.10	105.35	107.28
29	B	309	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
32	f	804	BCR	C21-C20-C19	-2.10	117.11	123.20
29	b	703	CLA	C3B-C4B-NB	-2.10	108.65	110.53
36	B	302	DD6	C-C1-C24	2.10	121.30	118.09
36	G	307	DD6	C37-C36-C31	-2.10	120.23	124.16
29	L	308	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
29	E	315	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
36	K	205	DD6	C7-C6-C8	2.10	121.30	118.09
29	N	309	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
29	K	211	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
29	O	308	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
29	D	308	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
36	L	303	DD6	C28-C27-C26	-2.10	120.11	124.18
29	a	830	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
38	F	305	UIX	C-C7-C10	-2.10	121.56	125.99
38	B	304	UIX	C35-C36-C38	-2.10	117.12	123.20
29	b	708	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
29	f	805	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
29	H	307	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
36	K	221	DD6	C-C1-C2	-2.10	119.42	122.82
29	M	306	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
36	A	204	DD6	C3-C4-C5	-2.10	119.23	123.52
36	E	302	DD6	C-C1-C24	2.10	121.29	118.09
29	I	217	CLA	C1-C2-C3	-2.10	122.76	126.20
37	h	204	PID	C8-C9-C10	2.10	127.70	123.60
36	L	303	DD6	C21-C20-C15	-2.10	118.85	122.30
36	J	302	DD6	C23-C16-C22	2.09	110.41	107.37
32	f	804	BCR	C38-C26-C27	2.09	118.06	113.60
35	j	106	DGD	O2G-C1B-O1B	-2.09	118.81	123.70
29	A	218	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
36	A	201	DD6	C37-C36-C35	2.09	118.27	114.42
38	A	203	UIX	C41-C40-C38	2.09	121.28	118.09
29	l	502	CLA	O2D-CGD-CBD	2.09	114.89	111.23
38	E	304	UIX	C37-C34-C30	-2.09	119.24	123.52
29	a	829	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
37	O	307	PID	CM4-C14-C13	2.09	123.66	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	807	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
39	Q	311	KC1	CAC-C3C-C4C	2.09	127.51	124.79
29	A	211	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
29	T	314	CLA	O2D-CGD-CBD	2.09	114.88	111.23
38	E	304	UIX	C12-C11-C10	2.09	121.28	118.09
29	b	717	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
29	E	311	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
32	a	834	BCR	C15-C16-C17	-2.09	119.25	123.52
29	b	731	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
29	K	213	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
37	T	302	PID	C28-C27-C26	2.09	113.64	109.89
36	K	204	DD6	C37-C36-C35	2.09	118.26	114.42
29	h	201	CLA	CMB-C2B-C3B	2.09	131.46	126.55
36	P	204	DD6	C4-C3-C2	-2.09	119.25	123.52
39	T	310	KC1	O2D-CGD-O1D	-2.09	119.79	123.85
39	P	211	KC1	O2D-CGD-O1D	-2.09	119.79	123.85
36	K	203	DD6	C25-C26-C27	-2.09	120.78	126.61
29	L	316	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
29	P	209	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
37	Q	306	PID	CM2-C5-C4	-2.08	105.31	108.97
37	G	309	PID	CM4-C14-C13	2.08	123.65	119.05
29	b	703	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	G	316	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	I	211	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
37	C	302	PID	O1-C6-C7	-2.08	110.91	116.88
29	l	504	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
34	b	732	LMG	O3-C3-C2	-2.08	105.47	110.38
32	b	729	BCR	C33-C5-C4	2.08	118.03	113.60
36	I	203	DD6	C9-C8-C6	-2.08	120.66	126.36
29	E	311	CLA	O2D-CGD-CBD	2.08	114.87	111.23
36	B	303	DD6	C12-C11-C13	2.08	121.27	118.09
32	f	801	BCR	C11-C12-C13	-2.08	120.66	126.36
29	Q	308	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
37	F	306	PID	C8-C9-C10	2.08	127.67	123.60
36	A	202	DD6	C10-C9-C8	-2.08	117.17	123.20
29	H	313	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
37	N	307	PID	CM3-C5-C4	-2.08	105.31	108.97
29	b	716	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
37	E	301	PID	CM3-C5-C4	-2.08	105.31	108.97
36	G	308	DD6	C28-C27-C26	-2.08	120.14	124.18
39	M	305	KC1	C1A-C2A-C3A	-2.08	105.37	107.28
29	I	209	CLA	O2A-CGA-O1A	-2.08	118.43	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	812	CLA	C1-C2-C3	-2.08	122.79	126.20
32	b	729	BCR	C35-C13-C12	2.08	121.26	118.09
29	a	803	CLA	CMB-C2B-C3B	2.08	131.44	126.55
38	C	306	UIX	C3-C5-C4	-2.08	106.91	110.79
34	P	201	LMG	O1-C7-C8	-2.08	105.77	110.82
39	T	315	KC1	O2D-CGD-O1D	-2.08	119.81	123.85
29	a	824	CLA	C1-C2-C3	-2.08	122.79	126.20
29	l	501	CLA	C1-C2-C3	-2.08	122.79	126.20
29	i	203	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
32	a	835	BCR	C20-C19-C18	-2.08	120.67	126.36
29	i	203	CLA	O2D-CGD-CBD	2.08	114.86	111.23
29	a	802	CLA	CHB-C1B-NB	2.08	127.16	124.05
29	a	831	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
29	N	313	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
36	O	303	DD6	C37-C36-C31	-2.07	120.28	124.16
39	G	318	KC1	C2A-C3A-C4A	2.07	107.97	106.41
37	O	301	PID	C17-C18-C19	2.07	129.52	124.72
36	G	308	DD6	C37-C36-C35	2.07	118.23	114.42
37	D	306	PID	O4-C12-C13	2.07	127.31	122.89
36	E	303	DD6	C21-C20-C15	-2.07	118.89	122.30
36	L	305	DD6	C25-C24-C1	-2.07	120.69	126.36
36	A	201	DD6	C3-C4-C5	-2.07	119.28	123.52
29	C	314	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
36	K	203	DD6	C28-C27-C26	-2.07	120.16	124.18
36	m	101	DD6	C10-C9-C8	-2.07	117.20	123.20
32	a	838	BCR	C33-C5-C4	2.07	118.01	113.60
32	f	801	BCR	C19-C18-C17	2.07	122.26	119.01
29	b	709	CLA	C1-C2-C3	-2.07	122.81	126.20
29	l	502	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
32	l	507	BCR	C11-C12-C13	-2.07	120.69	126.36
39	H	311	KC1	C2A-C3A-C4A	2.07	107.96	106.41
29	A	208	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
29	G	301	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
29	B	310	CLA	C1-C2-C3	-2.07	122.81	126.20
36	I	204	DD6	C28-C27-C26	-2.07	120.17	124.18
29	F	307	CLA	O2D-CGD-CBD	2.06	114.84	111.23
36	I	205	DD6	C12-C11-C10	-2.06	119.47	122.82
29	B	308	CLA	O2D-CGD-CBD	2.06	114.84	111.23
32	b	729	BCR	C16-C15-C14	-2.06	119.30	123.52
29	b	703	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
29	T	309	CLA	O2A-CGA-O1A	-2.06	117.04	123.20
29	T	314	CLA	O2A-CGA-O1A	-2.06	118.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	207	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
29	K	210	CLA	CMB-C2B-C3B	2.06	131.40	126.55
37	E	301	PID	CM5-C21-C22	-2.06	114.37	118.94
36	L	304	DD6	C25-C26-C27	-2.06	120.85	126.61
38	C	306	UIX	C21-C15-C20	-2.06	108.63	110.47
29	a	802	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
39	O	312	KC1	CAC-C3C-C4C	2.06	127.47	124.79
29	b	724	CLA	O2D-CGD-CBD	2.06	114.83	111.23
29	L	312	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
29	b	709	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
36	A	204	DD6	C14-C13-C11	-2.06	122.34	125.53
36	I	206	DD6	C25-C26-C27	-2.06	120.86	126.61
36	B	302	DD6	C3-C4-C5	-2.06	119.31	123.52
37	Q	304	PID	C8-C9-C10	2.05	127.62	123.60
36	M	301	DD6	C25-C26-C27	-2.05	120.87	126.61
35	j	105	DGD	O6D-C5D-C6D	2.05	110.77	106.69
29	b	721	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
35	h	203	DGD	O2G-C1B-O1B	-2.05	118.91	123.70
29	a	829	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
29	h	201	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
29	M	307	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
36	L	303	DD6	C25-C24-C1	-2.05	120.74	126.36
29	a	824	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
29	K	207	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
36	K	203	DD6	C4-C3-C2	-2.05	119.33	123.52
29	B	310	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
29	B	312	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
29	b	726	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
37	T	305	PID	C26-C25-C24	2.05	111.20	109.21
29	b	718	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
38	T	306	UIX	C33-C32-C35	-2.05	119.50	122.82
34	K	220	LMG	O7-C10-O9	-2.05	118.92	123.70
39	E	307	KC1	O2D-CGD-O1D	-2.05	119.86	123.85
29	T	314	CLA	CMB-C2B-C3B	2.05	131.36	126.55
34	K	201	LMG	O7-C10-O9	-2.05	118.92	123.70
29	a	831	CLA	C1-C2-C3	-2.05	122.85	126.20
36	K	204	DD6	C21-C20-C19	2.04	116.54	114.24
29	T	314	CLA	CED-O2D-CGD	2.04	120.55	115.92
29	M	306	CLA	C1-C2-C3	-2.04	122.85	126.20
29	H	312	CLA	CMB-C2B-C3B	2.04	131.36	126.55
29	G	317	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
36	L	303	DD6	C3-C4-C5	-2.04	119.34	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	I	215	KC1	O2A-CGA-O1A	-2.04	118.54	122.70
32	b	735	BCR	C37-C22-C21	-2.04	119.51	122.82
36	H	303	DD6	O1-C20-C21	-2.04	112.77	115.05
39	N	312	KC1	O2D-CGD-O1D	-2.04	119.87	123.85
36	G	308	DD6	C9-C8-C6	-2.04	120.77	126.36
34	A	219	LMG	O7-C10-O9	-2.04	118.93	123.70
32	a	835	BCR	C10-C11-C12	-2.04	117.29	123.20
29	b	714	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
37	P	205	PID	C15-C14-C13	2.04	122.05	116.80
36	M	304	DD6	C19-C18-C17	2.04	114.60	110.79
36	G	307	DD6	C28-C27-C26	-2.04	120.22	124.18
36	M	302	DD6	C25-C26-C27	-2.04	120.91	126.61
29	a	813	CLA	C1-C2-C3	-2.04	122.86	126.20
36	B	305	DD6	C14-C13-C11	-2.04	122.37	125.53
29	B	306	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
30	a	832	PQN	C2M-C2-C1	2.04	120.43	116.68
29	L	309	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
36	G	305	DD6	C7-C6-C5	-2.04	119.52	122.82
29	a	811	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
36	I	204	DD6	C25-C26-C27	-2.04	120.92	126.61
35	b	733	DGD	O6D-C5D-C4D	-2.04	106.03	109.70
36	E	302	DD6	C34-C35-C36	-2.04	107.11	112.18
29	A	218	CLA	C1-C2-C3	-2.03	122.86	126.20
32	l	507	BCR	C38-C26-C27	2.03	117.93	113.60
38	B	304	UIX	C37-C34-C30	-2.03	119.36	123.52
29	a	806	CLA	C1-C2-C3	-2.03	122.86	126.20
36	I	206	DD6	C26-C25-C24	-2.03	117.31	123.20
29	B	311	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
38	T	306	UIX	C10-C11-C13	2.03	122.21	119.01
29	J	308	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
37	C	305	PID	CM5-C21-C22	-2.03	114.42	118.94
29	a	813	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
29	b	719	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
29	O	314	CLA	CHB-C1B-NB	2.03	127.10	124.05
35	j	103	DGD	O1G-C1A-O1A	-2.03	118.54	123.63
36	I	206	DD6	C4-C3-C2	-2.03	119.36	123.52
29	b	718	CLA	CMB-C2B-C3B	2.03	131.33	126.55
29	a	815	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
29	L	310	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
29	b	702	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
29	A	211	CLA	C1-C2-C3	-2.03	122.87	126.20
29	b	713	CLA	O2A-CGA-O1A	-2.03	118.55	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	K	204	DD6	C25-C26-C27	-2.03	120.94	126.61
29	A	217	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
38	C	306	UIX	C10-C11-C13	2.03	122.20	119.01
39	O	315	KC1	O2A-CGA-O1A	-2.03	118.57	122.70
37	O	304	PID	C15-C14-C13	2.03	122.01	116.80
29	l	504	CLA	O1D-CGD-CBD	2.03	128.51	124.52
29	I	207	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
29	O	309	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
36	C	303	DD6	C25-C24-C1	-2.03	120.81	126.36
36	B	319	DD6	C26-C25-C24	-2.03	117.33	123.20
37	F	306	PID	C6-C7-C8	-2.02	121.71	125.99
32	b	729	BCR	C37-C22-C23	2.02	121.18	118.09
36	P	204	DD6	C37-C36-C31	-2.02	120.37	124.16
32	b	735	BCR	C31-C1-C6	-2.02	107.07	110.24
39	C	312	KC1	C1A-C2A-C3A	-2.02	105.42	107.28
29	b	716	CLA	C3B-C4B-NB	-2.02	108.72	110.53
32	a	838	BCR	C15-C16-C17	-2.02	119.38	123.52
36	D	304	DD6	C28-C27-C26	-2.02	120.25	124.18
39	Q	311	KC1	O2A-CGA-O1A	-2.02	118.58	122.70
29	H	308	CLA	O2D-CGD-CBD	2.02	114.77	111.23
29	M	310	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
29	N	311	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
29	a	837	CLA	C1-C2-C3	-2.02	122.88	126.20
29	a	822	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
36	B	301	DD6	C25-C24-C1	-2.02	120.82	126.36
35	B	318	DGD	C3E-C4E-C5E	2.02	113.90	110.23
36	F	301	DD6	C12-C11-C10	-2.02	119.54	122.82
38	Q	305	UIX	C36-C38-C40	-2.02	120.82	126.36
36	B	302	DD6	C10-C9-C8	-2.02	117.35	123.20
29	b	713	CLA	C1-C2-C3	-2.02	122.89	126.20
29	A	215	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
35	h	203	DGD	O1G-C1A-O1A	-2.02	118.58	123.63
29	G	317	CLA	C1-C2-C3	-2.02	122.89	126.20
29	I	216	CLA	O2D-CGD-CBD	2.02	114.76	111.23
36	I	202	DD6	C14-C13-C11	-2.02	122.40	125.53
39	K	215	KC1	CAA-CBA-CGA	-2.02	116.78	127.05
36	B	303	DD6	O1-C20-C19	-2.02	111.60	113.49
37	D	307	PID	C17-C18-C19	2.02	129.38	124.72
36	B	303	DD6	C37-C36-C35	2.02	118.13	114.42
37	F	304	PID	CM1-C1-C6	-2.02	118.98	122.30
32	b	735	BCR	C2-C1-C6	2.02	113.37	110.44
34	E	316	LMG	C1-O6-C5	2.02	117.66	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	l	509	CLA	O2D-CGD-CBD	2.02	114.76	111.23
29	b	704	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
34	j	102	LMG	O1-C7-C8	-2.02	105.91	110.82
36	E	302	DD6	C-C1-C2	-2.01	119.55	122.82
29	N	314	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
39	L	314	KC1	O2D-CGD-O1D	-2.01	119.93	123.85
29	b	704	CLA	CHB-C4A-NA	2.01	127.31	124.40
29	a	805	CLA	C1-C2-C3	-2.01	122.90	126.20
29	M	310	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
29	O	314	CLA	CHB-C4A-NA	2.01	127.30	124.40
36	N	303	DD6	C28-C27-C26	-2.01	120.28	124.18
29	a	809	CLA	O2D-CGD-CBD	2.01	114.75	111.23
37	N	302	PID	O1-C6-C7	-2.01	111.12	116.88
29	l	509	CLA	CMA-C3A-C2A	-2.01	111.62	116.23
29	b	716	CLA	CMB-C2B-C3B	2.01	131.28	126.55
34	P	201	LMG	O1-C1-C2	-2.01	105.22	108.27
36	J	302	DD6	C25-C26-C27	-2.01	120.99	126.61
29	a	826	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
38	T	306	UIX	C21-C15-C20	-2.01	108.67	110.47
37	D	305	PID	CM4-C14-C13	2.01	123.48	119.05
36	h	202	DD6	C25-C24-C1	-2.01	120.86	126.36
36	B	302	DD6	C32-C33-C34	-2.01	109.19	113.59
29	a	803	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
36	m	101	DD6	C12-C11-C13	2.01	121.15	118.09
37	N	305	PID	C8-C9-C10	2.01	127.53	123.60
39	D	310	KC1	O2D-CGD-O1D	-2.01	119.94	123.85
29	O	314	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
36	m	101	DD6	C14-C13-C11	-2.01	122.42	125.53
29	b	716	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
36	K	204	DD6	C28-C27-C26	-2.00	120.29	124.18
36	B	319	DD6	C28-C27-C26	-2.00	120.29	124.18
29	N	314	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
37	E	301	PID	CM4-C14-C13	2.00	123.47	119.05
36	L	301	DD6	O1-C20-C21	-2.00	112.81	115.05
38	L	302	UIX	C7-C10-C11	-2.00	122.42	125.53
37	N	304	PID	C15-C14-C13	2.00	121.95	116.80
29	T	314	CLA	C3B-C4B-NB	-2.00	108.74	110.53

All (220) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	a	801	CLA	ND

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Mol	Chain	Res	Type	Atom
29	a	802	CLA	ND
29	a	803	CLA	ND
29	a	804	CLA	ND
29	a	805	CLA	ND
29	a	806	CLA	ND
29	a	807	CLA	ND
29	a	808	CLA	ND
29	a	809	CLA	ND
29	a	810	CLA	ND
29	a	811	CLA	ND
29	a	812	CLA	ND
29	a	813	CLA	ND
29	a	814	CLA	ND
29	a	815	CLA	ND
29	a	816	CLA	ND
29	a	817	CLA	ND
29	a	818	CLA	ND
29	a	819	CLA	ND
29	a	820	CLA	ND
29	a	821	CLA	ND
29	a	822	CLA	ND
29	a	823	CLA	ND
29	a	824	CLA	ND
29	a	825	CLA	ND
29	a	826	CLA	ND
29	a	827	CLA	ND
29	a	828	CLA	ND
29	a	829	CLA	ND
29	a	830	CLA	ND
29	a	831	CLA	ND
29	a	837	CLA	ND
29	b	701	CLA	ND
29	b	702	CLA	ND
29	b	703	CLA	ND
29	b	704	CLA	ND
29	b	705	CLA	ND
29	b	706	CLA	ND
29	b	707	CLA	ND
29	b	708	CLA	ND
29	b	709	CLA	ND
29	b	710	CLA	ND
29	b	711	CLA	ND

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Mol	Chain	Res	Type	Atom
29	b	712	CLA	ND
29	b	713	CLA	ND
29	b	714	CLA	ND
29	b	715	CLA	ND
29	b	716	CLA	ND
29	b	717	CLA	ND
29	b	718	CLA	ND
29	b	719	CLA	ND
29	b	720	CLA	ND
29	b	721	CLA	ND
29	b	722	CLA	ND
29	b	723	CLA	ND
29	b	724	CLA	ND
29	b	725	CLA	ND
29	b	726	CLA	ND
29	b	731	CLA	ND
29	b	736	CLA	ND
29	f	802	CLA	ND
29	f	803	CLA	ND
29	f	805	CLA	ND
29	h	201	CLA	ND
29	i	201	CLA	ND
29	i	202	CLA	ND
29	i	203	CLA	ND
29	j	104	CLA	ND
29	l	501	CLA	ND
29	l	502	CLA	ND
29	l	503	CLA	ND
29	l	504	CLA	ND
29	l	505	CLA	ND
29	l	508	CLA	ND
29	l	509	CLA	ND
29	l	510	CLA	ND
29	A	206	CLA	ND
29	A	207	CLA	ND
29	A	208	CLA	ND
29	A	209	CLA	ND
29	A	210	CLA	ND
29	A	211	CLA	ND
29	A	212	CLA	ND
29	A	214	CLA	ND
29	A	215	CLA	ND

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Mol	Chain	Res	Type	Atom
29	A	216	CLA	ND
29	A	217	CLA	ND
29	A	218	CLA	ND
29	G	301	CLA	ND
29	G	302	CLA	ND
29	G	304	CLA	ND
29	G	311	CLA	ND
29	G	312	CLA	ND
29	G	313	CLA	ND
29	G	314	CLA	ND
29	G	316	CLA	ND
29	G	317	CLA	ND
29	G	319	CLA	ND
29	I	201	CLA	ND
29	I	207	CLA	ND
29	I	208	CLA	ND
29	I	209	CLA	ND
29	I	210	CLA	ND
29	I	211	CLA	ND
29	I	212	CLA	ND
29	I	213	CLA	ND
29	I	214	CLA	ND
29	I	216	CLA	ND
29	I	217	CLA	ND
29	K	207	CLA	ND
29	K	208	CLA	ND
29	K	209	CLA	ND
29	K	210	CLA	ND
29	K	211	CLA	ND
29	K	212	CLA	ND
29	K	213	CLA	ND
29	K	214	CLA	ND
29	K	216	CLA	ND
29	K	217	CLA	ND
29	K	218	CLA	ND
29	F	307	CLA	ND
29	F	308	CLA	ND
29	F	310	CLA	ND
29	F	311	CLA	ND
29	F	312	CLA	ND
29	F	313	CLA	ND
29	F	315	CLA	ND

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Mol	Chain	Res	Type	Atom
29	F	316	CLA	ND
29	J	305	CLA	ND
29	J	306	CLA	ND
29	J	307	CLA	ND
29	J	308	CLA	ND
29	J	309	CLA	ND
29	J	310	CLA	ND
29	J	311	CLA	ND
29	J	313	CLA	ND
29	M	306	CLA	ND
29	M	307	CLA	ND
29	M	308	CLA	ND
29	M	309	CLA	ND
29	M	310	CLA	ND
29	M	311	CLA	ND
29	M	313	CLA	ND
29	M	314	CLA	ND
29	M	315	CLA	ND
29	L	307	CLA	ND
29	L	308	CLA	ND
29	L	309	CLA	ND
29	L	310	CLA	ND
29	L	311	CLA	ND
29	L	312	CLA	ND
29	L	313	CLA	ND
29	L	315	CLA	ND
29	L	316	CLA	ND
29	L	317	CLA	ND
29	D	308	CLA	ND
29	D	309	CLA	ND
29	D	311	CLA	ND
29	D	312	CLA	ND
29	D	313	CLA	ND
29	D	314	CLA	ND
29	D	316	CLA	ND
29	B	306	CLA	ND
29	B	307	CLA	ND
29	B	308	CLA	ND
29	B	309	CLA	ND
29	B	310	CLA	ND
29	B	311	CLA	ND
29	B	312	CLA	ND

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Mol	Chain	Res	Type	Atom
29	B	314	CLA	ND
29	B	315	CLA	ND
29	B	316	CLA	ND
29	H	307	CLA	ND
29	H	308	CLA	ND
29	H	310	CLA	ND
29	H	312	CLA	ND
29	H	313	CLA	ND
29	H	315	CLA	ND
29	N	308	CLA	ND
29	N	309	CLA	ND
29	N	311	CLA	ND
29	N	313	CLA	ND
29	N	314	CLA	ND
29	N	316	CLA	ND
29	O	308	CLA	ND
29	O	311	CLA	ND
29	O	313	CLA	ND
29	O	316	CLA	ND
29	T	308	CLA	ND
29	T	309	CLA	ND
29	T	311	CLA	ND
29	T	313	CLA	ND
29	T	314	CLA	ND
29	T	316	CLA	ND
29	Q	307	CLA	ND
29	Q	308	CLA	ND
29	Q	310	CLA	ND
29	Q	312	CLA	ND
29	Q	313	CLA	ND
29	Q	315	CLA	ND
29	C	308	CLA	ND
29	C	309	CLA	ND
29	C	311	CLA	ND
29	C	313	CLA	ND
29	C	314	CLA	ND
29	C	316	CLA	ND
29	P	209	CLA	ND
29	P	210	CLA	ND
29	P	212	CLA	ND
29	P	214	CLA	ND
29	P	215	CLA	ND

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Mol	Chain	Res	Type	Atom
29	P	217	CLA	ND
29	E	305	CLA	ND
29	E	306	CLA	ND
29	E	308	CLA	ND
29	E	309	CLA	ND
29	E	310	CLA	ND
29	E	311	CLA	ND
29	E	313	CLA	ND
29	E	315	CLA	ND

All (2645) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	a	801	CLA	CBD-CGD-O2D-CED
29	a	805	CLA	C1A-C2A-CAA-CBA
29	a	805	CLA	C3A-C2A-CAA-CBA
29	a	805	CLA	CBD-CGD-O2D-CED
29	a	807	CLA	C1A-C2A-CAA-CBA
29	a	808	CLA	C2B-C3B-CAB-CBB
29	a	808	CLA	C4B-C3B-CAB-CBB
29	a	809	CLA	C1A-C2A-CAA-CBA
29	a	809	CLA	C3A-C2A-CAA-CBA
29	a	809	CLA	CHA-CBD-CGD-O1D
29	a	809	CLA	CHA-CBD-CGD-O2D
29	a	811	CLA	C1A-C2A-CAA-CBA
29	a	812	CLA	C1A-C2A-CAA-CBA
29	a	813	CLA	C1A-C2A-CAA-CBA
29	a	813	CLA	C3A-C2A-CAA-CBA
29	a	814	CLA	CBA-CGA-O2A-C1
29	a	815	CLA	C1A-C2A-CAA-CBA
29	a	815	CLA	C3A-C2A-CAA-CBA
29	a	815	CLA	CHA-CBD-CGD-O1D
29	a	815	CLA	CHA-CBD-CGD-O2D
29	a	818	CLA	C3A-C2A-CAA-CBA
29	a	819	CLA	C1A-C2A-CAA-CBA
29	a	819	CLA	C3A-C2A-CAA-CBA
29	a	821	CLA	C3A-C2A-CAA-CBA
29	a	821	CLA	CBD-CGD-O2D-CED
29	a	823	CLA	CBD-CGD-O2D-CED
29	a	825	CLA	CHA-CBD-CGD-O1D
29	a	825	CLA	CHA-CBD-CGD-O2D
29	a	825	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	a	826	CLA	C1A-C2A-CAA-CBA
29	a	826	CLA	C3A-C2A-CAA-CBA
29	a	826	CLA	C2B-C3B-CAB-CBB
29	a	826	CLA	C4B-C3B-CAB-CBB
29	a	827	CLA	C2B-C3B-CAB-CBB
29	a	827	CLA	C4B-C3B-CAB-CBB
29	a	828	CLA	CHA-CBD-CGD-O1D
29	a	828	CLA	CHA-CBD-CGD-O2D
29	a	828	CLA	CBD-CGD-O2D-CED
29	a	837	CLA	C1A-C2A-CAA-CBA
29	a	837	CLA	C3A-C2A-CAA-CBA
29	b	704	CLA	C2-C3-C5-C6
29	b	704	CLA	C4-C3-C5-C6
29	b	705	CLA	C1A-C2A-CAA-CBA
29	b	705	CLA	C3A-C2A-CAA-CBA
29	b	705	CLA	CBD-CGD-O2D-CED
29	b	706	CLA	C1A-C2A-CAA-CBA
29	b	707	CLA	CBD-CGD-O2D-CED
29	b	709	CLA	CHA-CBD-CGD-O1D
29	b	709	CLA	CHA-CBD-CGD-O2D
29	b	710	CLA	C1A-C2A-CAA-CBA
29	b	710	CLA	C3A-C2A-CAA-CBA
29	b	712	CLA	C3A-C2A-CAA-CBA
29	b	713	CLA	C3A-C2A-CAA-CBA
29	b	714	CLA	CHA-CBD-CGD-O1D
29	b	714	CLA	CHA-CBD-CGD-O2D
29	b	715	CLA	C1A-C2A-CAA-CBA
29	b	715	CLA	C3A-C2A-CAA-CBA
29	b	715	CLA	CBA-CGA-O2A-C1
29	b	717	CLA	C1A-C2A-CAA-CBA
29	b	719	CLA	C1A-C2A-CAA-CBA
29	b	719	CLA	C3A-C2A-CAA-CBA
29	b	719	CLA	CHA-CBD-CGD-O1D
29	b	719	CLA	CHA-CBD-CGD-O2D
29	b	720	CLA	CBD-CGD-O2D-CED
29	b	721	CLA	C6-C7-C8-C9
29	b	722	CLA	CBD-CGD-O2D-CED
29	b	722	CLA	C2-C3-C5-C6
29	b	722	CLA	C4-C3-C5-C6
29	b	726	CLA	C11-C12-C13-C14
29	b	731	CLA	CBD-CGD-O2D-CED
29	b	736	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	f	805	CLA	C1A-C2A-CAA-CBA
29	h	201	CLA	C1A-C2A-CAA-CBA
29	h	201	CLA	C3A-C2A-CAA-CBA
29	h	201	CLA	C2-C3-C5-C6
29	h	201	CLA	C4-C3-C5-C6
29	i	202	CLA	C6-C7-C8-C9
29	i	203	CLA	CHA-CBD-CGD-O1D
29	i	203	CLA	CHA-CBD-CGD-O2D
29	l	501	CLA	C1A-C2A-CAA-CBA
29	l	501	CLA	C3A-C2A-CAA-CBA
29	l	502	CLA	C4B-C3B-CAB-CBB
29	l	502	CLA	CHA-CBD-CGD-O1D
29	l	502	CLA	CHA-CBD-CGD-O2D
29	l	504	CLA	CBD-CGD-O2D-CED
29	l	510	CLA	C1A-C2A-CAA-CBA
29	A	210	CLA	CBD-CGD-O2D-CED
29	A	214	CLA	CAD-CBD-CGD-O2D
29	A	217	CLA	CBD-CGD-O2D-CED
29	G	302	CLA	C1A-C2A-CAA-CBA
29	G	302	CLA	CHA-CBD-CGD-O1D
29	G	302	CLA	CHA-CBD-CGD-O2D
29	G	304	CLA	C1A-C2A-CAA-CBA
29	G	304	CLA	C3A-C2A-CAA-CBA
29	G	304	CLA	C2B-C3B-CAB-CBB
29	G	304	CLA	C4B-C3B-CAB-CBB
29	G	304	CLA	CBD-CGD-O2D-CED
29	G	304	CLA	O1D-CGD-O2D-CED
29	G	314	CLA	CBD-CGD-O2D-CED
29	G	316	CLA	CBD-CGD-O2D-CED
29	G	317	CLA	CHA-CBD-CGD-O1D
29	G	317	CLA	CHA-CBD-CGD-O2D
29	I	207	CLA	CHA-CBD-CGD-O1D
29	I	207	CLA	CHA-CBD-CGD-O2D
29	I	208	CLA	C1A-C2A-CAA-CBA
29	I	208	CLA	C3A-C2A-CAA-CBA
29	I	208	CLA	CBA-CGA-O2A-C1
29	I	208	CLA	O1A-CGA-O2A-C1
29	I	212	CLA	C1A-C2A-CAA-CBA
29	I	216	CLA	CAD-CBD-CGD-O1D
29	I	216	CLA	CAD-CBD-CGD-O2D
29	I	217	CLA	CHA-CBD-CGD-O1D
29	I	217	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	I	217	CLA	CBD-CGD-O2D-CED
29	K	207	CLA	C1A-C2A-CAA-CBA
29	K	207	CLA	C3A-C2A-CAA-CBA
29	K	209	CLA	O1A-CGA-O2A-C1
29	K	209	CLA	C2-C3-C5-C6
29	K	209	CLA	C4-C3-C5-C6
29	K	212	CLA	C4B-C3B-CAB-CBB
29	K	213	CLA	CBD-CGD-O2D-CED
29	K	214	CLA	C2B-C3B-CAB-CBB
29	K	214	CLA	C4B-C3B-CAB-CBB
29	K	216	CLA	CBD-CGD-O2D-CED
29	K	217	CLA	CBA-CGA-O2A-C1
29	K	218	CLA	C1A-C2A-CAA-CBA
29	K	218	CLA	C3A-C2A-CAA-CBA
29	K	218	CLA	CBD-CGD-O2D-CED
29	F	310	CLA	C1A-C2A-CAA-CBA
29	F	310	CLA	CHA-CBD-CGD-O1D
29	F	310	CLA	CHA-CBD-CGD-O2D
29	F	313	CLA	C1A-C2A-CAA-CBA
29	F	313	CLA	C3A-C2A-CAA-CBA
29	F	313	CLA	CBA-CGA-O2A-C1
29	F	313	CLA	CBD-CGD-O2D-CED
29	F	313	CLA	O1D-CGD-O2D-CED
29	J	305	CLA	CBD-CGD-O2D-CED
29	J	306	CLA	C1A-C2A-CAA-CBA
29	J	306	CLA	C3A-C2A-CAA-CBA
29	J	306	CLA	CBD-CGD-O2D-CED
29	J	306	CLA	C4-C3-C5-C6
29	J	308	CLA	CHA-CBD-CGD-O1D
29	J	308	CLA	CHA-CBD-CGD-O2D
29	J	310	CLA	C1A-C2A-CAA-CBA
29	J	313	CLA	CBD-CGD-O2D-CED
29	M	308	CLA	CHA-CBD-CGD-O1D
29	M	308	CLA	CHA-CBD-CGD-O2D
29	M	309	CLA	CBA-CGA-O2A-C1
29	M	313	CLA	CHA-CBD-CGD-O2D
29	M	315	CLA	C1A-C2A-CAA-CBA
29	M	315	CLA	C3A-C2A-CAA-CBA
29	M	315	CLA	CBD-CGD-O2D-CED
29	M	315	CLA	O1D-CGD-O2D-CED
29	L	307	CLA	C1A-C2A-CAA-CBA
29	L	307	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	L	307	CLA	CBD-CGD-O2D-CED
29	L	311	CLA	C1A-C2A-CAA-CBA
29	L	311	CLA	C3A-C2A-CAA-CBA
29	L	312	CLA	C1A-C2A-CAA-CBA
29	L	312	CLA	C3A-C2A-CAA-CBA
29	L	315	CLA	CBD-CGD-O2D-CED
29	D	308	CLA	CBD-CGD-O2D-CED
29	D	309	CLA	CBD-CGD-O2D-CED
29	D	311	CLA	CBD-CGD-O2D-CED
29	D	312	CLA	CBA-CGA-O2A-C1
29	D	312	CLA	O1A-CGA-O2A-C1
29	D	313	CLA	CBD-CGD-O2D-CED
29	D	314	CLA	CBD-CGD-O2D-CED
29	B	307	CLA	CBD-CGD-O2D-CED
29	B	309	CLA	CHA-CBD-CGD-O1D
29	B	309	CLA	CHA-CBD-CGD-O2D
29	B	310	CLA	C1A-C2A-CAA-CBA
29	B	310	CLA	C3A-C2A-CAA-CBA
29	B	314	CLA	CAD-CBD-CGD-O1D
29	B	314	CLA	CAD-CBD-CGD-O2D
29	H	310	CLA	CBD-CGD-O2D-CED
29	H	310	CLA	C2-C3-C5-C6
29	H	310	CLA	C4-C3-C5-C6
29	H	312	CLA	C1A-C2A-CAA-CBA
29	H	312	CLA	C3A-C2A-CAA-CBA
29	H	312	CLA	CBD-CGD-O2D-CED
29	H	313	CLA	CBD-CGD-O2D-CED
29	H	315	CLA	CBD-CGD-O2D-CED
29	N	313	CLA	C1A-C2A-CAA-CBA
29	N	313	CLA	C3A-C2A-CAA-CBA
29	N	313	CLA	CHA-CBD-CGD-O1D
29	N	314	CLA	CBD-CGD-O2D-CED
29	O	313	CLA	CBD-CGD-O2D-CED
29	O	314	CLA	CBD-CGD-O2D-CED
29	O	314	CLA	O1D-CGD-O2D-CED
29	O	316	CLA	CAD-CBD-CGD-O1D
29	O	316	CLA	CAD-CBD-CGD-O2D
29	T	308	CLA	CBD-CGD-O2D-CED
29	T	311	CLA	CAD-CBD-CGD-O1D
29	T	311	CLA	CAD-CBD-CGD-O2D
29	T	311	CLA	CBD-CGD-O2D-CED
29	T	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	T	314	CLA	CBD-CGD-O2D-CED
29	T	314	CLA	O1D-CGD-O2D-CED
29	T	316	CLA	CAD-CBD-CGD-O1D
29	T	316	CLA	CAD-CBD-CGD-O2D
29	Q	308	CLA	C1A-C2A-CAA-CBA
29	Q	308	CLA	C3A-C2A-CAA-CBA
29	Q	312	CLA	CBA-CGA-O2A-C1
29	Q	313	CLA	C1A-C2A-CAA-CBA
29	Q	315	CLA	CAD-CBD-CGD-O1D
29	Q	315	CLA	CAD-CBD-CGD-O2D
29	C	311	CLA	CAD-CBD-CGD-O1D
29	C	311	CLA	CAD-CBD-CGD-O2D
29	C	311	CLA	CBD-CGD-O2D-CED
29	C	313	CLA	CBA-CGA-O2A-C1
29	C	313	CLA	CBD-CGD-O2D-CED
29	C	314	CLA	CBD-CGD-O2D-CED
29	C	316	CLA	CAD-CBD-CGD-O1D
29	C	316	CLA	CAD-CBD-CGD-O2D
29	P	209	CLA	O1A-CGA-O2A-C1
29	P	214	CLA	C1A-C2A-CAA-CBA
29	P	214	CLA	C3A-C2A-CAA-CBA
29	P	214	CLA	CBD-CGD-O2D-CED
29	P	215	CLA	CBD-CGD-O2D-CED
29	E	305	CLA	CBD-CGD-O2D-CED
29	E	308	CLA	CAD-CBD-CGD-O1D
29	E	308	CLA	CAD-CBD-CGD-O2D
29	E	309	CLA	C1A-C2A-CAA-CBA
29	E	310	CLA	CBD-CGD-O2D-CED
29	E	315	CLA	C1A-C2A-CAA-CBA
29	E	315	CLA	C3A-C2A-CAA-CBA
32	a	838	BCR	C7-C8-C9-C10
32	a	838	BCR	C7-C8-C9-C34
32	i	204	BCR	C21-C22-C23-C24
32	i	204	BCR	C37-C22-C23-C24
32	l	507	BCR	C7-C8-C9-C10
32	l	507	BCR	C7-C8-C9-C34
32	m	103	BCR	C7-C8-C9-C10
32	m	103	BCR	C7-C8-C9-C34
32	m	103	BCR	C21-C22-C23-C24
34	b	734	LMG	O7-C8-C9-O8
34	h	205	LMG	O9-C10-O7-C8
34	A	219	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	A	219	LMG	O9-C10-O7-C8
34	A	219	LMG	C11-C10-O7-C8
34	K	219	LMG	C11-C10-O7-C8
35	b	733	DGD	C2B-C1B-O2G-C2G
35	b	733	DGD	O6D-C1D-O3G-C3G
35	j	103	DGD	C2B-C1B-O2G-C2G
35	j	103	DGD	O6E-C1E-O5D-C6D
36	A	201	DD6	C5-C6-C8-C9
36	A	201	DD6	C7-C6-C8-C9
36	G	305	DD6	C10-C11-C13-C14
36	G	305	DD6	C5-C6-C8-C9
36	G	305	DD6	C7-C6-C8-C9
36	I	202	DD6	C13-C14-C15-O1
36	I	203	DD6	C5-C6-C8-C9
36	I	203	DD6	C7-C6-C8-C9
36	I	205	DD6	C5-C6-C8-C9
36	I	205	DD6	C7-C6-C8-C9
36	I	206	DD6	C13-C14-C15-O1
36	K	202	DD6	C1-C2-C3-C4
36	K	202	DD6	C5-C6-C8-C9
36	K	202	DD6	C7-C6-C8-C9
36	K	203	DD6	C13-C14-C15-O1
36	K	204	DD6	C10-C11-C13-C14
36	K	204	DD6	C12-C11-C13-C14
36	K	204	DD6	C13-C14-C15-C20
36	K	221	DD6	C11-C10-C9-C8
36	K	221	DD6	C5-C6-C8-C9
36	K	221	DD6	C7-C6-C8-C9
36	F	301	DD6	C1-C2-C3-C4
36	F	301	DD6	C24-C25-C26-C27
36	F	301	DD6	C5-C6-C8-C9
36	J	301	DD6	C10-C11-C13-C14
36	J	301	DD6	C12-C11-C13-C14
36	M	301	DD6	C10-C11-C13-C14
36	M	301	DD6	C12-C11-C13-C14
36	M	303	DD6	C7-C6-C8-C9
36	M	304	DD6	C10-C11-C13-C14
36	M	304	DD6	C12-C11-C13-C14
36	L	301	DD6	C13-C14-C15-O1
36	L	305	DD6	C5-C6-C8-C9
36	L	305	DD6	C7-C6-C8-C9
36	D	301	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
36	D	301	DD6	C12-C11-C13-C14
36	D	301	DD6	C5-C6-C8-C9
36	D	301	DD6	C7-C6-C8-C9
36	D	304	DD6	C10-C11-C13-C14
36	D	304	DD6	C12-C11-C13-C14
36	B	319	DD6	C5-C6-C8-C9
36	O	303	DD6	C1-C2-C3-C4
36	T	303	DD6	C13-C14-C15-O1
37	h	204	PID	O7-C30-O6-C27
37	G	303	PID	C13-C14-C15-C16
37	G	303	PID	CM4-C14-C15-C16
37	G	309	PID	O7-C30-O6-C27
37	F	302	PID	O7-C30-O6-C27
37	F	304	PID	C1-C6-C7-C8
37	F	304	PID	C6-C7-C8-C9
37	F	304	PID	C7-C8-C9-C10
37	F	304	PID	C7-C8-C9-C11
37	F	304	PID	O4-C12-C13-C14
37	F	304	PID	C18-C19-C20-C21
37	F	304	PID	C19-C20-C21-C22
37	F	304	PID	C19-C20-C21-CM5
37	F	304	PID	C20-C21-C22-C23
37	D	305	PID	C19-C20-C21-C22
37	D	305	PID	C19-C20-C21-CM5
37	D	305	PID	C20-C21-C22-C23
37	D	305	PID	CM5-C21-C22-C23
37	D	306	PID	O7-C30-O6-C27
37	D	307	PID	O1-C6-C7-C8
37	H	301	PID	O7-C30-O6-C27
37	H	302	PID	O7-C30-O6-C27
37	H	305	PID	O7-C30-O6-C27
37	H	306	PID	C1-C6-C7-C8
37	H	306	PID	O7-C30-O6-C27
37	N	301	PID	O1-C6-C7-C8
37	N	301	PID	O7-C30-O6-C27
37	N	304	PID	O4-C12-C13-C14
37	N	305	PID	C1-C6-C7-C8
37	N	305	PID	O1-C6-C7-C8
37	N	305	PID	C6-C7-C8-C9
37	N	305	PID	C7-C8-C9-C10
37	N	305	PID	C7-C8-C9-C11
37	N	305	PID	O4-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
37	N	305	PID	C13-C14-C15-C16
37	N	305	PID	CM4-C14-C15-C16
37	N	305	PID	C15-C16-C17-C18
37	N	305	PID	C17-C18-C19-C20
37	N	305	PID	C19-C20-C21-C22
37	N	305	PID	C19-C20-C21-CM5
37	N	305	PID	C31-C30-O6-C27
37	N	305	PID	O7-C30-O6-C27
37	N	307	PID	C1-C6-C7-C8
37	N	307	PID	C5-C6-C7-C8
37	N	307	PID	O1-C6-C7-C8
37	N	307	PID	C6-C7-C8-C9
37	O	301	PID	O1-C6-C7-C8
37	O	301	PID	O7-C30-O6-C27
37	O	302	PID	O7-C30-O6-C27
37	O	304	PID	O4-C12-C13-C14
37	O	305	PID	C6-C7-C8-C9
37	O	305	PID	C19-C20-C21-C22
37	O	305	PID	C19-C20-C21-CM5
37	O	305	PID	O7-C30-O6-C27
37	O	307	PID	C1-C6-C7-C8
37	O	307	PID	C5-C6-C7-C8
37	T	301	PID	O1-C6-C7-C8
37	T	301	PID	O4-C12-C13-C14
37	T	304	PID	O1-C6-C7-C8
37	T	307	PID	C7-C8-C9-C11
37	T	307	PID	O7-C30-O6-C27
37	T	317	PID	C1-C6-C7-C8
37	T	317	PID	C7-C8-C9-C10
37	T	317	PID	C7-C8-C9-C11
37	T	317	PID	O4-C12-C13-C14
37	T	317	PID	C31-C30-O6-C27
37	Q	304	PID	O7-C30-O6-C27
37	Q	306	PID	O1-C6-C7-C8
37	C	301	PID	O7-C30-O6-C27
37	C	302	PID	O7-C30-O6-C27
37	C	304	PID	O4-C12-C13-C14
37	C	304	PID	C19-C20-C21-C22
37	C	304	PID	C19-C20-C21-CM5
37	C	305	PID	C1-C6-C7-C8
37	C	305	PID	O1-C6-C7-C8
37	C	305	PID	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	C	305	PID	O7-C30-O6-C27
37	C	307	PID	O7-C30-O6-C27
37	P	202	PID	O1-C6-C7-C8
37	P	202	PID	O7-C30-O6-C27
37	P	203	PID	O7-C30-O6-C27
37	P	206	PID	C19-C20-C21-C22
37	P	206	PID	C19-C20-C21-CM5
37	P	206	PID	O7-C30-O6-C27
37	P	208	PID	O1-C6-C7-C8
37	P	208	PID	O7-C30-O6-C27
37	E	301	PID	O1-C6-C7-C8
37	E	301	PID	C14-C15-C16-C17
37	E	301	PID	C18-C19-C20-C21
37	E	301	PID	C20-C21-C22-C23
38	F	305	UIX	C7-C10-C11-C12
38	F	305	UIX	C14-C23-C26-C29
38	F	305	UIX	C14-C23-C26-C30
38	F	305	UIX	C31-C27-O2-C18
38	F	305	UIX	C25-C28-C32-C33
38	F	305	UIX	C25-C28-C32-C35
38	F	305	UIX	C36-C38-C40-C39
38	J	304	UIX	C11-C13-C14-C23
38	J	304	UIX	C14-C23-C26-C29
38	J	304	UIX	C14-C23-C26-C30
38	L	302	UIX	C31-C27-O2-C18
38	B	304	UIX	O4-C27-O2-C18
38	N	306	UIX	C31-C27-O2-C18
38	N	306	UIX	C36-C38-C40-C39
38	N	306	UIX	C36-C38-C40-C41
38	O	306	UIX	C31-C27-O2-C18
38	O	306	UIX	C25-C28-C32-C33
38	O	306	UIX	C25-C28-C32-C35
38	T	306	UIX	C31-C27-O2-C18
38	Q	305	UIX	C25-C28-C32-C33
38	Q	305	UIX	C25-C28-C32-C35
38	C	306	UIX	C25-C28-C32-C33
38	C	306	UIX	C25-C28-C32-C35
38	C	306	UIX	C36-C38-C40-C39
39	A	205	KC1	C2B-C3B-CAB-CBB
39	A	205	KC1	C4B-C3B-CAB-CBB
39	A	205	KC1	CHA-CBD-CGD-O2D
39	A	213	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	A	213	KC1	C2A-CAA-CBA-CGA
39	G	315	KC1	C1A-C2A-CAA-CBA
39	G	315	KC1	C2B-C3B-CAB-CBB
39	G	318	KC1	C2B-C3B-CAB-CBB
39	G	318	KC1	C2A-CAA-CBA-CGA
39	I	215	KC1	C2B-C3B-CAB-CBB
39	I	215	KC1	C2A-CAA-CBA-CGA
39	I	215	KC1	CHA-CBD-CGD-O1D
39	I	215	KC1	CHA-CBD-CGD-O2D
39	I	215	KC1	CBD-CGD-O2D-CED
39	K	215	KC1	C1A-C2A-CAA-CBA
39	K	215	KC1	CHA-CBD-CGD-O1D
39	K	215	KC1	CHA-CBD-CGD-O2D
39	F	309	KC1	C3A-C2A-CAA-CBA
39	F	309	KC1	C2B-C3B-CAB-CBB
39	F	309	KC1	CHA-CBD-CGD-O1D
39	F	309	KC1	CHA-CBD-CGD-O2D
39	F	314	KC1	C1A-C2A-CAA-CBA
39	F	314	KC1	C2B-C3B-CAB-CBB
39	F	314	KC1	CBD-CGD-O2D-CED
39	F	314	KC1	O1D-CGD-O2D-CED
39	J	312	KC1	C2B-C3B-CAB-CBB
39	J	312	KC1	C4B-C3B-CAB-CBB
39	J	312	KC1	C2A-CAA-CBA-CGA
39	M	305	KC1	C2B-C3B-CAB-CBB
39	M	305	KC1	C4B-C3B-CAB-CBB
39	M	312	KC1	C3A-C2A-CAA-CBA
39	M	312	KC1	C2B-C3B-CAB-CBB
39	M	312	KC1	CBD-CGD-O2D-CED
39	M	312	KC1	O1D-CGD-O2D-CED
39	L	306	KC1	C2B-C3B-CAB-CBB
39	L	314	KC1	C3A-C2A-CAA-CBA
39	L	314	KC1	CBD-CGD-O2D-CED
39	L	314	KC1	O1D-CGD-O2D-CED
39	D	310	KC1	C3A-C2A-CAA-CBA
39	D	310	KC1	C2B-C3B-CAB-CBB
39	D	315	KC1	C3A-C2A-CAA-CBA
39	D	315	KC1	C2B-C3B-CAB-CBB
39	D	315	KC1	C4B-C3B-CAB-CBB
39	D	315	KC1	CBD-CGD-O2D-CED
39	D	315	KC1	O1D-CGD-O2D-CED
39	B	313	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	B	313	KC1	C2A-CAA-CBA-CGA
39	B	313	KC1	CBD-CGD-O2D-CED
39	H	309	KC1	C1A-C2A-CAA-CBA
39	H	309	KC1	C2B-C3B-CAB-CBB
39	H	311	KC1	C2B-C3B-CAB-CBB
39	H	311	KC1	C4B-C3B-CAB-CBB
39	H	311	KC1	CHA-CBD-CGD-O2D
39	H	311	KC1	CBD-CGD-O2D-CED
39	H	314	KC1	C3A-C2A-CAA-CBA
39	H	314	KC1	CBD-CGD-O2D-CED
39	H	314	KC1	O1D-CGD-O2D-CED
39	N	310	KC1	C3A-C2A-CAA-CBA
39	N	310	KC1	C2B-C3B-CAB-CBB
39	N	312	KC1	C2B-C3B-CAB-CBB
39	N	312	KC1	C4B-C3B-CAB-CBB
39	N	312	KC1	CHA-CBD-CGD-O1D
39	N	312	KC1	CHA-CBD-CGD-O2D
39	N	312	KC1	CBD-CGD-O2D-CED
39	N	315	KC1	C3A-C2A-CAA-CBA
39	N	315	KC1	CBD-CGD-O2D-CED
39	N	315	KC1	O1D-CGD-O2D-CED
39	O	310	KC1	C3A-C2A-CAA-CBA
39	O	312	KC1	C2B-C3B-CAB-CBB
39	O	315	KC1	C1A-C2A-CAA-CBA
39	O	315	KC1	C3A-C2A-CAA-CBA
39	O	315	KC1	C2A-CAA-CBA-CGA
39	T	310	KC1	C1A-C2A-CAA-CBA
39	T	310	KC1	C3A-C2A-CAA-CBA
39	T	310	KC1	C2B-C3B-CAB-CBB
39	T	310	KC1	CHA-CBD-CGD-O1D
39	T	312	KC1	C1A-C2A-CAA-CBA
39	T	312	KC1	C2B-C3B-CAB-CBB
39	T	312	KC1	C4B-C3B-CAB-CBB
39	T	315	KC1	C1A-C2A-CAA-CBA
39	T	315	KC1	C3A-C2A-CAA-CBA
39	Q	309	KC1	C1A-C2A-CAA-CBA
39	Q	309	KC1	C3A-C2A-CAA-CBA
39	Q	309	KC1	C2B-C3B-CAB-CBB
39	Q	309	KC1	C4B-C3B-CAB-CBB
39	Q	311	KC1	C2B-C3B-CAB-CBB
39	Q	311	KC1	C4B-C3B-CAB-CBB
39	Q	314	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	Q	314	KC1	CBD-CGD-O2D-CED
39	Q	314	KC1	O1D-CGD-O2D-CED
39	C	310	KC1	C3A-C2A-CAA-CBA
39	C	310	KC1	C2B-C3B-CAB-CBB
39	C	312	KC1	C2B-C3B-CAB-CBB
39	C	312	KC1	CHA-CBD-CGD-O1D
39	C	312	KC1	CHA-CBD-CGD-O2D
39	C	315	KC1	C1A-C2A-CAA-CBA
39	C	315	KC1	C3A-C2A-CAA-CBA
39	C	315	KC1	CBD-CGD-O2D-CED
39	P	211	KC1	C1A-C2A-CAA-CBA
39	P	211	KC1	C3A-C2A-CAA-CBA
39	P	211	KC1	C2A-CAA-CBA-CGA
39	P	211	KC1	CHA-CBD-CGD-O2D
39	P	213	KC1	C2B-C3B-CAB-CBB
39	P	213	KC1	CHA-CBD-CGD-O1D
39	P	213	KC1	CHA-CBD-CGD-O2D
39	P	216	KC1	C1A-C2A-CAA-CBA
39	P	216	KC1	C3A-C2A-CAA-CBA
39	P	216	KC1	C2A-CAA-CBA-CGA
39	E	307	KC1	C3A-C2A-CAA-CBA
39	E	307	KC1	C2B-C3B-CAB-CBB
39	E	312	KC1	C1A-C2A-CAA-CBA
39	E	312	KC1	C2B-C3B-CAB-CBB
40	B	317	SQD	O5-C1-O6-C44
29	b	731	CLA	O1D-CGD-O2D-CED
29	b	736	CLA	O1D-CGD-O2D-CED
29	A	217	CLA	O1D-CGD-O2D-CED
29	G	311	CLA	O1D-CGD-O2D-CED
29	G	316	CLA	O1D-CGD-O2D-CED
29	M	308	CLA	O1D-CGD-O2D-CED
29	L	307	CLA	O1D-CGD-O2D-CED
29	L	315	CLA	O1D-CGD-O2D-CED
29	D	309	CLA	O1D-CGD-O2D-CED
29	D	313	CLA	O1D-CGD-O2D-CED
29	D	316	CLA	O1D-CGD-O2D-CED
29	N	314	CLA	O1D-CGD-O2D-CED
29	O	316	CLA	O1D-CGD-O2D-CED
29	T	313	CLA	O1D-CGD-O2D-CED
29	E	310	CLA	O1D-CGD-O2D-CED
39	C	315	KC1	O1D-CGD-O2D-CED
37	j	101	PID	C31-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
37	G	309	PID	C31-C30-O6-C27
37	F	302	PID	C31-C30-O6-C27
37	F	304	PID	C31-C30-O6-C27
37	H	305	PID	C31-C30-O6-C27
37	O	301	PID	C31-C30-O6-C27
37	O	302	PID	C31-C30-O6-C27
37	O	305	PID	C31-C30-O6-C27
37	Q	304	PID	C31-C30-O6-C27
37	C	302	PID	C31-C30-O6-C27
37	C	305	PID	C31-C30-O6-C27
37	P	203	PID	C31-C30-O6-C27
37	P	206	PID	C31-C30-O6-C27
37	P	208	PID	C31-C30-O6-C27
38	C	306	UIX	C31-C27-O2-C18
38	P	207	UIX	C31-C27-O2-C18
29	a	801	CLA	O1D-CGD-O2D-CED
29	a	803	CLA	O1D-CGD-O2D-CED
29	a	812	CLA	O1D-CGD-O2D-CED
29	a	817	CLA	O1D-CGD-O2D-CED
29	a	830	CLA	O1D-CGD-O2D-CED
29	a	831	CLA	O1D-CGD-O2D-CED
29	b	708	CLA	O1D-CGD-O2D-CED
29	A	210	CLA	O1D-CGD-O2D-CED
29	I	208	CLA	O1D-CGD-O2D-CED
29	I	212	CLA	O1D-CGD-O2D-CED
29	F	312	CLA	O1D-CGD-O2D-CED
29	L	310	CLA	O1D-CGD-O2D-CED
29	H	312	CLA	O1D-CGD-O2D-CED
29	N	313	CLA	O1D-CGD-O2D-CED
29	N	316	CLA	O1D-CGD-O2D-CED
29	Q	310	CLA	O1D-CGD-O2D-CED
29	Q	315	CLA	O1D-CGD-O2D-CED
29	C	313	CLA	O1D-CGD-O2D-CED
29	C	316	CLA	O1D-CGD-O2D-CED
29	P	214	CLA	O1D-CGD-O2D-CED
29	P	215	CLA	O1D-CGD-O2D-CED
29	E	305	CLA	O1D-CGD-O2D-CED
39	I	215	KC1	O1D-CGD-O2D-CED
39	B	313	KC1	O1D-CGD-O2D-CED
37	H	301	PID	C31-C30-O6-C27
37	N	301	PID	C31-C30-O6-C27
37	T	317	PID	O7-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
37	C	301	PID	C31-C30-O6-C27
38	A	203	UIX	C31-C27-O2-C18
38	F	305	UIX	O4-C27-O2-C18
38	L	302	UIX	O4-C27-O2-C18
38	T	306	UIX	O4-C27-O2-C18
38	Q	305	UIX	C31-C27-O2-C18
29	a	803	CLA	CBD-CGD-O2D-CED
29	a	812	CLA	CBD-CGD-O2D-CED
29	a	813	CLA	CBD-CGD-O2D-CED
29	a	817	CLA	CBD-CGD-O2D-CED
29	a	819	CLA	CBD-CGD-O2D-CED
29	a	820	CLA	CBD-CGD-O2D-CED
29	a	830	CLA	CBD-CGD-O2D-CED
29	a	831	CLA	CBD-CGD-O2D-CED
29	b	702	CLA	CBD-CGD-O2D-CED
29	b	704	CLA	CBD-CGD-O2D-CED
29	b	708	CLA	CBD-CGD-O2D-CED
29	b	719	CLA	CBD-CGD-O2D-CED
29	f	802	CLA	CBD-CGD-O2D-CED
29	l	502	CLA	CBD-CGD-O2D-CED
29	A	212	CLA	CBD-CGD-O2D-CED
29	G	311	CLA	CBD-CGD-O2D-CED
29	I	201	CLA	CBD-CGD-O2D-CED
29	I	208	CLA	CBD-CGD-O2D-CED
29	I	210	CLA	CBD-CGD-O2D-CED
29	I	212	CLA	CBD-CGD-O2D-CED
29	I	216	CLA	CBD-CGD-O2D-CED
29	F	310	CLA	CBD-CGD-O2D-CED
29	F	312	CLA	CBD-CGD-O2D-CED
29	M	306	CLA	CBD-CGD-O2D-CED
29	M	308	CLA	CBD-CGD-O2D-CED
29	L	310	CLA	CBD-CGD-O2D-CED
29	L	312	CLA	CBD-CGD-O2D-CED
29	D	316	CLA	CBD-CGD-O2D-CED
29	B	316	CLA	CBD-CGD-O2D-CED
29	N	309	CLA	CBD-CGD-O2D-CED
29	N	311	CLA	CBD-CGD-O2D-CED
29	N	313	CLA	CBD-CGD-O2D-CED
29	N	316	CLA	CBD-CGD-O2D-CED
29	O	316	CLA	CBD-CGD-O2D-CED
29	T	309	CLA	CBD-CGD-O2D-CED
29	Q	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	Q	315	CLA	CBD-CGD-O2D-CED
29	C	316	CLA	CBD-CGD-O2D-CED
29	P	209	CLA	CBD-CGD-O2D-CED
29	E	306	CLA	CBD-CGD-O2D-CED
39	O	315	KC1	CBD-CGD-O2D-CED
29	a	806	CLA	O1A-CGA-O2A-C1
29	a	813	CLA	O1A-CGA-O2A-C1
29	b	707	CLA	O1A-CGA-O2A-C1
29	b	709	CLA	O1A-CGA-O2A-C1
29	f	805	CLA	O1A-CGA-O2A-C1
29	I	209	CLA	O1A-CGA-O2A-C1
29	I	213	CLA	O1A-CGA-O2A-C1
29	J	310	CLA	O1A-CGA-O2A-C1
29	Q	313	CLA	O1A-CGA-O2A-C1
29	a	814	CLA	O1A-CGA-O2A-C1
29	a	816	CLA	O1A-CGA-O2A-C1
29	b	715	CLA	O1A-CGA-O2A-C1
29	K	217	CLA	O1A-CGA-O2A-C1
29	F	313	CLA	O1A-CGA-O2A-C1
29	M	309	CLA	O1A-CGA-O2A-C1
29	Q	312	CLA	O1A-CGA-O2A-C1
29	a	823	CLA	O1D-CGD-O2D-CED
29	l	504	CLA	O1D-CGD-O2D-CED
29	D	314	CLA	O1D-CGD-O2D-CED
37	h	204	PID	C31-C30-O6-C27
37	D	306	PID	C31-C30-O6-C27
37	H	302	PID	C31-C30-O6-C27
37	H	306	PID	C31-C30-O6-C27
37	T	307	PID	C31-C30-O6-C27
37	C	307	PID	C31-C30-O6-C27
37	P	202	PID	C31-C30-O6-C27
38	B	304	UIX	C31-C27-O2-C18
37	D	303	PID	C26-C27-O6-C30
37	N	305	PID	C26-C27-O6-C30
37	T	302	PID	C26-C27-O6-C30
29	a	816	CLA	CBA-CGA-O2A-C1
29	J	309	CLA	CBA-CGA-O2A-C1
29	L	317	CLA	CBA-CGA-O2A-C1
29	a	813	CLA	O1D-CGD-O2D-CED
29	b	702	CLA	O1D-CGD-O2D-CED
29	b	704	CLA	O1D-CGD-O2D-CED
29	l	502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	I	209	CLA	O1D-CGD-O2D-CED
29	I	210	CLA	O1D-CGD-O2D-CED
29	L	308	CLA	O1D-CGD-O2D-CED
29	B	316	CLA	O1D-CGD-O2D-CED
29	H	313	CLA	O1D-CGD-O2D-CED
29	N	309	CLA	O1D-CGD-O2D-CED
29	N	311	CLA	O1D-CGD-O2D-CED
29	C	314	CLA	O1D-CGD-O2D-CED
29	a	806	CLA	CBA-CGA-O2A-C1
29	b	707	CLA	CBA-CGA-O2A-C1
29	b	709	CLA	CBA-CGA-O2A-C1
29	f	805	CLA	CBA-CGA-O2A-C1
29	I	209	CLA	CBA-CGA-O2A-C1
29	J	310	CLA	CBA-CGA-O2A-C1
29	Q	313	CLA	CBA-CGA-O2A-C1
34	K	219	LMG	C29-C28-O8-C9
37	N	307	PID	C31-C30-O6-C27
37	N	307	PID	O7-C30-O6-C27
38	N	306	UIX	O4-C27-O2-C18
38	O	306	UIX	O4-C27-O2-C18
29	b	702	CLA	O1A-CGA-O2A-C1
29	l	504	CLA	O1A-CGA-O2A-C1
29	M	310	CLA	O1A-CGA-O2A-C1
29	D	314	CLA	O1A-CGA-O2A-C1
29	B	306	CLA	O1A-CGA-O2A-C1
29	N	308	CLA	O1A-CGA-O2A-C1
29	N	314	CLA	O1A-CGA-O2A-C1
29	O	308	CLA	O1A-CGA-O2A-C1
29	T	314	CLA	O1A-CGA-O2A-C1
29	C	308	CLA	O1A-CGA-O2A-C1
29	C	314	CLA	O1A-CGA-O2A-C1
29	P	215	CLA	O1A-CGA-O2A-C1
29	E	305	CLA	O1A-CGA-O2A-C1
34	b	732	LMG	O10-C28-O8-C9
34	K	219	LMG	O10-C28-O8-C9
34	E	316	LMG	O10-C28-O8-C9
35	j	106	DGD	O1A-C1A-O1G-C1G
29	C	313	CLA	O1A-CGA-O2A-C1
29	b	705	CLA	O1D-CGD-O2D-CED
29	I	217	CLA	O1D-CGD-O2D-CED
29	K	213	CLA	O1D-CGD-O2D-CED
29	B	307	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	A	213	KC1	CAA-CBA-CGA-O2A
29	a	805	CLA	O1D-CGD-O2D-CED
29	a	828	CLA	O1D-CGD-O2D-CED
29	b	707	CLA	O1D-CGD-O2D-CED
29	b	722	CLA	O1D-CGD-O2D-CED
29	G	314	CLA	O1D-CGD-O2D-CED
29	K	216	CLA	O1D-CGD-O2D-CED
29	K	218	CLA	O1D-CGD-O2D-CED
29	J	305	CLA	O1D-CGD-O2D-CED
29	J	306	CLA	O1D-CGD-O2D-CED
29	D	308	CLA	O1D-CGD-O2D-CED
29	D	311	CLA	O1D-CGD-O2D-CED
29	H	310	CLA	O1D-CGD-O2D-CED
29	H	315	CLA	O1D-CGD-O2D-CED
29	O	313	CLA	O1D-CGD-O2D-CED
29	T	311	CLA	O1D-CGD-O2D-CED
29	a	827	CLA	CBD-CGD-O2D-CED
34	P	201	LMG	O9-C10-O7-C8
35	b	733	DGD	O1B-C1B-O2G-C2G
35	j	103	DGD	O1B-C1B-O2G-C2G
29	f	803	CLA	O1A-CGA-O2A-C1
29	T	313	CLA	O1A-CGA-O2A-C1
29	P	214	CLA	O1A-CGA-O2A-C1
29	a	829	CLA	C3-C5-C6-C7
29	b	703	CLA	C3-C5-C6-C7
29	b	706	CLA	C3-C5-C6-C7
29	b	711	CLA	C3-C5-C6-C7
29	b	713	CLA	C3-C5-C6-C7
29	b	716	CLA	C3-C5-C6-C7
29	b	717	CLA	C3-C5-C6-C7
29	f	805	CLA	C3-C5-C6-C7
29	i	201	CLA	C3-C5-C6-C7
29	A	211	CLA	C3-C5-C6-C7
29	A	212	CLA	C3-C5-C6-C7
29	A	218	CLA	C3-C5-C6-C7
29	G	317	CLA	C3-C5-C6-C7
29	I	210	CLA	C3-C5-C6-C7
29	I	213	CLA	C3-C5-C6-C7
29	J	311	CLA	C3-C5-C6-C7
29	L	312	CLA	C3-C5-C6-C7
29	B	309	CLA	C3-C5-C6-C7
29	a	821	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	b	720	CLA	O1D-CGD-O2D-CED
29	J	313	CLA	O1D-CGD-O2D-CED
29	a	813	CLA	CBA-CGA-O2A-C1
29	b	702	CLA	CBA-CGA-O2A-C1
29	I	213	CLA	CBA-CGA-O2A-C1
29	K	209	CLA	CBA-CGA-O2A-C1
29	N	308	CLA	CBA-CGA-O2A-C1
29	N	314	CLA	CBA-CGA-O2A-C1
29	O	308	CLA	CBA-CGA-O2A-C1
29	T	314	CLA	CBA-CGA-O2A-C1
29	C	314	CLA	CBA-CGA-O2A-C1
29	P	209	CLA	CBA-CGA-O2A-C1
34	b	732	LMG	C29-C28-O8-C9
34	E	316	LMG	C29-C28-O8-C9
38	C	306	UIX	O4-C27-O2-C18
29	a	802	CLA	CBD-CGD-O2D-CED
29	a	814	CLA	CBD-CGD-O2D-CED
29	a	816	CLA	CBD-CGD-O2D-CED
29	a	826	CLA	CBD-CGD-O2D-CED
29	a	837	CLA	CBD-CGD-O2D-CED
29	b	717	CLA	CBD-CGD-O2D-CED
29	i	202	CLA	CBD-CGD-O2D-CED
29	l	503	CLA	CBD-CGD-O2D-CED
29	A	209	CLA	CBD-CGD-O2D-CED
29	I	209	CLA	CBD-CGD-O2D-CED
29	F	308	CLA	CBD-CGD-O2D-CED
29	J	310	CLA	CBD-CGD-O2D-CED
29	M	313	CLA	CBD-CGD-O2D-CED
29	L	308	CLA	CBD-CGD-O2D-CED
29	L	317	CLA	CBD-CGD-O2D-CED
29	E	311	CLA	CBD-CGD-O2D-CED
39	Q	309	KC1	CBD-CGD-O2D-CED
39	P	213	KC1	CBD-CGD-O2D-CED
34	h	205	LMG	C11-C10-O7-C8
29	T	308	CLA	O1D-CGD-O2D-CED
29	C	311	CLA	O1D-CGD-O2D-CED
39	N	312	KC1	O1D-CGD-O2D-CED
37	F	304	PID	O7-C30-O6-C27
38	P	207	UIX	O4-C27-O2-C18
29	H	307	CLA	O1A-CGA-O2A-C1
29	F	310	CLA	O1A-CGA-O2A-C1
29	F	312	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	j	101	PID	O7-C30-O6-C27
39	B	313	KC1	CAA-CBA-CGA-O1A
29	b	706	CLA	C4-C3-C5-C6
29	b	716	CLA	C4-C3-C5-C6
29	b	717	CLA	C4-C3-C5-C6
29	b	718	CLA	C4-C3-C5-C6
29	A	212	CLA	C4-C3-C5-C6
29	G	302	CLA	C4-C3-C5-C6
29	J	311	CLA	C4-C3-C5-C6
29	L	313	CLA	C4-C3-C5-C6
29	Q	308	CLA	C4-C3-C5-C6
29	Q	310	CLA	C4-C3-C5-C6
29	E	305	CLA	C4-C3-C5-C6
29	a	825	CLA	C2-C3-C5-C6
29	b	706	CLA	C2-C3-C5-C6
29	b	718	CLA	C2-C3-C5-C6
29	A	212	CLA	C2-C3-C5-C6
29	J	306	CLA	C2-C3-C5-C6
29	L	313	CLA	C2-C3-C5-C6
29	Q	310	CLA	C2-C3-C5-C6
29	E	305	CLA	C2-C3-C5-C6
29	a	828	CLA	CBA-CGA-O2A-C1
29	f	802	CLA	CBA-CGA-O2A-C1
29	f	803	CLA	CBA-CGA-O2A-C1
29	F	310	CLA	CBA-CGA-O2A-C1
29	F	312	CLA	CBA-CGA-O2A-C1
29	T	313	CLA	CBA-CGA-O2A-C1
29	P	214	CLA	CBA-CGA-O2A-C1
29	i	203	CLA	CBD-CGD-O2D-CED
29	a	819	CLA	O1D-CGD-O2D-CED
29	F	310	CLA	O1D-CGD-O2D-CED
37	G	310	PID	C31-C30-O6-C27
29	b	715	CLA	C2A-CAA-CBA-CGA
29	M	314	CLA	C3-C5-C6-C7
29	A	215	CLA	O1A-CGA-O2A-C1
29	b	722	CLA	C3-C5-C6-C7
29	b	736	CLA	C3-C5-C6-C7
29	i	203	CLA	C3-C5-C6-C7
29	l	505	CLA	C3-C5-C6-C7
29	H	308	CLA	C3-C5-C6-C7
30	b	727	PQN	C13-C15-C16-C17
29	a	819	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	l	504	CLA	CBA-CGA-O2A-C1
29	A	217	CLA	CBA-CGA-O2A-C1
29	M	306	CLA	CBA-CGA-O2A-C1
29	M	310	CLA	CBA-CGA-O2A-C1
29	L	316	CLA	CBA-CGA-O2A-C1
29	D	314	CLA	CBA-CGA-O2A-C1
29	B	306	CLA	CBA-CGA-O2A-C1
29	C	308	CLA	CBA-CGA-O2A-C1
29	P	215	CLA	CBA-CGA-O2A-C1
29	E	305	CLA	CBA-CGA-O2A-C1
35	j	106	DGD	C2A-C1A-O1G-C1G
38	Q	305	UIX	O4-C27-O2-C18
29	a	828	CLA	O1A-CGA-O2A-C1
29	C	314	CLA	C2-C1-O2A-CGA
36	I	203	DD6	C1-C2-C3-C4
36	K	202	DD6	C3-C4-C5-C6
36	L	305	DD6	C11-C10-C9-C8
36	D	304	DD6	C3-C4-C5-C6
36	O	303	DD6	C24-C25-C26-C27
37	G	303	PID	C14-C15-C16-C17
37	N	305	PID	C14-C15-C16-C17
37	C	305	PID	C14-C15-C16-C17
37	P	208	PID	C18-C19-C20-C21
29	a	819	CLA	O1A-CGA-O2A-C1
29	b	712	CLA	O1A-CGA-O2A-C1
29	A	217	CLA	O1A-CGA-O2A-C1
29	L	313	CLA	O1A-CGA-O2A-C1
29	L	316	CLA	O1A-CGA-O2A-C1
34	A	219	LMG	O10-C28-O8-C9
29	b	705	CLA	C2C-C3C-CAC-CBC
29	E	306	CLA	O1D-CGD-O2D-CED
29	J	309	CLA	O1A-CGA-O2A-C1
29	L	317	CLA	O1A-CGA-O2A-C1
38	E	304	UIX	C31-C27-O2-C18
29	a	801	CLA	C3-C5-C6-C7
29	a	804	CLA	C3-C5-C6-C7
29	a	837	CLA	C3-C5-C6-C7
29	b	704	CLA	C3-C5-C6-C7
29	b	709	CLA	C3-C5-C6-C7
29	b	718	CLA	C3-C5-C6-C7
29	G	313	CLA	C3-C5-C6-C7
29	b	721	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	M	310	CLA	CBD-CGD-O2D-CED
29	B	312	CLA	CBD-CGD-O2D-CED
39	E	312	KC1	CBD-CGD-O2D-CED
29	f	802	CLA	O1D-CGD-O2D-CED
29	A	212	CLA	O1D-CGD-O2D-CED
29	T	309	CLA	O1D-CGD-O2D-CED
29	P	209	CLA	O1D-CGD-O2D-CED
29	a	820	CLA	CBA-CGA-O2A-C1
29	b	720	CLA	CBA-CGA-O2A-C1
29	l	505	CLA	CBA-CGA-O2A-C1
29	A	215	CLA	CBA-CGA-O2A-C1
29	I	207	CLA	CBA-CGA-O2A-C1
29	H	307	CLA	CBA-CGA-O2A-C1
34	b	730	LMG	C29-C28-O8-C9
34	A	219	LMG	C29-C28-O8-C9
34	j	102	LMG	O6-C5-C6-O5
34	K	201	LMG	O6-C5-C6-O5
35	b	733	DGD	O6E-C5E-C6E-O5E
29	M	306	CLA	O1A-CGA-O2A-C1
29	b	719	CLA	O1D-CGD-O2D-CED
29	I	216	CLA	O1D-CGD-O2D-CED
37	N	302	PID	C31-C30-O6-C27
37	N	302	PID	O7-C30-O6-C27
38	E	304	UIX	O4-C27-O2-C18
29	b	709	CLA	CBD-CGD-O2D-CED
29	C	308	CLA	CBD-CGD-O2D-CED
29	P	210	CLA	CBD-CGD-O2D-CED
34	P	201	LMG	C11-C10-O7-C8
29	K	208	CLA	CBA-CGA-O2A-C1
29	E	309	CLA	CBA-CGA-O2A-C1
29	M	306	CLA	O1D-CGD-O2D-CED
29	L	312	CLA	O1D-CGD-O2D-CED
29	b	712	CLA	CBD-CGD-O2D-CED
29	K	210	CLA	CBD-CGD-O2D-CED
29	M	314	CLA	CBD-CGD-O2D-CED
29	P	217	CLA	CBD-CGD-O2D-CED
29	E	309	CLA	CBD-CGD-O2D-CED
29	a	820	CLA	O1D-CGD-O2D-CED
29	b	712	CLA	CBA-CGA-O2A-C1
29	L	313	CLA	CBA-CGA-O2A-C1
29	E	306	CLA	CBA-CGA-O2A-C1
39	C	310	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	a	820	CLA	C4-C3-C5-C6
29	a	823	CLA	C4-C3-C5-C6
29	i	201	CLA	C4-C3-C5-C6
29	H	308	CLA	C4-C3-C5-C6
29	N	309	CLA	C4-C3-C5-C6
29	C	309	CLA	C4-C3-C5-C6
29	a	820	CLA	C2-C3-C5-C6
29	b	716	CLA	C2-C3-C5-C6
29	i	201	CLA	C2-C3-C5-C6
29	J	311	CLA	C2-C3-C5-C6
29	N	309	CLA	C2-C3-C5-C6
29	Q	308	CLA	C2-C3-C5-C6
29	a	820	CLA	O1A-CGA-O2A-C1
29	b	720	CLA	O1A-CGA-O2A-C1
29	l	505	CLA	O1A-CGA-O2A-C1
34	b	730	LMG	O10-C28-O8-C9
29	O	309	CLA	CBD-CGD-O2D-CED
29	f	802	CLA	O1A-CGA-O2A-C1
38	A	203	UIX	O4-C27-O2-C18
34	A	219	LMG	O6-C5-C6-O5
29	M	314	CLA	C2A-CAA-CBA-CGA
29	I	201	CLA	O1D-CGD-O2D-CED
29	I	207	CLA	O1A-CGA-O2A-C1
29	E	306	CLA	O1A-CGA-O2A-C1
34	K	219	LMG	O6-C1-O1-C7
35	G	320	DGD	O6E-C1E-O5D-C6D
29	a	824	CLA	CBA-CGA-O2A-C1
29	L	312	CLA	CBA-CGA-O2A-C1
29	B	311	CLA	CBA-CGA-O2A-C1
34	j	102	LMG	C29-C28-O8-C9
35	b	733	DGD	C2A-C1A-O1G-C1G
29	b	710	CLA	CBD-CGD-O2D-CED
29	b	711	CLA	CBD-CGD-O2D-CED
29	K	214	CLA	CBD-CGD-O2D-CED
29	F	315	CLA	CBD-CGD-O2D-CED
29	L	316	CLA	CBD-CGD-O2D-CED
29	N	308	CLA	CBD-CGD-O2D-CED
29	P	212	CLA	CBD-CGD-O2D-CED
39	C	310	KC1	CBD-CGD-O2D-CED
34	E	316	LMG	O6-C5-C6-O5
29	M	311	CLA	CBA-CGA-O2A-C1
29	E	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
34	K	220	LMG	O6-C5-C6-O5
29	a	827	CLA	O1D-CGD-O2D-CED
35	b	733	DGD	C4E-C5E-C6E-O5E
29	L	311	CLA	CBD-CGD-O2D-CED
29	O	311	CLA	CBD-CGD-O2D-CED
34	b	730	LMG	C11-C10-O7-C8
29	b	721	CLA	C3-C5-C6-C7
36	I	203	DD6	C11-C10-C9-C8
36	F	301	DD6	C3-C4-C5-C6
36	T	303	DD6	C24-C25-C26-C27
38	F	305	UIX	C11-C13-C14-C23
38	P	207	UIX	C34-C37-C39-C40
29	L	312	CLA	O1A-CGA-O2A-C1
29	a	807	CLA	CBA-CGA-O2A-C1
29	a	811	CLA	CBA-CGA-O2A-C1
29	a	829	CLA	CBA-CGA-O2A-C1
29	a	830	CLA	CBA-CGA-O2A-C1
29	b	724	CLA	CBA-CGA-O2A-C1
29	j	104	CLA	CBA-CGA-O2A-C1
29	G	304	CLA	CBA-CGA-O2A-C1
29	G	317	CLA	CBA-CGA-O2A-C1
29	K	214	CLA	CBA-CGA-O2A-C1
29	L	308	CLA	CBA-CGA-O2A-C1
29	O	314	CLA	CBA-CGA-O2A-C1
29	B	315	CLA	CBA-CGA-O2A-C1
29	M	311	CLA	CBD-CGD-O2D-CED
39	H	309	KC1	CBD-CGD-O2D-CED
34	K	220	LMG	C4-C5-C6-O5
34	K	219	LMG	C4-C5-C6-O5
39	A	213	KC1	CAA-CBA-CGA-O1A
39	K	215	KC1	CAA-CBA-CGA-O2A
39	E	307	KC1	CAA-CBA-CGA-O2A
29	b	711	CLA	C4-C3-C5-C6
29	G	312	CLA	C4-C3-C5-C6
29	L	308	CLA	C4-C3-C5-C6
29	b	711	CLA	C2-C3-C5-C6
29	b	717	CLA	C2-C3-C5-C6
29	G	302	CLA	C2-C3-C5-C6
29	G	312	CLA	C2-C3-C5-C6
29	L	308	CLA	C2-C3-C5-C6
29	H	308	CLA	C2-C3-C5-C6
29	A	206	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	F	316	CLA	CBD-CGD-O2D-CED
29	a	807	CLA	C11-C10-C8-C9
29	a	807	CLA	C11-C12-C13-C14
29	a	823	CLA	C6-C7-C8-C9
29	a	824	CLA	C6-C7-C8-C9
29	a	829	CLA	C6-C7-C8-C9
29	a	829	CLA	C11-C12-C13-C14
29	a	829	CLA	C14-C13-C15-C16
29	b	704	CLA	C6-C7-C8-C9
29	b	705	CLA	C14-C13-C15-C16
29	l	505	CLA	C6-C7-C8-C9
29	A	218	CLA	C6-C7-C8-C9
29	I	213	CLA	C11-C12-C13-C14
29	B	310	CLA	C6-C7-C8-C9
29	Q	308	CLA	C6-C7-C8-C9
34	K	201	LMG	C4-C5-C6-O5
29	l	503	CLA	O1D-CGD-O2D-CED
29	H	313	CLA	C2-C1-O2A-CGA
34	A	219	LMG	C2-C1-O1-C7
34	K	219	LMG	C2-C1-O1-C7
29	E	309	CLA	O1A-CGA-O2A-C1
29	a	814	CLA	O1D-CGD-O2D-CED
29	a	826	CLA	O1D-CGD-O2D-CED
29	b	724	CLA	O1A-CGA-O2A-C1
29	G	317	CLA	O1A-CGA-O2A-C1
32	l	506	BCR	C37-C22-C23-C24
32	m	103	BCR	C37-C22-C23-C24
36	G	305	DD6	C12-C11-C13-C14
36	G	307	DD6	C12-C11-C13-C14
36	I	202	DD6	C-C1-C24-C25
36	I	203	DD6	C-C1-C24-C25
36	F	301	DD6	C12-C11-C13-C14
36	F	301	DD6	C7-C6-C8-C9
36	M	303	DD6	C12-C11-C13-C14
36	L	301	DD6	C12-C11-C13-C14
36	L	304	DD6	C12-C11-C13-C14
36	B	301	DD6	C12-C11-C13-C14
36	B	319	DD6	C-C1-C24-C25
36	B	319	DD6	C7-C6-C8-C9
36	E	302	DD6	C12-C11-C13-C14
38	F	305	UIX	C36-C38-C40-C41
38	C	306	UIX	C36-C38-C40-C41

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Mol	Chain	Res	Type	Atoms
32	l	506	BCR	C21-C22-C23-C24
36	G	307	DD6	C10-C11-C13-C14
36	I	203	DD6	C2-C1-C24-C25
36	K	202	DD6	C10-C11-C13-C14
36	F	301	DD6	C10-C11-C13-C14
36	M	303	DD6	C10-C11-C13-C14
36	M	303	DD6	C5-C6-C8-C9
36	L	301	DD6	C10-C11-C13-C14
36	L	304	DD6	C10-C11-C13-C14
36	B	301	DD6	C10-C11-C13-C14
36	B	319	DD6	C2-C1-C24-C25
36	E	302	DD6	C10-C11-C13-C14
38	F	305	UIX	C7-C10-C11-C13
29	a	837	CLA	O1D-CGD-O2D-CED
29	i	202	CLA	O1D-CGD-O2D-CED
29	K	208	CLA	O1A-CGA-O2A-C1
29	a	811	CLA	O1A-CGA-O2A-C1
29	a	830	CLA	O1A-CGA-O2A-C1
29	K	214	CLA	O1A-CGA-O2A-C1
29	L	308	CLA	O1A-CGA-O2A-C1
29	O	314	CLA	O1A-CGA-O2A-C1
34	K	201	LMG	C11-C10-O7-C8
39	A	205	KC1	CAA-CBA-CGA-O2A
39	M	305	KC1	CAA-CBA-CGA-O2A
39	L	314	KC1	CAA-CBA-CGA-O1A
39	H	309	KC1	CAA-CBA-CGA-O2A
39	Q	311	KC1	CAA-CBA-CGA-O2A
39	C	312	KC1	CAA-CBA-CGA-O1A
39	C	312	KC1	CAA-CBA-CGA-O2A
29	J	307	CLA	CBA-CGA-O2A-C1
34	b	730	LMG	O7-C8-C9-O8
29	l	501	CLA	CBA-CGA-O2A-C1
29	l	503	CLA	CBA-CGA-O2A-C1
29	Q	308	CLA	CBA-CGA-O2A-C1
29	l	504	CLA	C13-C15-C16-C17
29	A	209	CLA	O1D-CGD-O2D-CED
29	M	313	CLA	O1D-CGD-O2D-CED
29	L	317	CLA	O1D-CGD-O2D-CED
34	K	219	LMG	O6-C5-C6-O5
34	j	102	LMG	C4-C5-C6-O5
37	G	303	PID	C31-C30-O6-C27
29	a	829	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	i	201	CLA	C10-C11-C12-C13
29	l	502	CLA	C8-C10-C11-C12
29	l	501	CLA	C3-C5-C6-C7
29	l	504	CLA	C3-C5-C6-C7
29	a	816	CLA	O1D-CGD-O2D-CED
39	H	311	KC1	O1D-CGD-O2D-CED
29	j	104	CLA	O1A-CGA-O2A-C1
29	B	310	CLA	C5-C6-C7-C8
29	b	718	CLA	CBD-CGD-O2D-CED
29	b	706	CLA	C6-C7-C8-C10
29	E	308	CLA	C11-C10-C8-C7
39	L	306	KC1	CAA-CBA-CGA-O2A
29	a	831	CLA	C4-C3-C5-C6
29	b	718	CLA	C8-C10-C11-C12
29	F	308	CLA	O1D-CGD-O2D-CED
36	I	202	DD6	C24-C25-C26-C27
36	I	203	DD6	C24-C25-C26-C27
36	F	301	DD6	C11-C10-C9-C8
36	B	319	DD6	C1-C2-C3-C4
36	B	319	DD6	C3-C4-C5-C6
38	P	207	UIX	C32-C35-C36-C38
29	M	308	CLA	O2A-C1-C2-C3
29	J	310	CLA	O1D-CGD-O2D-CED
30	a	832	PQN	C13-C15-C16-C17
29	a	829	CLA	C13-C15-C16-C17
34	b	730	LMG	O6-C5-C6-O5
34	b	732	LMG	C10-C11-C12-C13
34	E	316	LMG	C28-C29-C30-C31
29	a	829	CLA	O1A-CGA-O2A-C1
29	G	304	CLA	O1A-CGA-O2A-C1
29	b	702	CLA	C10-C11-C12-C13
29	b	707	CLA	C8-C10-C11-C12
29	b	725	CLA	C15-C16-C17-C18
29	l	504	CLA	C10-C11-C12-C13
29	a	813	CLA	C2A-CAA-CBA-CGA
29	b	717	CLA	C2A-CAA-CBA-CGA
29	b	719	CLA	C2A-CAA-CBA-CGA
29	b	725	CLA	C2A-CAA-CBA-CGA
29	b	736	CLA	C2A-CAA-CBA-CGA
29	h	201	CLA	C2A-CAA-CBA-CGA
29	A	215	CLA	C2A-CAA-CBA-CGA
29	G	301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	I	209	CLA	C2A-CAA-CBA-CGA
29	D	308	CLA	C2A-CAA-CBA-CGA
29	N	313	CLA	C2A-CAA-CBA-CGA
39	B	313	KC1	CAA-CBA-CGA-O2A
39	O	310	KC1	CAA-CBA-CGA-O2A
39	O	315	KC1	CAA-CBA-CGA-O2A
29	a	824	CLA	C13-C15-C16-C17
29	b	703	CLA	C10-C11-C12-C13
29	b	707	CLA	C15-C16-C17-C18
29	b	709	CLA	C5-C6-C7-C8
29	i	202	CLA	C5-C6-C7-C8
29	E	306	CLA	C13-C15-C16-C17
34	b	732	LMG	C28-C29-C30-C31
35	h	203	DGD	C1B-C2B-C3B-C4B
35	j	103	DGD	C1B-C2B-C3B-C4B
29	a	802	CLA	O1D-CGD-O2D-CED
29	b	717	CLA	O1D-CGD-O2D-CED
29	a	807	CLA	O1A-CGA-O2A-C1
29	E	311	CLA	C3-C5-C6-C7
34	K	201	LMG	O6-C1-O1-C7
29	a	807	CLA	C5-C6-C7-C8
29	b	701	CLA	C8-C10-C11-C12
29	G	312	CLA	C5-C6-C7-C8
29	J	306	CLA	C8-C10-C11-C12
29	a	808	CLA	CBA-CGA-O2A-C1
29	A	212	CLA	CBA-CGA-O2A-C1
29	D	308	CLA	CBA-CGA-O2A-C1
35	m	102	DGD	C4D-C5D-C6D-O5D
29	a	824	CLA	O1A-CGA-O2A-C1
29	B	311	CLA	O1A-CGA-O2A-C1
29	Q	308	CLA	O1A-CGA-O2A-C1
35	b	733	DGD	O1A-C1A-O1G-C1G
35	j	106	DGD	C1B-C2B-C3B-C4B
29	b	703	CLA	C13-C15-C16-C17
29	B	310	CLA	C10-C11-C12-C13
29	b	721	CLA	O1D-CGD-O2D-CED
29	G	312	CLA	C10-C11-C12-C13
29	E	311	CLA	C5-C6-C7-C8
39	M	305	KC1	CAA-CBA-CGA-O1A
29	C	309	CLA	C2-C3-C5-C6
35	b	733	DGD	C1A-C2A-C3A-C4A
35	j	106	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
29	i	203	CLA	O1D-CGD-O2D-CED
29	M	310	CLA	O1D-CGD-O2D-CED
29	B	312	CLA	O1D-CGD-O2D-CED
29	E	311	CLA	O1D-CGD-O2D-CED
29	a	806	CLA	C15-C16-C17-C18
29	b	718	CLA	C5-C6-C7-C8
29	l	505	CLA	C5-C6-C7-C8
29	I	210	CLA	C5-C6-C7-C8
29	E	315	CLA	C5-C6-C7-C8
29	I	211	CLA	CBA-CGA-O2A-C1
29	J	306	CLA	CBA-CGA-O2A-C1
34	P	201	LMG	C29-C28-O8-C9
39	K	215	KC1	C2A-CAA-CBA-CGA
39	D	310	KC1	C2A-CAA-CBA-CGA
39	H	309	KC1	C2A-CAA-CBA-CGA
39	N	315	KC1	C2A-CAA-CBA-CGA
37	G	310	PID	O7-C30-O6-C27
29	i	201	CLA	C5-C6-C7-C8
29	l	501	CLA	C10-C11-C12-C13
29	a	810	CLA	C3-C5-C6-C7
29	K	211	CLA	C3-C5-C6-C7
29	E	305	CLA	C3-C5-C6-C7
36	G	305	DD6	C1-C2-C3-C4
36	G	305	DD6	C3-C4-C5-C6
36	D	304	DD6	C1-C2-C3-C4
38	F	305	UIX	C32-C35-C36-C38
38	O	306	UIX	C26-C30-C34-C37
38	O	306	UIX	C32-C35-C36-C38
39	T	315	KC1	CAA-CBA-CGA-O2A
29	E	306	CLA	C2A-CAA-CBA-CGA
29	a	809	CLA	CBA-CGA-O2A-C1
29	a	826	CLA	CBA-CGA-O2A-C1
29	b	736	CLA	CBA-CGA-O2A-C1
29	b	718	CLA	C10-C11-C12-C13
29	i	201	CLA	C15-C16-C17-C18
29	I	211	CLA	C5-C6-C7-C8
29	I	213	CLA	C13-C15-C16-C17
29	I	213	CLA	C15-C16-C17-C18
29	L	312	CLA	C5-C6-C7-C8
29	C	308	CLA	O1D-CGD-O2D-CED
29	P	210	CLA	O1D-CGD-O2D-CED
29	I	209	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	K	211	CLA	C5-C6-C7-C8
29	B	308	CLA	C5-C6-C7-C8
29	E	306	CLA	C15-C16-C17-C18
29	J	311	CLA	CBD-CGD-O2D-CED
29	a	807	CLA	C10-C11-C12-C13
29	a	826	CLA	C15-C16-C17-C18
29	b	736	CLA	C15-C16-C17-C18
29	A	209	CLA	C8-C10-C11-C12
29	G	312	CLA	C13-C15-C16-C17
29	G	316	CLA	C13-C15-C16-C17
35	m	102	DGD	O6D-C5D-C6D-O5D
39	G	318	KC1	CAA-CBA-CGA-O2A
29	a	823	CLA	C2-C3-C5-C6
29	B	310	CLA	C15-C16-C17-C18
29	E	305	CLA	C10-C11-C12-C13
29	M	307	CLA	CBD-CGD-O2D-CED
29	b	709	CLA	O1D-CGD-O2D-CED
29	l	501	CLA	O1A-CGA-O2A-C1
29	b	705	CLA	C4C-C3C-CAC-CBC
29	K	213	CLA	O2A-C1-C2-C3
34	K	201	LMG	C2-C1-O1-C7
35	b	733	DGD	C2D-C1D-O3G-C3G
40	J	314	SQD	C2-C1-O6-C44
29	l	503	CLA	C8-C10-C11-C12
35	b	733	DGD	O6D-C5D-C6D-O5D
29	L	307	CLA	CBA-CGA-O2A-C1
29	l	502	CLA	C16-C17-C18-C20
37	O	304	PID	C19-C20-C21-CM5
37	Q	306	PID	C19-C20-C21-CM5
29	a	827	CLA	C3-C5-C6-C7
29	N	309	CLA	C3-C5-C6-C7
39	I	215	KC1	CAA-CBA-CGA-O2A
39	N	315	KC1	CAA-CBA-CGA-O2A
29	K	210	CLA	O1D-CGD-O2D-CED
29	b	723	CLA	C5-C6-C7-C8
32	b	728	BCR	C37-C22-C23-C24
32	f	801	BCR	C7-C8-C9-C34
32	l	507	BCR	C11-C12-C13-C35
36	h	202	DD6	C12-C11-C13-C14
36	I	205	DD6	C12-C11-C13-C14
36	K	202	DD6	C12-C11-C13-C14
36	J	302	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
36	J	303	DD6	C12-C11-C13-C14
32	b	728	BCR	C21-C22-C23-C24
36	I	205	DD6	C10-C11-C13-C14
36	J	302	DD6	C10-C11-C13-C14
36	J	303	DD6	C10-C11-C13-C14
29	b	736	CLA	O1A-CGA-O2A-C1
29	l	503	CLA	O1A-CGA-O2A-C1
34	j	102	LMG	O10-C28-O8-C9
29	a	837	CLA	C2A-CAA-CBA-CGA
29	b	702	CLA	C2A-CAA-CBA-CGA
29	l	510	CLA	C2A-CAA-CBA-CGA
29	L	307	CLA	C2A-CAA-CBA-CGA
29	L	311	CLA	CBA-CGA-O2A-C1
37	P	202	PID	C16-C17-C18-C19
29	M	314	CLA	O1D-CGD-O2D-CED
29	I	212	CLA	C6-C7-C8-C10
29	L	312	CLA	C6-C7-C8-C10
29	N	309	CLA	C16-C17-C18-C19
29	P	217	CLA	O1D-CGD-O2D-CED
29	I	211	CLA	O1A-CGA-O2A-C1
29	i	202	CLA	C3-C5-C6-C7
29	G	302	CLA	C3-C5-C6-C7
29	I	211	CLA	C3-C5-C6-C7
37	O	304	PID	C19-C20-C21-C22
37	Q	306	PID	C19-C20-C21-C22
34	K	219	LMG	O9-C10-O7-C8
39	J	312	KC1	CAA-CBA-CGA-O2A
39	L	306	KC1	CAA-CBA-CGA-O1A
39	Q	311	KC1	CAA-CBA-CGA-O1A
39	C	315	KC1	CAA-CBA-CGA-O2A
39	E	307	KC1	CAA-CBA-CGA-O1A
29	b	717	CLA	C5-C6-C7-C8
29	O	309	CLA	O1D-CGD-O2D-CED
29	E	309	CLA	O1D-CGD-O2D-CED
29	b	712	CLA	O1D-CGD-O2D-CED
29	a	821	CLA	CBA-CGA-O2A-C1
29	b	711	CLA	CBA-CGA-O2A-C1
29	B	308	CLA	CBA-CGA-O2A-C1
29	M	309	CLA	CBD-CGD-O2D-CED
29	a	810	CLA	C6-C7-C8-C10
29	G	314	CLA	C11-C12-C13-C15
29	I	210	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	I	212	CLA	C6-C7-C8-C9
29	L	312	CLA	C6-C7-C8-C9
29	H	308	CLA	C16-C17-C18-C20
29	P	210	CLA	C16-C17-C18-C19
29	P	210	CLA	C16-C17-C18-C20
29	a	809	CLA	O1A-CGA-O2A-C1
29	a	826	CLA	O1A-CGA-O2A-C1
37	Q	301	PID	C26-C27-O6-C30
37	Q	301	PID	C28-C27-O6-C30
29	N	308	CLA	O1D-CGD-O2D-CED
34	b	730	LMG	C38-C39-C40-C41
34	b	732	LMG	C32-C33-C34-C35
37	P	206	PID	C17-C18-C19-C20
34	K	220	LMG	C30-C31-C32-C33
34	K	220	LMG	C28-C29-C30-C31
39	A	205	KC1	CAA-CBA-CGA-O1A
35	j	103	DGD	C2B-C3B-C4B-C5B
29	E	310	CLA	O1A-CGA-O2A-C1
29	A	212	CLA	O1A-CGA-O2A-C1
29	D	308	CLA	O1A-CGA-O2A-C1
29	a	827	CLA	CBA-CGA-O2A-C1
29	b	719	CLA	CBA-CGA-O2A-C1
35	b	733	DGD	C9B-CAB-CBB-CCB
29	F	315	CLA	O1D-CGD-O2D-CED
29	a	825	CLA	C13-C15-C16-C17
29	b	704	CLA	C4B-C3B-CAB-CBB
29	b	725	CLA	C4B-C3B-CAB-CBB
29	l	510	CLA	C4B-C3B-CAB-CBB
29	G	311	CLA	C4B-C3B-CAB-CBB
29	J	311	CLA	C4B-C3B-CAB-CBB
29	L	307	CLA	C4B-C3B-CAB-CBB
29	L	317	CLA	C4B-C3B-CAB-CBB
29	b	717	CLA	C16-C17-C18-C19
29	b	717	CLA	C16-C17-C18-C20
29	G	314	CLA	C11-C12-C13-C14
29	H	308	CLA	C16-C17-C18-C19
29	N	309	CLA	C16-C17-C18-C20
29	a	808	CLA	O1A-CGA-O2A-C1
29	a	809	CLA	C2A-CAA-CBA-CGA
29	a	823	CLA	C2A-CAA-CBA-CGA
29	b	711	CLA	C2A-CAA-CBA-CGA
29	I	211	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	K	209	CLA	C2A-CAA-CBA-CGA
29	L	308	CLA	C2A-CAA-CBA-CGA
35	G	320	DGD	C2A-C3A-C4A-C5A
29	b	706	CLA	C8-C10-C11-C12
29	P	210	CLA	C5-C6-C7-C8
34	K	220	LMG	C11-C10-O7-C8
34	b	732	LMG	O6-C5-C6-O5
29	a	807	CLA	C12-C13-C15-C16
29	b	702	CLA	C6-C7-C8-C10
29	l	505	CLA	C6-C7-C8-C10
29	b	714	CLA	C5-C6-C7-C8
34	j	102	LMG	C18-C19-C20-C21
35	b	733	DGD	C7B-C8B-C9B-CAB
29	J	306	CLA	O1A-CGA-O2A-C1
39	K	215	KC1	CAA-CBA-CGA-O1A
39	C	310	KC1	CAA-CBA-CGA-O1A
29	a	806	CLA	C3A-C2A-CAA-CBA
29	a	811	CLA	C3A-C2A-CAA-CBA
29	a	812	CLA	C3A-C2A-CAA-CBA
29	a	828	CLA	C3A-C2A-CAA-CBA
29	b	706	CLA	C3A-C2A-CAA-CBA
29	b	717	CLA	C3A-C2A-CAA-CBA
29	f	803	CLA	C3A-C2A-CAA-CBA
29	F	310	CLA	C3A-C2A-CAA-CBA
29	L	316	CLA	C3A-C2A-CAA-CBA
29	D	314	CLA	C3A-C2A-CAA-CBA
29	H	313	CLA	C3A-C2A-CAA-CBA
29	N	314	CLA	C3A-C2A-CAA-CBA
29	T	314	CLA	C3A-C2A-CAA-CBA
29	Q	313	CLA	C3A-C2A-CAA-CBA
29	C	314	CLA	C3A-C2A-CAA-CBA
29	P	215	CLA	C3A-C2A-CAA-CBA
29	K	212	CLA	CBD-CGD-O2D-CED
39	A	205	KC1	CBD-CGD-O2D-CED
29	N	313	CLA	CBA-CGA-O2A-C1
29	a	803	CLA	C15-C16-C17-C18
29	b	704	CLA	C13-C15-C16-C17
29	b	712	CLA	C5-C6-C7-C8
36	D	301	DD6	C24-C25-C26-C27
29	a	810	CLA	C6-C7-C8-C9
29	B	315	CLA	O1A-CGA-O2A-C1
34	b	732	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
34	K	201	LMG	C31-C32-C33-C34
29	E	314	CLA	CBD-CGD-O2D-CED
29	a	805	CLA	CBA-CGA-O2A-C1
29	l	502	CLA	CBA-CGA-O2A-C1
29	b	702	CLA	C5-C6-C7-C8
29	b	711	CLA	O1D-CGD-O2D-CED
29	L	316	CLA	O1D-CGD-O2D-CED
34	A	219	LMG	C30-C31-C32-C33
34	K	201	LMG	C34-C35-C36-C37
29	M	311	CLA	O1A-CGA-O2A-C1
29	b	710	CLA	O1D-CGD-O2D-CED
29	L	307	CLA	O1A-CGA-O2A-C1
29	b	725	CLA	C2B-C3B-CAB-CBB
29	b	736	CLA	C2B-C3B-CAB-CBB
29	l	502	CLA	C2B-C3B-CAB-CBB
29	l	510	CLA	C2B-C3B-CAB-CBB
29	A	216	CLA	C2B-C3B-CAB-CBB
29	K	212	CLA	C2B-C3B-CAB-CBB
29	L	317	CLA	C2B-C3B-CAB-CBB
32	b	735	BCR	C1-C6-C7-C8
32	l	506	BCR	C23-C24-C25-C30
34	b	734	LMG	C11-C12-C13-C14
29	G	302	CLA	CBA-CGA-O2A-C1
35	j	106	DGD	C2A-C3A-C4A-C5A
29	P	212	CLA	O1D-CGD-O2D-CED
29	L	317	CLA	C2A-CAA-CBA-CGA
35	b	733	DGD	C1B-C2B-C3B-C4B
29	a	821	CLA	O1A-CGA-O2A-C1
29	a	827	CLA	O1A-CGA-O2A-C1
29	b	711	CLA	O1A-CGA-O2A-C1
29	b	719	CLA	O1A-CGA-O2A-C1
29	B	308	CLA	O1A-CGA-O2A-C1
34	b	730	LMG	C36-C37-C38-C39
34	b	730	LMG	O9-C10-O7-C8
29	G	304	CLA	C4-C3-C5-C6
29	M	314	CLA	C4-C3-C5-C6
35	m	102	DGD	C6A-C7A-C8A-C9A
29	a	831	CLA	C2-C3-C5-C6
29	I	210	CLA	C6-C7-C8-C10
34	b	732	LMG	C31-C32-C33-C34
29	G	312	CLA	CBA-CGA-O2A-C1
29	H	313	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	a	833	LHG	C24-C23-O8-C6
29	a	824	CLA	C14-C13-C15-C16
29	O	314	CLA	C2-C1-O2A-CGA
34	K	220	LMG	C14-C15-C16-C17
29	a	812	CLA	C8-C10-C11-C12
29	G	316	CLA	C5-C6-C7-C8
34	b	734	LMG	C18-C19-C20-C21
29	J	309	CLA	C2C-C3C-CAC-CBC
29	I	213	CLA	C10-C11-C12-C13
34	b	730	LMG	C14-C15-C16-C17
29	a	807	CLA	C8-C10-C11-C12
36	O	303	DD6	C3-C4-C5-C6
29	l	502	CLA	C16-C17-C18-C19
35	G	320	DGD	C2B-C1B-O2G-C2G
29	J	307	CLA	O1A-CGA-O2A-C1
34	b	730	LMG	C37-C38-C39-C40
34	j	102	LMG	C34-C35-C36-C37
37	N	305	PID	C28-C27-O6-C30
32	a	838	BCR	C37-C22-C23-C24
32	b	728	BCR	C36-C18-C19-C20
36	I	204	DD6	C12-C11-C13-C14
36	K	203	DD6	C12-C11-C13-C14
35	G	320	DGD	C1A-C2A-C3A-C4A
29	L	313	CLA	C3-C5-C6-C7
29	Q	308	CLA	C3-C5-C6-C7
36	I	204	DD6	C10-C11-C13-C14
36	K	203	DD6	C10-C11-C13-C14
40	B	317	SQD	C45-C44-O6-C1
34	j	102	LMG	C17-C18-C19-C20
29	a	803	CLA	C2A-CAA-CBA-CGA
29	i	202	CLA	C16-C17-C18-C19
29	i	202	CLA	C16-C17-C18-C20
29	E	308	CLA	C16-C17-C18-C19
39	C	312	KC1	CBD-CGD-O2D-CED
29	I	209	CLA	C4-C3-C5-C6
39	N	315	KC1	C2B-C3B-CAB-CBB
39	O	310	KC1	C2B-C3B-CAB-CBB
29	l	502	CLA	O1A-CGA-O2A-C1
29	b	709	CLA	C8-C10-C11-C12
29	l	503	CLA	C5-C6-C7-C8
29	I	217	CLA	C5-C6-C7-C8
29	E	314	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	h	203	DGD	CAB-CBB-CCB-CDB
35	j	106	DGD	C2B-C1B-O2G-C2G
29	A	212	CLA	C5-C6-C7-C8
39	G	315	KC1	C4B-C3B-CAB-CBB
39	G	318	KC1	C4B-C3B-CAB-CBB
39	F	309	KC1	C4B-C3B-CAB-CBB
39	F	314	KC1	C4B-C3B-CAB-CBB
39	M	312	KC1	C4B-C3B-CAB-CBB
39	D	310	KC1	C4B-C3B-CAB-CBB
39	B	313	KC1	C4B-C3B-CAB-CBB
39	H	309	KC1	C4B-C3B-CAB-CBB
39	N	310	KC1	C4B-C3B-CAB-CBB
39	N	310	KC1	C2A-CAA-CBA-CGA
39	O	312	KC1	C4B-C3B-CAB-CBB
39	C	310	KC1	C4B-C3B-CAB-CBB
39	C	312	KC1	C4B-C3B-CAB-CBB
39	P	213	KC1	C4B-C3B-CAB-CBB
39	E	307	KC1	C4B-C3B-CAB-CBB
29	E	308	CLA	C16-C17-C18-C20
29	a	805	CLA	O1A-CGA-O2A-C1
29	O	311	CLA	O1D-CGD-O2D-CED
34	K	219	LMG	C30-C31-C32-C33
34	j	102	LMG	C28-C29-C30-C31
29	b	736	CLA	C10-C11-C12-C13
29	A	218	CLA	C5-C6-C7-C8
29	K	214	CLA	O1D-CGD-O2D-CED
34	P	201	LMG	O6-C5-C6-O5
34	K	219	LMG	O7-C8-C9-O8
37	G	303	PID	O7-C30-O6-C27
34	K	219	LMG	C32-C33-C34-C35
29	F	316	CLA	O1D-CGD-O2D-CED
29	G	302	CLA	O1A-CGA-O2A-C1
29	J	306	CLA	C13-C15-C16-C17
34	j	102	LMG	C31-C32-C33-C34
34	K	201	LMG	C17-C18-C19-C20
29	A	210	CLA	CBA-CGA-O2A-C1
29	F	307	CLA	CBA-CGA-O2A-C1
31	a	833	LHG	C2-C3-O3-P
39	H	309	KC1	CAA-CBA-CGA-O1A
29	b	726	CLA	C3-C5-C6-C7
29	G	314	CLA	C2-C3-C5-C6
34	K	201	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	b	734	LMG	C17-C18-C19-C20
29	b	713	CLA	C2A-CAA-CBA-CGA
29	G	312	CLA	C2A-CAA-CBA-CGA
29	J	308	CLA	C2A-CAA-CBA-CGA
29	B	310	CLA	C2A-CAA-CBA-CGA
29	P	214	CLA	C2A-CAA-CBA-CGA
29	b	723	CLA	CBA-CGA-O2A-C1
29	I	212	CLA	CBA-CGA-O2A-C1
29	L	311	CLA	O1D-CGD-O2D-CED
29	a	820	CLA	C13-C15-C16-C17
29	G	312	CLA	C8-C10-C11-C12
37	F	304	PID	C16-C17-C18-C19
29	H	313	CLA	O1A-CGA-O2A-C1
29	L	308	CLA	C3-C5-C6-C7
29	a	806	CLA	C1A-C2A-CAA-CBA
29	a	818	CLA	C1A-C2A-CAA-CBA
29	a	820	CLA	C1A-C2A-CAA-CBA
29	a	821	CLA	C1A-C2A-CAA-CBA
29	a	828	CLA	C1A-C2A-CAA-CBA
29	b	712	CLA	C1A-C2A-CAA-CBA
29	b	713	CLA	C1A-C2A-CAA-CBA
29	b	720	CLA	C1A-C2A-CAA-CBA
29	b	721	CLA	C1A-C2A-CAA-CBA
29	f	803	CLA	C1A-C2A-CAA-CBA
29	A	212	CLA	C1A-C2A-CAA-CBA
29	G	316	CLA	C1A-C2A-CAA-CBA
29	I	217	CLA	C1A-C2A-CAA-CBA
29	F	308	CLA	C1A-C2A-CAA-CBA
29	L	316	CLA	C1A-C2A-CAA-CBA
29	D	314	CLA	C1A-C2A-CAA-CBA
29	H	313	CLA	C1A-C2A-CAA-CBA
29	N	314	CLA	C1A-C2A-CAA-CBA
29	T	309	CLA	C1A-C2A-CAA-CBA
29	T	314	CLA	C1A-C2A-CAA-CBA
29	C	314	CLA	C1A-C2A-CAA-CBA
29	P	215	CLA	C1A-C2A-CAA-CBA
29	a	810	CLA	CBD-CGD-O2D-CED
29	b	722	CLA	C8-C10-C11-C12
29	Q	310	CLA	C10-C11-C12-C13
29	T	311	CLA	CBA-CGA-O2A-C1
29	G	312	CLA	O1A-CGA-O2A-C1
34	K	220	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
35	j	103	DGD	C4D-C5D-C6D-O5D
29	a	802	CLA	C11-C10-C8-C7
29	a	829	CLA	C6-C7-C8-C10
29	a	829	CLA	C11-C10-C8-C7
29	b	706	CLA	C12-C13-C15-C16
29	b	736	CLA	C11-C12-C13-C15
29	i	202	CLA	C11-C10-C8-C7
29	l	504	CLA	C6-C7-C8-C10
29	A	209	CLA	C12-C13-C15-C16
29	G	316	CLA	C12-C13-C15-C16
29	I	211	CLA	C6-C7-C8-C10
29	B	312	CLA	C11-C10-C8-C7
29	N	309	CLA	C11-C12-C13-C15
29	E	306	CLA	C6-C7-C8-C10
29	E	308	CLA	C11-C12-C13-C15
29	E	315	CLA	C11-C10-C8-C7
30	a	832	PQN	C22-C23-C25-C26
29	J	306	CLA	C16-C17-C18-C20
39	H	311	KC1	CAA-CBA-CGA-O2A
29	a	809	CLA	C4-C3-C5-C6
29	a	809	CLA	C2-C3-C5-C6
40	J	314	SQD	C8-C7-O47-C45
29	a	802	CLA	C11-C12-C13-C14
29	a	827	CLA	C6-C7-C8-C9
29	b	705	CLA	C11-C10-C8-C9
29	b	711	CLA	C11-C10-C8-C9
29	b	718	CLA	C11-C12-C13-C14
29	b	736	CLA	C11-C12-C13-C14
29	A	218	CLA	C11-C10-C8-C9
29	G	316	CLA	C14-C13-C15-C16
29	Q	308	CLA	C11-C10-C8-C9
29	E	308	CLA	C11-C12-C13-C14
29	E	315	CLA	C11-C10-C8-C9
30	b	727	PQN	C21-C22-C23-C24
29	A	207	CLA	CBA-CGA-O2A-C1
29	B	312	CLA	CBA-CGA-O2A-C1
29	T	316	CLA	CBD-CGD-O2D-CED
29	M	310	CLA	O2A-C1-C2-C3
34	b	734	LMG	C7-C8-C9-O8
34	K	201	LMG	C7-C8-C9-O8
34	E	316	LMG	O1-C7-C8-C9
35	j	103	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
29	J	308	CLA	C5-C6-C7-C8
35	h	203	DGD	C7B-C8B-C9B-CAB
34	b	734	LMG	C29-C28-O8-C9
29	a	837	CLA	C6-C7-C8-C9
29	b	702	CLA	C16-C17-C18-C20
29	C	309	CLA	C16-C17-C18-C19
34	A	219	LMG	C28-C29-C30-C31
35	j	106	DGD	C3A-C4A-C5A-C6A
29	G	314	CLA	C4-C3-C5-C6
29	b	703	CLA	C8-C10-C11-C12
29	O	309	CLA	C13-C15-C16-C17
32	l	506	BCR	C7-C8-C9-C34
29	P	215	CLA	C2-C1-O2A-CGA
34	K	201	LMG	C33-C34-C35-C36
29	l	501	CLA	C8-C10-C11-C12
29	I	209	CLA	C8-C10-C11-C12
29	Q	310	CLA	C8-C10-C11-C12
30	a	832	PQN	C23-C25-C26-C27
29	a	802	CLA	C13-C15-C16-C17
34	b	730	LMG	C34-C35-C36-C37
29	I	212	CLA	O1A-CGA-O2A-C1
29	b	718	CLA	O1D-CGD-O2D-CED
29	M	311	CLA	O1D-CGD-O2D-CED
39	O	315	KC1	O1D-CGD-O2D-CED
29	I	212	CLA	O2A-C1-C2-C3
34	P	201	LMG	C9-C8-O7-C10
29	i	201	CLA	C8-C10-C11-C12
36	G	305	DD6	C11-C10-C9-C8
36	G	306	DD6	C11-C10-C9-C8
36	D	301	DD6	C11-C10-C9-C8
38	N	306	UIX	C34-C37-C39-C40
29	J	306	CLA	C16-C17-C18-C19
29	C	309	CLA	C16-C17-C18-C20
29	b	723	CLA	O1A-CGA-O2A-C1
29	A	206	CLA	O1D-CGD-O2D-CED
37	T	317	PID	C19-C20-C21-C22
34	E	316	LMG	C29-C30-C31-C32
35	h	203	DGD	C8B-C9B-CAB-CBB
34	b	730	LMG	C11-C12-C13-C14
29	l	505	CLA	C4-C3-C5-C6
37	N	305	PID	C16-C17-C18-C19
34	A	219	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	A	207	CLA	O1A-CGA-O2A-C1
34	b	732	LMG	C14-C15-C16-C17
35	b	733	DGD	C2B-C3B-C4B-C5B
35	h	203	DGD	C9B-CAB-CBB-CCB
29	J	309	CLA	C4C-C3C-CAC-CBC
34	b	732	LMG	C38-C39-C40-C41
29	l	505	CLA	CAA-CBA-CGA-O2A
34	b	730	LMG	C32-C33-C34-C35
29	a	816	CLA	C2A-CAA-CBA-CGA
29	b	720	CLA	C2A-CAA-CBA-CGA
29	J	309	CLA	C2A-CAA-CBA-CGA
29	b	716	CLA	C5-C6-C7-C8
29	a	806	CLA	C2-C1-O2A-CGA
35	b	733	DGD	C4B-C5B-C6B-C7B
29	a	837	CLA	C6-C7-C8-C10
34	K	220	LMG	C29-C28-O8-C9
39	L	314	KC1	C2C-C3C-CAC-CBC
29	G	304	CLA	C11-C12-C13-C14
37	D	305	PID	C17-C18-C19-C20
37	P	206	PID	C15-C16-C17-C18
39	E	312	KC1	C2C-C3C-CAC-CBC
34	b	732	LMG	C37-C38-C39-C40
29	a	826	CLA	C13-C15-C16-C17
29	E	314	CLA	O1D-CGD-O2D-CED
37	P	206	PID	C14-C15-C16-C17
39	O	315	KC1	CAA-CBA-CGA-O1A
29	a	812	CLA	C4-C3-C5-C6
29	b	701	CLA	C4-C3-C5-C6
29	A	209	CLA	C4-C3-C5-C6
29	K	211	CLA	C4-C3-C5-C6
34	K	220	LMG	C32-C33-C34-C35
29	a	822	CLA	CBA-CGA-O2A-C1
36	A	202	DD6	C27-C29-C30-C31
36	A	204	DD6	C27-C29-C30-C31
36	I	204	DD6	C27-C29-C30-C31
36	M	304	DD6	C27-C29-C30-C31
36	L	301	DD6	C27-C29-C30-C31
36	L	305	DD6	C27-C29-C30-C31
36	B	305	DD6	C27-C29-C30-C31
36	H	303	DD6	C27-C29-C30-C31
36	N	303	DD6	C27-C29-C30-C31
36	O	303	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	Q	302	DD6	C27-C29-C30-C31
36	P	204	DD6	C27-C29-C30-C31
29	L	311	CLA	O1A-CGA-O2A-C1
29	a	802	CLA	C11-C10-C8-C9
29	a	806	CLA	C6-C7-C8-C9
29	a	809	CLA	C14-C13-C15-C16
29	a	829	CLA	C11-C10-C8-C9
29	b	701	CLA	C11-C10-C8-C9
29	b	706	CLA	C6-C7-C8-C9
29	b	706	CLA	C14-C13-C15-C16
29	i	202	CLA	C11-C10-C8-C9
29	A	209	CLA	C14-C13-C15-C16
29	B	308	CLA	C6-C7-C8-C9
29	B	310	CLA	C11-C10-C8-C9
29	B	312	CLA	C11-C10-C8-C9
29	H	308	CLA	C11-C12-C13-C14
29	N	309	CLA	C11-C12-C13-C14
29	E	306	CLA	C6-C7-C8-C9
29	l	503	CLA	C10-C11-C12-C13
29	a	801	CLA	C4B-C3B-CAB-CBB
29	b	721	CLA	C4B-C3B-CAB-CBB
29	b	736	CLA	C4B-C3B-CAB-CBB
29	A	210	CLA	C4B-C3B-CAB-CBB
29	A	216	CLA	C4B-C3B-CAB-CBB
29	G	312	CLA	C4B-C3B-CAB-CBB
29	I	213	CLA	C4B-C3B-CAB-CBB
29	F	313	CLA	C4B-C3B-CAB-CBB
29	L	315	CLA	C4B-C3B-CAB-CBB
29	N	308	CLA	C4B-C3B-CAB-CBB
29	Q	312	CLA	C4B-C3B-CAB-CBB
29	C	313	CLA	C4B-C3B-CAB-CBB
29	P	209	CLA	C4B-C3B-CAB-CBB
29	P	214	CLA	C4B-C3B-CAB-CBB
34	j	102	LMG	C14-C15-C16-C17
29	a	837	CLA	C5-C6-C7-C8
29	A	209	CLA	C13-C15-C16-C17
39	G	318	KC1	CAA-CBA-CGA-O1A
29	I	201	CLA	C2A-CAA-CBA-CGA
29	M	311	CLA	C2A-CAA-CBA-CGA
40	B	317	SQD	C2-C1-O6-C44
29	b	721	CLA	C5-C6-C7-C8
29	a	802	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	a	806	CLA	C6-C7-C8-C10
29	a	809	CLA	C12-C13-C15-C16
29	a	820	CLA	C11-C10-C8-C7
29	a	822	CLA	C11-C12-C13-C15
29	a	827	CLA	C6-C7-C8-C10
29	b	701	CLA	C11-C10-C8-C7
29	b	705	CLA	C11-C10-C8-C7
29	b	711	CLA	C11-C10-C8-C7
29	b	712	CLA	C12-C13-C15-C16
29	b	718	CLA	C11-C12-C13-C15
29	A	218	CLA	C11-C10-C8-C7
29	G	312	CLA	C11-C12-C13-C15
29	J	308	CLA	C6-C7-C8-C10
29	B	308	CLA	C6-C7-C8-C10
29	B	310	CLA	C11-C10-C8-C7
29	H	308	CLA	C11-C12-C13-C15
29	Q	308	CLA	C11-C10-C8-C7
29	E	306	CLA	C11-C12-C13-C15
30	b	727	PQN	C21-C22-C23-C25
34	b	730	LMG	C17-C18-C19-C20
34	j	102	LMG	C19-C20-C21-C22
29	a	825	CLA	C15-C16-C17-C18
34	j	102	LMG	C30-C31-C32-C33
29	a	807	CLA	C3A-C2A-CAA-CBA
29	b	721	CLA	C3A-C2A-CAA-CBA
29	i	203	CLA	C3A-C2A-CAA-CBA
29	G	302	CLA	C3A-C2A-CAA-CBA
29	I	212	CLA	C3A-C2A-CAA-CBA
29	J	310	CLA	C3A-C2A-CAA-CBA
29	D	311	CLA	C3A-C2A-CAA-CBA
29	H	310	CLA	C3A-C2A-CAA-CBA
29	B	310	CLA	C8-C10-C11-C12
29	M	309	CLA	O1D-CGD-O2D-CED
29	b	701	CLA	C2-C3-C5-C6
34	b	732	LMG	C36-C37-C38-C39
35	b	733	DGD	CAB-CBB-CCB-CDB
29	B	312	CLA	O1A-CGA-O2A-C1
31	a	833	LHG	O10-C23-O8-C6
29	a	812	CLA	CBA-CGA-O2A-C1
29	A	211	CLA	CBA-CGA-O2A-C1
36	K	202	DD6	C11-C10-C9-C8
36	M	303	DD6	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
36	I	202	DD6	C2-C1-C24-C25
34	j	102	LMG	C33-C34-C35-C36
34	A	219	LMG	C34-C35-C36-C37
35	h	203	DGD	C2A-C3A-C4A-C5A
35	G	320	DGD	O1B-C1B-O2G-C2G
29	K	218	CLA	C2A-CAA-CBA-CGA
34	b	730	LMG	O1-C7-C8-C9
34	b	730	LMG	C7-C8-C9-O8
34	K	219	LMG	C7-C8-C9-O8
35	j	106	DGD	C1G-C2G-C3G-O3G
29	P	210	CLA	C3-C5-C6-C7
35	b	733	DGD	C7A-C8A-C9A-CAA
34	P	201	LMG	O10-C28-O8-C9
29	a	803	CLA	C4-C3-C5-C6
34	K	219	LMG	C28-C29-C30-C31
34	j	102	LMG	O7-C10-C11-C12
29	A	209	CLA	C2-C3-C5-C6
29	b	701	CLA	CBD-CGD-O2D-CED
29	J	308	CLA	CBD-CGD-O2D-CED
29	M	307	CLA	O1D-CGD-O2D-CED
29	L	315	CLA	C2B-C3B-CAB-CBB
29	N	308	CLA	C2B-C3B-CAB-CBB
29	P	209	CLA	C2B-C3B-CAB-CBB
29	P	214	CLA	C2B-C3B-CAB-CBB
32	a	838	BCR	C23-C24-C25-C30
32	b	729	BCR	C1-C6-C7-C8
32	l	506	BCR	C1-C6-C7-C8
29	A	218	CLA	C8-C10-C11-C12
39	N	315	KC1	CAA-CBA-CGA-O1A
35	b	733	DGD	C4D-C5D-C6D-O5D
29	A	207	CLA	CBD-CGD-O2D-CED
29	J	311	CLA	O1D-CGD-O2D-CED
29	a	812	CLA	C2A-CAA-CBA-CGA
29	J	306	CLA	C15-C16-C17-C18
34	b	730	LMG	O1-C7-C8-O7
34	E	316	LMG	O1-C7-C8-O7
35	j	103	DGD	O2G-C2G-C3G-O3G
35	j	106	DGD	O1G-C1G-C2G-O2G
34	A	219	LMG	C4-C5-C6-O5
35	B	318	DGD	C2B-C3B-C4B-C5B
39	O	310	KC1	CAA-CBA-CGA-O1A
29	a	803	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	O	309	CLA	C15-C16-C17-C18
29	a	824	CLA	CBD-CGD-O2D-CED
29	a	802	CLA	C14-C13-C15-C16
29	a	820	CLA	C11-C10-C8-C9
29	b	707	CLA	C6-C7-C8-C9
29	b	712	CLA	C14-C13-C15-C16
29	i	201	CLA	C6-C7-C8-C9
29	A	209	CLA	C11-C10-C8-C9
29	G	312	CLA	C11-C12-C13-C14
29	E	306	CLA	C11-C12-C13-C14
29	E	311	CLA	C11-C10-C8-C9
34	K	201	LMG	C18-C19-C20-C21
29	G	302	CLA	CAA-CBA-CGA-O2A
39	T	315	KC1	CAA-CBA-CGA-O1A
35	B	318	DGD	C4D-C5D-C6D-O5D
37	F	304	PID	C17-C18-C19-C20
29	K	212	CLA	O1D-CGD-O2D-CED
29	I	207	CLA	O2A-C1-C2-C3
29	K	207	CLA	O2A-C1-C2-C3
29	a	810	CLA	C2A-CAA-CBA-CGA
39	Q	314	KC1	CAA-CBA-CGA-O2A
29	i	203	CLA	CBA-CGA-O2A-C1
29	L	310	CLA	C4-C3-C5-C6
36	B	319	DD6	C11-C10-C9-C8
37	O	305	PID	C18-C19-C20-C21
29	K	211	CLA	C2-C3-C5-C6
34	K	219	LMG	C33-C34-C35-C36
37	D	306	PID	CM4-C14-C15-C16
37	T	317	PID	C19-C20-C21-CM5
29	b	736	CLA	C8-C10-C11-C12
39	F	309	KC1	CAA-CBA-CGA-O1A
29	b	702	CLA	C16-C17-C18-C19
36	K	203	DD6	C7-C6-C8-C9
36	K	221	DD6	C12-C11-C13-C14
36	T	303	DD6	C12-C11-C13-C14
29	a	809	CLA	C11-C10-C8-C7
29	b	704	CLA	C6-C7-C8-C10
29	b	707	CLA	C6-C7-C8-C10
29	b	720	CLA	C11-C10-C8-C7
29	i	201	CLA	C6-C7-C8-C10
29	A	209	CLA	C11-C10-C8-C7
29	Q	310	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	E	311	CLA	C11-C10-C8-C7
32	a	838	BCR	C21-C22-C23-C24
32	b	728	BCR	C17-C18-C19-C20
32	f	801	BCR	C7-C8-C9-C10
32	l	506	BCR	C7-C8-C9-C10
36	h	202	DD6	C10-C11-C13-C14
36	K	221	DD6	C10-C11-C13-C14
36	T	303	DD6	C10-C11-C13-C14
34	E	316	LMG	C8-C7-O1-C1
29	i	201	CLA	C2A-CAA-CBA-CGA
29	l	503	CLA	C2A-CAA-CBA-CGA
29	b	712	CLA	C4-C3-C5-C6
29	M	314	CLA	C2-C3-C5-C6
39	H	314	KC1	C2B-C3B-CAB-CBB
39	O	315	KC1	C2B-C3B-CAB-CBB
39	T	315	KC1	C2B-C3B-CAB-CBB
39	Q	314	KC1	C2B-C3B-CAB-CBB
39	C	315	KC1	C2B-C3B-CAB-CBB
39	P	211	KC1	C2B-C3B-CAB-CBB
29	K	209	CLA	C3-C5-C6-C7
29	M	307	CLA	C3-C5-C6-C7
34	b	732	LMG	C13-C14-C15-C16
35	m	102	DGD	CCA-CDA-CEA-CFA
35	b	733	DGD	C3G-C2G-O2G-C1B
29	a	822	CLA	O1A-CGA-O2A-C1
29	b	707	CLA	C16-C17-C18-C20
29	A	209	CLA	C16-C17-C18-C20
29	I	217	CLA	C6-C7-C8-C9
34	b	732	LMG	C17-C18-C19-C20
35	B	318	DGD	O6D-C5D-C6D-O5D
29	Q	310	CLA	C3-C5-C6-C7
35	j	106	DGD	O1B-C1B-O2G-C2G
35	G	320	DGD	C1G-C2G-C3G-O3G
39	A	213	KC1	C4B-C3B-CAB-CBB
39	I	215	KC1	C4B-C3B-CAB-CBB
39	L	306	KC1	C4B-C3B-CAB-CBB
39	N	315	KC1	C4B-C3B-CAB-CBB
39	O	310	KC1	C4B-C3B-CAB-CBB
39	T	310	KC1	C4B-C3B-CAB-CBB
39	C	312	KC1	C2A-CAA-CBA-CGA
39	E	312	KC1	C4B-C3B-CAB-CBB
29	A	211	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	b	714	CLA	C8-C10-C11-C12
29	b	702	CLA	C4-C3-C5-C6
29	I	213	CLA	C4-C3-C5-C6
29	O	309	CLA	C4-C3-C5-C6
29	b	725	CLA	CBD-CGD-O2D-CED
29	G	304	CLA	C2-C3-C5-C6
29	I	209	CLA	C2-C3-C5-C6
29	L	310	CLA	C2-C3-C5-C6
37	G	303	PID	C12-C13-C14-CM4
37	F	304	PID	CM5-C21-C22-C23
37	P	206	PID	CM5-C21-C22-C23
37	E	301	PID	CM5-C21-C22-C23
38	N	306	UIX	C25-C28-C32-C33
38	T	306	UIX	C25-C28-C32-C33
29	a	831	CLA	C5-C6-C7-C8
29	b	731	CLA	C3-C5-C6-C7
34	b	732	LMG	O7-C8-C9-O8
34	K	201	LMG	O7-C8-C9-O8
35	j	106	DGD	O2G-C2G-C3G-O3G
29	i	201	CLA	C13-C15-C16-C17
29	G	302	CLA	C15-C16-C17-C18
29	a	809	CLA	C11-C10-C8-C9
29	a	822	CLA	C11-C12-C13-C14
29	b	701	CLA	C11-C12-C13-C14
29	b	718	CLA	C11-C10-C8-C9
29	N	313	CLA	O1A-CGA-O2A-C1
35	b	733	DGD	C8A-C9A-CAA-CBA
29	a	812	CLA	O1A-CGA-O2A-C1
29	i	203	CLA	O1A-CGA-O2A-C1
34	j	102	LMG	C32-C33-C34-C35
29	a	812	CLA	C11-C12-C13-C15
39	P	216	KC1	CAA-CBA-CGA-O2A
29	a	810	CLA	O1D-CGD-O2D-CED
29	l	502	CLA	C3-C5-C6-C7
29	a	829	CLA	C5-C6-C7-C8
29	b	725	CLA	C16-C17-C18-C20
29	a	806	CLA	C13-C15-C16-C17
29	T	316	CLA	O1D-CGD-O2D-CED
34	b	734	LMG	C16-C17-C18-C19
36	A	201	DD6	C27-C29-C30-C31
36	K	203	DD6	C27-C29-C30-C31
36	T	303	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
29	a	811	CLA	C4B-C3B-CAB-CBB
29	a	813	CLA	C4B-C3B-CAB-CBB
29	a	817	CLA	C4B-C3B-CAB-CBB
29	a	818	CLA	C4B-C3B-CAB-CBB
29	a	820	CLA	C4B-C3B-CAB-CBB
29	a	837	CLA	C4B-C3B-CAB-CBB
29	b	707	CLA	C4B-C3B-CAB-CBB
29	b	711	CLA	C1A-C2A-CAA-CBA
29	b	713	CLA	C4B-C3B-CAB-CBB
29	b	715	CLA	C4B-C3B-CAB-CBB
29	b	726	CLA	C4B-C3B-CAB-CBB
29	i	203	CLA	C1A-C2A-CAA-CBA
29	l	503	CLA	C4B-C3B-CAB-CBB
29	A	206	CLA	C4B-C3B-CAB-CBB
29	A	214	CLA	C4B-C3B-CAB-CBB
29	A	217	CLA	C4B-C3B-CAB-CBB
29	I	208	CLA	C4B-C3B-CAB-CBB
29	I	212	CLA	C4B-C3B-CAB-CBB
29	I	214	CLA	C1A-C2A-CAA-CBA
29	K	207	CLA	C4B-C3B-CAB-CBB
29	K	213	CLA	C4B-C3B-CAB-CBB
29	K	218	CLA	C4B-C3B-CAB-CBB
29	F	311	CLA	C4B-C3B-CAB-CBB
29	J	305	CLA	C4B-C3B-CAB-CBB
29	M	311	CLA	C1A-C2A-CAA-CBA
29	D	312	CLA	C4B-C3B-CAB-CBB
29	B	306	CLA	C4B-C3B-CAB-CBB
29	B	307	CLA	C4B-C3B-CAB-CBB
29	B	312	CLA	C1A-C2A-CAA-CBA
29	B	316	CLA	C4B-C3B-CAB-CBB
29	H	307	CLA	C4B-C3B-CAB-CBB
29	O	308	CLA	C4B-C3B-CAB-CBB
29	T	308	CLA	C4B-C3B-CAB-CBB
29	Q	307	CLA	C4B-C3B-CAB-CBB
29	C	308	CLA	C4B-C3B-CAB-CBB
29	E	305	CLA	C4B-C3B-CAB-CBB
29	E	309	CLA	C4B-C3B-CAB-CBB
29	E	315	CLA	C4B-C3B-CAB-CBB
29	b	736	CLA	C4-C3-C5-C6
29	K	211	CLA	C2A-CAA-CBA-CGA
29	D	312	CLA	C2A-CAA-CBA-CGA
34	K	220	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
29	G	311	CLA	C2-C3-C5-C6
29	B	311	CLA	C2-C3-C5-C6
40	B	317	SQD	C12-C13-C14-C15
29	J	306	CLA	C3-C5-C6-C7
29	l	501	CLA	C6-C7-C8-C10
29	l	502	CLA	C12-C13-C15-C16
29	B	312	CLA	C12-C13-C15-C16
35	G	320	DGD	O6D-C5D-C6D-O5D
29	G	312	CLA	C16-C17-C18-C20
29	E	309	CLA	C3A-C2A-CAA-CBA
29	b	707	CLA	C16-C17-C18-C19
29	A	209	CLA	C16-C17-C18-C19
29	I	217	CLA	C6-C7-C8-C10
35	h	203	DGD	CBB-CCB-CDB-CEB
29	P	212	CLA	C2A-CAA-CBA-CGA
29	Q	310	CLA	C11-C10-C8-C9
29	F	307	CLA	O1A-CGA-O2A-C1
36	I	205	DD6	C11-C10-C9-C8
29	G	301	CLA	C1-C2-C3-C4
38	N	306	UIX	C25-C28-C32-C35
39	G	315	KC1	C3A-C2A-CAA-CBA
39	I	215	KC1	C1A-C2A-CAA-CBA
39	F	309	KC1	C1A-C2A-CAA-CBA
39	F	314	KC1	C3A-C2A-CAA-CBA
39	L	314	KC1	C1A-C2A-CAA-CBA
39	H	309	KC1	C3A-C2A-CAA-CBA
39	H	314	KC1	C1A-C2A-CAA-CBA
39	N	310	KC1	C1A-C2A-CAA-CBA
39	T	312	KC1	C3A-C2A-CAA-CBA
39	E	312	KC1	C3A-C2A-CAA-CBA
29	A	210	CLA	O1A-CGA-O2A-C1
34	K	201	LMG	C14-C15-C16-C17
34	j	102	LMG	O7-C8-C9-O8
35	G	320	DGD	O2G-C2G-C3G-O3G
35	B	318	DGD	O2G-C2G-C3G-O3G
29	A	212	CLA	C6-C7-C8-C10
34	b	732	LMG	C7-C8-C9-O8
34	j	102	LMG	C7-C8-C9-O8
35	B	318	DGD	C1G-C2G-C3G-O3G
29	b	703	CLA	CAD-CBD-CGD-O2D
29	A	209	CLA	CAD-CBD-CGD-O2D
29	G	314	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	K	216	CLA	CAD-CBD-CGD-O2D
29	D	311	CLA	CAD-CBD-CGD-O2D
29	D	316	CLA	CAD-CBD-CGD-O2D
29	H	315	CLA	CAD-CBD-CGD-O2D
29	N	316	CLA	CAD-CBD-CGD-O2D
29	P	212	CLA	CAD-CBD-CGD-O2D
37	D	307	PID	O4-C12-C13-C14
37	N	301	PID	O4-C12-C13-C14
37	C	301	PID	O4-C12-C13-C14
37	P	205	PID	O4-C12-C13-C14
29	A	207	CLA	O1D-CGD-O2D-CED
29	G	319	CLA	CBD-CGD-O2D-CED
40	J	314	SQD	C23-C24-C25-C26
29	b	701	CLA	C2A-CAA-CBA-CGA
29	N	309	CLA	C2A-CAA-CBA-CGA
29	T	311	CLA	C2A-CAA-CBA-CGA
29	E	311	CLA	C2A-CAA-CBA-CGA
40	J	314	SQD	O49-C7-O47-C45
29	a	830	CLA	CHA-CBD-CGD-O1D
29	b	703	CLA	CAD-CBD-CGD-O1D
29	b	710	CLA	CHA-CBD-CGD-O1D
29	b	710	CLA	CHA-CBD-CGD-O2D
29	l	503	CLA	CHA-CBD-CGD-O1D
29	A	209	CLA	CAD-CBD-CGD-O1D
29	A	214	CLA	CAD-CBD-CGD-O1D
29	G	314	CLA	CAD-CBD-CGD-O1D
29	I	212	CLA	CHA-CBD-CGD-O1D
29	K	216	CLA	CAD-CBD-CGD-O1D
29	M	313	CLA	CHA-CBD-CGD-O1D
29	L	307	CLA	CHA-CBD-CGD-O1D
29	D	311	CLA	CAD-CBD-CGD-O1D
29	D	316	CLA	CAD-CBD-CGD-O1D
29	H	315	CLA	CAD-CBD-CGD-O1D
29	N	316	CLA	CAD-CBD-CGD-O1D
29	O	311	CLA	CHA-CBD-CGD-O1D
29	O	311	CLA	CHA-CBD-CGD-O2D
29	Q	310	CLA	CHA-CBD-CGD-O1D
29	Q	310	CLA	CHA-CBD-CGD-O2D
29	P	212	CLA	CAD-CBD-CGD-O1D
32	l	507	BCR	C9-C10-C11-C12
36	B	301	DD6	C24-C25-C26-C27
36	E	303	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
38	N	306	UIX	C26-C30-C34-C37
39	A	205	KC1	CHA-CBD-CGD-O1D
39	T	310	KC1	CHA-CBD-CGD-O2D
39	Q	311	KC1	CHA-CBD-CGD-O2D
39	P	211	KC1	CHA-CBD-CGD-O1D
29	a	801	CLA	C16-C17-C18-C19
29	a	811	CLA	C2B-C3B-CAB-CBB
29	a	817	CLA	C2B-C3B-CAB-CBB
29	a	818	CLA	C2B-C3B-CAB-CBB
29	b	704	CLA	C2B-C3B-CAB-CBB
29	b	726	CLA	C2B-C3B-CAB-CBB
29	l	503	CLA	C2B-C3B-CAB-CBB
29	A	217	CLA	C2B-C3B-CAB-CBB
29	G	311	CLA	C2B-C3B-CAB-CBB
29	I	208	CLA	C2B-C3B-CAB-CBB
29	I	213	CLA	C2B-C3B-CAB-CBB
29	F	311	CLA	C2B-C3B-CAB-CBB
29	J	311	CLA	C2B-C3B-CAB-CBB
29	L	307	CLA	C2B-C3B-CAB-CBB
29	D	312	CLA	C2B-C3B-CAB-CBB
29	B	306	CLA	C2B-C3B-CAB-CBB
29	B	307	CLA	C2B-C3B-CAB-CBB
29	B	316	CLA	C2B-C3B-CAB-CBB
29	T	308	CLA	C2B-C3B-CAB-CBB
29	Q	307	CLA	C2B-C3B-CAB-CBB
29	C	308	CLA	C2B-C3B-CAB-CBB
29	E	309	CLA	C2B-C3B-CAB-CBB
29	E	315	CLA	C2B-C3B-CAB-CBB
29	T	311	CLA	O1A-CGA-O2A-C1
32	a	835	BCR	C7-C8-C9-C34
32	b	728	BCR	C7-C8-C9-C34
29	D	311	CLA	CBA-CGA-O2A-C1
34	b	730	LMG	C16-C17-C18-C19
34	E	316	LMG	C31-C32-C33-C34
34	K	220	LMG	C10-C11-C12-C13
29	b	725	CLA	O1D-CGD-O2D-CED
29	A	211	CLA	C5-C6-C7-C8
29	f	805	CLA	C5-C6-C7-C8
32	f	801	BCR	C15-C16-C17-C18
31	a	833	LHG	C14-C15-C16-C17
29	Q	310	CLA	CBA-CGA-O2A-C1
29	Q	310	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	b	723	CLA	CBD-CGD-O2D-CED
29	a	812	CLA	C11-C10-C8-C9
29	a	831	CLA	C11-C12-C13-C14
29	b	714	CLA	C11-C10-C8-C9
29	b	718	CLA	C6-C7-C8-C9
29	l	505	CLA	C11-C10-C8-C9
29	G	304	CLA	C11-C10-C8-C9
29	J	308	CLA	C6-C7-C8-C9
29	a	812	CLA	C11-C10-C8-C7
29	A	218	CLA	C6-C7-C8-C10
29	B	310	CLA	C6-C7-C8-C10
29	Q	308	CLA	C11-C12-C13-C15
29	J	308	CLA	O1D-CGD-O2D-CED
29	M	315	CLA	CAA-CBA-CGA-O2A
35	G	320	DGD	C4D-C5D-C6D-O5D
29	a	807	CLA	C4-C3-C5-C6
29	l	505	CLA	C2-C3-C5-C6
29	a	818	CLA	CAA-CBA-CGA-O2A
29	K	212	CLA	CAA-CBA-CGA-O2A
29	b	701	CLA	O1D-CGD-O2D-CED
32	l	506	BCR	C13-C14-C15-C16
29	L	310	CLA	C2A-CAA-CBA-CGA
29	a	825	CLA	C5-C6-C7-C8
34	K	219	LMG	C34-C35-C36-C37
29	a	824	CLA	O1D-CGD-O2D-CED
39	G	315	KC1	CAA-CBA-CGA-O2A
29	l	504	CLA	C4-C3-C5-C6
29	G	317	CLA	C4-C3-C5-C6
29	B	306	CLA	O2A-C1-C2-C3
35	h	203	DGD	C4B-C5B-C6B-C7B
35	B	318	DGD	C5D-C6D-O5D-C1E
29	i	202	CLA	C15-C16-C17-C18
29	a	818	CLA	C2A-CAA-CBA-CGA
29	b	703	CLA	C2A-CAA-CBA-CGA
29	j	104	CLA	C2A-CAA-CBA-CGA
29	A	209	CLA	C2A-CAA-CBA-CGA
36	P	204	DD6	C24-C25-C26-C27
29	I	213	CLA	C16-C17-C18-C20
29	M	307	CLA	C4-C3-C5-C6
29	i	203	CLA	CAA-CBA-CGA-O2A
29	G	311	CLA	O1A-CGA-O2A-C1
37	T	317	PID	C28-C27-O6-C30

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Mol	Chain	Res	Type	Atoms
36	I	206	DD6	C27-C29-C30-C31
36	B	301	DD6	C27-C29-C30-C31
36	B	302	DD6	C27-C29-C30-C31
36	T	303	DD6	C27-C29-C30-C31
29	f	805	CLA	C11-C12-C13-C15
29	a	825	CLA	C6-C7-C8-C9
29	b	725	CLA	C6-C7-C8-C9
29	l	501	CLA	C6-C7-C8-C9
29	A	209	CLA	C11-C12-C13-C14
29	G	312	CLA	C6-C7-C8-C9
29	E	308	CLA	C11-C10-C8-C9
29	a	825	CLA	CBA-CGA-O2A-C1
29	G	311	CLA	CBA-CGA-O2A-C1
29	K	213	CLA	CBA-CGA-O2A-C1
29	K	217	CLA	C4B-C3B-CAB-CBB
29	P	212	CLA	C4B-C3B-CAB-CBB
29	B	314	CLA	CBD-CGD-O2D-CED
29	b	726	CLA	C16-C17-C18-C20
29	b	716	CLA	CBA-CGA-O2A-C1
29	a	801	CLA	C5-C6-C7-C8
29	b	716	CLA	O1A-CGA-O2A-C1
29	N	311	CLA	C2A-CAA-CBA-CGA
29	l	503	CLA	C4-C3-C5-C6
29	I	212	CLA	C4-C3-C5-C6
36	K	202	DD6	C24-C25-C26-C27
29	G	301	CLA	CBA-CGA-O2A-C1
39	H	314	KC1	C4B-C3B-CAB-CBB
39	P	211	KC1	C4B-C3B-CAB-CBB
34	E	316	LMG	C30-C31-C32-C33
35	b	733	DGD	C8B-C9B-CAB-CBB
29	b	723	CLA	O1D-CGD-O2D-CED
29	b	704	CLA	CAA-CBA-CGA-O2A
29	a	829	CLA	C11-C12-C13-C15
29	b	703	CLA	C11-C10-C8-C7
29	G	302	CLA	C12-C13-C15-C16
29	K	213	CLA	O1A-CGA-O2A-C1
29	a	810	CLA	C5-C6-C7-C8
29	a	801	CLA	C16-C17-C18-C20
34	b	732	LMG	C35-C36-C37-C38
29	a	825	CLA	O1A-CGA-O2A-C1
34	K	220	LMG	O1-C7-C8-O7
35	b	733	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
29	b	708	CLA	C3A-C2A-CAA-CBA
29	l	510	CLA	C3A-C2A-CAA-CBA
29	M	309	CLA	C3A-C2A-CAA-CBA
29	O	313	CLA	C3A-C2A-CAA-CBA
34	A	219	LMG	C33-C34-C35-C36
29	M	308	CLA	CBA-CGA-O2A-C1
32	b	735	BCR	C20-C21-C22-C37
32	f	801	BCR	C16-C17-C18-C36
32	f	804	BCR	C35-C13-C14-C15
40	J	314	SQD	O5-C1-O6-C44
31	a	833	LHG	C9-C10-C11-C12
29	l	510	CLA	CAA-CBA-CGA-O1A
29	G	319	CLA	O1D-CGD-O2D-CED
29	b	716	CLA	C2-C1-O2A-CGA
29	b	718	CLA	C2-C1-O2A-CGA
29	I	209	CLA	C2-C1-O2A-CGA
36	D	304	DD6	C24-C25-C26-C27
38	T	306	UIX	C34-C37-C39-C40
29	a	830	CLA	C3-C5-C6-C7
29	H	308	CLA	C15-C16-C17-C18
29	G	311	CLA	C4-C3-C5-C6
29	B	311	CLA	C4-C3-C5-C6
35	B	318	DGD	C1A-C2A-C3A-C4A
29	l	510	CLA	CAA-CBA-CGA-O2A
29	L	316	CLA	C2C-C3C-CAC-CBC
29	i	202	CLA	C2A-CAA-CBA-CGA
35	j	106	DGD	O1G-C1G-C2G-C3G
35	B	318	DGD	C2A-C3A-C4A-C5A
29	M	308	CLA	O1A-CGA-O2A-C1
29	a	803	CLA	C6-C7-C8-C9
29	a	825	CLA	C14-C13-C15-C16
29	b	701	CLA	C14-C13-C15-C16
29	b	703	CLA	C11-C10-C8-C9
29	b	725	CLA	C11-C12-C13-C14
29	b	736	CLA	C6-C7-C8-C9
29	b	736	CLA	C11-C10-C8-C9
29	J	306	CLA	C14-C13-C15-C16
29	C	309	CLA	C6-C7-C8-C9
30	a	832	PQN	C19-C18-C20-C21
34	K	220	LMG	C31-C32-C33-C34
34	A	219	LMG	C7-C8-O7-C10
29	b	704	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	m	102	DGD	CAA-CBA-CCA-CDA
29	f	805	CLA	C2A-CAA-CBA-CGA
29	A	207	CLA	C2A-CAA-CBA-CGA
29	I	208	CLA	C2A-CAA-CBA-CGA
29	H	310	CLA	C2A-CAA-CBA-CGA
39	I	215	KC1	CAA-CBA-CGA-O1A
29	a	808	CLA	C1A-C2A-CAA-CBA
29	a	816	CLA	C1A-C2A-CAA-CBA
29	b	708	CLA	C1A-C2A-CAA-CBA
29	b	709	CLA	C1A-C2A-CAA-CBA
29	G	317	CLA	C1A-C2A-CAA-CBA
29	K	214	CLA	C1A-C2A-CAA-CBA
29	D	311	CLA	C1A-C2A-CAA-CBA
29	O	313	CLA	C1A-C2A-CAA-CBA
32	b	735	BCR	C20-C21-C22-C23
32	f	801	BCR	C16-C17-C18-C19
32	f	804	BCR	C12-C13-C14-C15
35	j	106	DGD	O6D-C5D-C6D-O5D
29	a	801	CLA	C2B-C3B-CAB-CBB
29	a	813	CLA	C2B-C3B-CAB-CBB
29	a	820	CLA	C2B-C3B-CAB-CBB
29	a	822	CLA	C2B-C3B-CAB-CBB
29	a	837	CLA	C2B-C3B-CAB-CBB
29	b	707	CLA	C2B-C3B-CAB-CBB
29	b	713	CLA	C2B-C3B-CAB-CBB
29	b	715	CLA	C2B-C3B-CAB-CBB
29	A	206	CLA	C2B-C3B-CAB-CBB
29	A	214	CLA	C2B-C3B-CAB-CBB
29	G	312	CLA	C2B-C3B-CAB-CBB
29	I	212	CLA	C2B-C3B-CAB-CBB
29	K	207	CLA	C2B-C3B-CAB-CBB
29	K	213	CLA	C2B-C3B-CAB-CBB
29	K	218	CLA	C2B-C3B-CAB-CBB
29	F	313	CLA	C2B-C3B-CAB-CBB
29	J	305	CLA	C2B-C3B-CAB-CBB
29	H	307	CLA	C2B-C3B-CAB-CBB
29	O	308	CLA	C2B-C3B-CAB-CBB
29	Q	312	CLA	C2B-C3B-CAB-CBB
29	Q	313	CLA	C2B-C3B-CAB-CBB
29	P	212	CLA	C2B-C3B-CAB-CBB
29	E	305	CLA	C2B-C3B-CAB-CBB
32	a	838	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
32	b	729	BCR	C5-C6-C7-C8
32	b	729	BCR	C23-C24-C25-C30
32	b	735	BCR	C5-C6-C7-C8
32	l	506	BCR	C5-C6-C7-C8
32	l	506	BCR	C23-C24-C25-C26
32	m	103	BCR	C23-C24-C25-C26
29	G	301	CLA	O1A-CGA-O2A-C1
35	m	102	DGD	C5B-C6B-C7B-C8B
29	I	217	CLA	C4-C3-C5-C6
29	K	212	CLA	C4-C3-C5-C6
29	B	308	CLA	C4-C3-C5-C6
29	E	311	CLA	C4-C3-C5-C6
29	a	807	CLA	C2-C3-C5-C6
29	l	503	CLA	C2-C3-C5-C6
29	a	801	CLA	C6-C7-C8-C10
29	a	807	CLA	C11-C12-C13-C15
29	a	811	CLA	C6-C7-C8-C10
29	a	825	CLA	C12-C13-C15-C16
29	b	736	CLA	C6-C7-C8-C10
29	A	209	CLA	C11-C12-C13-C15
29	G	312	CLA	C6-C7-C8-C10
29	B	310	CLA	C12-C13-C15-C16
29	Q	308	CLA	C6-C7-C8-C10
29	Q	308	CLA	C12-C13-C15-C16
29	H	308	CLA	C2A-CAA-CBA-CGA
31	a	833	LHG	C11-C10-C9-C8
29	a	827	CLA	C13-C15-C16-C17
34	b	732	LMG	C16-C17-C18-C19
29	a	806	CLA	C5-C6-C7-C8
29	I	213	CLA	C16-C17-C18-C19
32	b	729	BCR	C37-C22-C23-C24
38	A	203	UIX	C14-C23-C26-C29
29	a	812	CLA	C2-C3-C5-C6
29	E	311	CLA	C2-C3-C5-C6
29	I	214	CLA	C6-C7-C8-C9
39	Q	314	KC1	C2A-CAA-CBA-CGA
29	D	311	CLA	C2A-CAA-CBA-CGA
29	b	709	CLA	C11-C10-C8-C9
29	E	306	CLA	C14-C13-C15-C16
34	b	734	LMG	C31-C32-C33-C34
36	B	319	DD6	C24-C25-C26-C27
37	N	305	PID	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
34	h	205	LMG	C11-C12-C13-C14
29	a	806	CLA	C4-C3-C5-C6
30	b	727	PQN	C14-C13-C15-C16
29	b	702	CLA	C2-C3-C5-C6
29	O	309	CLA	C2-C3-C5-C6
29	Q	308	CLA	C10-C11-C12-C13
29	l	505	CLA	CAA-CBA-CGA-O1A
34	b	734	LMG	C12-C13-C14-C15
34	j	102	LMG	O1-C7-C8-C9
34	b	732	LMG	C4-C5-C6-O5
29	a	829	CLA	C2A-CAA-CBA-CGA
29	G	314	CLA	C2A-CAA-CBA-CGA
29	J	311	CLA	C2A-CAA-CBA-CGA
29	L	313	CLA	C2A-CAA-CBA-CGA
29	T	314	CLA	C2A-CAA-CBA-CGA
29	C	309	CLA	C2A-CAA-CBA-CGA
29	N	314	CLA	C2-C1-O2A-CGA
36	K	204	DD6	C27-C29-C30-C31
36	K	205	DD6	C27-C29-C30-C31
29	M	306	CLA	C4-C3-C5-C6
29	B	309	CLA	C4-C3-C5-C6
29	a	806	CLA	C2-C3-C5-C6
29	N	309	CLA	C10-C11-C12-C13
29	a	822	CLA	C4B-C3B-CAB-CBB
29	b	702	CLA	C4B-C3B-CAB-CBB
29	Q	313	CLA	C4B-C3B-CAB-CBB
37	D	307	PID	C19-C20-C21-CM5
37	C	305	PID	C19-C20-C21-CM5
29	B	314	CLA	O1D-CGD-O2D-CED
29	a	810	CLA	C4-C3-C5-C6
29	a	801	CLA	CAA-CBA-CGA-O2A
29	N	309	CLA	C15-C16-C17-C18
29	a	823	CLA	C6-C7-C8-C10
29	B	316	CLA	CAA-CBA-CGA-O2A
29	L	316	CLA	C4C-C3C-CAC-CBC
29	l	502	CLA	C14-C13-C15-C16
29	l	503	CLA	C6-C7-C8-C9
29	B	312	CLA	C14-C13-C15-C16
29	P	210	CLA	C14-C13-C15-C16
29	E	311	CLA	C11-C12-C13-C14
34	h	205	LMG	C8-C7-O1-C1
29	i	203	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	I	214	CLA	C2A-CAA-CBA-CGA
29	T	313	CLA	C2A-CAA-CBA-CGA
29	a	822	CLA	C2-C1-O2A-CGA
29	a	823	CLA	C2-C1-O2A-CGA
29	a	826	CLA	C2-C1-O2A-CGA
29	a	829	CLA	C2-C1-O2A-CGA
29	i	203	CLA	C2-C1-O2A-CGA
29	K	210	CLA	C2-C1-O2A-CGA
29	M	314	CLA	C2-C1-O2A-CGA
29	B	308	CLA	C3-C5-C6-C7
29	f	805	CLA	C3A-C2A-CAA-CBA
34	b	734	LMG	C30-C31-C32-C33
39	P	216	KC1	C2B-C3B-CAB-CBB
29	a	825	CLA	C3-C5-C6-C7
29	b	702	CLA	C3-C5-C6-C7
29	O	309	CLA	C16-C17-C18-C20
39	C	315	KC1	CAA-CBA-CGA-O1A
29	b	736	CLA	O2A-C1-C2-C3
37	F	302	PID	C15-C16-C17-C18
29	I	214	CLA	C6-C7-C8-C10
29	a	809	CLA	C13-C15-C16-C17
29	O	314	CLA	C2A-CAA-CBA-CGA
29	a	809	CLA	C10-C11-C12-C13
29	l	502	CLA	C15-C16-C17-C18
29	E	308	CLA	C10-C11-C12-C13
29	E	306	CLA	C16-C17-C18-C20
36	A	204	DD6	C13-C14-C15-O1
36	G	308	DD6	C13-C14-C15-O1
36	I	205	DD6	C13-C14-C15-O1
36	K	204	DD6	C13-C14-C15-O1
36	K	206	DD6	C13-C14-C15-O1
36	M	303	DD6	C13-C14-C15-O1
36	D	304	DD6	C13-C14-C15-O1
36	B	302	DD6	C13-C14-C15-O1
36	B	305	DD6	C13-C14-C15-O1
36	B	319	DD6	C13-C14-C15-O1
37	D	302	PID	O1-C6-C7-C8
37	D	307	PID	C19-C20-C21-C22
37	O	307	PID	O1-C6-C7-C8
37	C	301	PID	O1-C6-C7-C8
37	C	305	PID	C19-C20-C21-C22
37	P	203	PID	O1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	a	817	CLA	CAA-CBA-CGA-O2A
29	B	316	CLA	CAA-CBA-CGA-O1A
29	G	301	CLA	O2A-C1-C2-C3
29	a	817	CLA	CAA-CBA-CGA-O1A
29	h	201	CLA	C8-C10-C11-C12
29	P	210	CLA	C15-C16-C17-C18
39	O	315	KC1	C4B-C3B-CAB-CBB
39	T	315	KC1	C4B-C3B-CAB-CBB
39	Q	314	KC1	C4B-C3B-CAB-CBB
39	C	315	KC1	C4B-C3B-CAB-CBB
39	P	216	KC1	C4B-C3B-CAB-CBB
29	O	308	CLA	O1D-CGD-O2D-CED
29	b	720	CLA	C4-C3-C5-C6
29	A	211	CLA	C4-C3-C5-C6
29	L	316	CLA	C2A-CAA-CBA-CGA
29	L	309	CLA	CAA-CBA-CGA-O2A
29	f	803	CLA	CBD-CGD-O2D-CED
37	O	305	PID	C14-C15-C16-C17
37	T	307	PID	C7-C8-C9-C10
38	P	207	UIX	C25-C28-C32-C33
29	a	812	CLA	C11-C12-C13-C14
30	a	832	PQN	C15-C16-C17-C18
29	K	209	CLA	C6-C7-C8-C9
35	m	102	DGD	C2B-C3B-C4B-C5B
34	j	102	LMG	O1-C7-C8-O7
29	I	213	CLA	C6-C7-C8-C9
29	B	312	CLA	C6-C7-C8-C9
29	N	309	CLA	C14-C13-C15-C16
29	a	821	CLA	CAA-CBA-CGA-O2A
29	b	703	CLA	CAA-CBA-CGA-O2A
35	j	106	DGD	O1G-C1A-C2A-C3A
32	a	835	BCR	C7-C8-C9-C10
36	K	203	DD6	C5-C6-C8-C9
36	T	303	DD6	C2-C1-C24-C25
29	B	308	CLA	CBD-CGD-O2D-CED
29	G	302	CLA	CAA-CBA-CGA-O1A
29	A	208	CLA	CAA-CBA-CGA-O2A
29	b	720	CLA	C2-C3-C5-C6
29	I	207	CLA	C2A-CAA-CBA-CGA
29	a	803	CLA	C11-C10-C8-C7
29	a	806	CLA	C11-C12-C13-C15
29	a	829	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	b	709	CLA	C11-C10-C8-C7
29	b	721	CLA	C6-C7-C8-C10
29	i	202	CLA	C6-C7-C8-C10
29	l	503	CLA	C6-C7-C8-C10
29	l	503	CLA	C11-C10-C8-C7
29	G	316	CLA	C11-C12-C13-C15
29	J	306	CLA	C12-C13-C15-C16
29	D	311	CLA	O1A-CGA-O2A-C1
29	b	717	CLA	O1A-CGA-O2A-C1
29	D	313	CLA	C4C-C3C-CAC-CBC
29	a	812	CLA	C2B-C3B-CAB-CBB
29	a	816	CLA	C2B-C3B-CAB-CBB
29	b	721	CLA	C2B-C3B-CAB-CBB
29	A	208	CLA	C2B-C3B-CAB-CBB
29	A	210	CLA	C2B-C3B-CAB-CBB
29	C	313	CLA	C2B-C3B-CAB-CBB
29	E	306	CLA	C2B-C3B-CAB-CBB
32	b	729	BCR	C23-C24-C25-C26
32	i	204	BCR	C1-C6-C7-C8
32	i	204	BCR	C5-C6-C7-C8
29	b	717	CLA	CAA-CBA-CGA-O2A
29	b	705	CLA	C2-C1-O2A-CGA
29	B	308	CLA	C2-C1-O2A-CGA
29	f	803	CLA	O1D-CGD-O2D-CED
29	b	707	CLA	C13-C15-C16-C17
36	D	301	DD6	C11-C13-C14-C15
37	H	305	PID	C6-C7-C8-C9
37	O	307	PID	C6-C7-C8-C9
37	T	317	PID	C6-C7-C8-C9
29	b	720	CLA	CAA-CBA-CGA-O2A
29	b	701	CLA	C13-C15-C16-C17
29	O	309	CLA	C16-C17-C18-C19
29	I	209	CLA	CAA-CBA-CGA-O2A
29	K	210	CLA	CAA-CBA-CGA-O2A
29	M	307	CLA	C2-C3-C5-C6
29	G	311	CLA	C2A-CAA-CBA-CGA
29	K	207	CLA	C2A-CAA-CBA-CGA
29	H	312	CLA	C2A-CAA-CBA-CGA
29	Q	310	CLA	C2A-CAA-CBA-CGA
29	I	211	CLA	C13-C15-C16-C17
29	b	710	CLA	CAA-CBA-CGA-O2A
29	G	313	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	K	217	CLA	CAA-CBA-CGA-O2A
34	K	201	LMG	C30-C31-C32-C33
29	F	311	CLA	CAA-CBA-CGA-O2A
29	L	316	CLA	CAA-CBA-CGA-O2A
35	b	733	DGD	O2G-C1B-C2B-C3B
40	J	314	SQD	C4-C5-C6-S
34	b	730	LMG	C40-C41-C42-C43
35	j	103	DGD	O1G-C1A-C2A-C3A
29	a	831	CLA	O1A-CGA-O2A-C1
29	b	709	CLA	C2-C3-C5-C6
29	G	317	CLA	C2-C3-C5-C6
34	j	102	LMG	O9-C10-C11-C12
35	B	318	DGD	C4B-C5B-C6B-C7B
39	N	310	KC1	CAA-CBA-CGA-O2A
39	P	211	KC1	CAA-CBA-CGA-O2A
29	a	802	CLA	C2A-CAA-CBA-CGA
29	b	706	CLA	C2A-CAA-CBA-CGA
31	a	833	LHG	C24-C25-C26-C27
29	L	307	CLA	CAA-CBA-CGA-O2A
29	b	720	CLA	C11-C10-C8-C9
29	b	726	CLA	C11-C10-C8-C9
29	l	503	CLA	C11-C10-C8-C9
29	B	308	CLA	C14-C13-C15-C16
29	B	310	CLA	C14-C13-C15-C16
30	a	832	PQN	C24-C23-C25-C26
29	D	311	CLA	CAA-CBA-CGA-O2A
34	K	201	LMG	O1-C7-C8-C9
34	j	102	LMG	C11-C12-C13-C14
29	a	816	CLA	C4B-C3B-CAB-CBB
29	b	703	CLA	C1A-C2A-CAA-CBA
29	b	722	CLA	C1A-C2A-CAA-CBA
29	A	215	CLA	C1A-C2A-CAA-CBA
29	A	215	CLA	C4B-C3B-CAB-CBB
29	I	207	CLA	C4B-C3B-CAB-CBB
29	I	209	CLA	C1A-C2A-CAA-CBA
29	K	212	CLA	C1A-C2A-CAA-CBA
29	F	307	CLA	C4B-C3B-CAB-CBB
29	F	312	CLA	C1A-C2A-CAA-CBA
29	J	307	CLA	C4B-C3B-CAB-CBB
29	M	309	CLA	C1A-C2A-CAA-CBA
29	B	308	CLA	C1A-C2A-CAA-CBA
29	H	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	Q	312	CLA	C1A-C2A-CAA-CBA
29	P	215	CLA	C4B-C3B-CAB-CBB
29	E	306	CLA	C4B-C3B-CAB-CBB
29	E	308	CLA	C4B-C3B-CAB-CBB
29	b	709	CLA	C4-C3-C5-C6
29	H	310	CLA	CAA-CBA-CGA-O2A
29	I	217	CLA	C2-C3-C5-C6
32	l	507	BCR	C11-C12-C13-C14
38	A	203	UIX	C14-C23-C26-C30
36	M	302	DD6	C3-C4-C5-C6
38	N	306	UIX	C32-C35-C36-C38
29	a	806	CLA	CAA-CBA-CGA-O2A
29	a	831	CLA	CAA-CBA-CGA-O2A
29	b	709	CLA	CAA-CBA-CGA-O2A
29	l	501	CLA	CAA-CBA-CGA-O2A
29	D	312	CLA	CAA-CBA-CGA-O2A
40	J	314	SQD	C9-C10-C11-C12
34	j	102	LMG	O8-C28-C29-C30
29	a	813	CLA	C2-C3-C5-C6
29	a	807	CLA	C15-C16-C17-C18
29	A	209	CLA	C15-C16-C17-C18
29	J	308	CLA	C4-C3-C5-C6
29	b	714	CLA	C2-C1-O2A-CGA
29	j	104	CLA	C2-C1-O2A-CGA
29	B	310	CLA	C2-C1-O2A-CGA
29	a	823	CLA	C11-C10-C8-C7
29	a	824	CLA	C6-C7-C8-C10
29	b	705	CLA	C12-C13-C15-C16
29	b	726	CLA	C11-C12-C13-C15
29	i	201	CLA	C12-C13-C15-C16
29	I	213	CLA	C11-C12-C13-C15
29	P	210	CLA	C12-C13-C15-C16
29	E	311	CLA	C11-C12-C13-C15
40	J	314	SQD	C13-C14-C15-C16
34	A	219	LMG	C9-C8-O7-C10
34	b	732	LMG	C30-C31-C32-C33
29	b	717	CLA	CBA-CGA-O2A-C1
29	C	311	CLA	C2A-CAA-CBA-CGA
29	G	302	CLA	C8-C10-C11-C12
29	I	211	CLA	C16-C17-C18-C19
29	P	212	CLA	CAA-CBA-CGA-O2A
29	G	316	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	E	305	CLA	C8-C10-C11-C12
29	b	703	CLA	CAA-CBA-CGA-O1A
29	Q	308	CLA	C16-C17-C18-C20
34	A	219	LMG	O9-C10-C11-C12
35	b	733	DGD	O1B-C1B-C2B-C3B
29	a	831	CLA	CBA-CGA-O2A-C1
34	K	201	LMG	C10-C11-C12-C13
29	K	218	CLA	CAA-CBA-CGA-O2A
29	a	821	CLA	CAA-CBA-CGA-O1A
29	K	217	CLA	CAA-CBA-CGA-O1A
29	a	811	CLA	C6-C7-C8-C9
29	l	504	CLA	C6-C7-C8-C9
29	G	316	CLA	C11-C12-C13-C14
29	Q	308	CLA	C14-C13-C15-C16
29	b	710	CLA	CAA-CBA-CGA-O1A
38	O	306	UIX	C34-C37-C39-C40
29	a	831	CLA	C3-C5-C6-C7
29	L	316	CLA	CAA-CBA-CGA-O1A
29	a	813	CLA	CAA-CBA-CGA-O2A
29	f	805	CLA	C8-C10-C11-C12
37	H	306	PID	C5-C6-C7-C8
37	Q	306	PID	C5-C6-C7-C8
37	C	305	PID	C5-C6-C7-C8
38	J	304	UIX	C2-C-C7-C10
38	P	207	UIX	C25-C28-C32-C35
39	G	318	KC1	C1A-C2A-CAA-CBA
39	I	215	KC1	C3A-C2A-CAA-CBA
39	K	215	KC1	C3A-C2A-CAA-CBA
39	J	312	KC1	C3A-C2A-CAA-CBA
39	M	312	KC1	C1A-C2A-CAA-CBA
39	D	310	KC1	C1A-C2A-CAA-CBA
39	D	315	KC1	C1A-C2A-CAA-CBA
39	N	315	KC1	C1A-C2A-CAA-CBA
39	O	310	KC1	C1A-C2A-CAA-CBA
39	O	312	KC1	C3A-C2A-CAA-CBA
39	Q	314	KC1	C1A-C2A-CAA-CBA
39	C	310	KC1	C1A-C2A-CAA-CBA
39	P	213	KC1	C1A-C2A-CAA-CBA
39	E	307	KC1	C1A-C2A-CAA-CBA
40	J	314	SQD	O5-C5-C6-S
29	A	208	CLA	CAA-CBA-CGA-O1A
29	I	209	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	D	311	CLA	CAA-CBA-CGA-O1A
29	B	309	CLA	C5-C6-C7-C8
29	O	308	CLA	CBD-CGD-O2D-CED
35	j	106	DGD	O1A-C1A-C2A-C3A
29	B	315	CLA	C4C-C3C-CAC-CBC
29	b	709	CLA	CAA-CBA-CGA-O1A
29	K	210	CLA	CAA-CBA-CGA-O1A
29	N	311	CLA	CAA-CBA-CGA-O2A
29	H	307	CLA	O1D-CGD-O2D-CED
34	K	219	LMG	O1-C7-C8-C9
29	b	720	CLA	CAA-CBA-CGA-O1A
29	L	309	CLA	CAA-CBA-CGA-O1A
34	j	102	LMG	O10-C28-C29-C30
35	j	103	DGD	O1A-C1A-C2A-C3A
29	A	218	CLA	CAA-CBA-CGA-O2A
29	G	313	CLA	CAA-CBA-CGA-O1A
29	F	311	CLA	CAA-CBA-CGA-O1A
29	a	811	CLA	CAD-CBD-CGD-O2D
29	b	720	CLA	CAD-CBD-CGD-O2D
29	b	722	CLA	CAD-CBD-CGD-O2D
29	f	805	CLA	CAD-CBD-CGD-O2D
29	i	203	CLA	CAD-CBD-CGD-O2D
29	K	217	CLA	CAD-CBD-CGD-O2D
29	C	313	CLA	CAD-CBD-CGD-O2D
37	P	206	PID	O4-C12-C13-C14
37	P	208	PID	O4-C12-C13-C14
39	L	306	KC1	CAD-CBD-CGD-O2D
39	H	309	KC1	CAD-CBD-CGD-O2D
39	N	310	KC1	CAD-CBD-CGD-O2D
34	K	219	LMG	O8-C28-C29-C30
29	a	806	CLA	CAA-CBA-CGA-O1A
29	H	310	CLA	CAA-CBA-CGA-O1A
37	T	317	PID	C26-C27-O6-C30
35	j	105	DGD	O6D-C5D-C6D-O5D
40	J	314	SQD	C30-C31-C32-C33
29	D	312	CLA	CAA-CBA-CGA-O1A
29	Q	308	CLA	C2A-CAA-CBA-CGA
29	a	813	CLA	CAA-CBA-CGA-O1A
29	P	212	CLA	CAA-CBA-CGA-O1A
29	a	810	CLA	CAA-CBA-CGA-O2A
29	B	309	CLA	CAA-CBA-CGA-O2A
29	P	209	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
34	A	219	LMG	O7-C10-C11-C12
29	b	717	CLA	C15-C16-C17-C18
29	b	715	CLA	CBD-CGD-O2D-CED
29	E	306	CLA	C16-C17-C18-C19
29	a	831	CLA	CAA-CBA-CGA-O1A
29	l	501	CLA	CAA-CBA-CGA-O1A
29	L	307	CLA	CAA-CBA-CGA-O1A
37	T	302	PID	O7-C30-O6-C27
29	b	719	CLA	CAA-CBA-CGA-O2A
29	K	209	CLA	CAA-CBA-CGA-O2A
29	N	309	CLA	C2C-C3C-CAC-CBC
29	B	308	CLA	O1D-CGD-O2D-CED

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	h	204	PID	C24-C25-C26-C27-C28-C29
37	T	317	PID	C24-C25-C26-C27-C28-C29
37	F	304	PID	C24-C25-C26-C27-C28-C29

331 monomers are involved in 958 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	D	315	KC1	2	0
29	C	311	CLA	2	0
29	N	311	CLA	1	0
36	J	303	DD6	1	0
29	M	314	CLA	1	0
37	N	301	PID	2	0
37	O	307	PID	5	0
37	Q	303	PID	2	0
36	B	301	DD6	2	0
29	D	312	CLA	4	0
36	G	307	DD6	3	0
36	I	205	DD6	3	0
29	a	804	CLA	6	0
37	T	301	PID	4	0
29	a	828	CLA	4	0
39	P	211	KC1	1	0
29	a	837	CLA	5	0
32	m	103	BCR	8	0
29	A	206	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	K	219	LMG	2	0
36	I	206	DD6	1	0
37	O	305	PID	7	0
29	Q	313	CLA	4	0
29	J	307	CLA	2	0
29	L	313	CLA	4	0
36	G	305	DD6	1	0
29	b	726	CLA	6	0
35	j	103	DGD	2	0
36	O	303	DD6	2	0
29	I	209	CLA	4	0
34	b	732	LMG	6	0
29	O	309	CLA	6	0
37	P	205	PID	3	0
29	a	801	CLA	4	0
29	b	713	CLA	1	0
36	P	204	DD6	1	0
29	H	315	CLA	2	0
38	B	304	UIX	1	0
29	a	825	CLA	4	0
39	P	216	KC1	1	0
29	H	308	CLA	5	0
36	L	305	DD6	1	0
36	N	303	DD6	1	0
35	m	102	DGD	5	0
29	M	315	CLA	1	0
29	I	217	CLA	4	0
29	G	301	CLA	2	0
29	J	306	CLA	5	0
37	h	204	PID	1	0
29	a	815	CLA	1	0
29	a	802	CLA	4	0
37	P	208	PID	3	0
29	A	207	CLA	1	0
29	G	312	CLA	4	0
36	K	204	DD6	2	0
29	a	817	CLA	1	0
29	I	208	CLA	1	0
29	i	202	CLA	8	0
29	N	314	CLA	5	0
37	P	206	PID	9	0
29	Q	308	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	K	211	CLA	3	0
37	P	203	PID	5	0
39	H	309	KC1	1	0
29	B	307	CLA	2	0
37	H	304	PID	4	0
39	E	307	KC1	2	0
36	K	221	DD6	2	0
29	b	704	CLA	2	0
29	E	305	CLA	6	0
35	j	106	DGD	4	0
29	L	310	CLA	3	0
35	b	733	DGD	2	0
34	j	102	LMG	3	0
29	J	313	CLA	1	0
29	F	307	CLA	3	0
29	T	311	CLA	1	0
29	M	309	CLA	2	0
29	E	313	CLA	2	0
35	j	105	DGD	4	0
29	a	826	CLA	5	0
36	M	303	DD6	1	0
29	a	823	CLA	5	0
32	b	729	BCR	5	0
29	K	217	CLA	1	0
34	P	201	LMG	1	0
32	l	507	BCR	4	0
32	a	838	BCR	5	0
29	I	214	CLA	4	0
29	a	811	CLA	2	0
29	N	308	CLA	1	0
29	b	725	CLA	3	0
37	Q	304	PID	5	0
29	B	309	CLA	1	0
29	H	312	CLA	2	0
29	a	819	CLA	4	0
36	B	303	DD6	1	0
29	b	702	CLA	11	0
29	A	217	CLA	2	0
29	M	308	CLA	1	0
29	b	701	CLA	5	0
29	a	827	CLA	4	0
29	b	736	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	G	304	CLA	7	0
29	a	820	CLA	4	0
29	L	315	CLA	2	0
29	h	201	CLA	7	0
29	C	308	CLA	2	0
29	a	806	CLA	11	0
37	O	302	PID	8	0
29	F	308	CLA	1	0
29	f	802	CLA	1	0
37	j	101	PID	5	0
29	I	212	CLA	3	0
29	Q	312	CLA	3	0
37	E	301	PID	7	0
37	H	305	PID	7	0
37	C	302	PID	4	0
29	I	210	CLA	3	0
29	b	731	CLA	2	0
37	N	302	PID	4	0
29	E	314	CLA	1	0
36	A	202	DD6	1	0
29	a	810	CLA	7	0
29	H	313	CLA	4	0
29	D	308	CLA	1	0
29	F	315	CLA	1	0
38	F	305	UIX	2	0
29	O	313	CLA	3	0
29	a	813	CLA	2	0
29	E	310	CLA	1	0
29	b	714	CLA	4	0
29	b	724	CLA	7	0
39	N	315	KC1	3	0
36	D	304	DD6	3	0
36	M	301	DD6	1	0
37	T	302	PID	4	0
29	F	313	CLA	4	0
29	Q	315	CLA	2	0
29	A	216	CLA	2	0
29	K	218	CLA	3	0
29	b	703	CLA	7	0
29	i	201	CLA	6	0
29	N	309	CLA	8	0
29	a	805	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	G	317	CLA	2	0
32	b	728	BCR	6	0
29	T	316	CLA	3	0
29	f	803	CLA	2	0
32	f	804	BCR	5	0
29	F	311	CLA	4	0
37	D	305	PID	5	0
34	K	220	LMG	1	0
29	a	822	CLA	2	0
33	c	102	SF4	3	0
29	b	712	CLA	5	0
29	i	203	CLA	5	0
29	b	707	CLA	7	0
29	A	215	CLA	2	0
29	P	210	CLA	7	0
36	L	301	DD6	1	0
39	G	315	KC1	1	0
29	b	715	CLA	4	0
29	G	316	CLA	1	0
33	a	836	SF4	2	0
37	H	301	PID	4	0
29	a	814	CLA	1	0
40	J	314	SQD	7	0
29	B	312	CLA	2	0
29	b	716	CLA	5	0
29	b	722	CLA	2	0
29	H	310	CLA	3	0
29	D	309	CLA	2	0
29	C	316	CLA	3	0
29	a	812	CLA	5	0
29	b	717	CLA	5	0
37	Q	301	PID	5	0
37	C	304	PID	4	0
37	T	305	PID	5	0
29	M	313	CLA	1	0
29	N	313	CLA	1	0
29	T	314	CLA	8	0
29	I	211	CLA	3	0
35	h	203	DGD	9	0
29	D	311	CLA	1	0
29	D	316	CLA	1	0
36	J	302	DD6	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	F	302	PID	1	0
29	a	830	CLA	1	0
29	l	505	CLA	6	0
34	h	205	LMG	2	0
29	C	313	CLA	1	0
29	E	311	CLA	3	0
32	a	835	BCR	4	0
40	B	317	SQD	3	0
29	C	309	CLA	3	0
37	H	302	PID	3	0
36	A	204	DD6	1	0
37	O	301	PID	2	0
29	l	510	CLA	3	0
29	B	316	CLA	1	0
34	b	734	LMG	1	0
37	T	307	PID	3	0
29	K	209	CLA	2	0
34	A	219	LMG	2	0
29	A	209	CLA	1	0
29	C	314	CLA	6	0
36	M	302	DD6	3	0
37	G	309	PID	2	0
29	L	316	CLA	4	0
29	P	214	CLA	2	0
37	C	305	PID	10	0
29	a	816	CLA	1	0
29	l	509	CLA	2	0
37	N	305	PID	7	0
29	b	708	CLA	3	0
39	C	310	KC1	1	0
37	D	306	PID	3	0
37	F	304	PID	15	0
39	Q	314	KC1	2	0
36	F	303	DD6	2	0
29	L	312	CLA	4	0
36	C	303	DD6	1	0
29	b	718	CLA	5	0
29	I	207	CLA	2	0
29	I	216	CLA	2	0
29	Q	310	CLA	3	0
37	C	301	PID	2	0
29	a	821	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	K	210	CLA	4	0
29	f	805	CLA	5	0
29	G	313	CLA	1	0
37	O	304	PID	3	0
34	K	201	LMG	4	0
29	B	310	CLA	5	0
37	Q	306	PID	5	0
29	a	808	CLA	3	0
29	E	308	CLA	3	0
29	A	208	CLA	2	0
34	b	730	LMG	6	0
37	G	310	PID	3	0
29	J	311	CLA	2	0
29	b	723	CLA	6	0
29	B	315	CLA	1	0
39	G	318	KC1	1	0
37	C	307	PID	3	0
29	M	307	CLA	2	0
32	i	204	BCR	7	0
29	b	706	CLA	3	0
29	K	214	CLA	7	0
37	N	307	PID	6	0
36	B	319	DD6	4	0
29	P	212	CLA	2	0
32	b	735	BCR	8	0
29	a	829	CLA	5	0
29	b	720	CLA	5	0
29	A	218	CLA	2	0
29	J	310	CLA	3	0
37	P	202	PID	4	0
29	D	313	CLA	2	0
29	A	214	CLA	2	0
39	H	314	KC1	1	0
29	L	308	CLA	2	0
29	b	721	CLA	5	0
29	a	809	CLA	6	0
37	T	304	PID	4	0
29	l	502	CLA	1	0
30	b	727	PQN	3	0
39	N	310	KC1	2	0
38	E	304	UIX	1	0
29	F	310	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	824	CLA	10	0
38	J	304	UIX	1	0
29	T	309	CLA	4	0
29	O	314	CLA	10	0
36	T	303	DD6	1	0
29	I	213	CLA	3	0
29	P	217	CLA	2	0
29	P	209	CLA	2	0
29	b	711	CLA	6	0
29	l	501	CLA	9	0
37	F	306	PID	5	0
29	L	311	CLA	1	0
29	a	803	CLA	8	0
32	l	506	BCR	4	0
29	E	306	CLA	9	0
29	A	212	CLA	3	0
29	L	317	CLA	1	0
29	F	312	CLA	4	0
37	G	303	PID	3	0
29	a	818	CLA	1	0
37	N	304	PID	2	0
29	K	212	CLA	4	0
36	M	304	DD6	1	0
32	a	834	BCR	8	0
29	a	807	CLA	7	0
37	T	317	PID	3	0
29	G	302	CLA	9	0
37	D	303	PID	10	0
30	a	832	PQN	6	0
29	D	314	CLA	9	0
29	b	719	CLA	10	0
31	a	833	LHG	5	0
29	L	307	CLA	1	0
32	f	801	BCR	8	0
29	J	305	CLA	1	0
29	Q	307	CLA	3	0
29	b	705	CLA	9	0
29	J	309	CLA	5	0
29	B	308	CLA	5	0
29	B	306	CLA	1	0
29	O	316	CLA	1	0
29	T	313	CLA	2	0

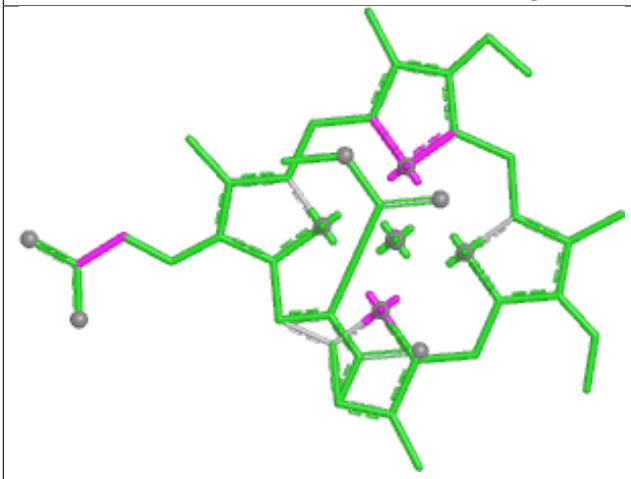
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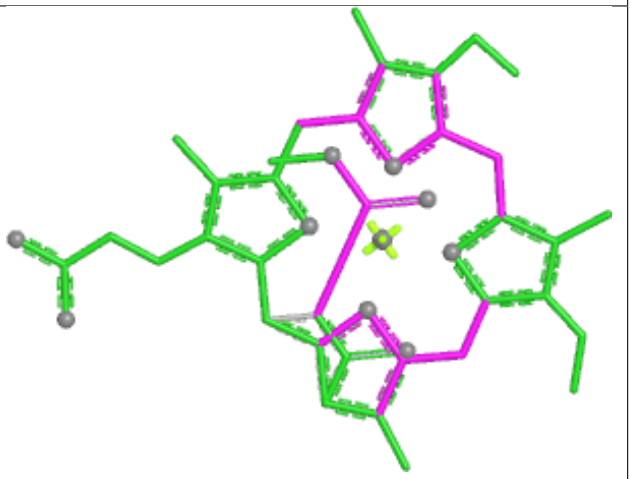
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	305	DD6	1	0
34	E	316	LMG	6	0
29	l	503	CLA	6	0
37	D	307	PID	2	0
29	P	215	CLA	5	0
29	A	211	CLA	2	0
29	M	306	CLA	1	0
29	K	213	CLA	6	0
29	a	831	CLA	4	0
37	H	306	PID	7	0
35	G	320	DGD	2	0
37	D	302	PID	1	0
29	b	709	CLA	3	0
29	l	504	CLA	10	0
29	M	311	CLA	8	0
29	G	314	CLA	4	0
29	E	315	CLA	5	0
39	I	215	KC1	1	0

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

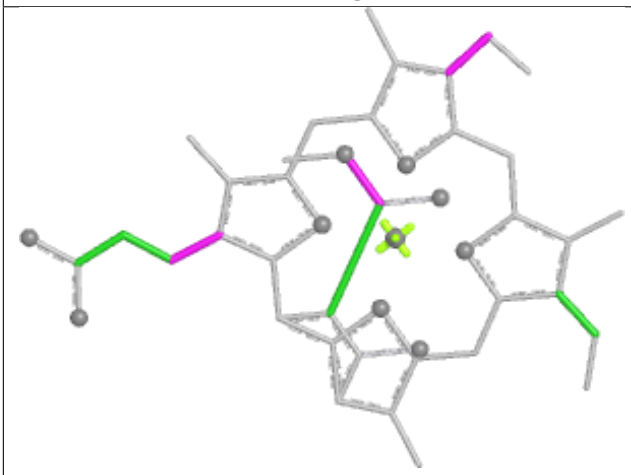
Ligand KC1 D 315



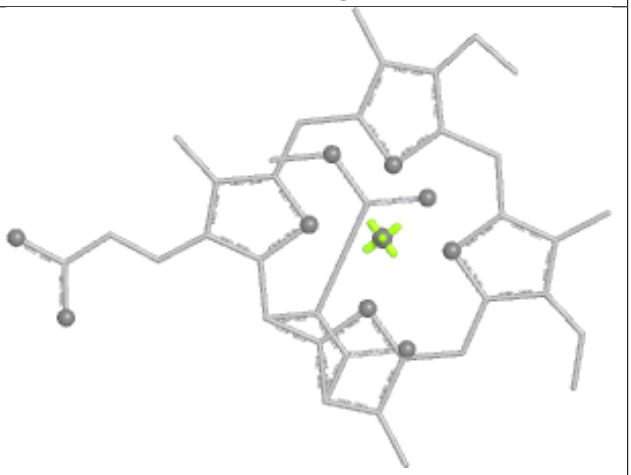
Bond lengths



Bond angles

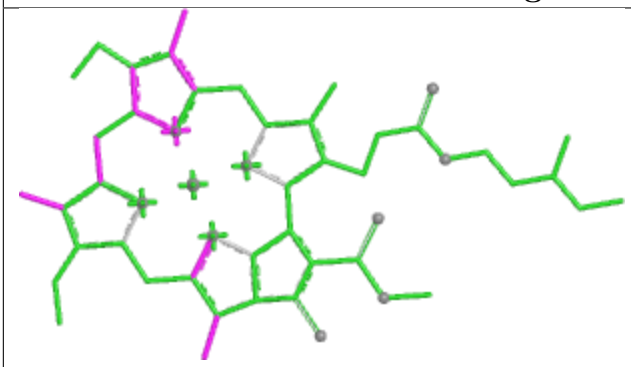


Torsions

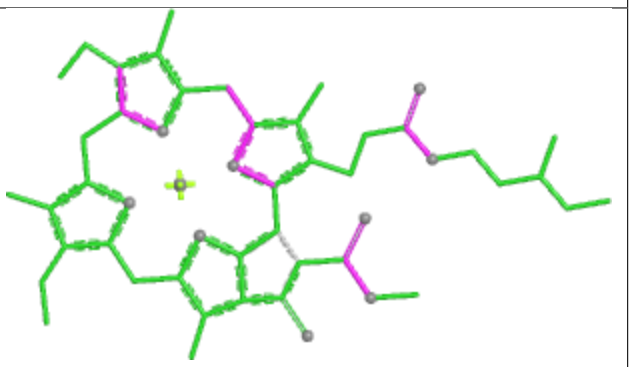


Rings

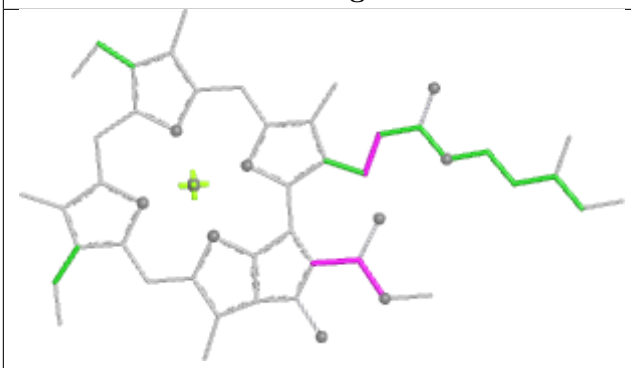
Ligand CLA C 311



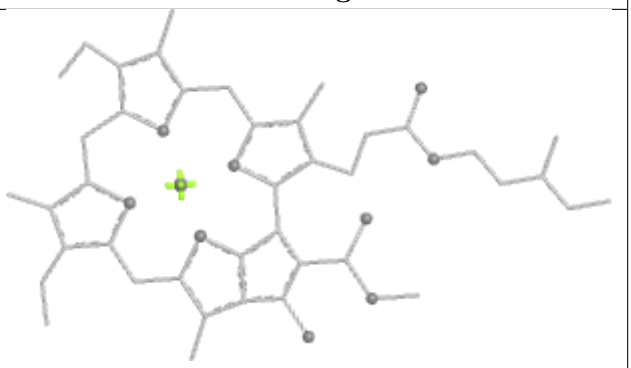
Bond lengths



Bond angles

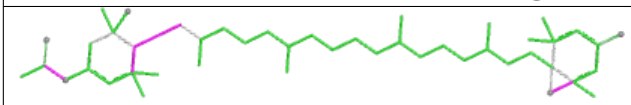


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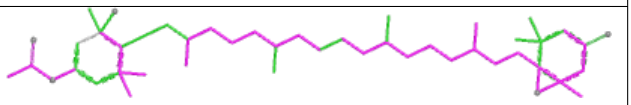


Rings

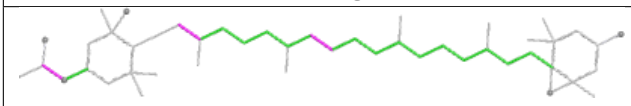
Ligand UIX T 306



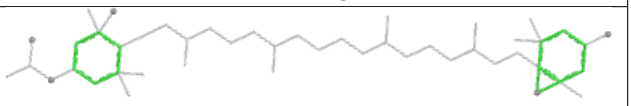
Bond lengths



Bond angles

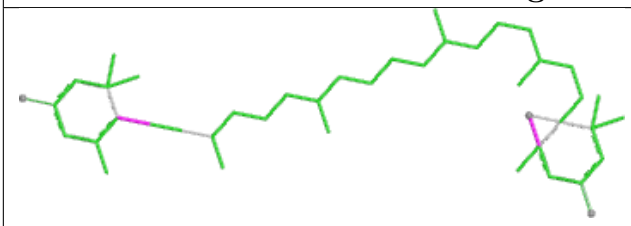


Torsions

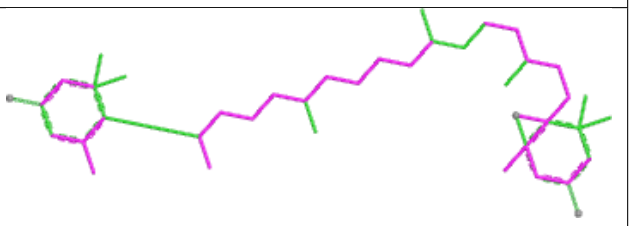


Rings

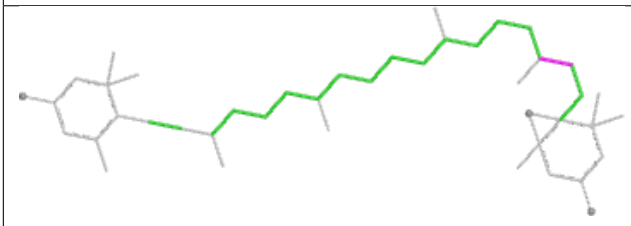
Ligand DD6 L 304



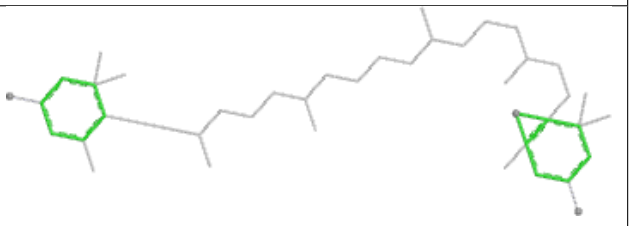
Bond lengths



Bond angles

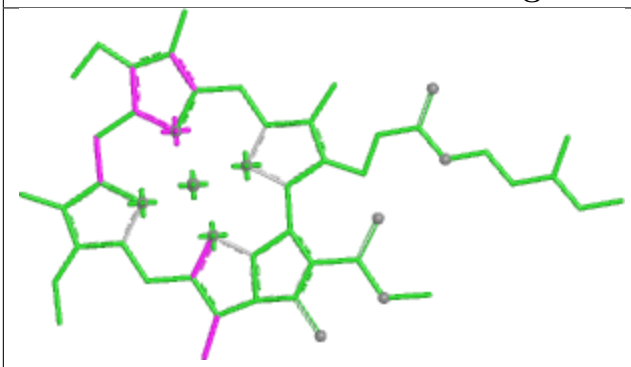


Torsions

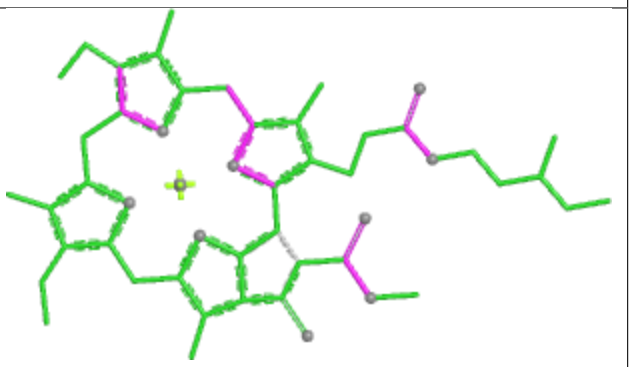


Rings

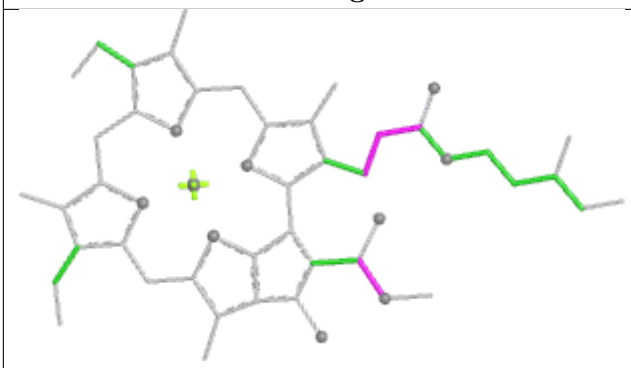
Ligand CLA N 311



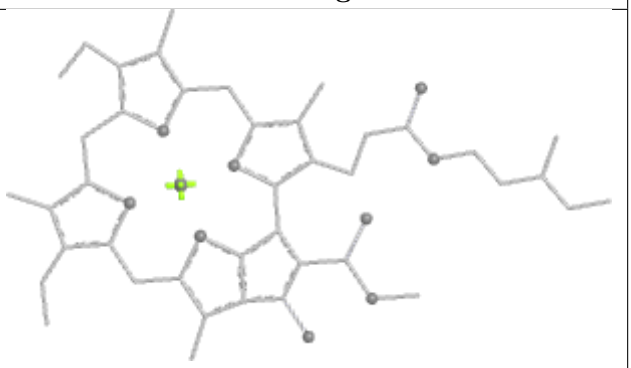
Bond lengths



Bond angles

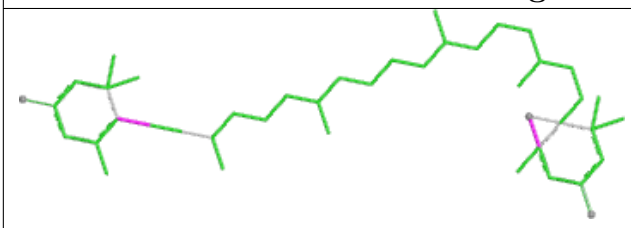


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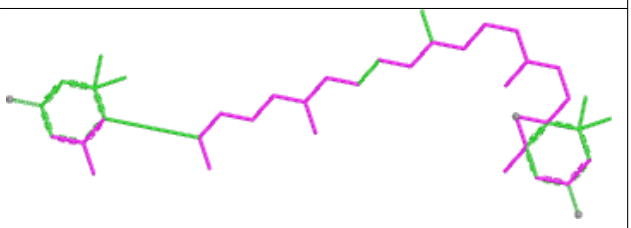


Rings

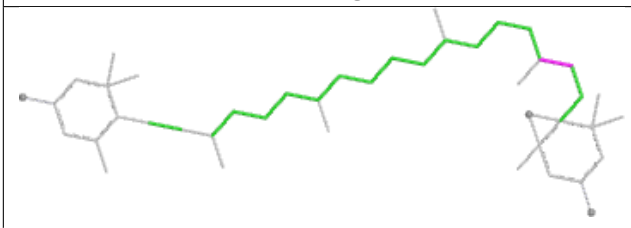
Ligand DD6 J 303



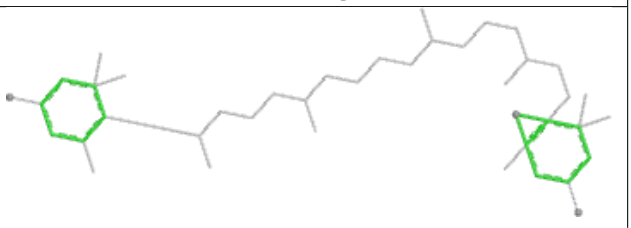
Bond lengths



Bond angles

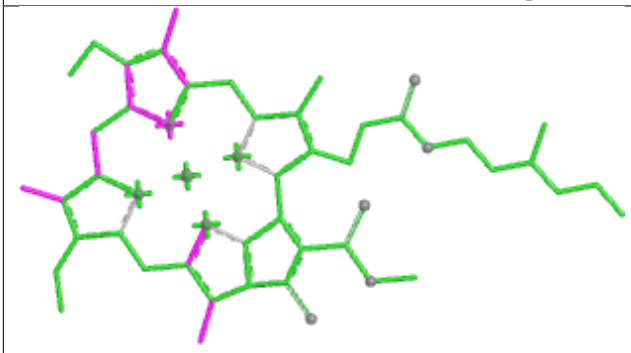


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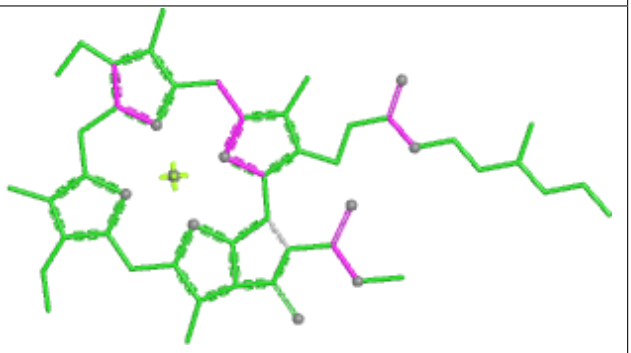


Rings

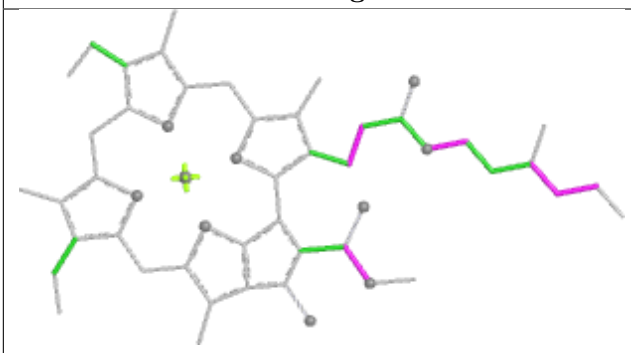
Ligand CLA M 314



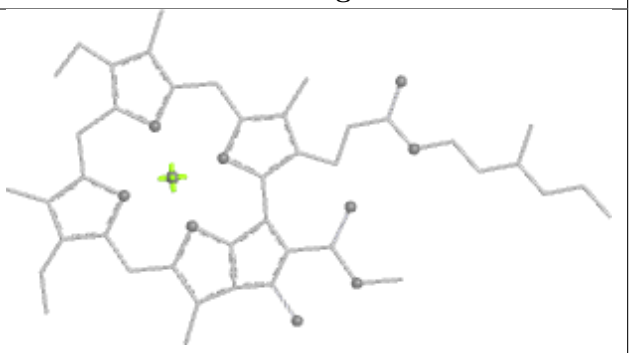
Bond lengths



Bond angles

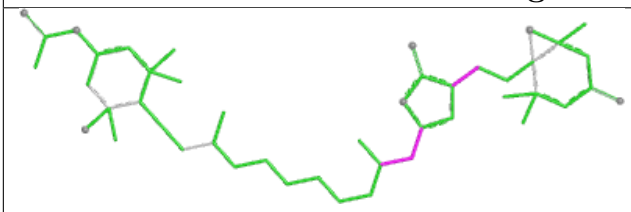


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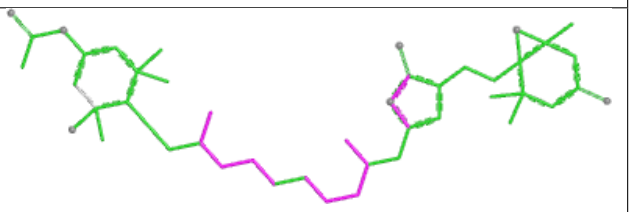


Rings

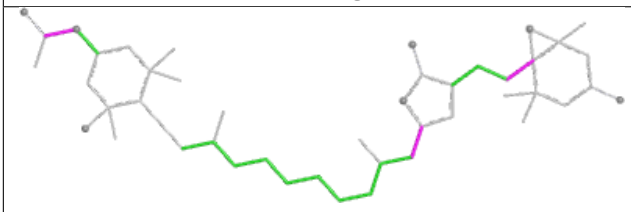
Ligand PID N 301



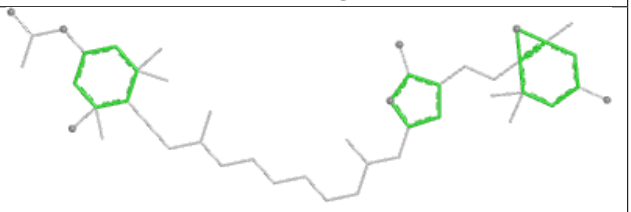
Bond lengths



Bond angles



Torsions



Rings

Ligand UIX P 207



Bond lengths



Bond angles

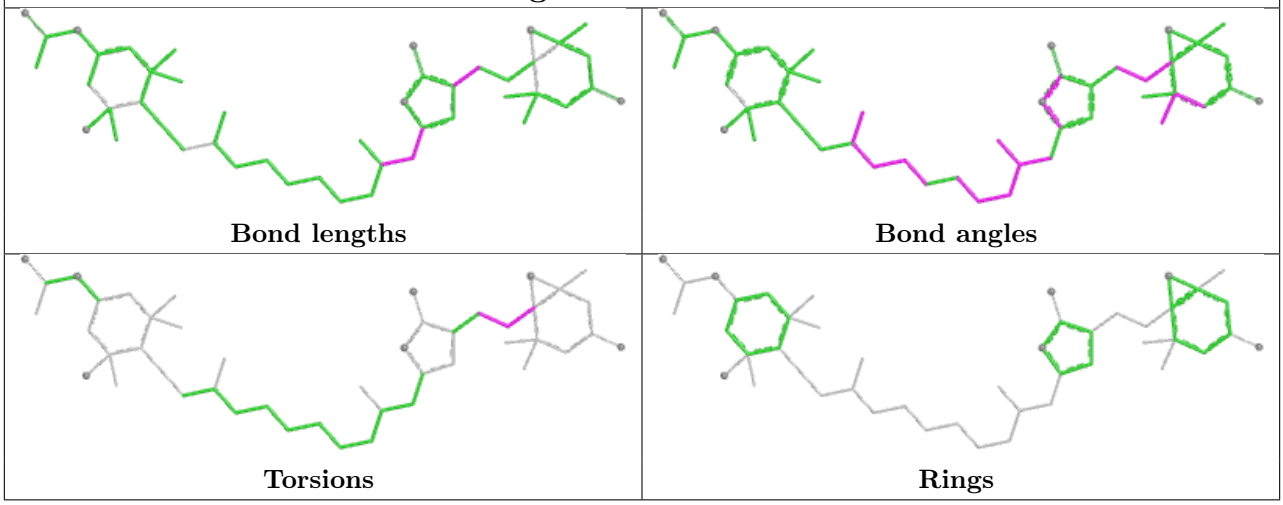


Torsions

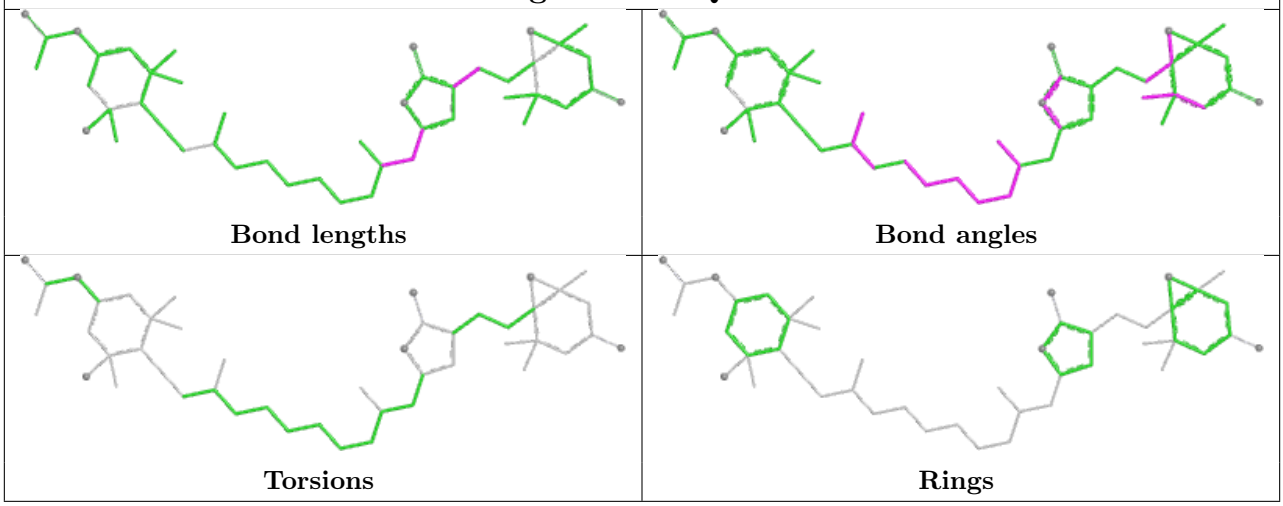


Rings

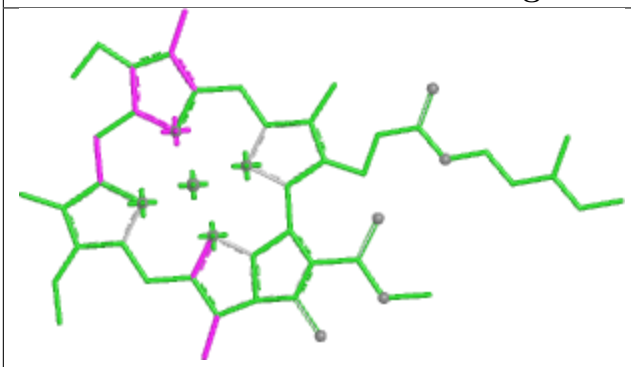
Ligand PID O 307



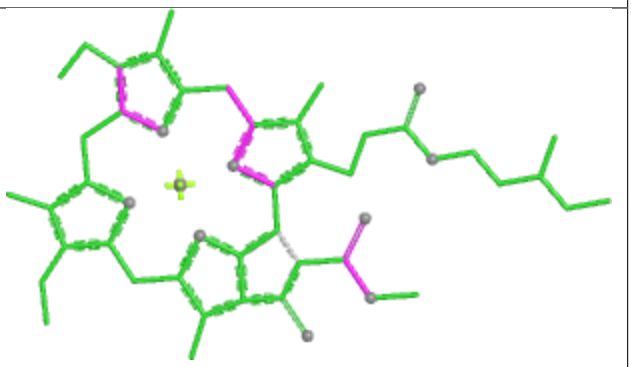
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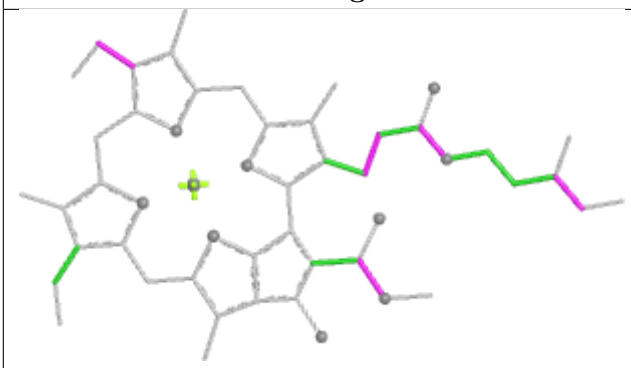
Ligand CLA G 311



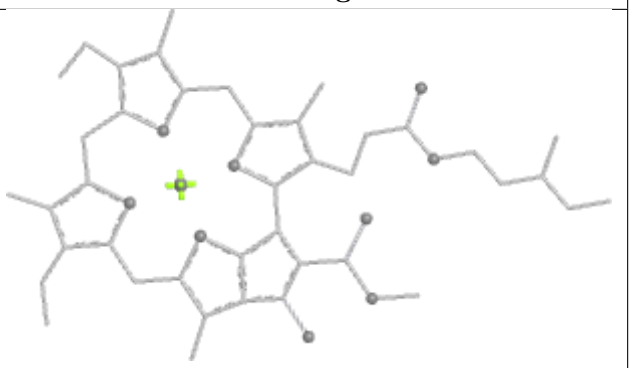
Bond lengths



Bond angles

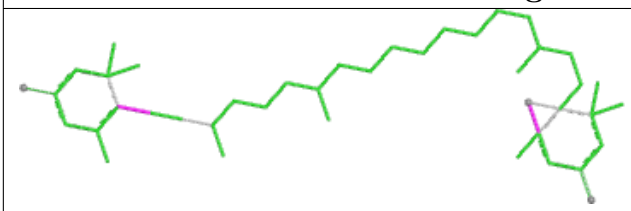


Torsions

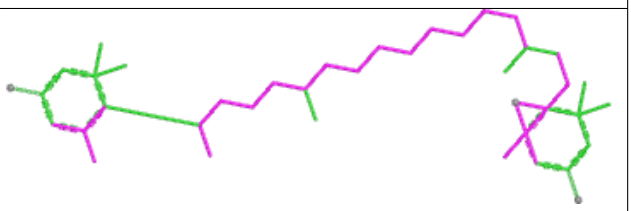


Rings

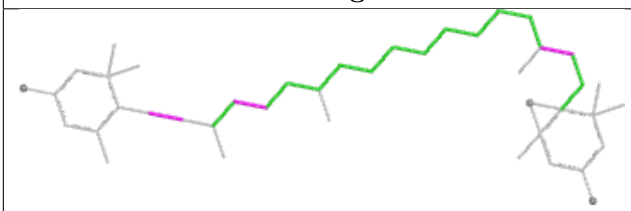
Ligand DD6 B 301



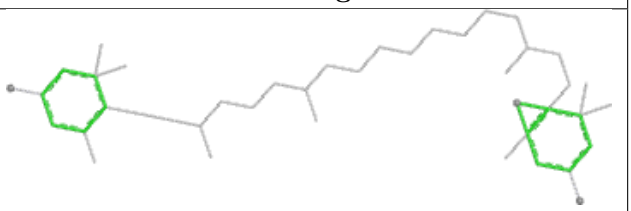
Bond lengths



Bond angles

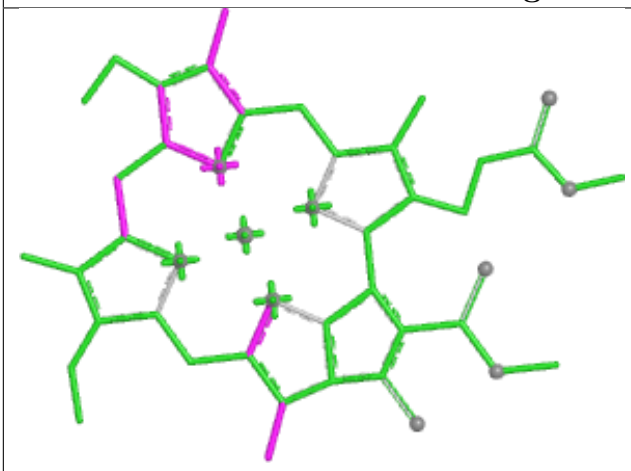


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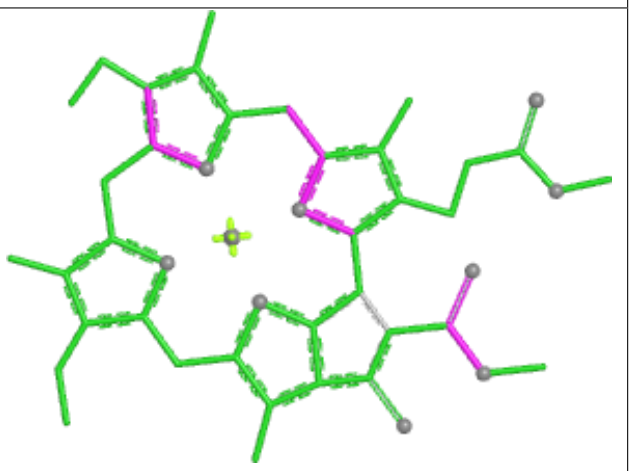


Rings

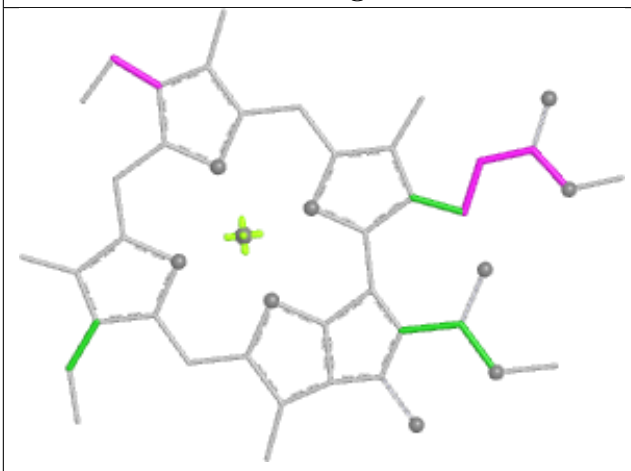
Ligand CLA D 312



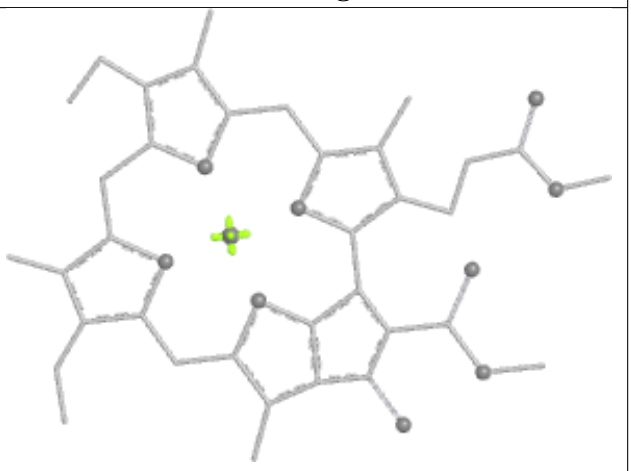
Bond lengths



Bond angles

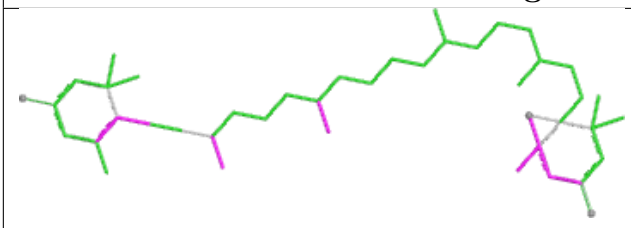


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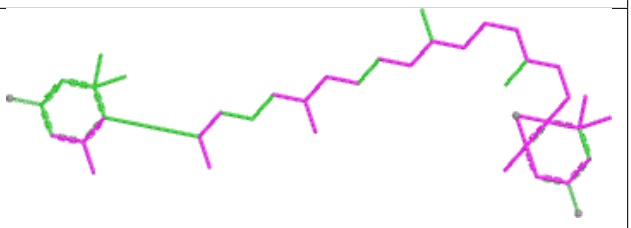


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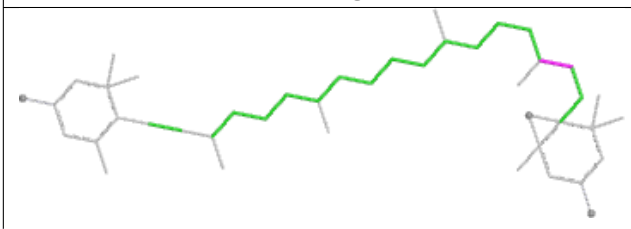
Ligand DD6 G 307



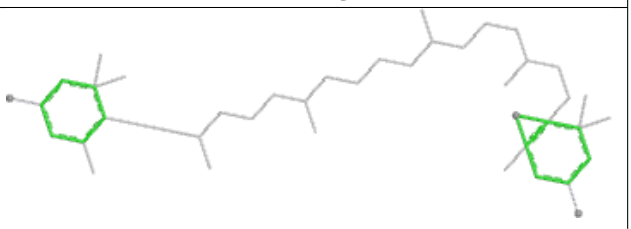
Bond lengths



Bond angles

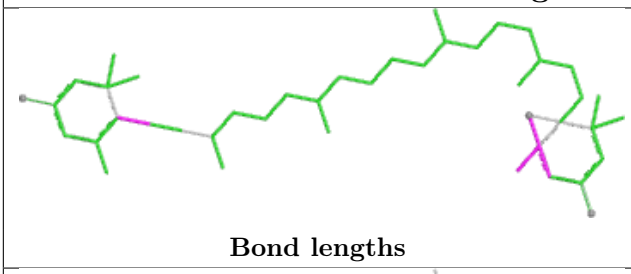


Torsions

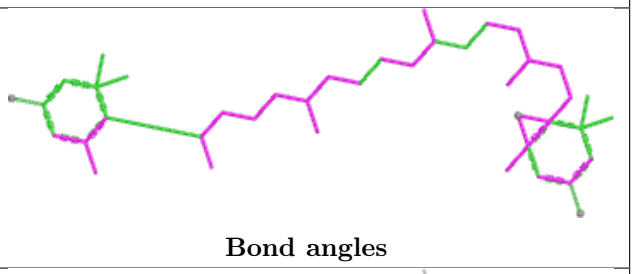


Rings

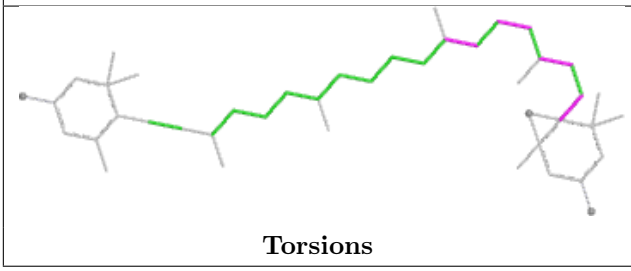
Ligand DD6 I 205



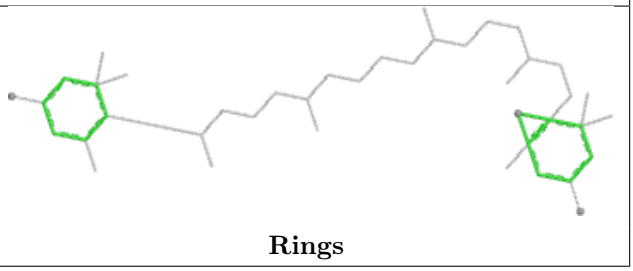
Bond lengths



Bond angles

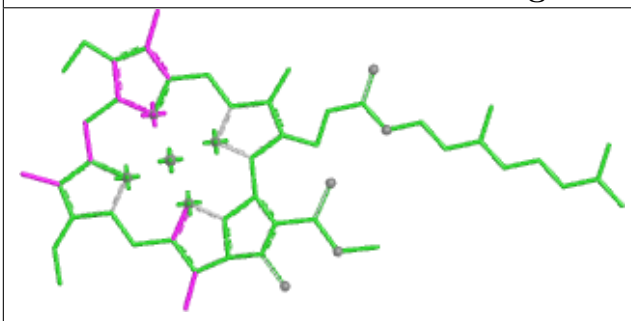


Torsions

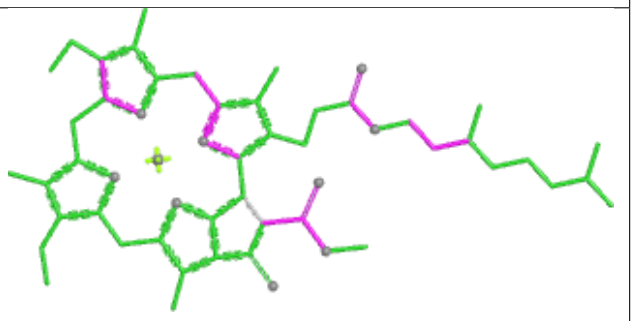


Rings

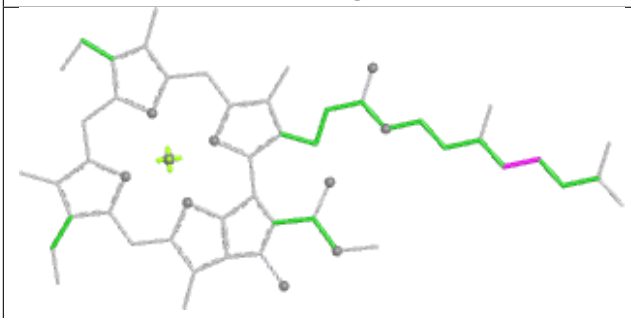
Ligand CLA a 804



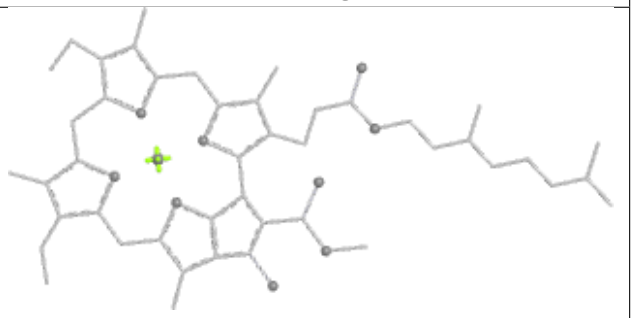
Bond lengths



Bond angles

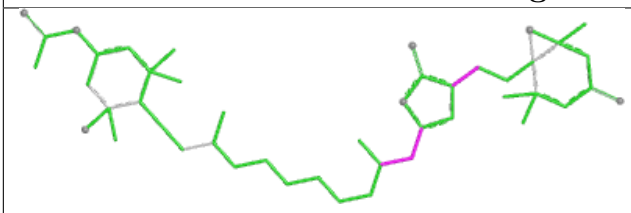


Torsions

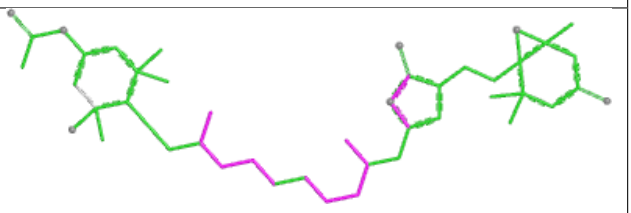


Rings

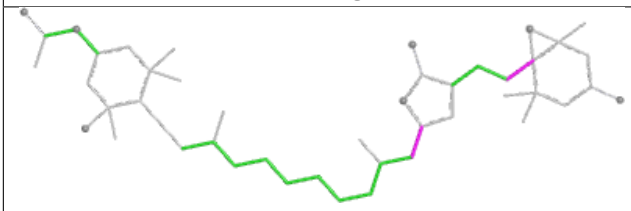
Ligand PID T 301



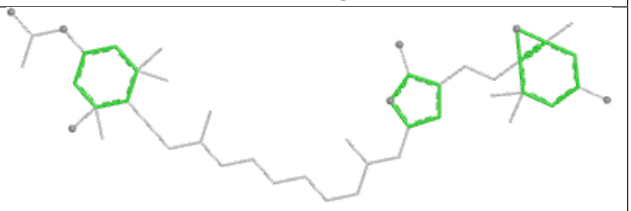
Bond lengths



Bond angles

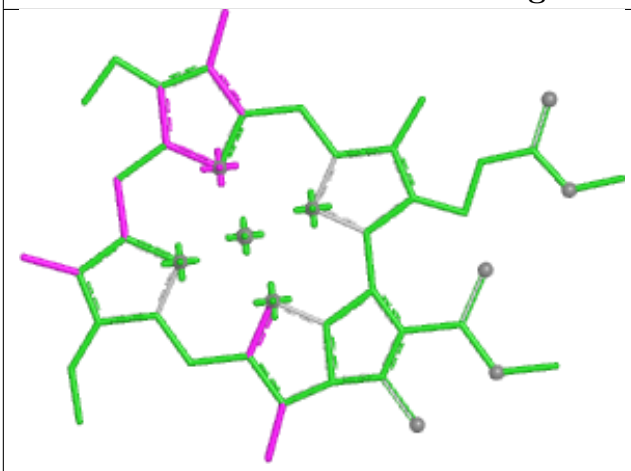


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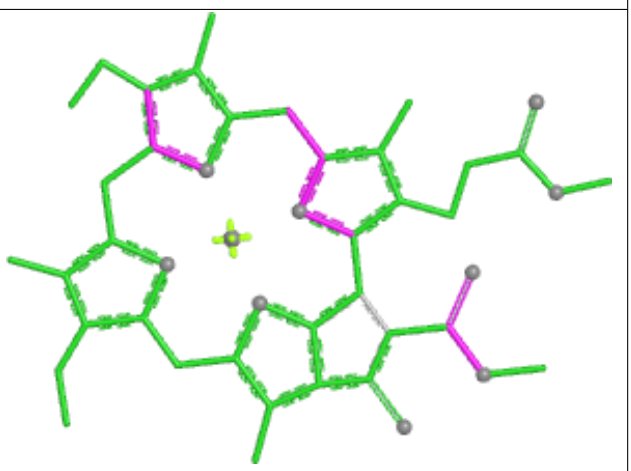


Rings

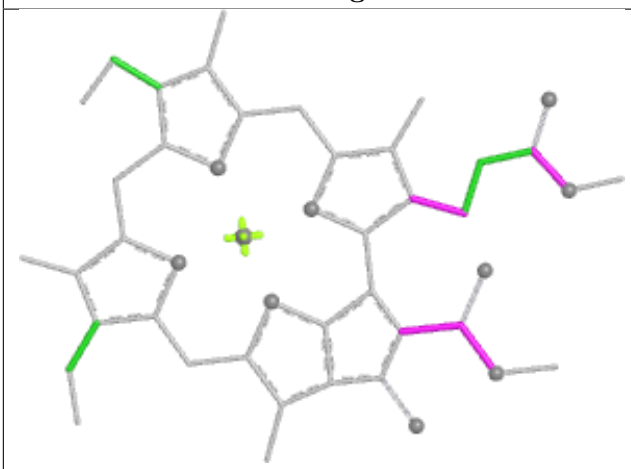
Ligand CLA a 828



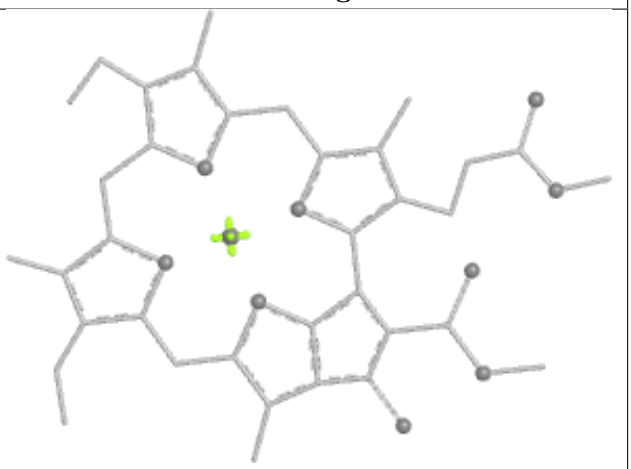
Bond lengths



Bond angles

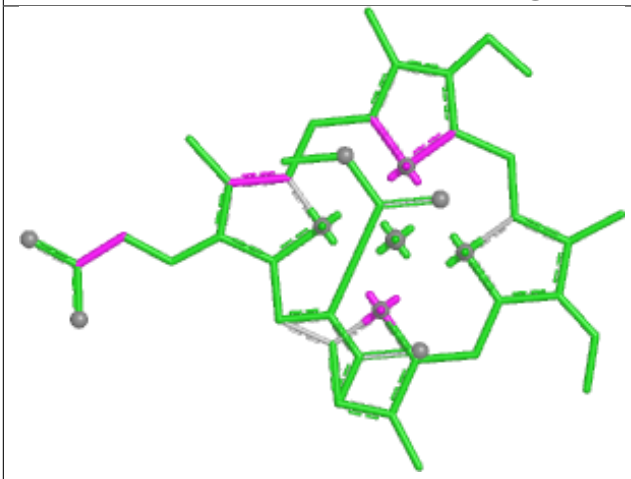


Torsions

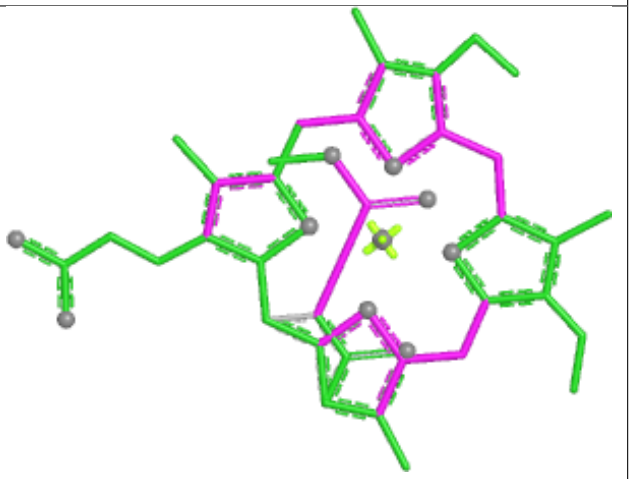


Rings

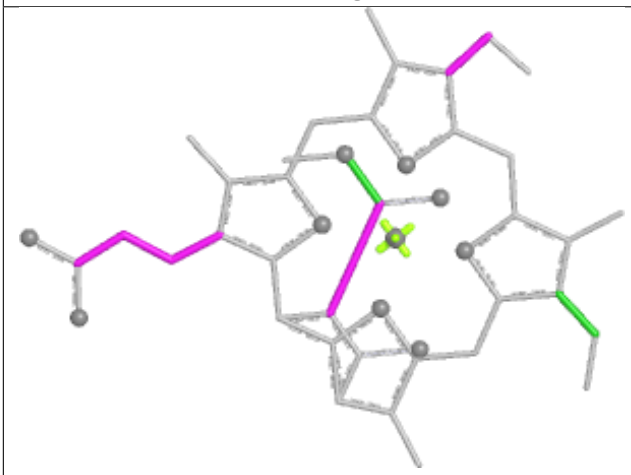
Ligand KC1 P 211



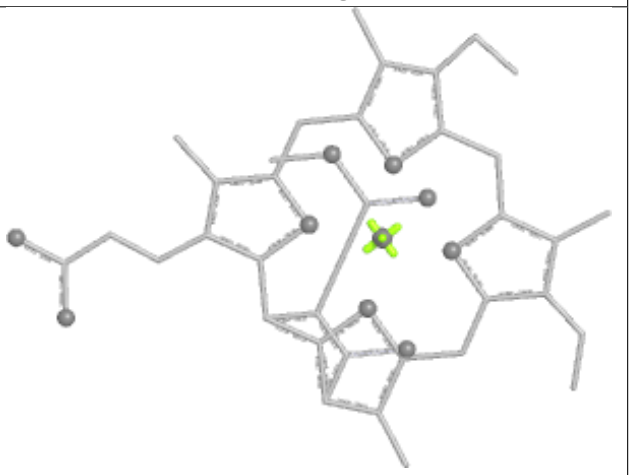
Bond lengths



Bond angles

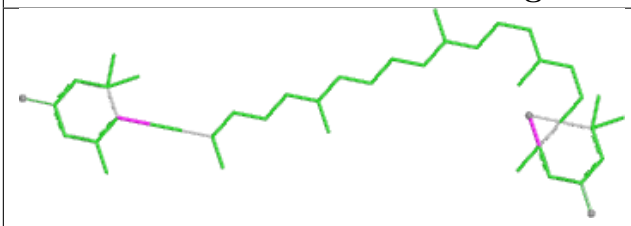


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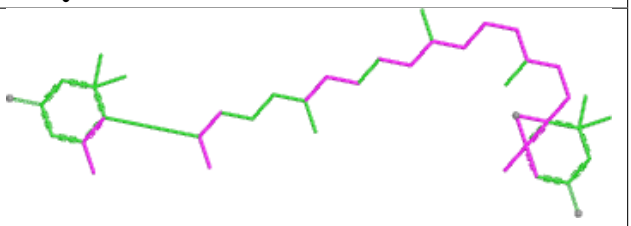


Rings

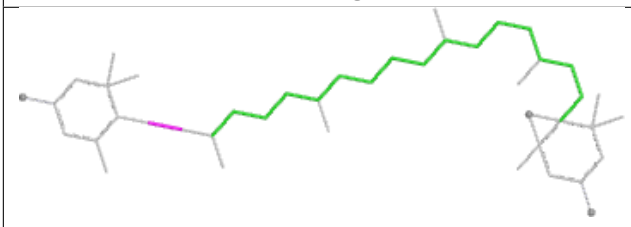
Ligand DD6 Q 302



Bond lengths



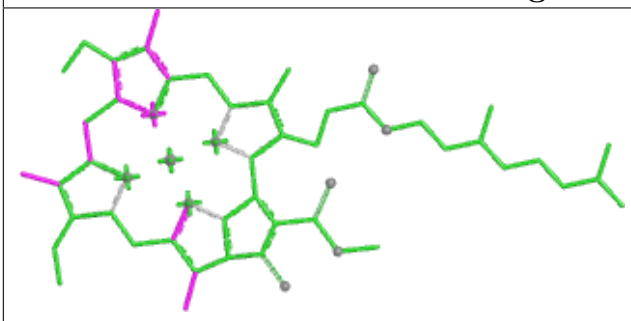
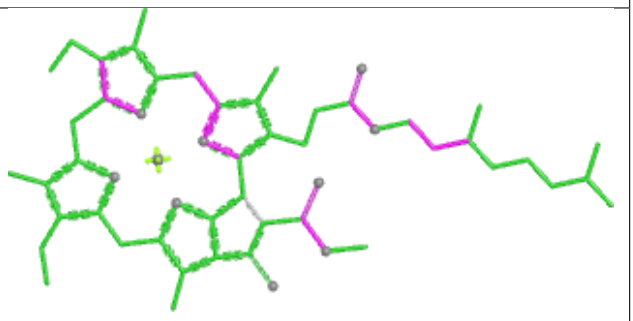
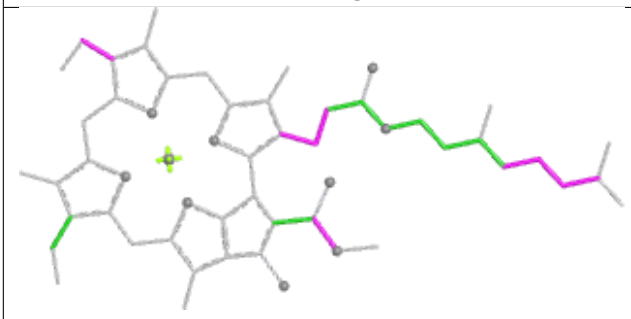
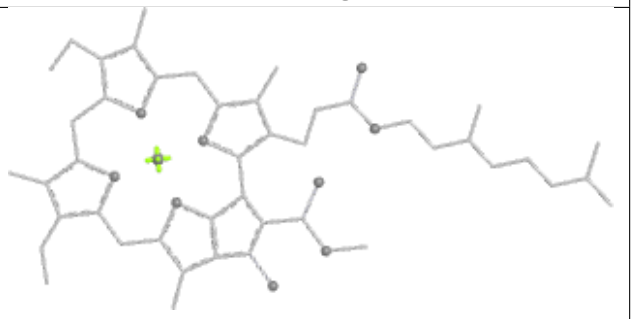
Bond angles

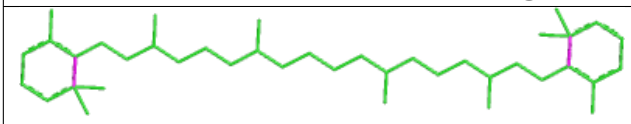
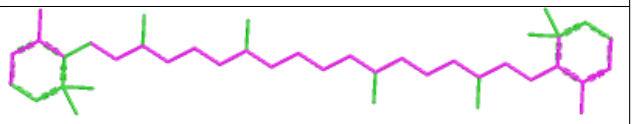
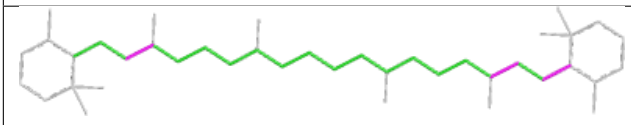
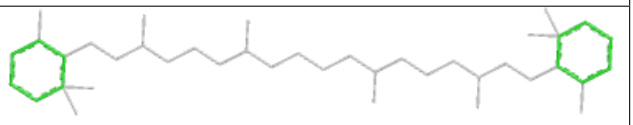


Torsions

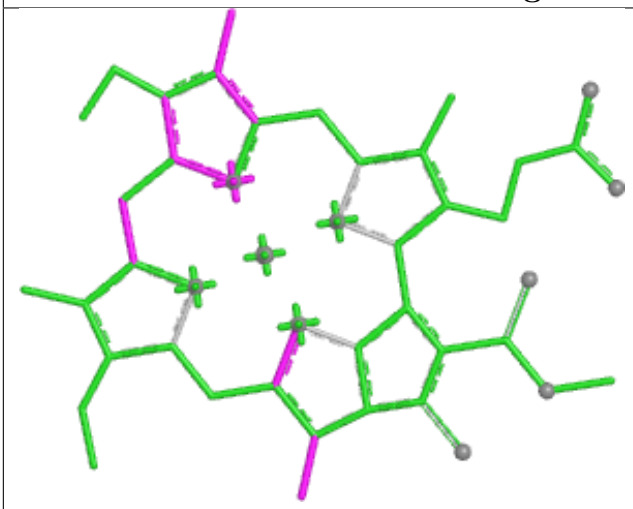


Rings

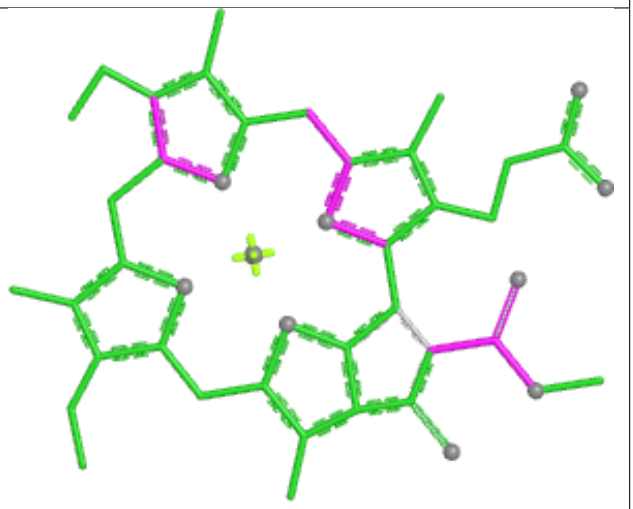
Ligand CLA a 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR m 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

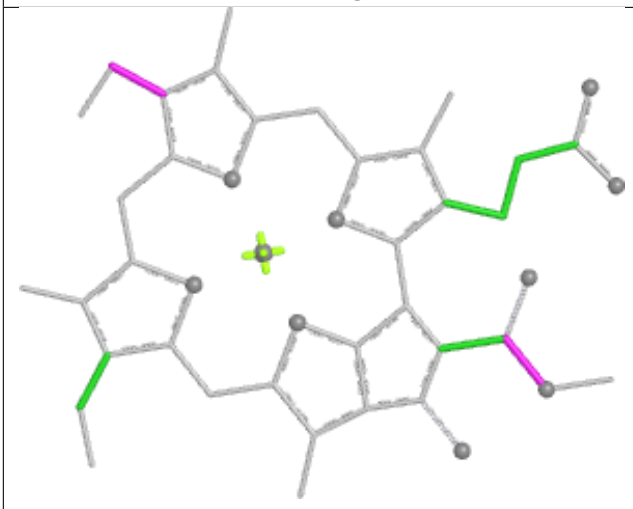
Ligand CLA A 206



Bond lengths



Bond angles

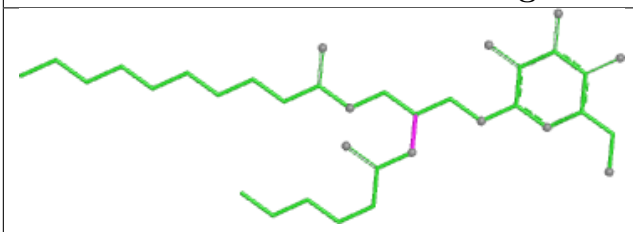


Torsions

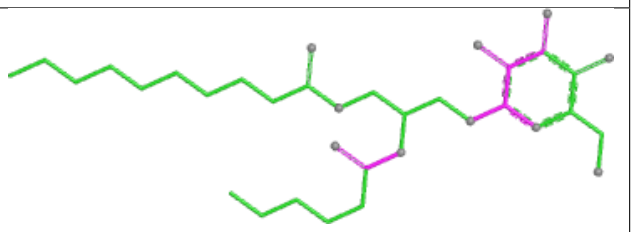


Rings

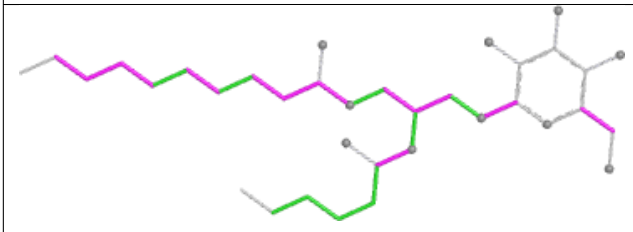
Ligand LMG K 219



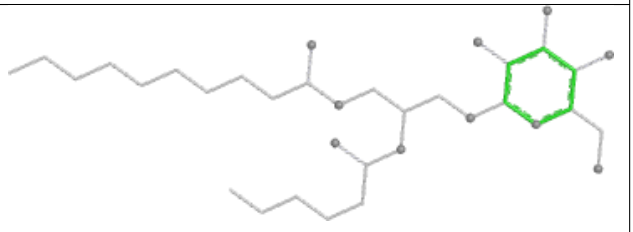
Bond lengths



Bond angles

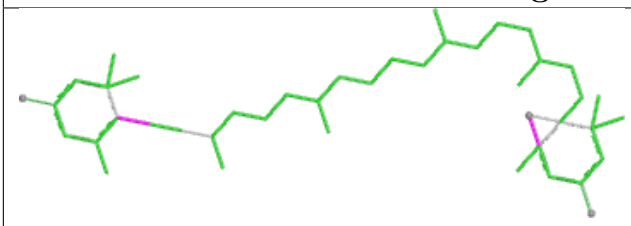


Torsions

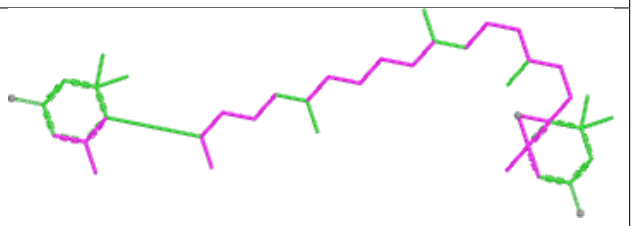


Rings

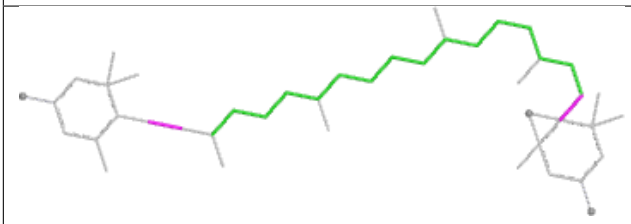
Ligand DD6 I 206



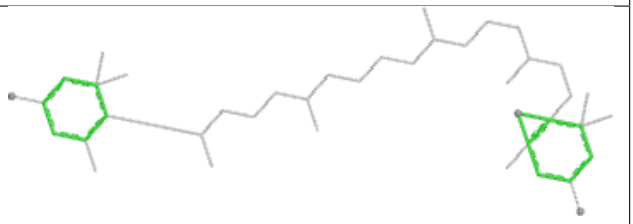
Bond lengths



Bond angles

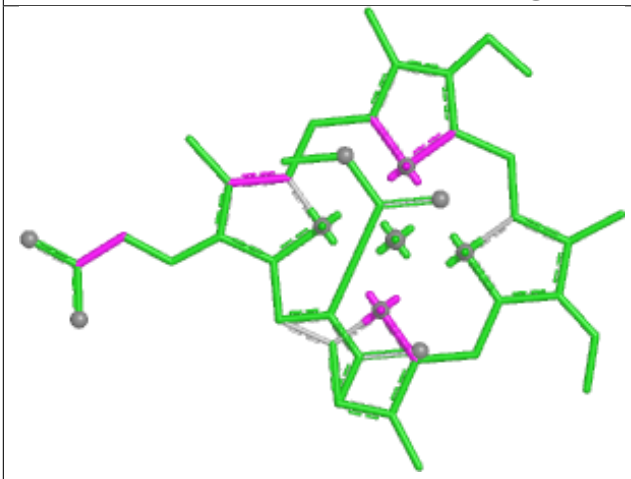


Torsions

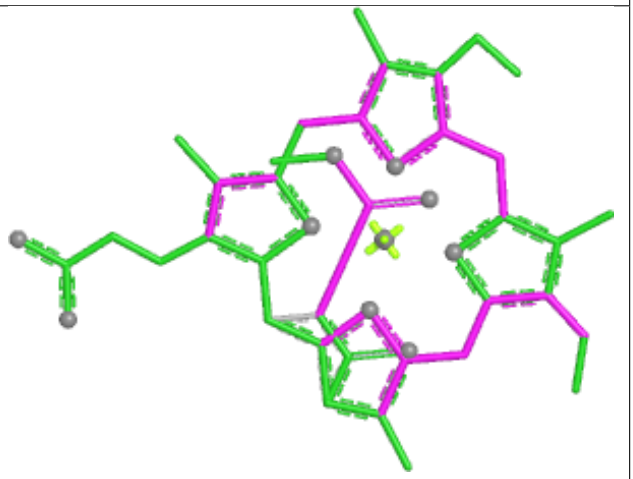


Rings

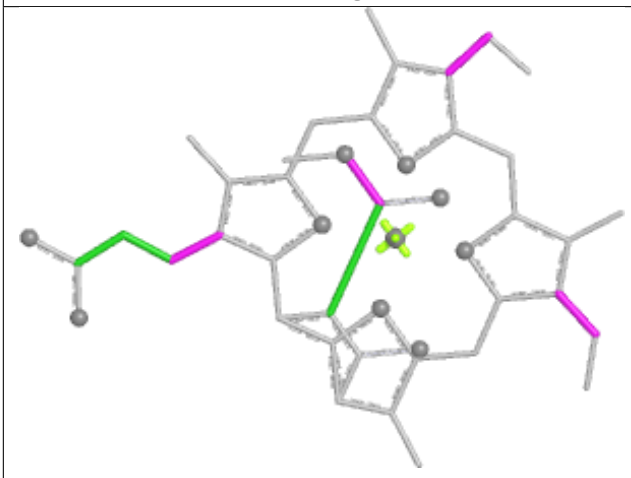
Ligand KC1 E 312



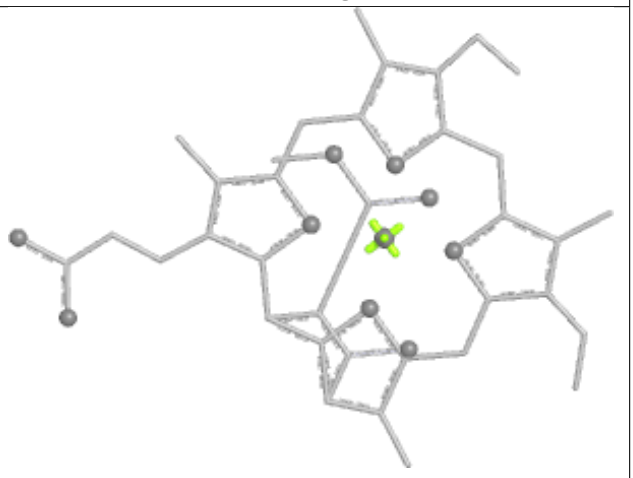
Bond lengths



Bond angles

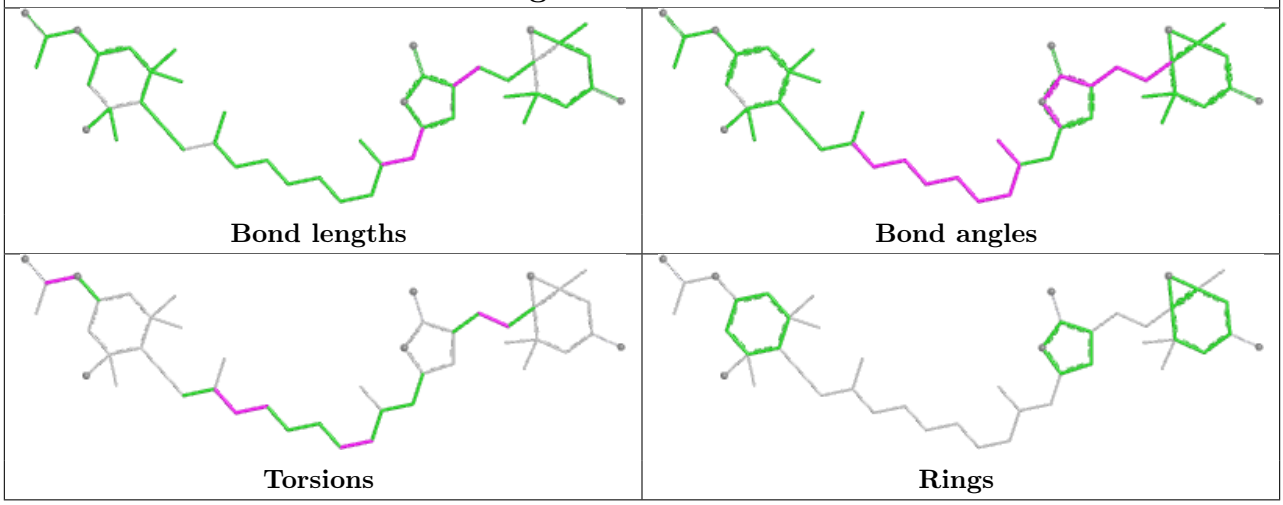


Torsions

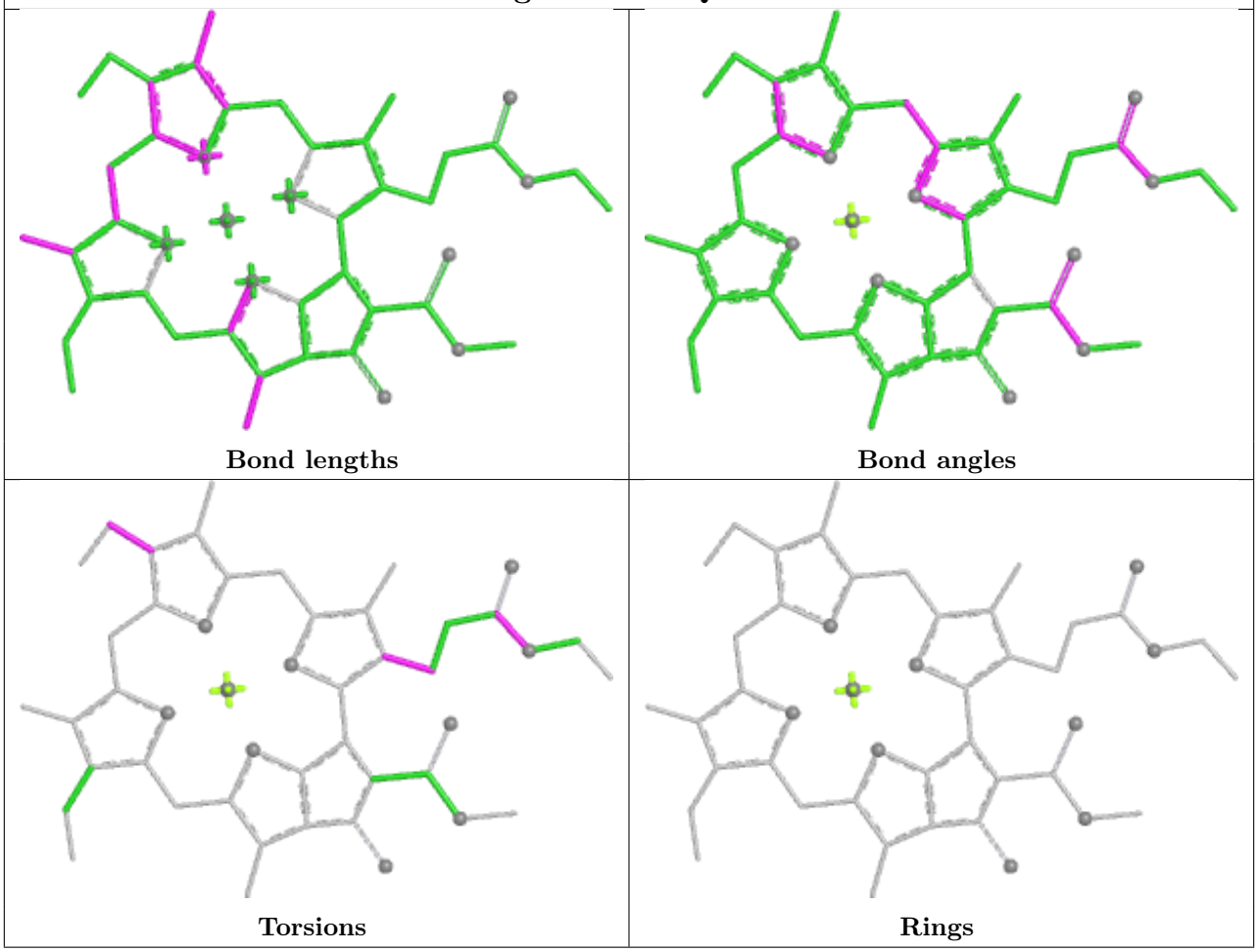


Rings

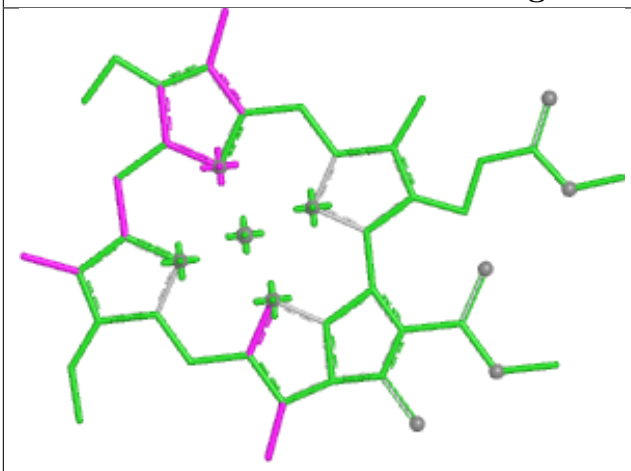
Ligand PID O 305



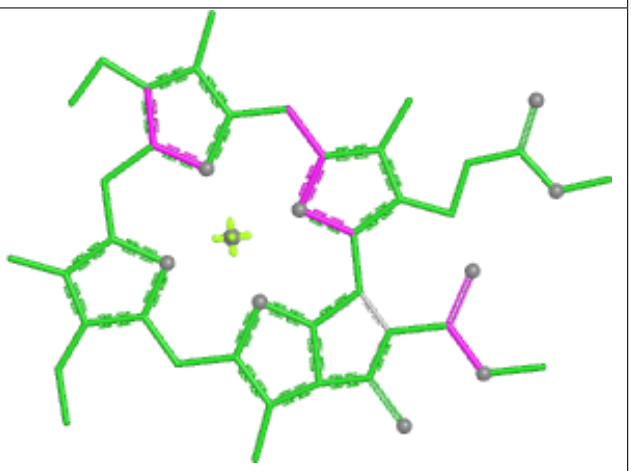
Ligand CLA Q 313



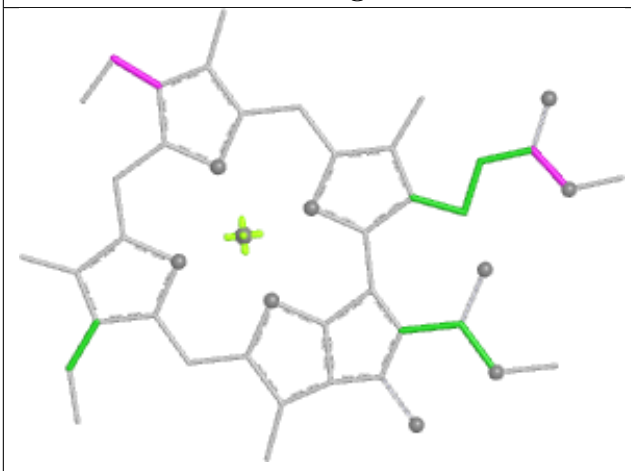
Ligand CLA J 307



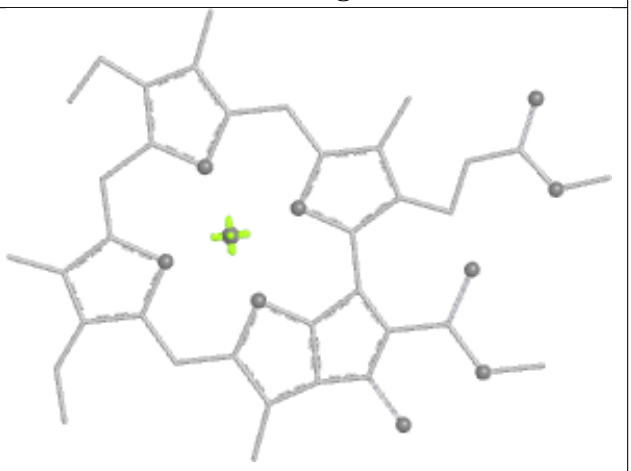
Bond lengths



Bond angles

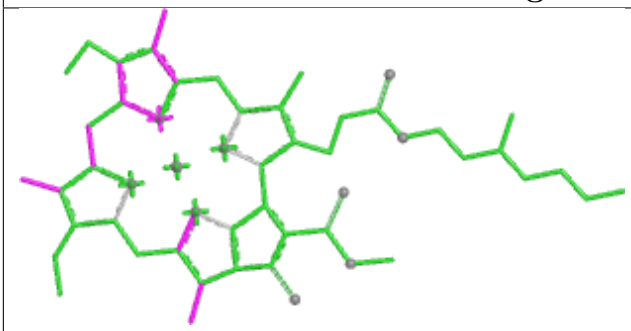


Torsions

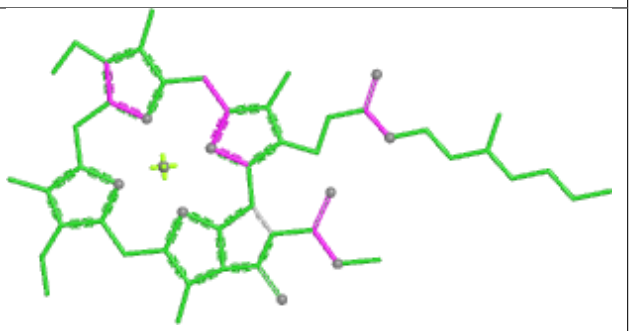


Rings

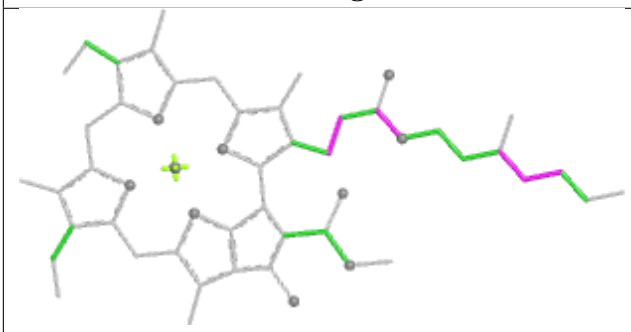
Ligand CLA L 313



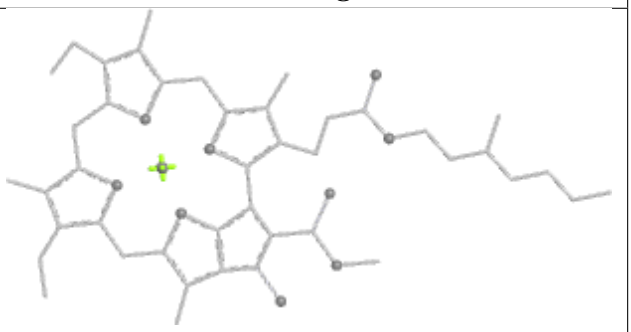
Bond lengths



Bond angles

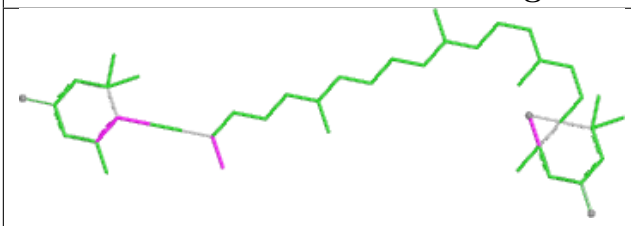


Torsions

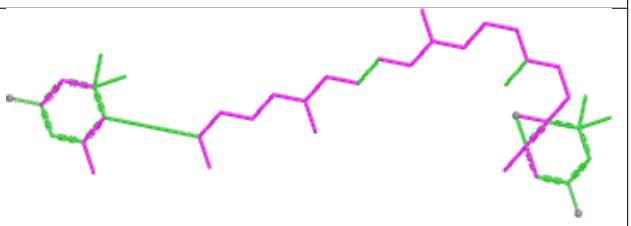


Rings

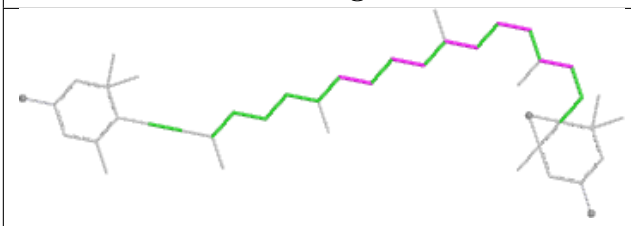
Ligand DD6 G 305



Bond lengths



Bond angles

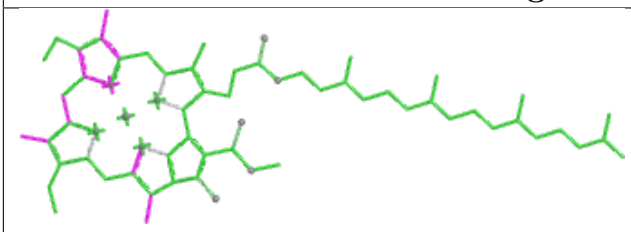


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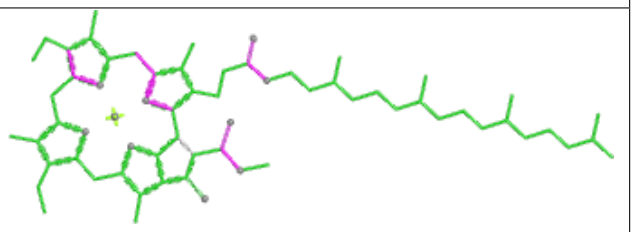


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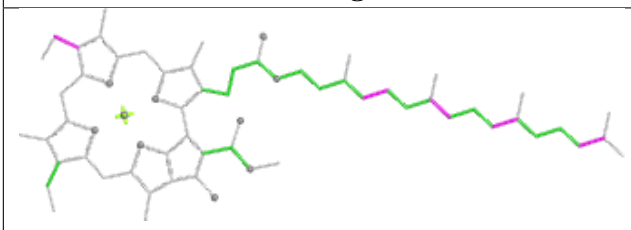
Ligand CLA b 726



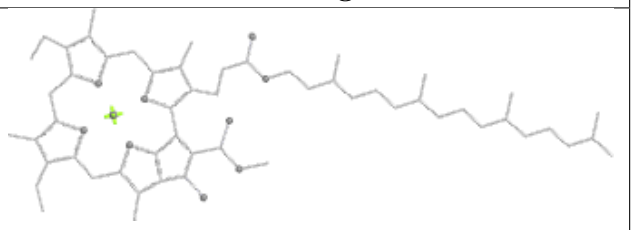
Bond lengths



Bond angles

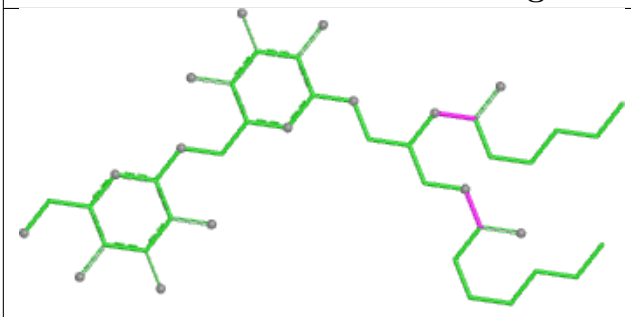


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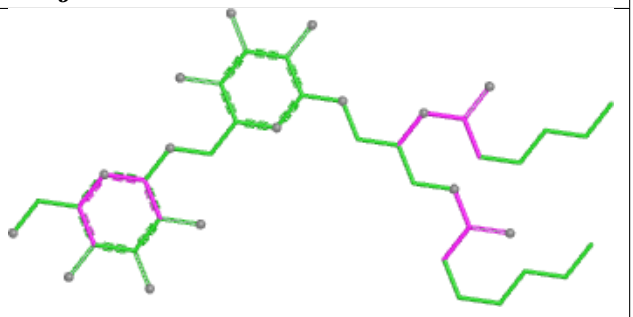


Rings

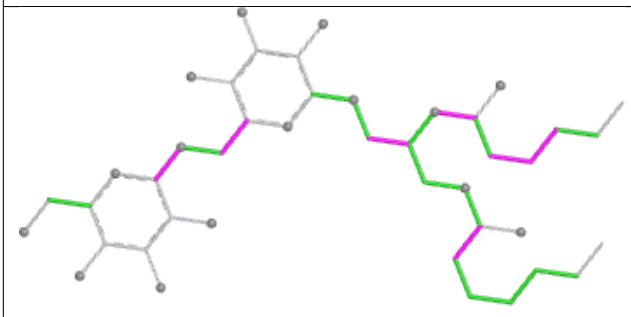
Ligand DGD j 103



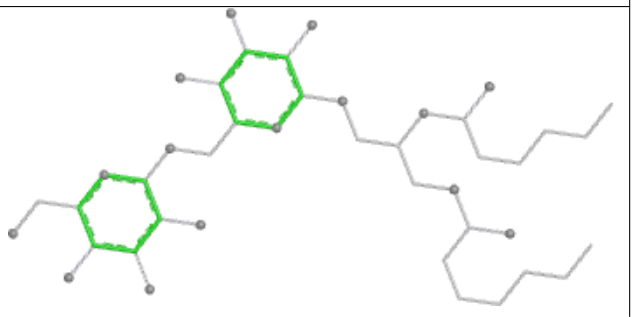
Bond lengths



Bond angles

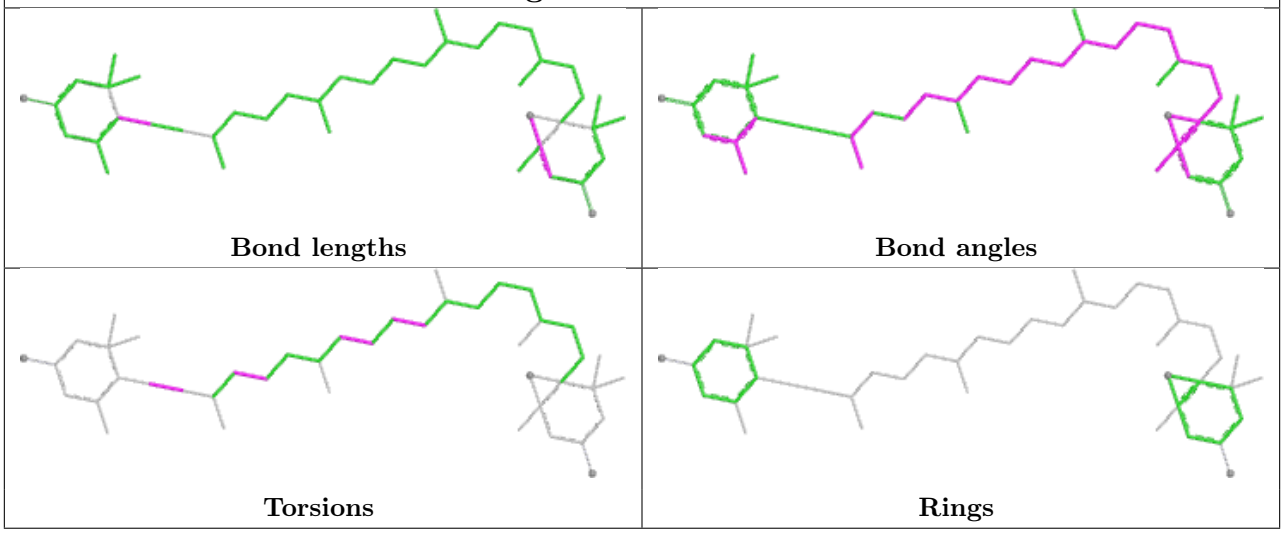


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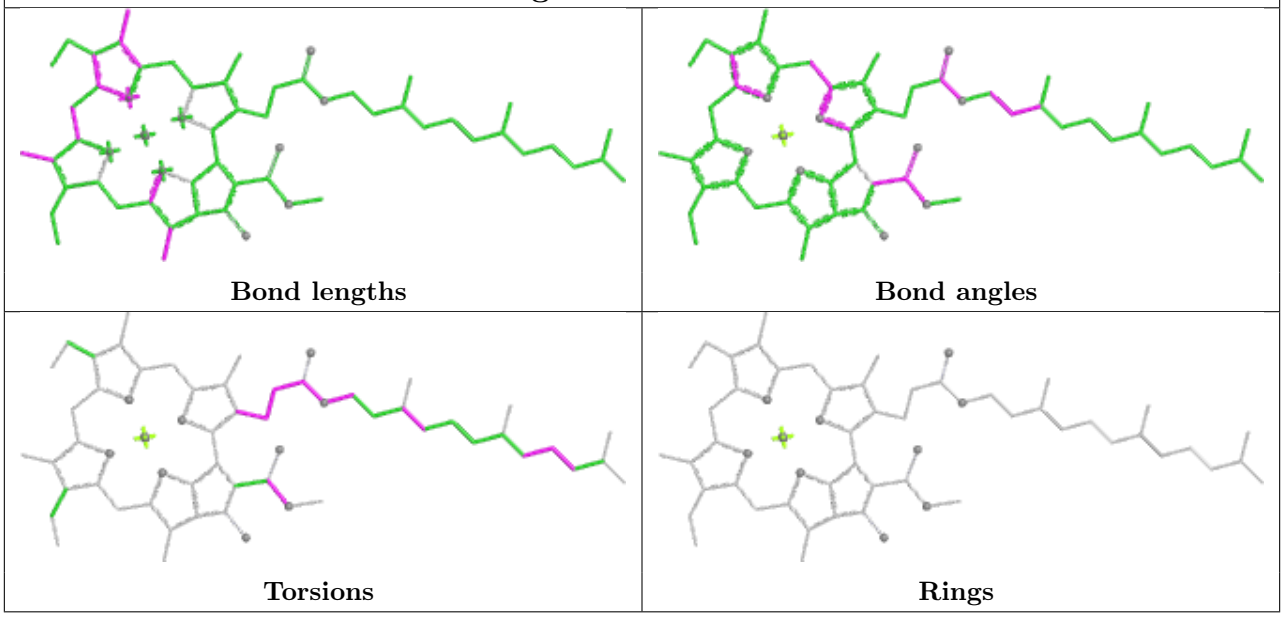


Rings

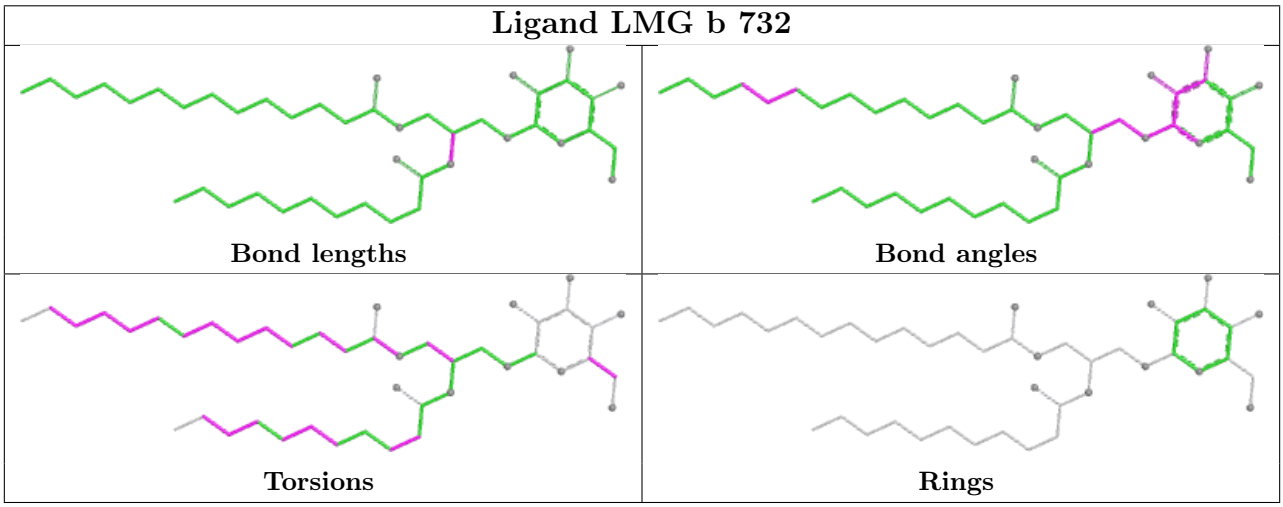
Ligand DD6 O 303



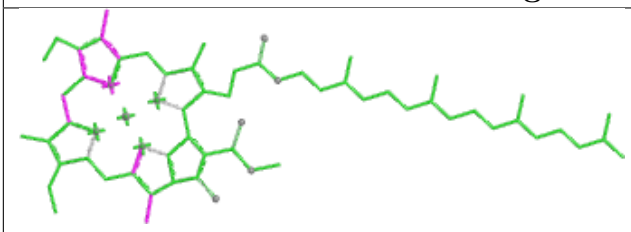
Ligand CLA I 209



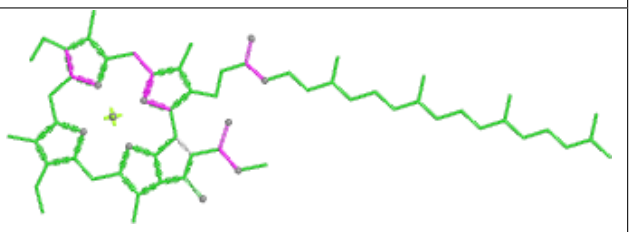
Ligand LMG b 732



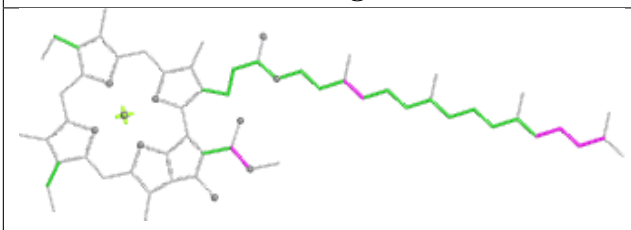
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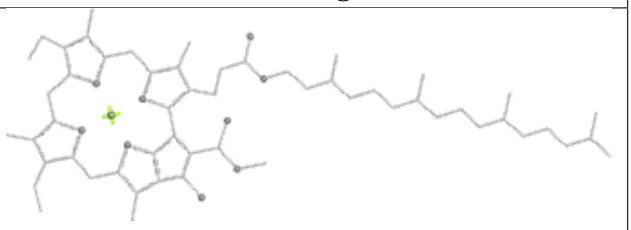
Bond lengths



Bond angles

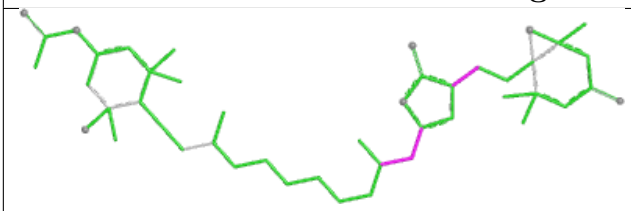


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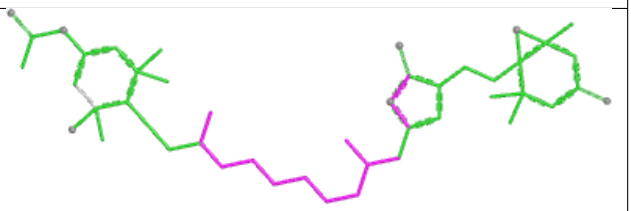


Rings

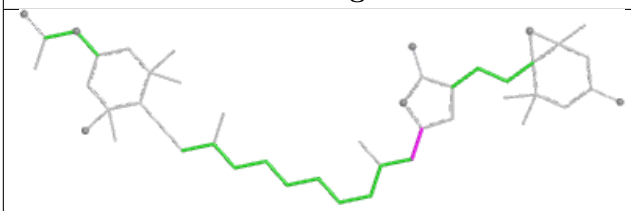
Ligand PID P 205



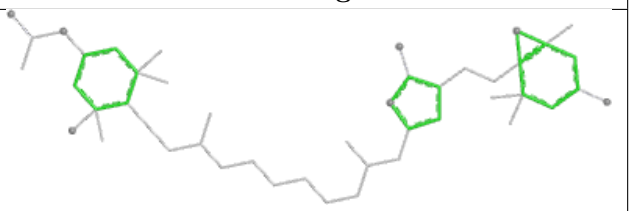
Bond lengths



Bond angles

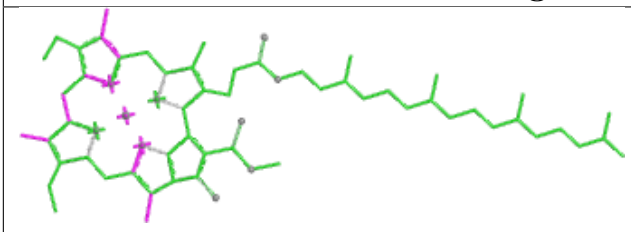


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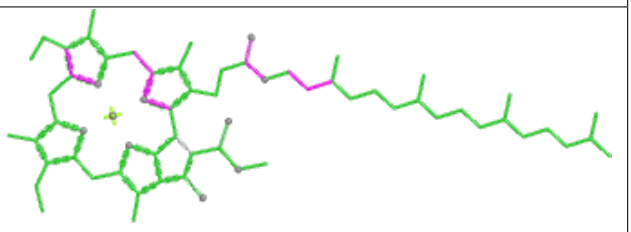


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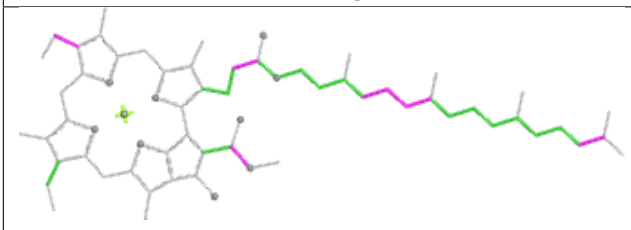
Ligand CLA a 801



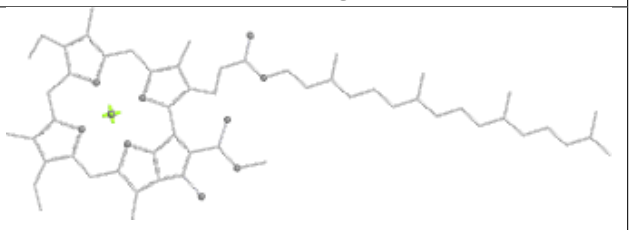
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Bond angles

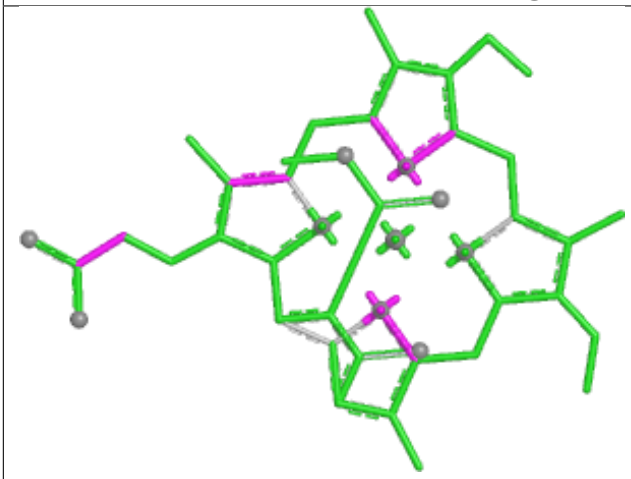


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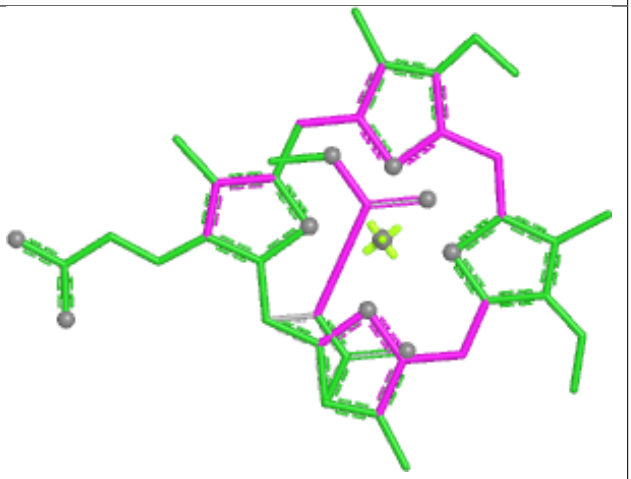


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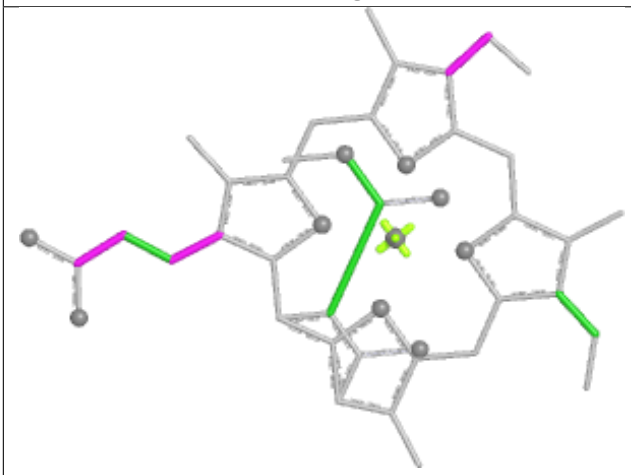
Ligand KC1 O 310



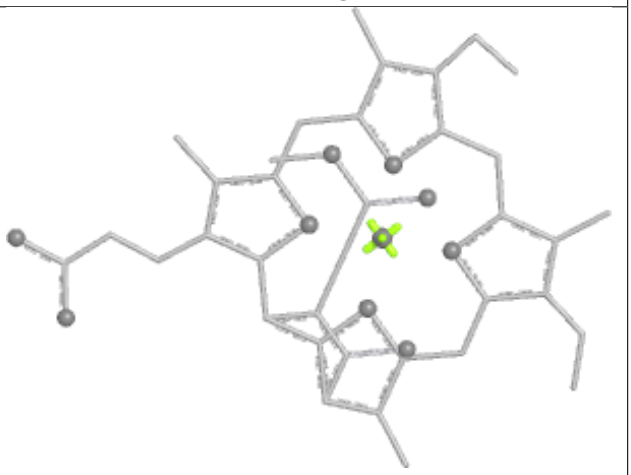
Bond lengths



Bond angles

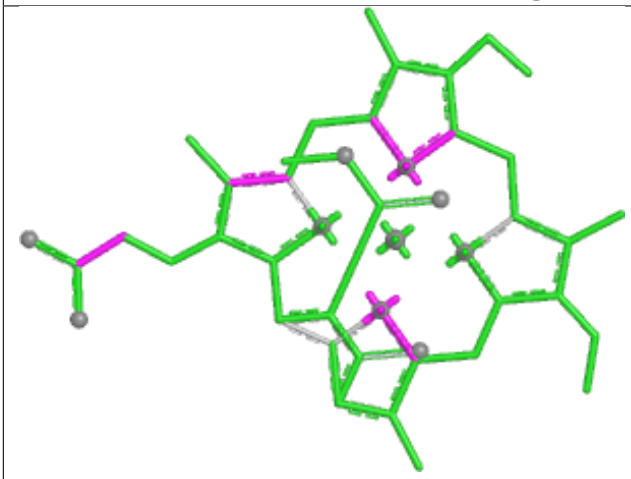


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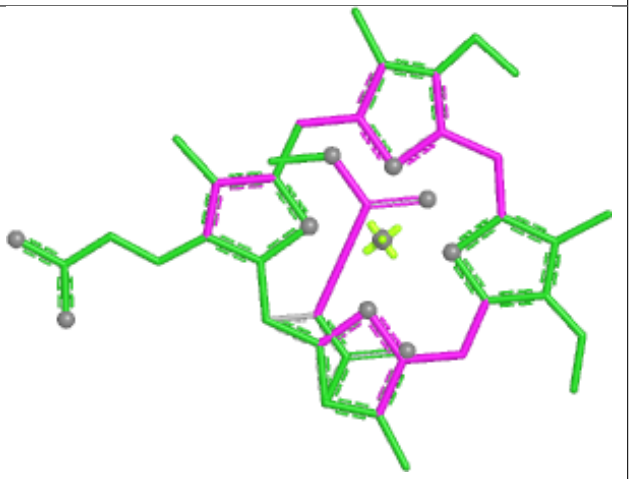


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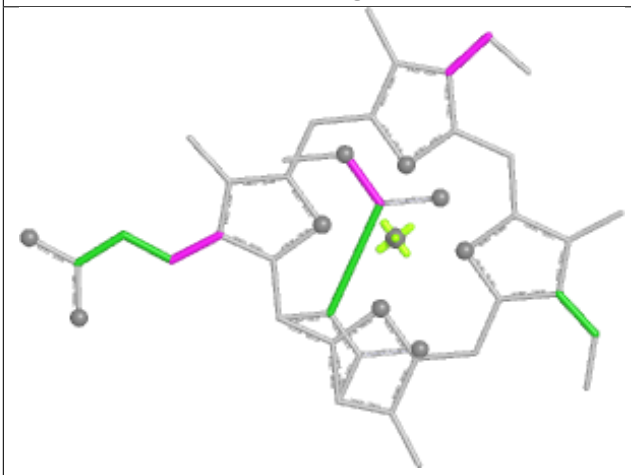
Ligand KC1 F 314



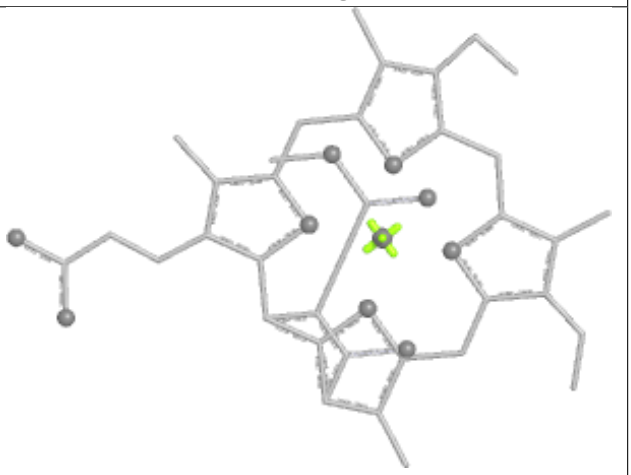
Bond lengths



Bond angles

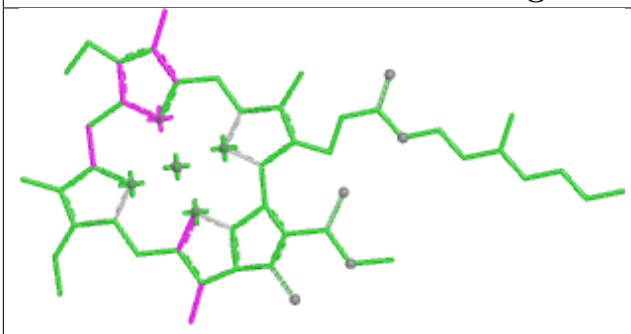


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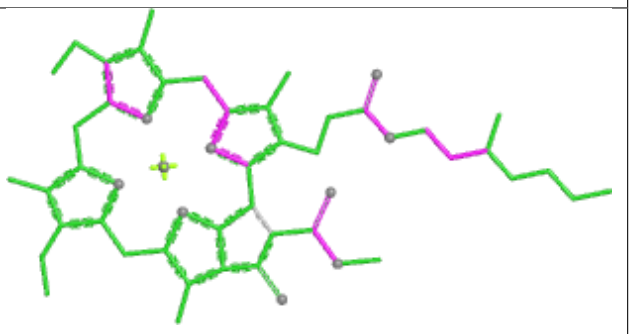


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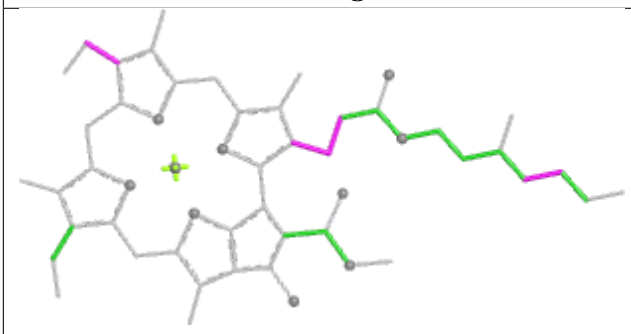
Ligand CLA b 713



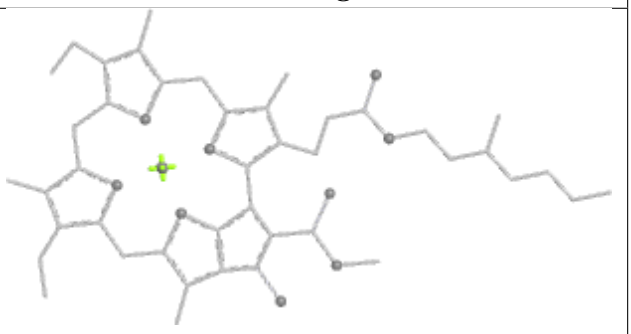
Bond lengths



Bond angles



Torsions

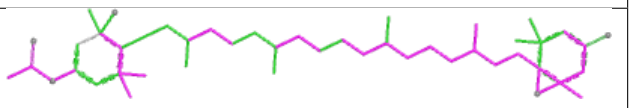


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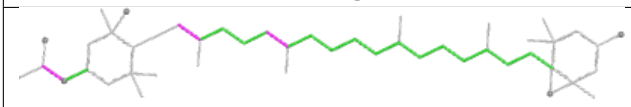
Ligand UIX C 306



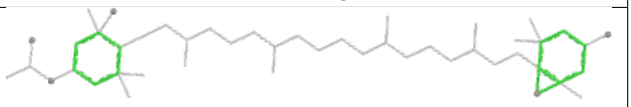
Bond lengths



Bond angles

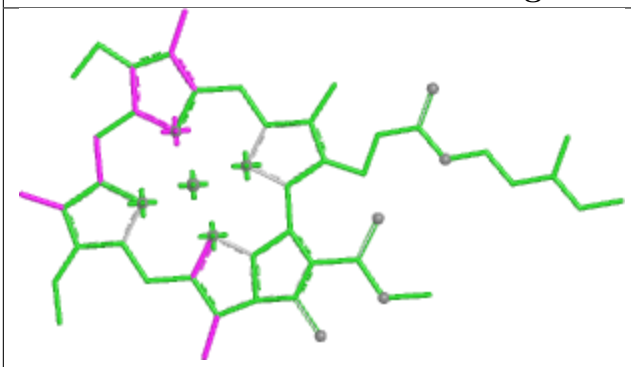


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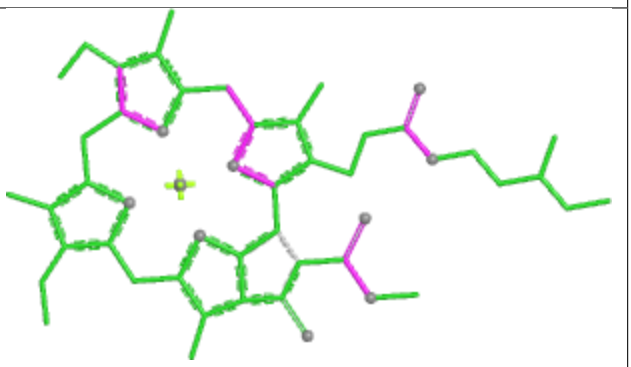


Rings

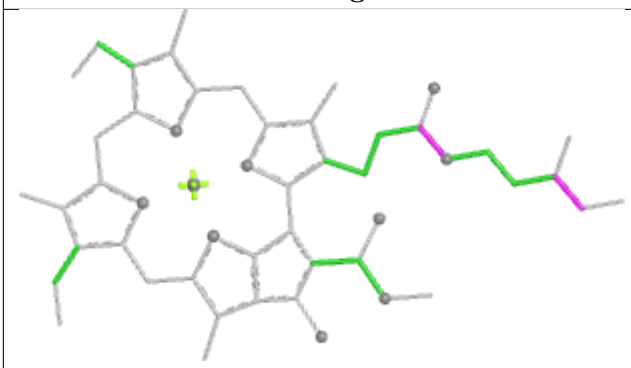
Ligand CLA B 311



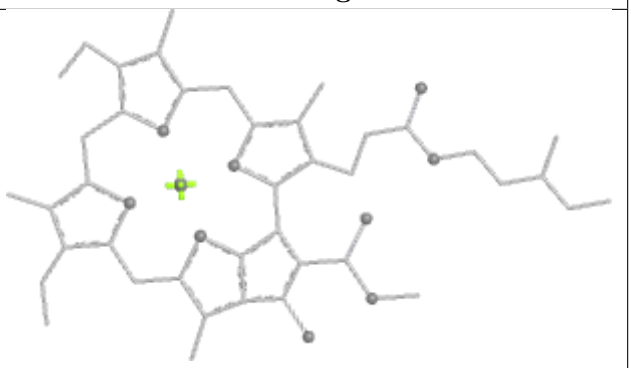
Bond lengths



Bond angles

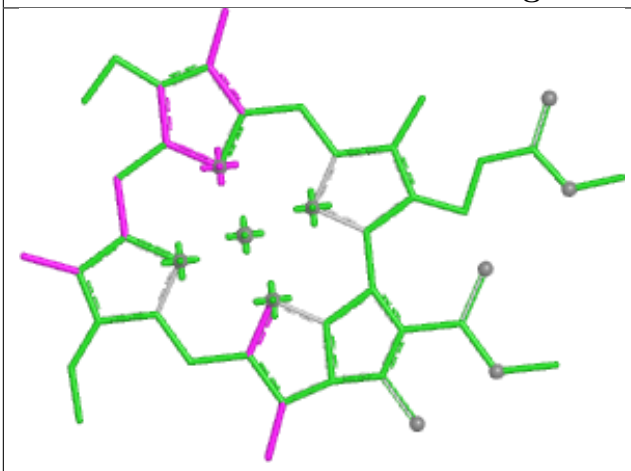


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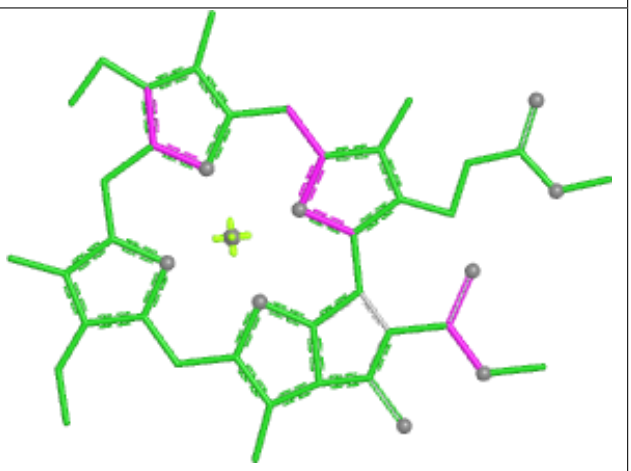


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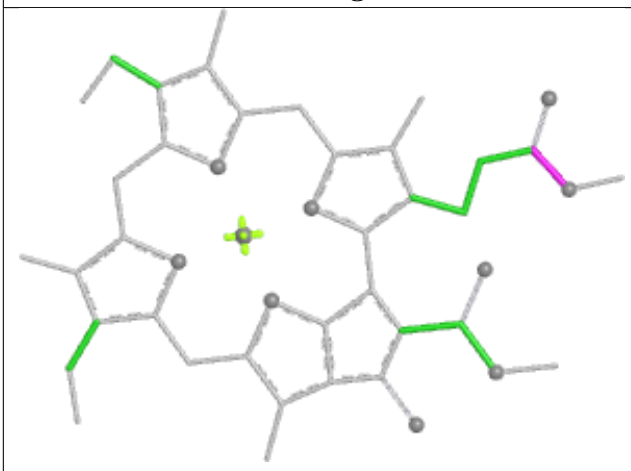
Ligand CLA K 208



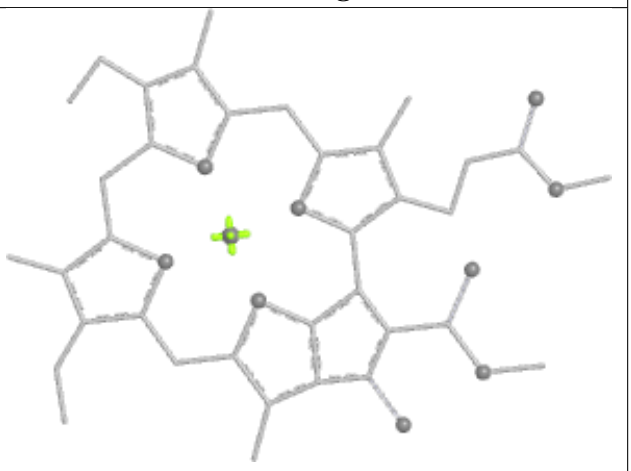
Bond lengths



Bond angles

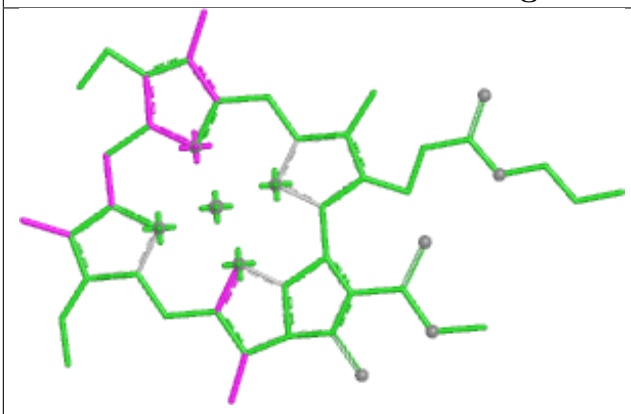


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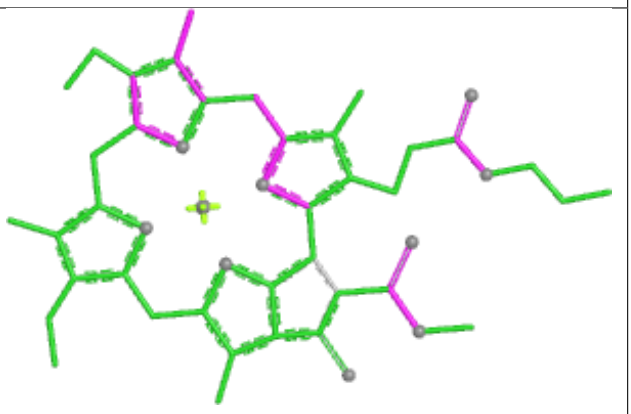


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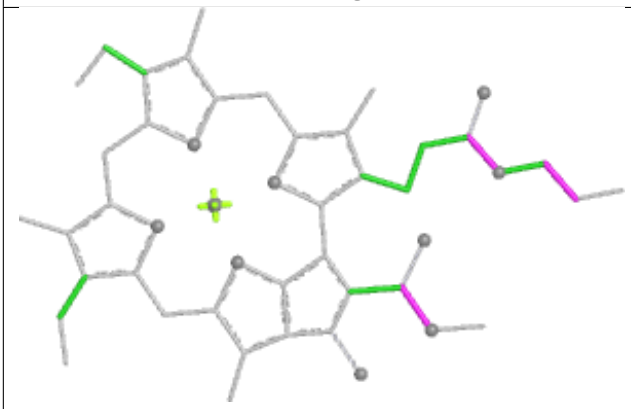
Ligand CLA M 310



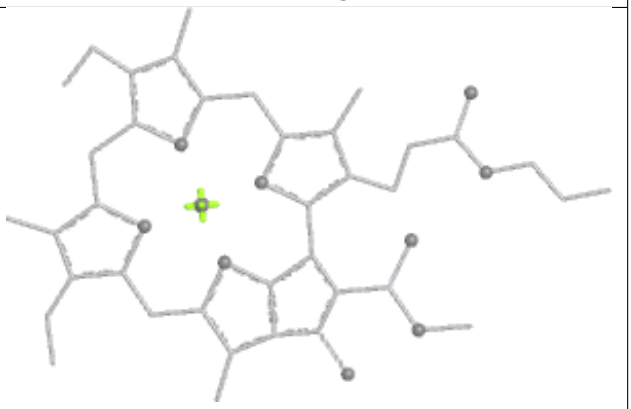
Bond lengths



Bond angles

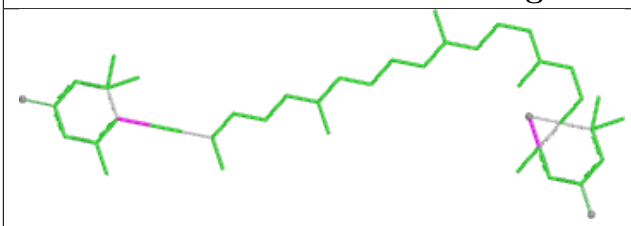


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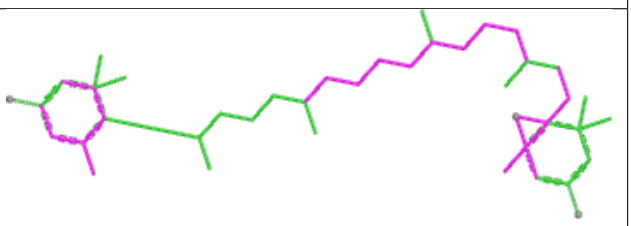


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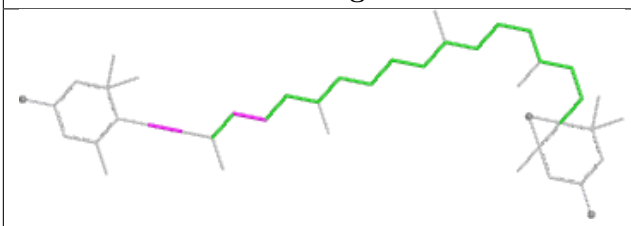
Ligand DD6 P 204



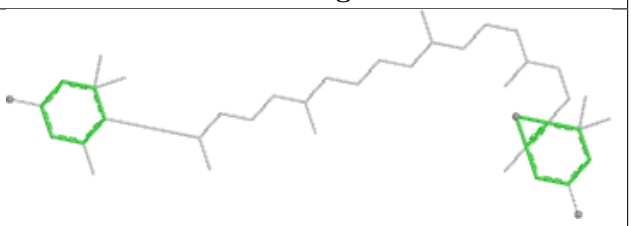
Bond lengths



Bond angles

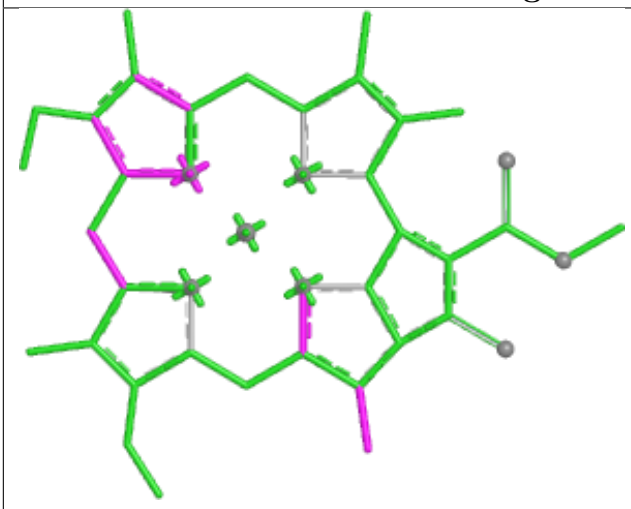


Torsions

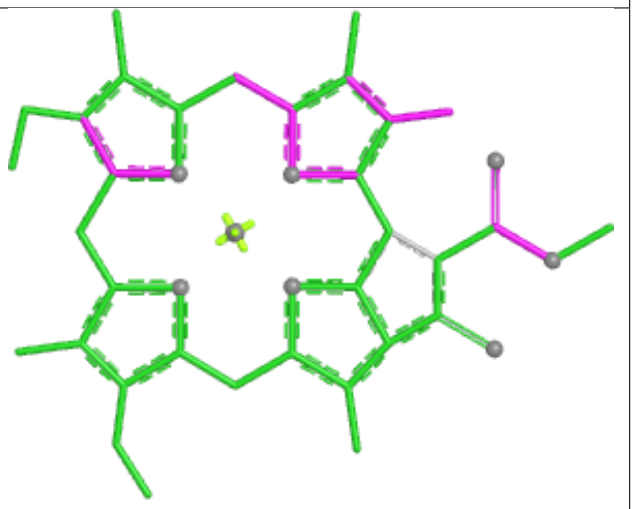


Rings

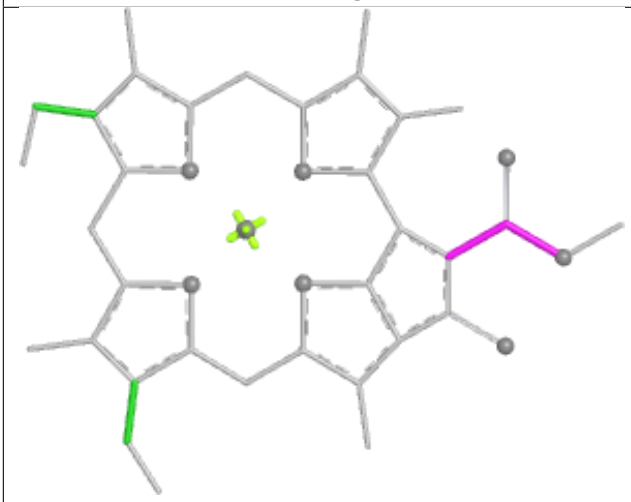
Ligand CLA H 315



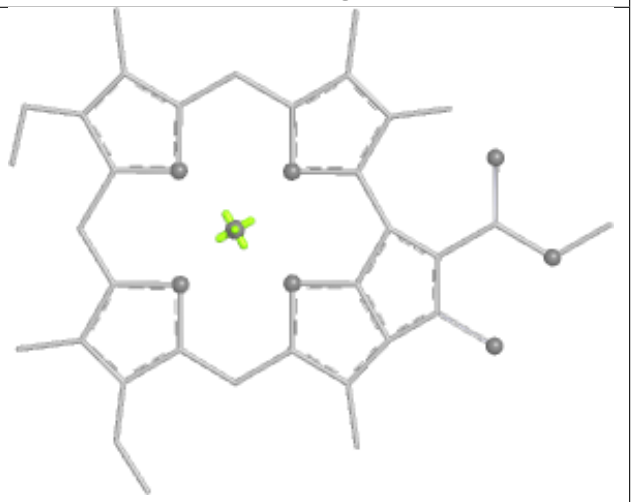
Bond lengths



Bond angles



Torsions

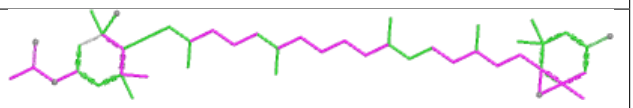


Rings

Ligand UIX B 304



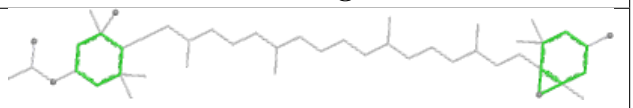
Bond lengths



Bond angles

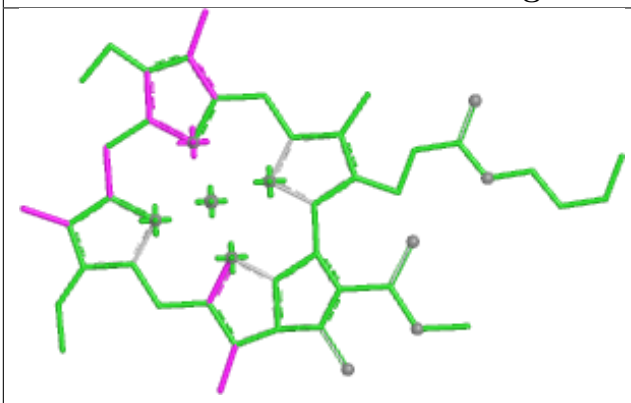


Torsions

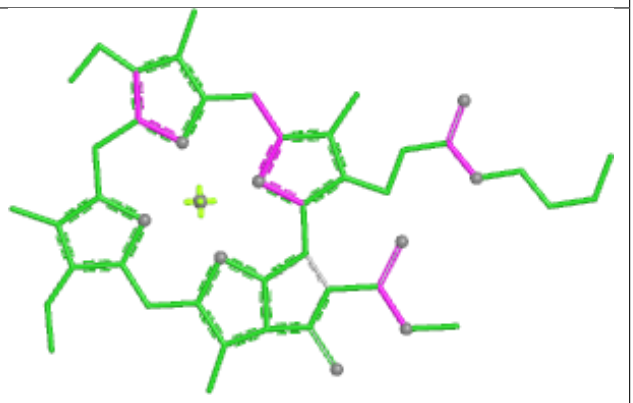


Rings

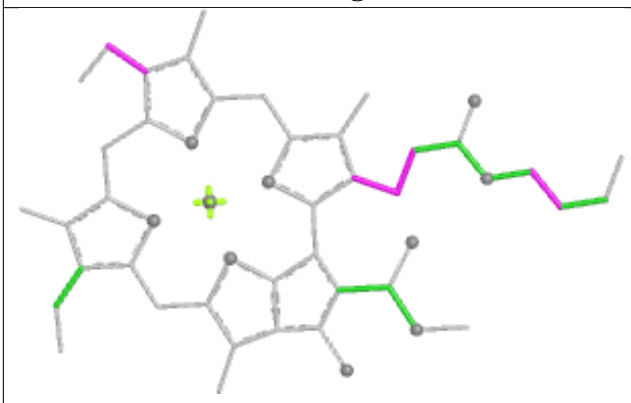
Ligand CLA K 207



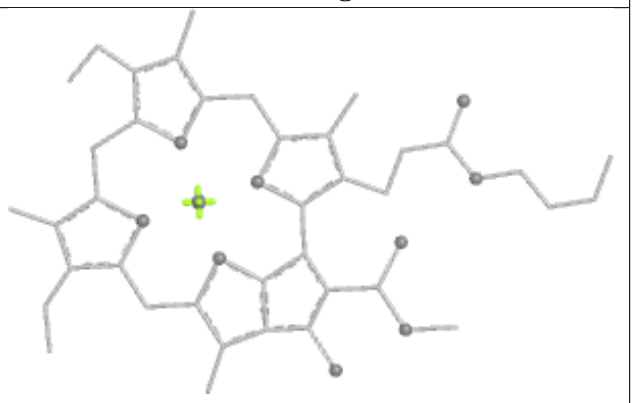
Bond lengths



Bond angles

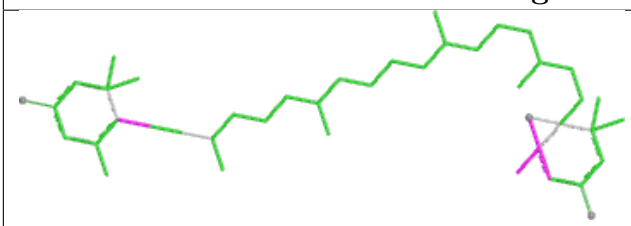


Torsions

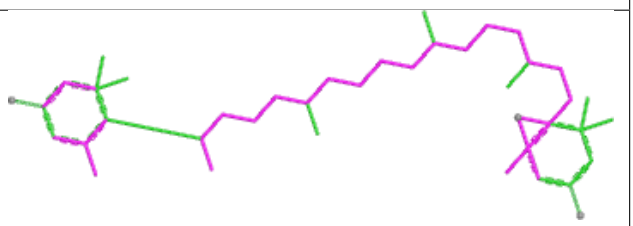


Rings

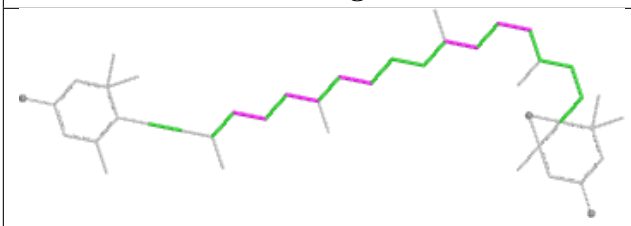
Ligand DD6 I 203



Bond lengths



Bond angles

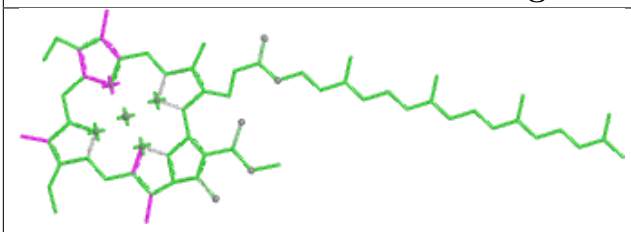


Torsions

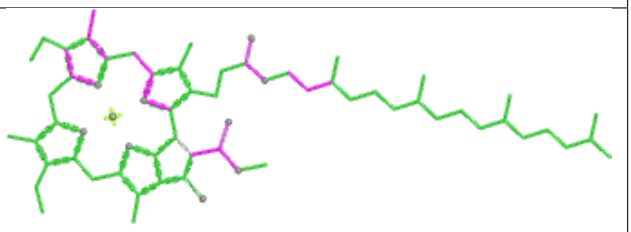


Rings

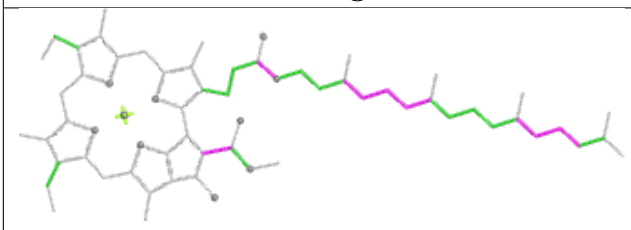
Ligand CLA a 825



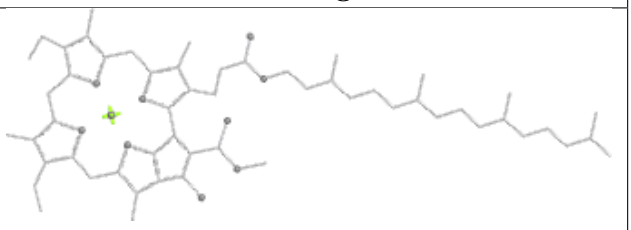
Bond lengths



Bond angles

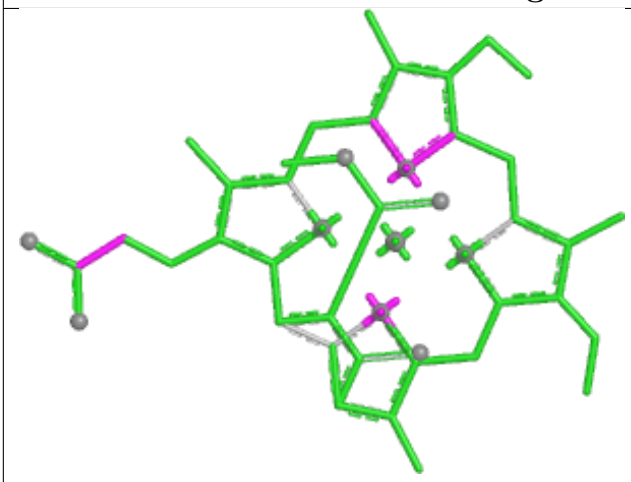


Torsions

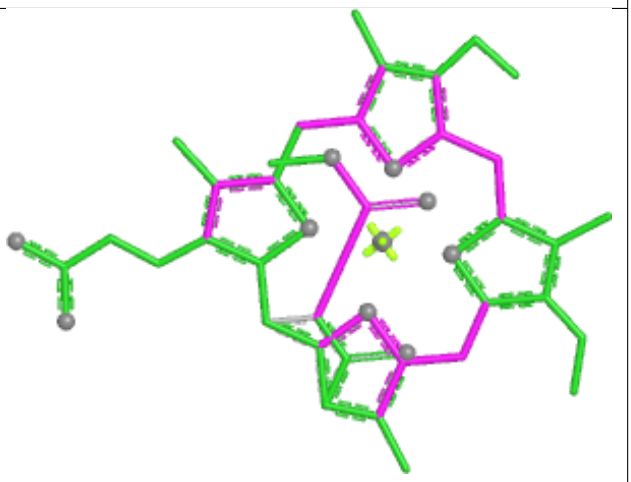


Rings

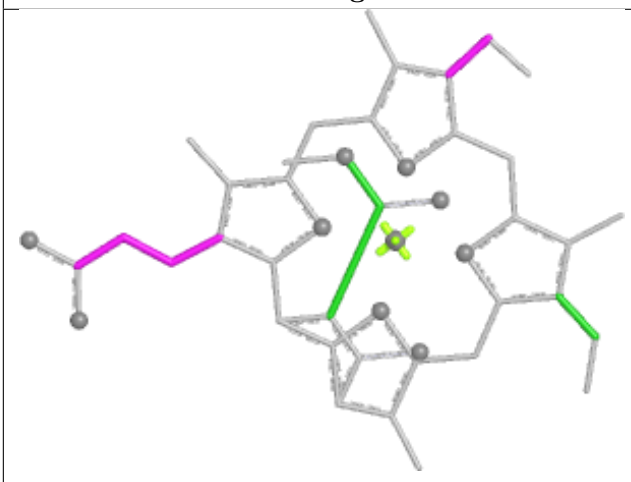
Ligand KC1 P 216



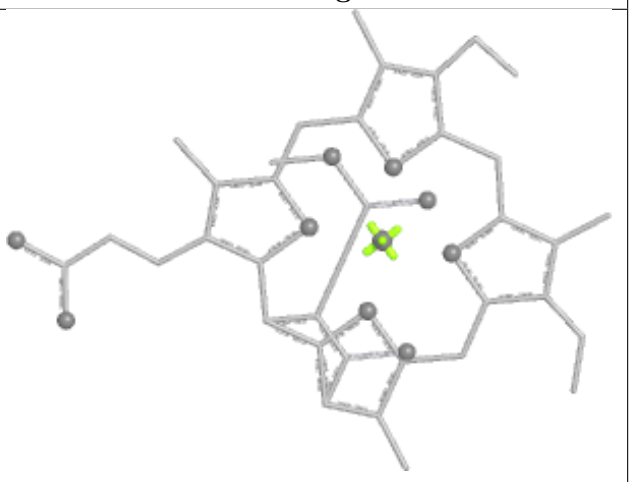
Bond lengths



Bond angles

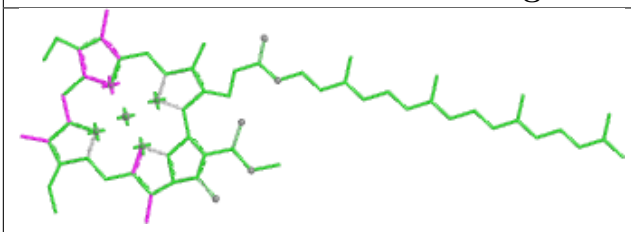


Torsions

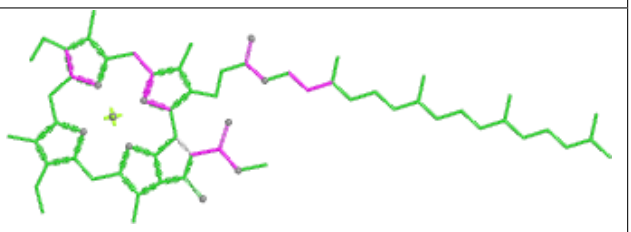


Rings

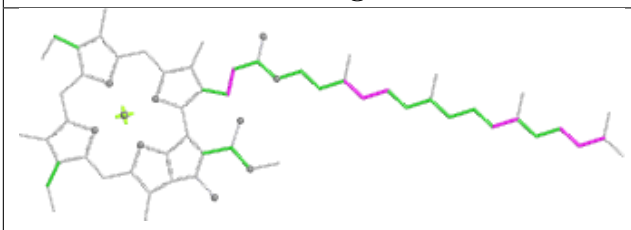
Ligand CLA H 308



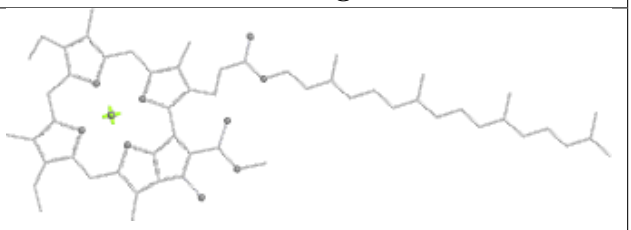
Bond lengths



Bond angles



Torsions

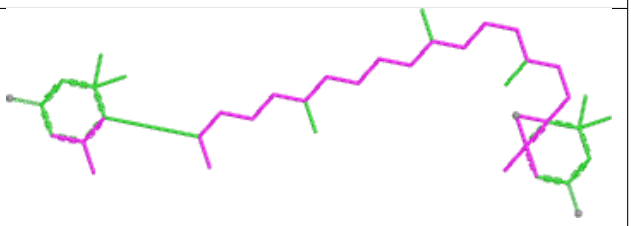


Rings

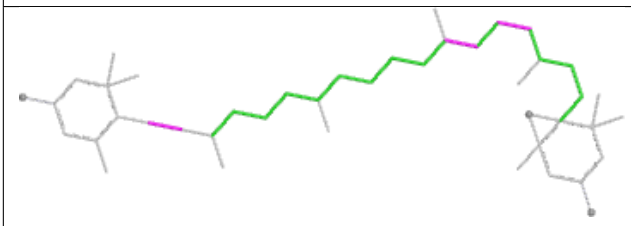
Ligand DD6 L 305



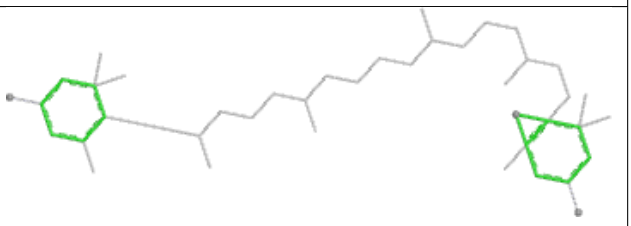
Bond lengths



Bond angles

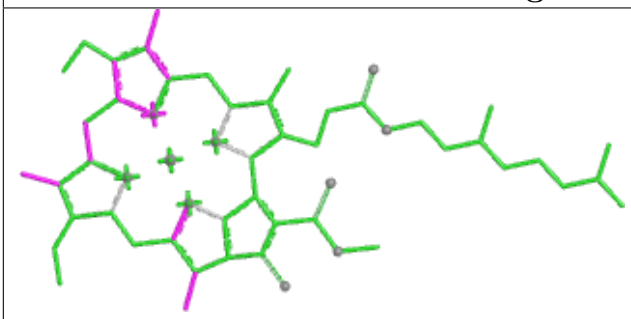


Torsions

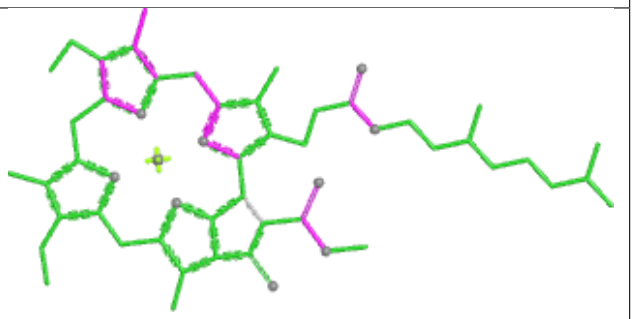


Rings

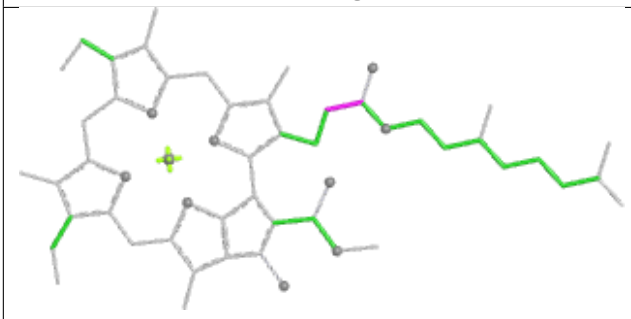
Ligand CLA L 309



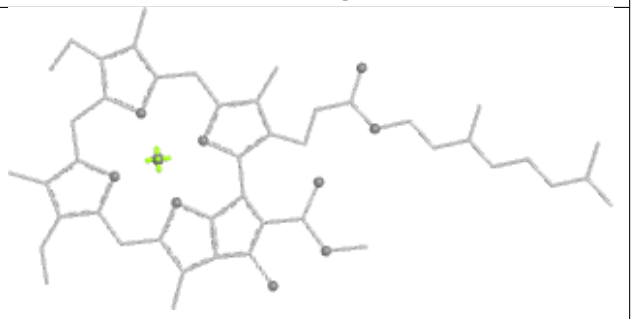
Bond lengths



Bond angles

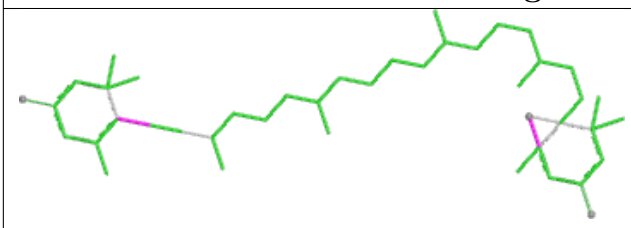


Torsions

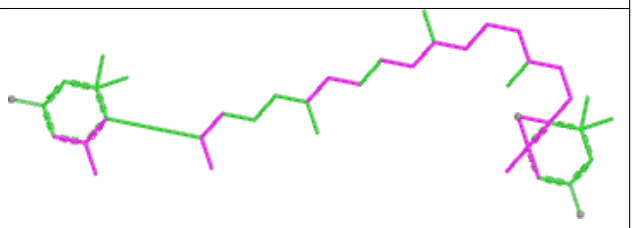


Rings

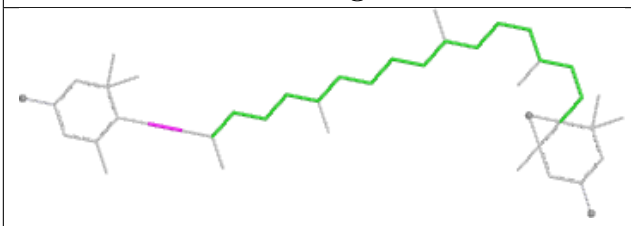
Ligand DD6 N 303



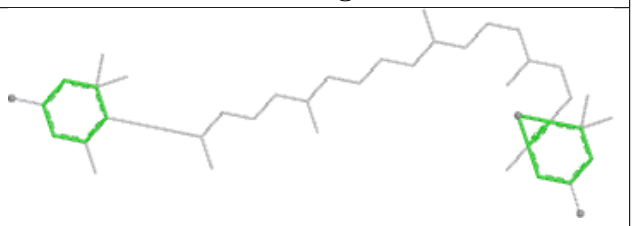
Bond lengths



Bond angles

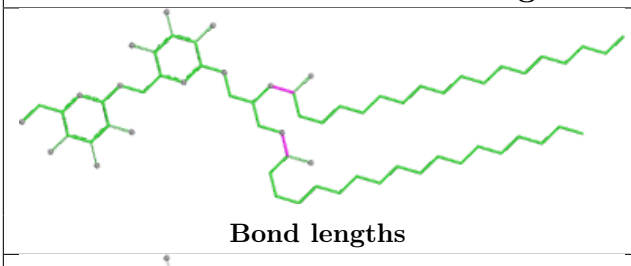


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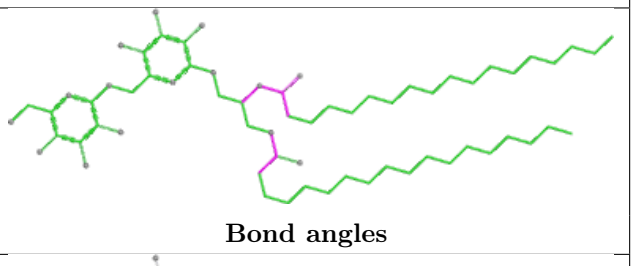


Rings

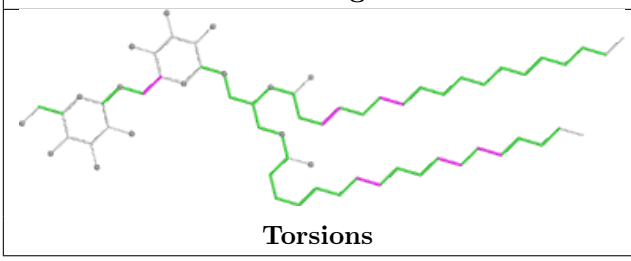
Ligand DGD m 102



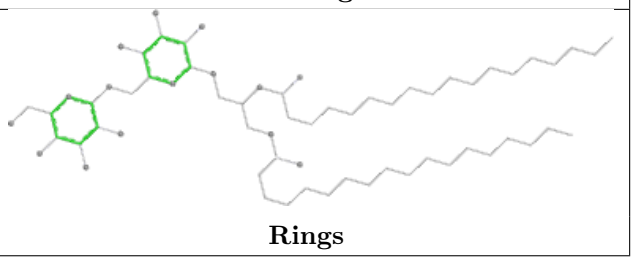
Bond lengths



Bond angles

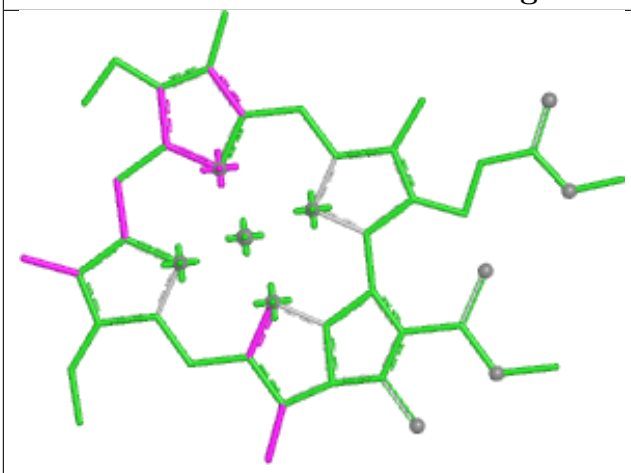


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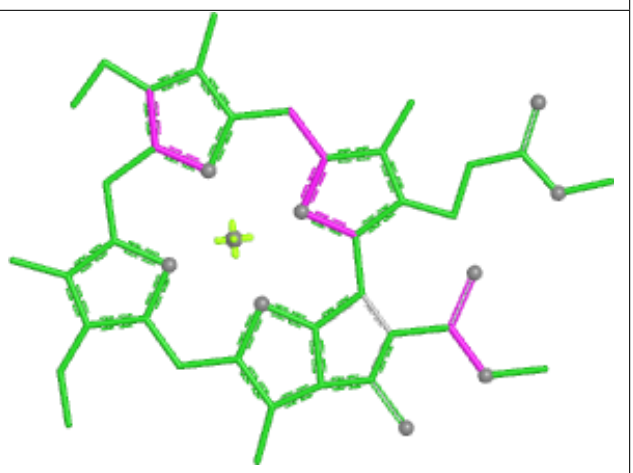


Rings

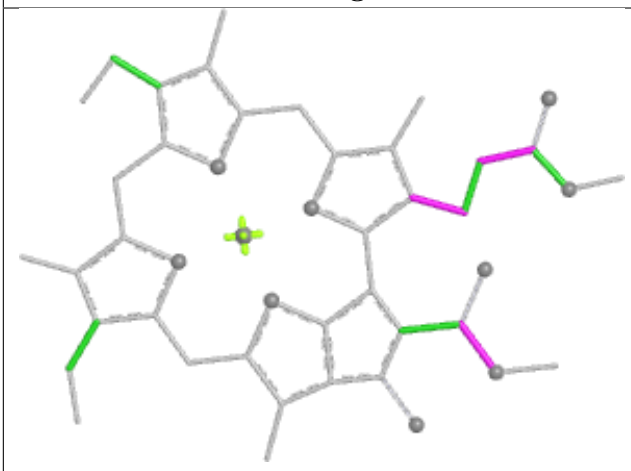
Ligand CLA M 315



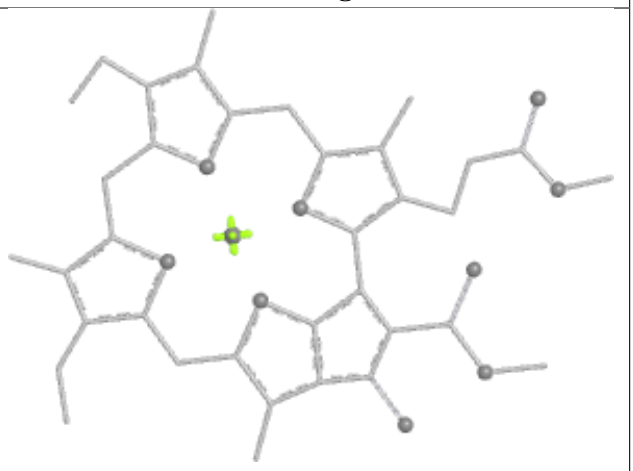
Bond lengths



Bond angles

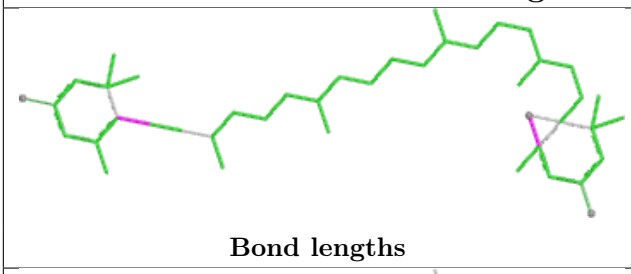


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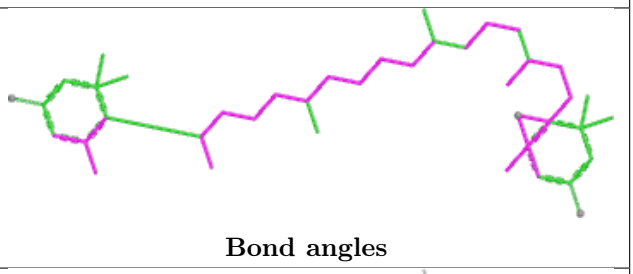


Rings

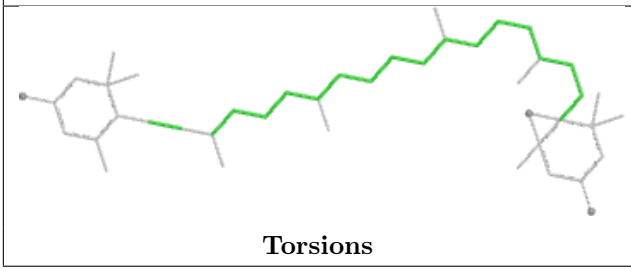
Ligand DD6 L 303



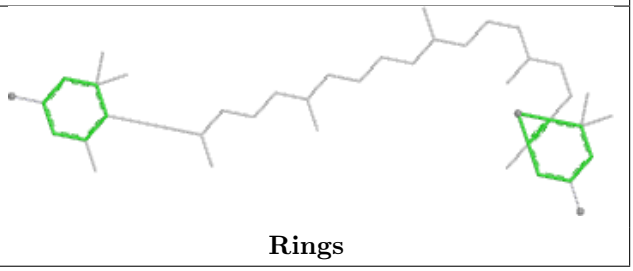
Bond lengths



Bond angles

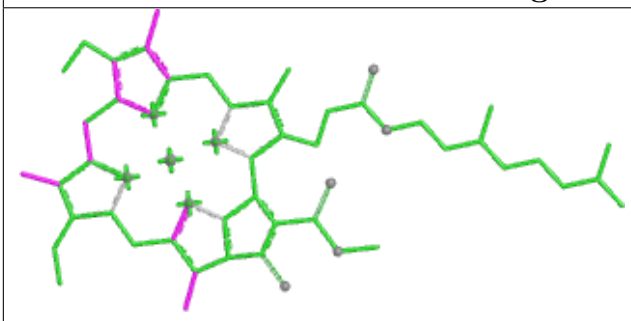


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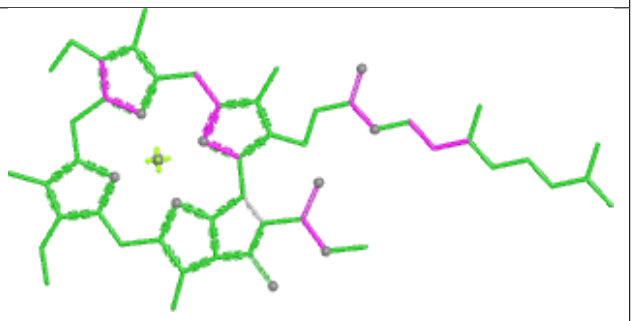


Rings

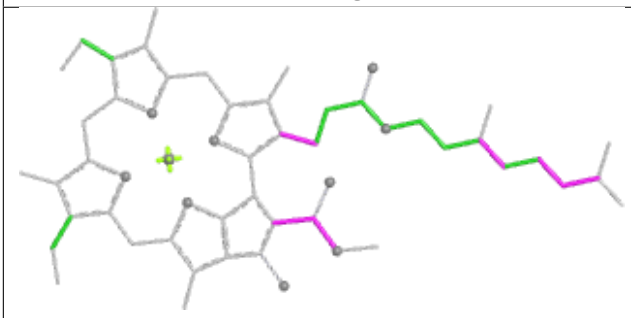
Ligand CLA I 217



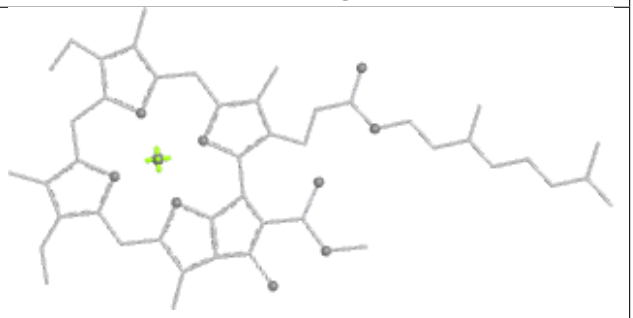
Bond lengths



Bond angles

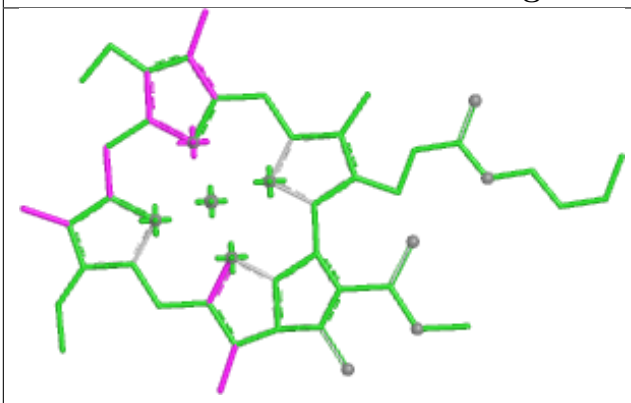


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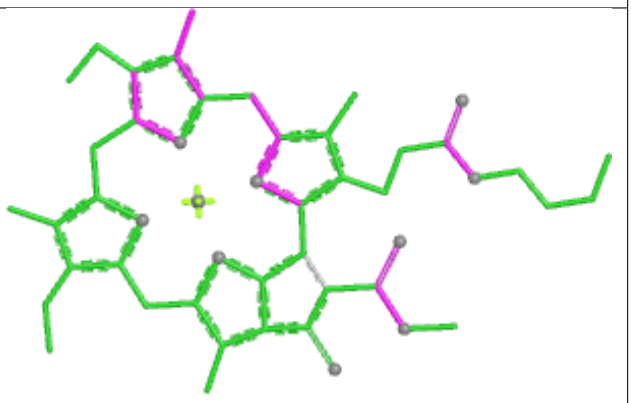


Rings

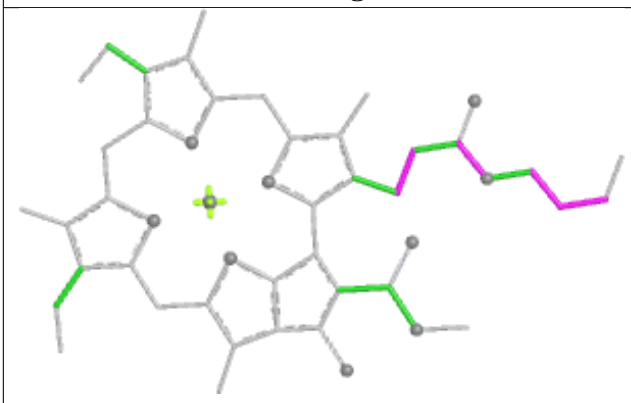
Ligand CLA G 301



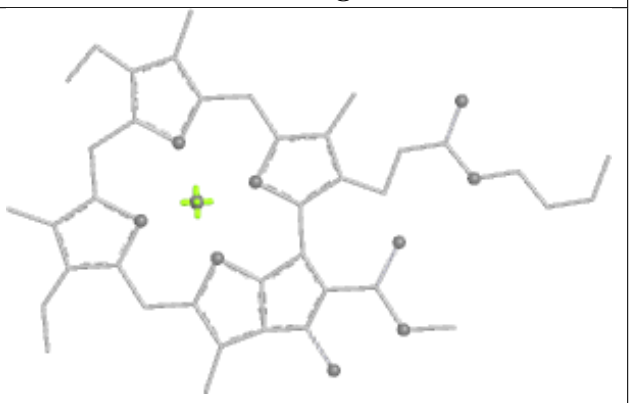
Bond lengths



Bond angles

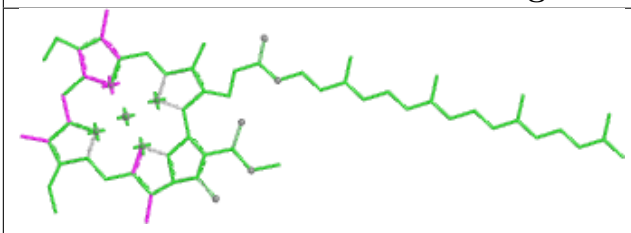


Torsions

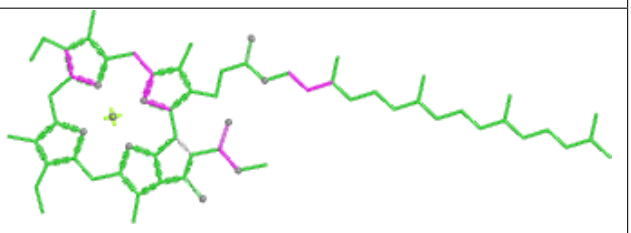


Rings

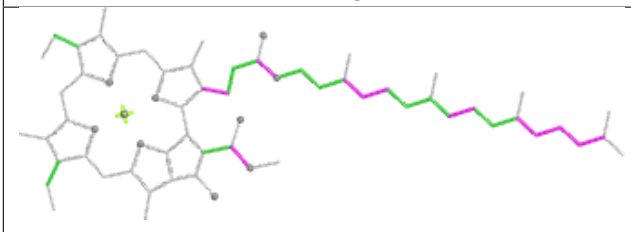
Ligand CLA J 306



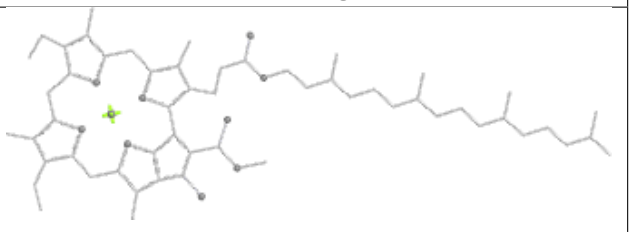
Bond lengths



Bond angles

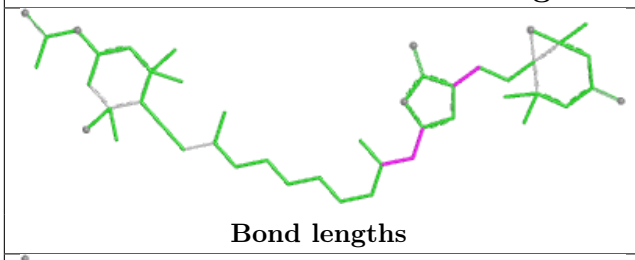


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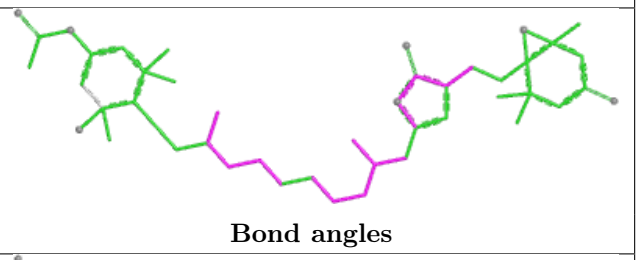


Rings

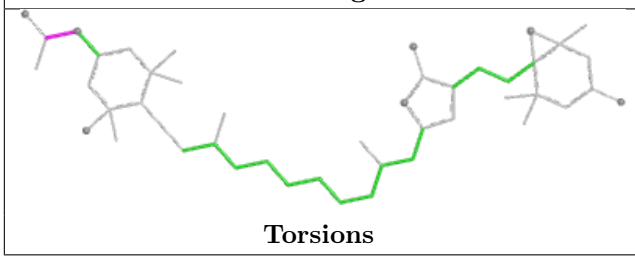
Ligand PID h 204



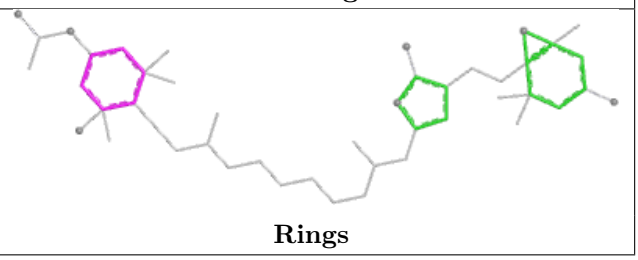
Bond lengths



Bond angles

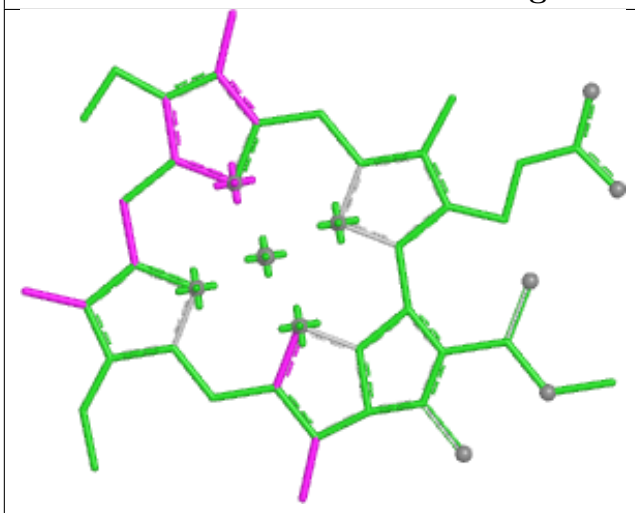


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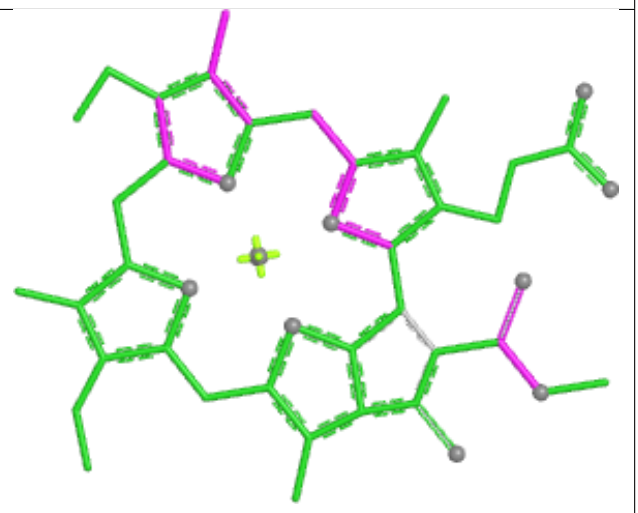


Rings

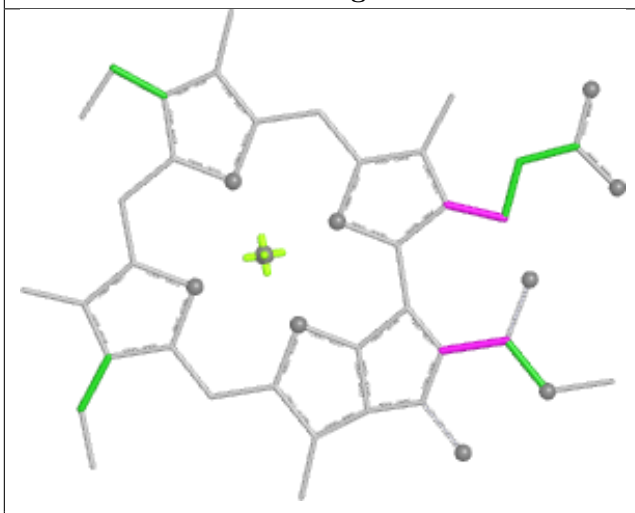
Ligand CLA a 815



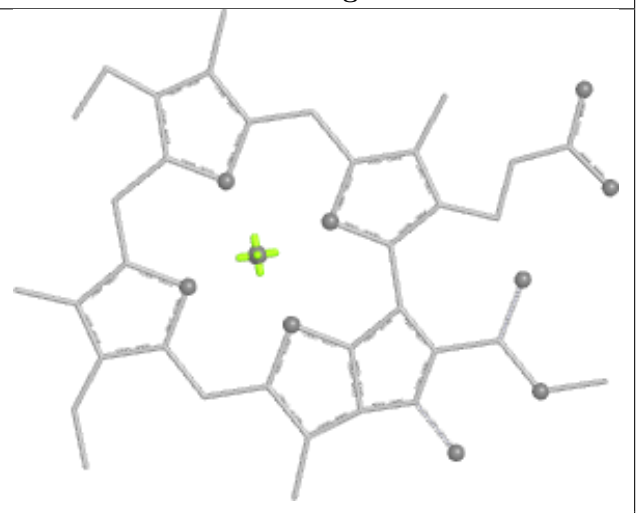
Bond lengths



Bond angles

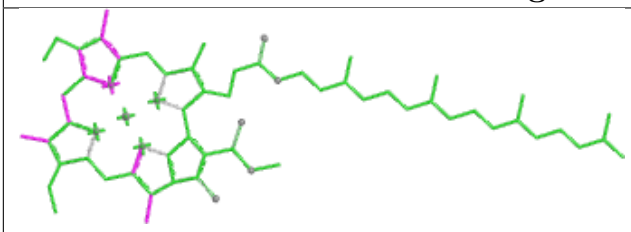


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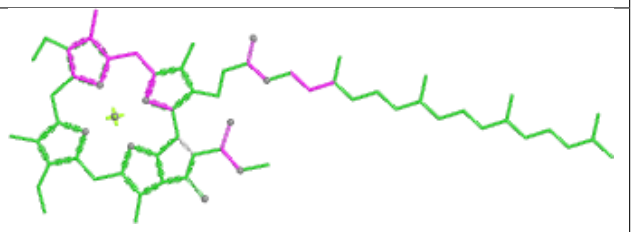


Rings

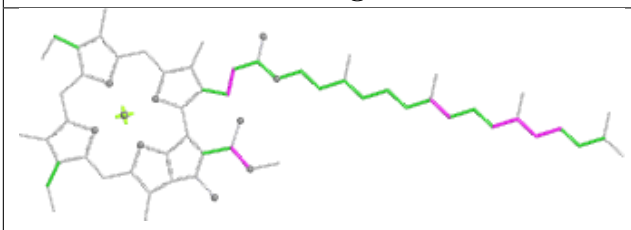
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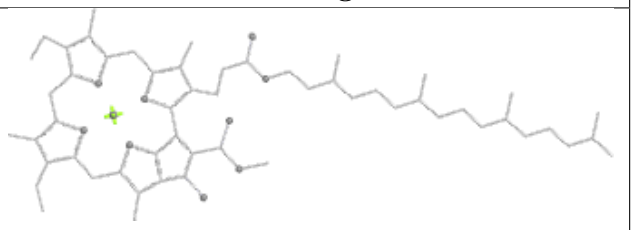
Bond lengths



Bond angles

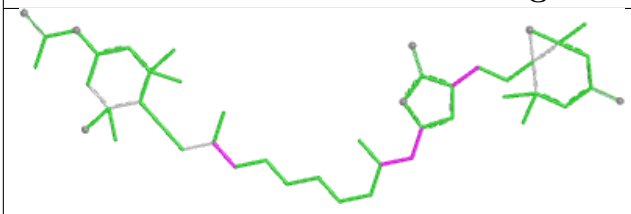


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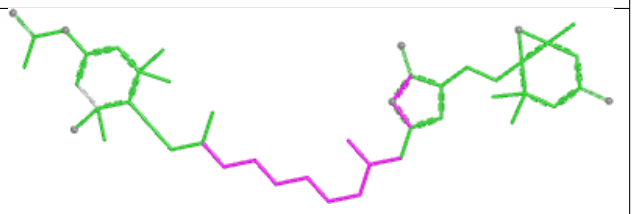


Rings

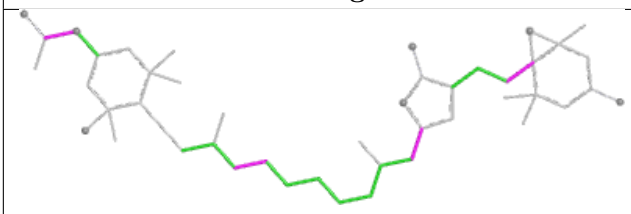
Ligand PID P 208



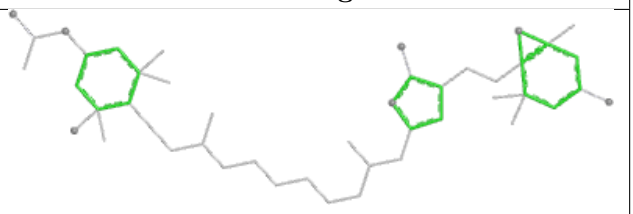
Bond lengths



Bond angles

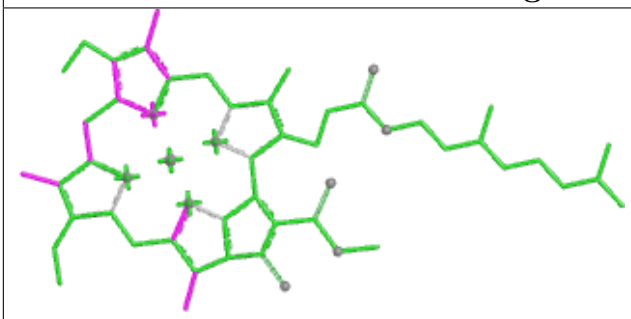


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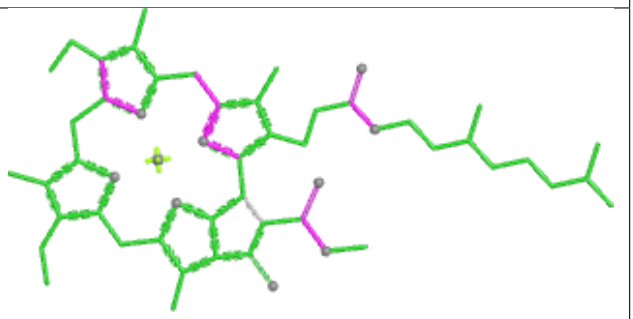


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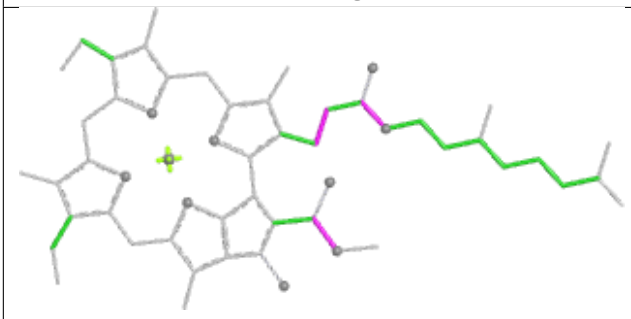
Ligand CLA A 207



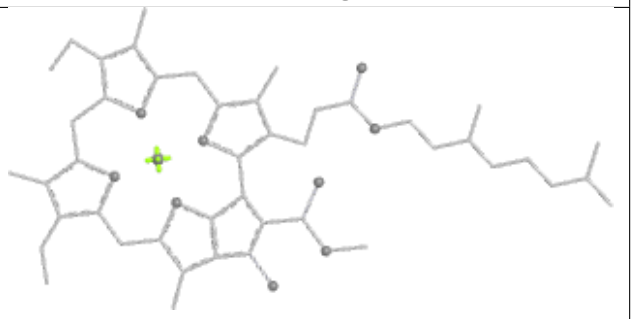
Bond lengths



Bond angles

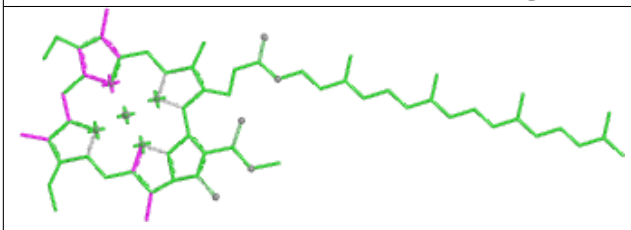


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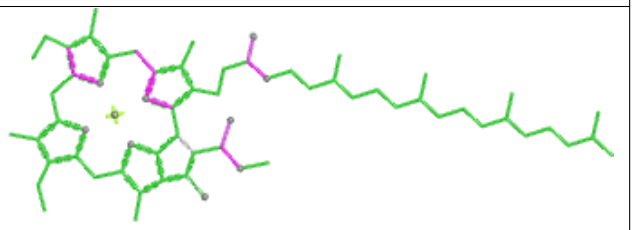


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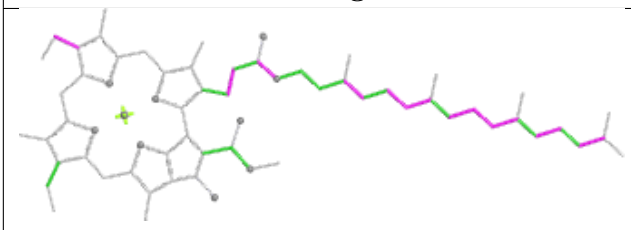
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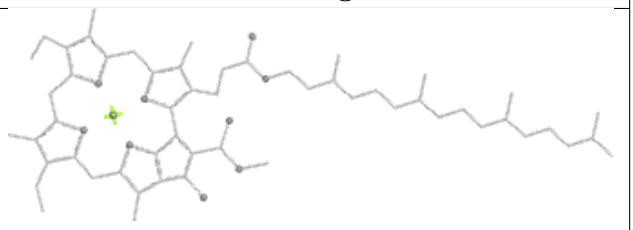
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Bond angles

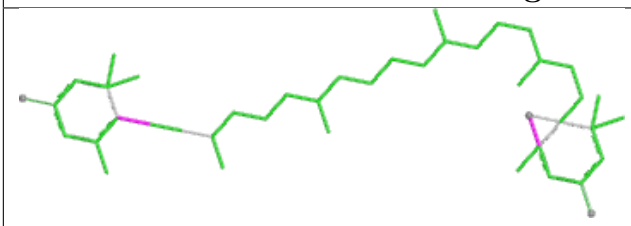


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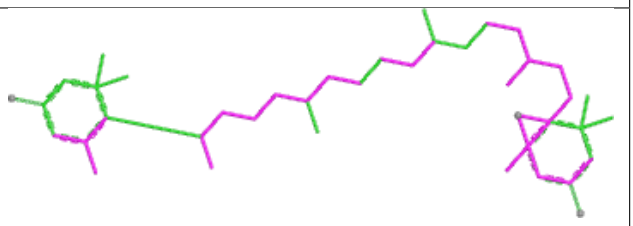


Rings

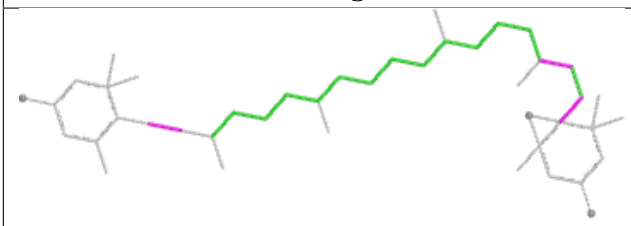
Ligand DD6 K 204



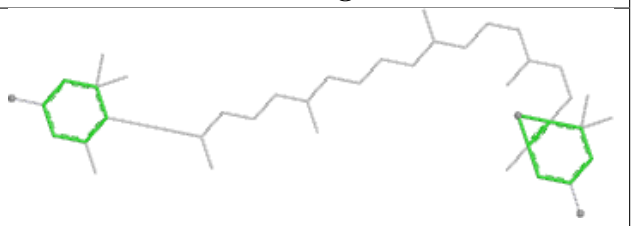
Bond lengths



Bond angles

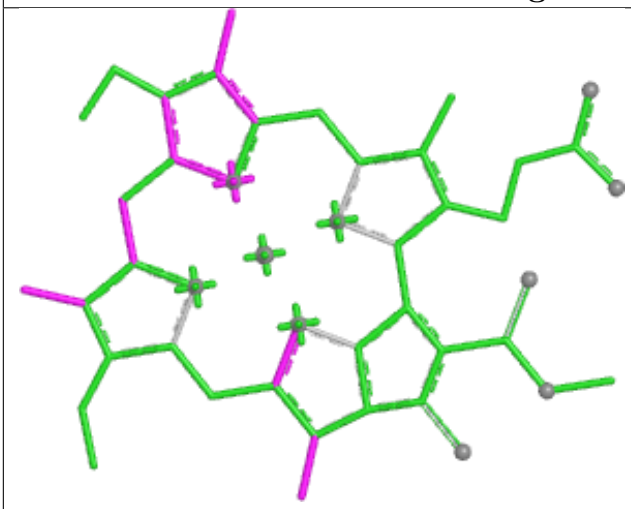


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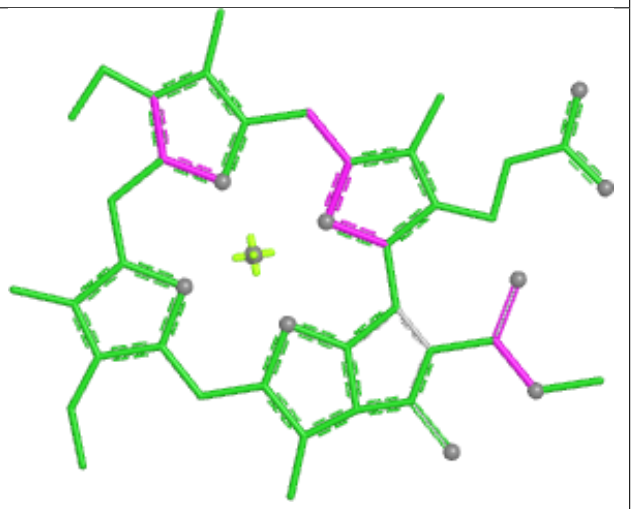


Rings

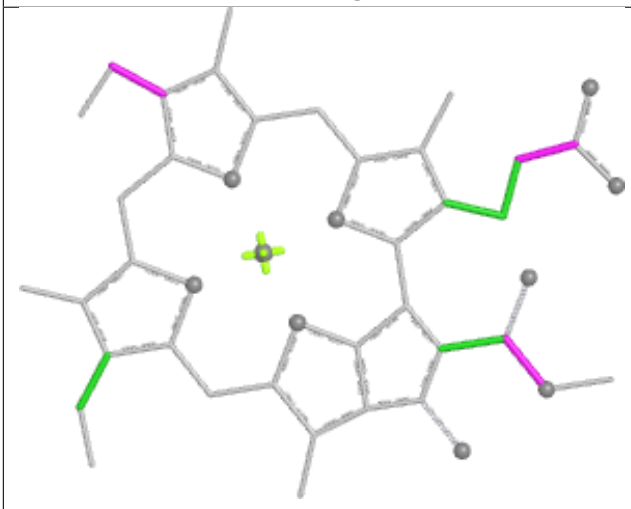
Ligand CLA a 817



Bond lengths



Bond angles

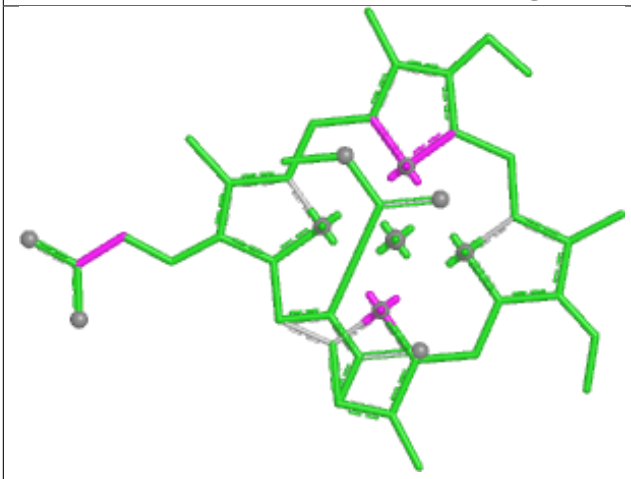


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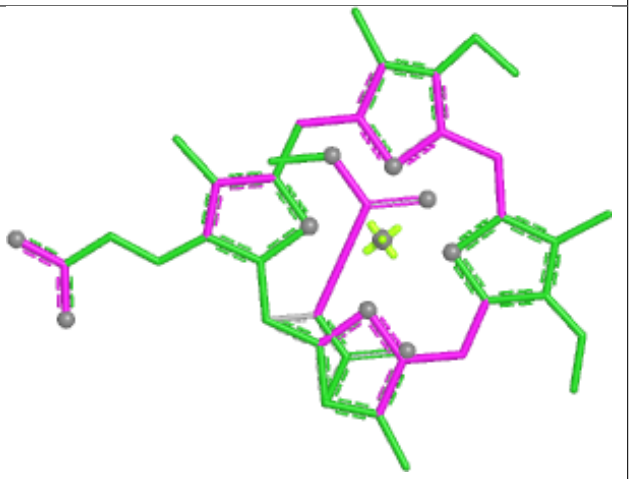


Rings

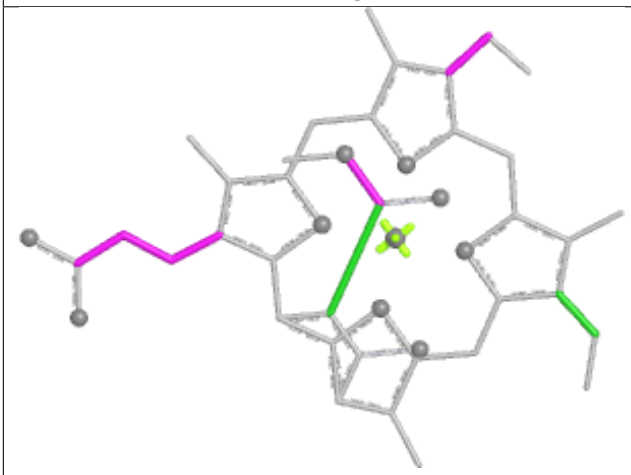
Ligand KC1 O 315



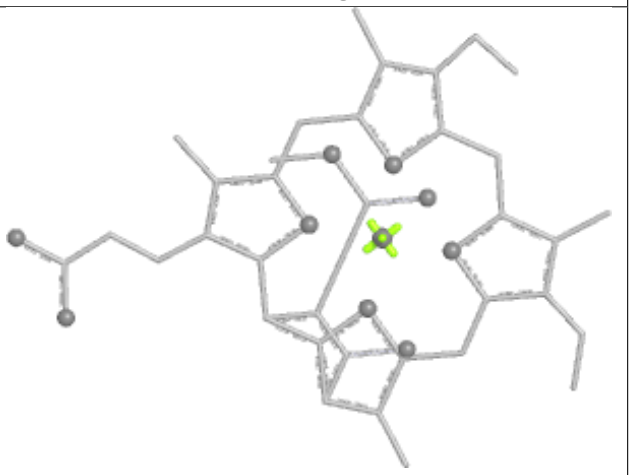
Bond lengths



Bond angles

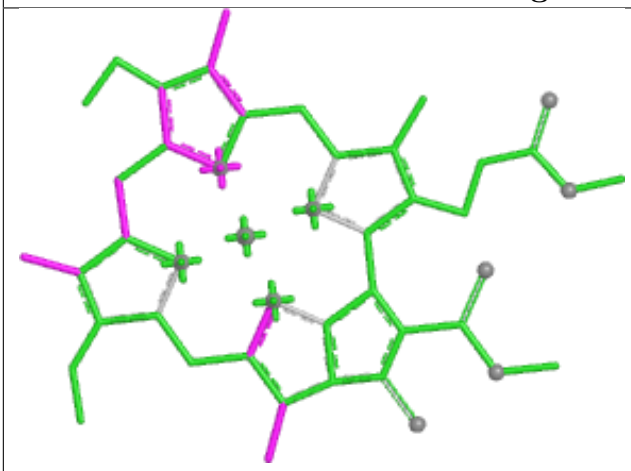


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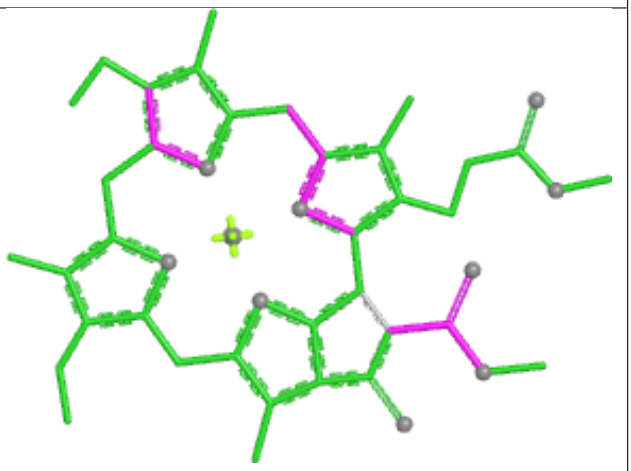


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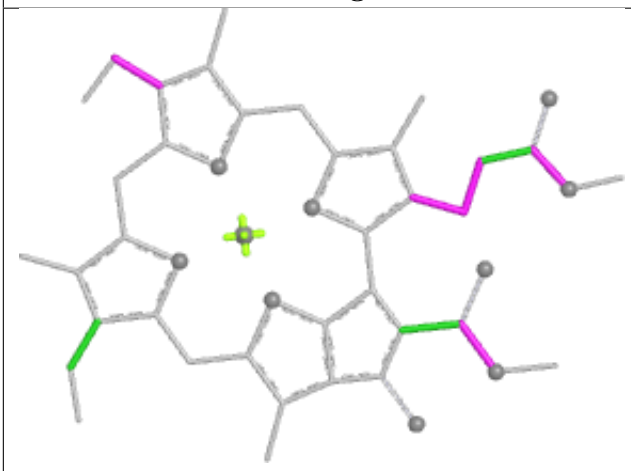
Ligand CLA I 208



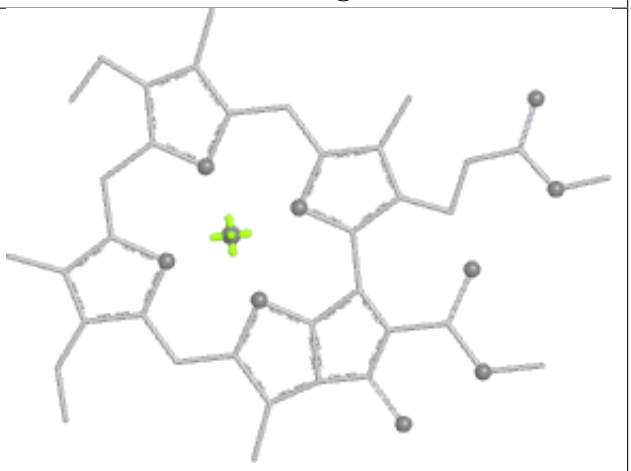
Bond lengths



Bond angles

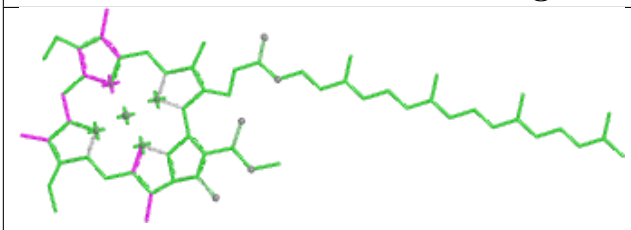


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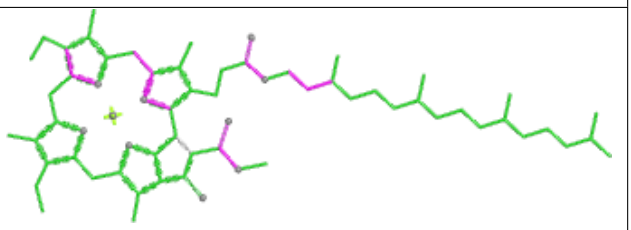


Rings

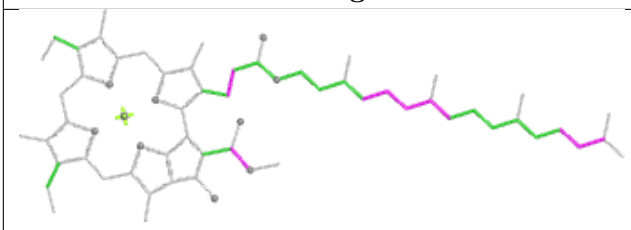
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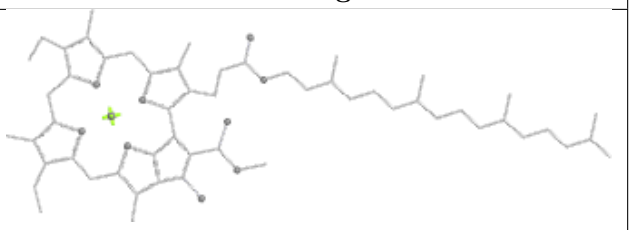
Bond lengths



Bond angles

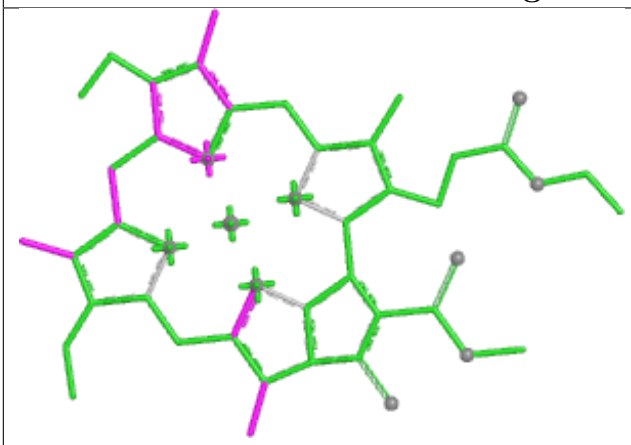


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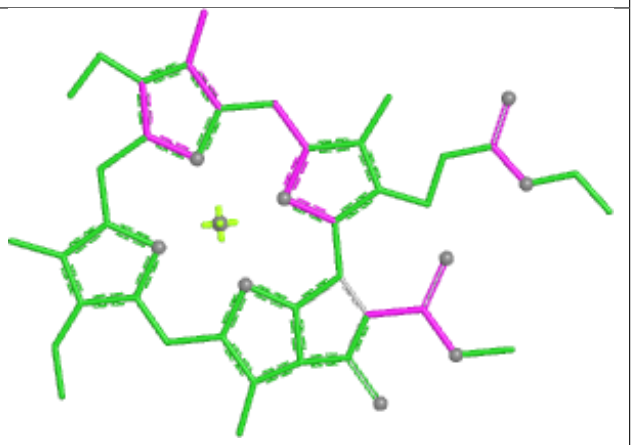


Rings

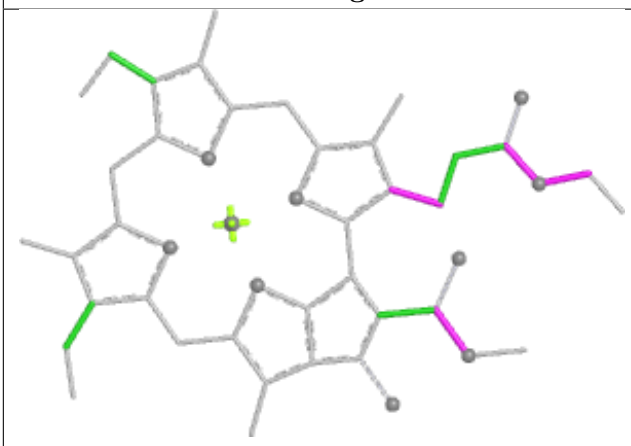
Ligand CLA N 314



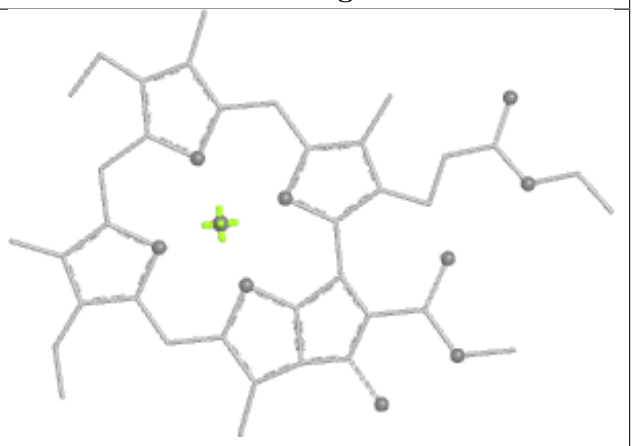
Bond lengths



Bond angles

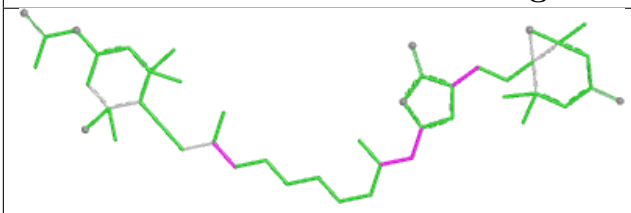


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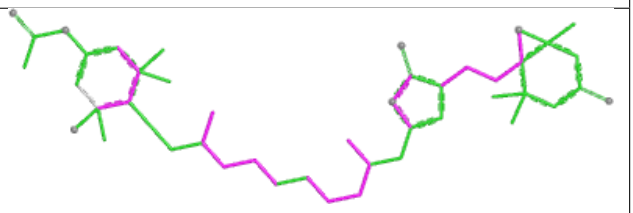


Rings

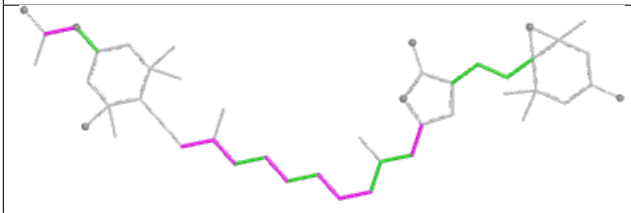
Ligand PID P 206



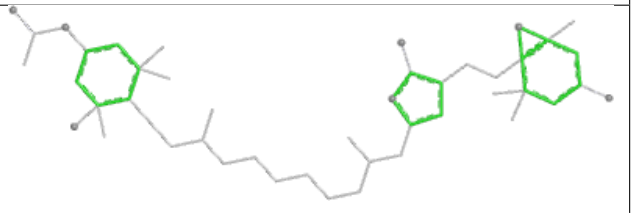
Bond lengths



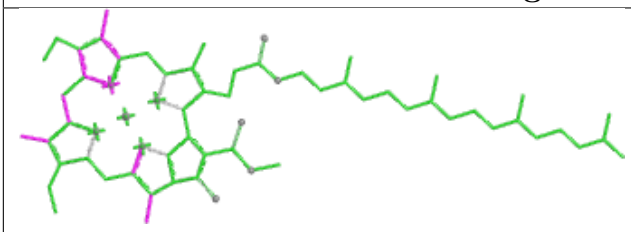
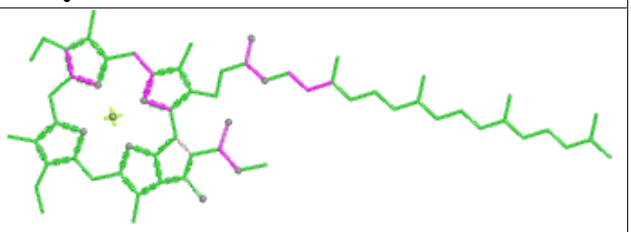
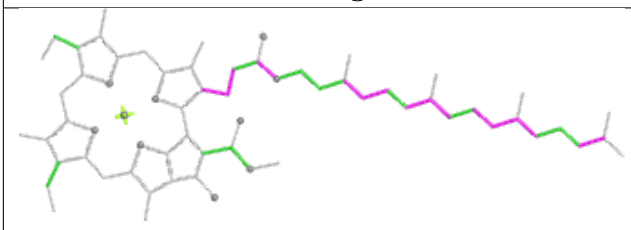
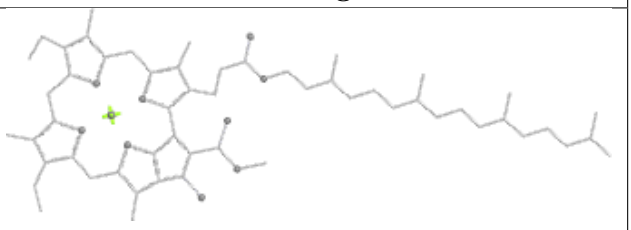
Bond angles

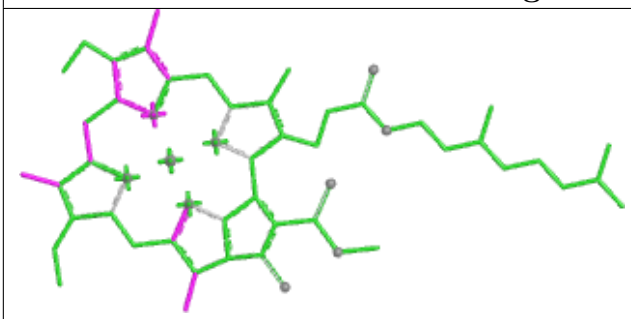
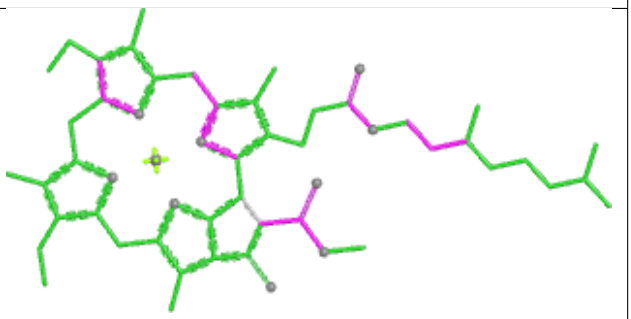
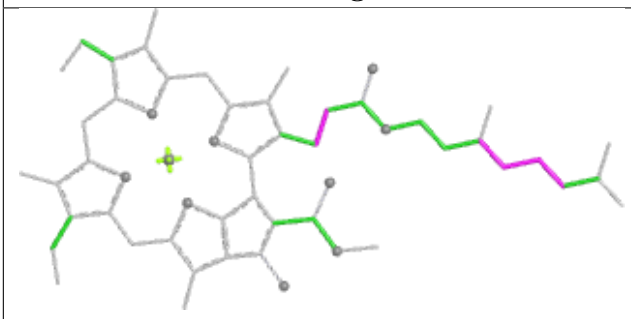
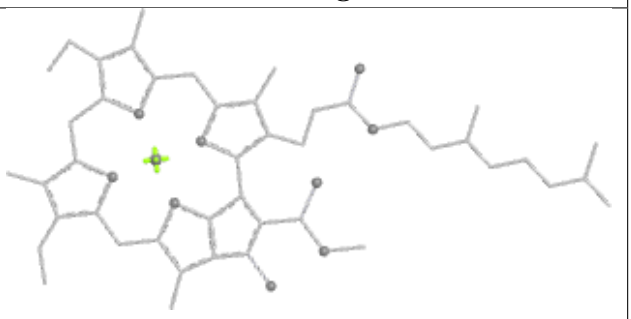


Torsions

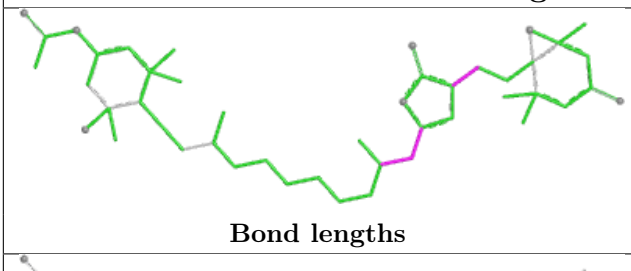


Rings

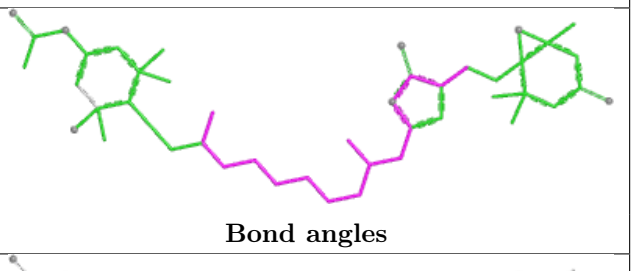
Ligand CLA Q 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

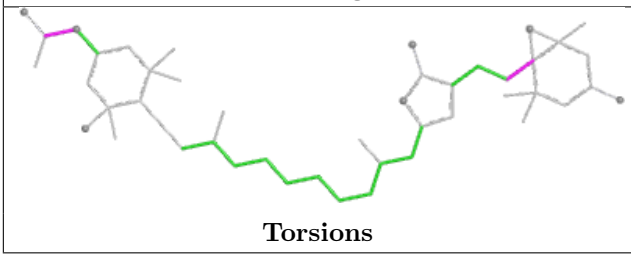
Ligand PID P 203



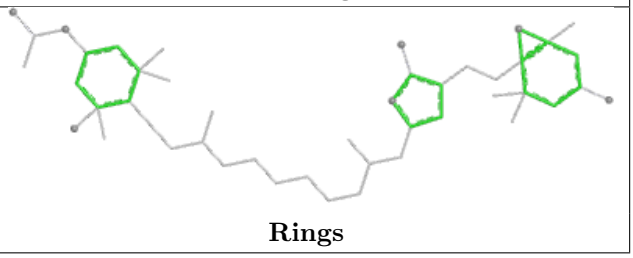
Bond lengths



Bond angles

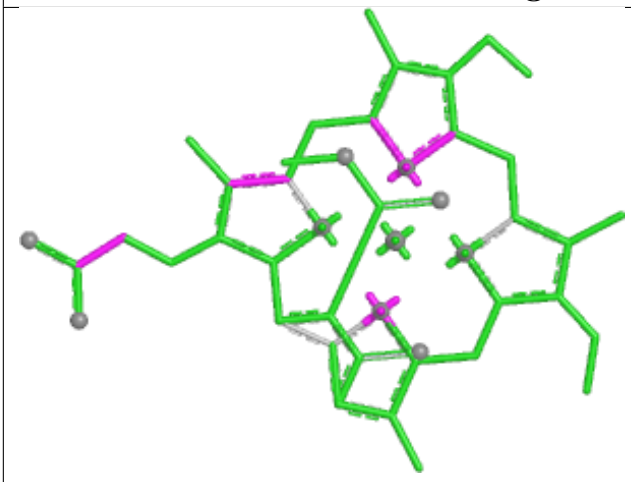


Torsions

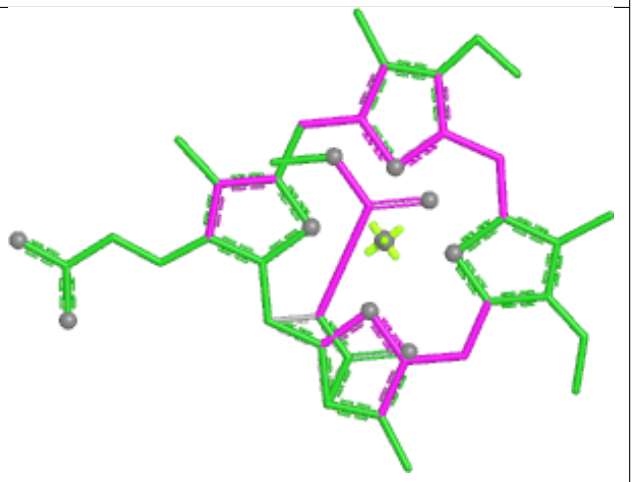


Rings

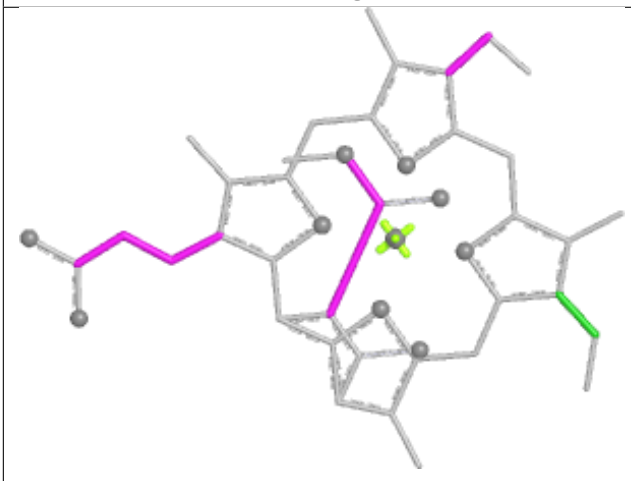
Ligand KC1 H 309



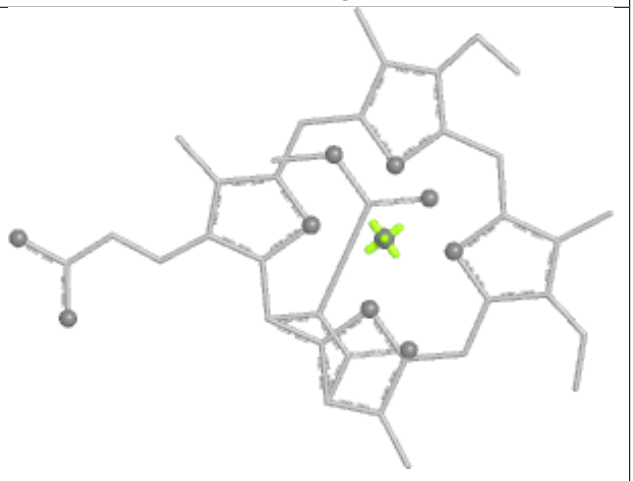
Bond lengths



Bond angles

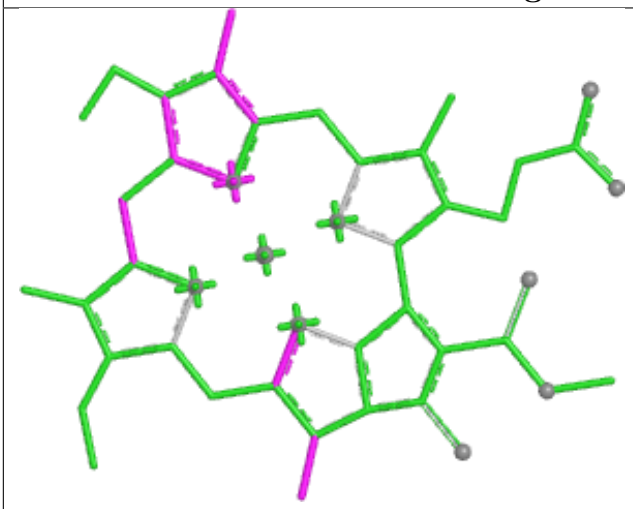


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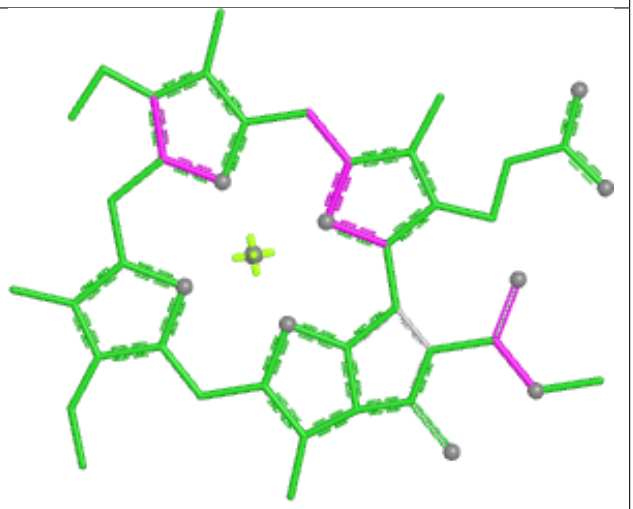


Rings

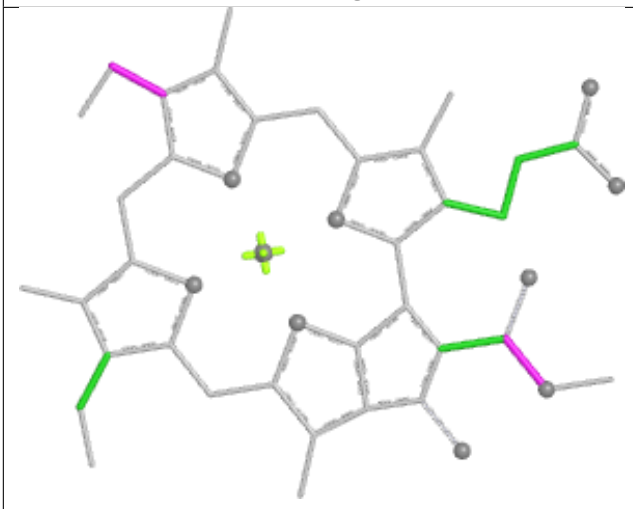
Ligand CLA B 307



Bond lengths



Bond angles

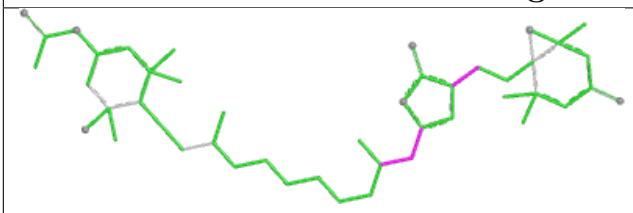


Torsions

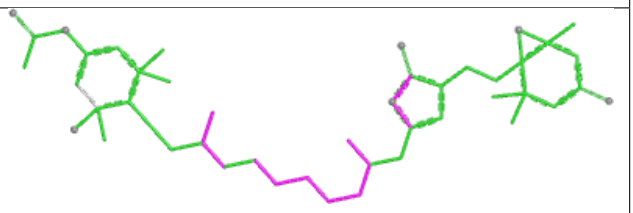


Rings

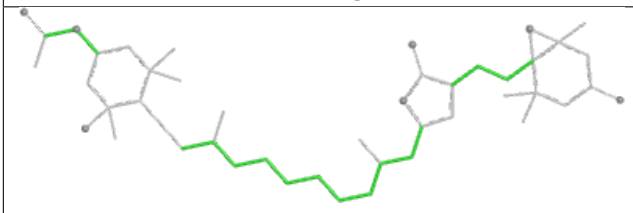
Ligand PID H 304



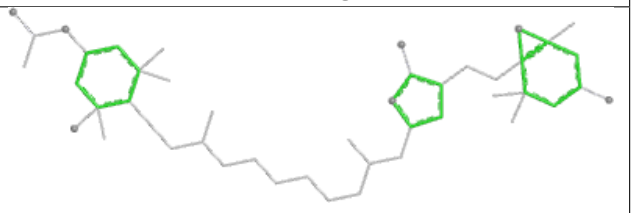
Bond lengths



Bond angles

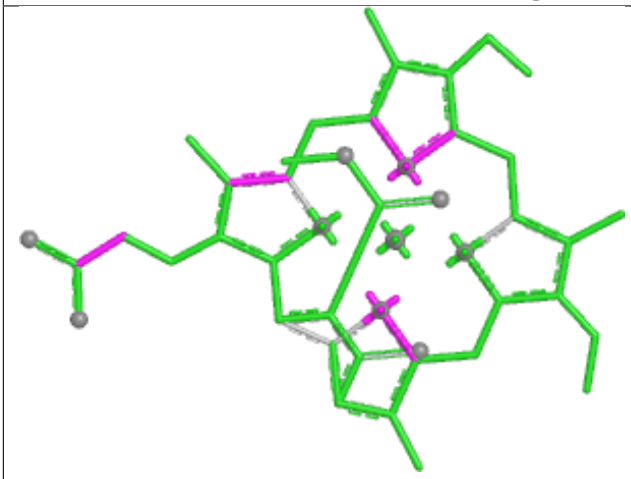


Torsions

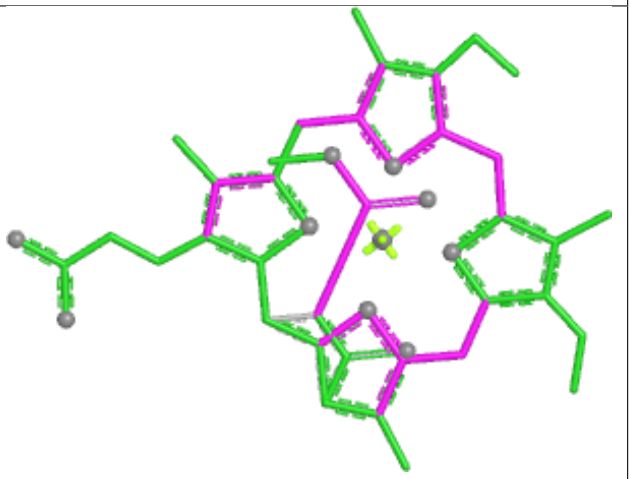


Rings

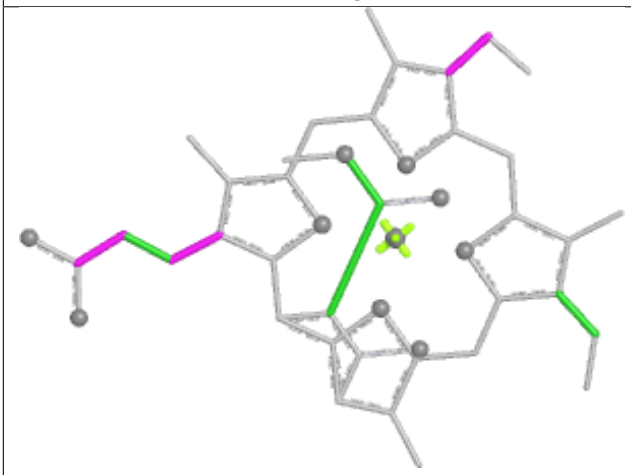
Ligand KC1 E 307



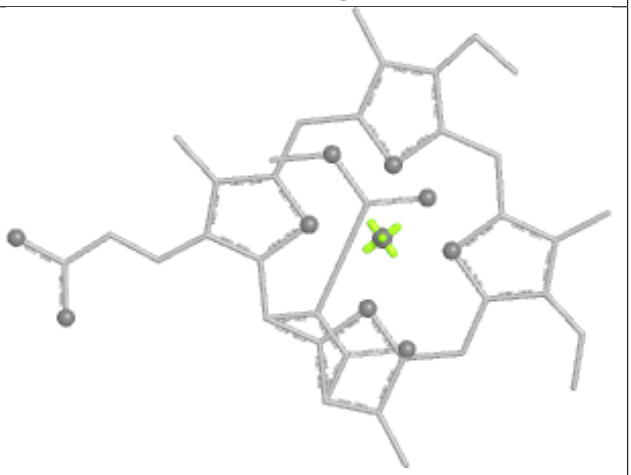
Bond lengths



Bond angles

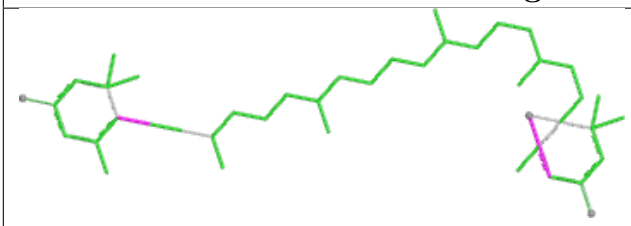


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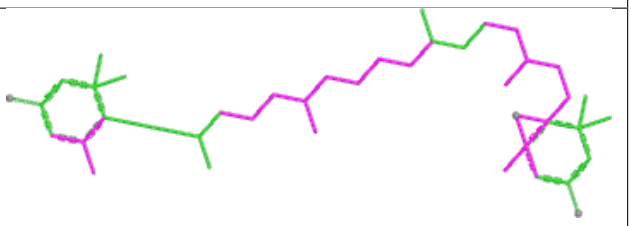


Rings

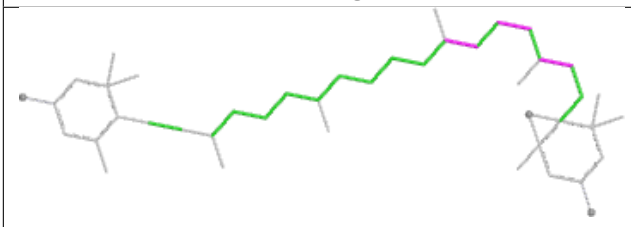
Ligand DD6 K 221



Bond lengths



Bond angles

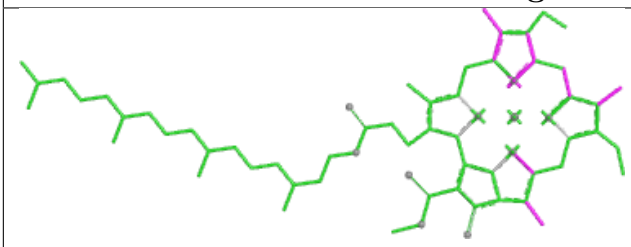


Torsions

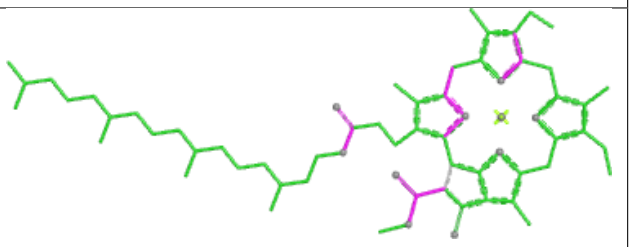


Rings

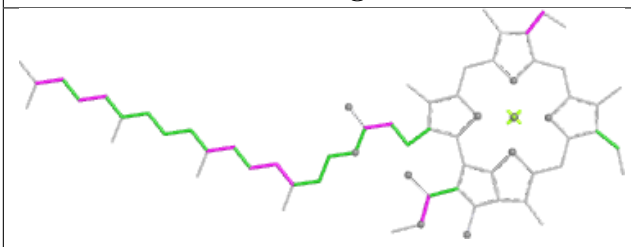
Ligand CLA b 704



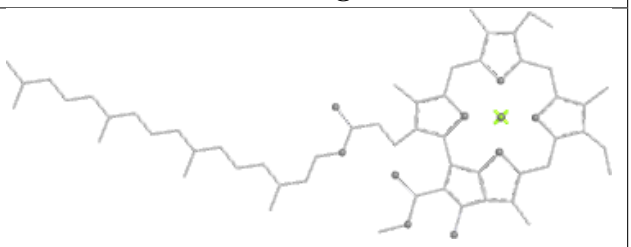
Bond lengths



Bond angles

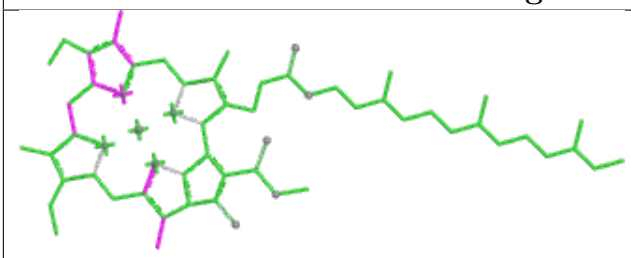


Torsions

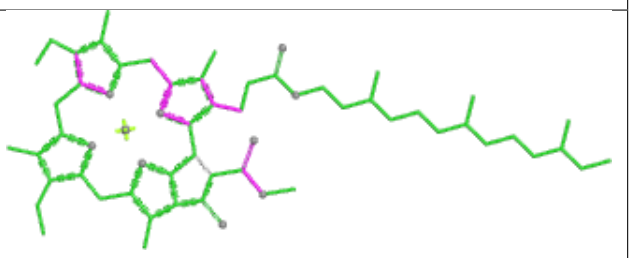


Rings

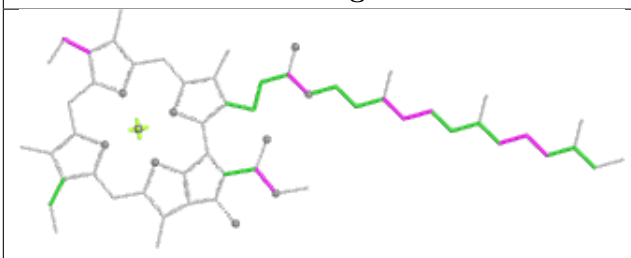
Ligand CLA E 305



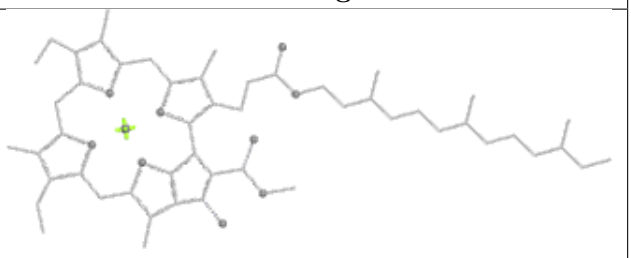
Bond lengths



Bond angles

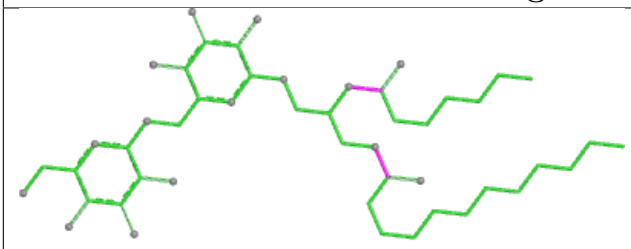


Torsions

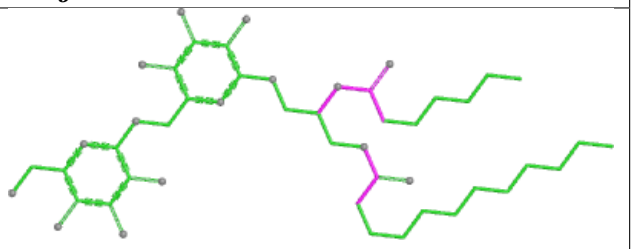


Rings

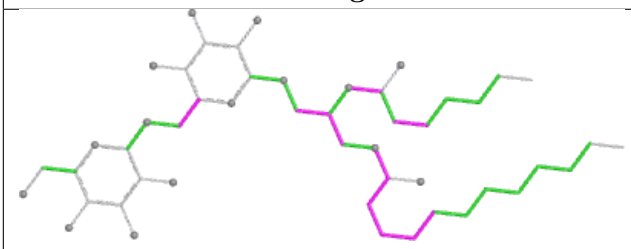
Ligand DGD j 106



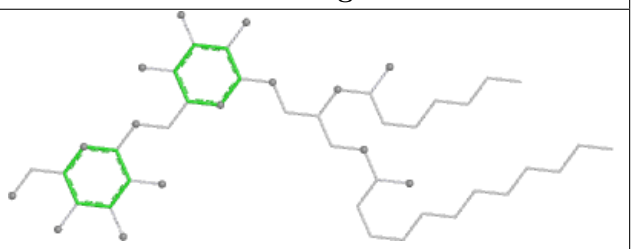
Bond lengths



Bond angles

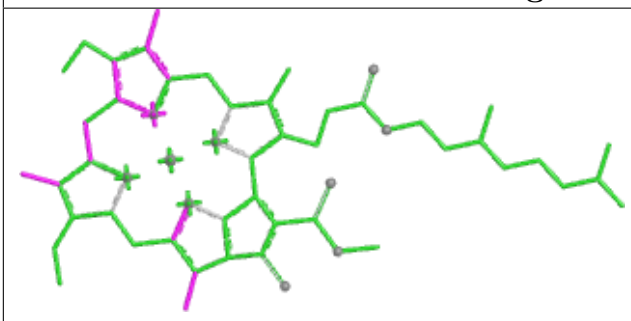


Torsions

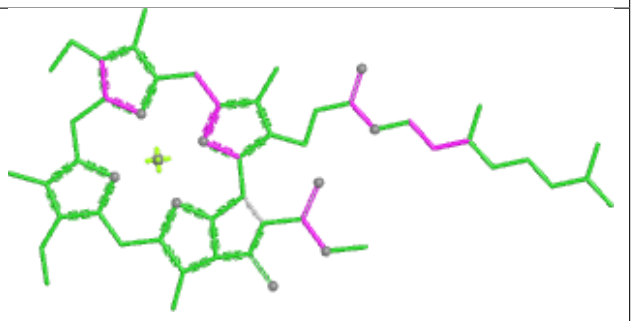


Rings

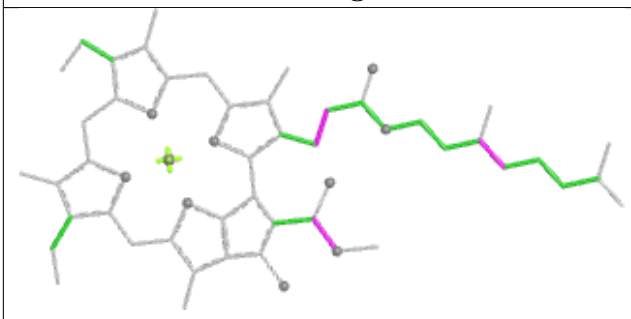
Ligand CLA L 310



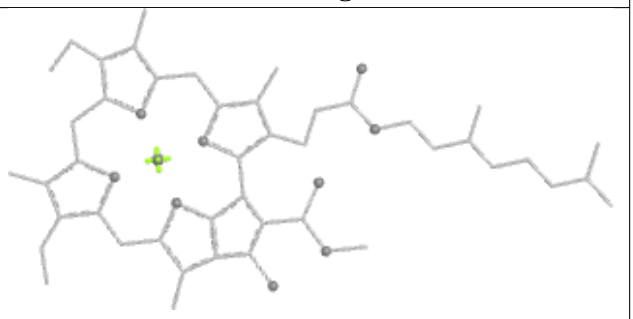
Bond lengths



Bond angles

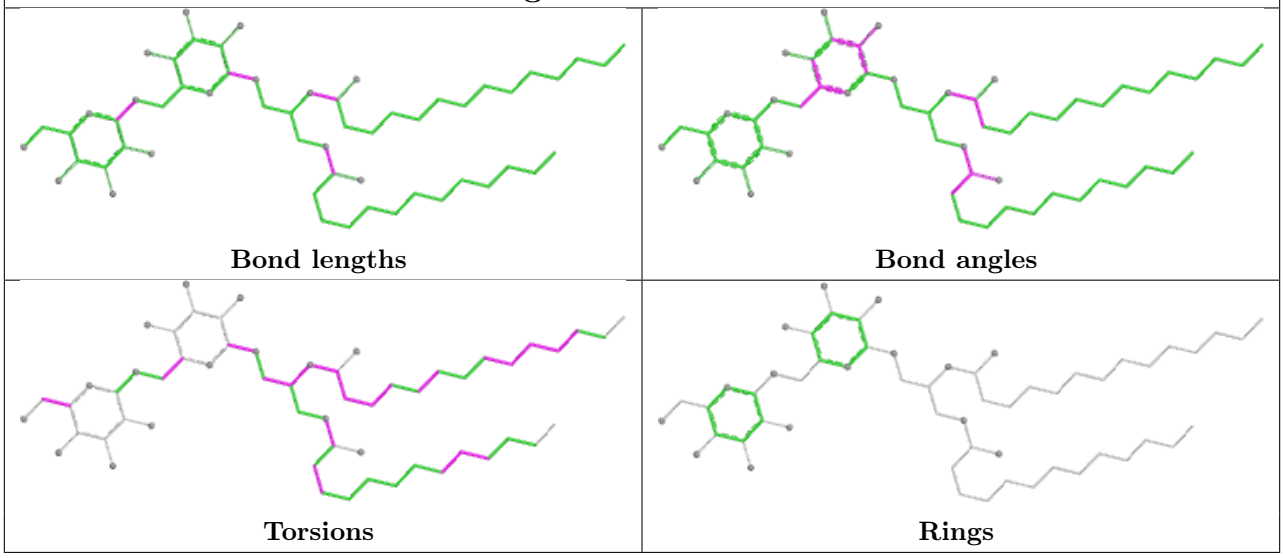


Torsions

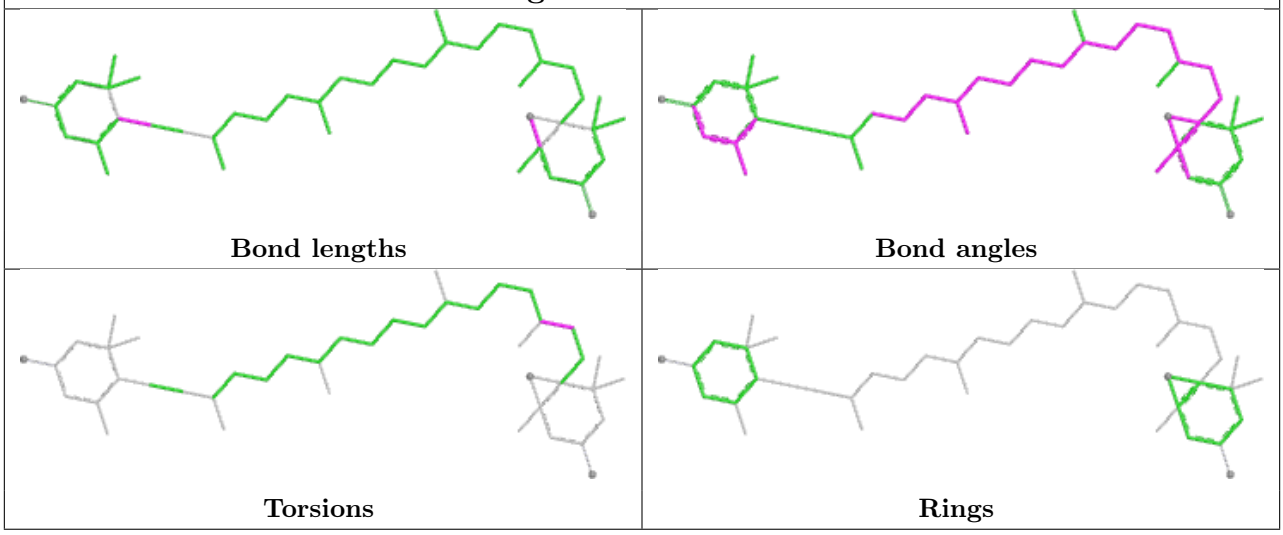


Rings

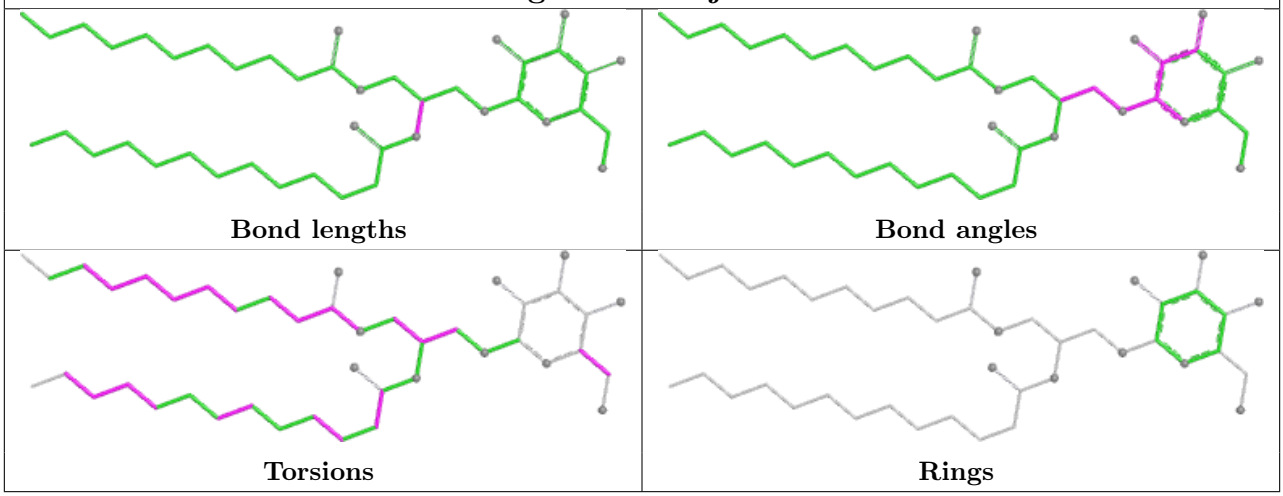
Ligand DGD b 733



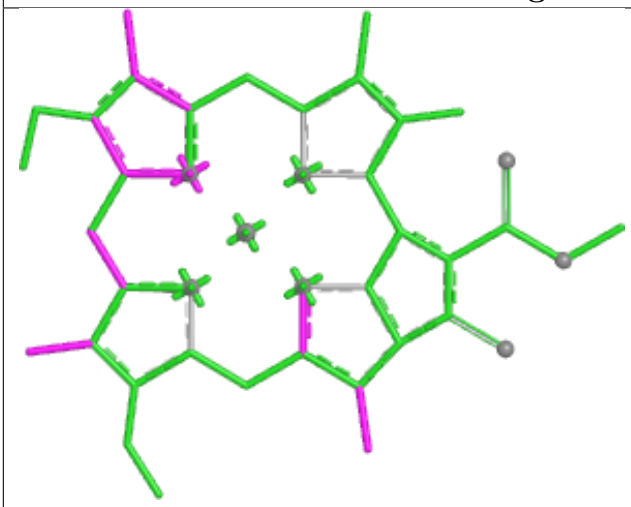
Ligand DD6 E 302



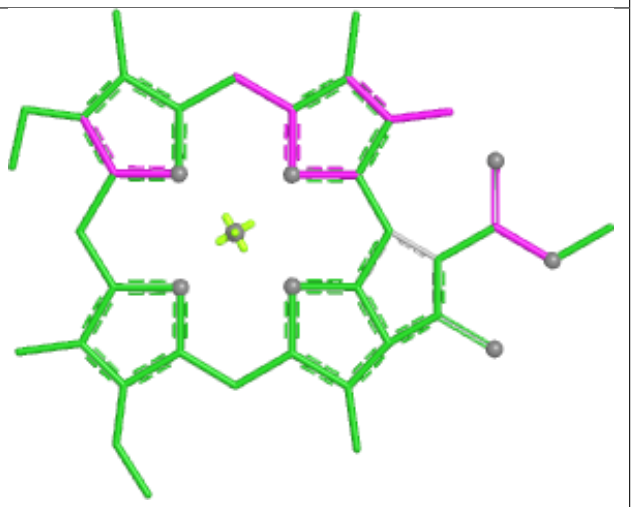
Ligand LMG j 102



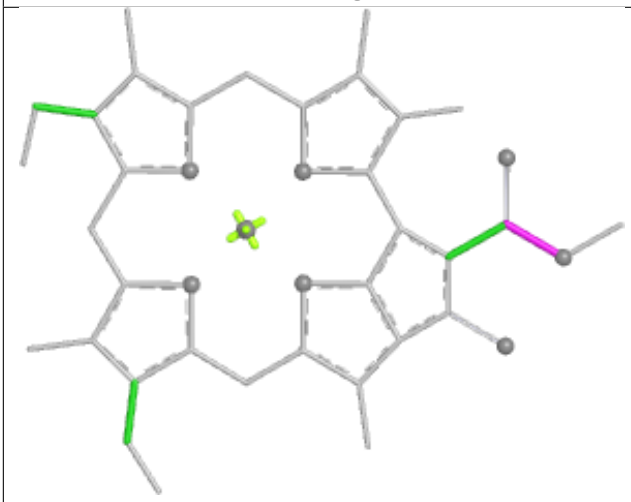
Ligand CLA J 313



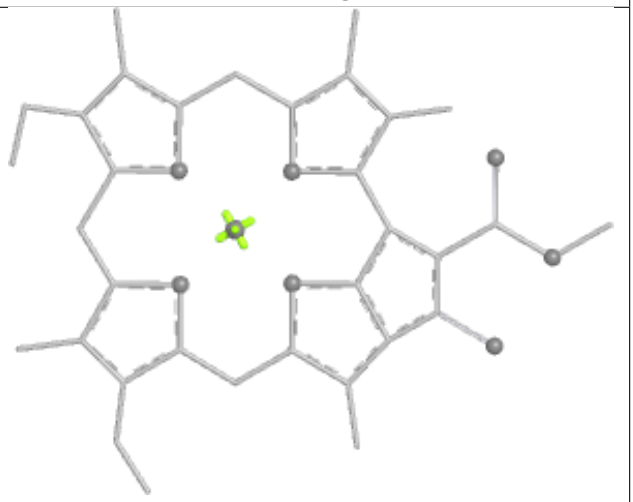
Bond lengths



Bond angles

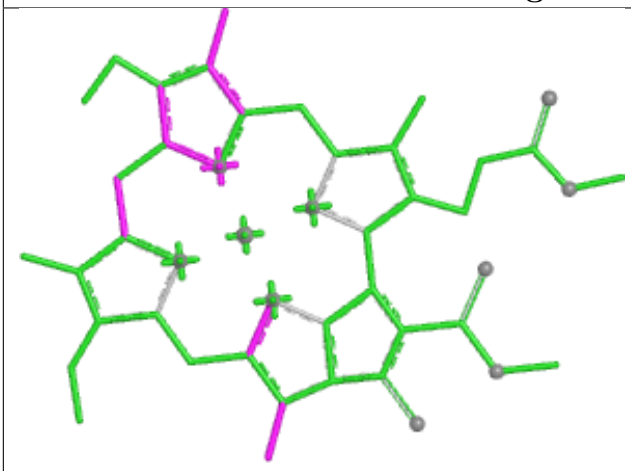


Torsions

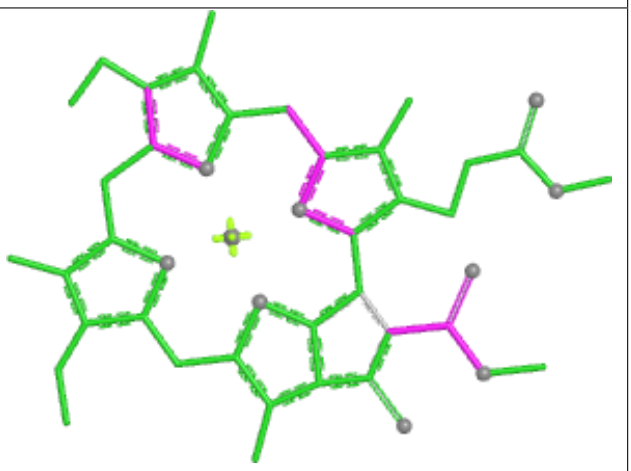


Rings

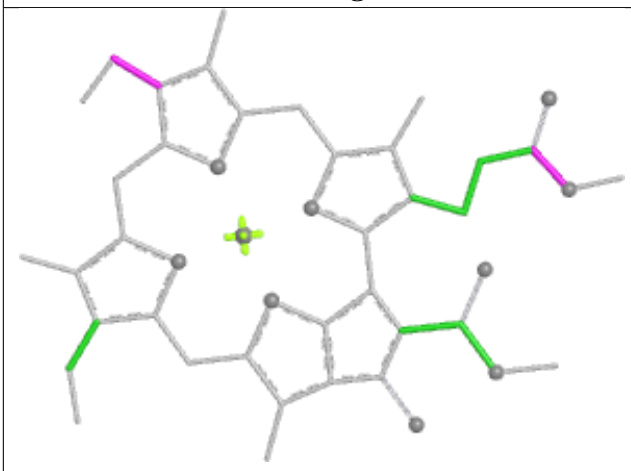
Ligand CLA F 307



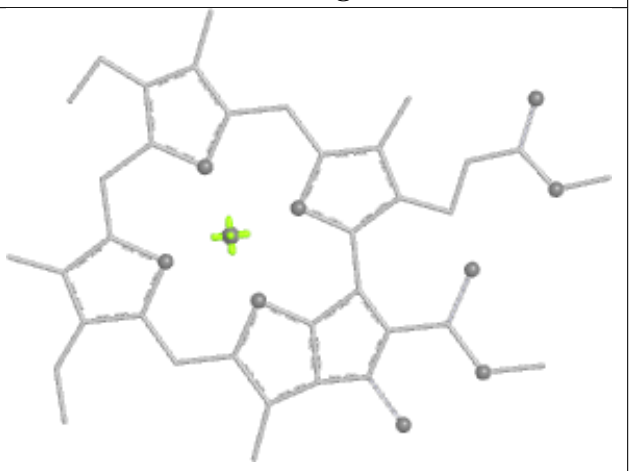
Bond lengths



Bond angles

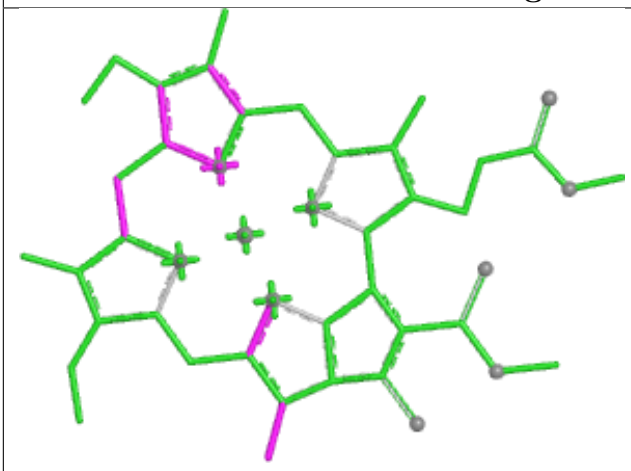


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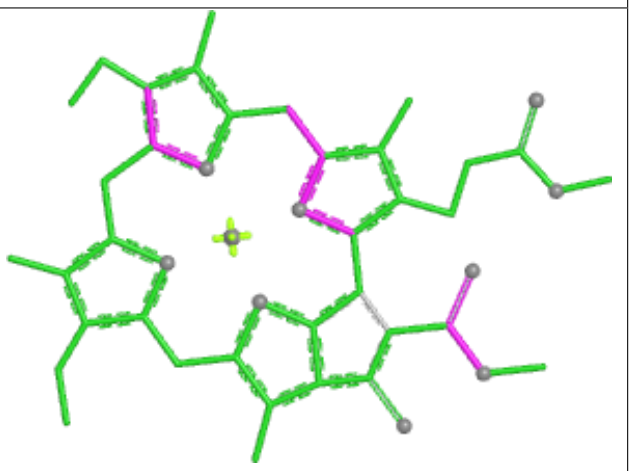


Rings

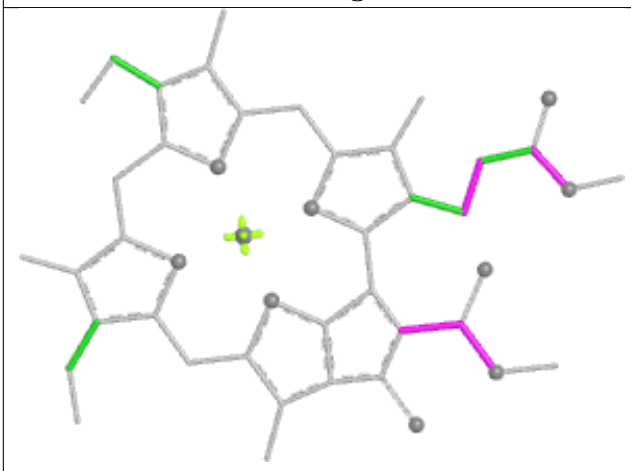
Ligand CLA T 311



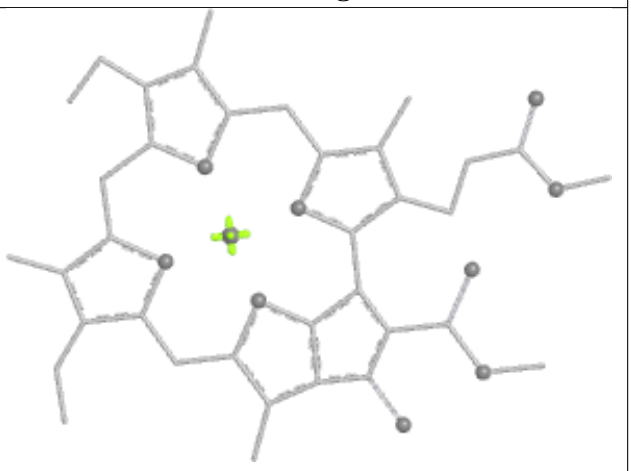
Bond lengths



Bond angles

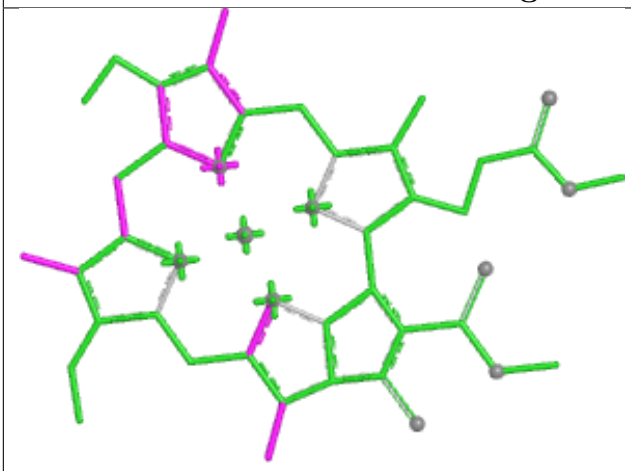


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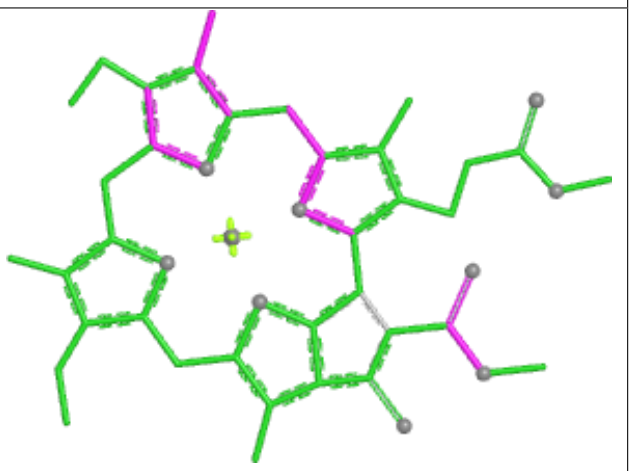


Rings

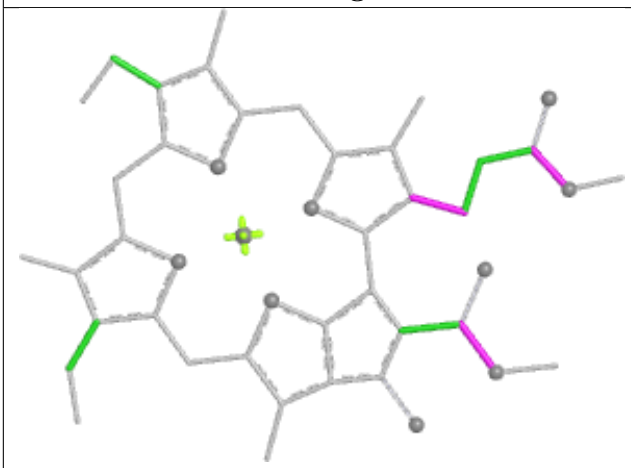
Ligand CLA M 309



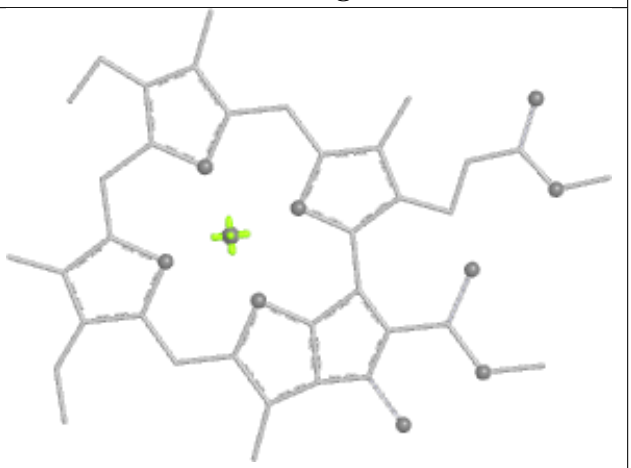
Bond lengths



Bond angles



Torsions



Rings

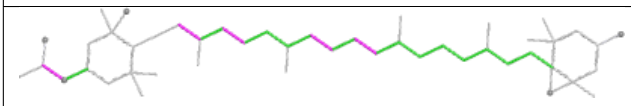
Ligand UIX O 306



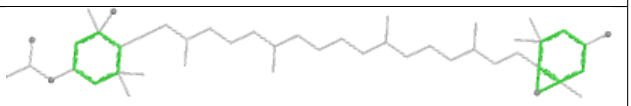
Bond lengths



Bond angles

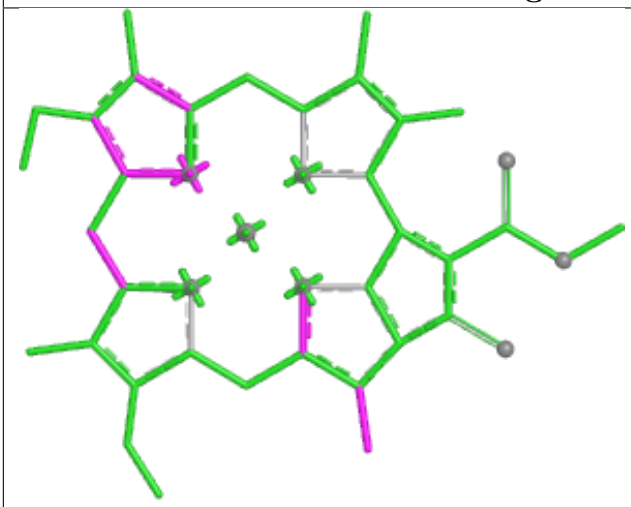


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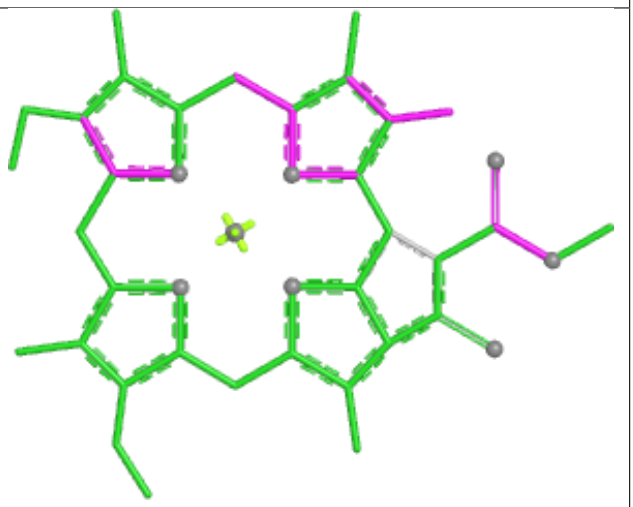


Rings

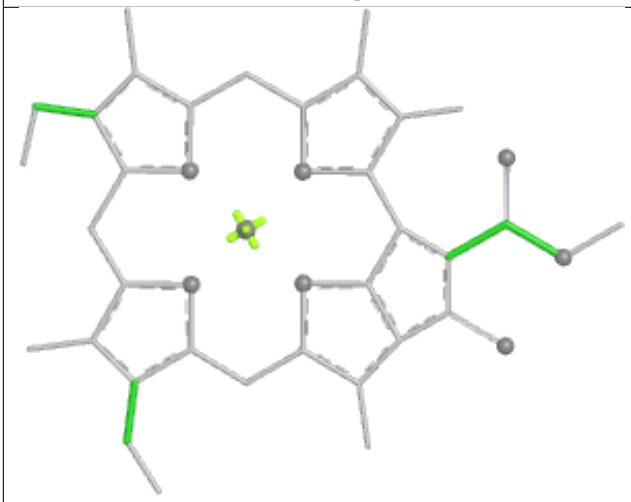
Ligand CLA E 313



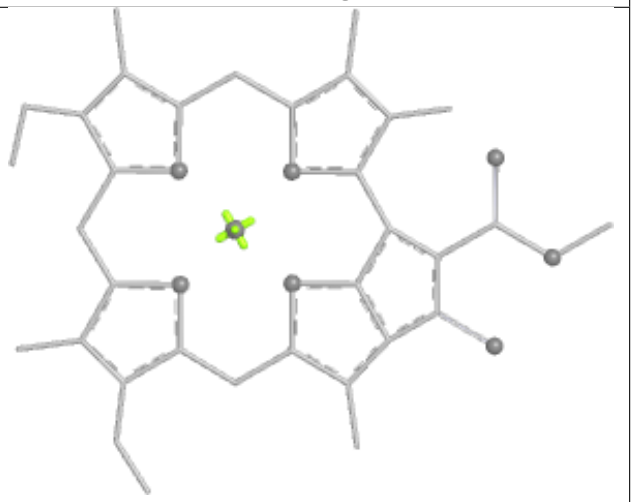
Bond lengths



Bond angles

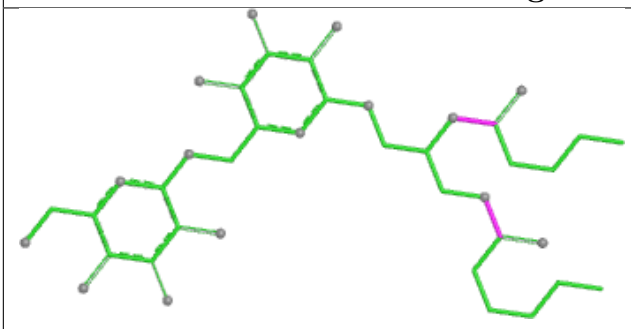


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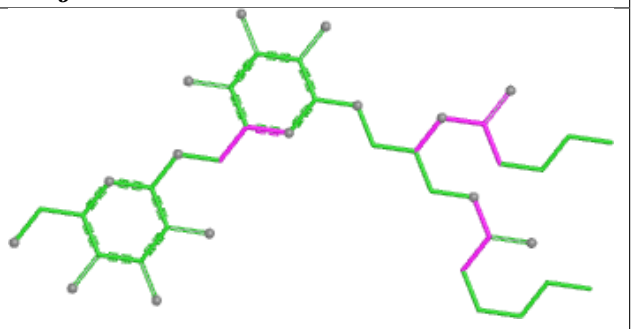


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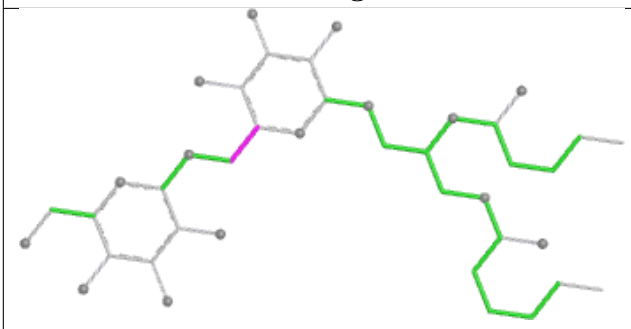
Ligand DGD j 105



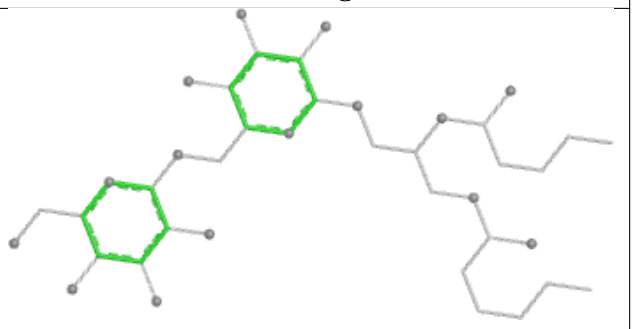
Bond lengths



Bond angles

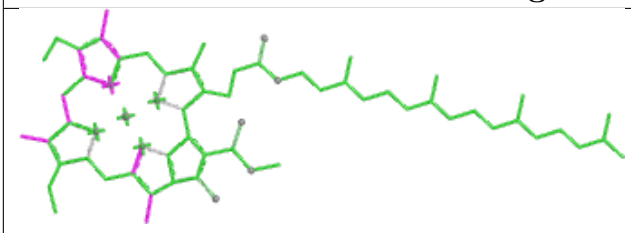


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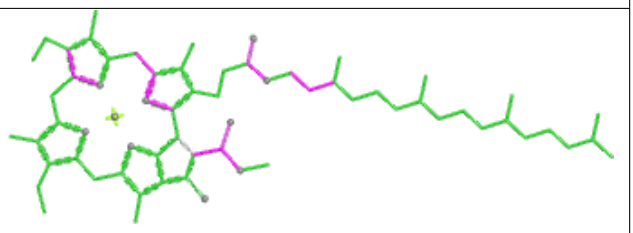


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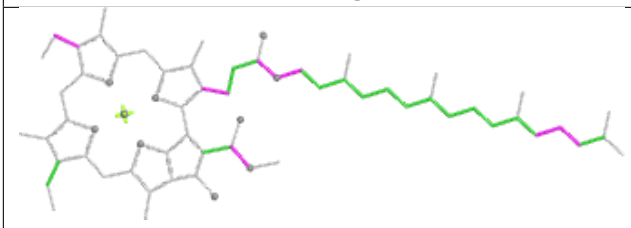
Ligand CLA a 826



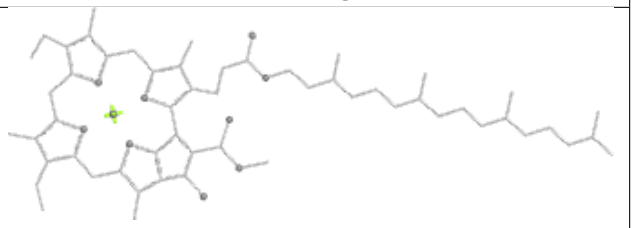
Bond lengths



Bond angles

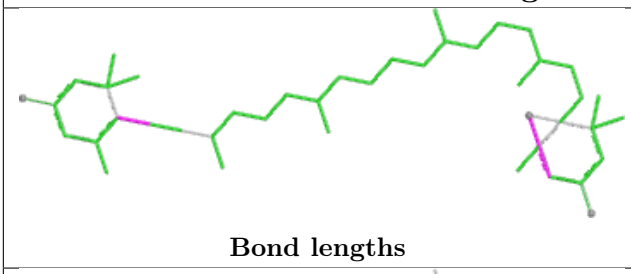


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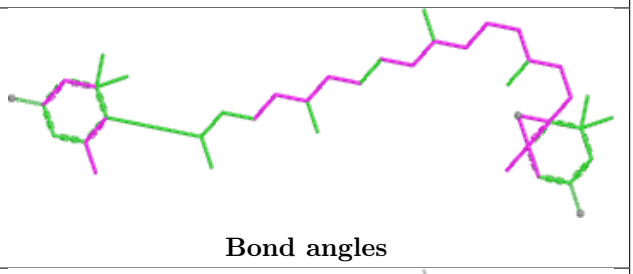


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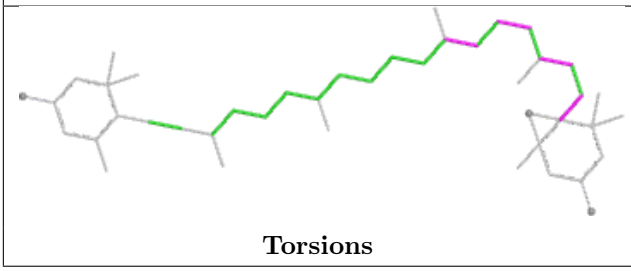
Ligand DD6 M 303



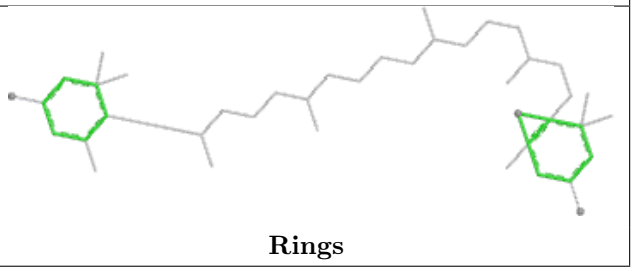
Bond lengths



Bond angles

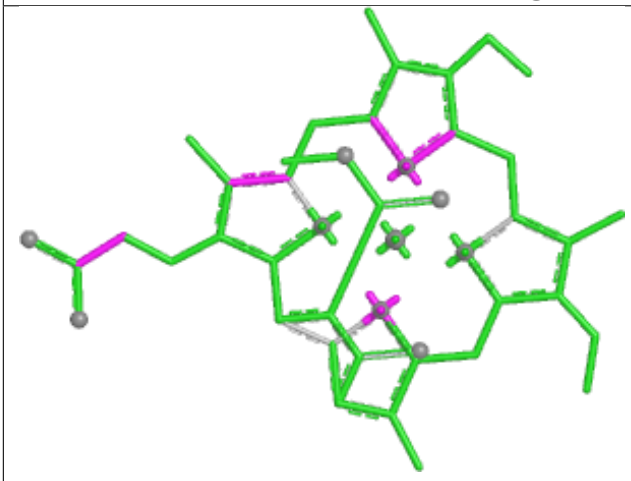


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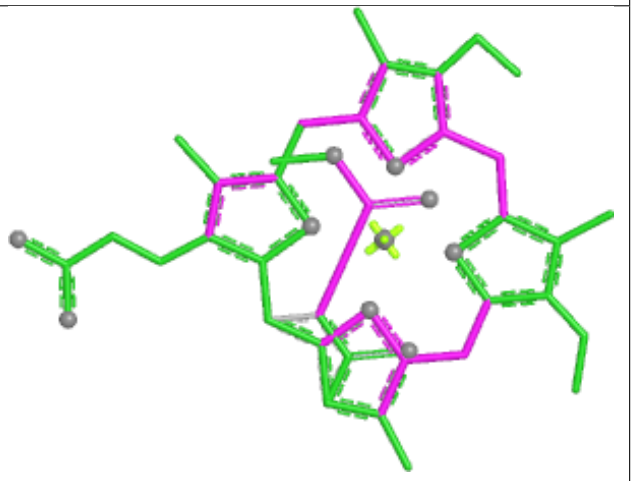


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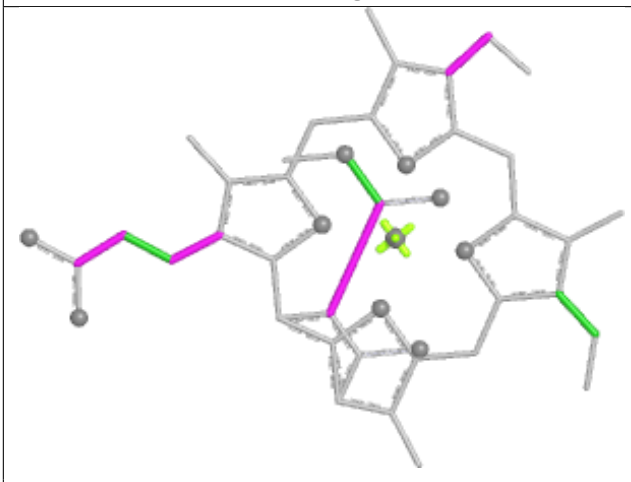
Ligand KC1 F 309



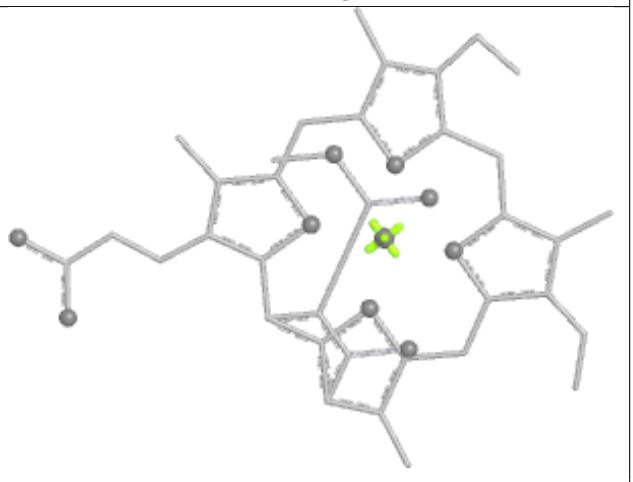
Bond lengths



Bond angles

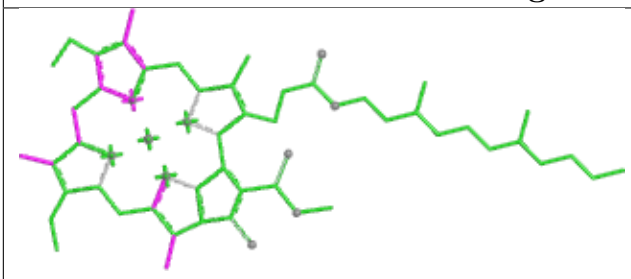


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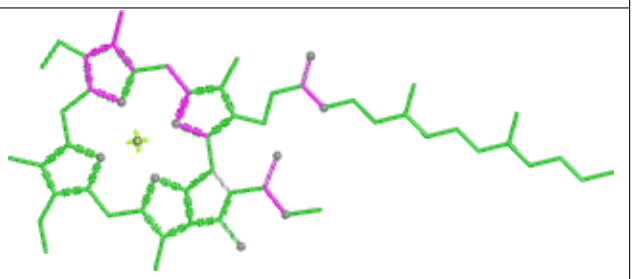


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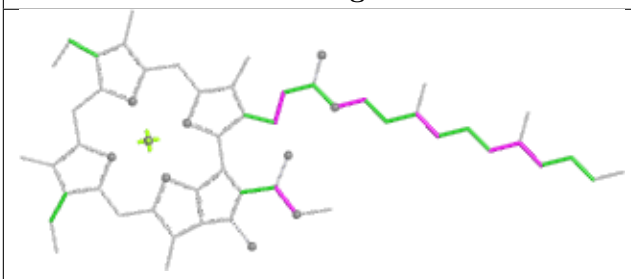
Ligand CLA a 823



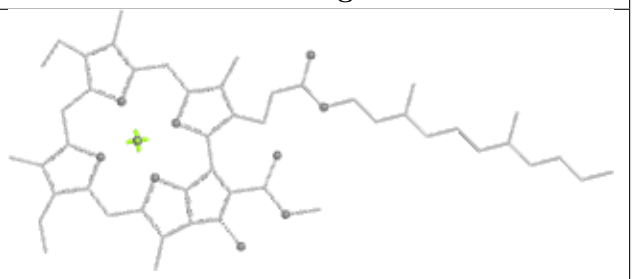
Bond lengths



Bond angles



Torsions

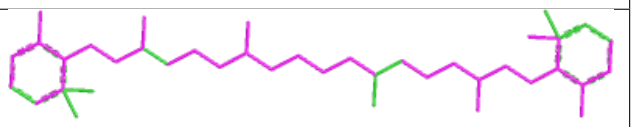


Rings

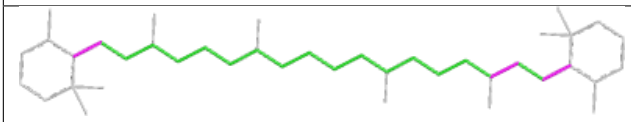
Ligand BCR b 729



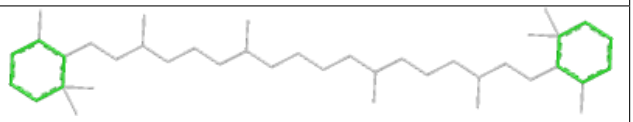
Bond lengths



Bond angles

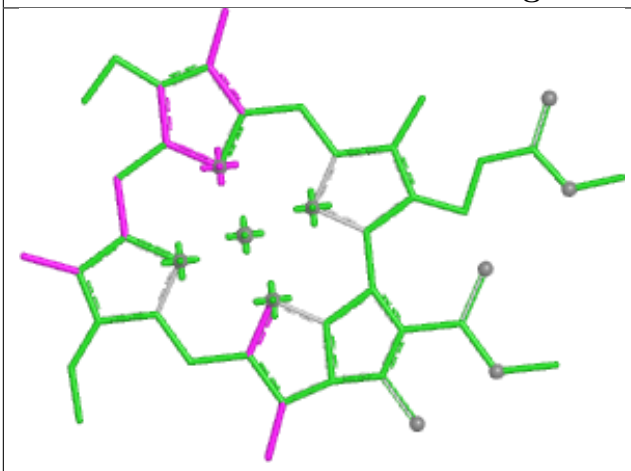


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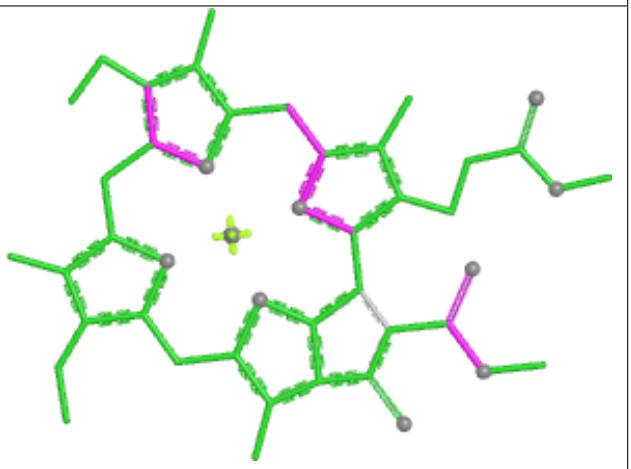


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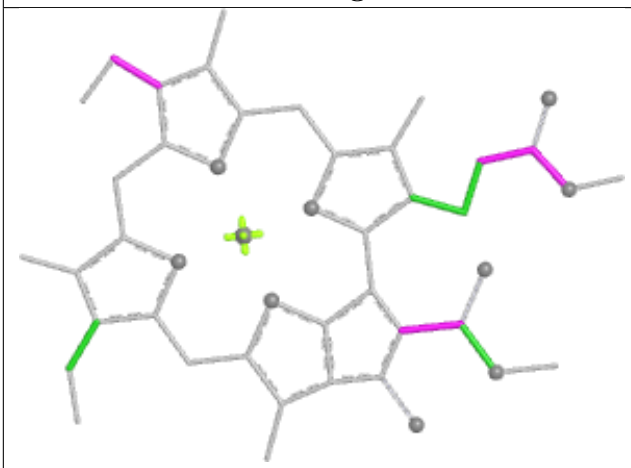
Ligand CLA K 217



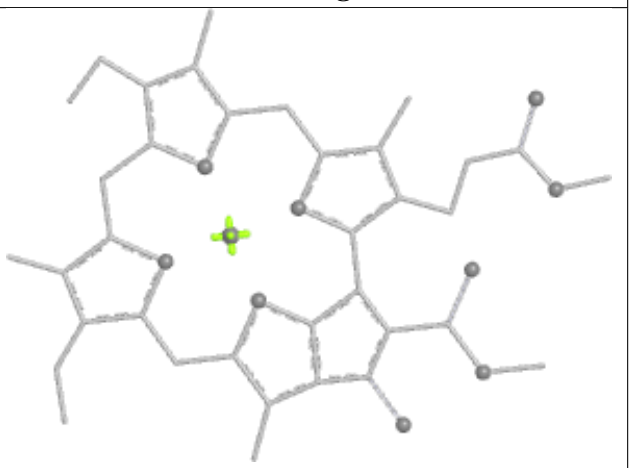
Bond lengths



Bond angles

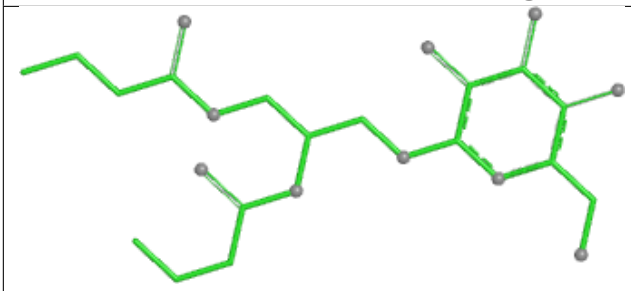


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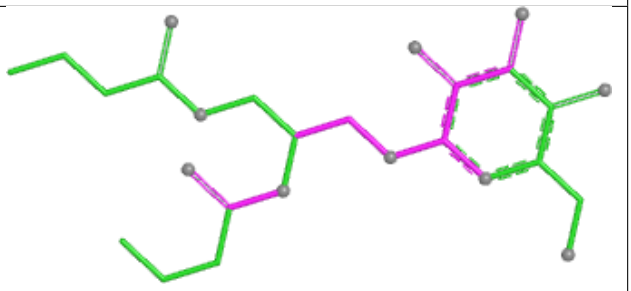


Rings

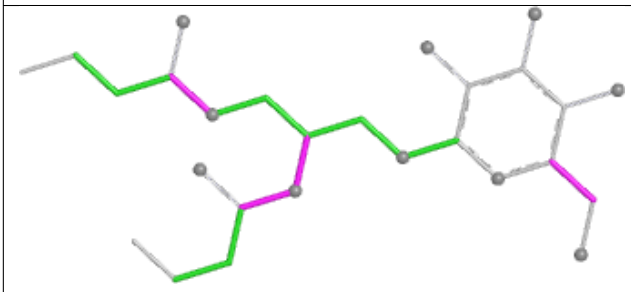
Ligand LMG P 201



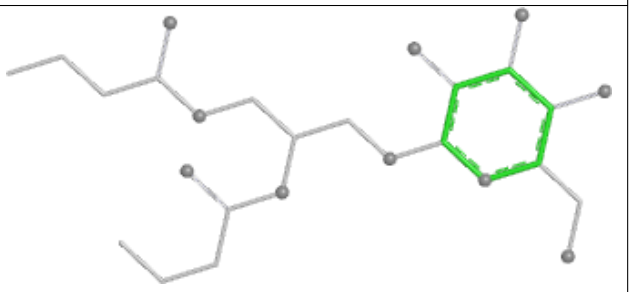
Bond lengths



Bond angles

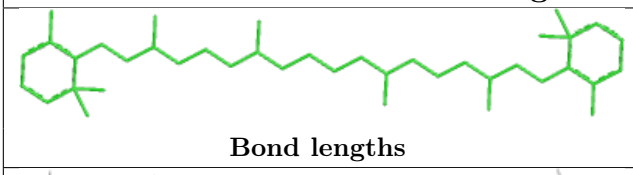


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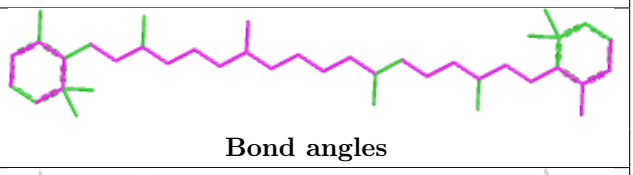


Rings

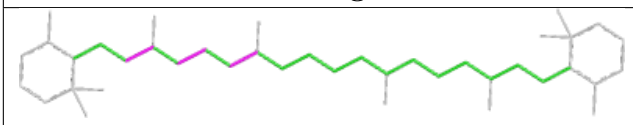
Ligand BCR l 507



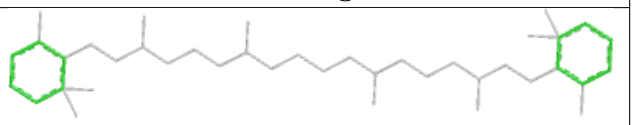
Bond lengths



Bond angles

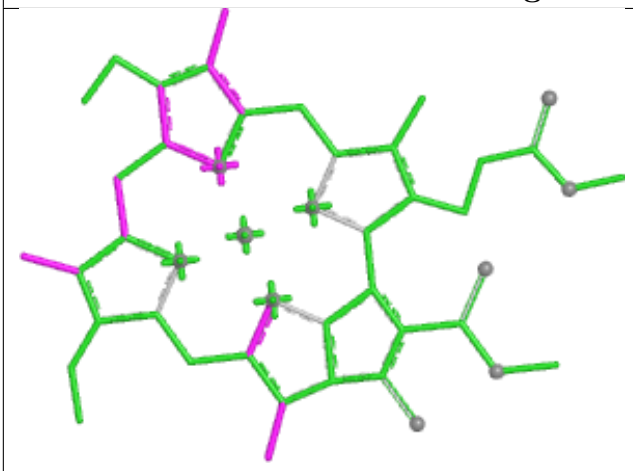


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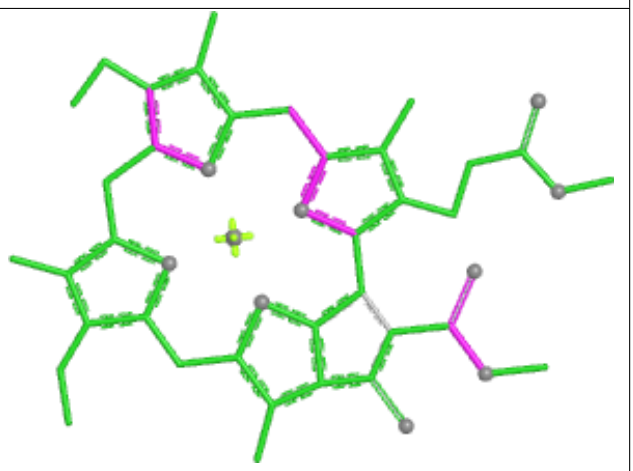


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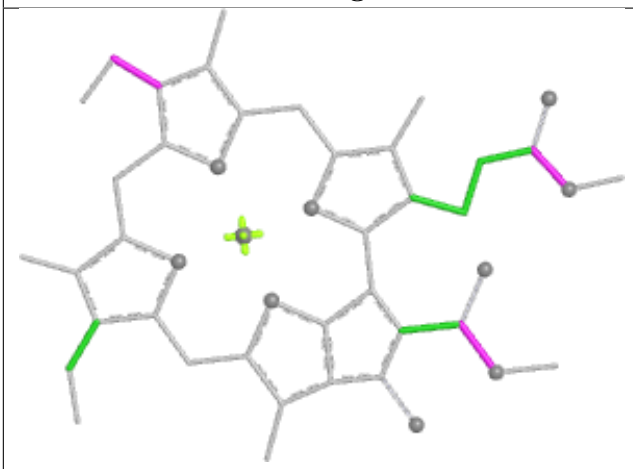
Ligand CLA A 210



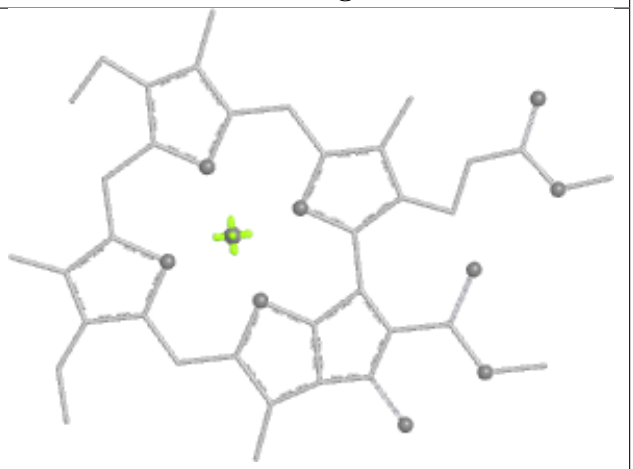
Bond lengths



Bond angles

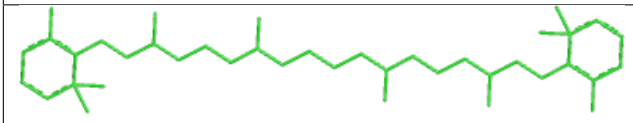


Torsions

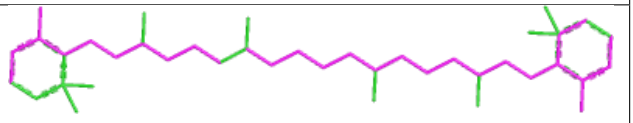


Rings

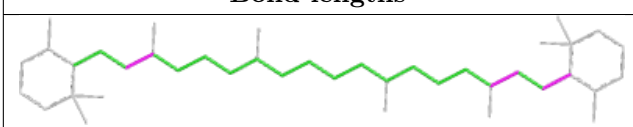
Ligand BCR a 838



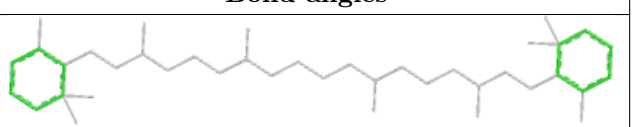
Bond lengths



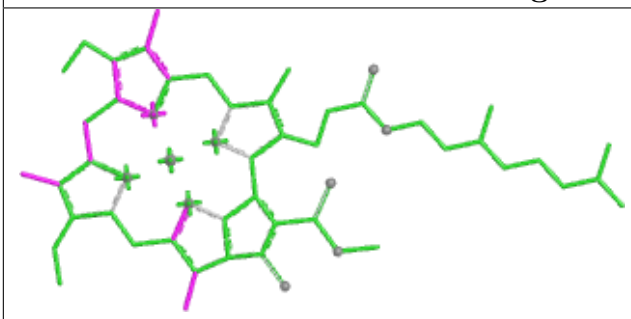
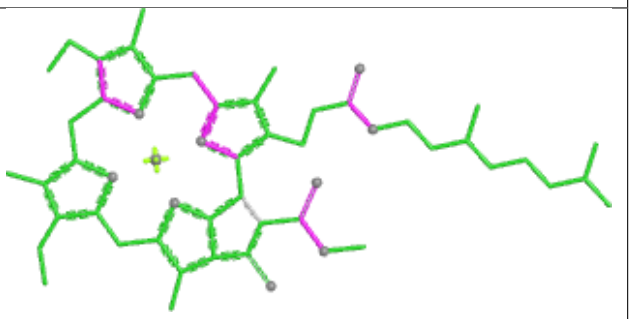
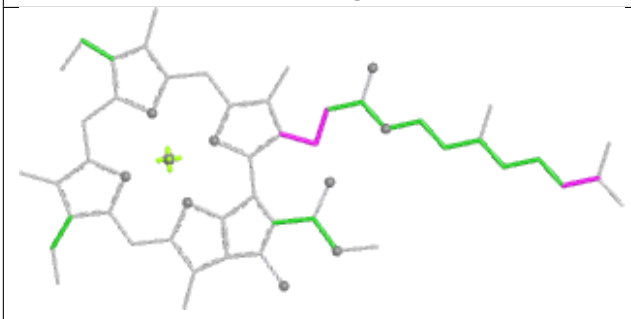
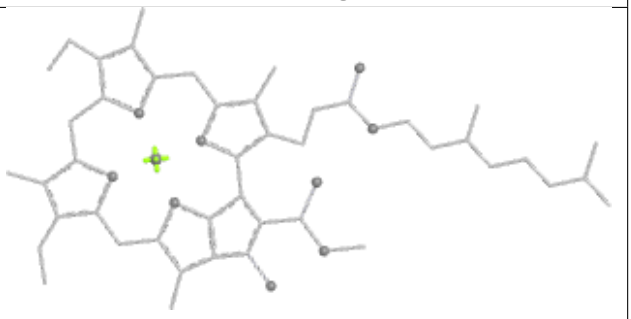
Bond angles

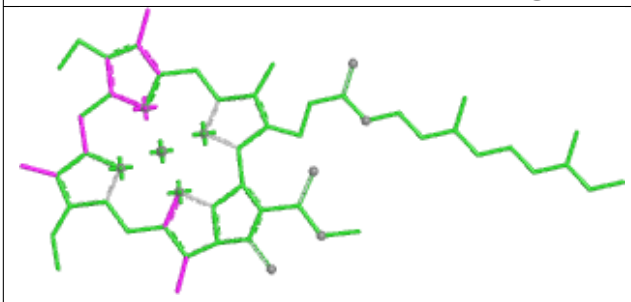
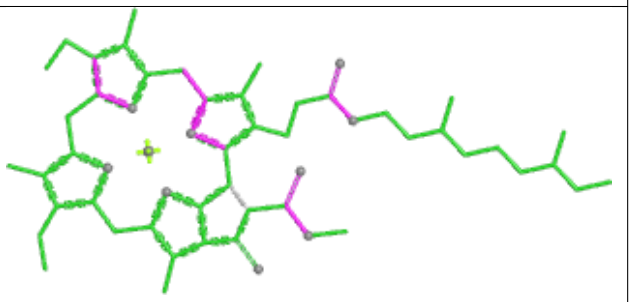
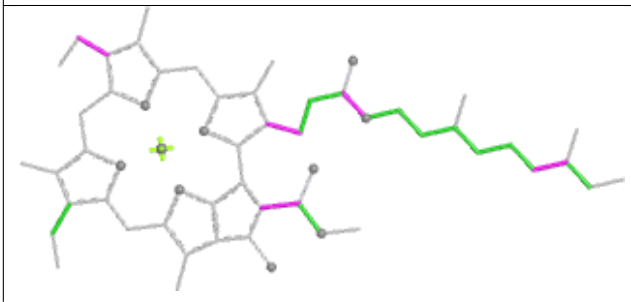
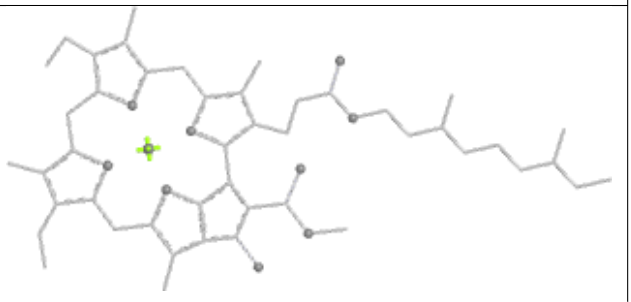


Torsions

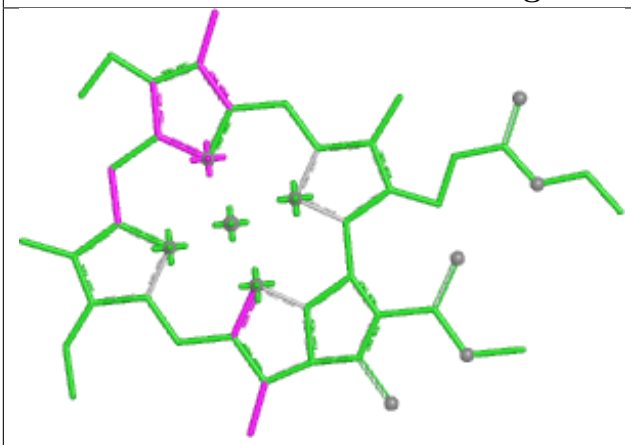


Rings

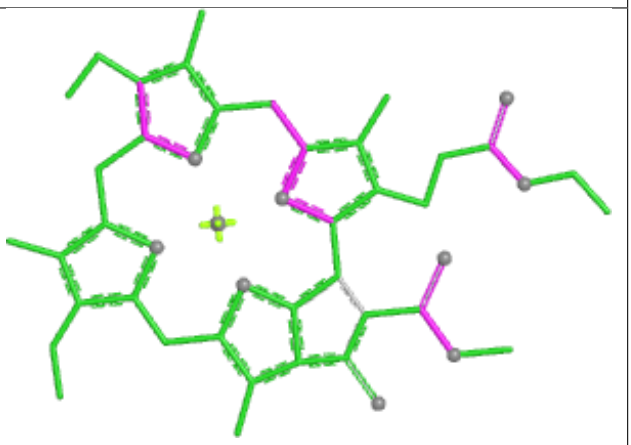
Ligand CLA I 214	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

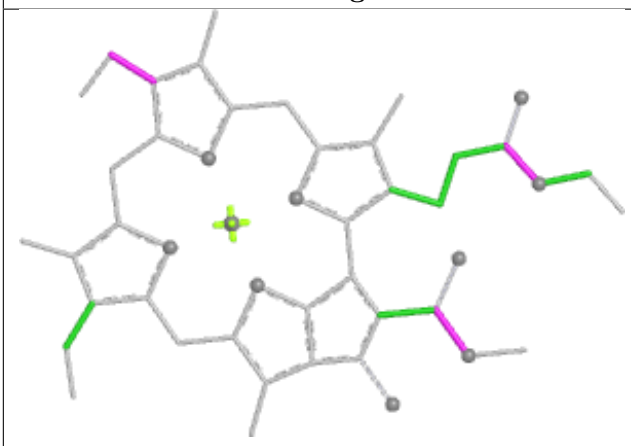
Ligand CLA N 308



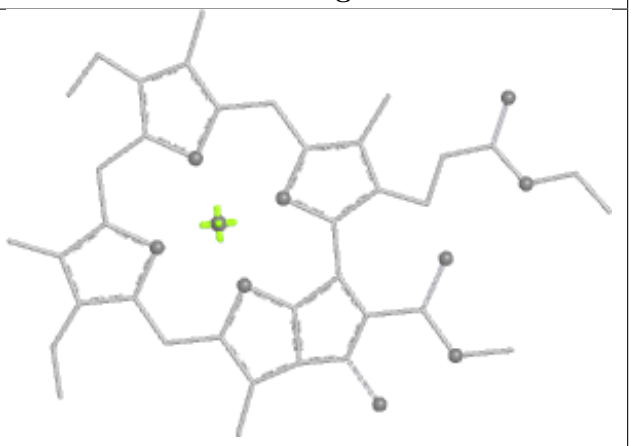
Bond lengths



Bond angles

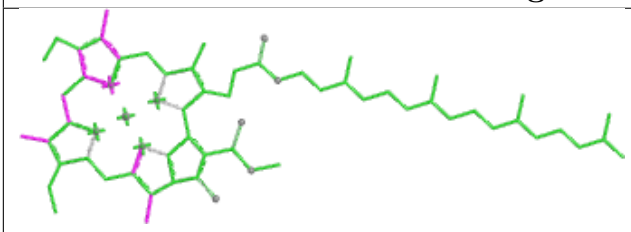


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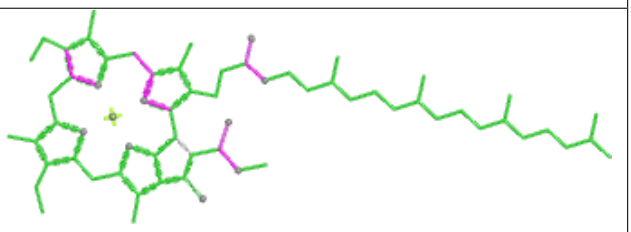


Rings

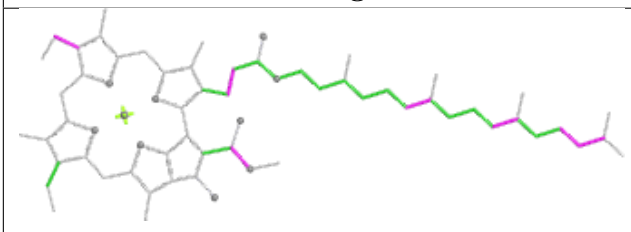
Ligand CLA b 725



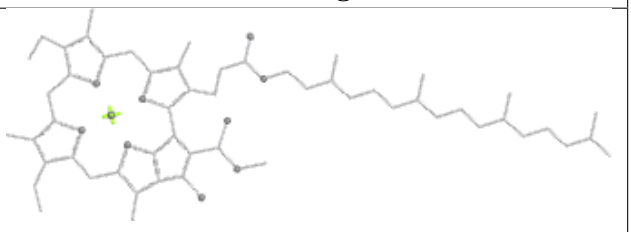
Bond lengths



Bond angles

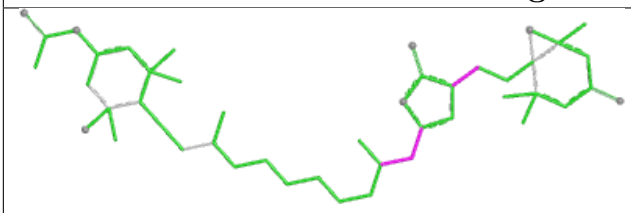


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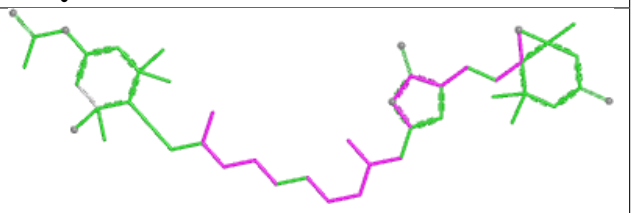


Rings

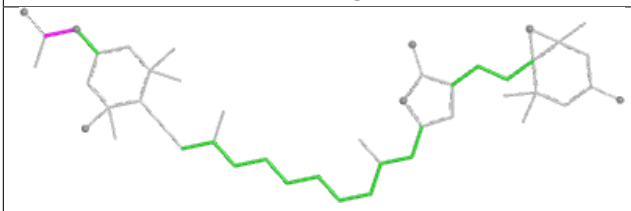
Ligand PID Q 304



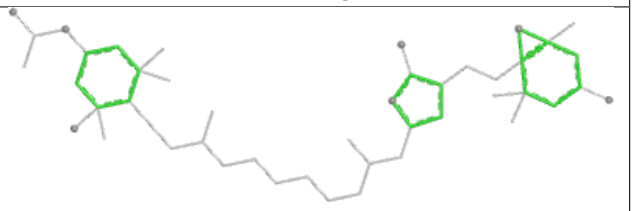
Bond lengths



Bond angles

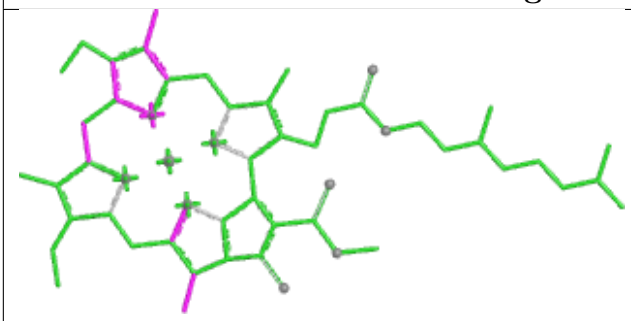


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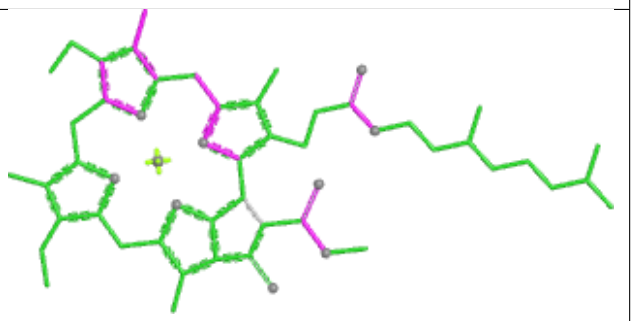


Rings

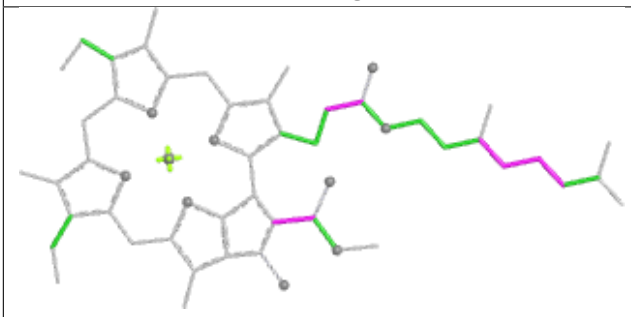
Ligand CLA B 309



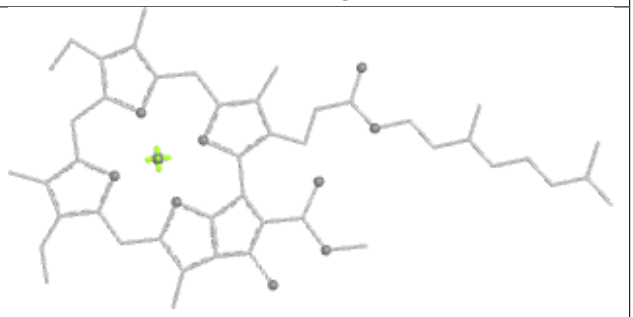
Bond lengths



Bond angles

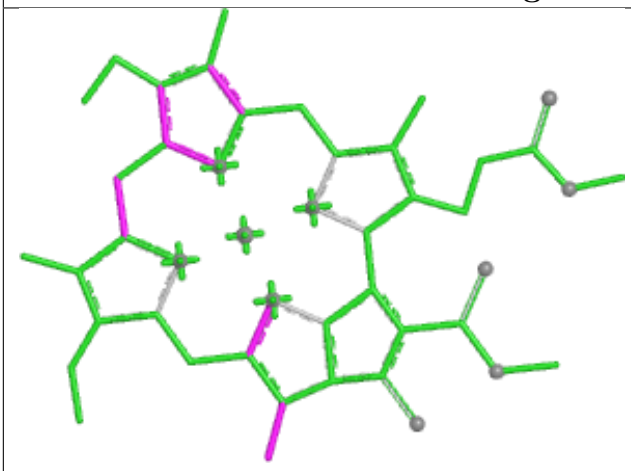


Torsions

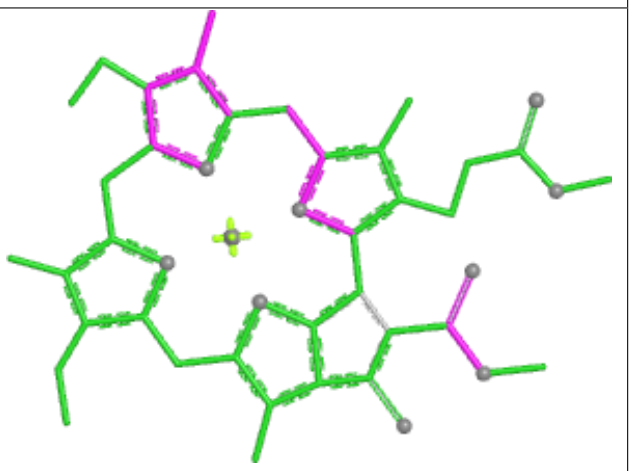


Rings

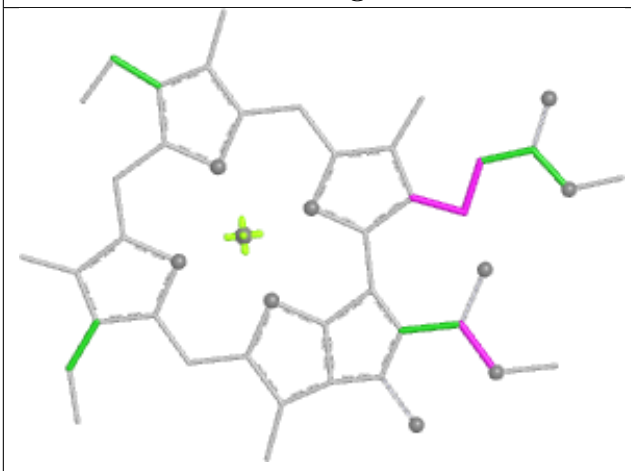
Ligand CLA H 312



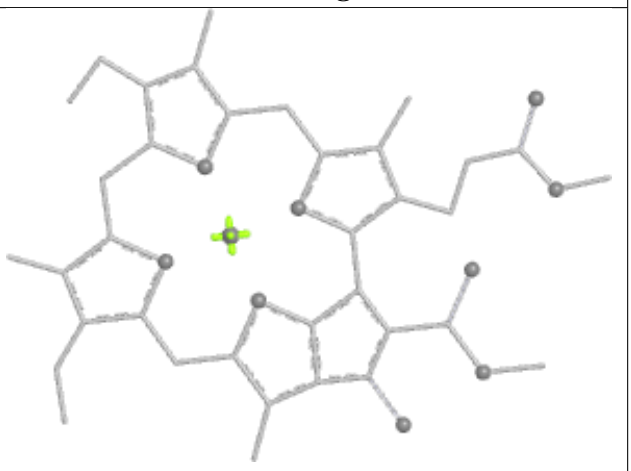
Bond lengths



Bond angles

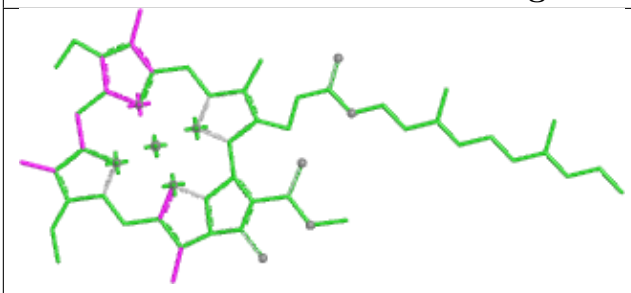


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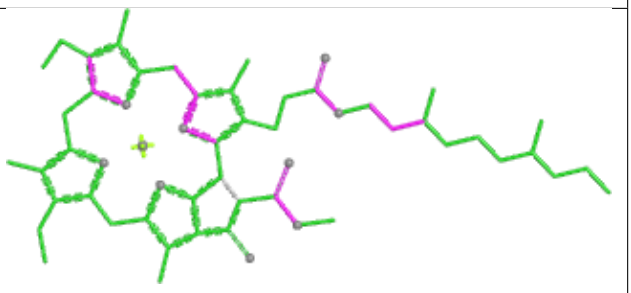


Rings

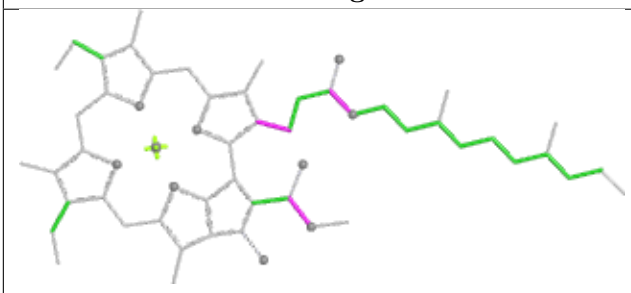
Ligand CLA a 819



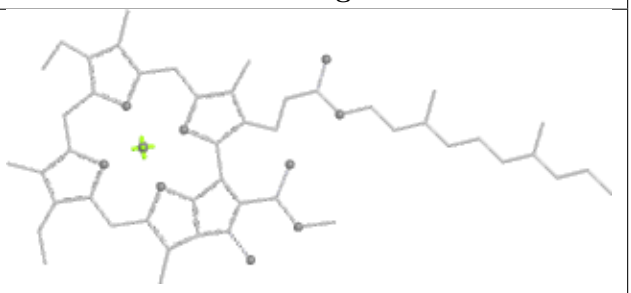
Bond lengths



Bond angles

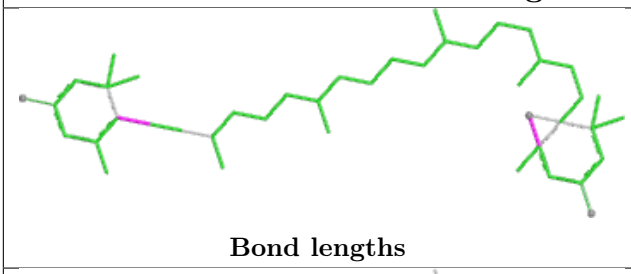


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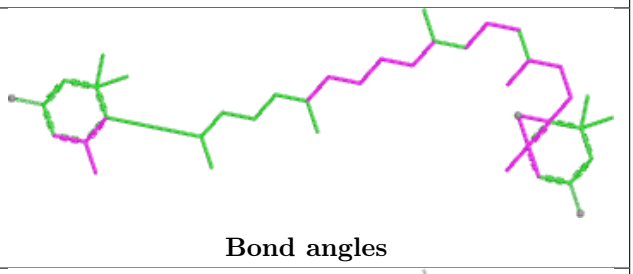


Rings

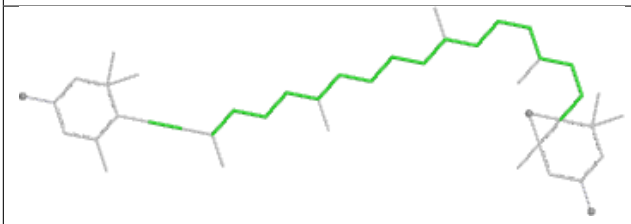
Ligand DD6 B 303



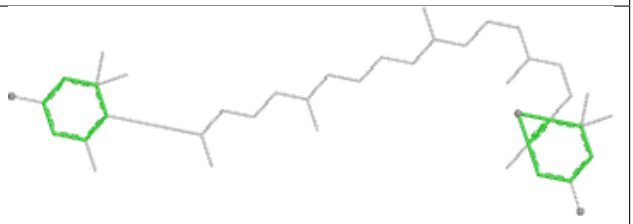
Bond lengths



Bond angles

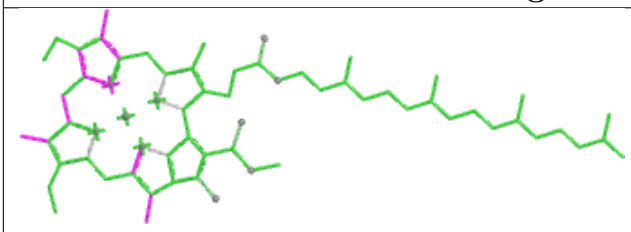


Torsions

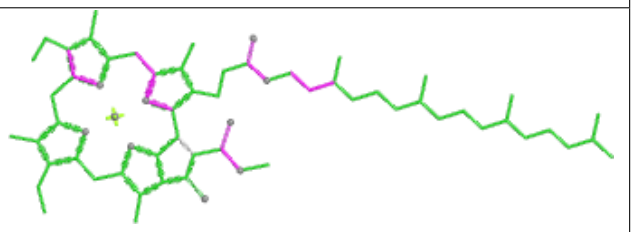


Rings

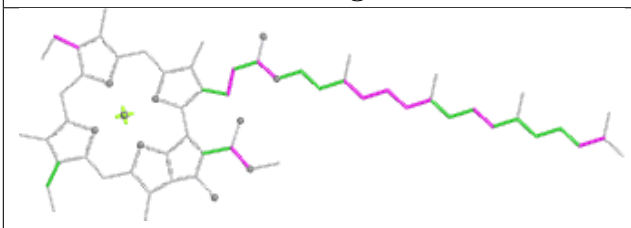
Ligand CLA b 702



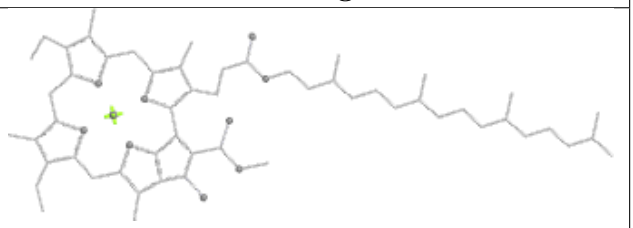
Bond lengths



Bond angles

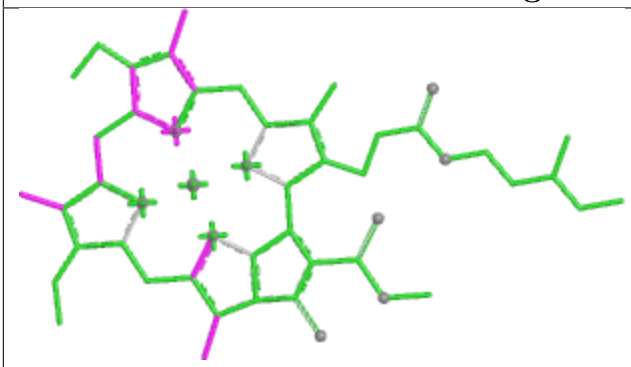


Torsions

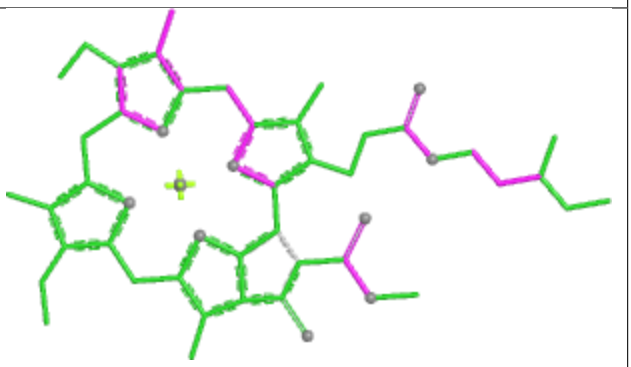


Rings

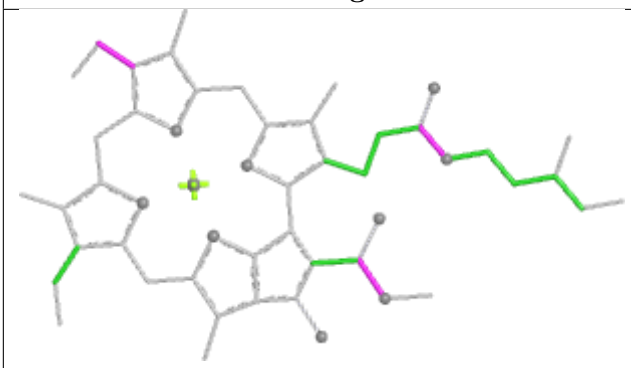
Ligand CLA A 217



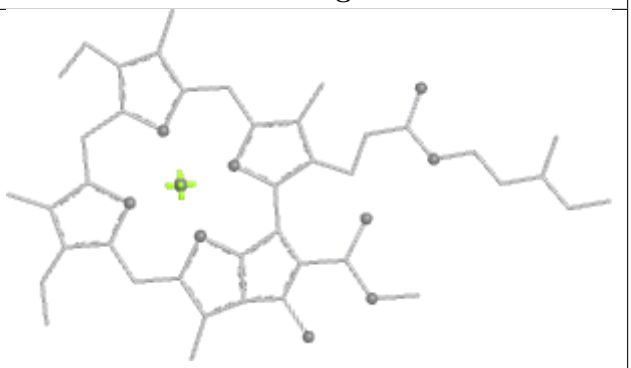
Bond lengths



Bond angles

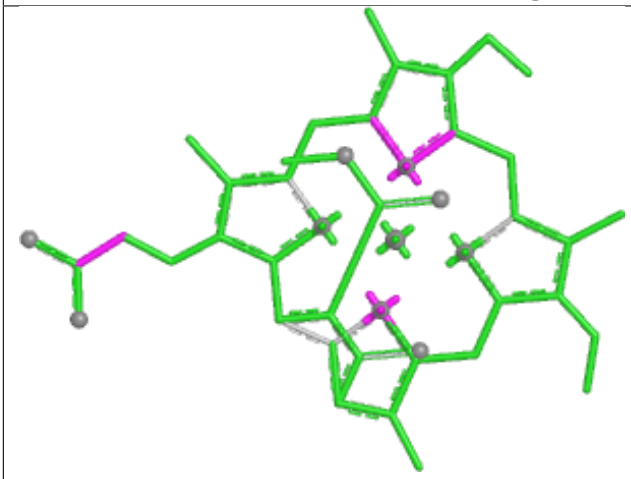


Torsions

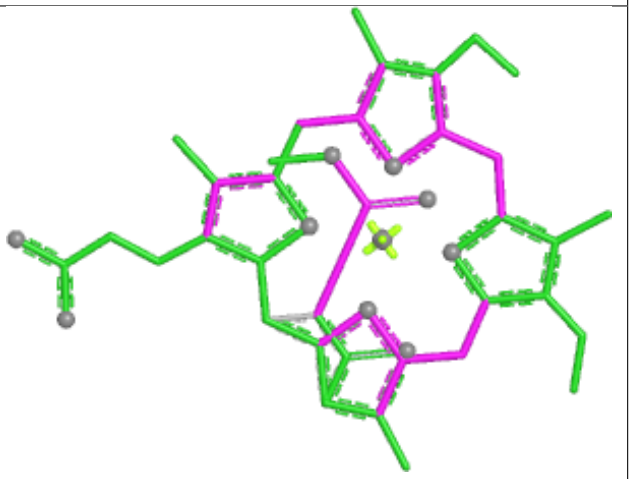


Rings

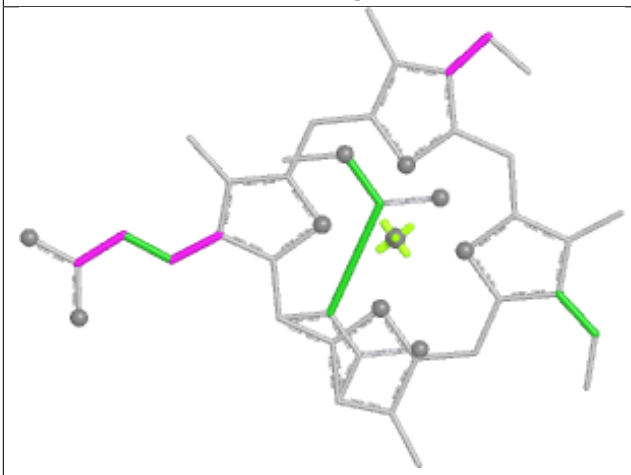
Ligand KC1 T 315



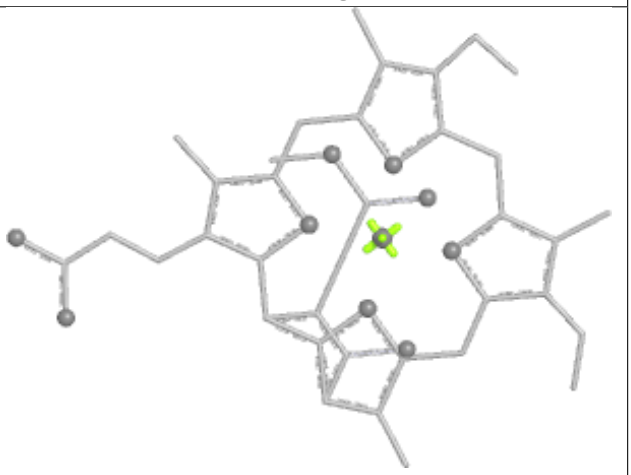
Bond lengths



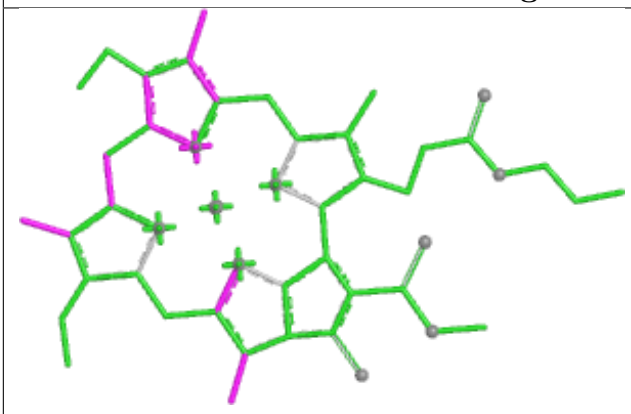
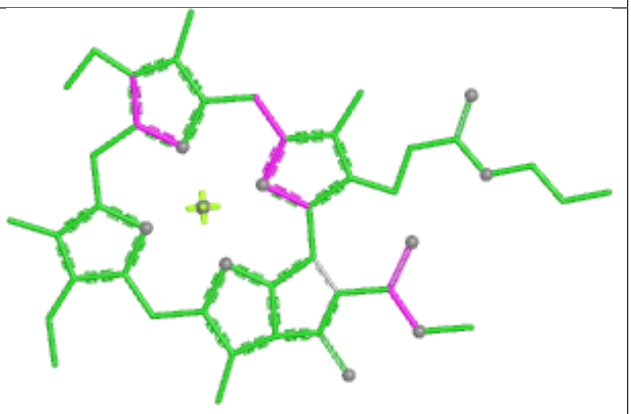
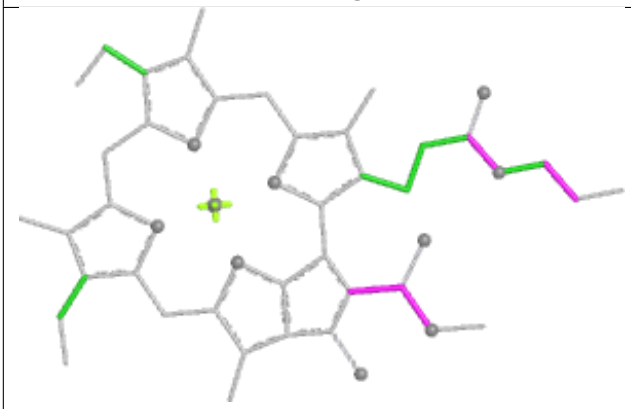
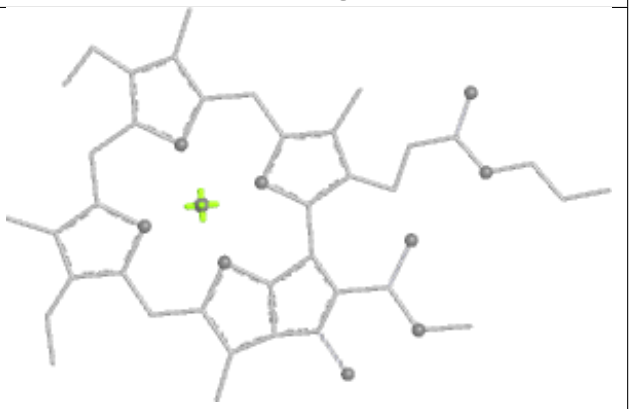
Bond angles

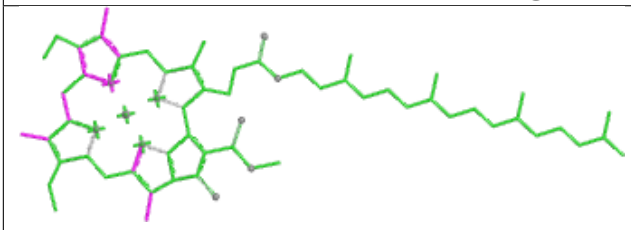
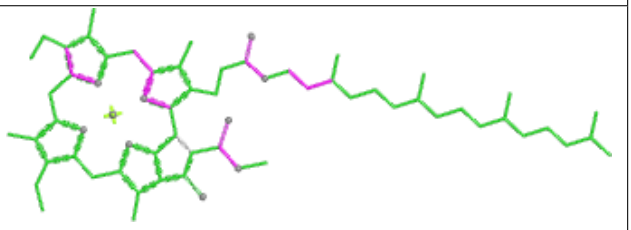
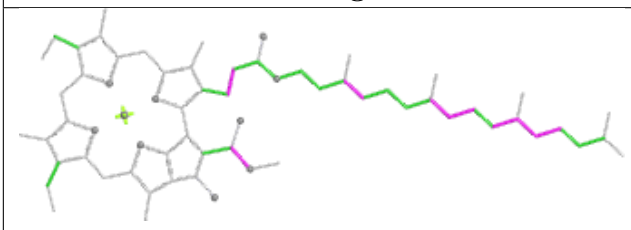
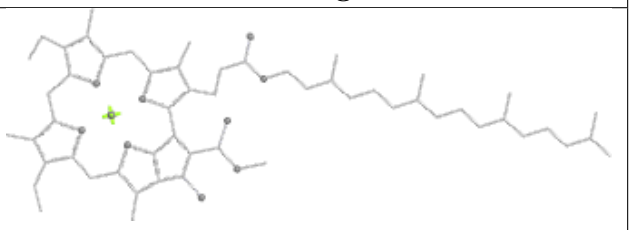


Torsions

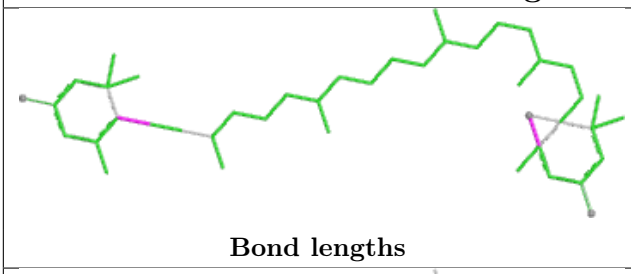


Rings

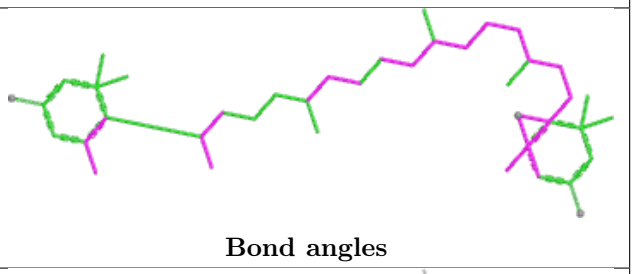
Ligand CLA M 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

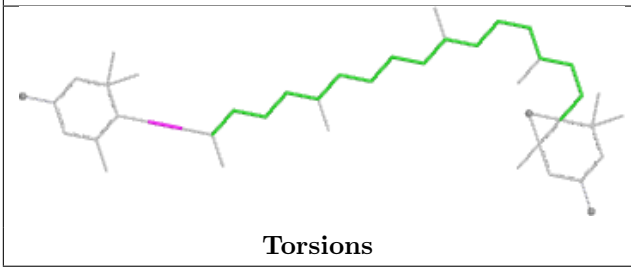
Ligand DD6 H 303



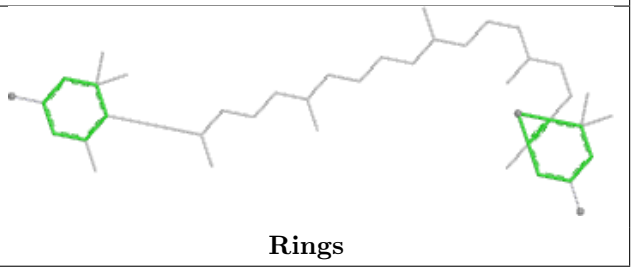
Bond lengths



Bond angles

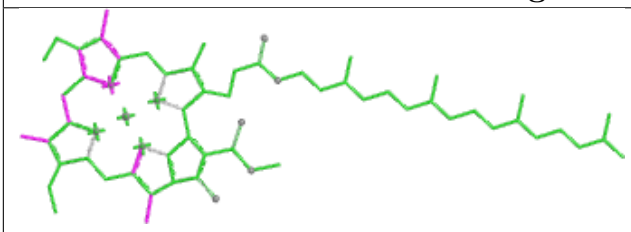


Torsions

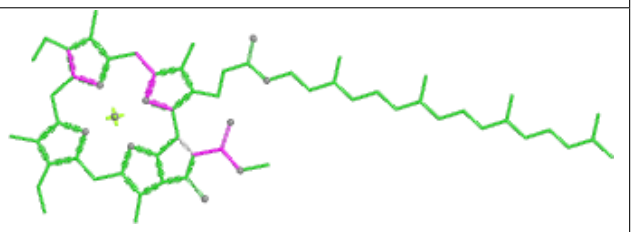


Rings

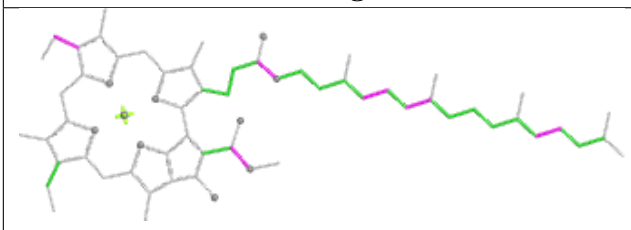
Ligand CLA a 827



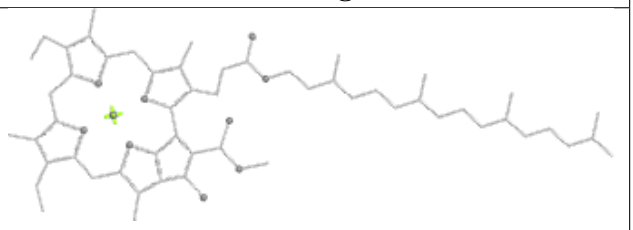
Bond lengths



Bond angles

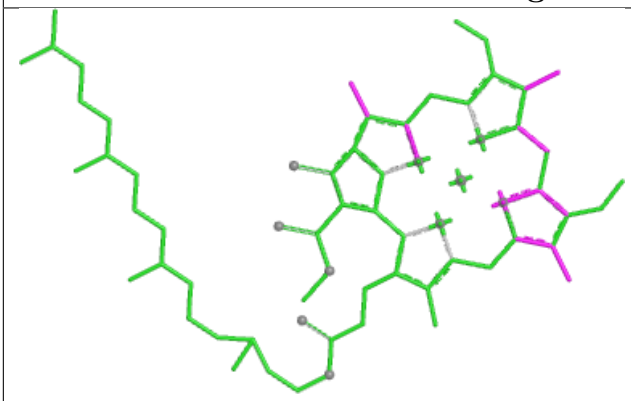


Torsions

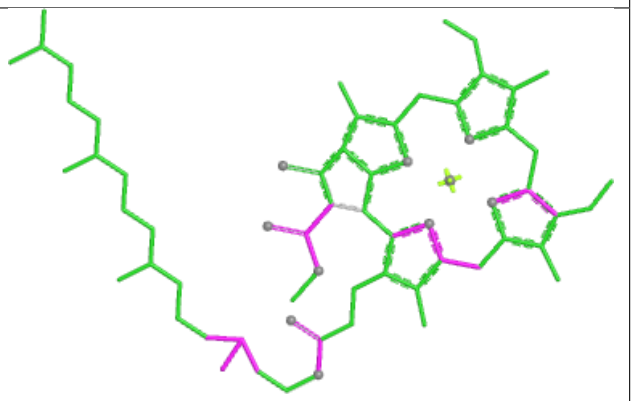


Rings

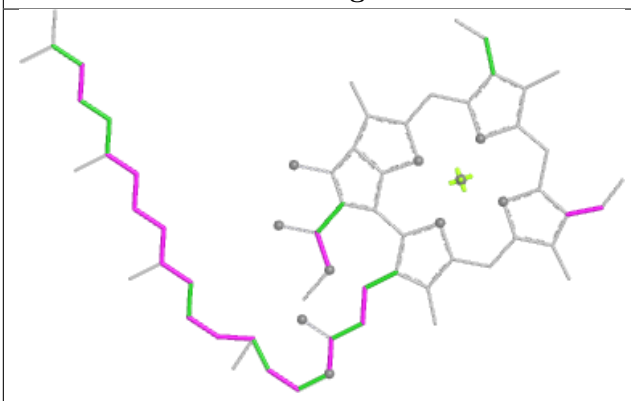
Ligand CLA b 736



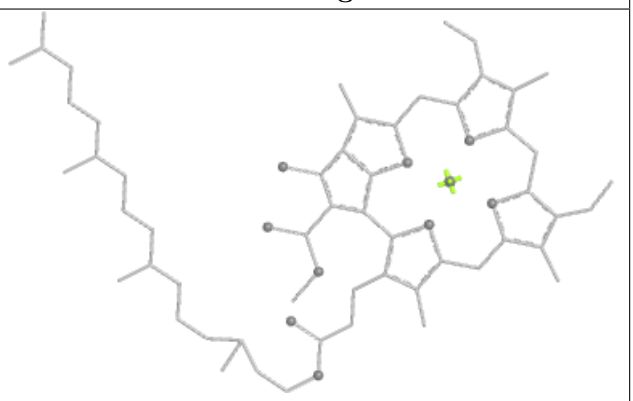
Bond lengths



Bond angles

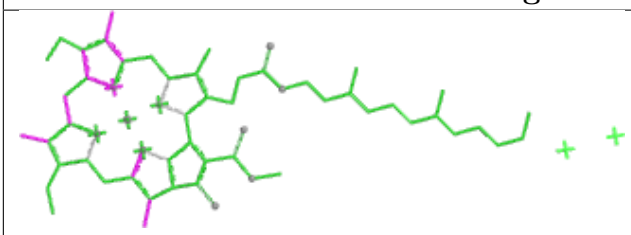


Torsions

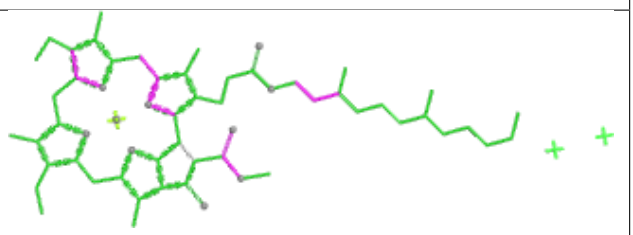


Rings

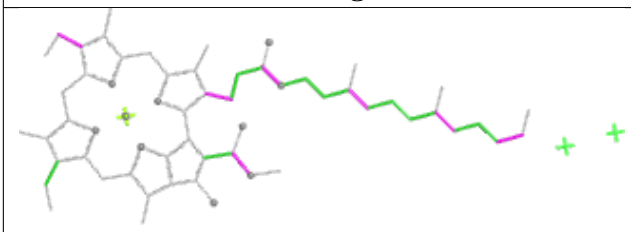
Ligand CLA G 304



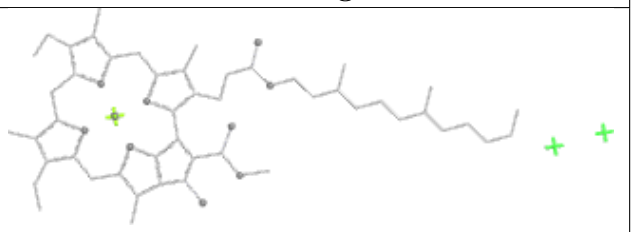
Bond lengths



Bond angles

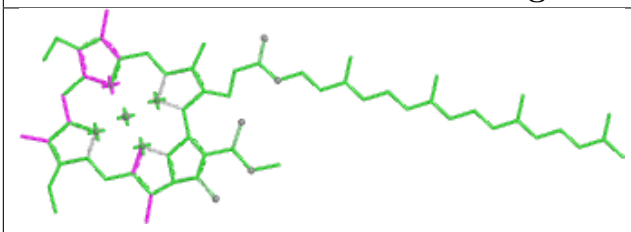


Torsions

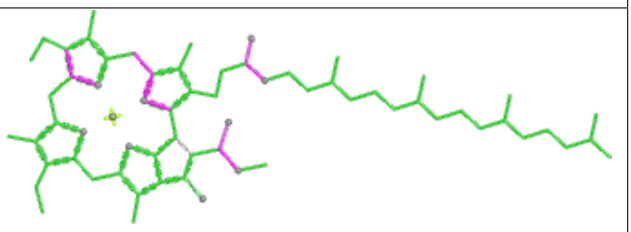


Rings

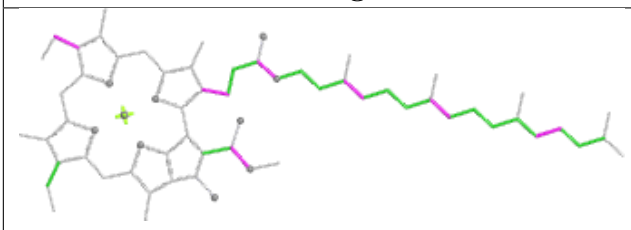
Ligand CLA a 820



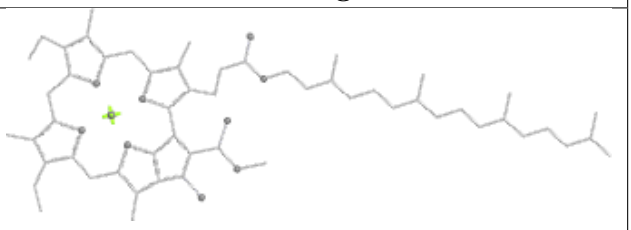
Bond lengths



Bond angles

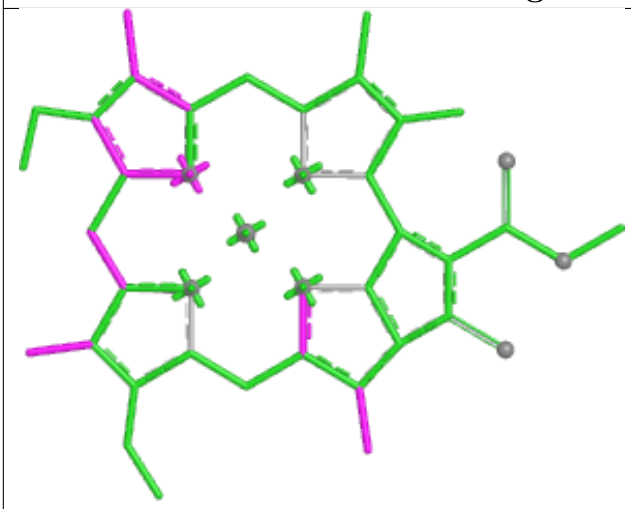


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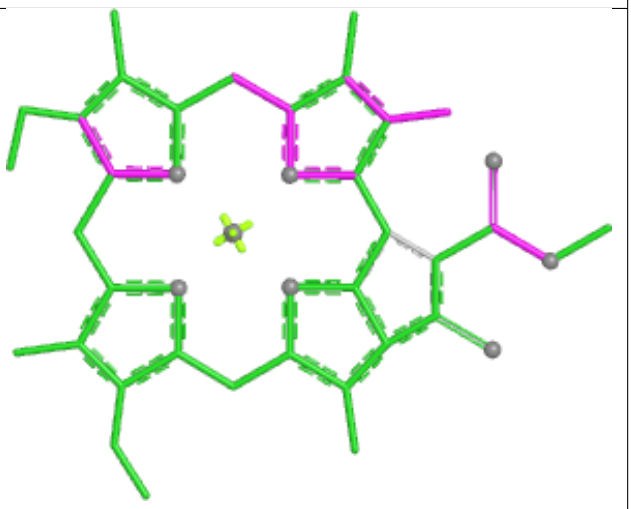


Rings

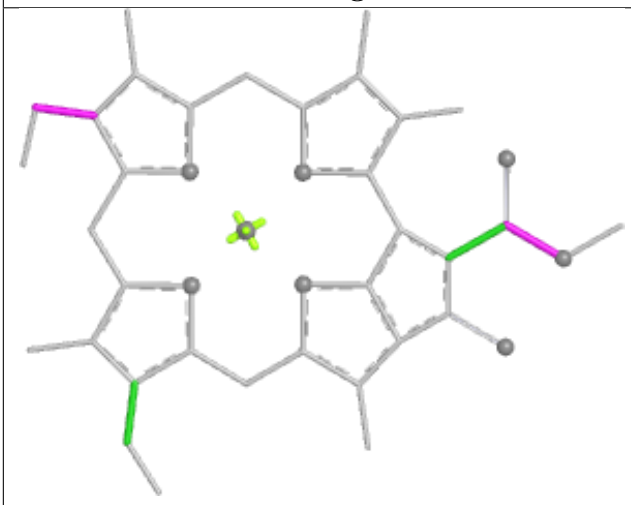
Ligand CLA L 315



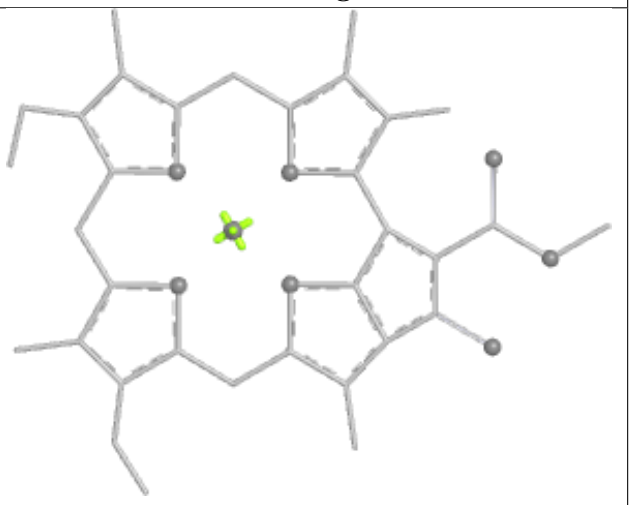
Bond lengths



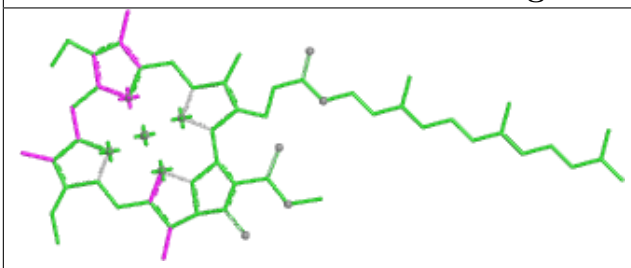
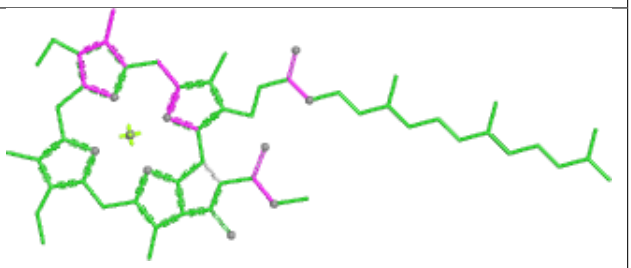
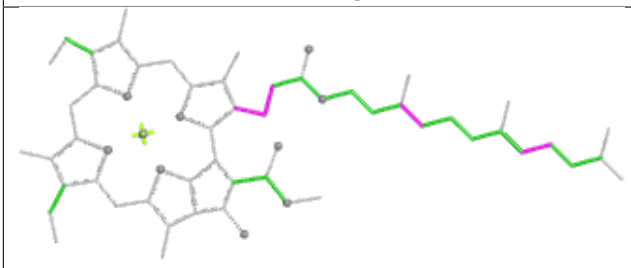
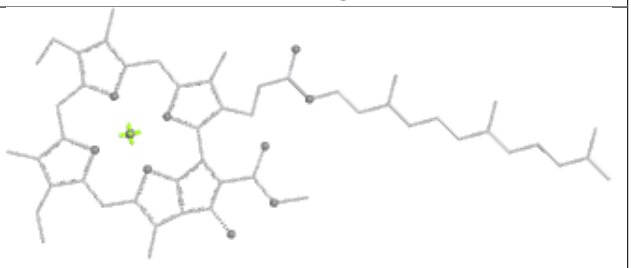
Bond angles

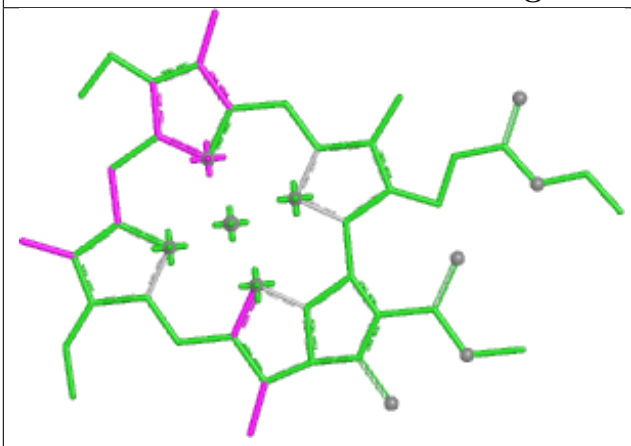
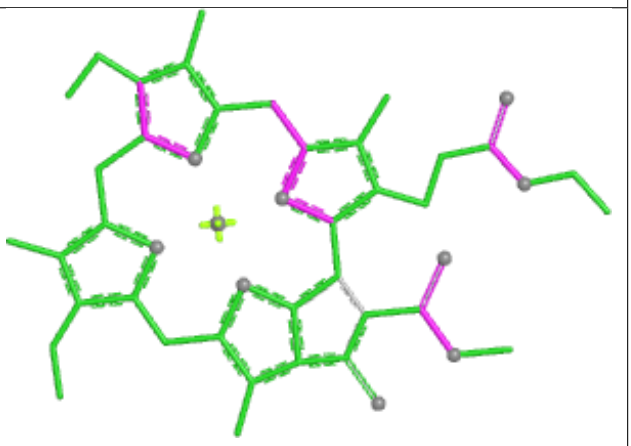
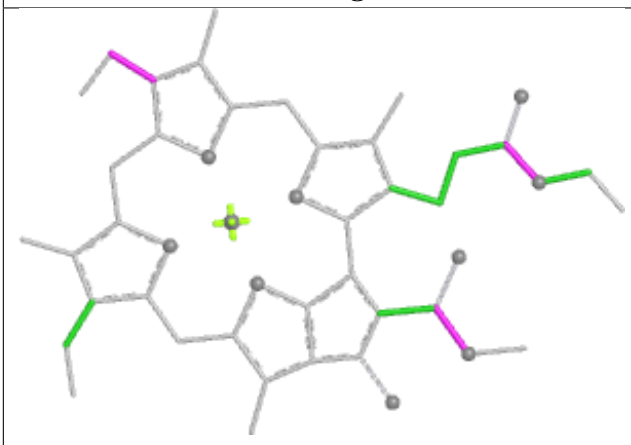
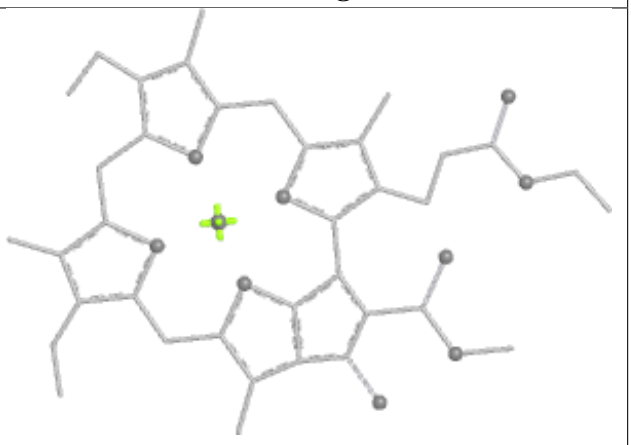


Torsions

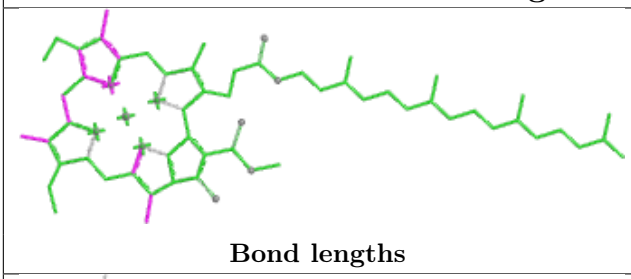


Rings

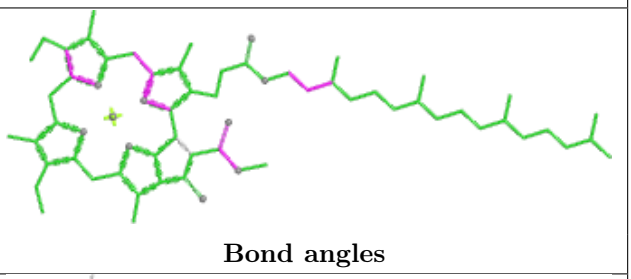
Ligand CLA h 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

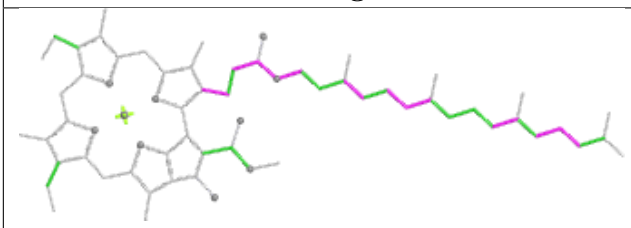
Ligand CLA a 806



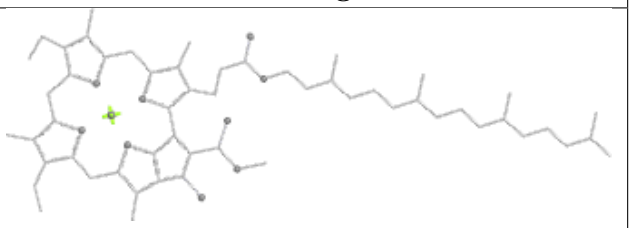
Bond lengths



Bond angles



Torsions

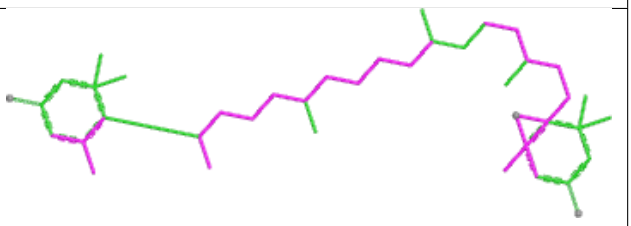


Rings

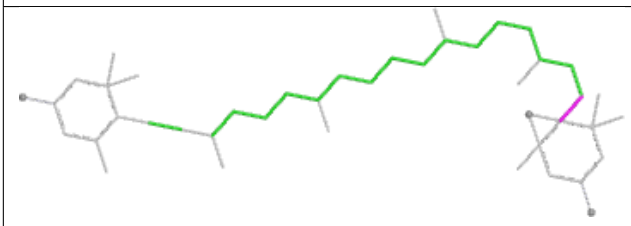
Ligand DD6 K 206



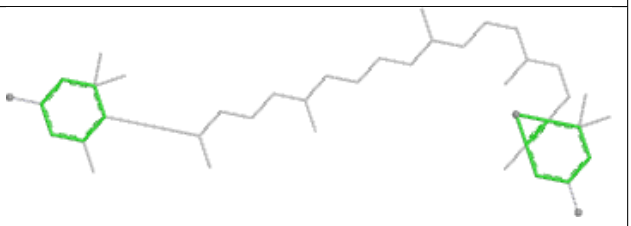
Bond lengths



Bond angles

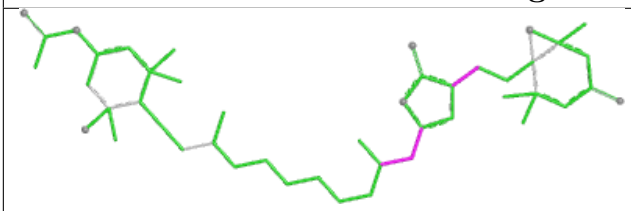


Torsions

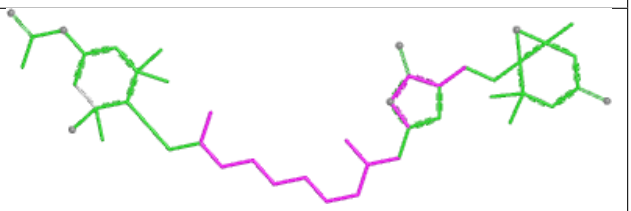


Rings

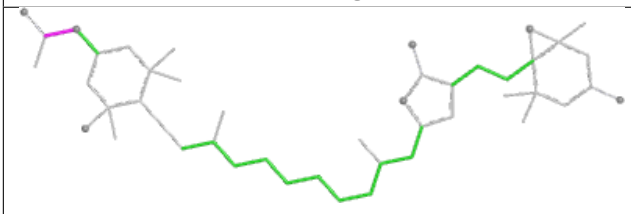
Ligand PID O 302



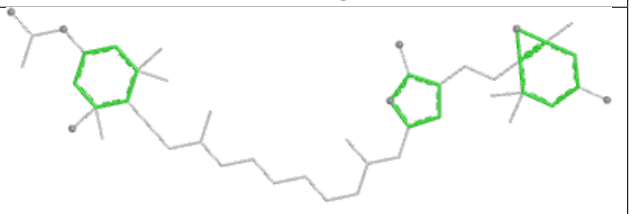
Bond lengths



Bond angles

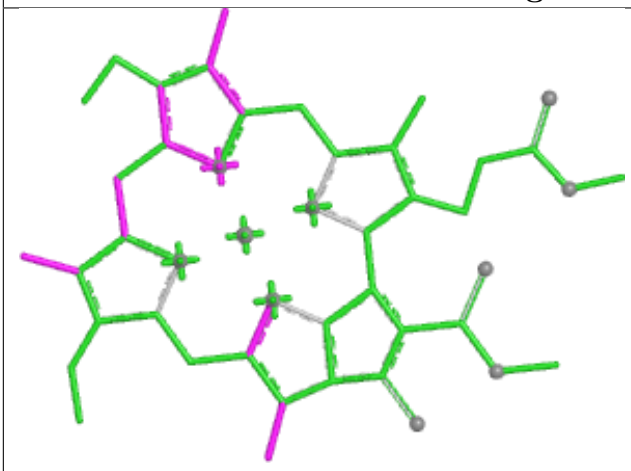


Torsions

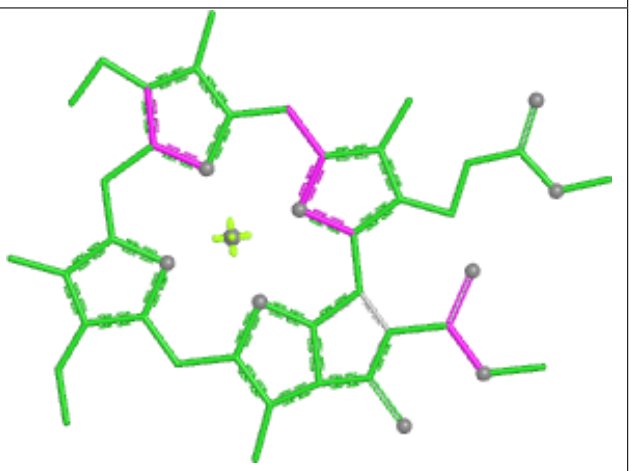


Rings

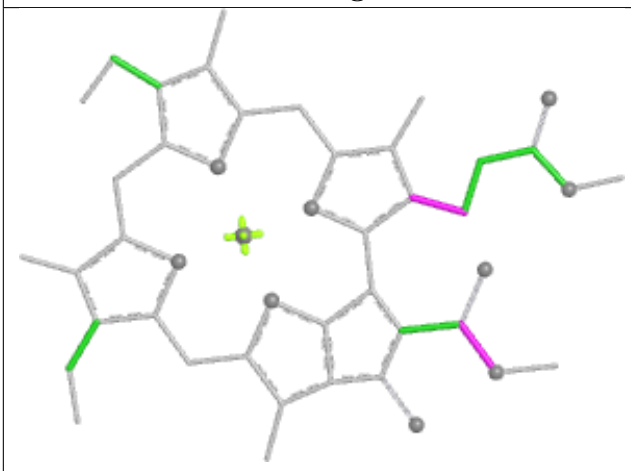
Ligand CLA F 308



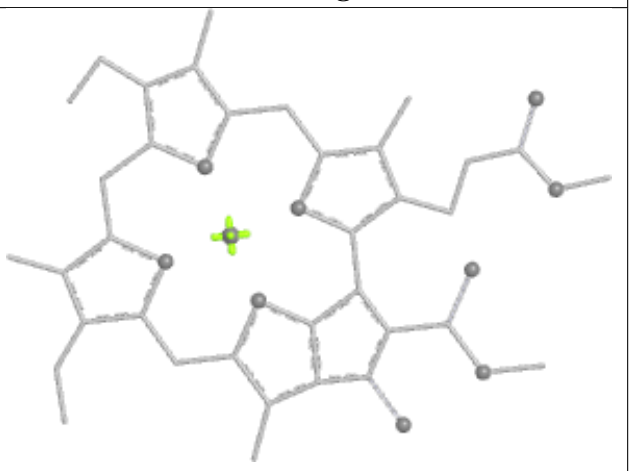
Bond lengths



Bond angles



Torsions

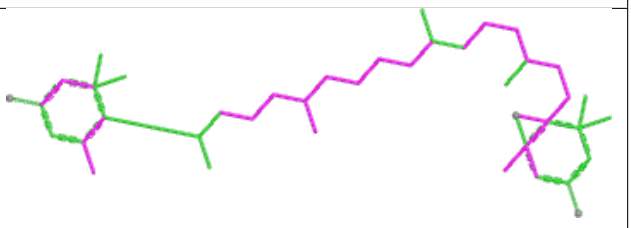


Rings

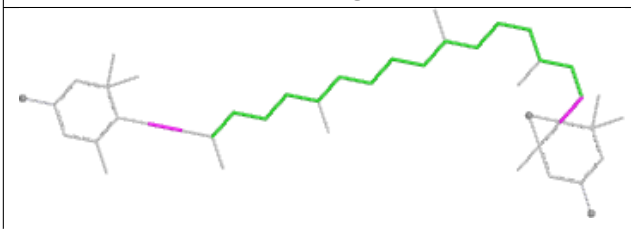
Ligand DD6 B 302



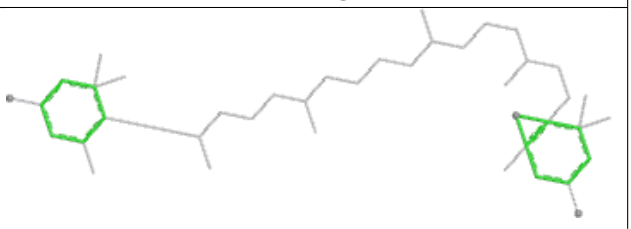
Bond lengths



Bond angles

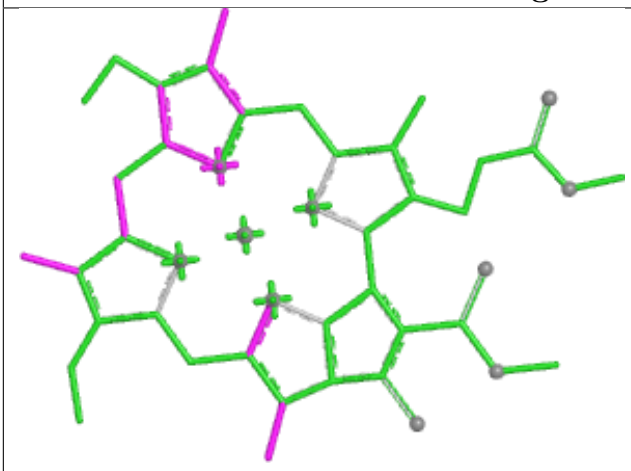


Torsions

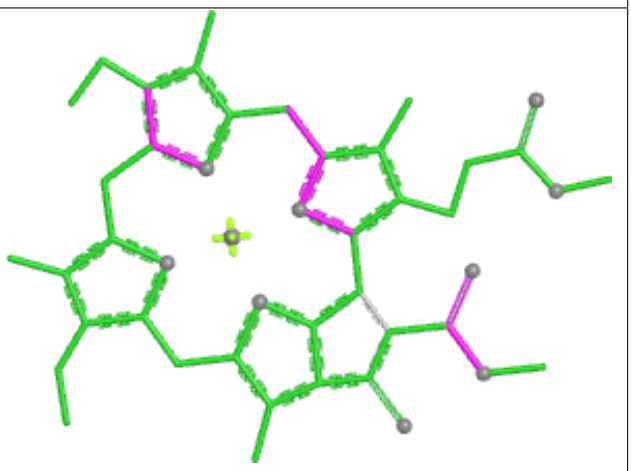


Rings

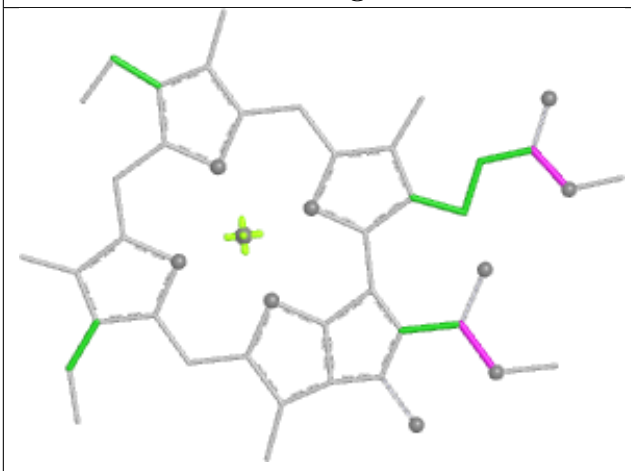
Ligand CLA f 802



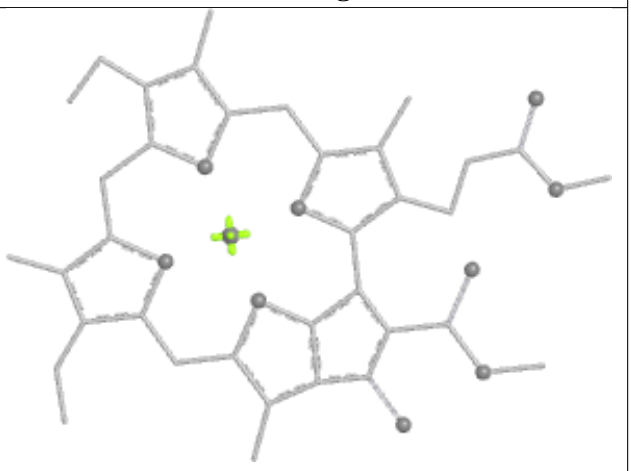
Bond lengths



Bond angles

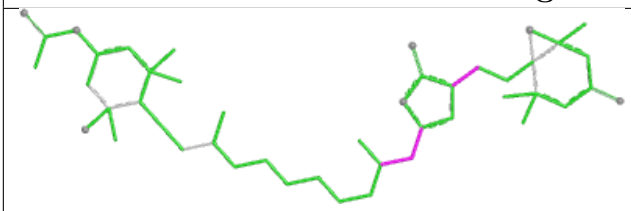


Torsions

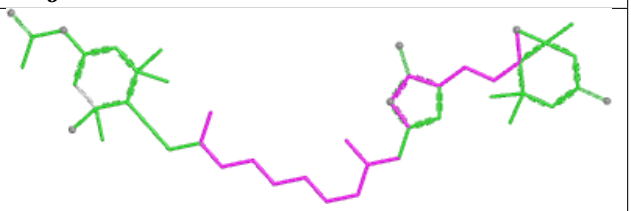


Rings

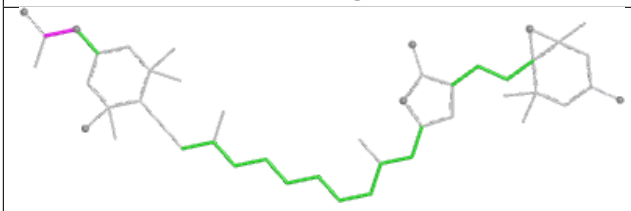
Ligand PID j 101



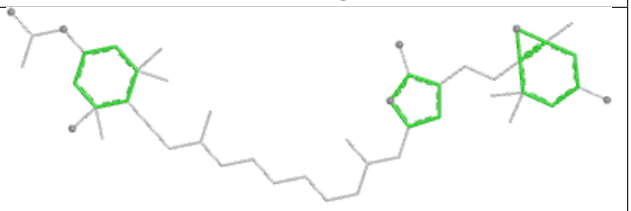
Bond lengths



Bond angles

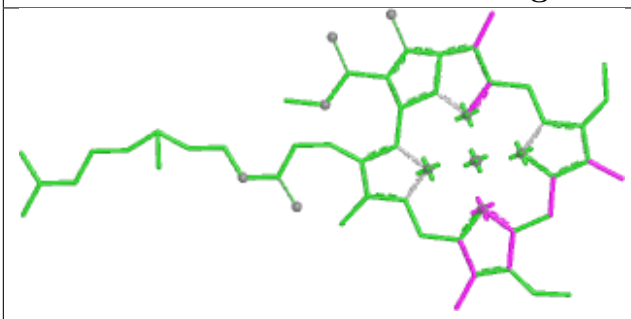


Torsions

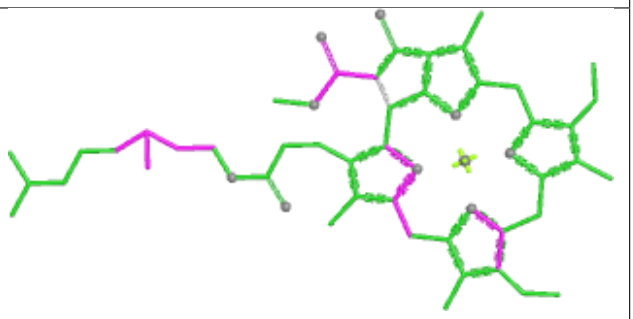


Rings

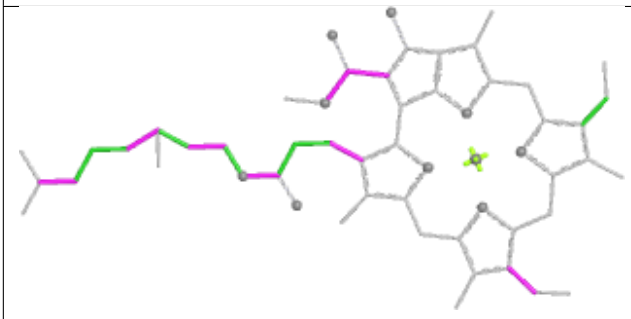
Ligand CLA I 212



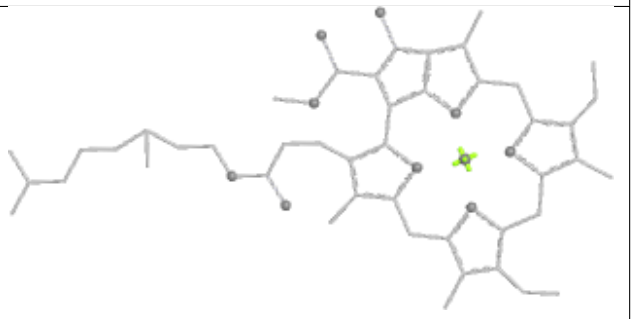
Bond lengths



Bond angles

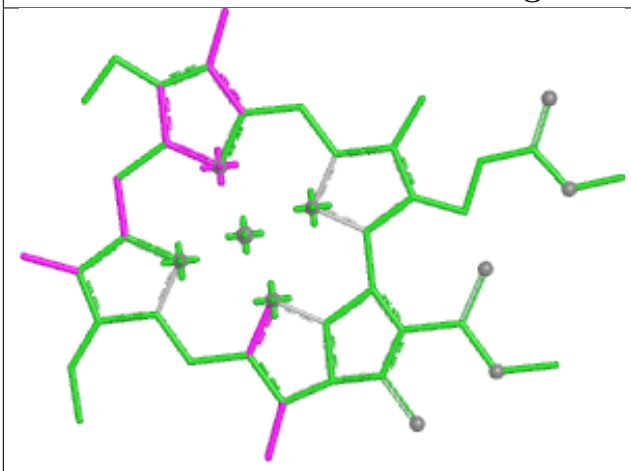


Torsions

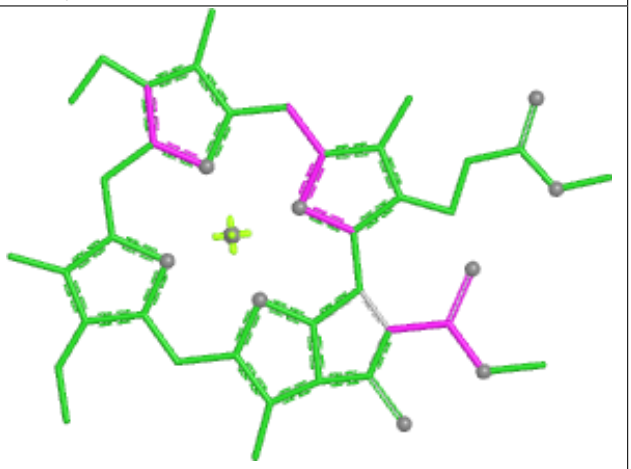


Rings

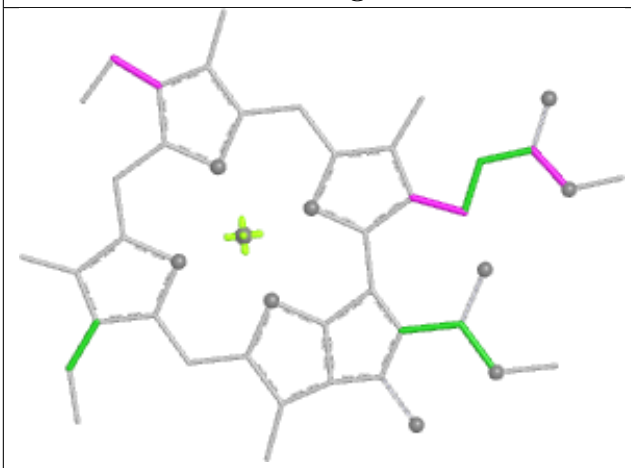
Ligand CLA Q 312



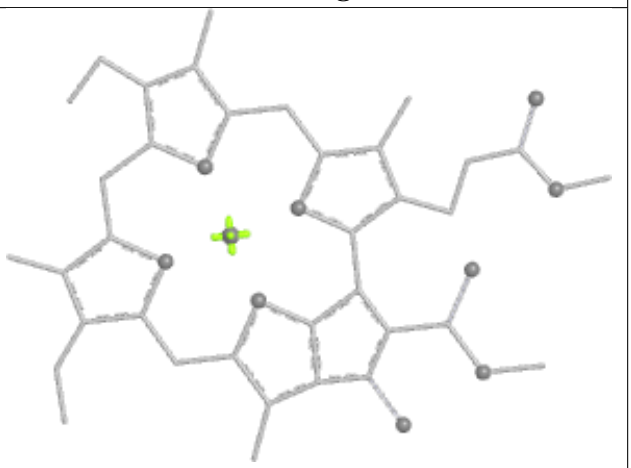
Bond lengths



Bond angles

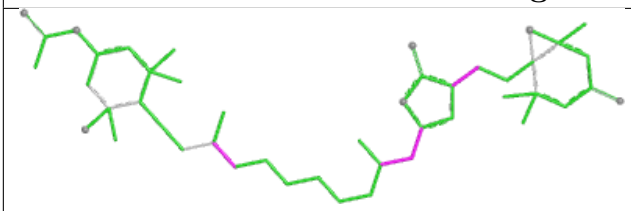


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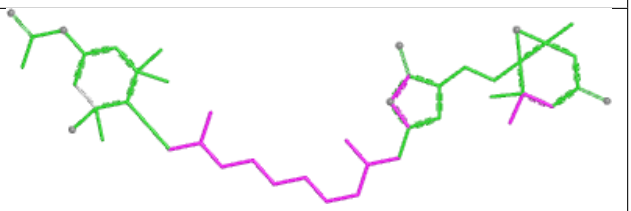


Rings

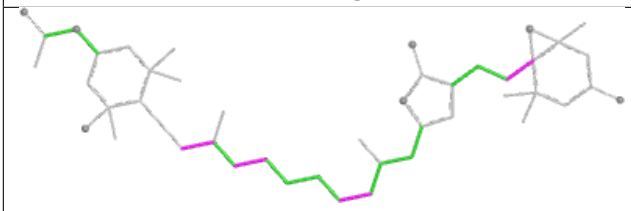
Ligand PID E 301



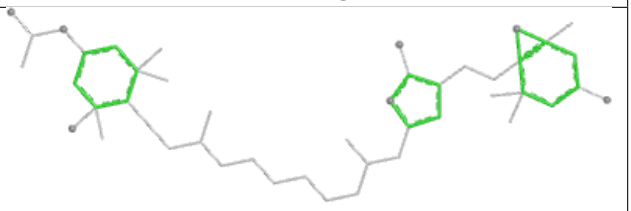
Bond lengths



Bond angles

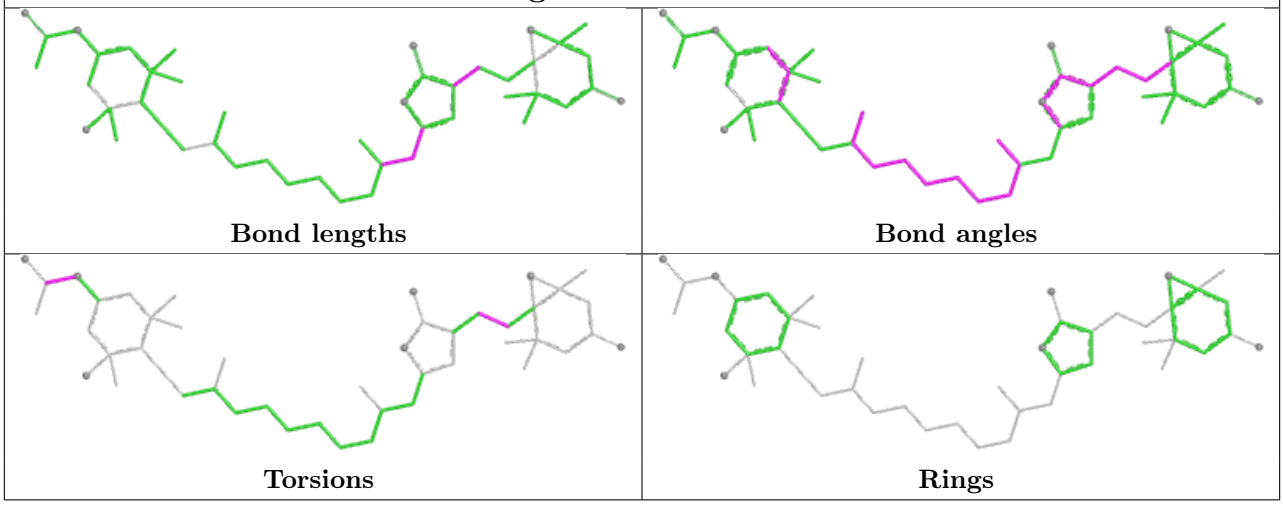


Torsions

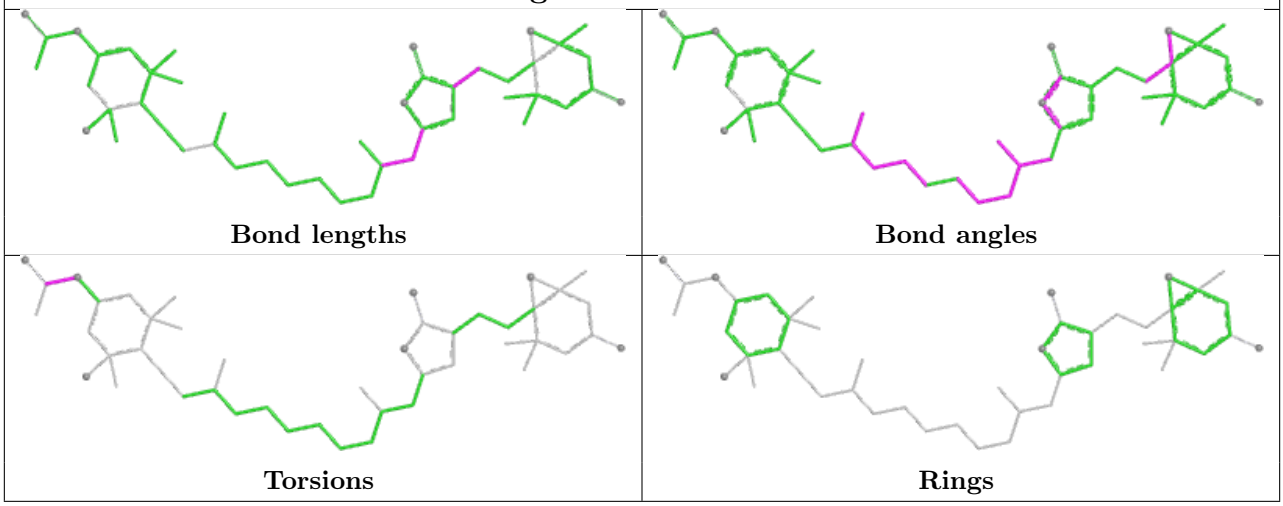


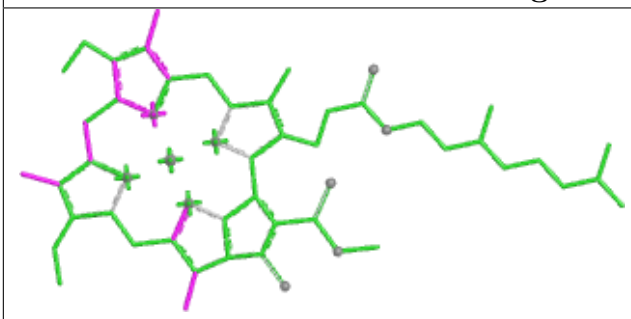
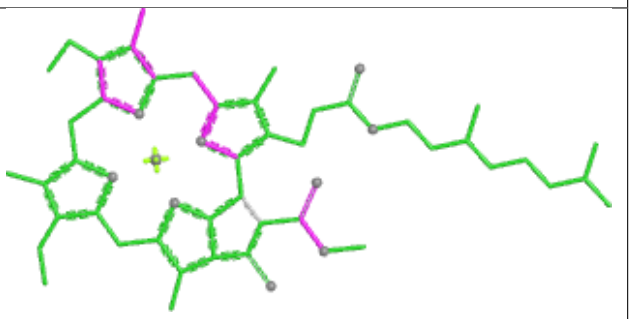
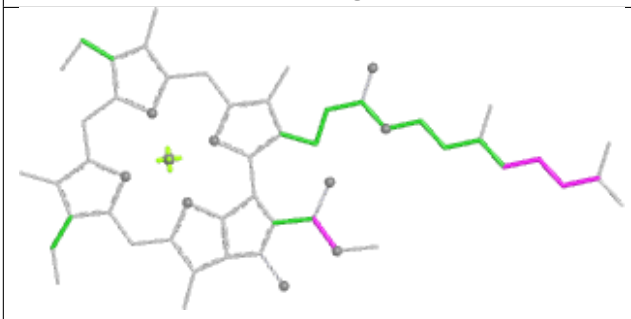
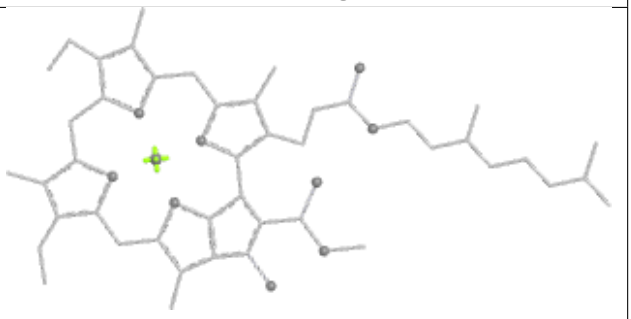
Rings

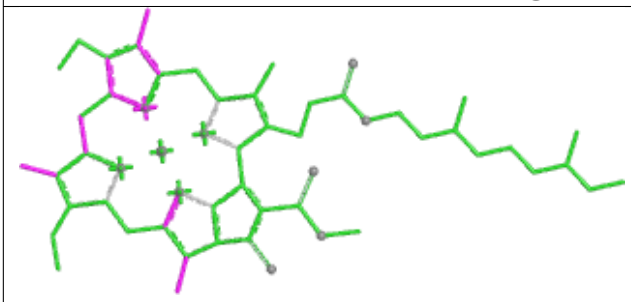
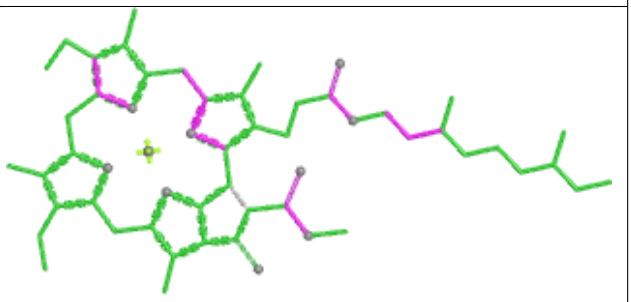
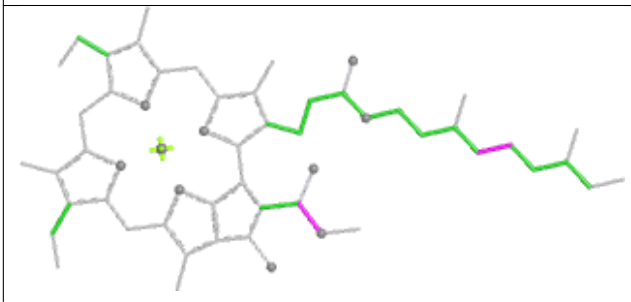
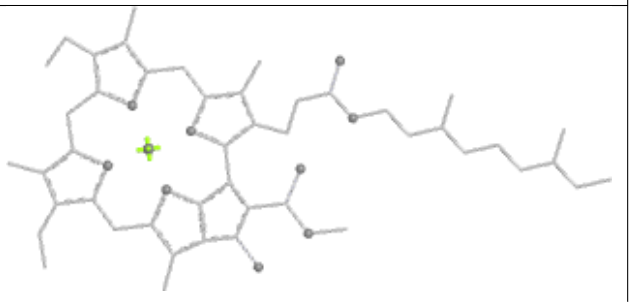
Ligand PID H 305

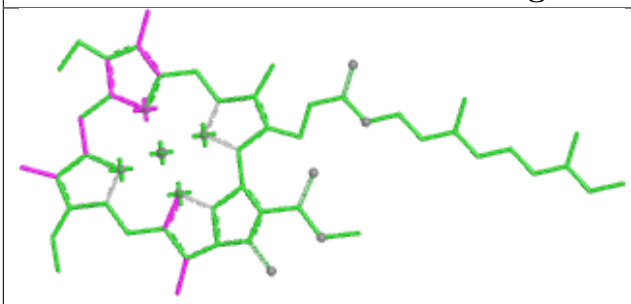
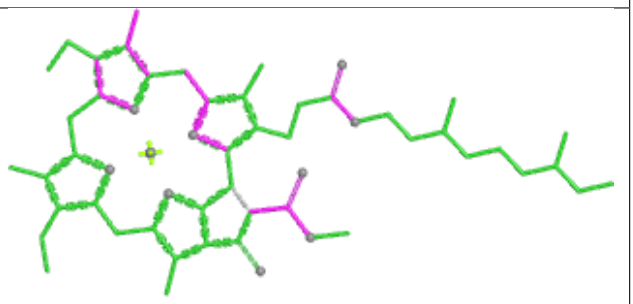
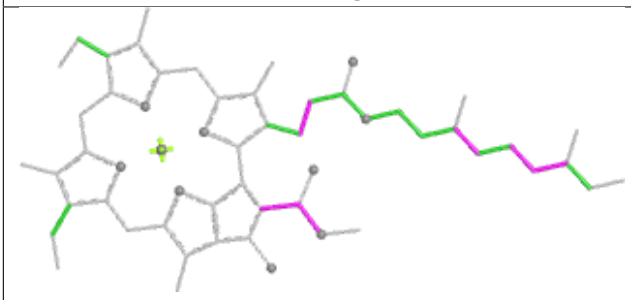
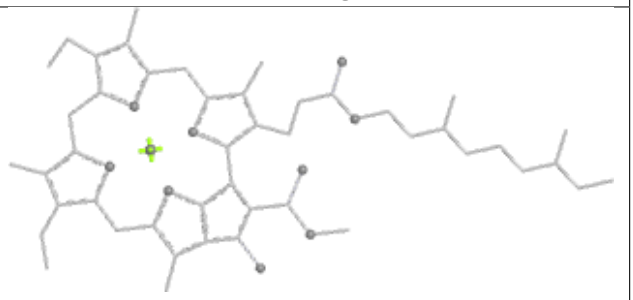


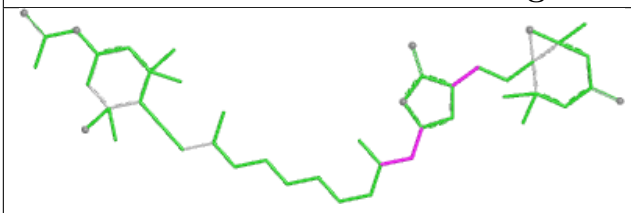
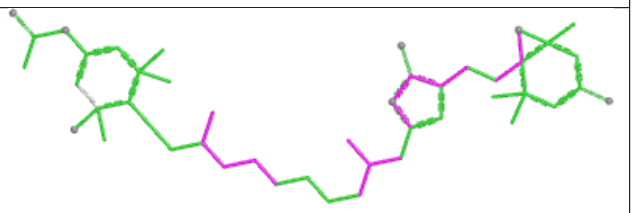
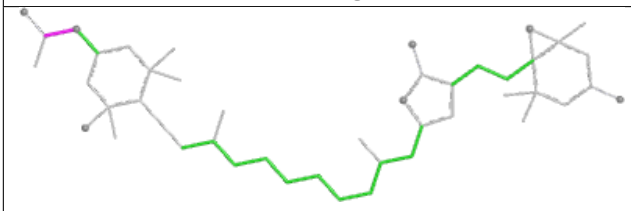
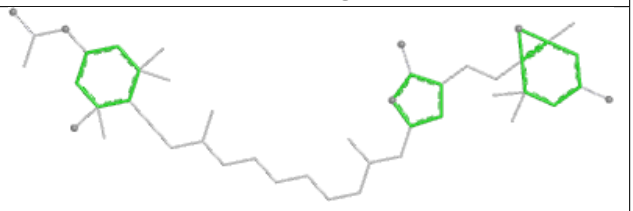
Ligand PID C 302



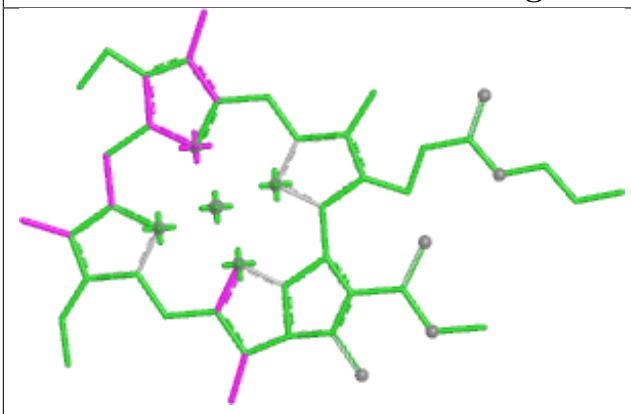
Ligand CLA I 210	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 731	
 Bond lengths	 Bond angles
 Torsions	 Rings

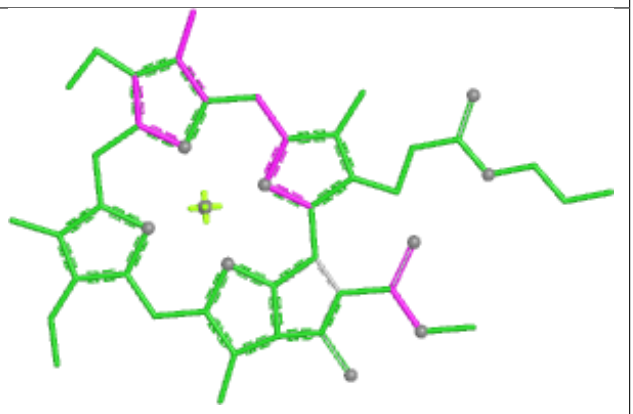
Ligand CLA J 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PID N 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

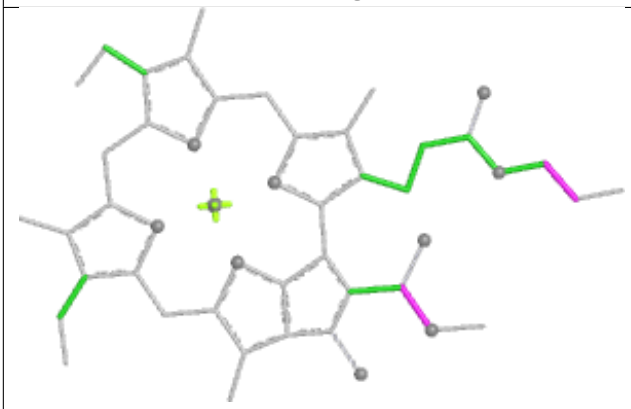
Ligand CLA E 314



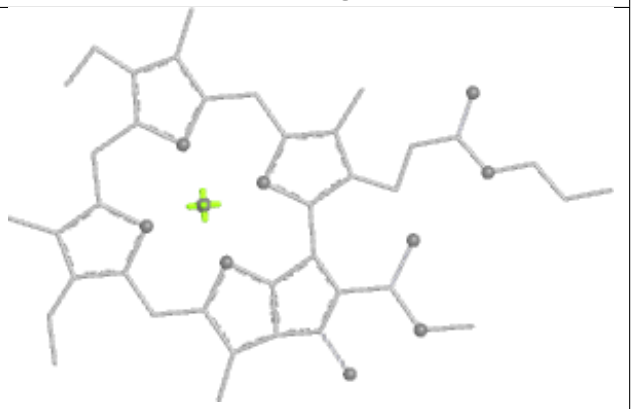
Bond lengths



Bond angles

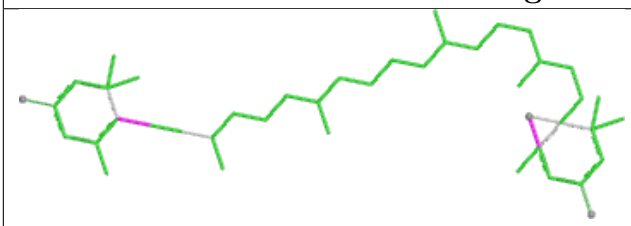


Torsions

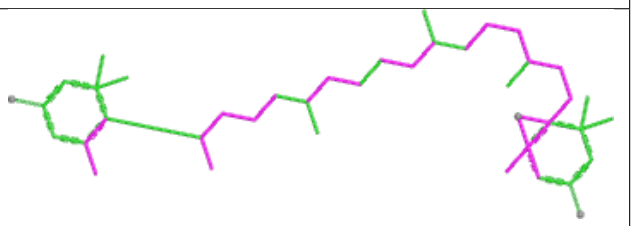


Rings

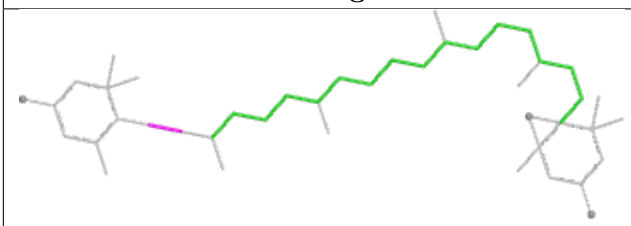
Ligand DD6 A 202



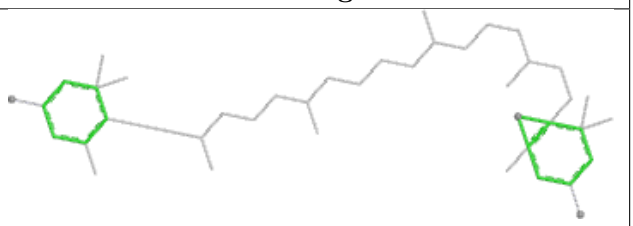
Bond lengths



Bond angles

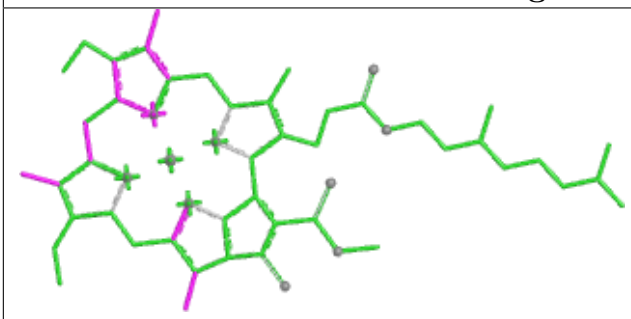


Torsions

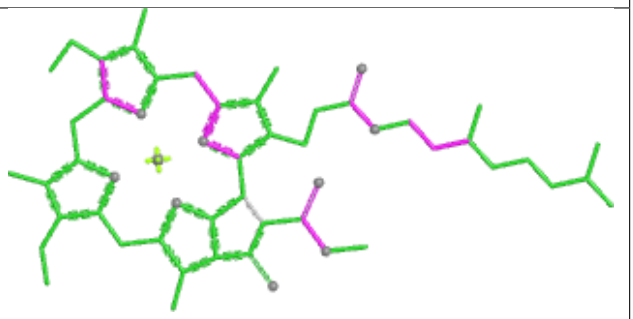


Rings

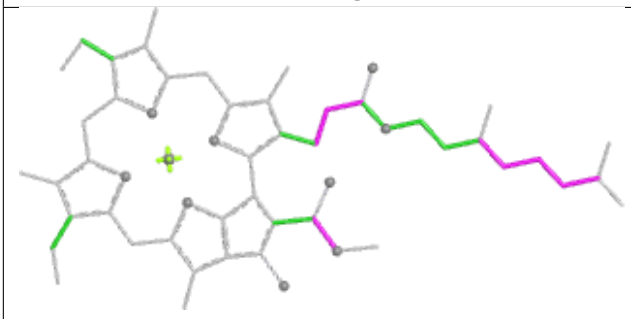
Ligand CLA a 810



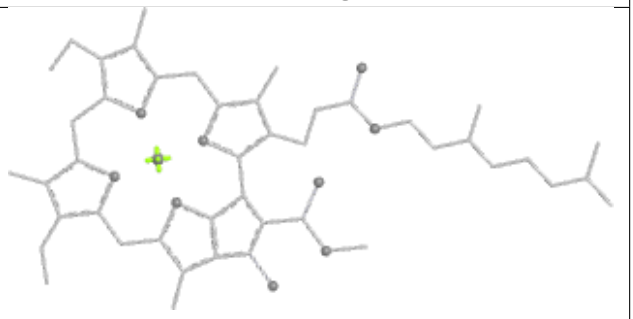
Bond lengths



Bond angles

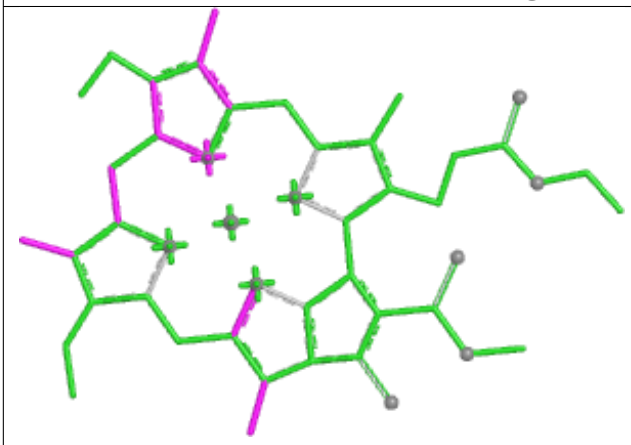


Torsions

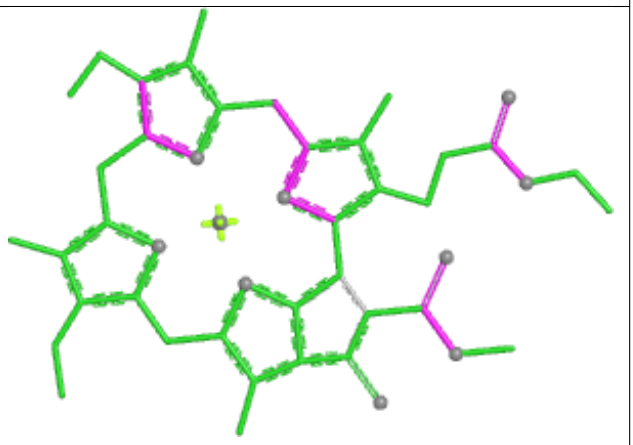


Rings

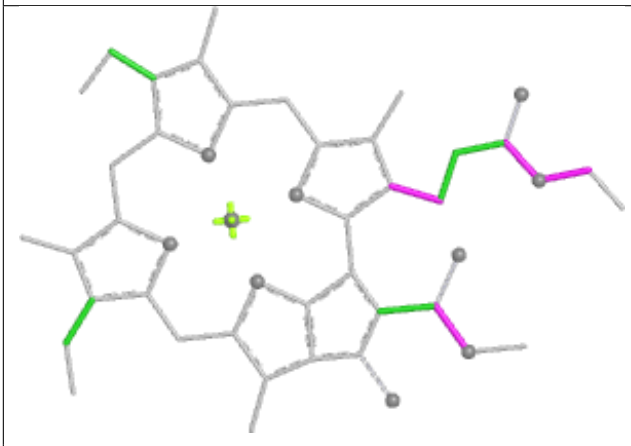
Ligand CLA H 313



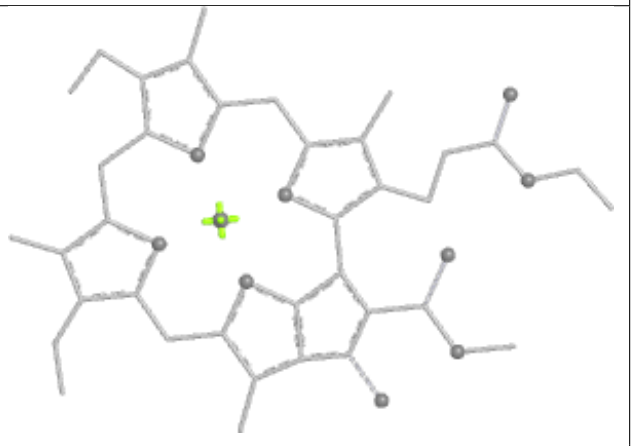
Bond lengths



Bond angles

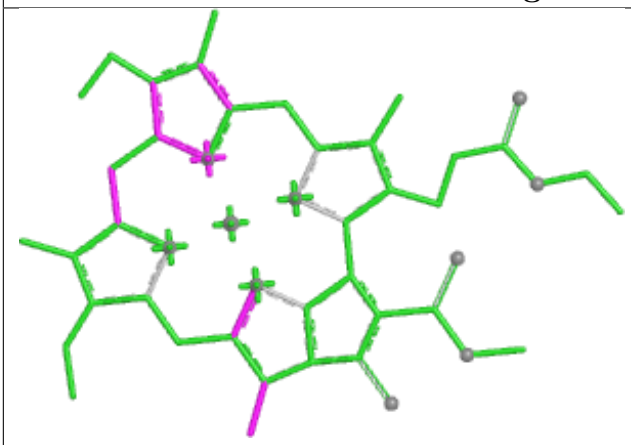


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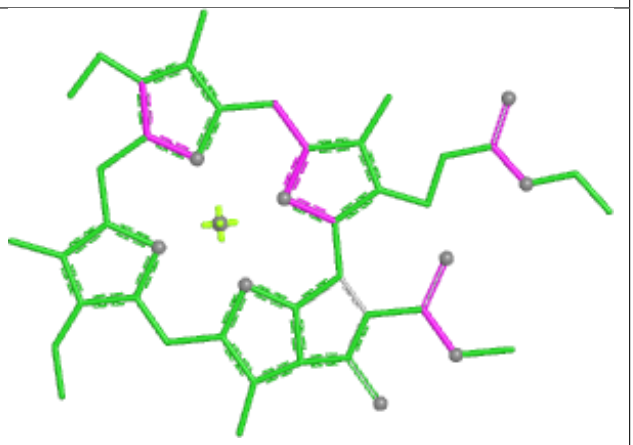


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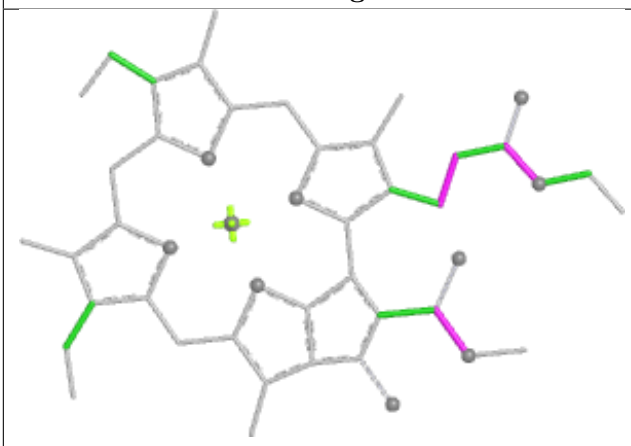
Ligand CLA D 308



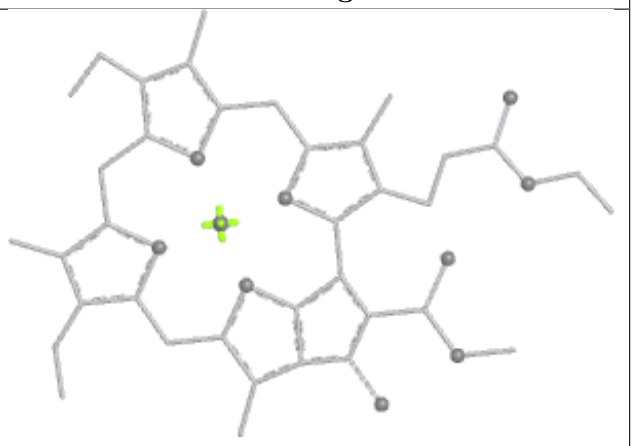
Bond lengths



Bond angles

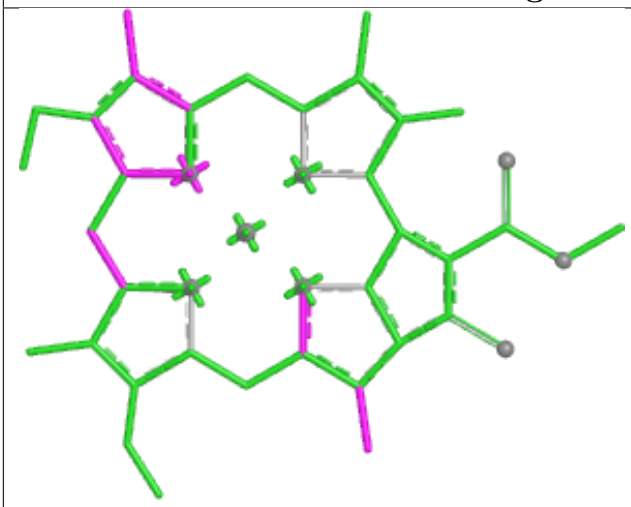


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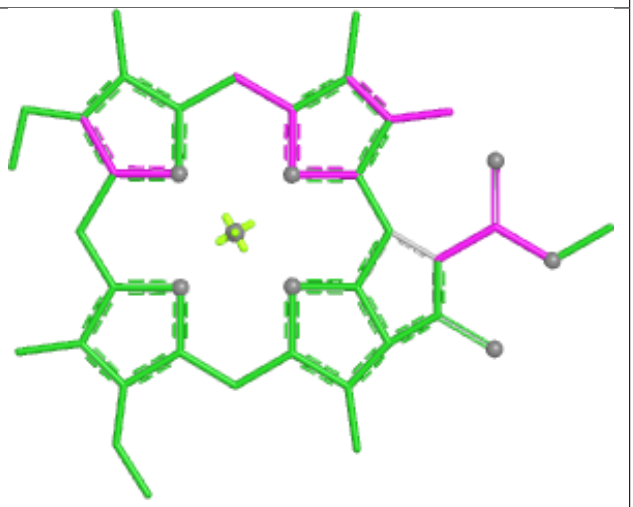


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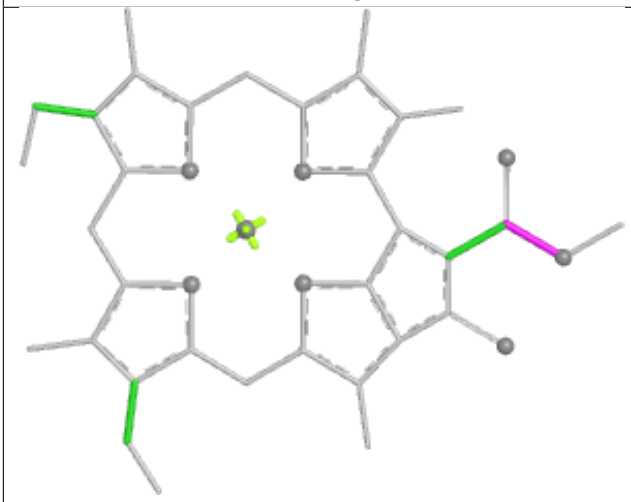
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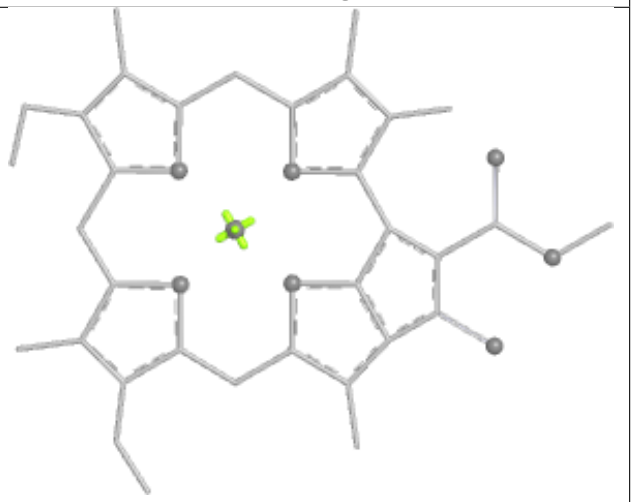
Bond lengths



Bond angles



Torsions

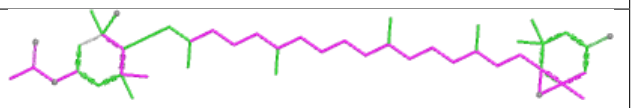


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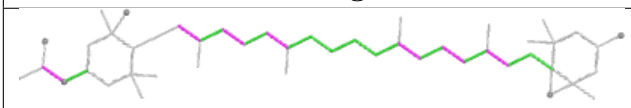
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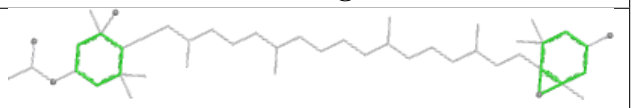
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Bond angles

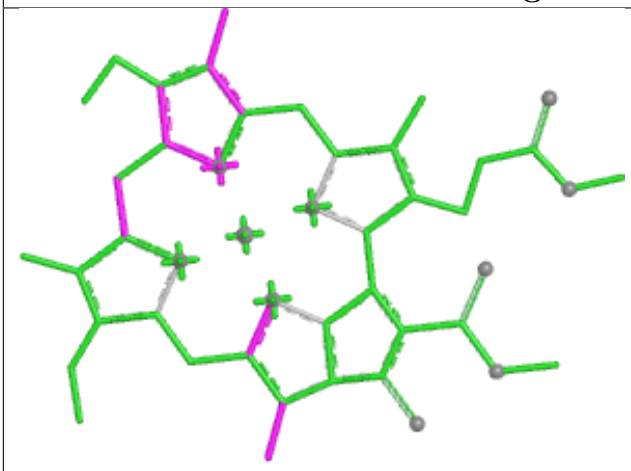


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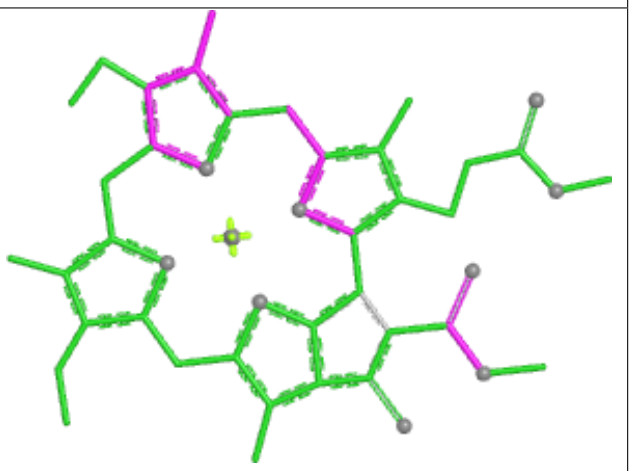


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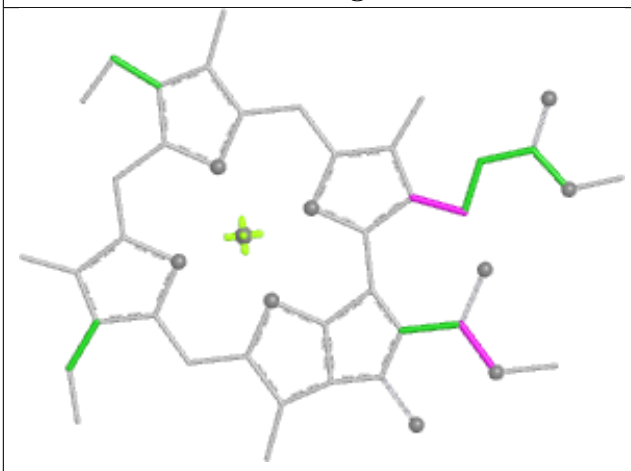
Ligand CLA O 313



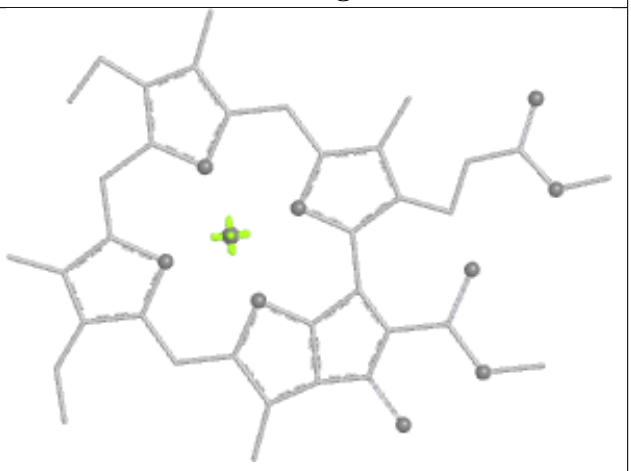
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Bond angles

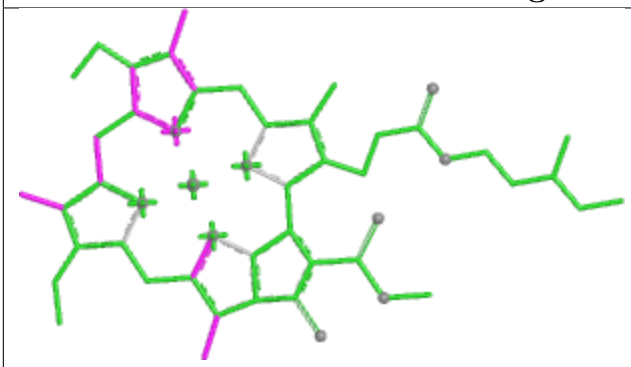


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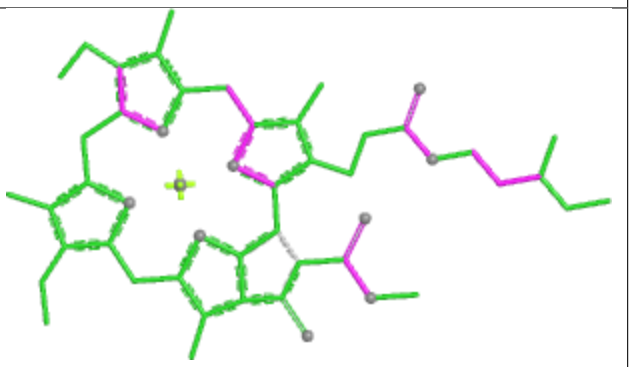


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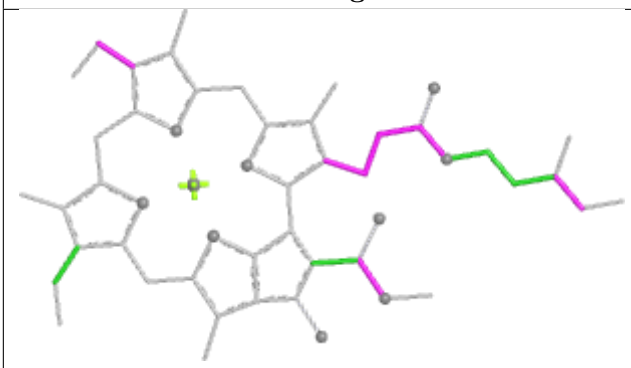
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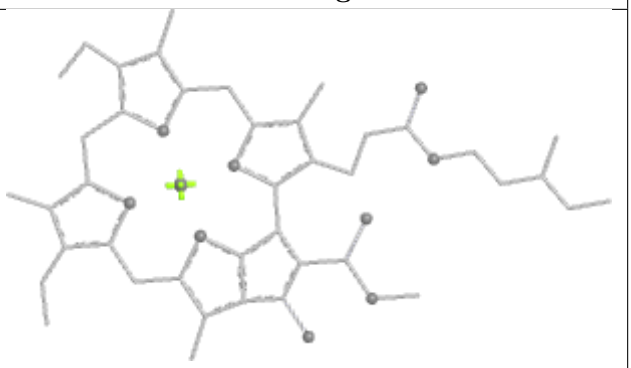
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Bond angles

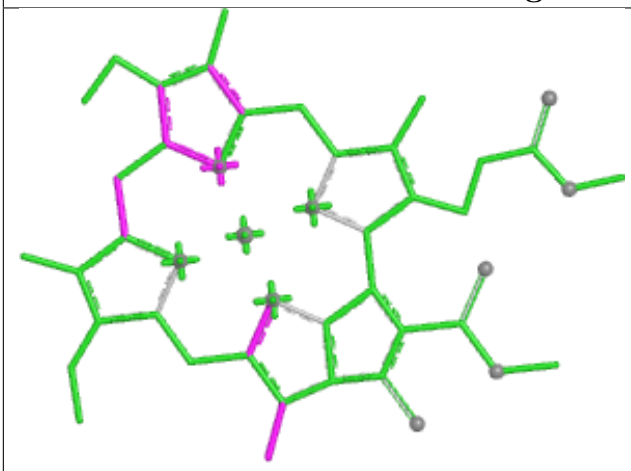


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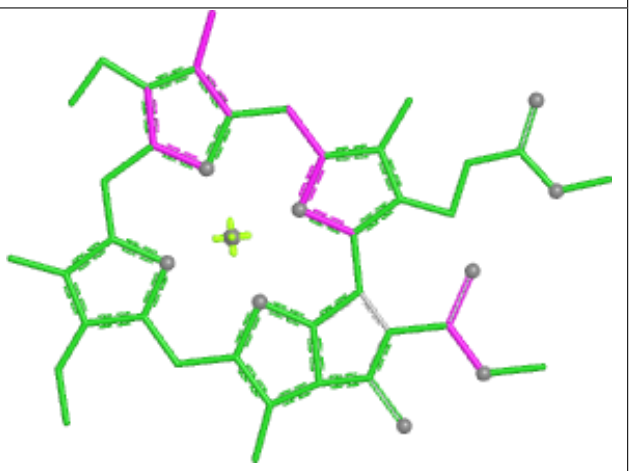


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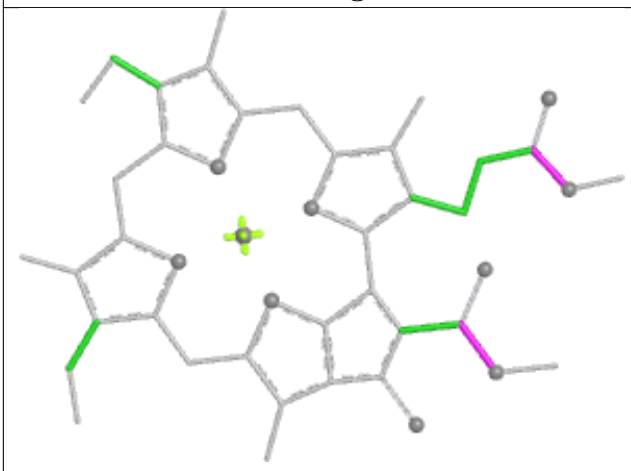
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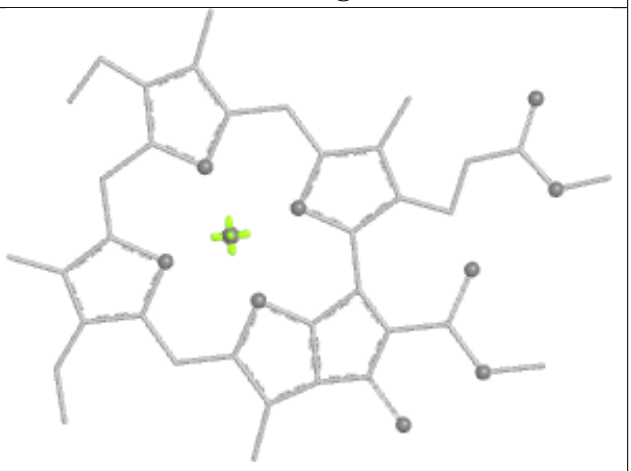
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Bond angles

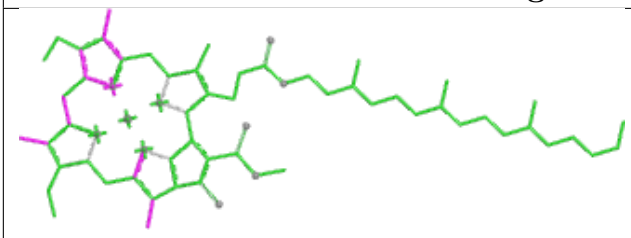


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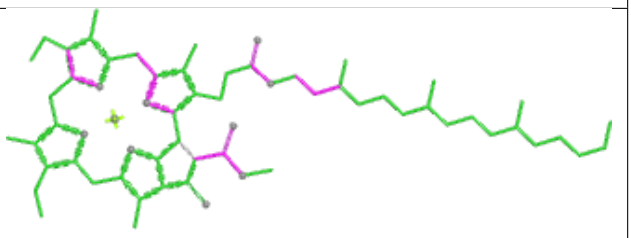


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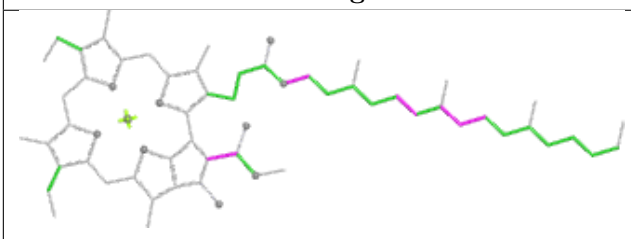
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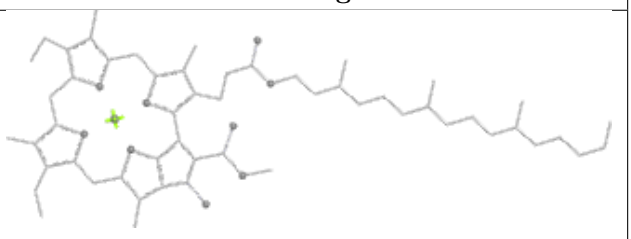
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Bond angles

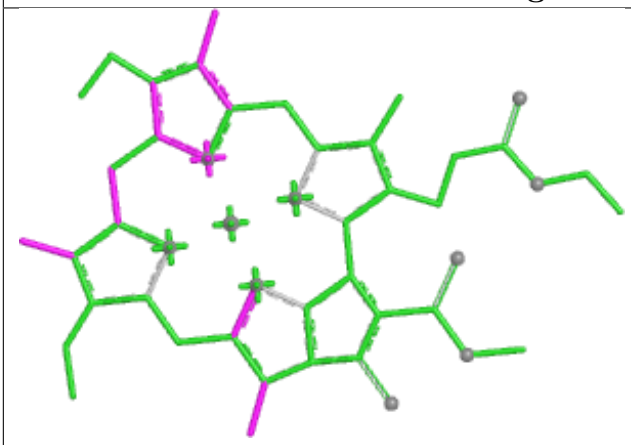


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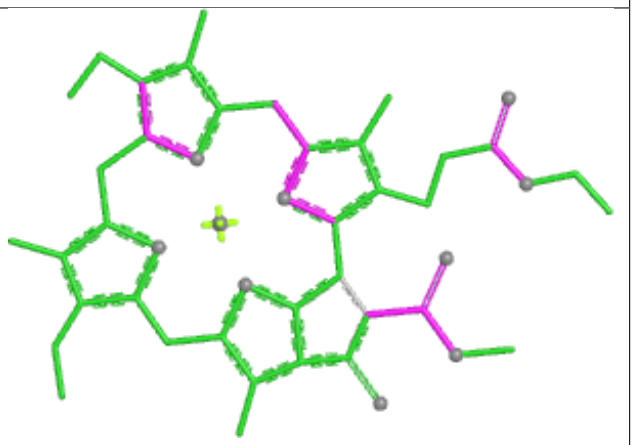


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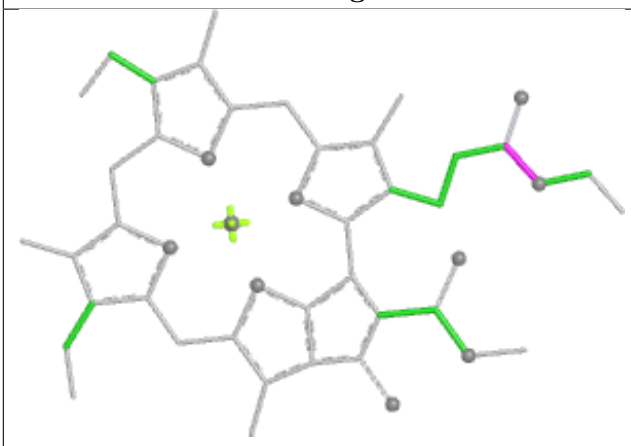
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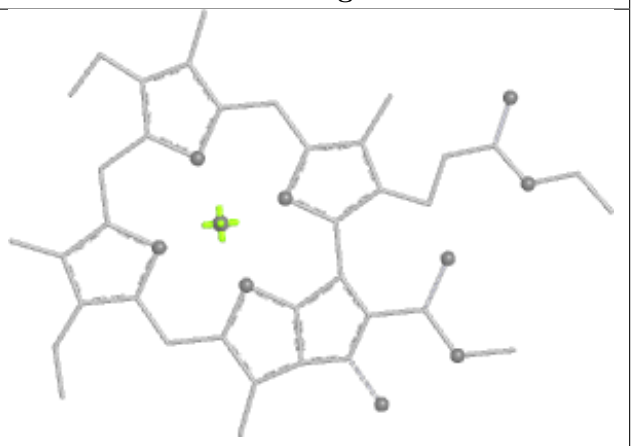
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Bond angles

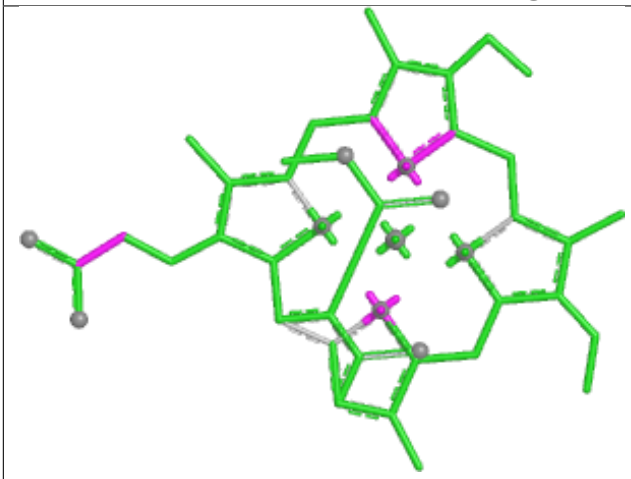


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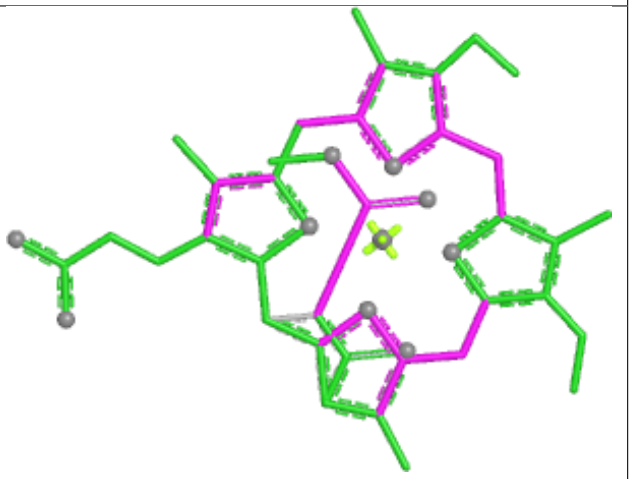


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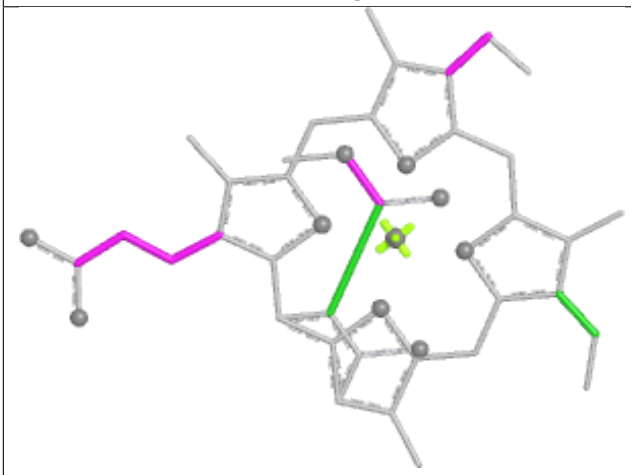
Ligand KC1 N 315



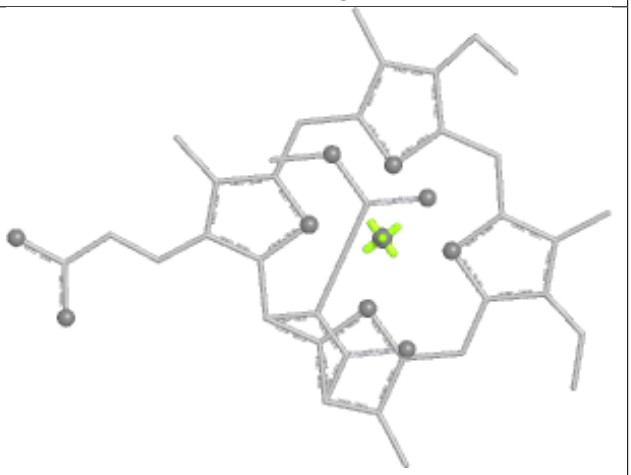
Bond lengths



Bond angles

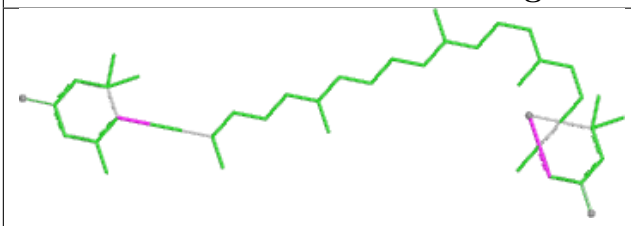


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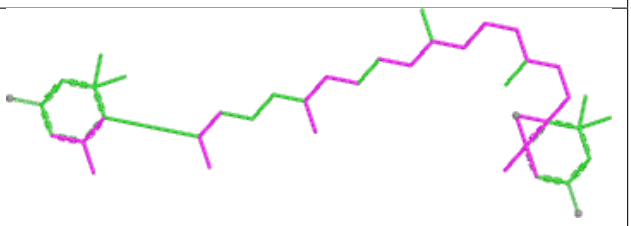


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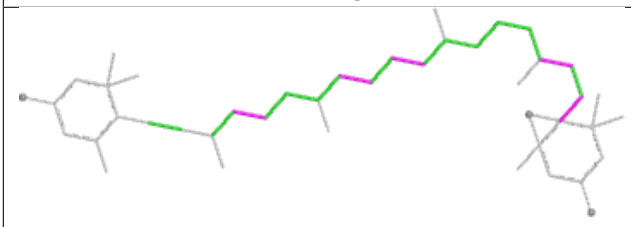
Ligand DD6 D 304



Bond lengths



Bond angles

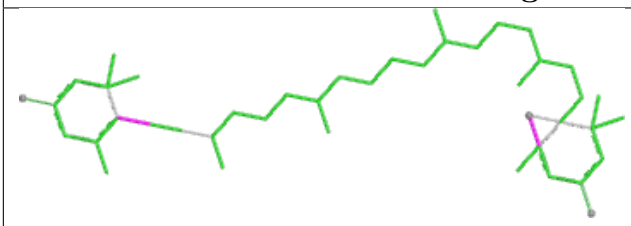


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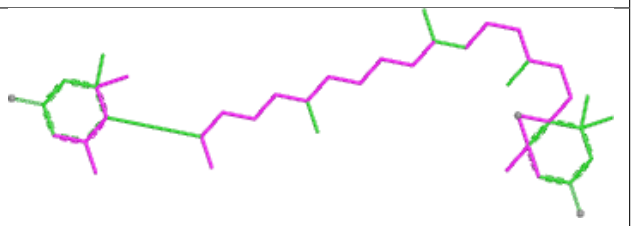


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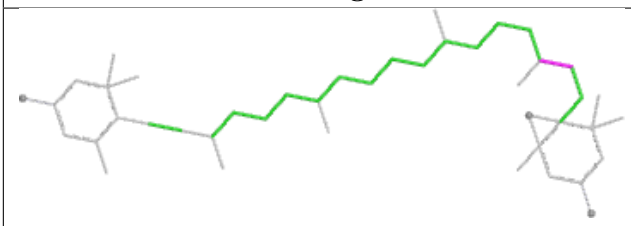
Ligand DD6 M 301



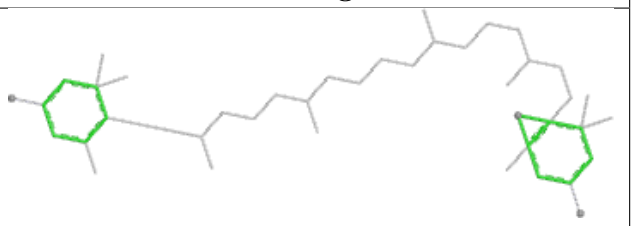
Bond lengths



Bond angles

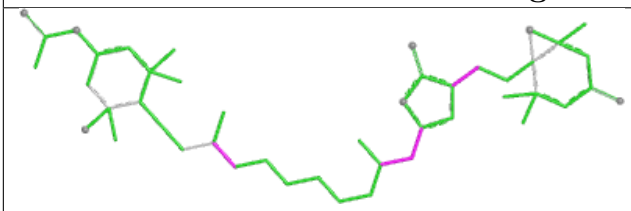


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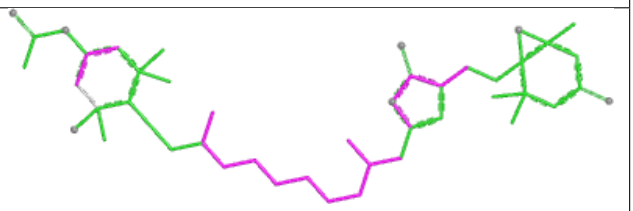


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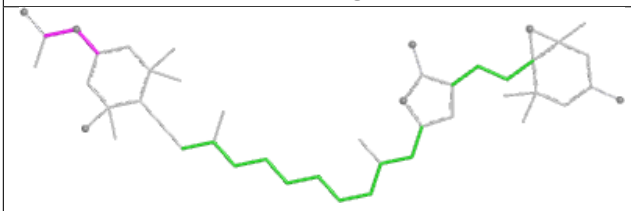
Ligand PID T 302



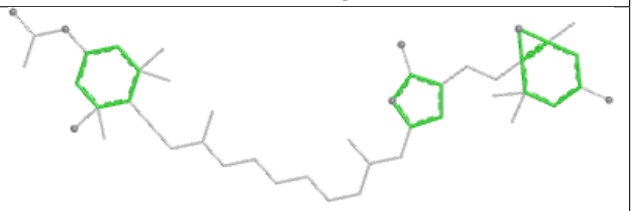
Bond lengths



Bond angles

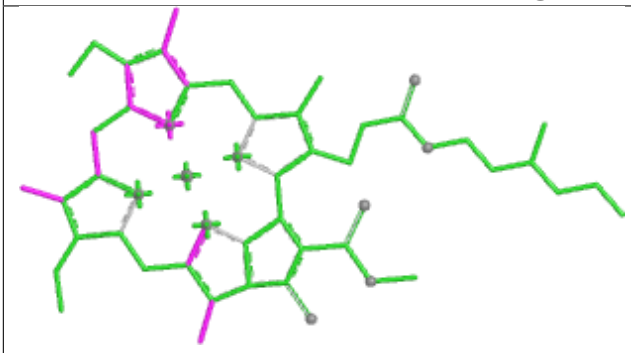


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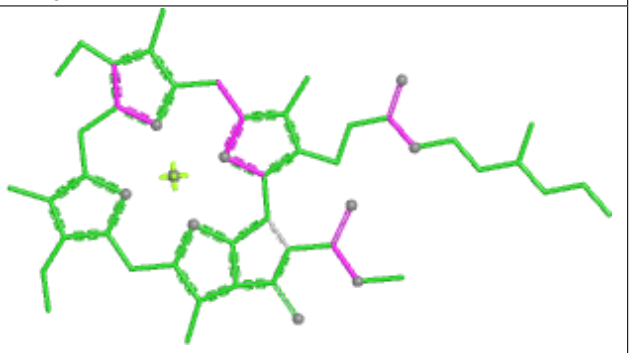


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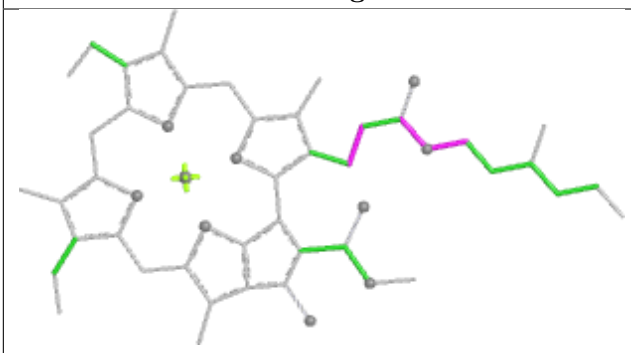
Ligand CLA j 104



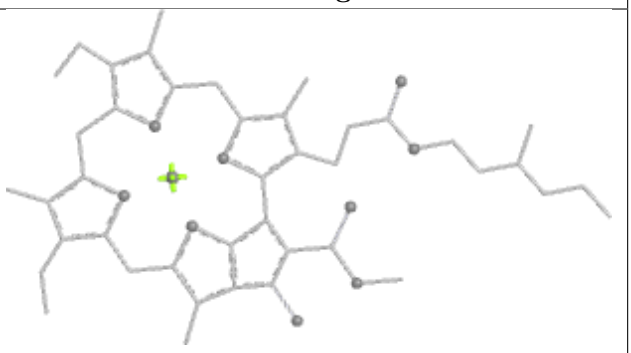
Bond lengths



Bond angles

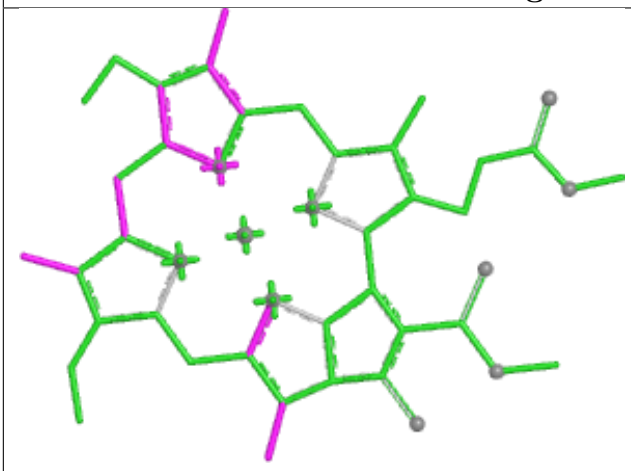


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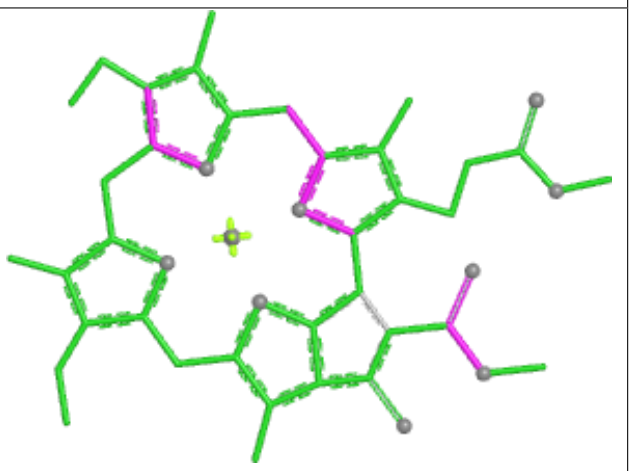


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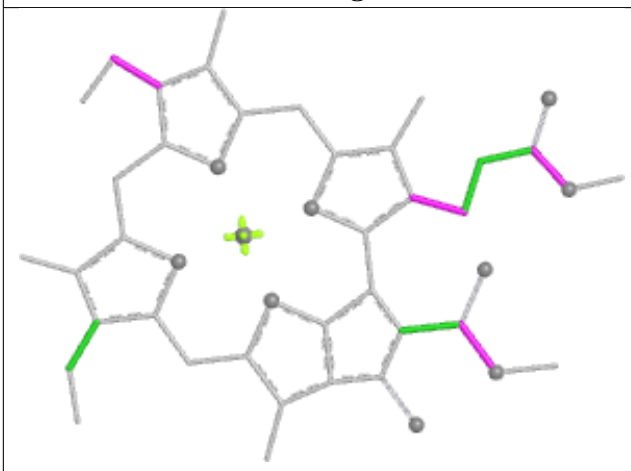
Ligand CLA F 313



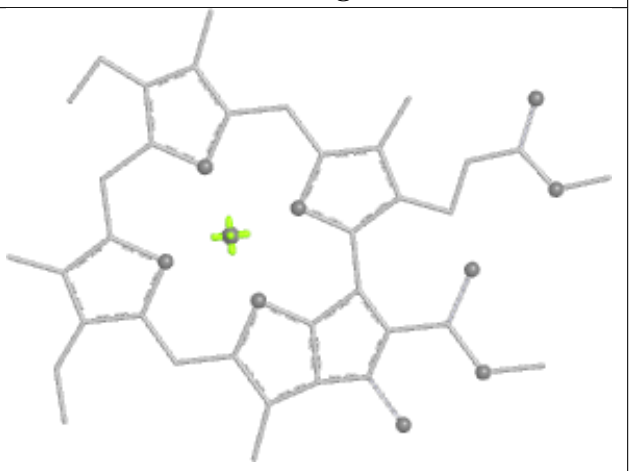
Bond lengths



Bond angles

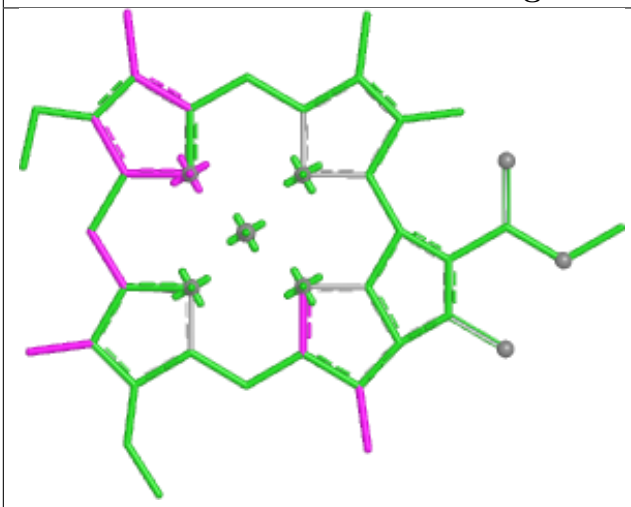


Torsions

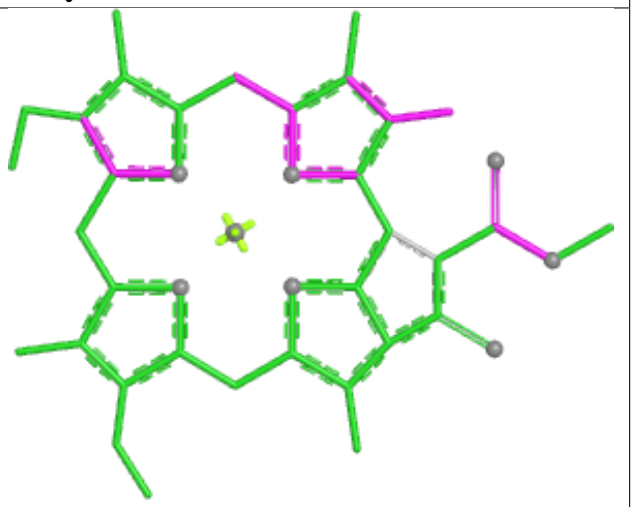


Rings

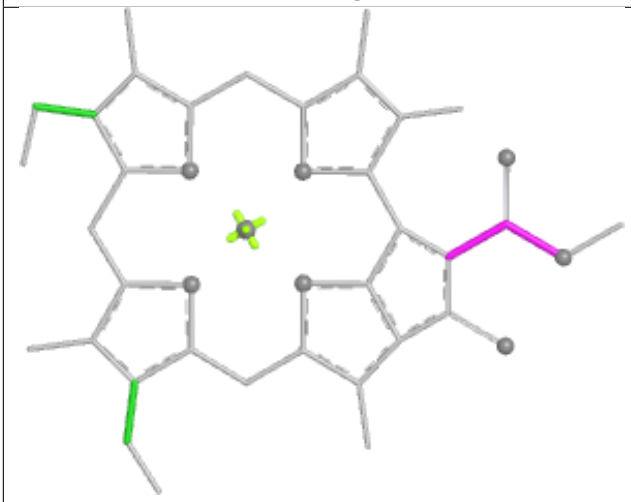
Ligand CLA Q 315



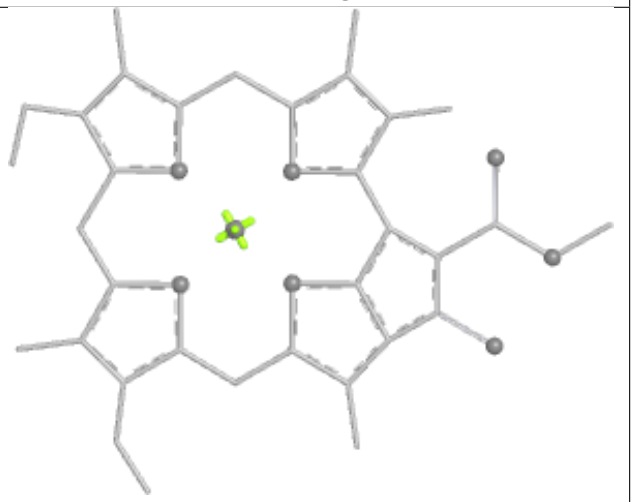
Bond lengths



Bond angles

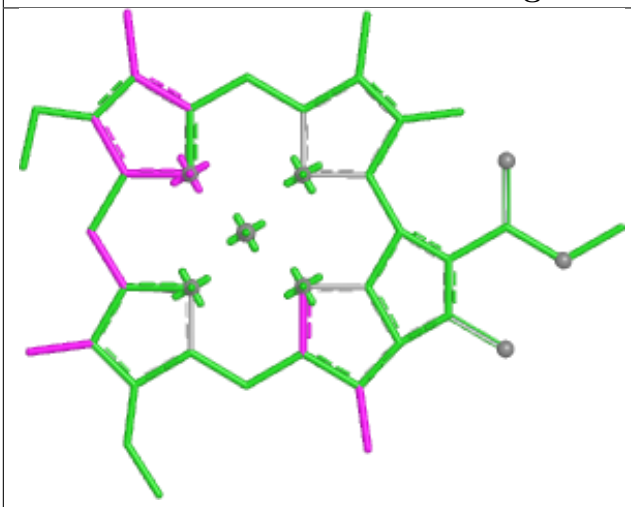


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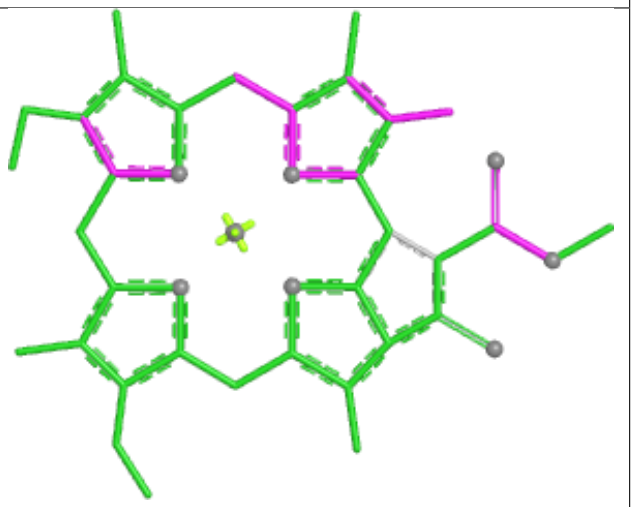


Rings

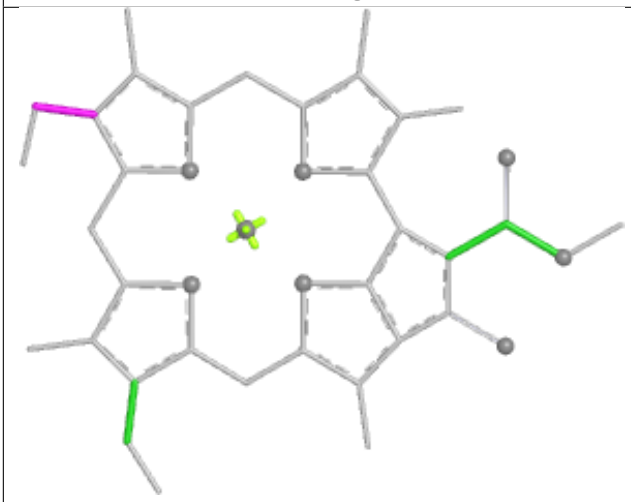
Ligand CLA A 216



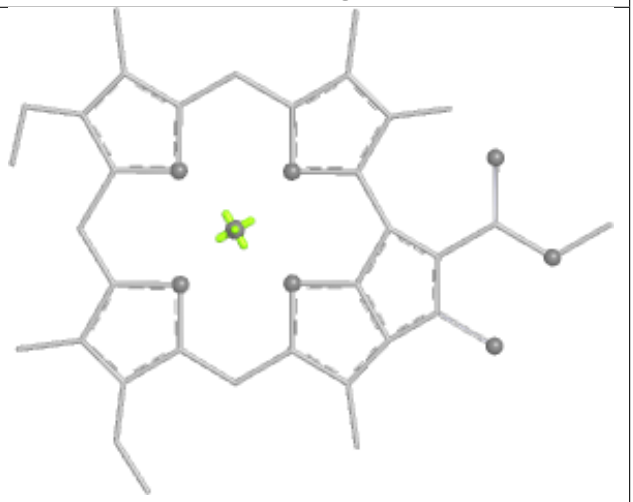
Bond lengths



Bond angles

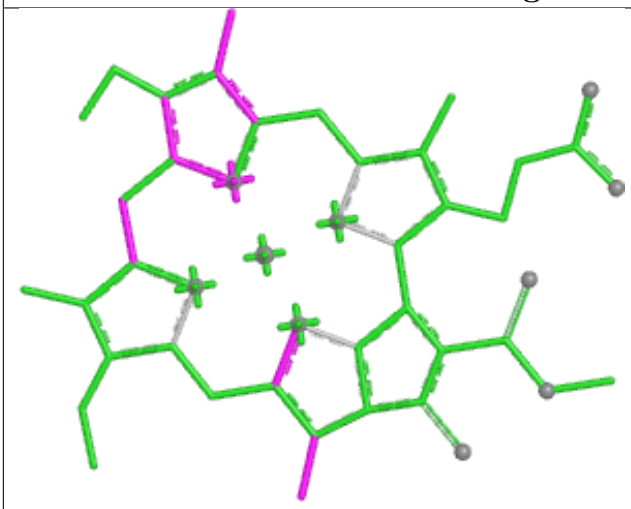


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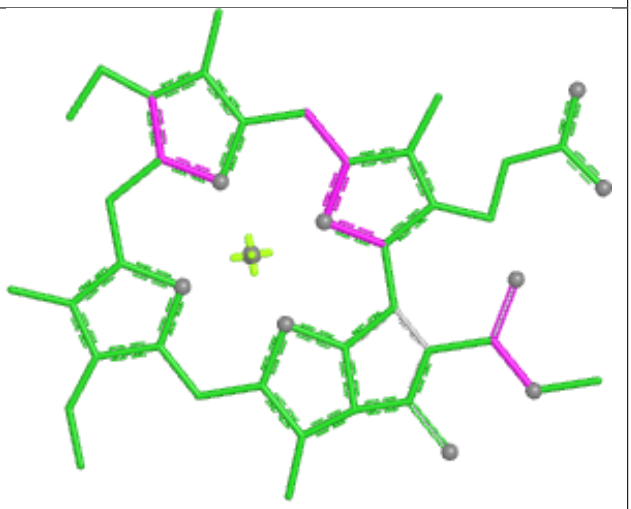


Rings

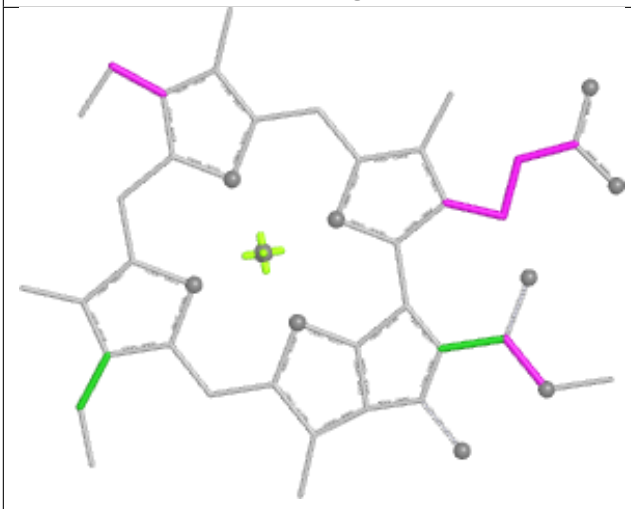
Ligand CLA K 218



Bond lengths



Bond angles

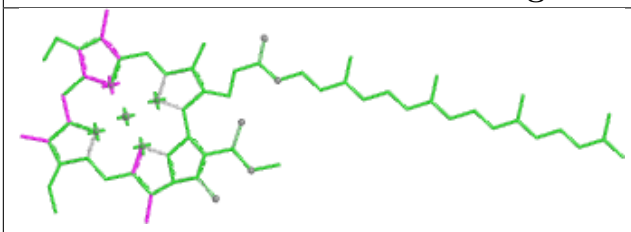


Torsions

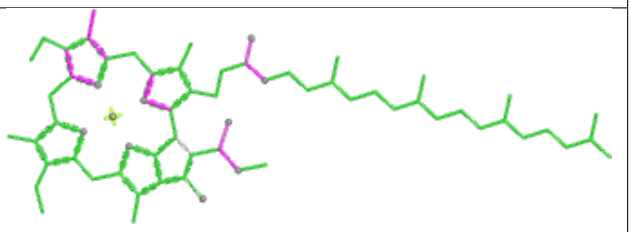


Rings

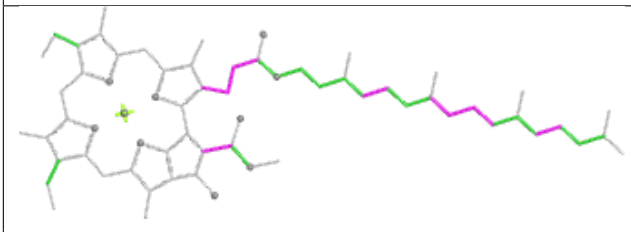
Ligand CLA b 703



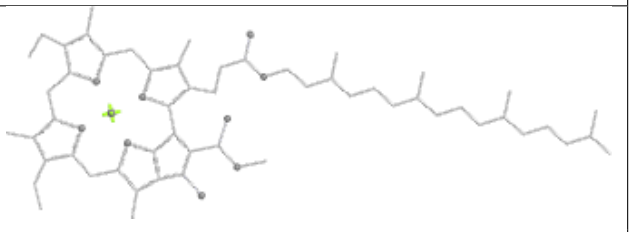
Bond lengths



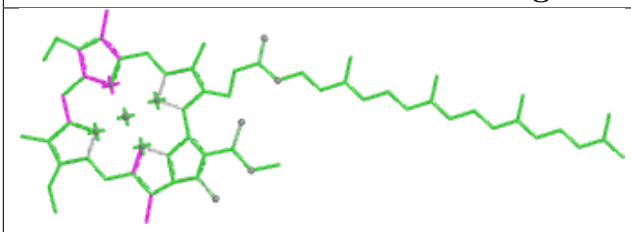
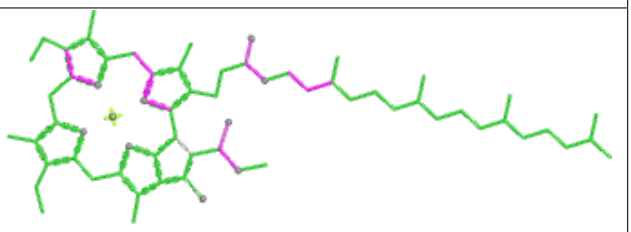
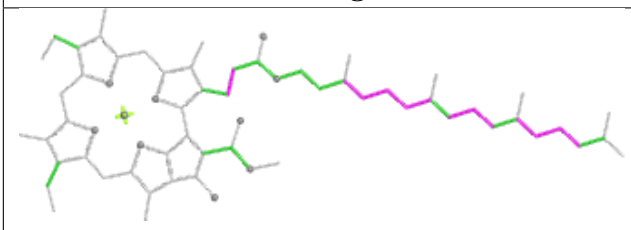
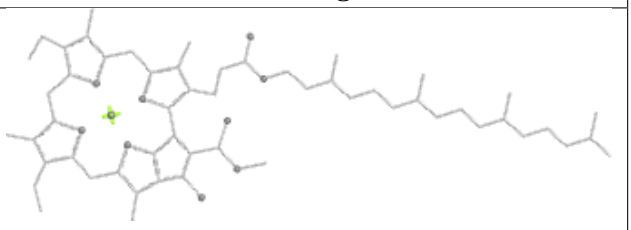
Bond angles

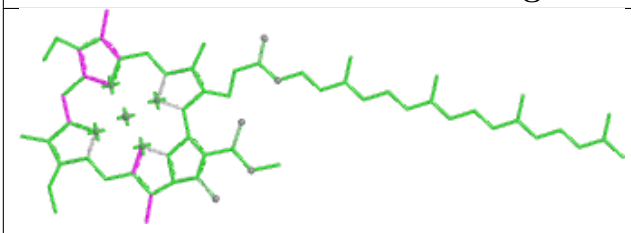
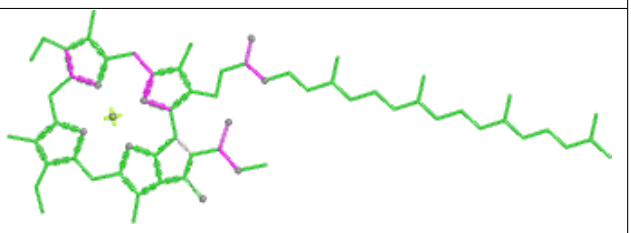
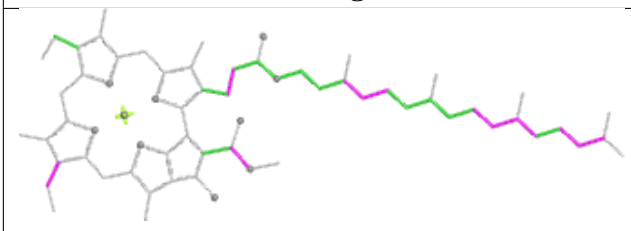
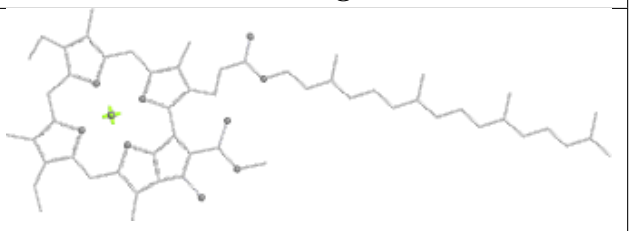


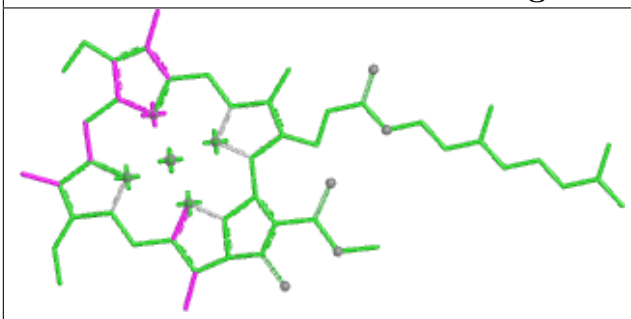
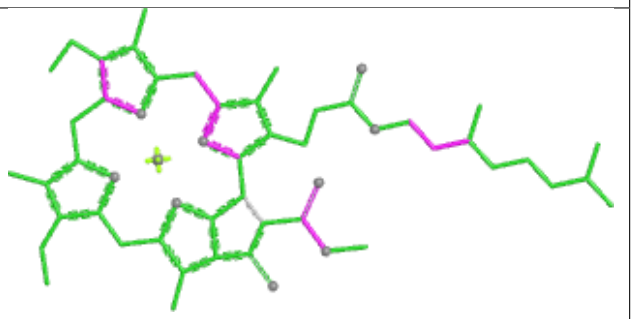
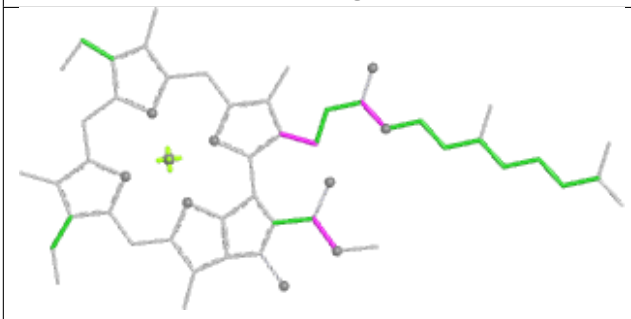
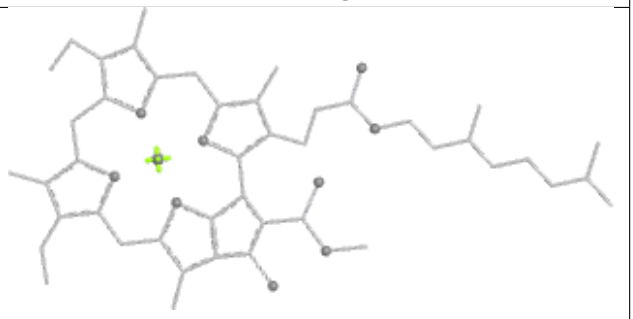
Torsions

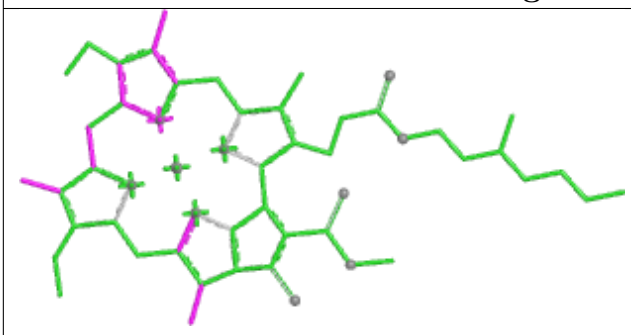
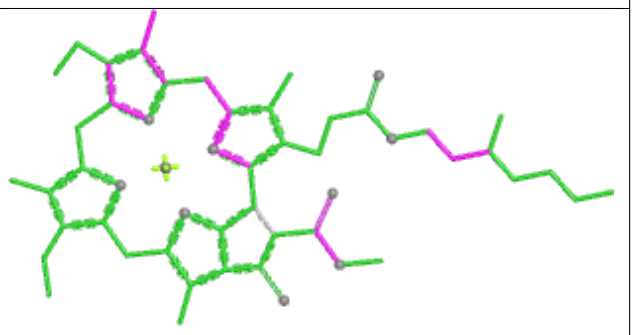
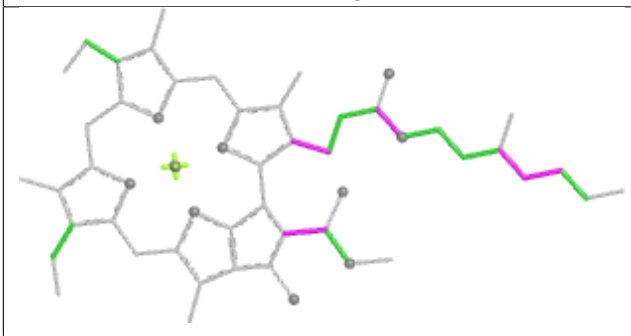
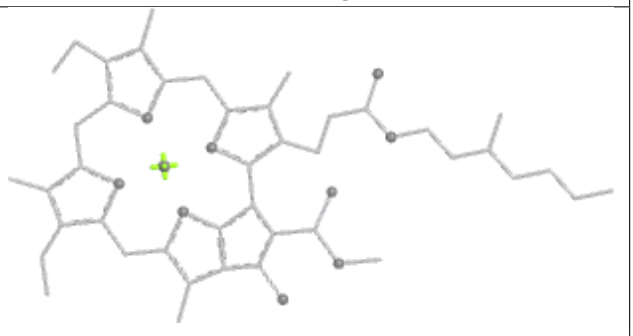


Rings

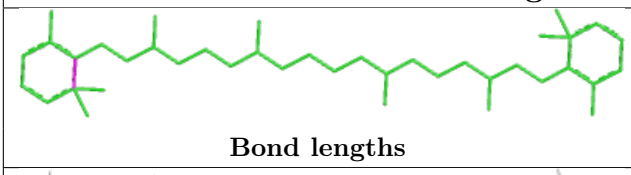
Ligand CLA i 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

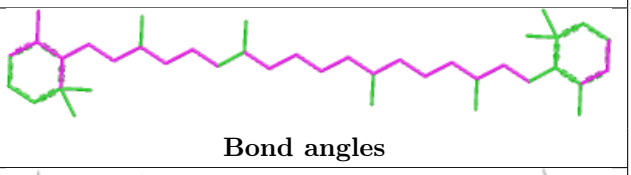
Ligand CLA a 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

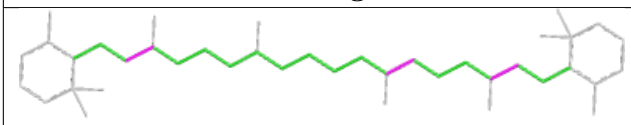
Ligand BCR b 728



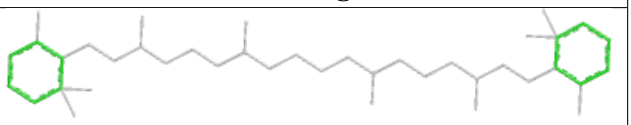
Bond lengths



Bond angles

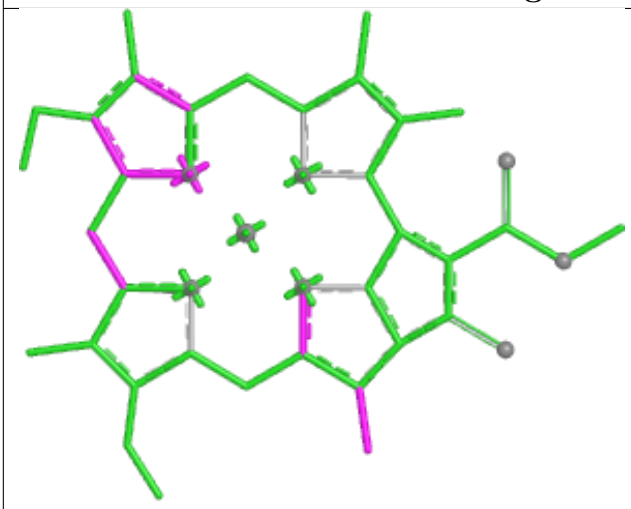


Torsions

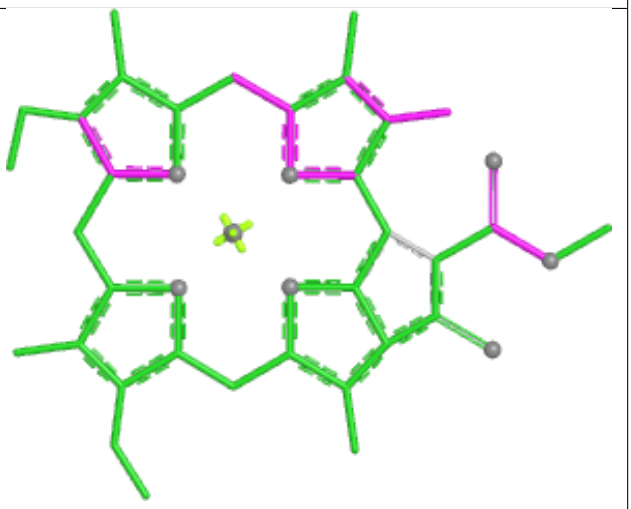


Rings

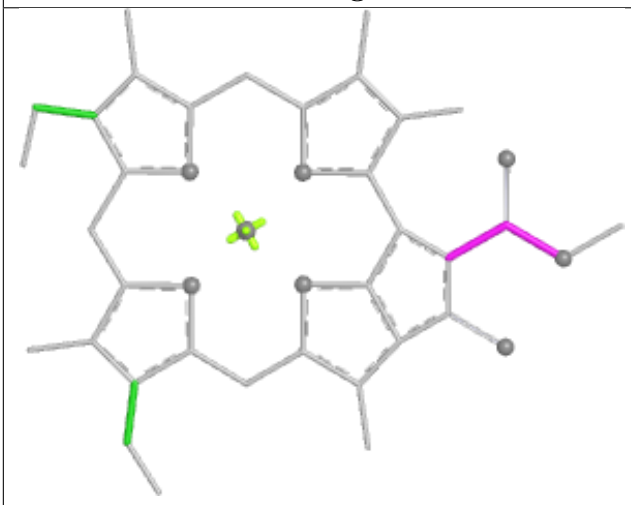
Ligand CLA T 316



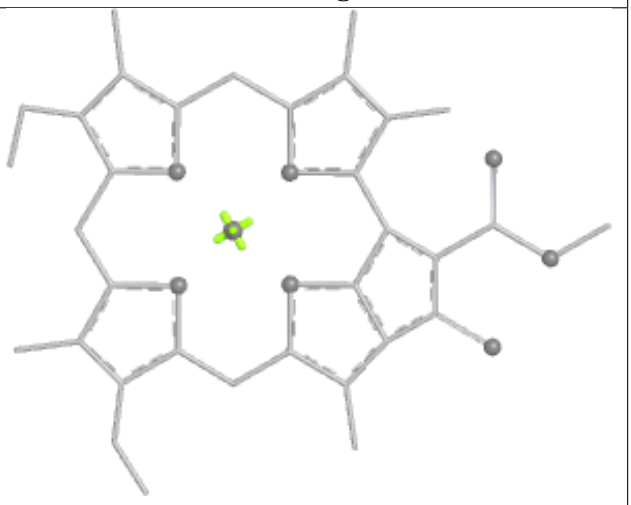
Bond lengths



Bond angles

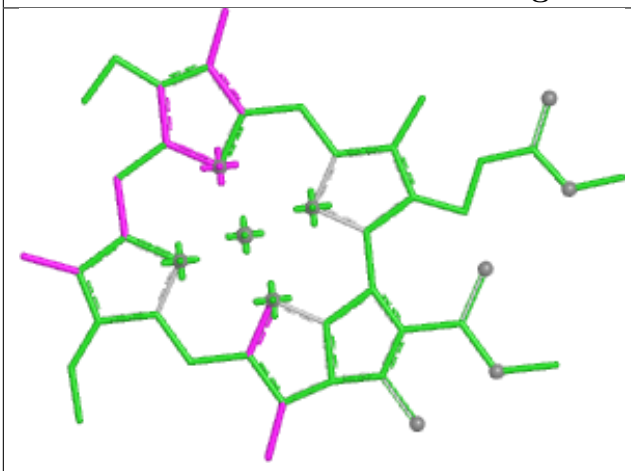


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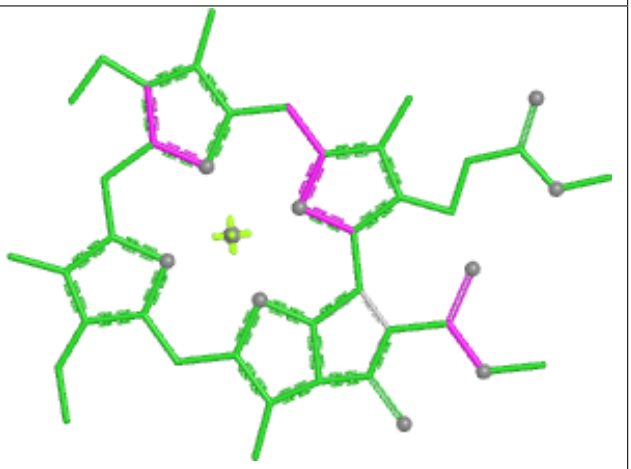


Rings

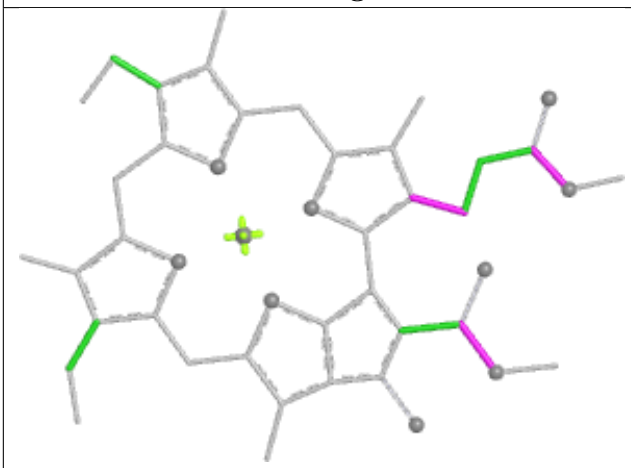
Ligand CLA f 803



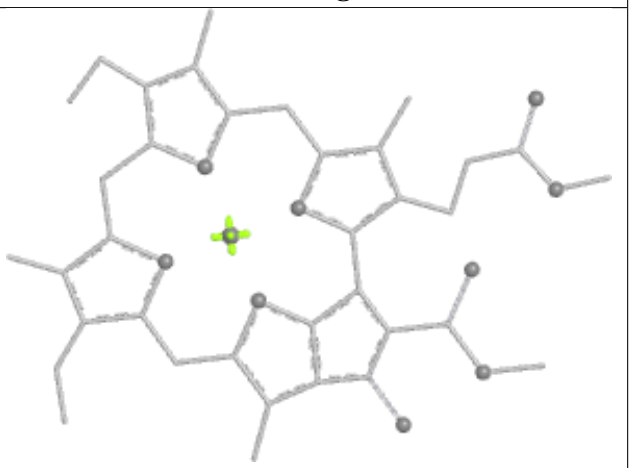
Bond lengths



Bond angles



Torsions

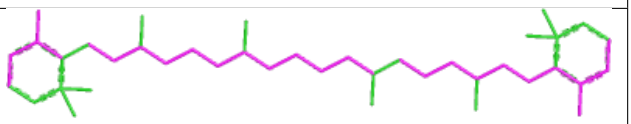


Rings

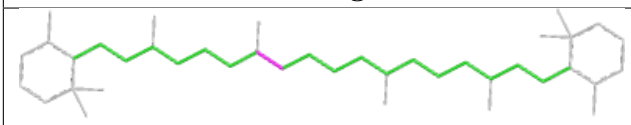
Ligand BCR f 804



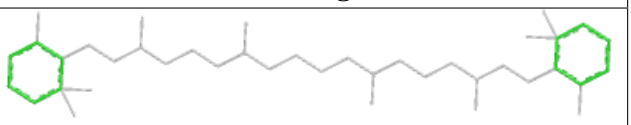
Bond lengths



Bond angles

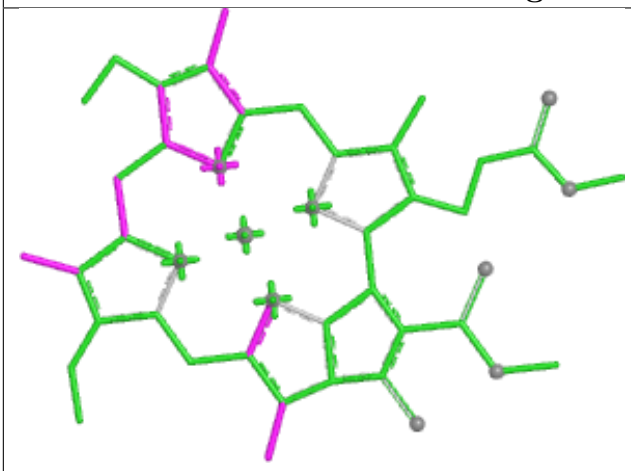


Torsions

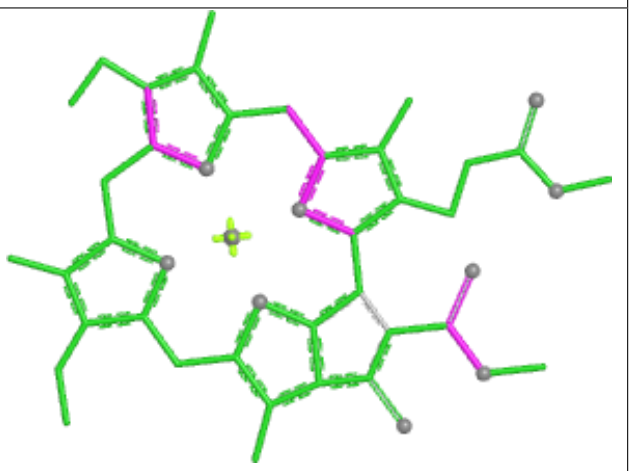


Rings

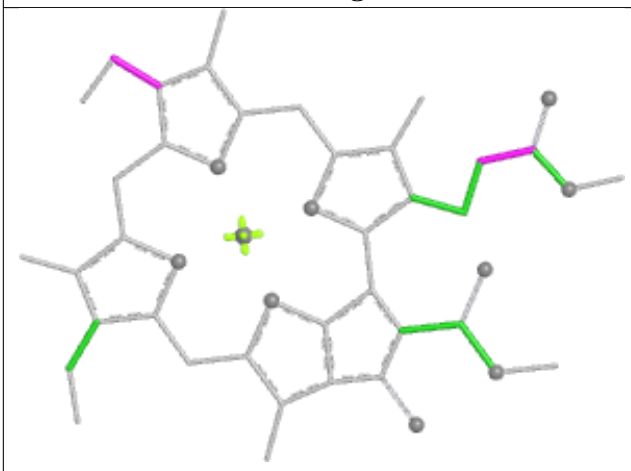
Ligand CLA F 311



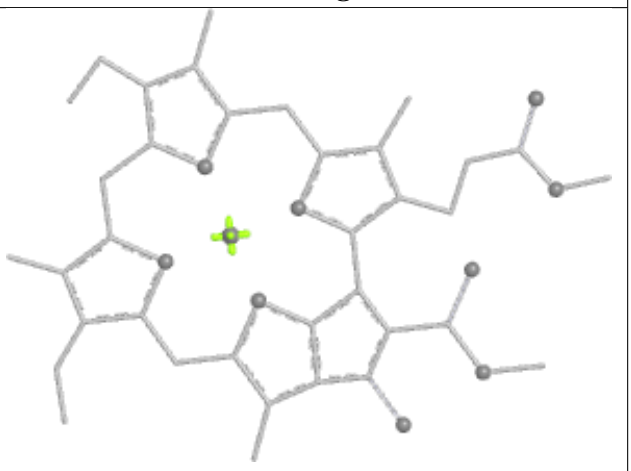
Bond lengths



Bond angles

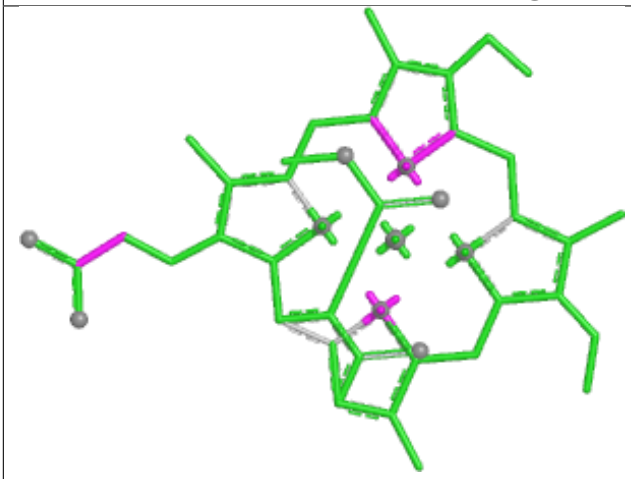


Torsions

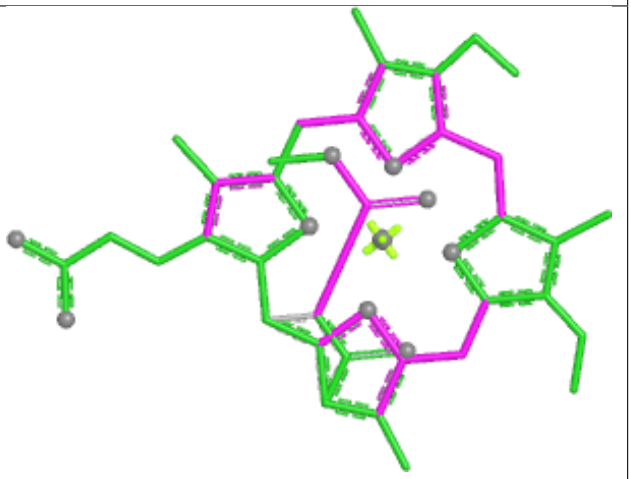


Rings

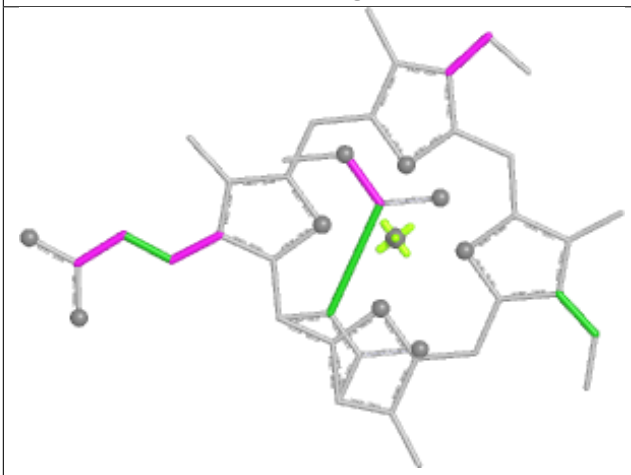
Ligand KC1 C 315



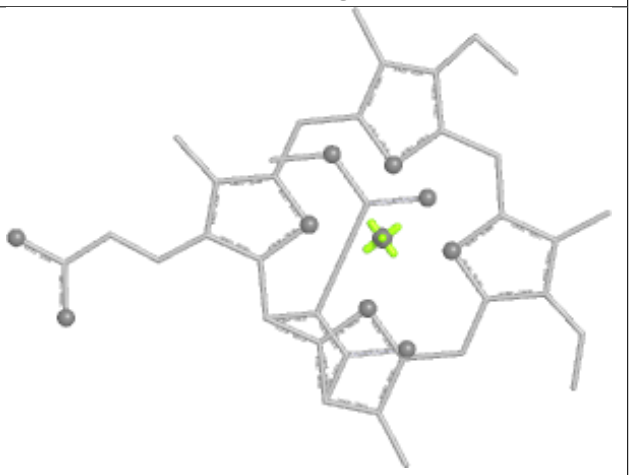
Bond lengths



Bond angles

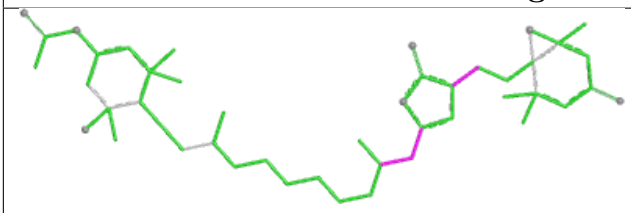


Torsions

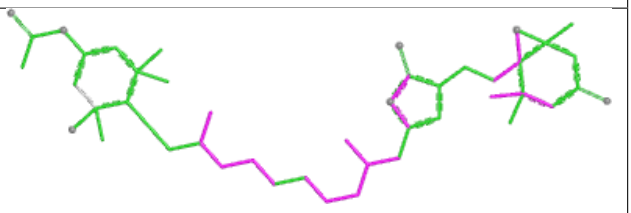


Rings

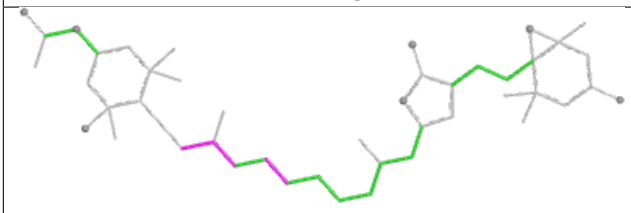
Ligand PID D 305



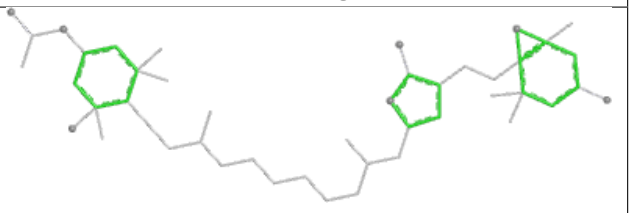
Bond lengths



Bond angles

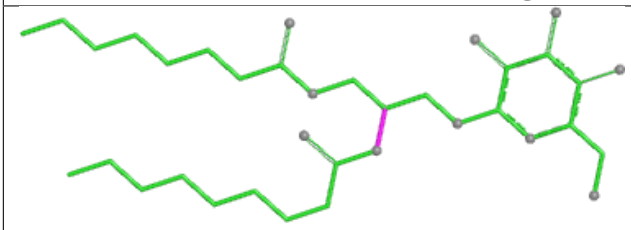


Torsions

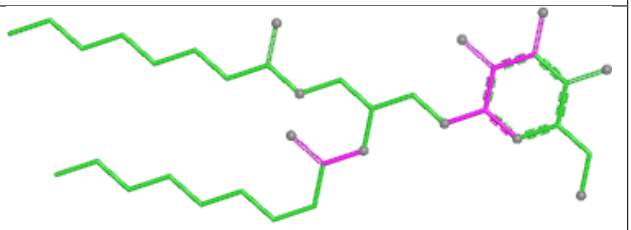


Rings

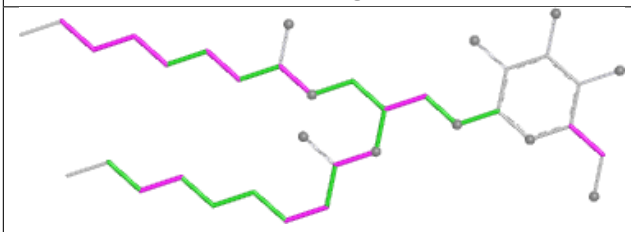
Ligand LMG K 220



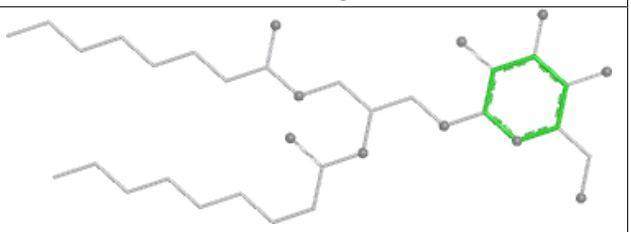
Bond lengths



Bond angles

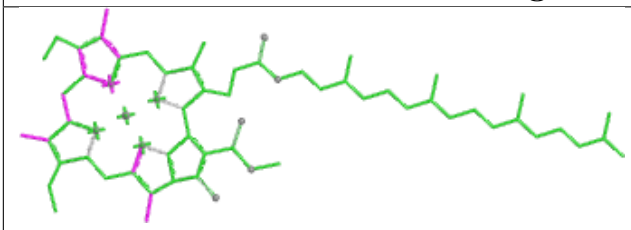


Torsions

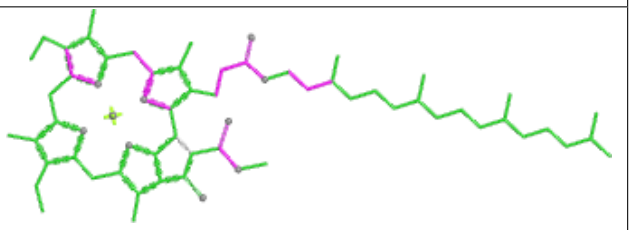


Rings

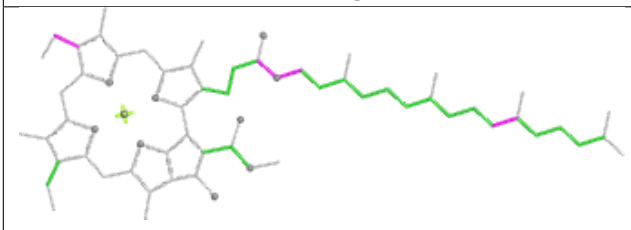
Ligand CLA a 822



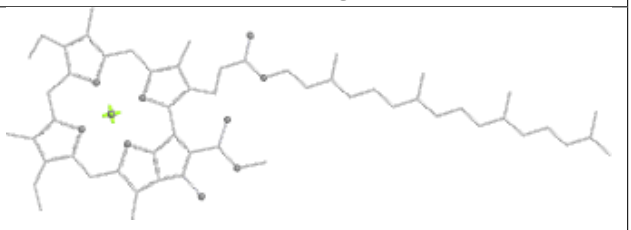
Bond lengths



Bond angles



Torsions



Rings

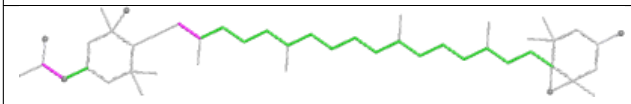
Ligand UIX Q 305



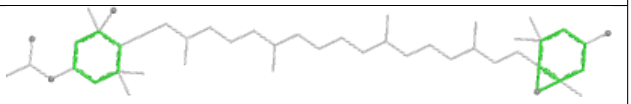
Bond lengths



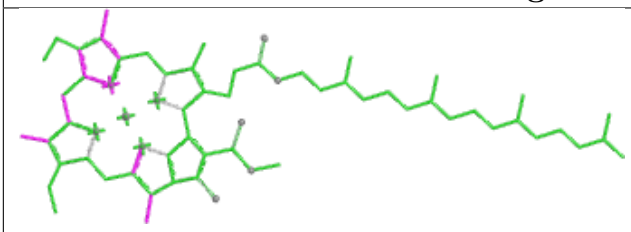
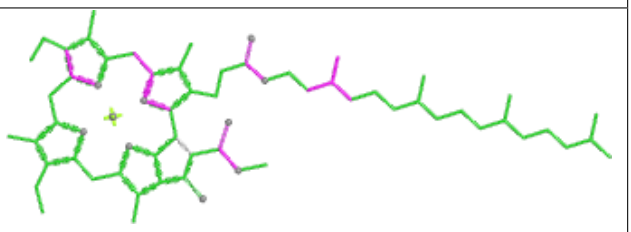
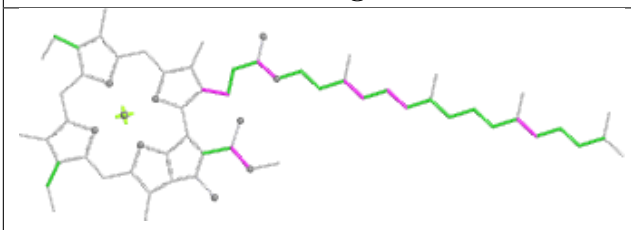
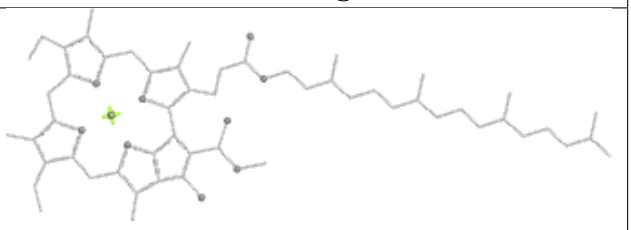
Bond angles

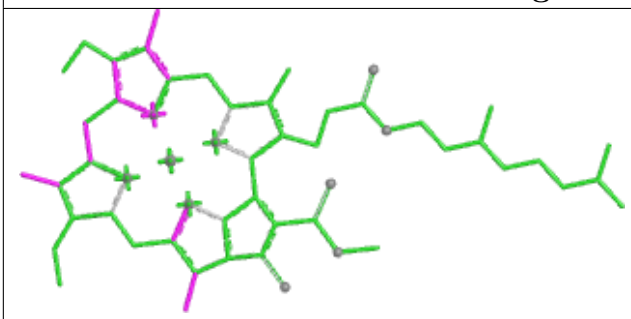
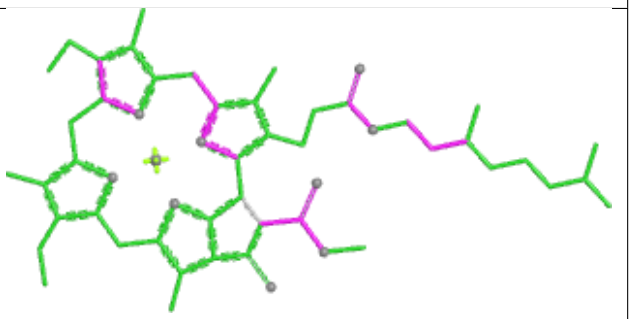
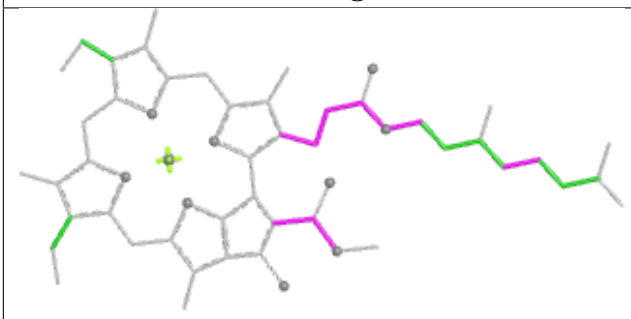
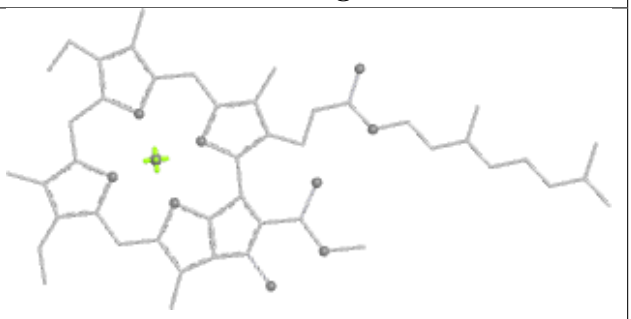


Torsions

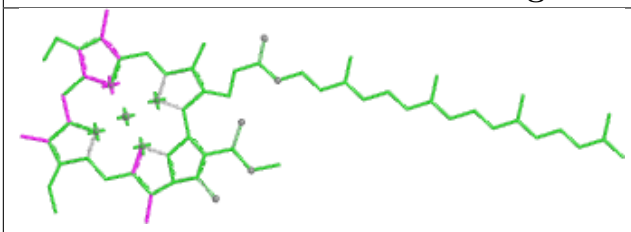


Rings

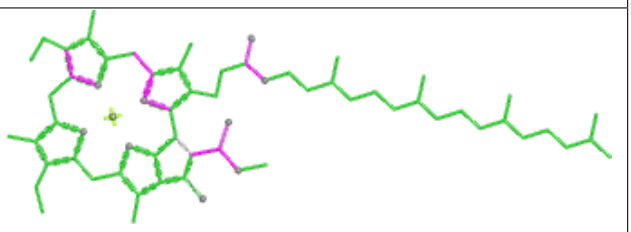
Ligand CLA b 712	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA i 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

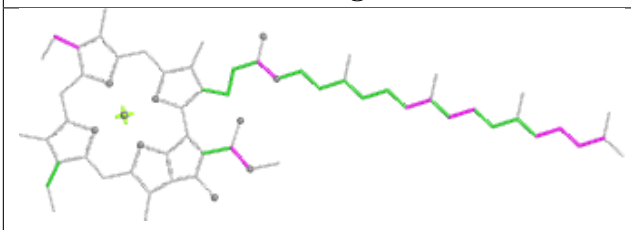
Ligand CLA b 707



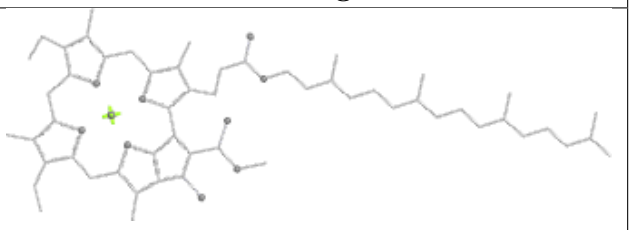
Bond lengths



Bond angles

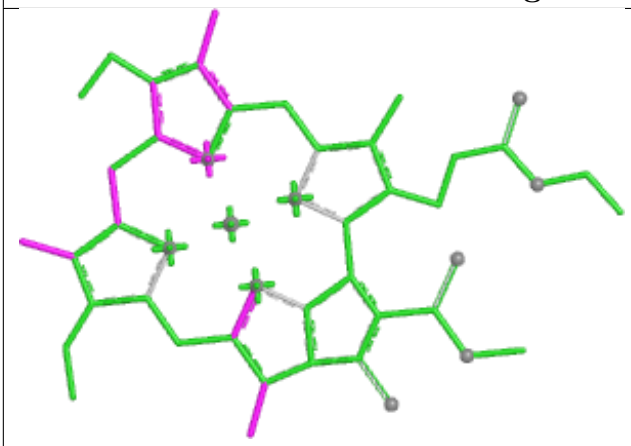


Torsions

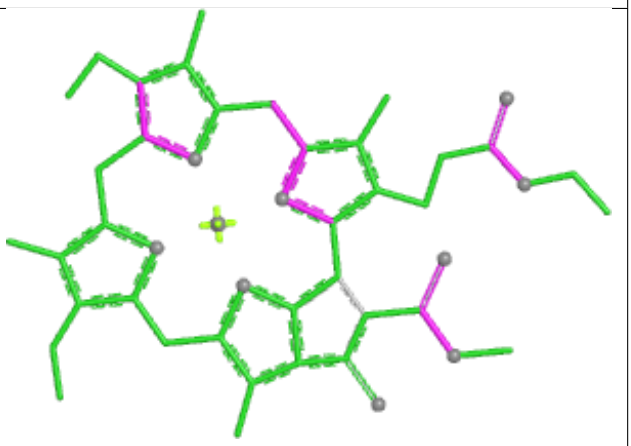


Rings

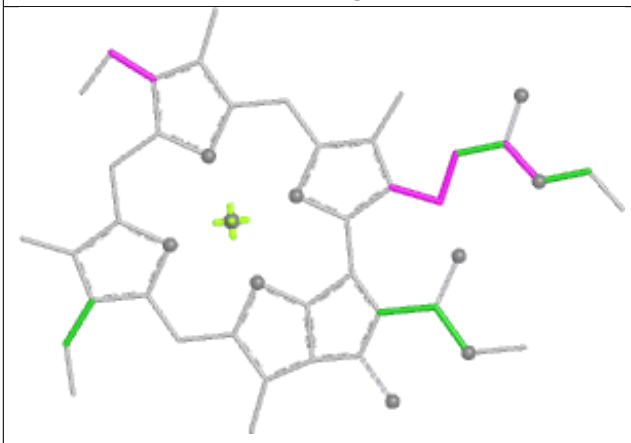
Ligand CLA A 215



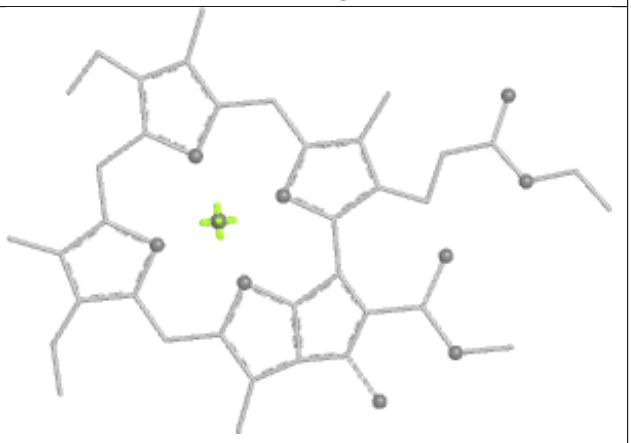
Bond lengths



Bond angles

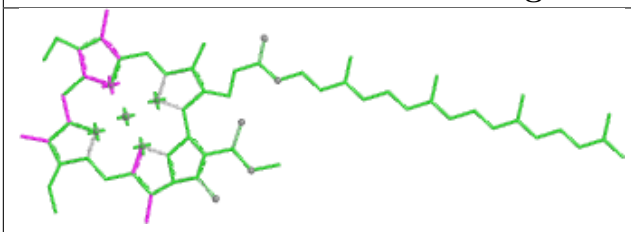


Torsions

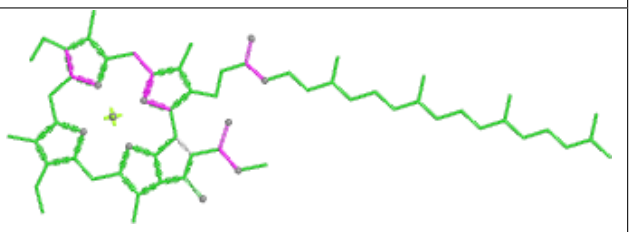


Rings

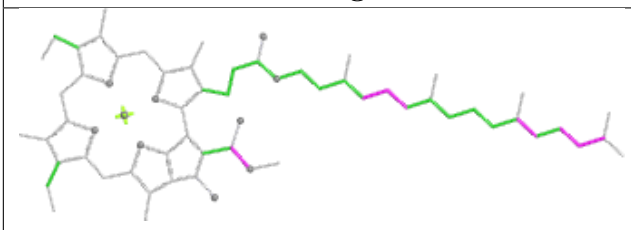
Ligand CLA P 210



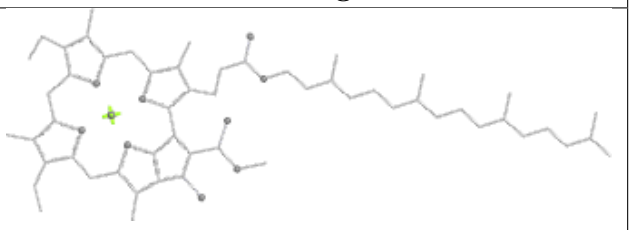
Bond lengths



Bond angles



Torsions

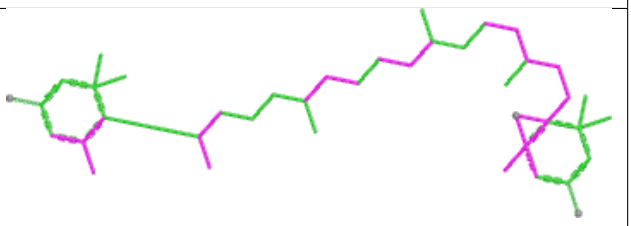


Rings

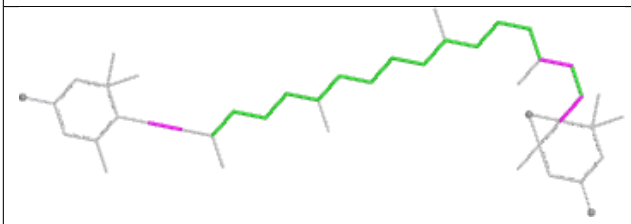
Ligand DD6 L 301



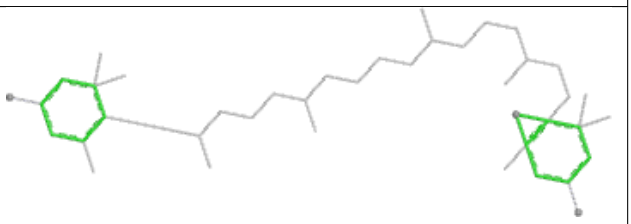
Bond lengths



Bond angles

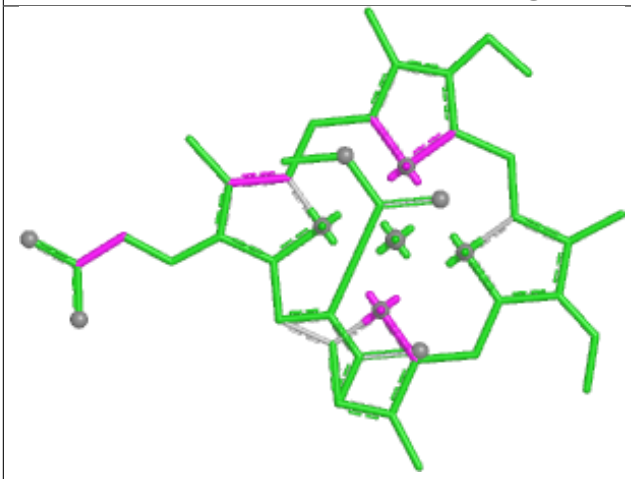


Torsions

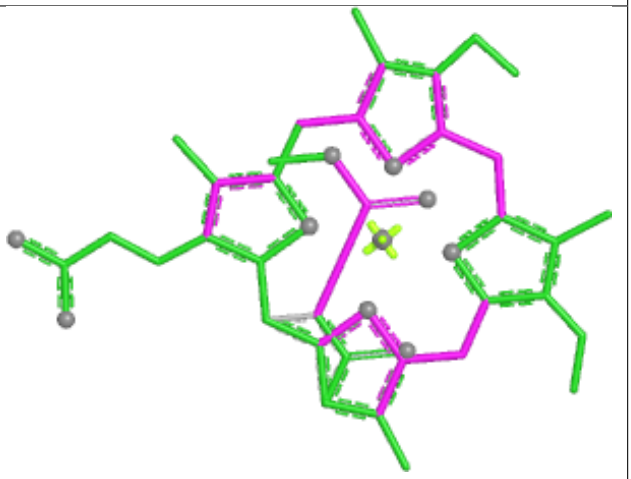


Rings

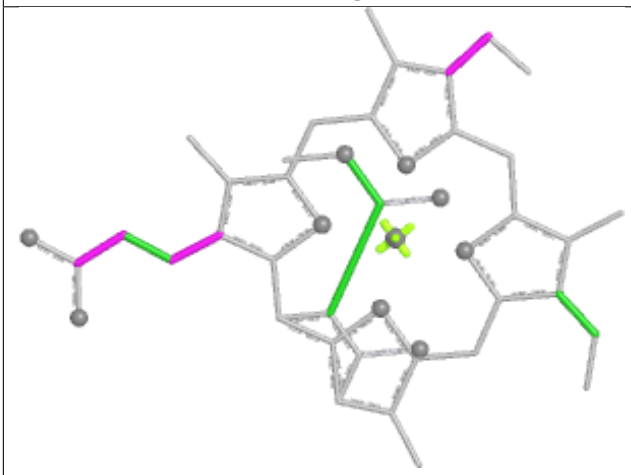
Ligand KC1 G 315



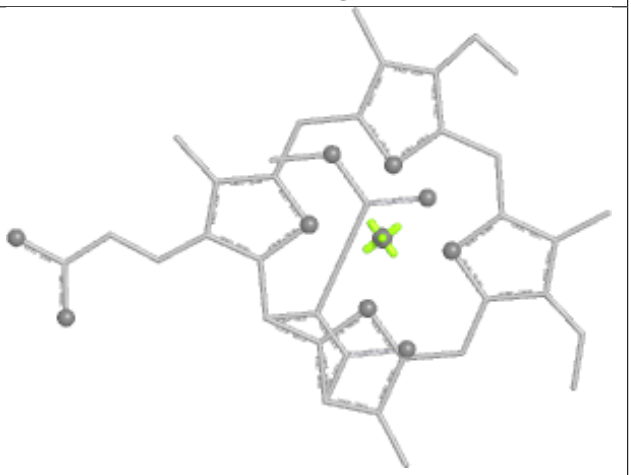
Bond lengths



Bond angles

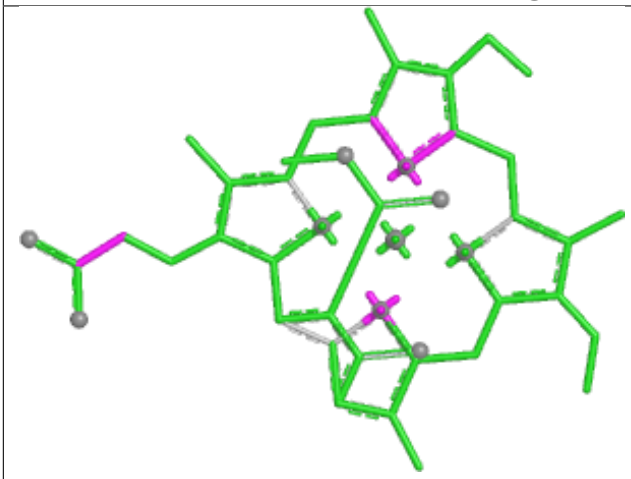


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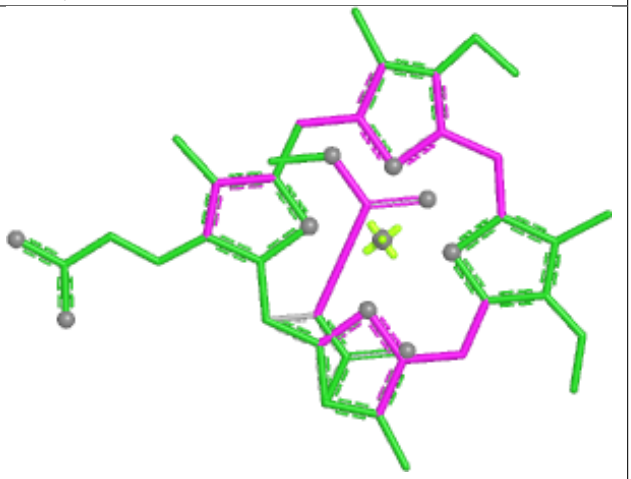


Rings

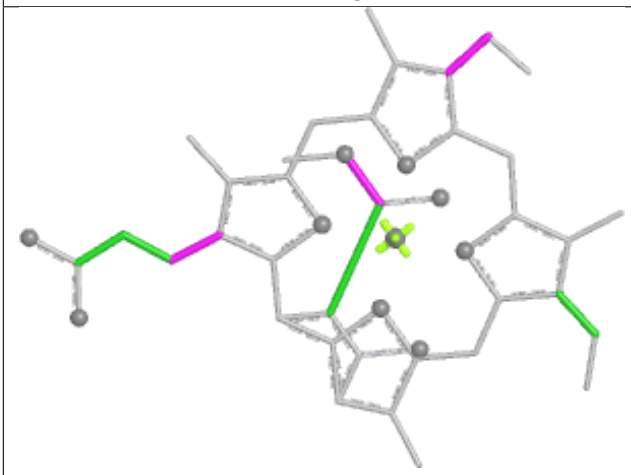
Ligand KC1 Q 309



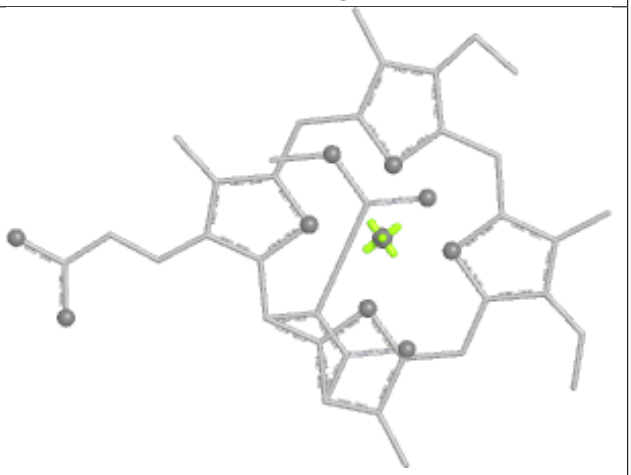
Bond lengths



Bond angles

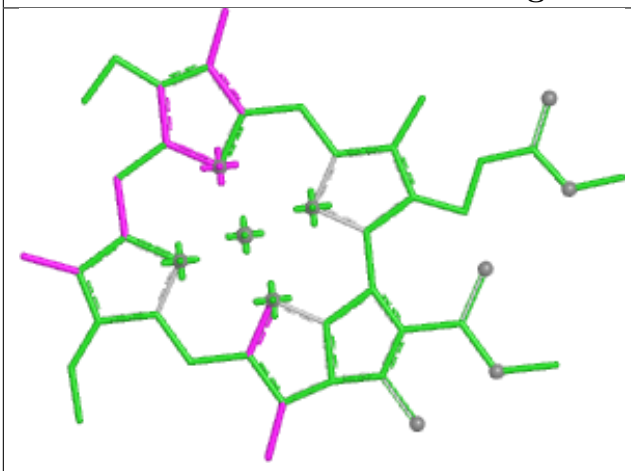


Torsions

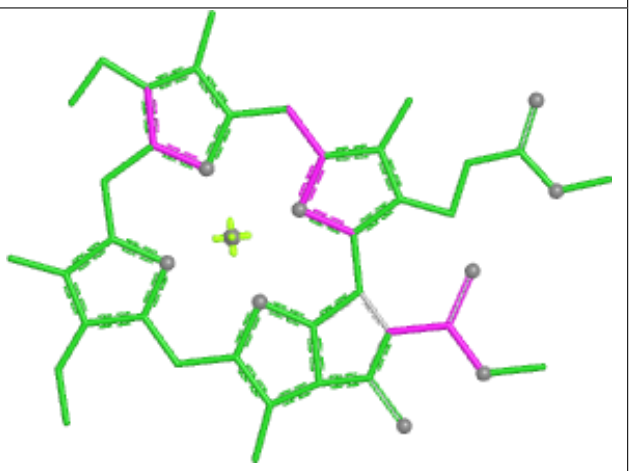


Rings

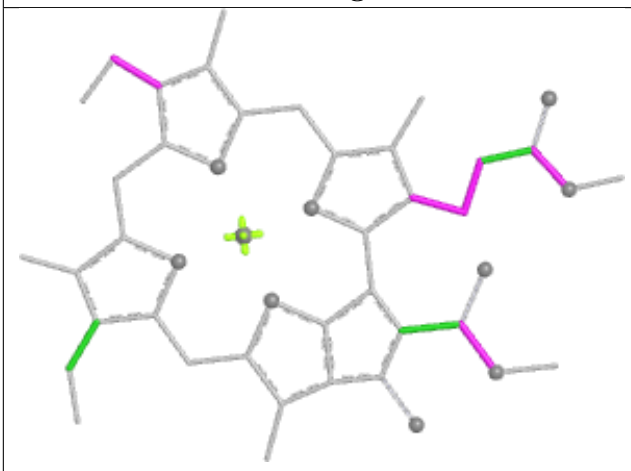
Ligand CLA b 715



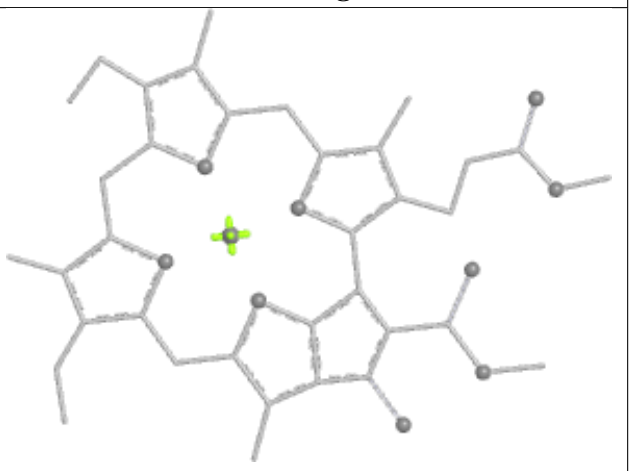
Bond lengths



Bond angles

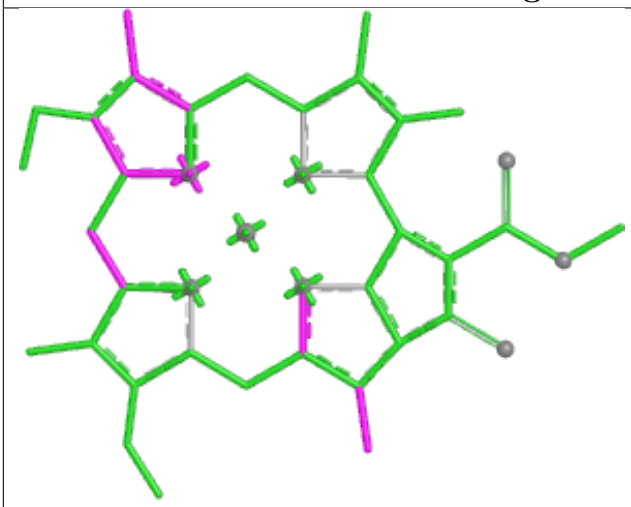


Torsions

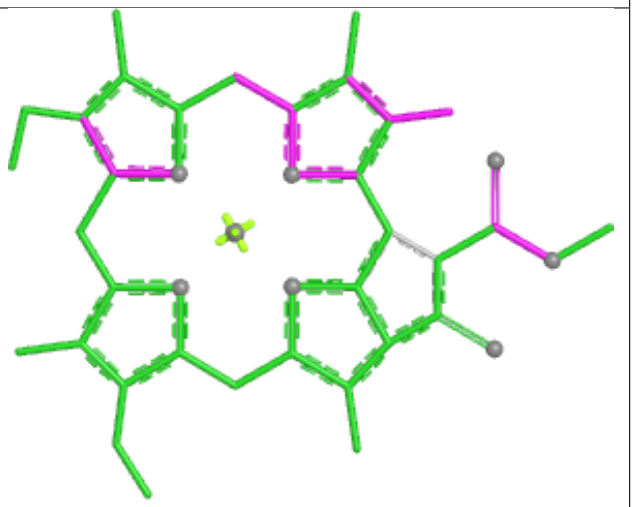


Rings

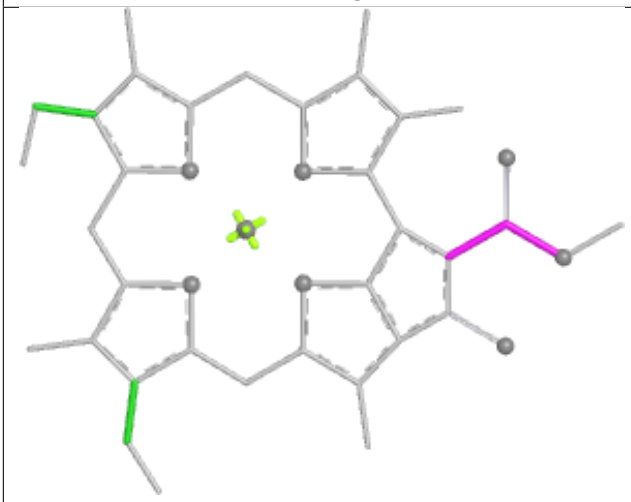
Ligand CLA N 316



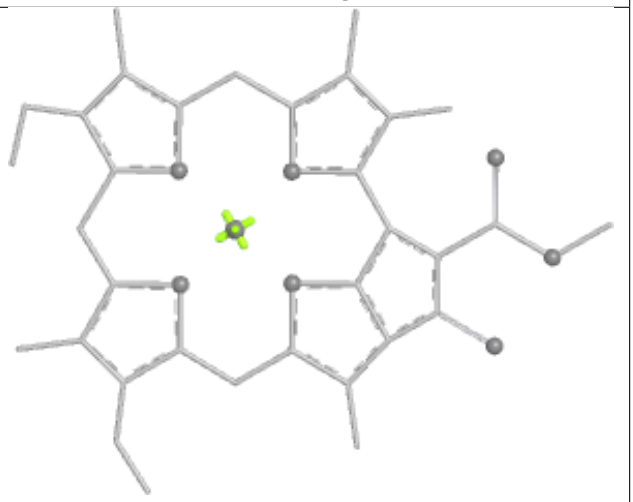
Bond lengths



Bond angles

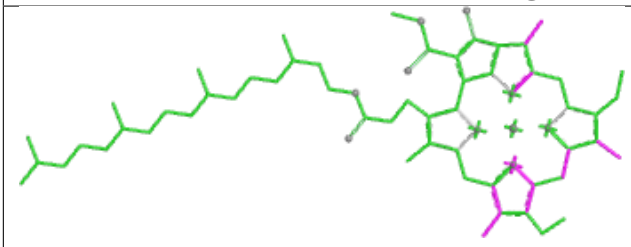


Torsions

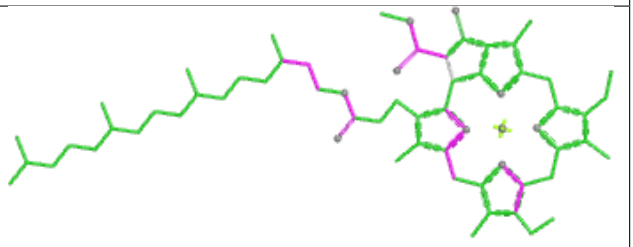


Rings

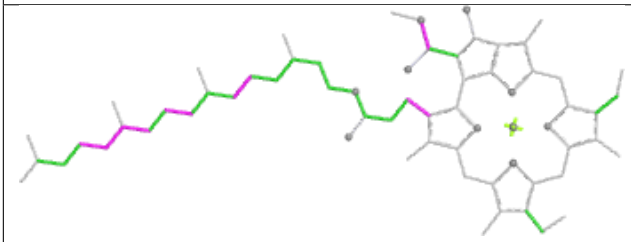
Ligand CLA G 316



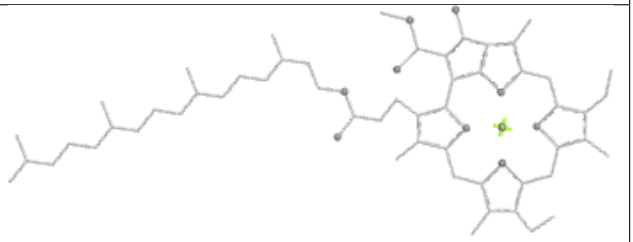
Bond lengths



Bond angles

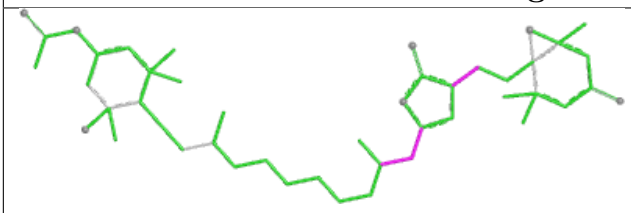


Torsions

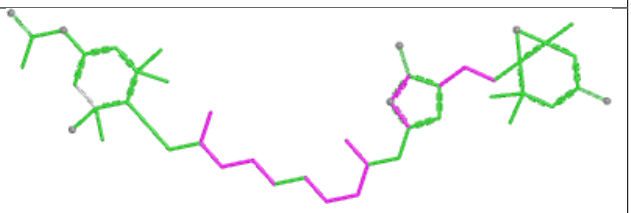


Rings

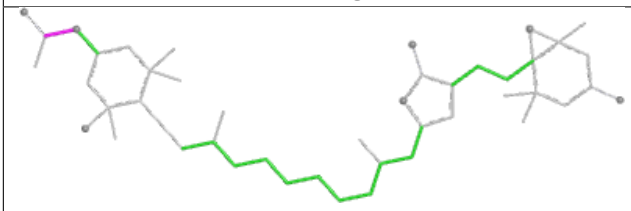
Ligand PID H 301



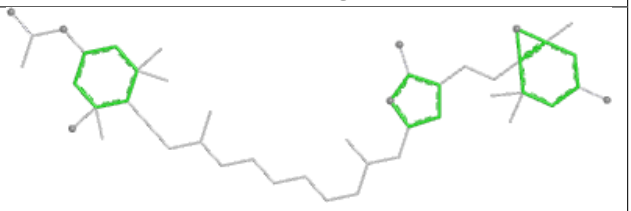
Bond lengths



Bond angles

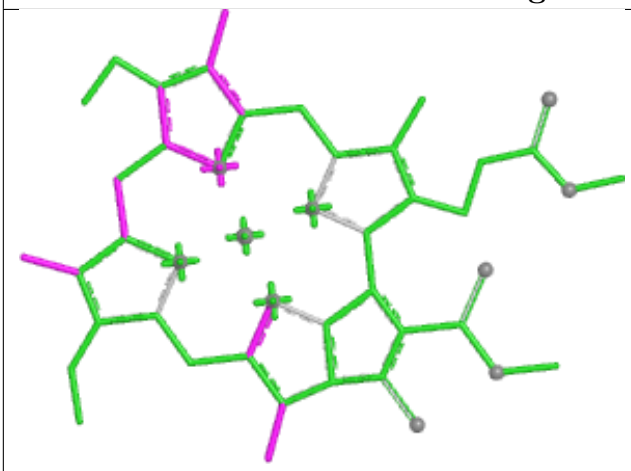


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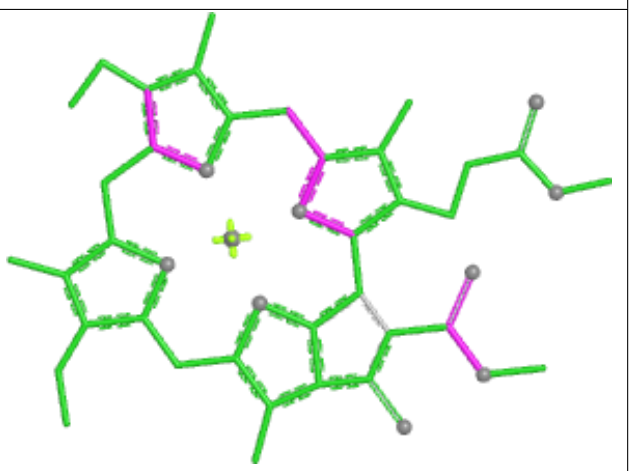


Rings

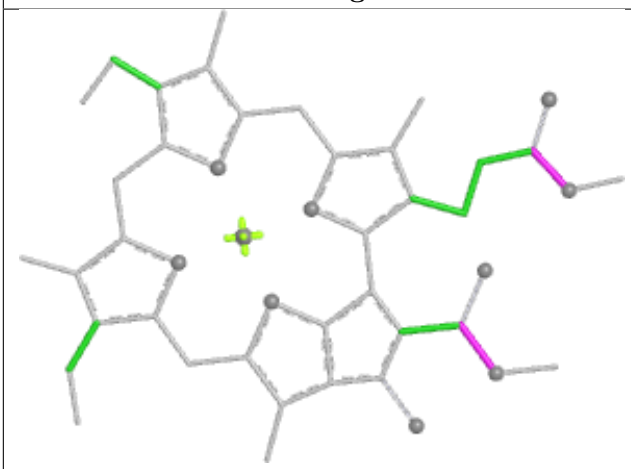
Ligand CLA a 814



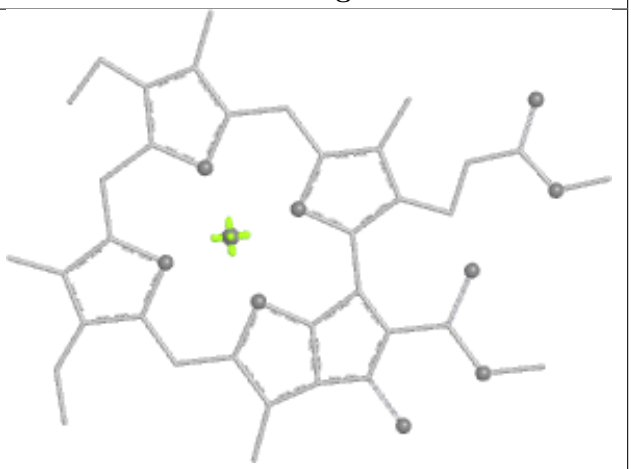
Bond lengths



Bond angles

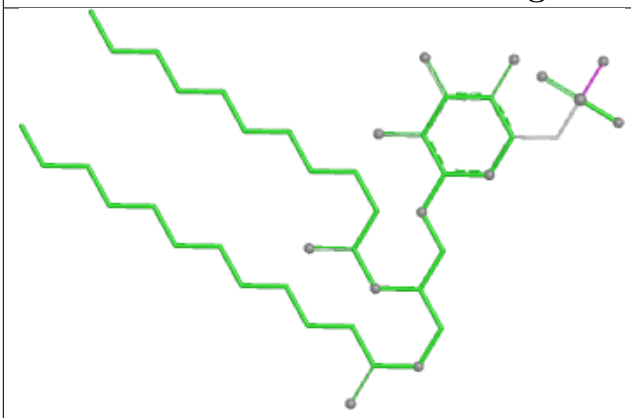


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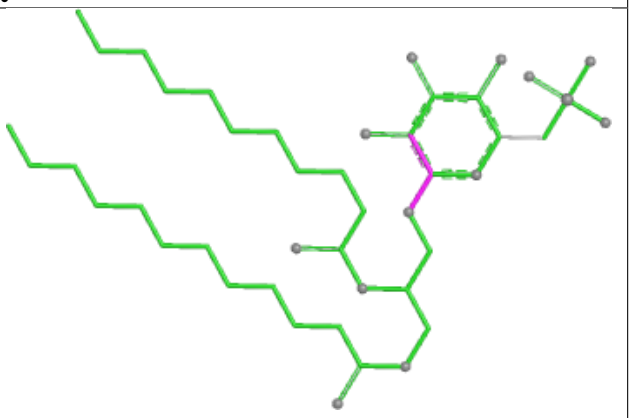


Rings

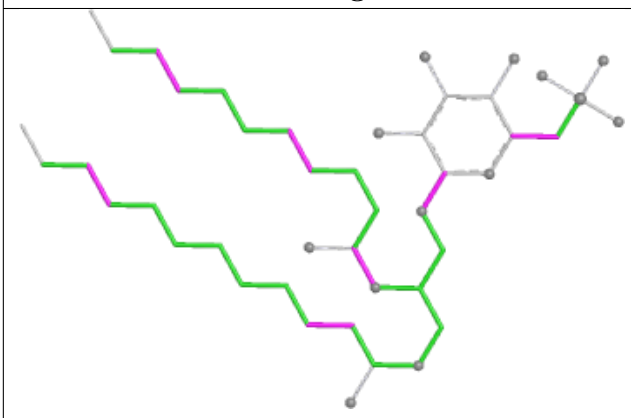
Ligand SQD J 314



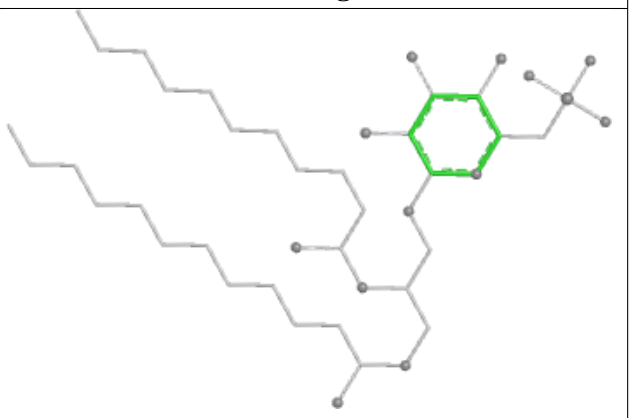
Bond lengths



Bond angles

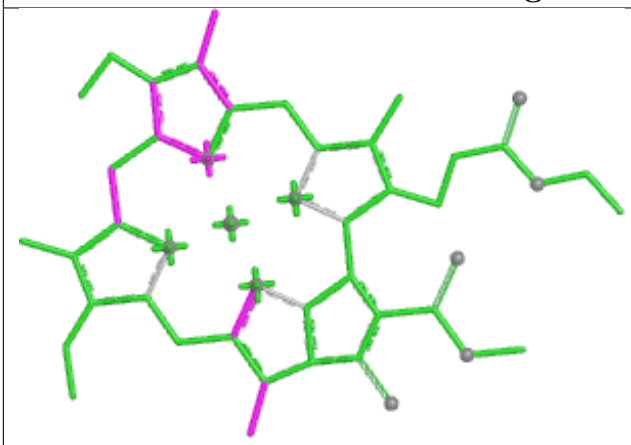


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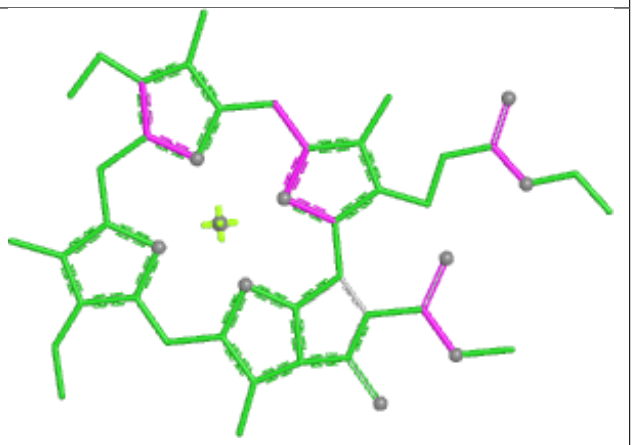


Rings

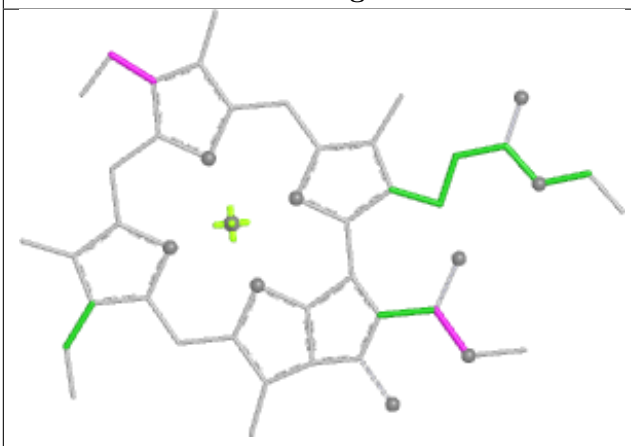
Ligand CLA T 308



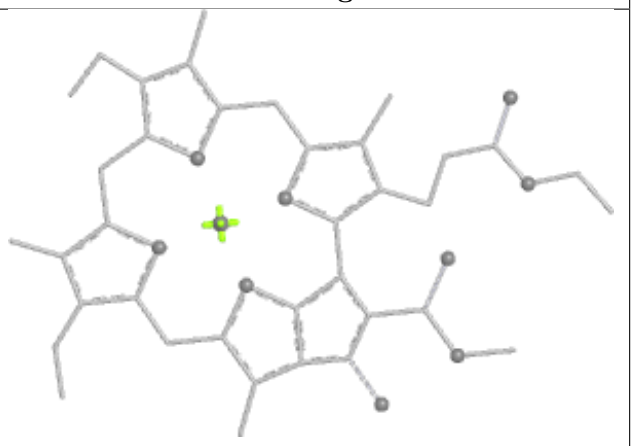
Bond lengths



Bond angles

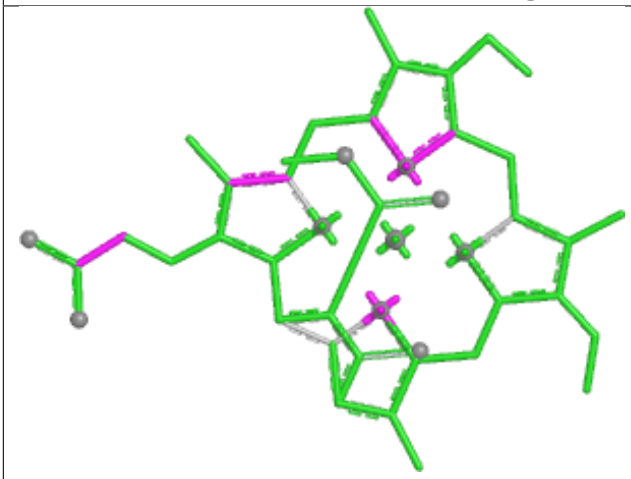


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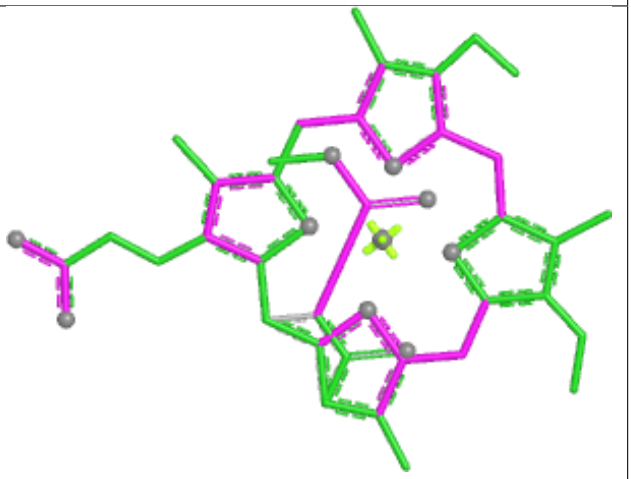


Rings

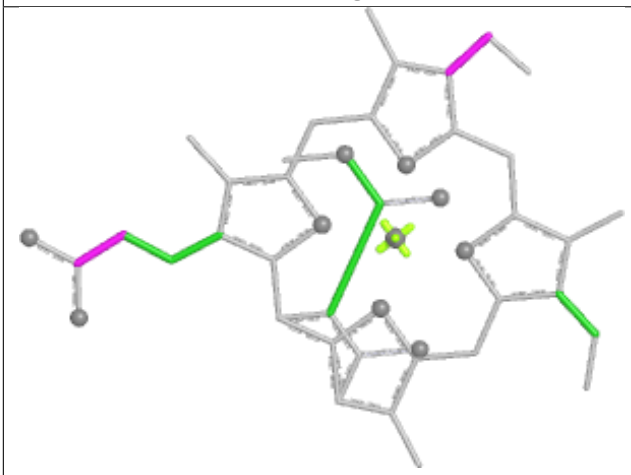
Ligand KC1 M 305



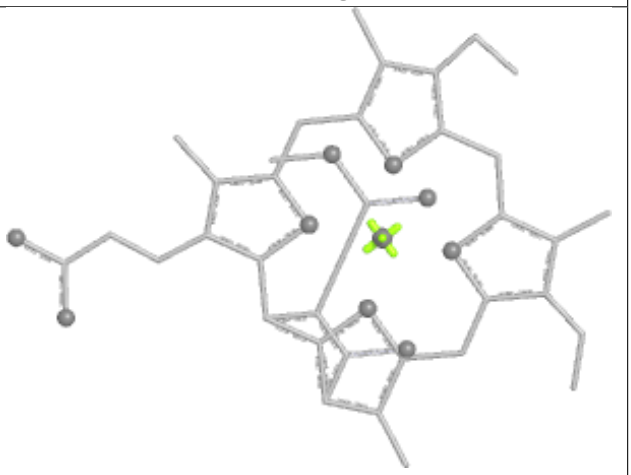
Bond lengths



Bond angles

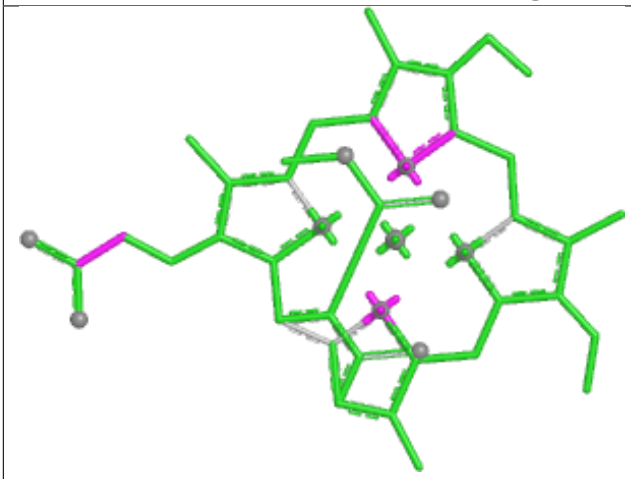


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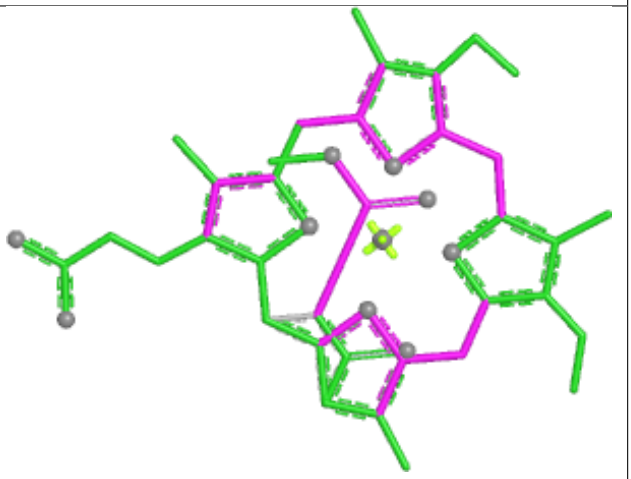


Rings

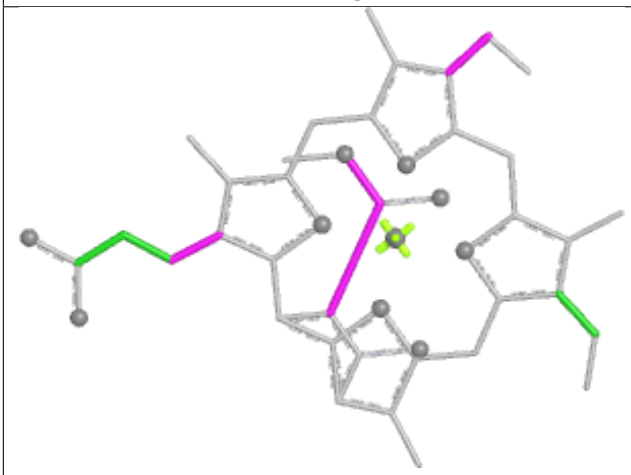
Ligand KC1 P 213



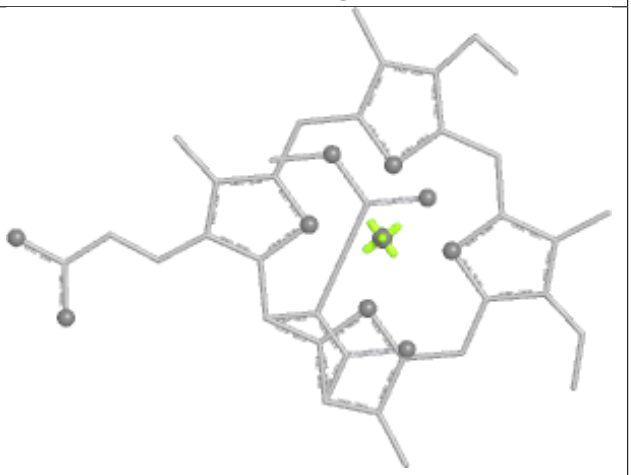
Bond lengths



Bond angles

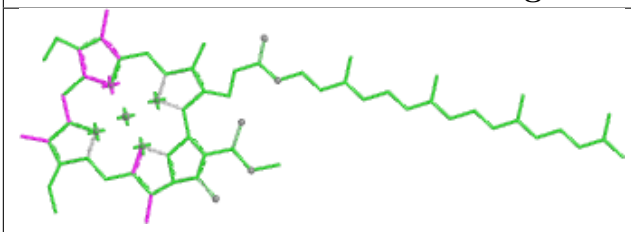


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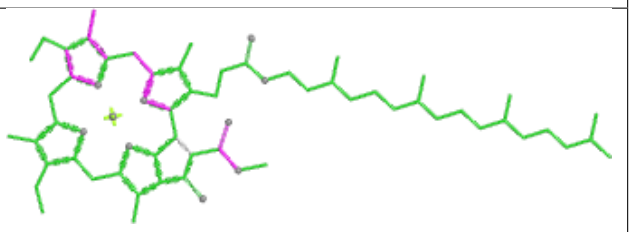


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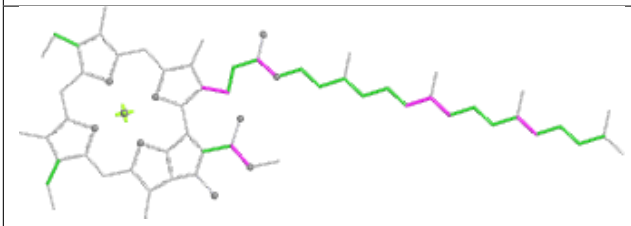
Ligand CLA B 312



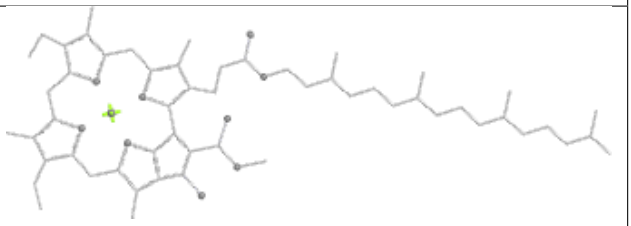
Bond lengths



Bond angles

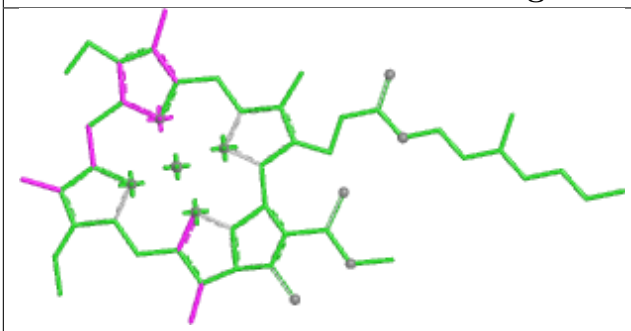


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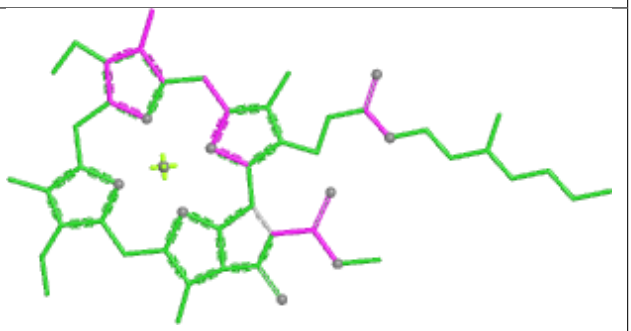


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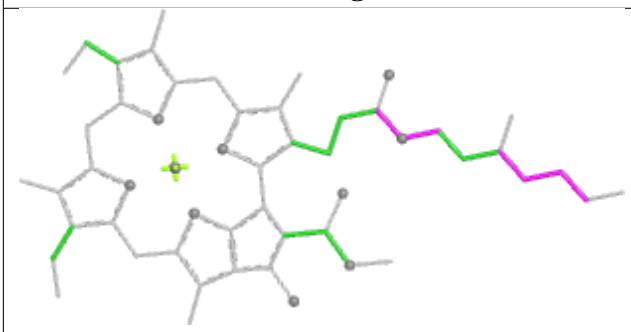
Ligand CLA b 716



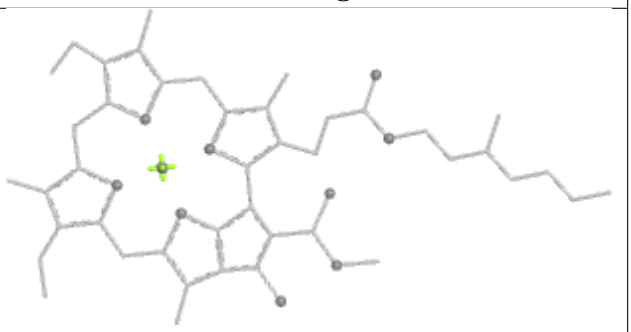
Bond lengths



Bond angles

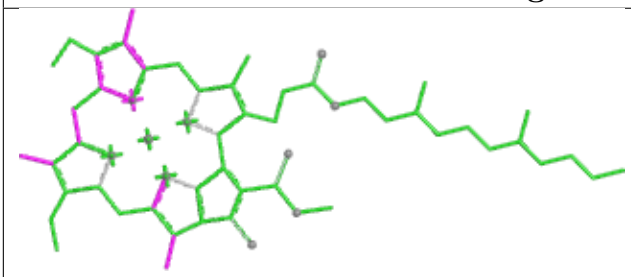


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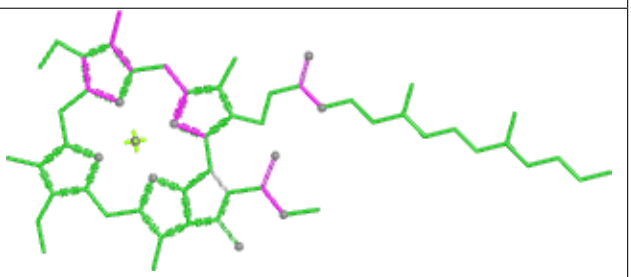


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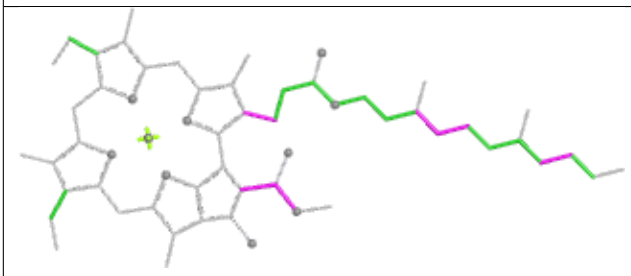
Ligand CLA b 722



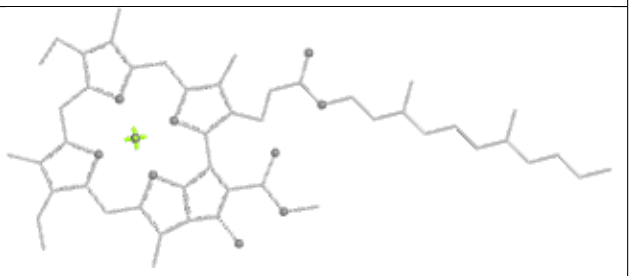
Bond lengths



Bond angles

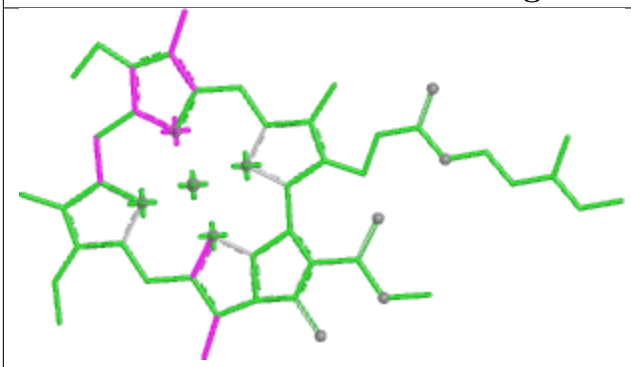


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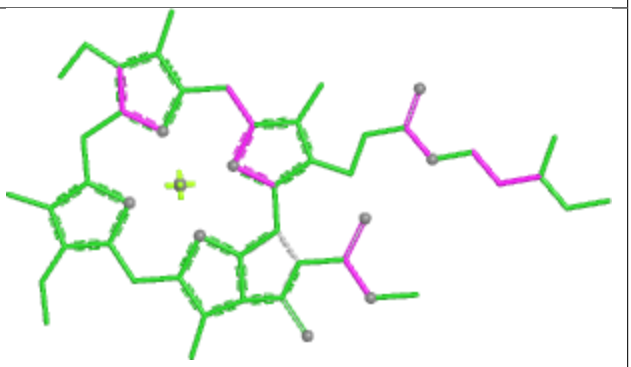


Rings

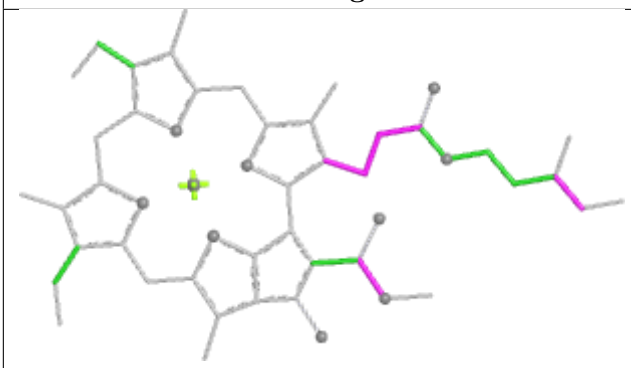
Ligand CLA H 310



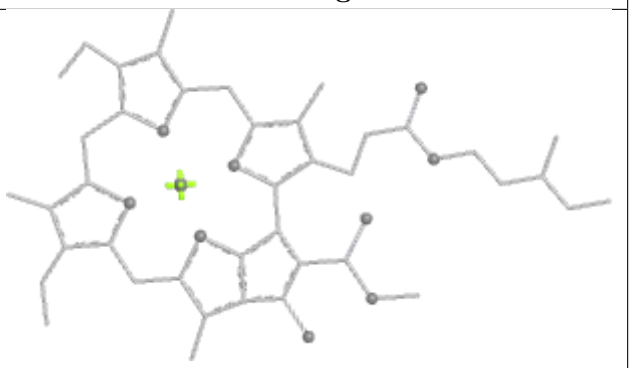
Bond lengths



Bond angles

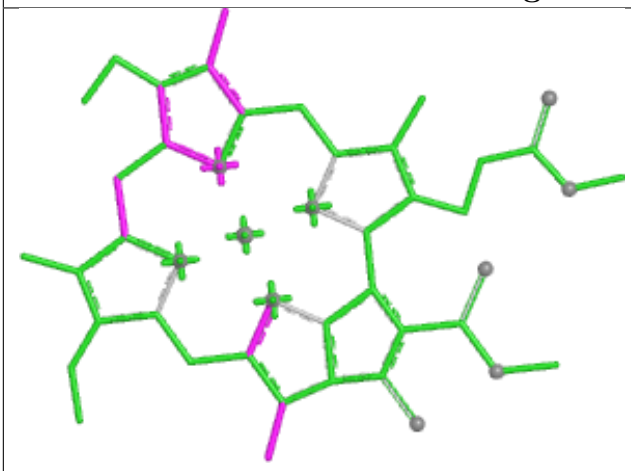


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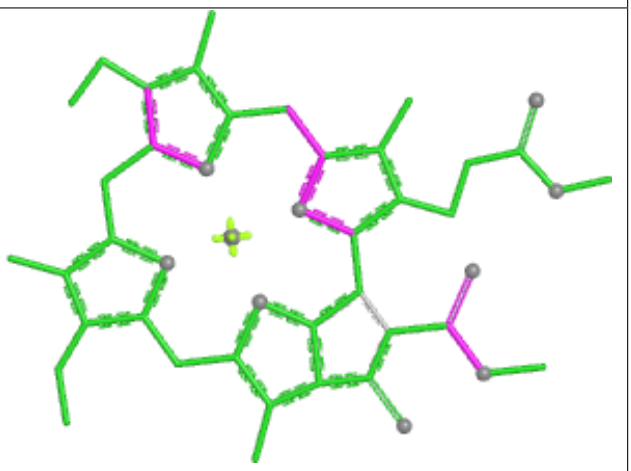


Rings

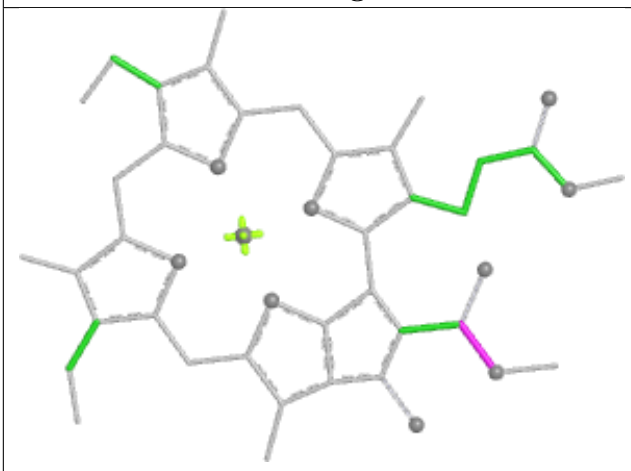
Ligand CLA D 309



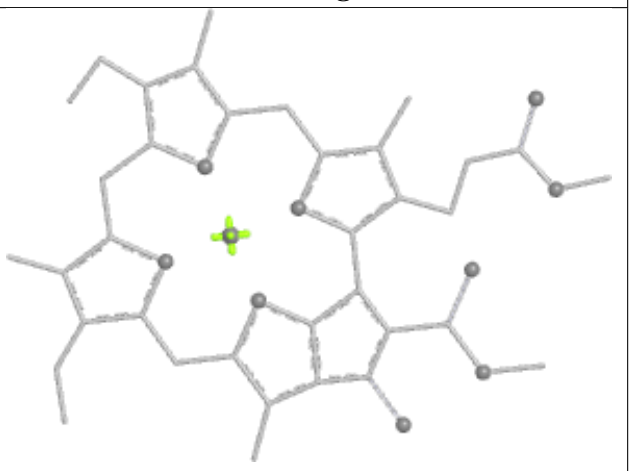
Bond lengths



Bond angles

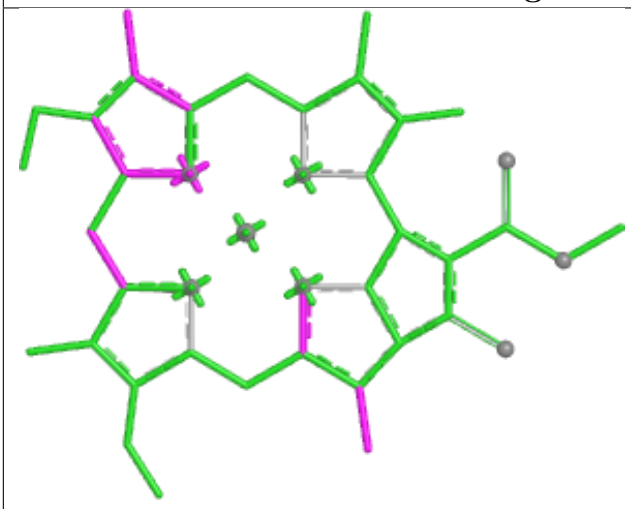


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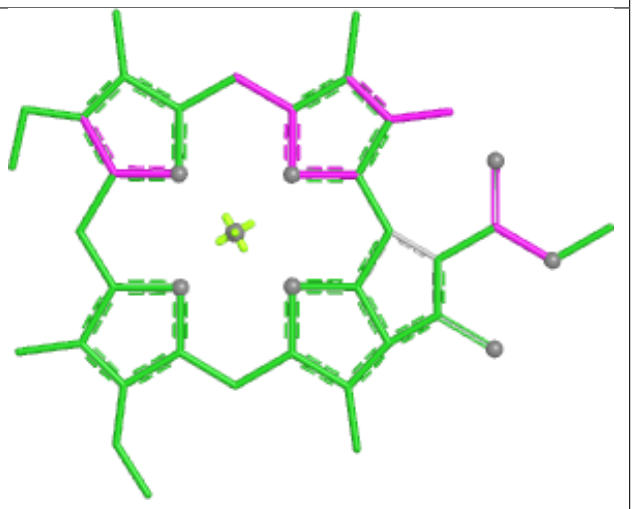


Rings

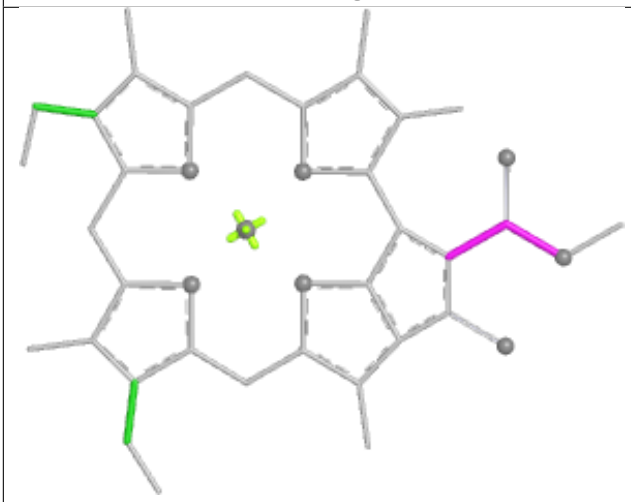
Ligand CLA C 316



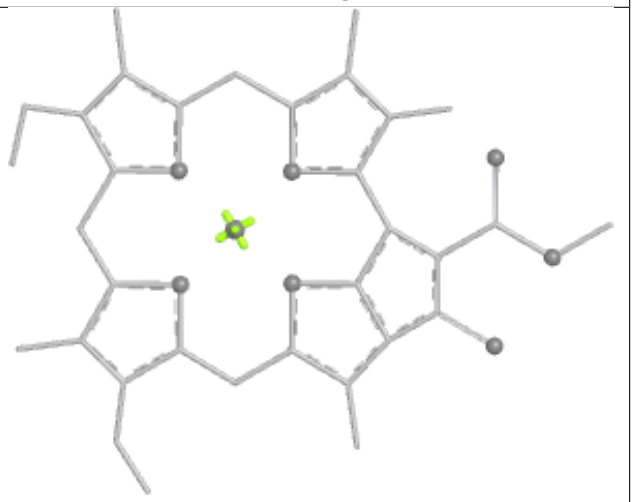
Bond lengths



Bond angles

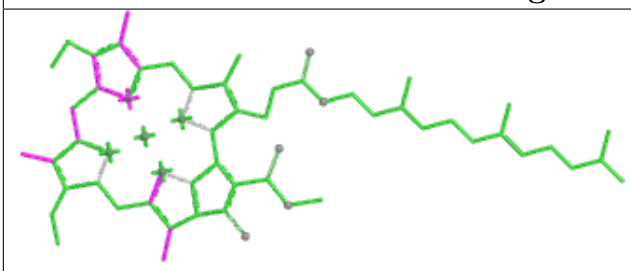


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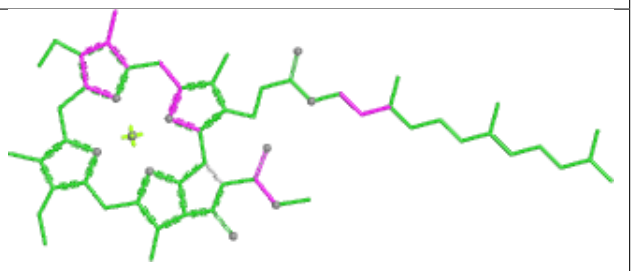


Rings

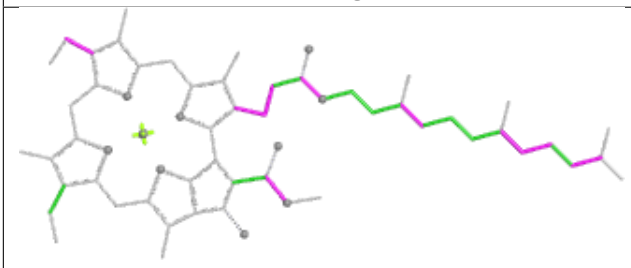
Ligand CLA a 812



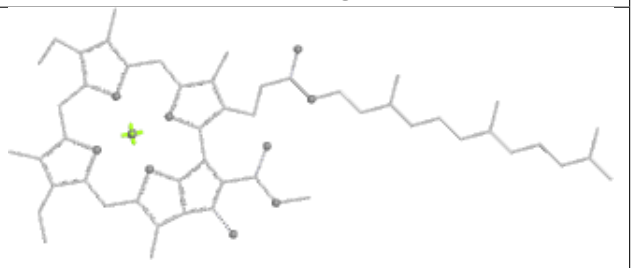
Bond lengths



Bond angles

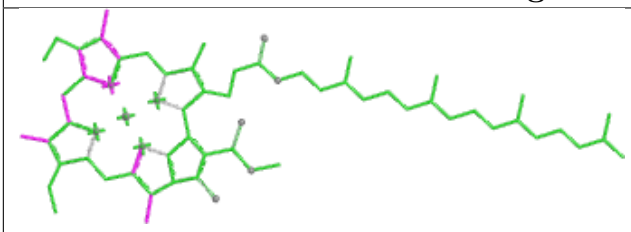


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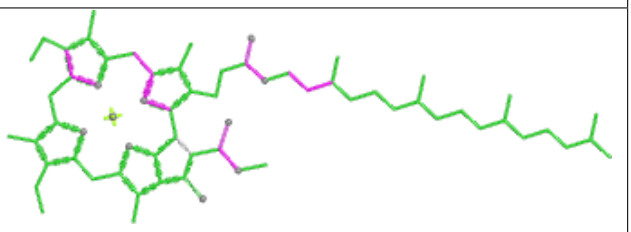


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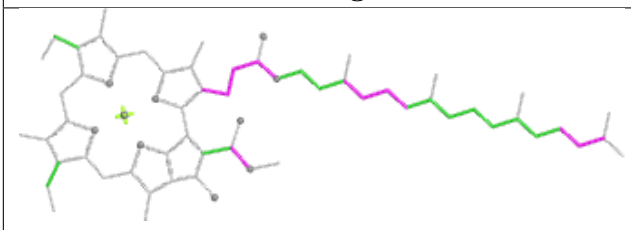
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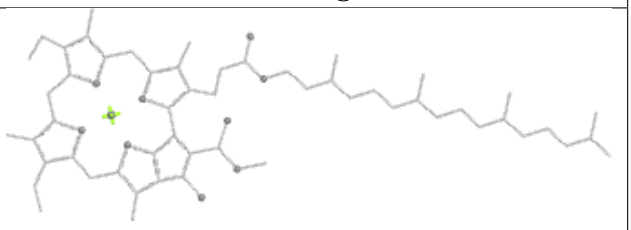
Bond lengths



Bond angles

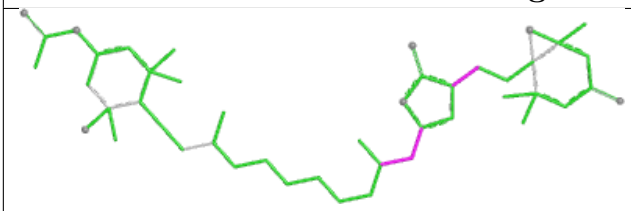


Torsions

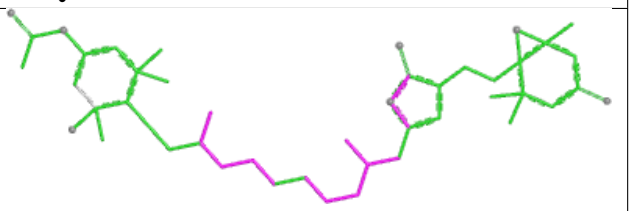


Rings

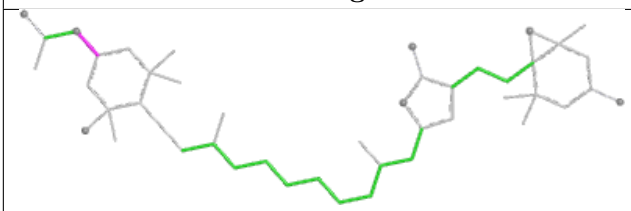
Ligand PID Q 301



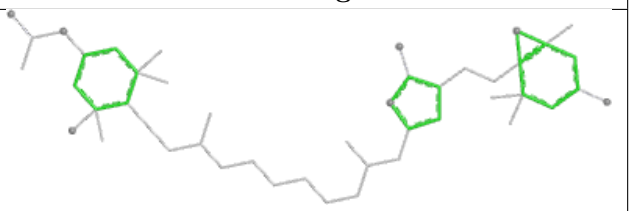
Bond lengths



Bond angles

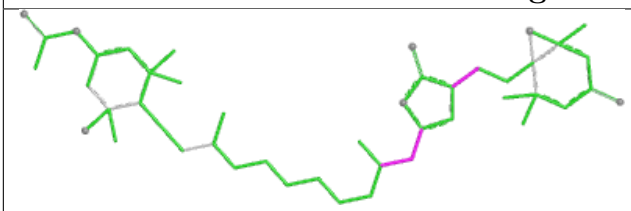


Torsions

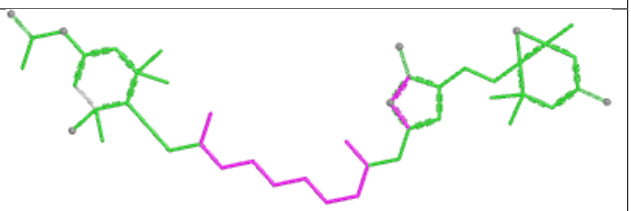


Rings

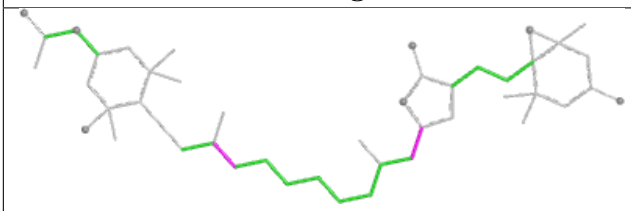
Ligand PID C 304



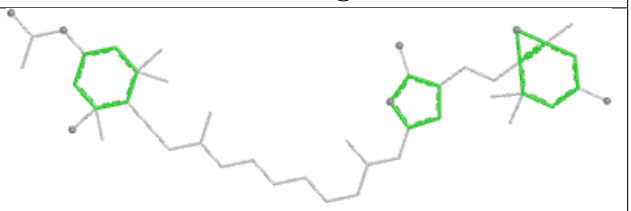
Bond lengths



Bond angles

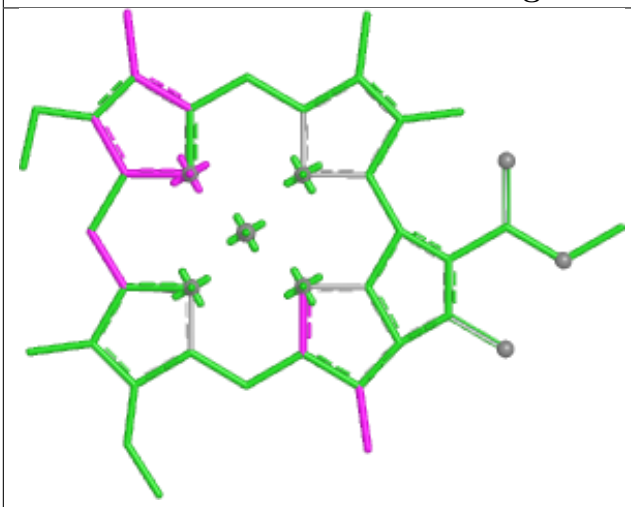


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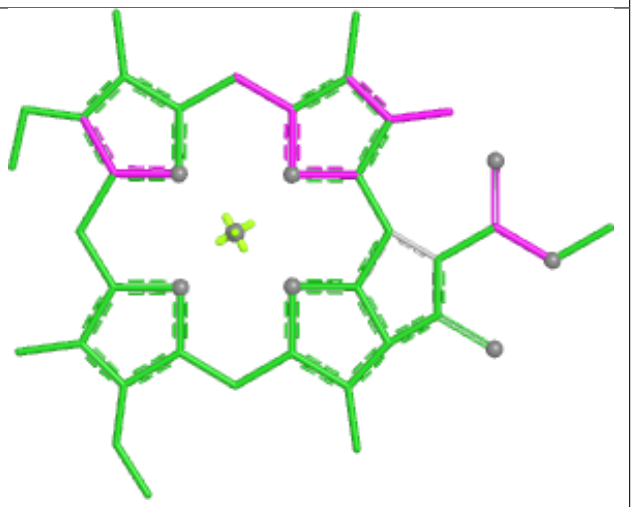


Rings

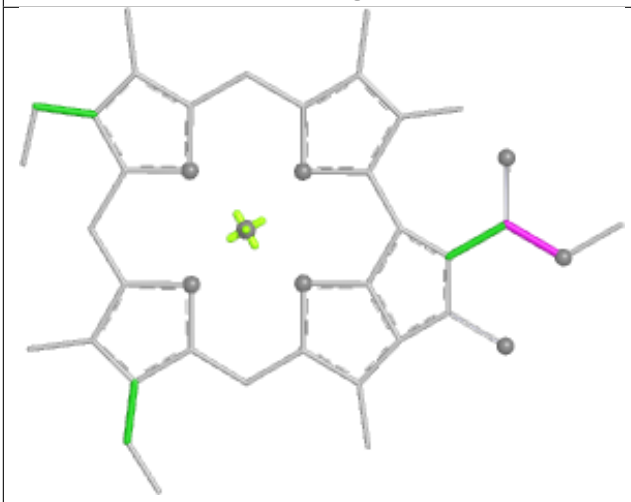
Ligand CLA G 319



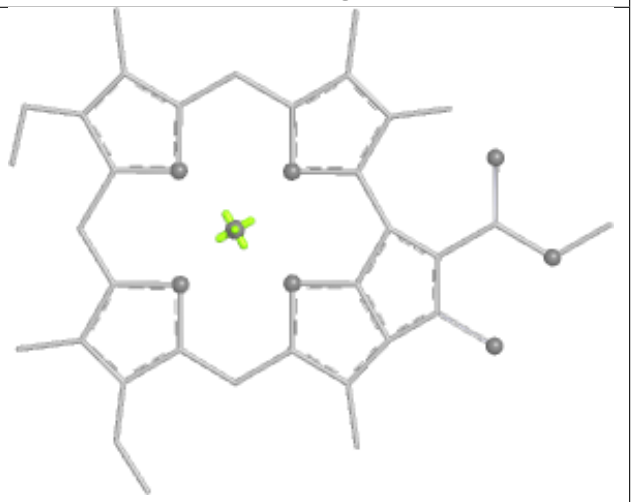
Bond lengths



Bond angles

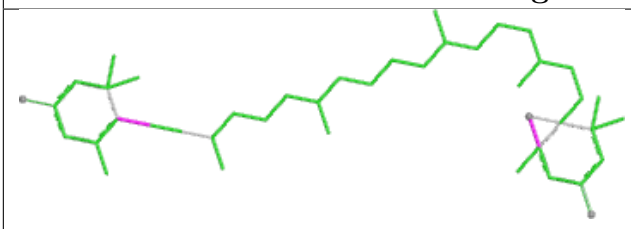


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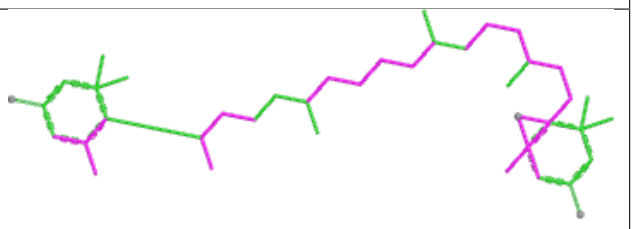


Rings

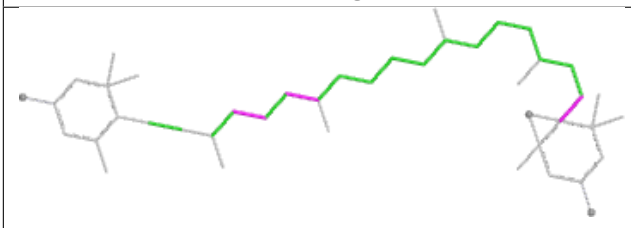
Ligand DD6 I 202



Bond lengths



Bond angles

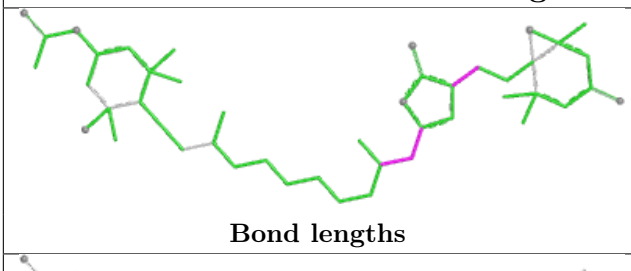


Torsions

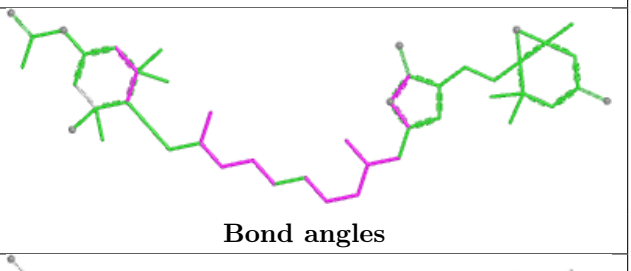


Rings

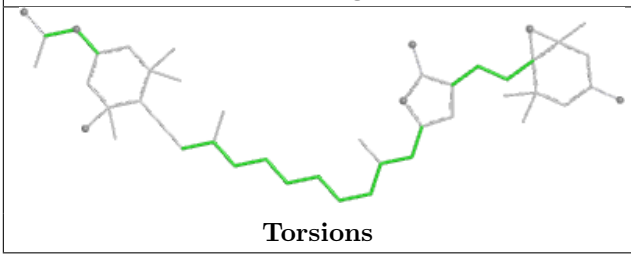
Ligand PID T 305



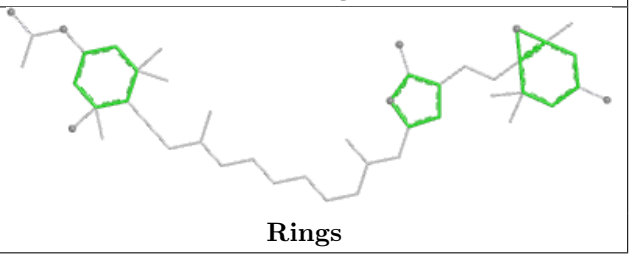
Bond lengths



Bond angles

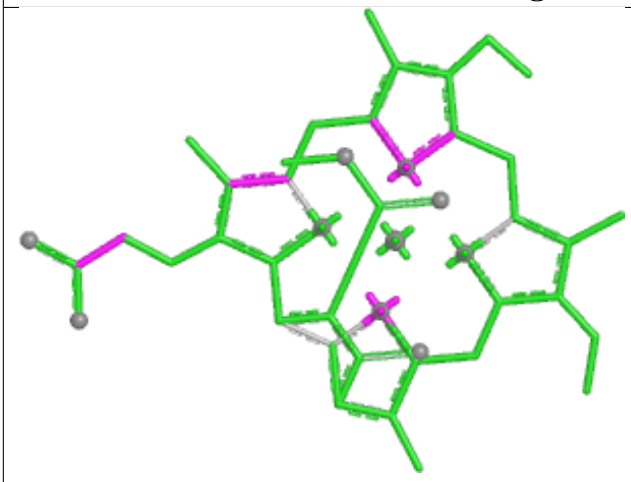


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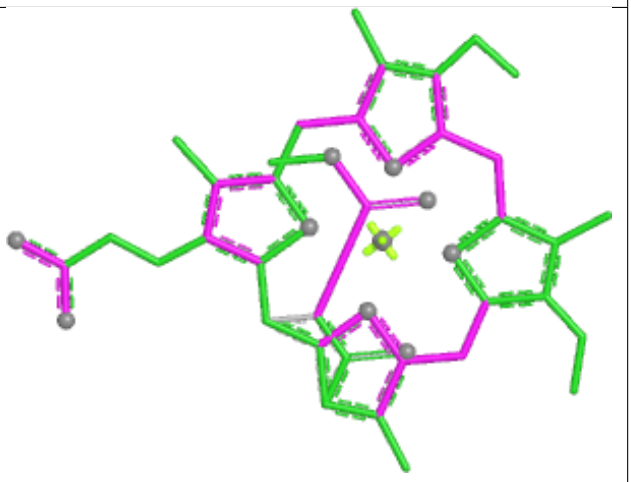


Rings

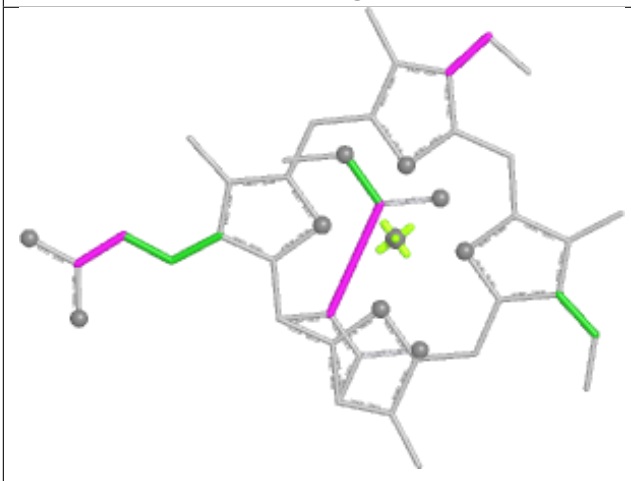
Ligand KC1 L 306



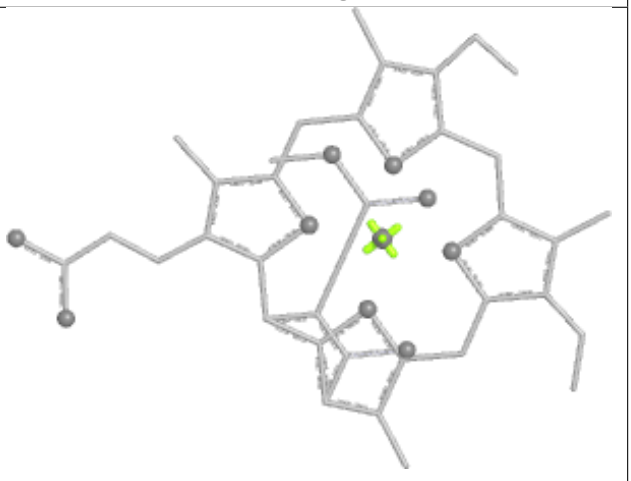
Bond lengths



Bond angles

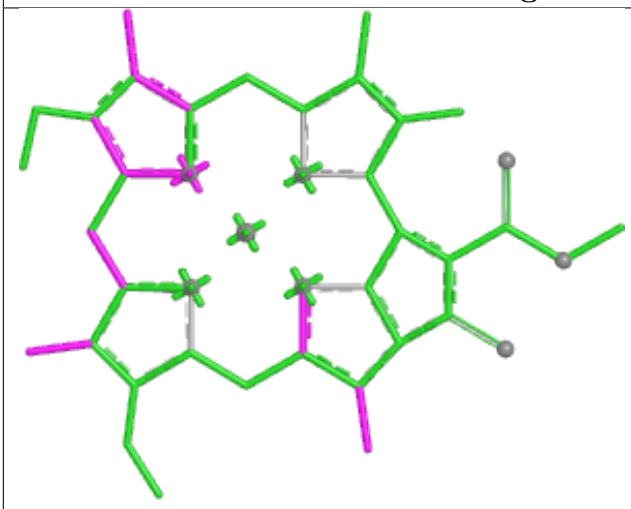


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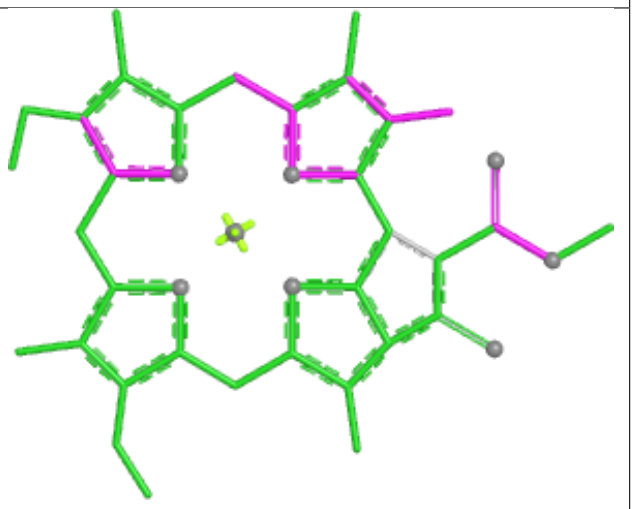


Rings

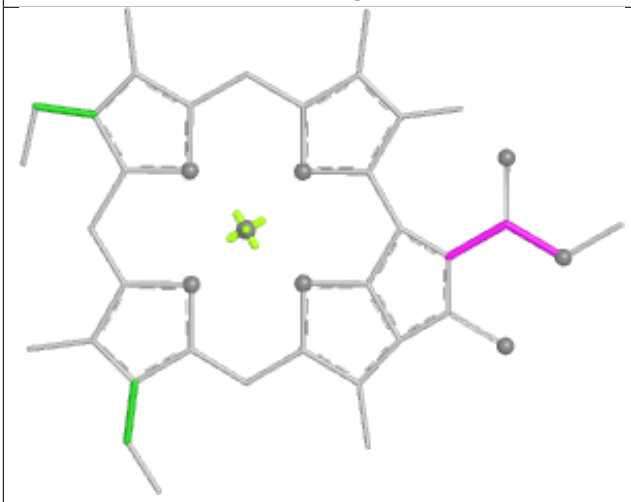
Ligand CLA M 313



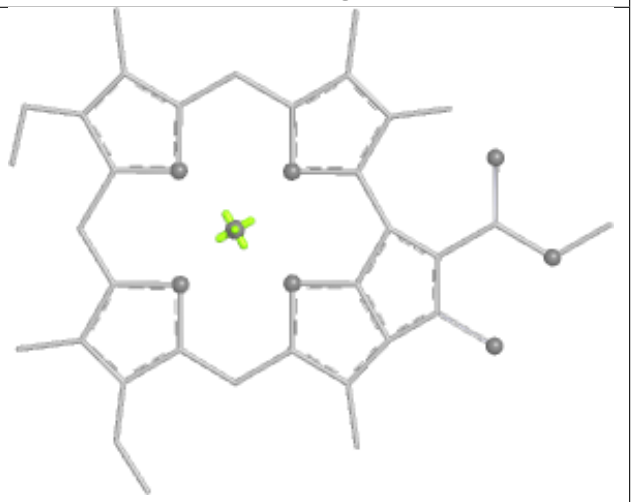
Bond lengths



Bond angles

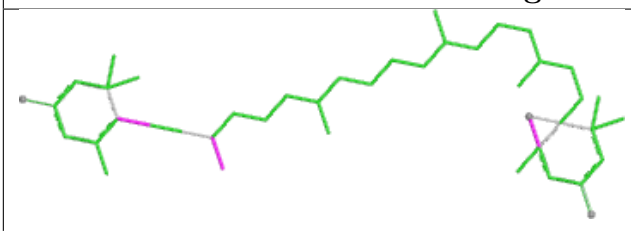


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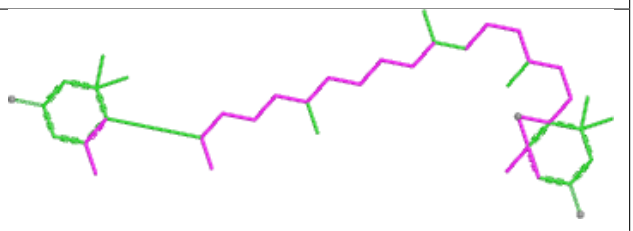


Rings

Ligand DD6 G 306



Bond lengths



Bond angles

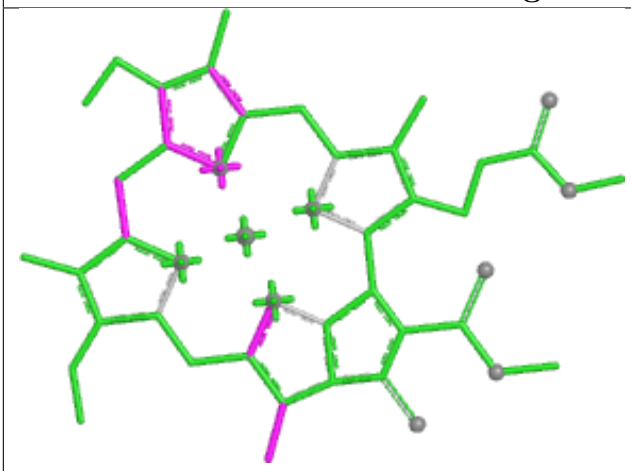


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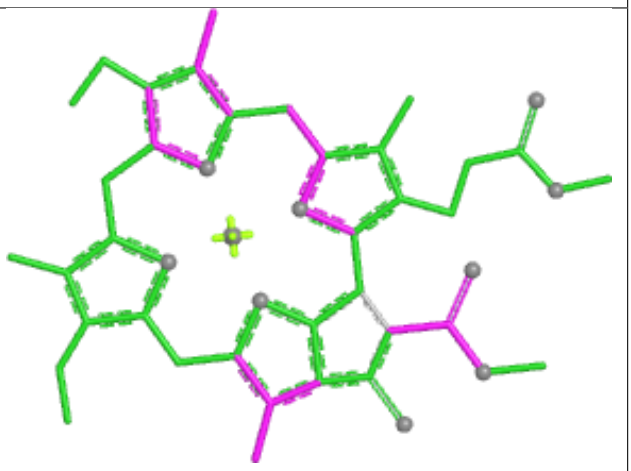


Rings

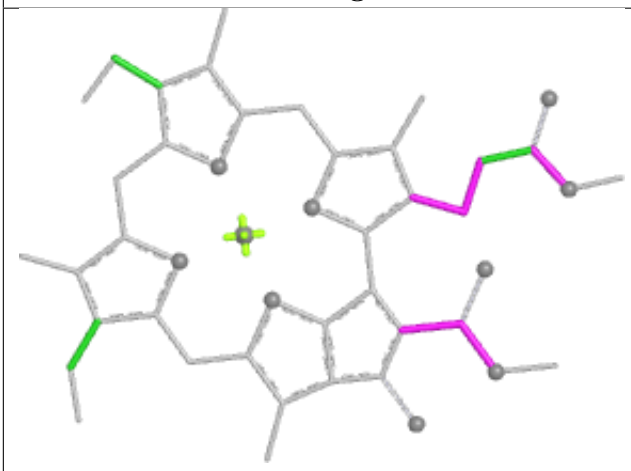
Ligand CLA N 313



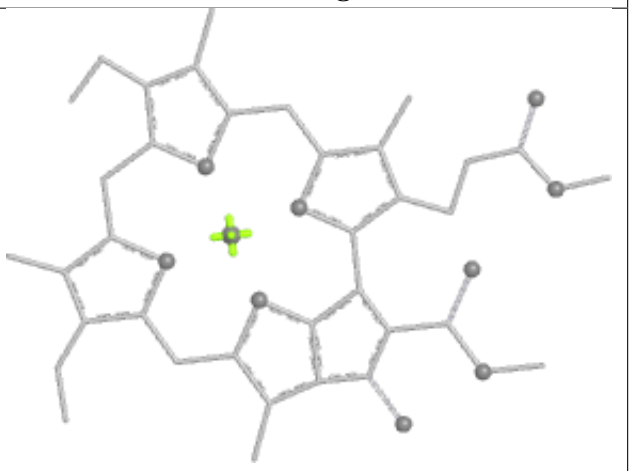
Bond lengths



Bond angles

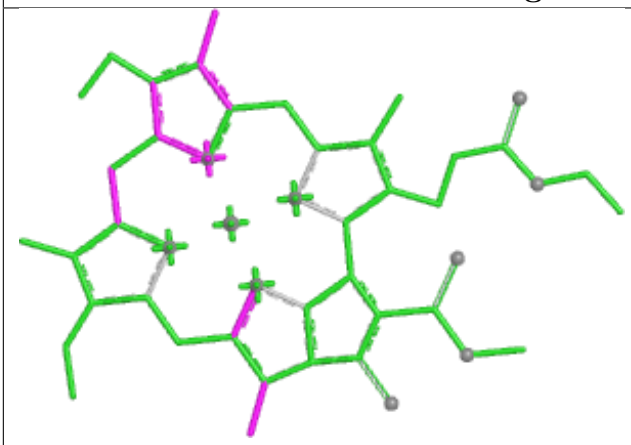


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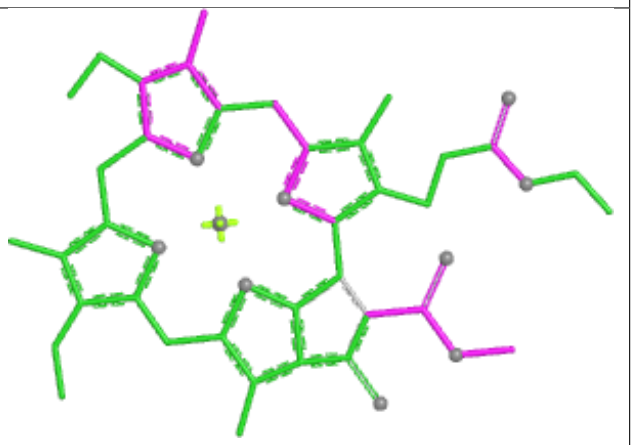


Rings

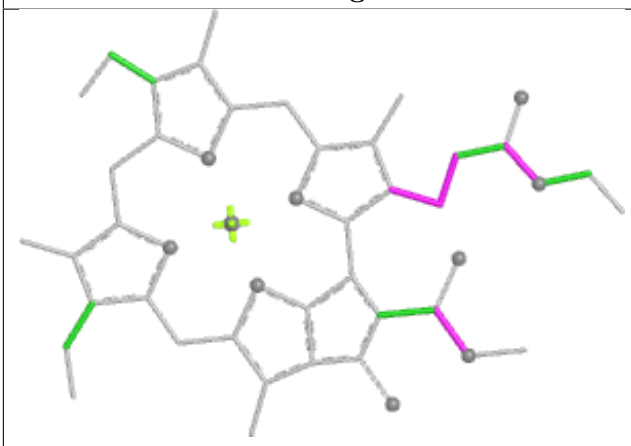
Ligand CLA T 314



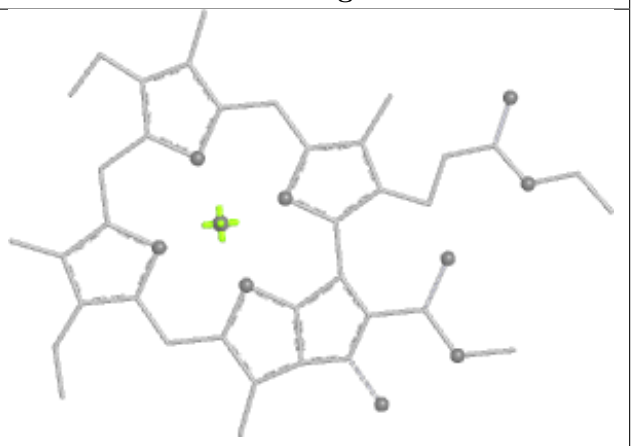
Bond lengths



Bond angles

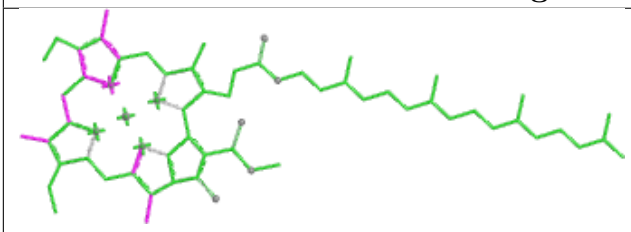


Torsions

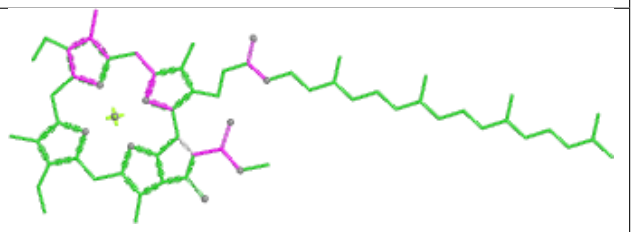


Rings

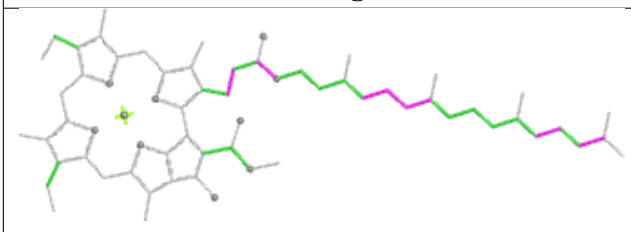
Ligand CLA I 211



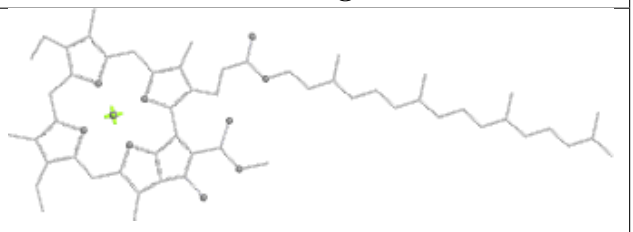
Bond lengths



Bond angles

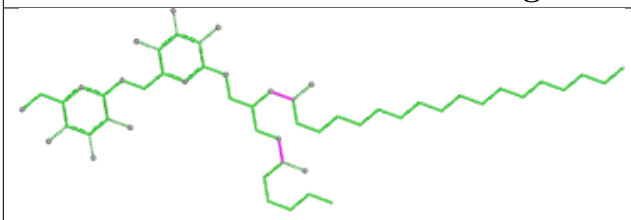


Torsions

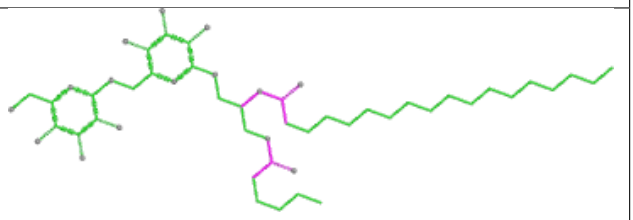


Rings

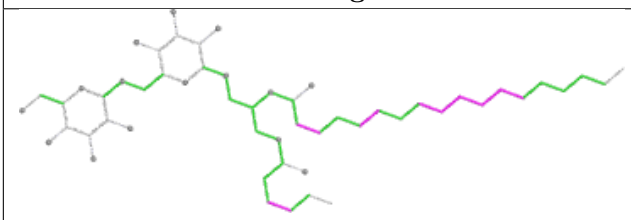
Ligand DGD h 203



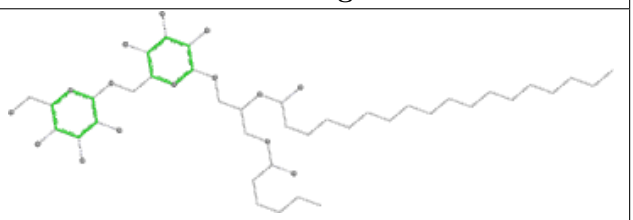
Bond lengths



Bond angles

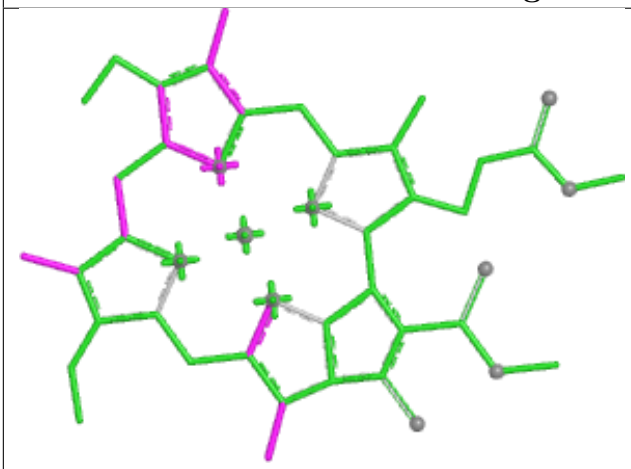


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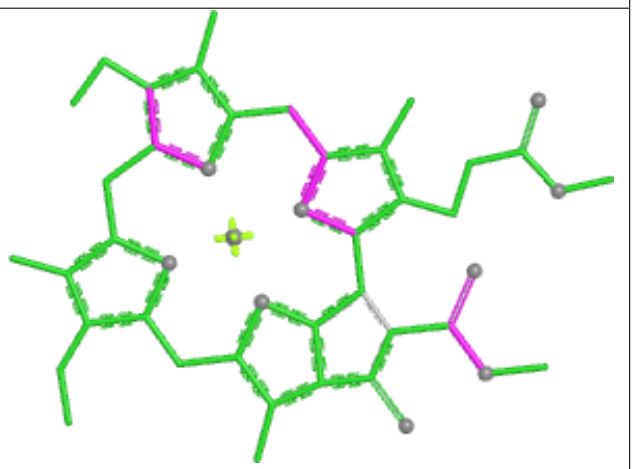


Rings

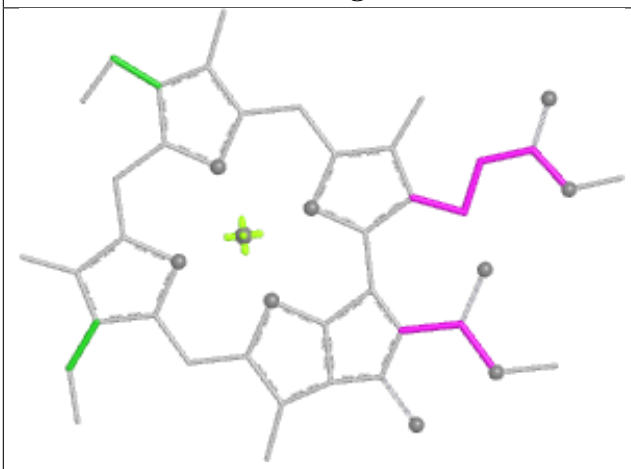
Ligand CLA D 311



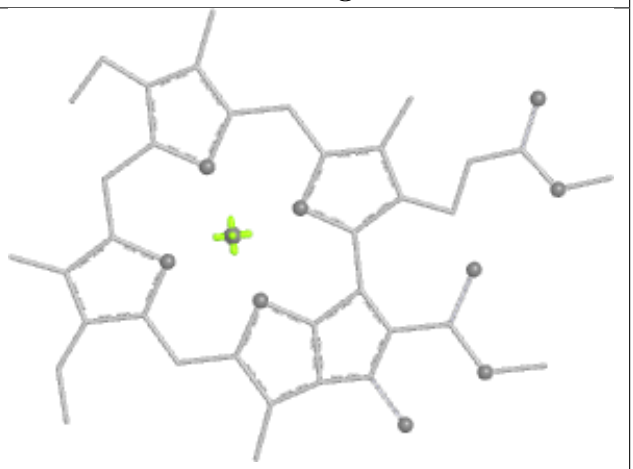
Bond lengths



Bond angles

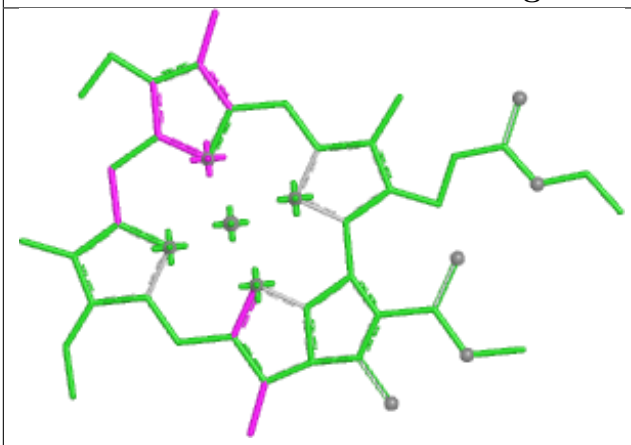


Torsions

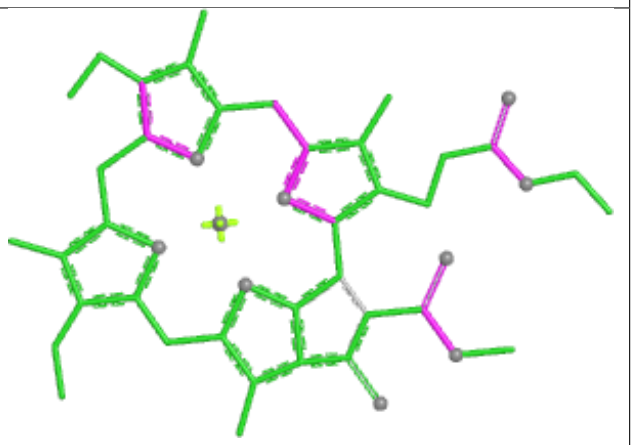


Rings

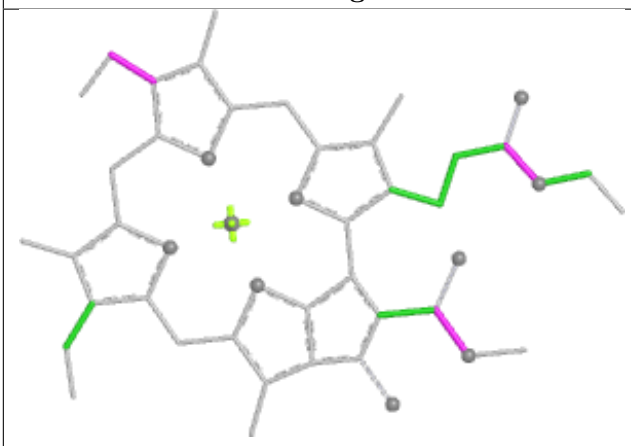
Ligand CLA H 307



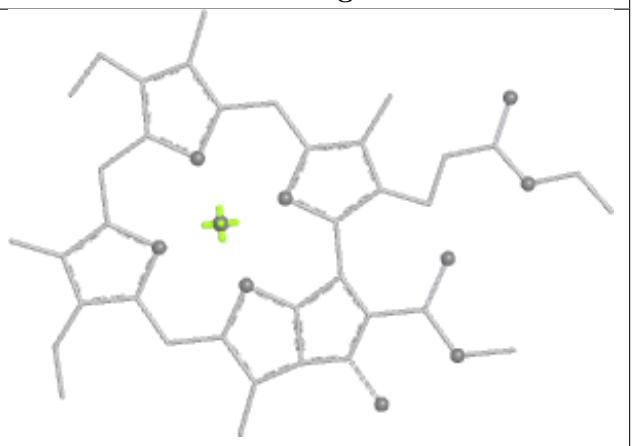
Bond lengths



Bond angles

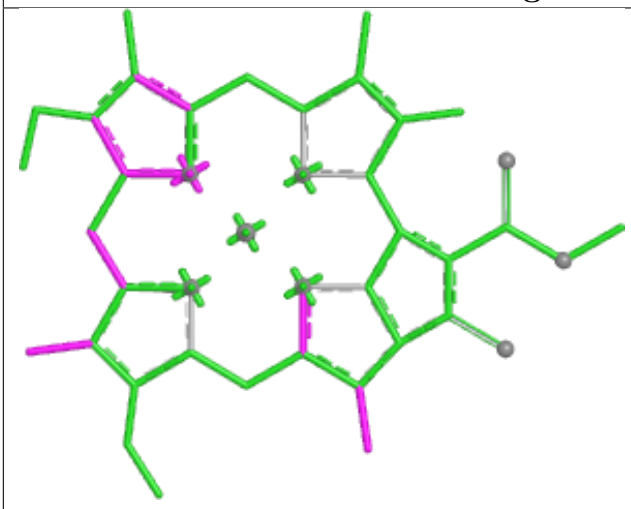


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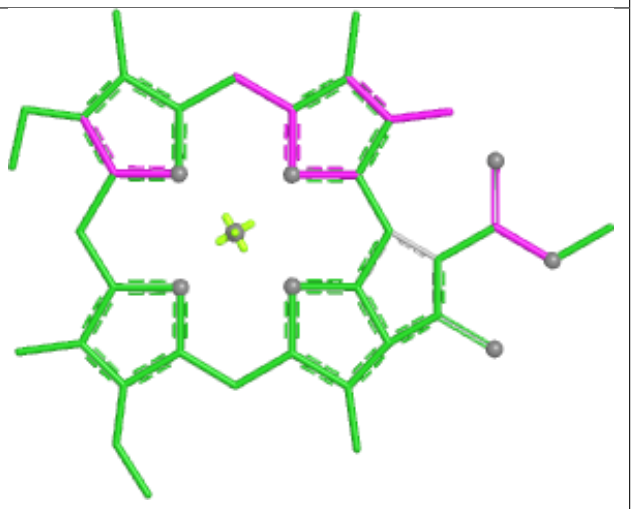


Rings

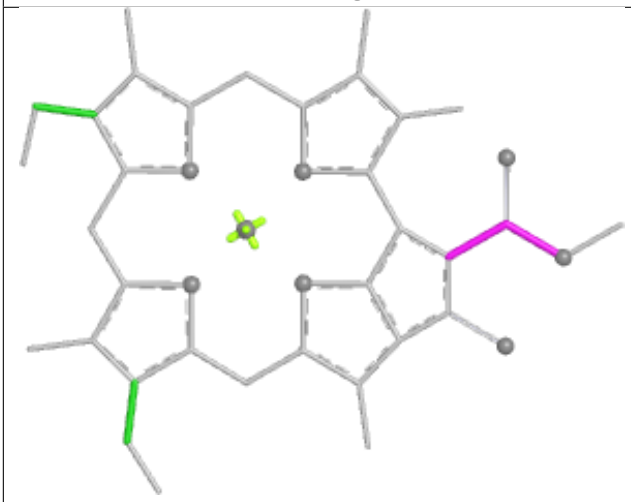
Ligand CLA D 316



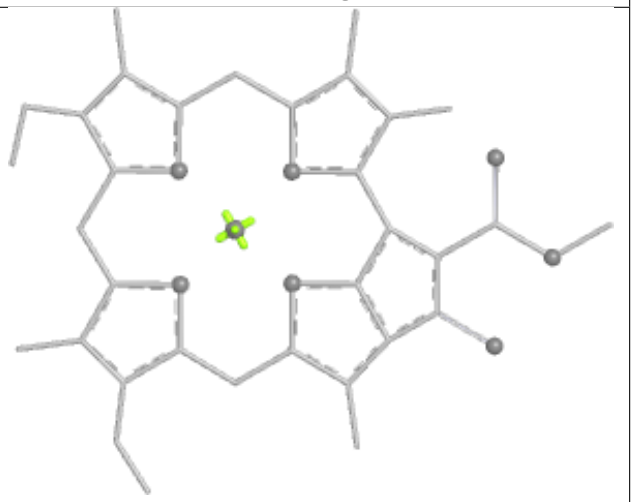
Bond lengths



Bond angles

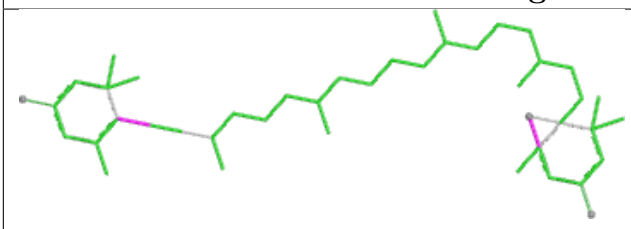


Torsions

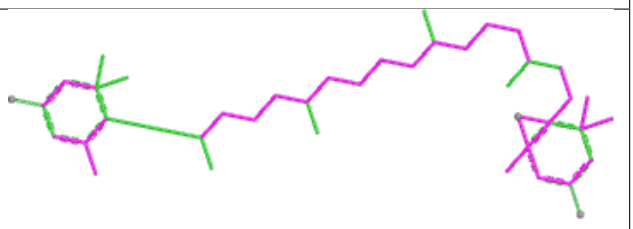


Rings

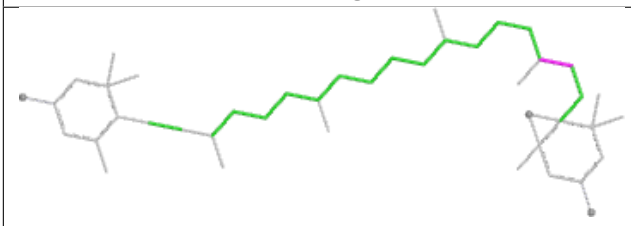
Ligand DD6 J 302



Bond lengths



Bond angles

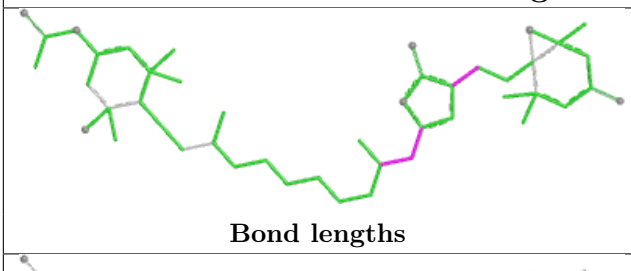


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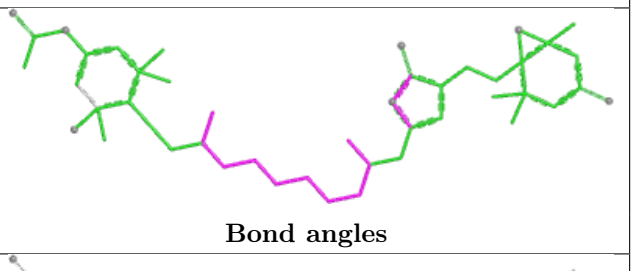


Rings

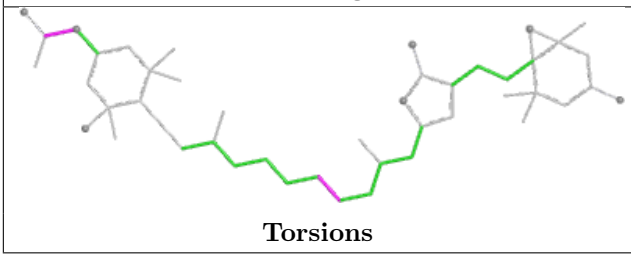
Ligand PID F 302



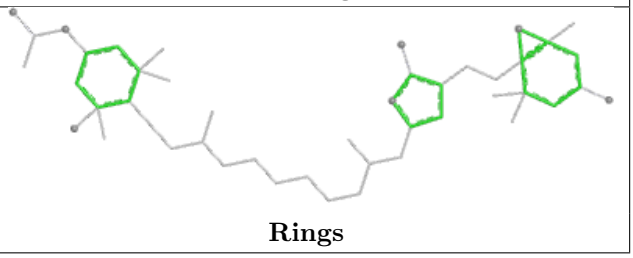
Bond lengths



Bond angles

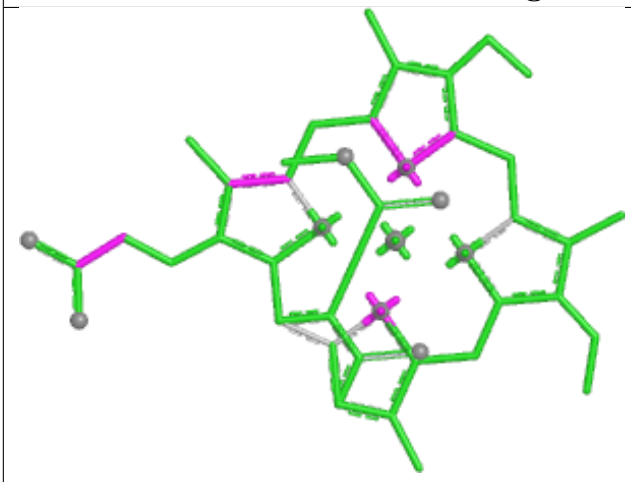


Torsions

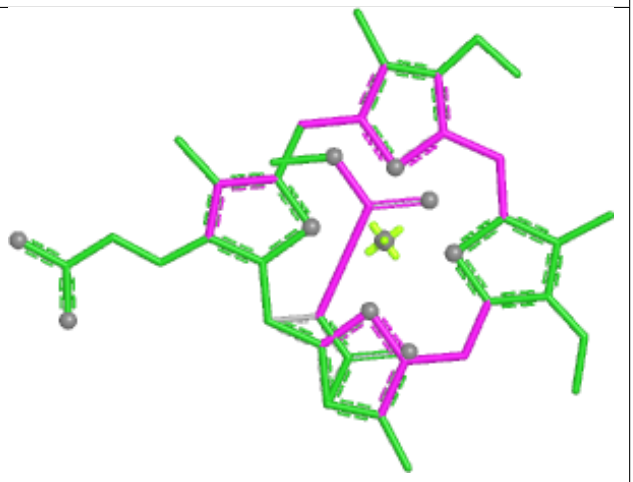


Rings

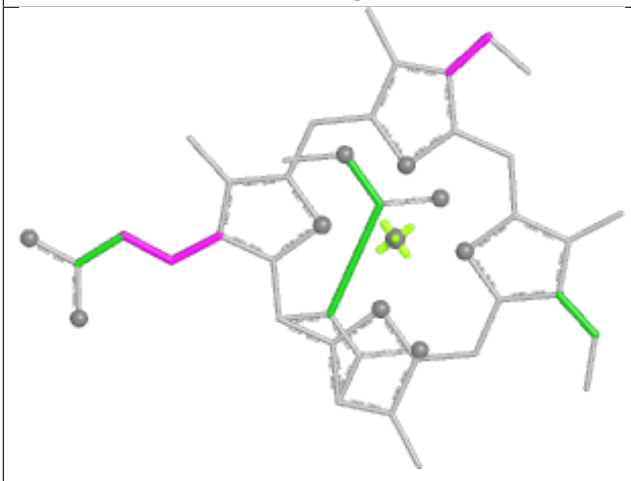
Ligand KC1 D 310



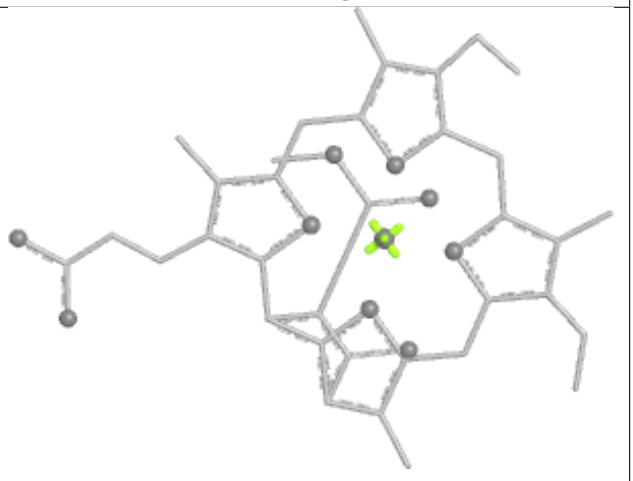
Bond lengths



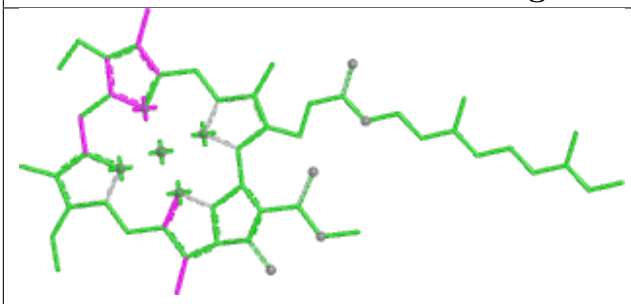
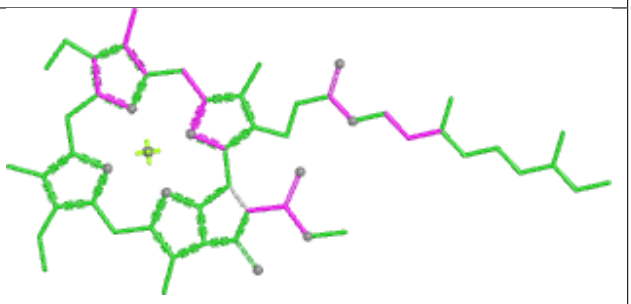
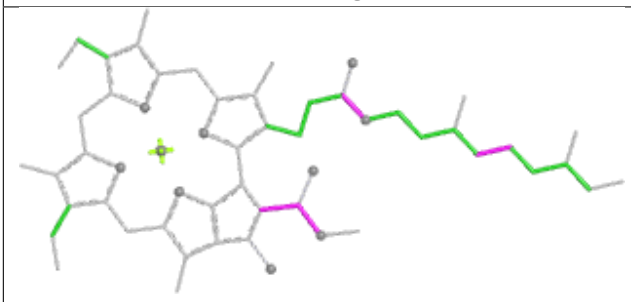
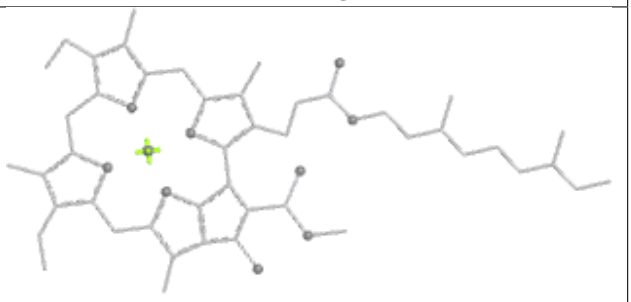
Bond angles

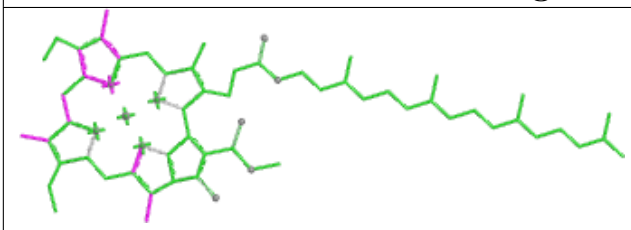
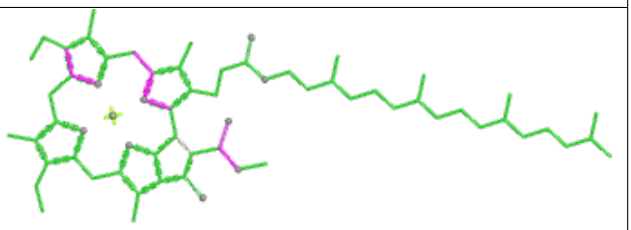
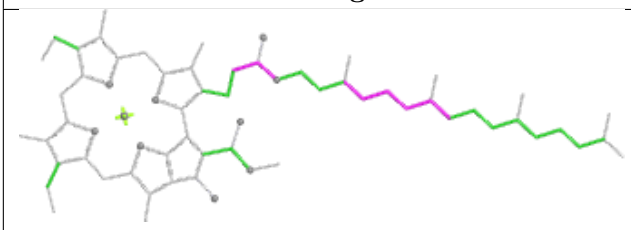
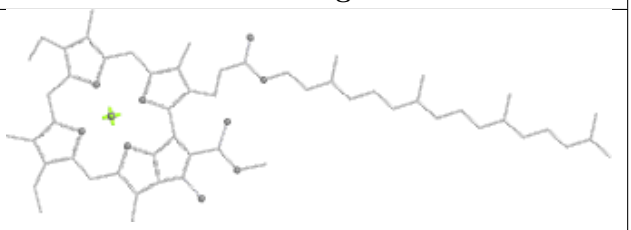


Torsions

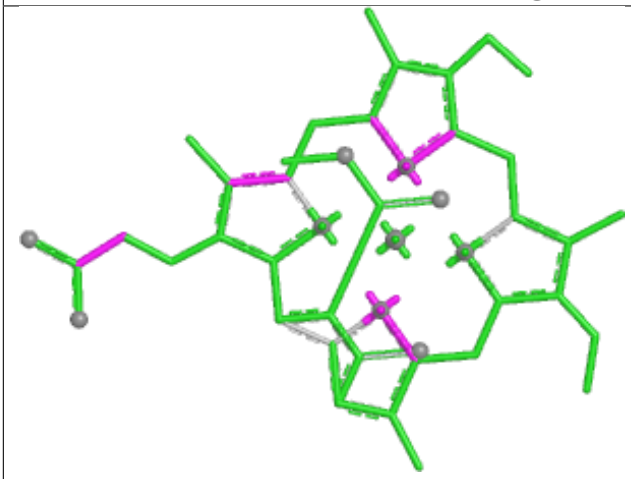


Rings

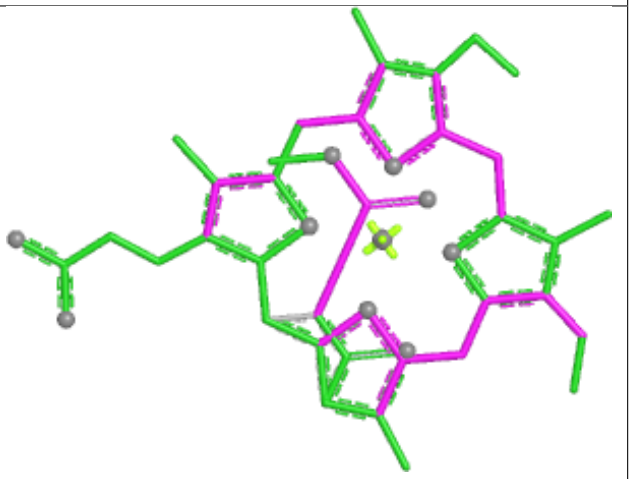
Ligand CLA a 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

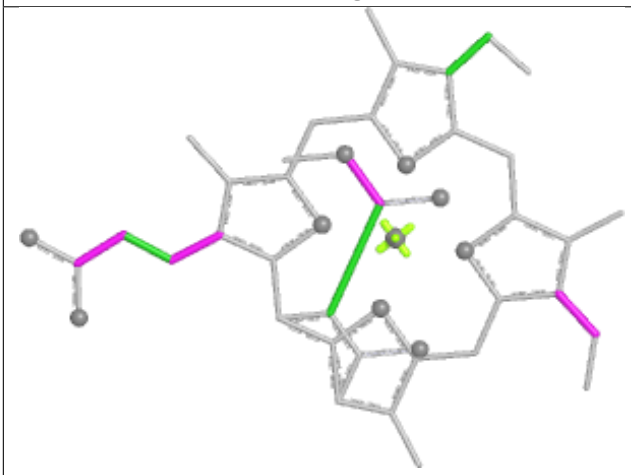
Ligand KC1 L 314



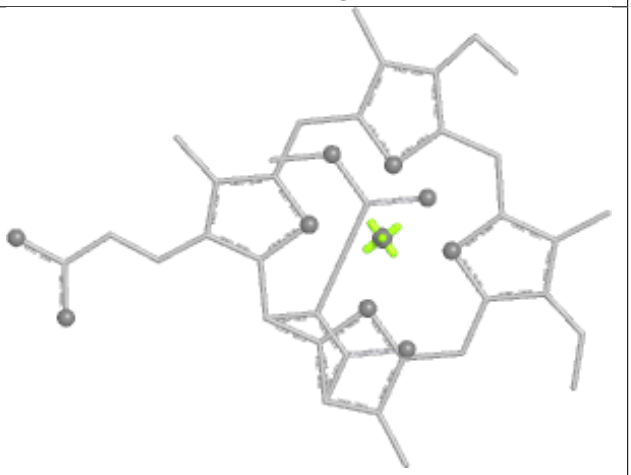
Bond lengths



Bond angles

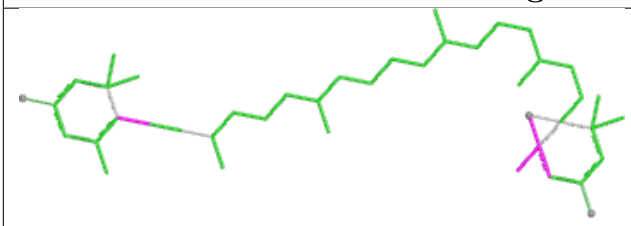


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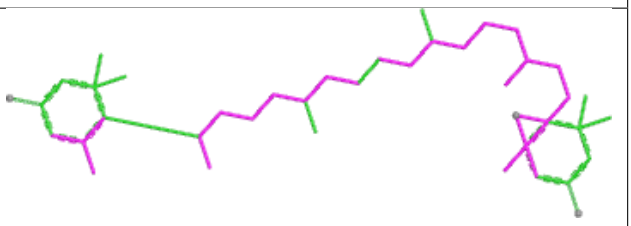


Rings

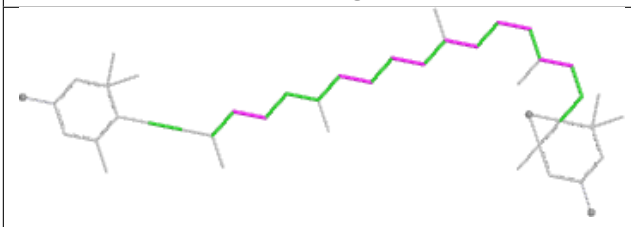
Ligand DD6 F 301



Bond lengths



Bond angles

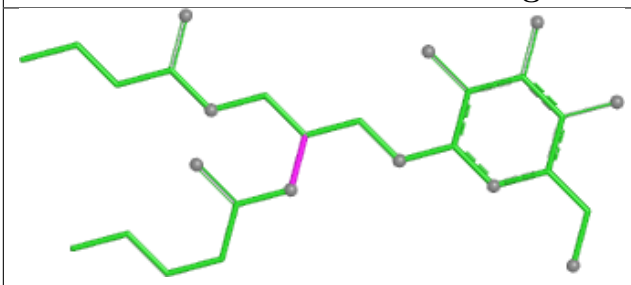


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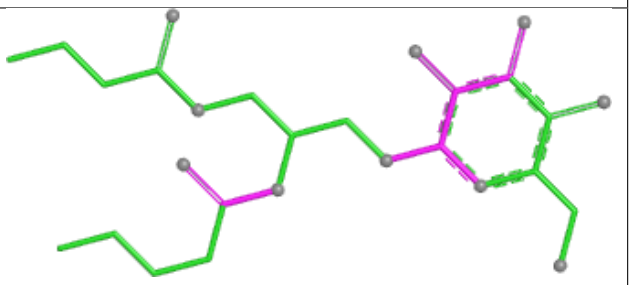


Rings

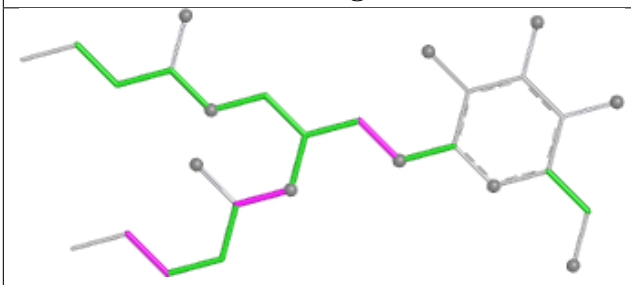
Ligand LMG h 205



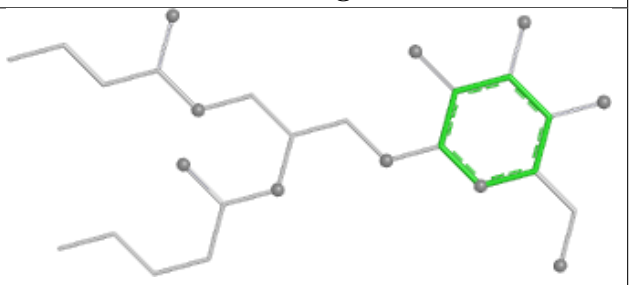
Bond lengths



Bond angles

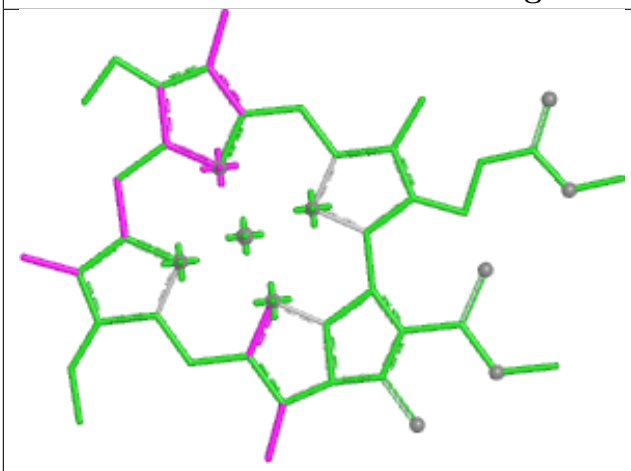


Torsions

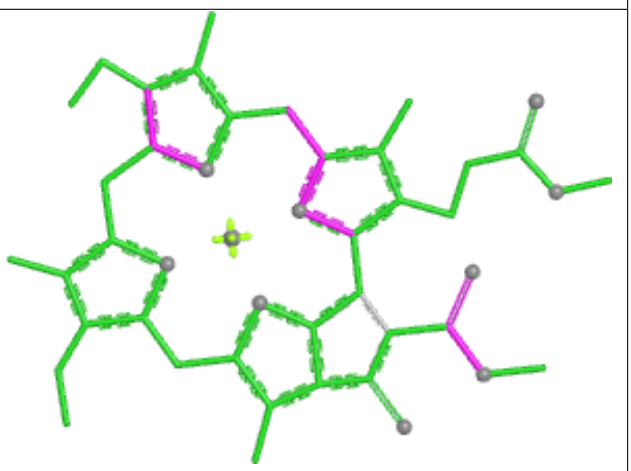


Rings

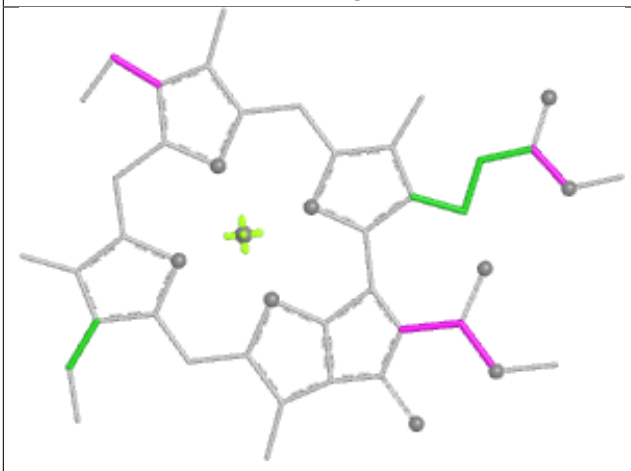
Ligand CLA C 313



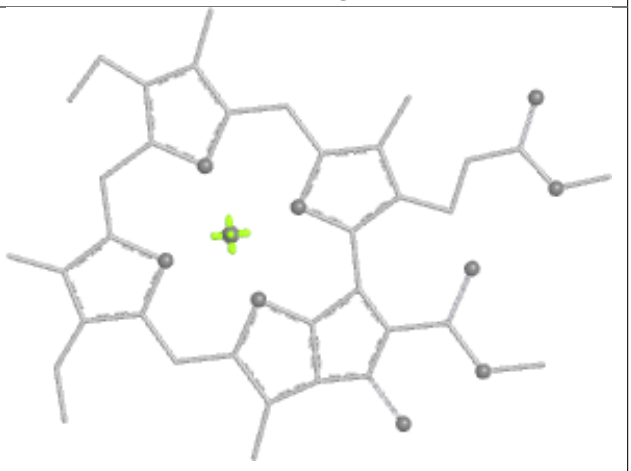
Bond lengths



Bond angles

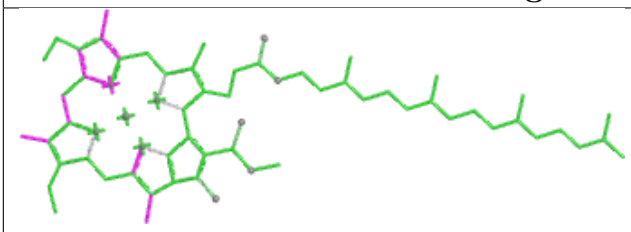


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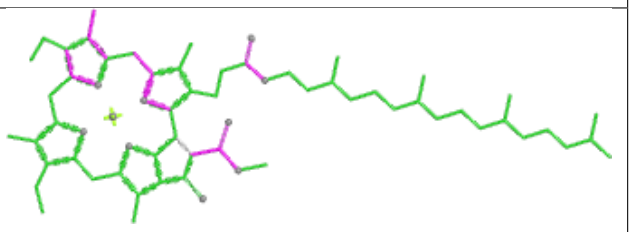


Rings

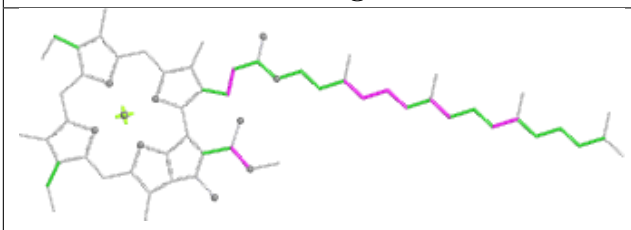
Ligand CLA E 311



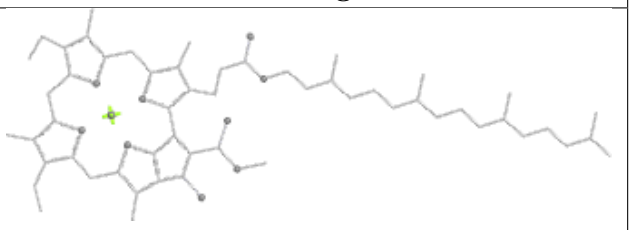
Bond lengths



Bond angles



Torsions

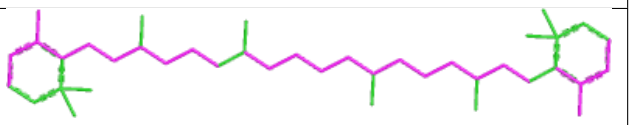


Rings

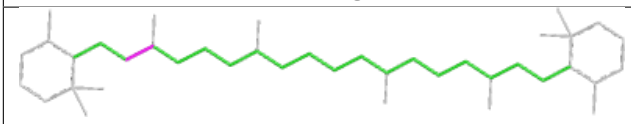
Ligand BCR a 835



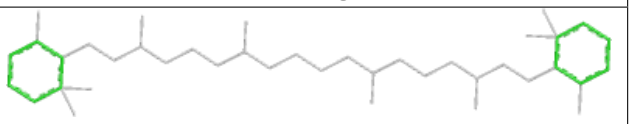
Bond lengths



Bond angles

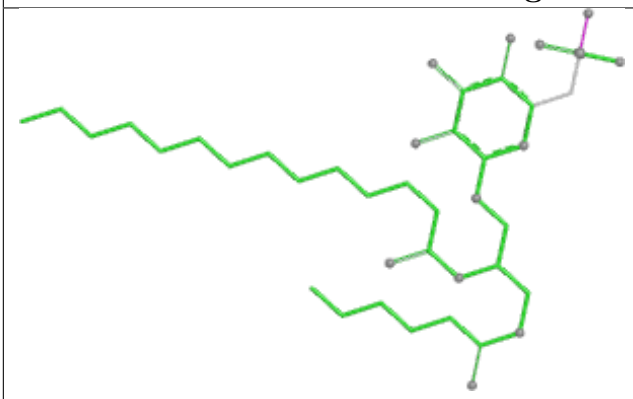


Torsions

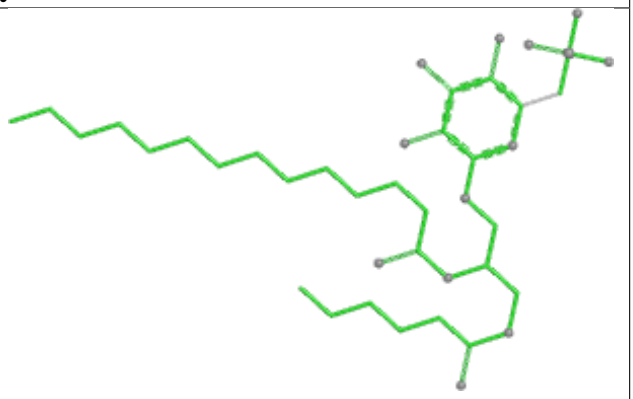


Rings

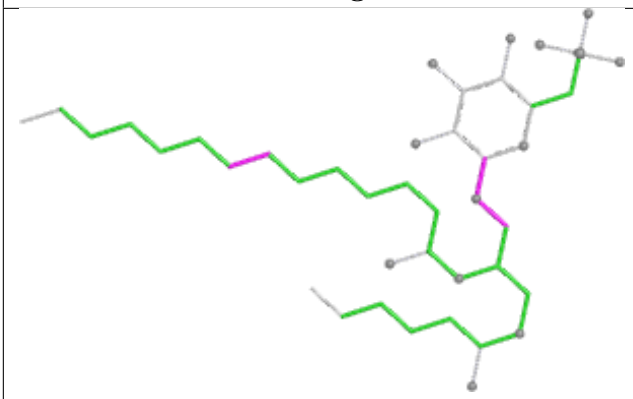
Ligand SQD B 317



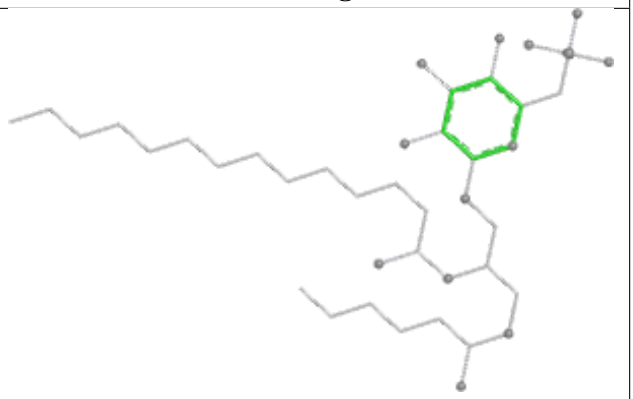
Bond lengths



Bond angles

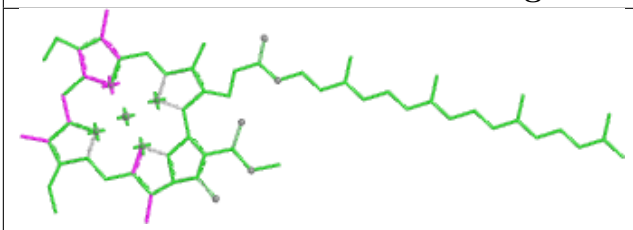


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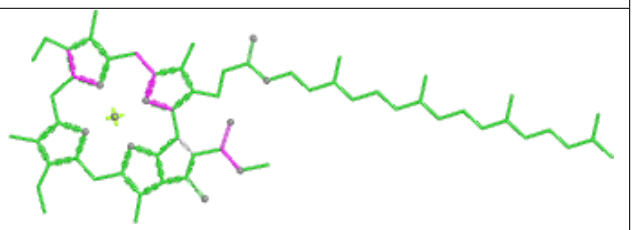


Rings

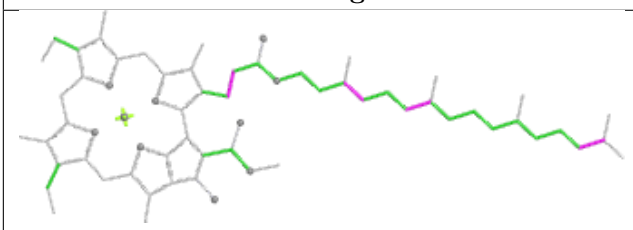
Ligand CLA C 309



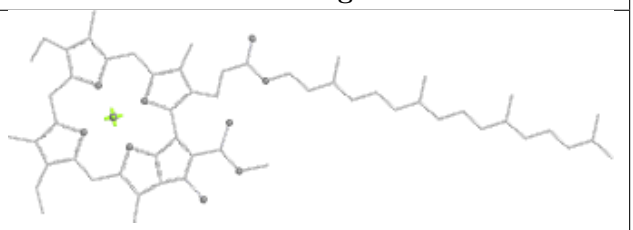
Bond lengths



Bond angles

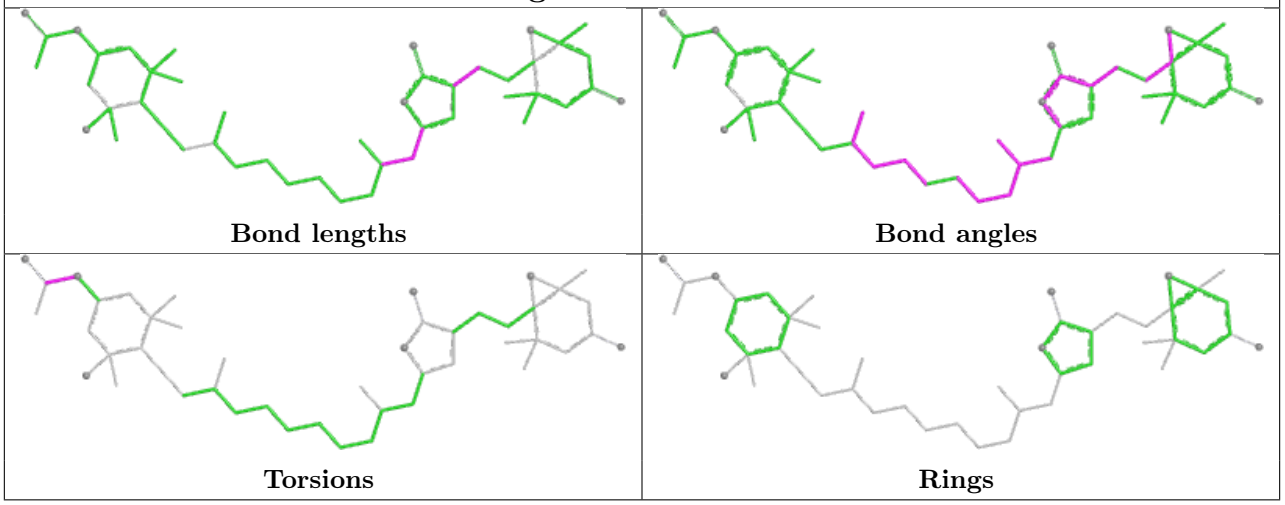


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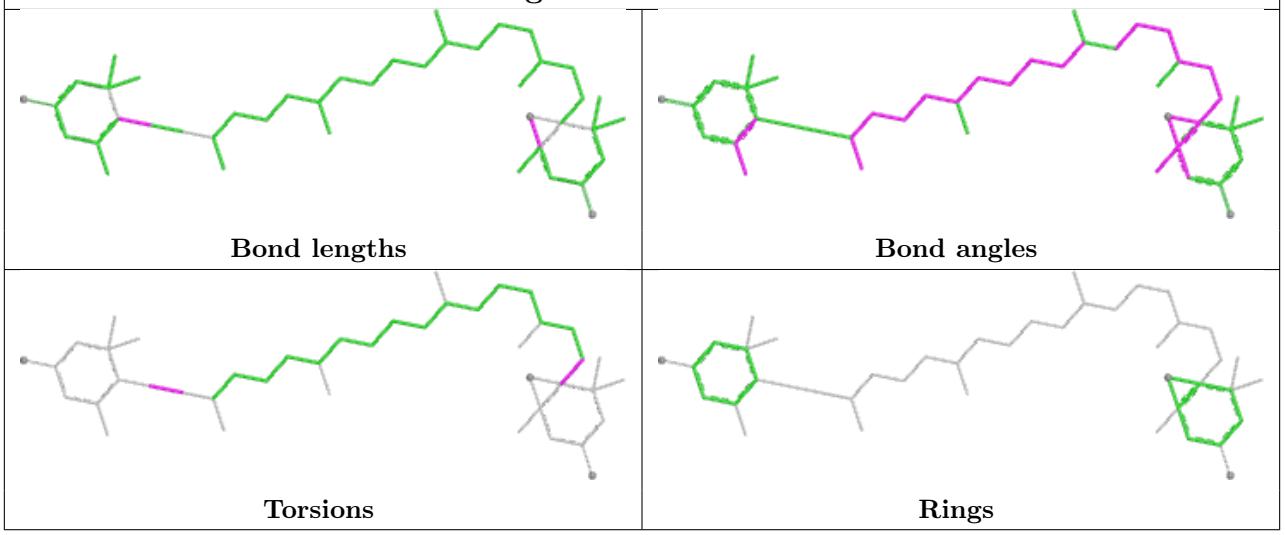


Rings

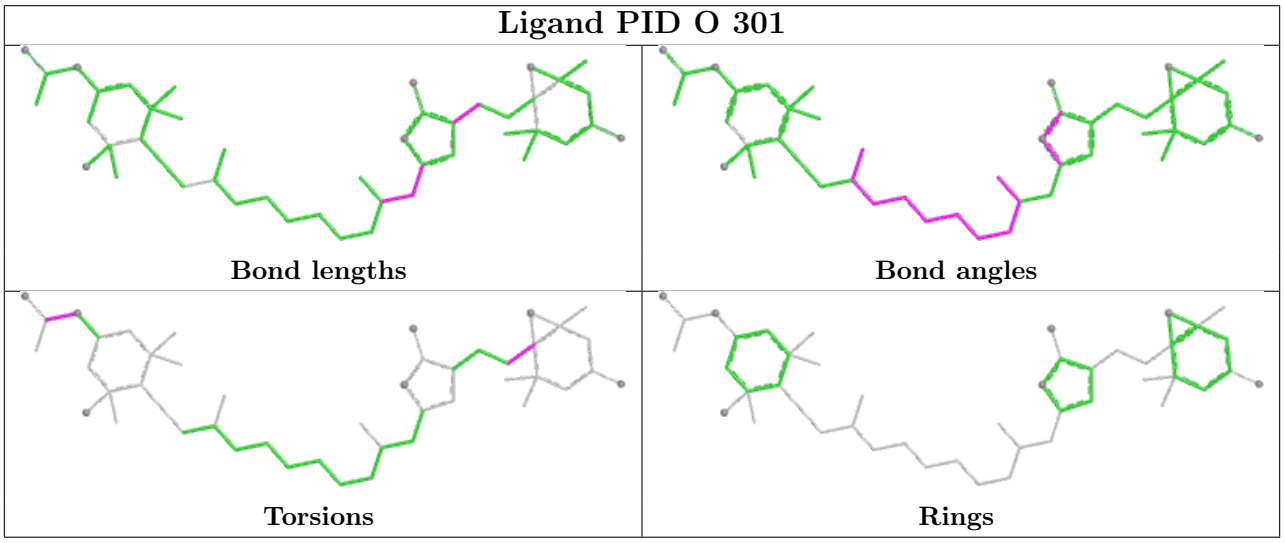
Ligand PID H 302



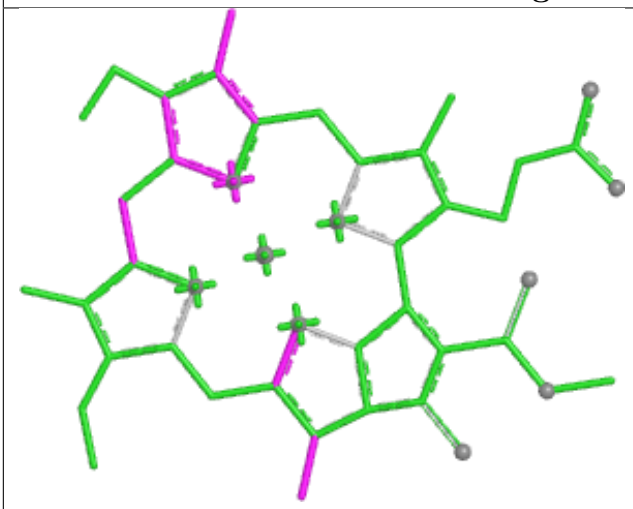
Ligand DD6 A 204



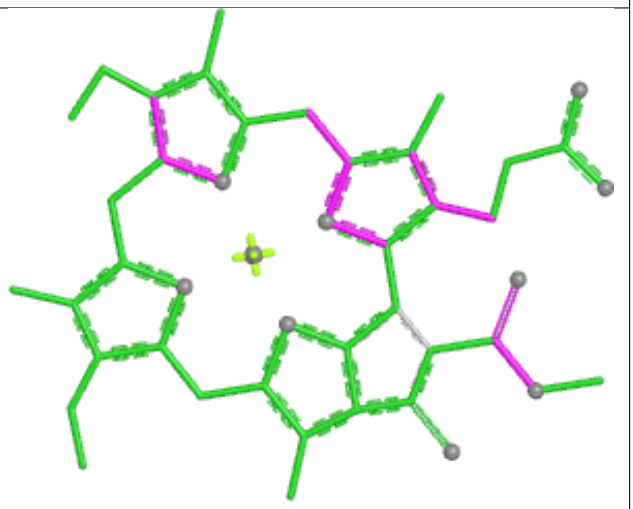
Ligand PID O 301



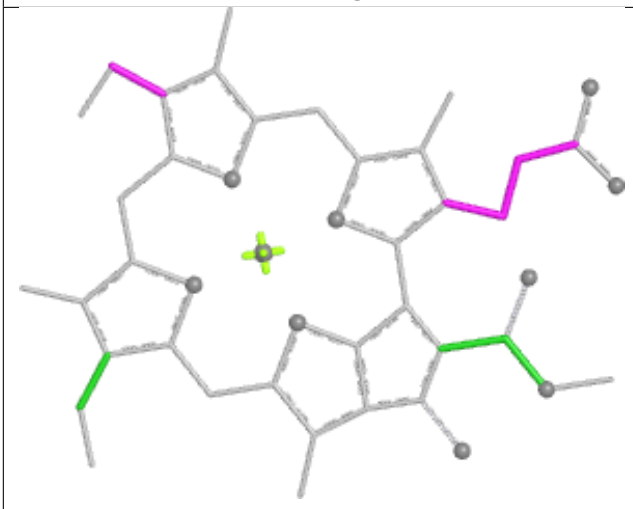
Ligand CLA l 510



Bond lengths



Bond angles

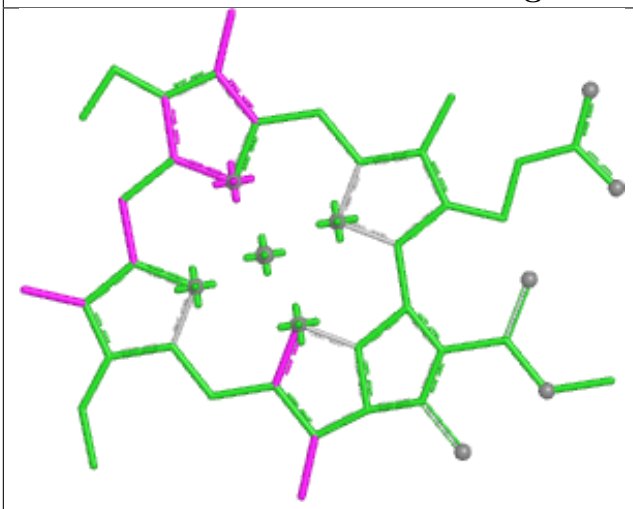


Torsions

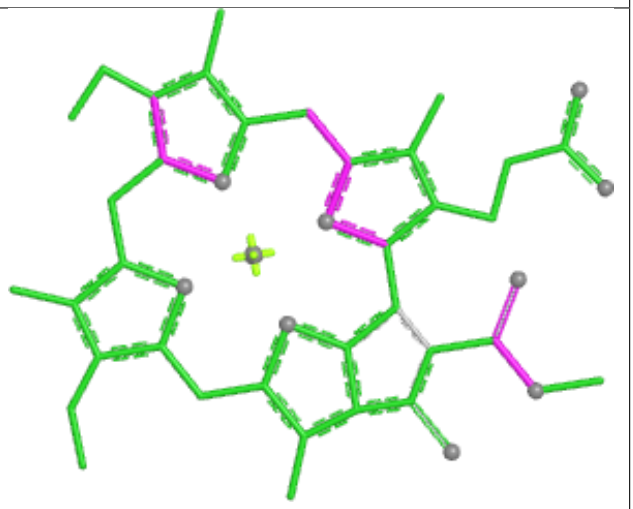


Rings

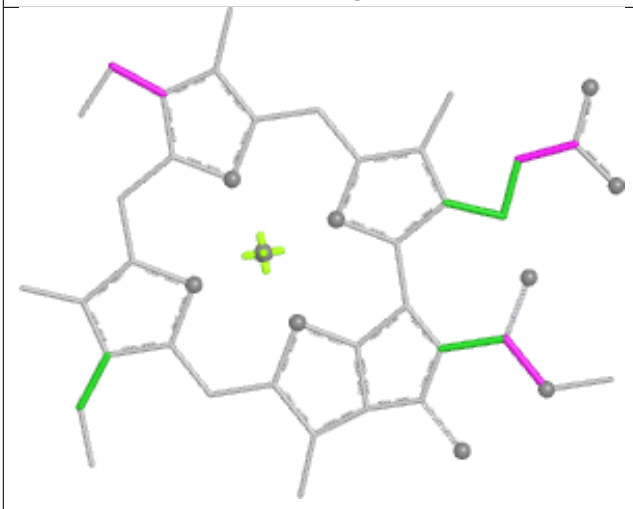
Ligand CLA B 316



Bond lengths



Bond angles

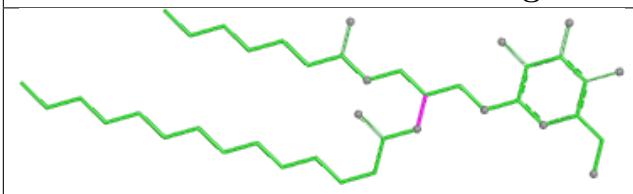


Torsions

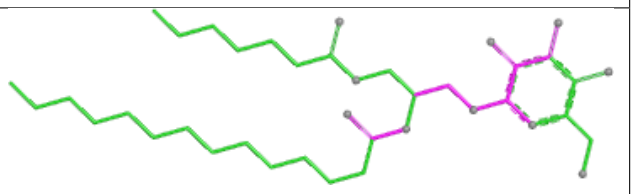


Rings

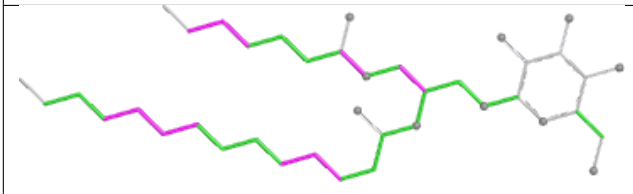
Ligand LMG b 734



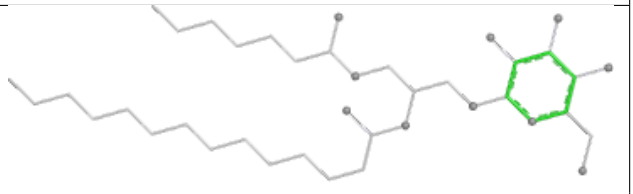
Bond lengths



Bond angles

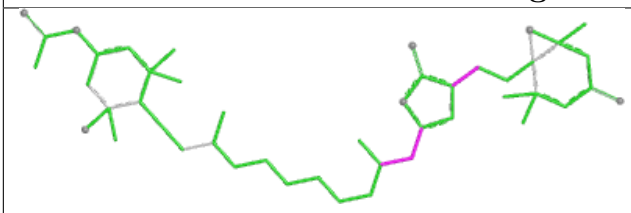


Torsions

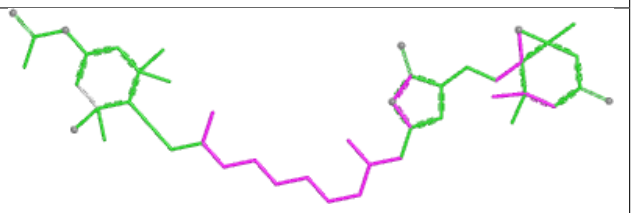


Rings

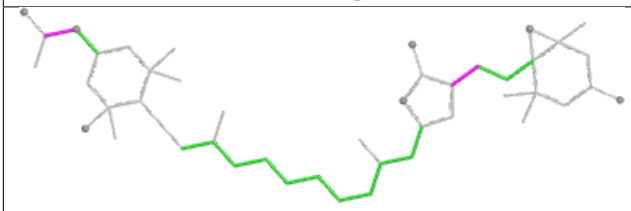
Ligand PID T 307



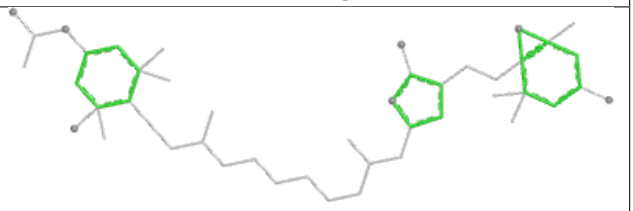
Bond lengths



Bond angles

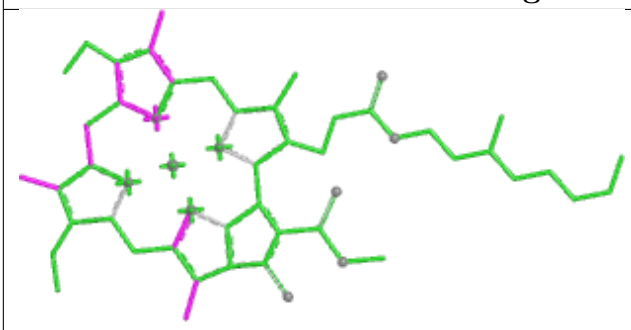


Torsions

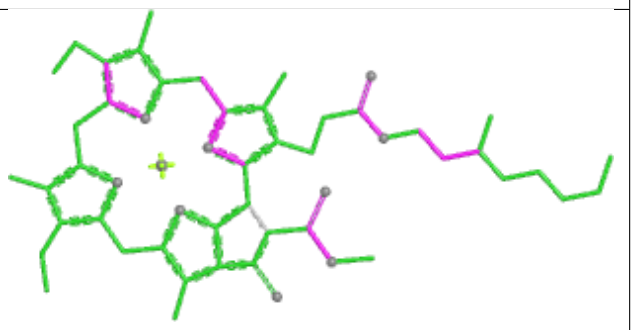


Rings

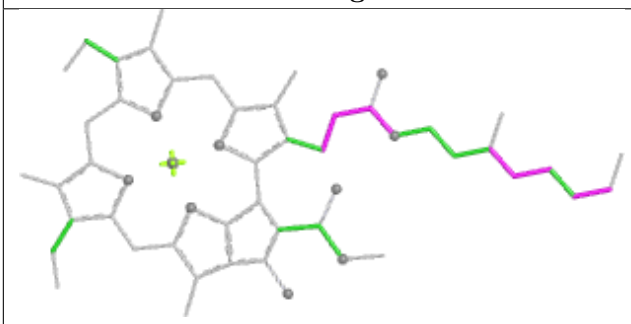
Ligand CLA K 209



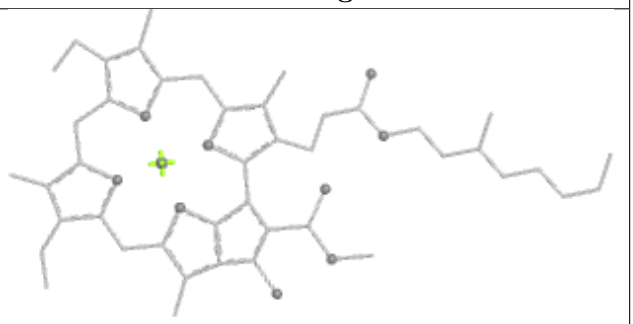
Bond lengths



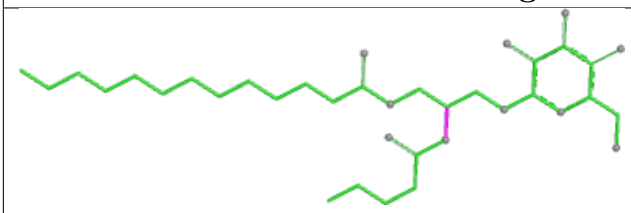
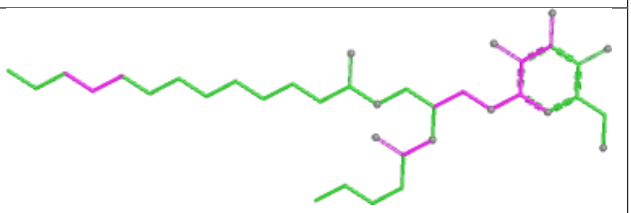
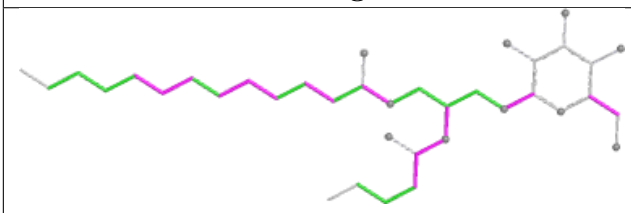
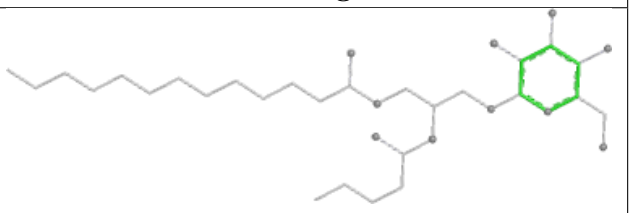
Bond angles

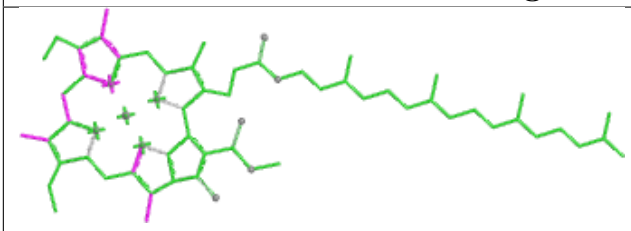
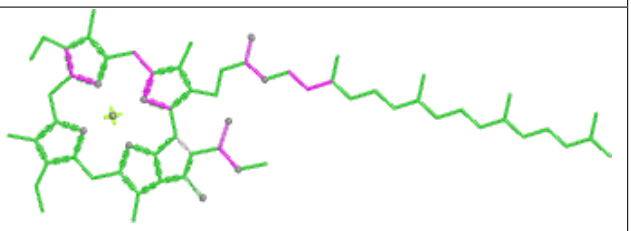
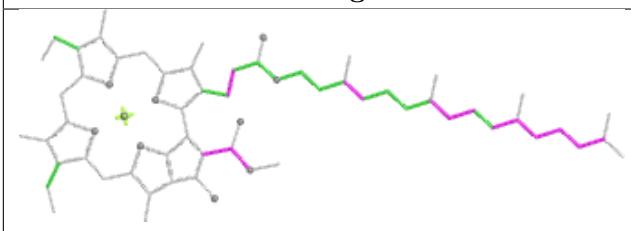
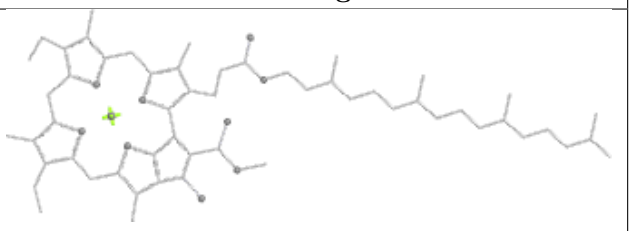


Torsions

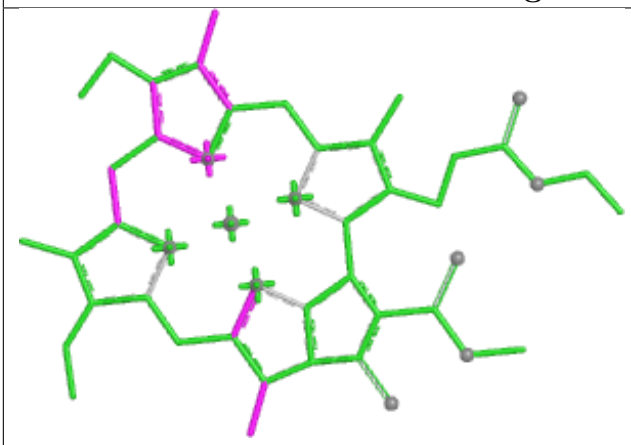


Rings

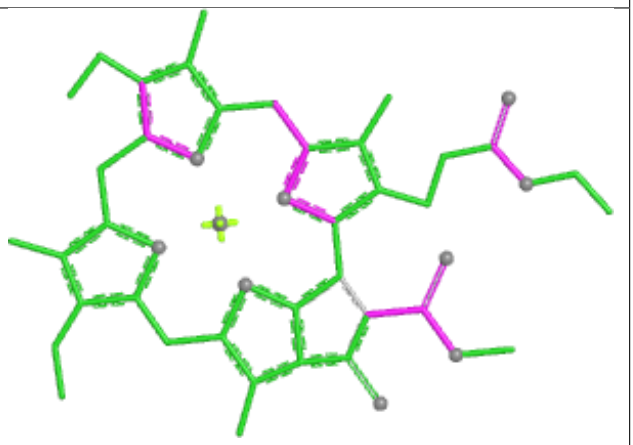
Ligand LMG A 219	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 209	
 Bond lengths	 Bond angles
 Torsions	 Rings

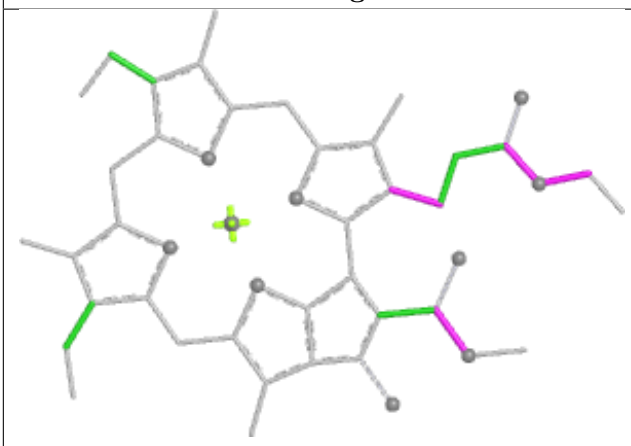
Ligand CLA C 314



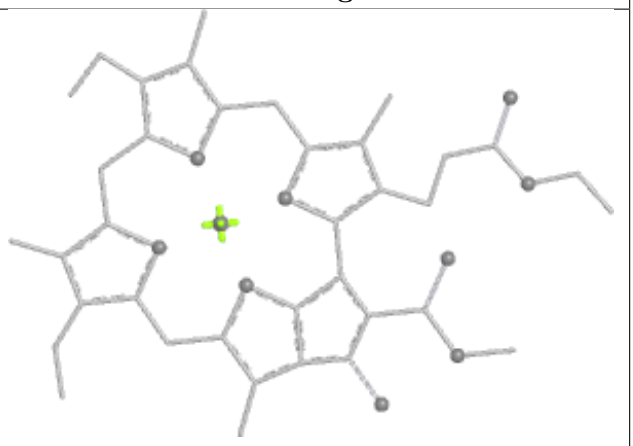
Bond lengths



Bond angles

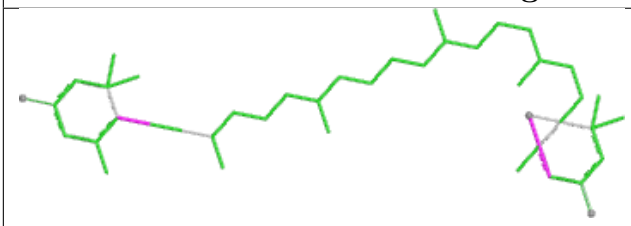


Torsions

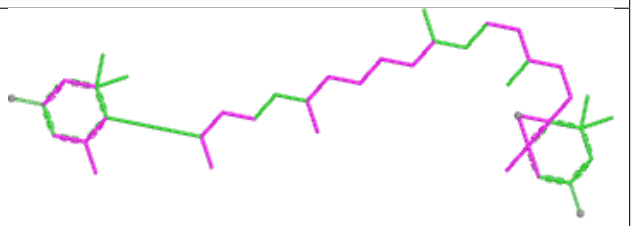


Rings

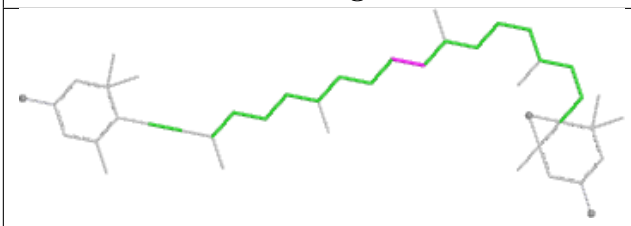
Ligand DD6 M 302



Bond lengths



Bond angles

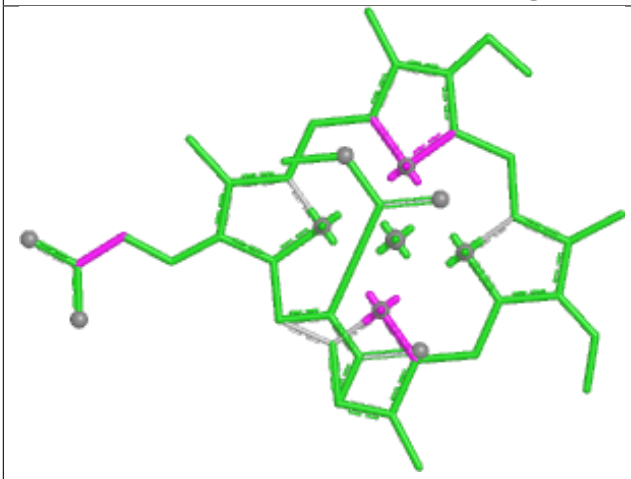


Torsions

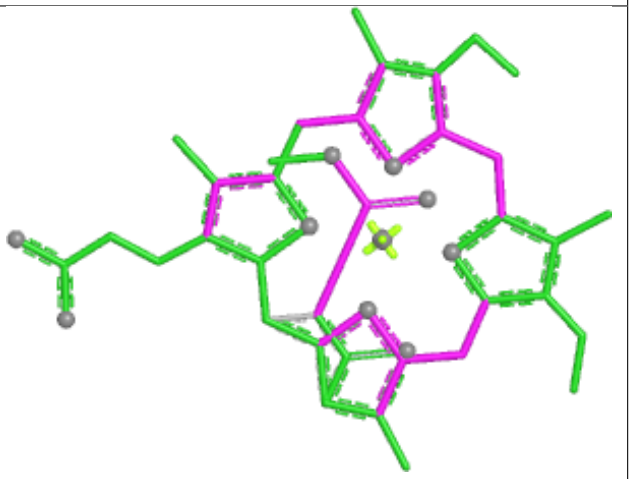


Rings

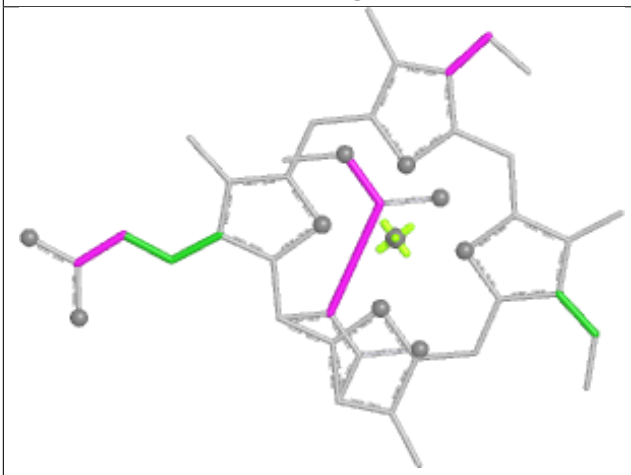
Ligand KC1 H 311



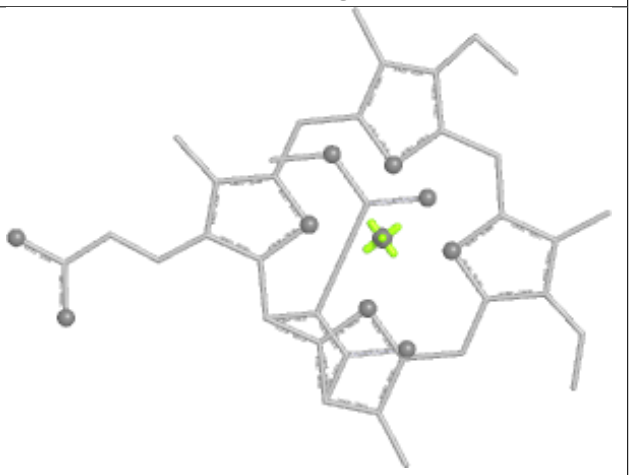
Bond lengths



Bond angles

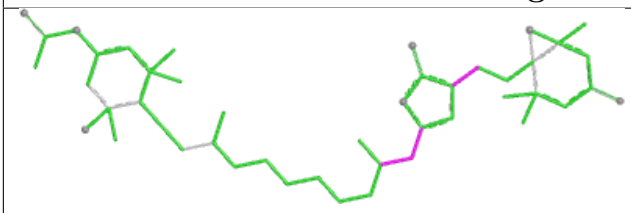


Torsions

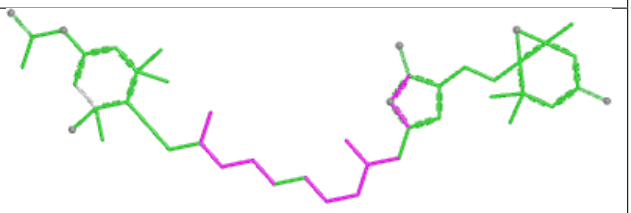


Rings

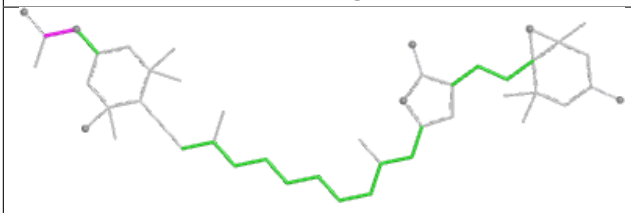
Ligand PID G 309



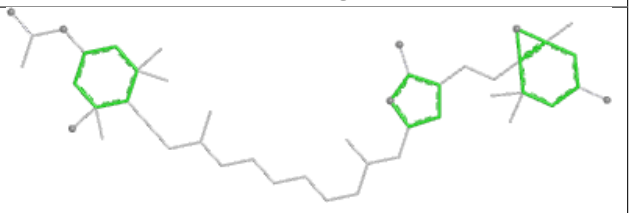
Bond lengths



Bond angles

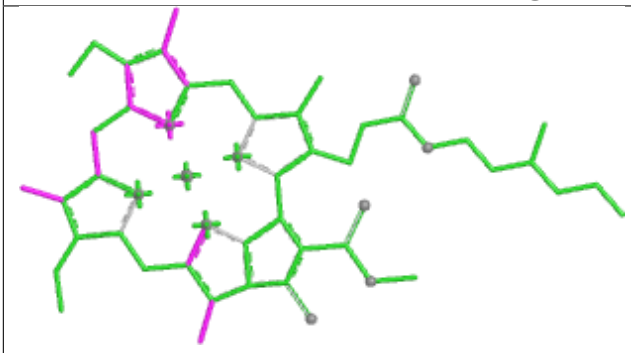


Torsions

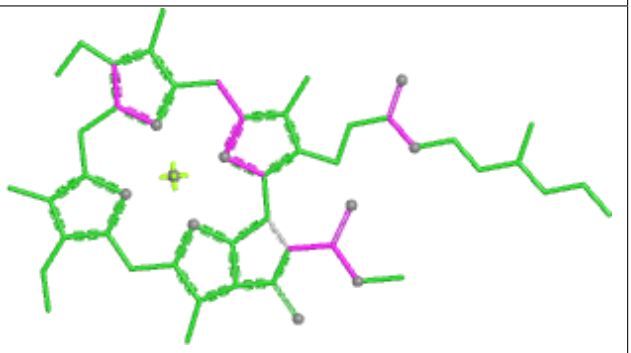


Rings

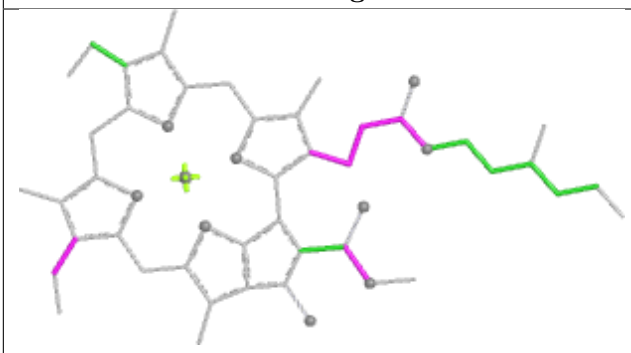
Ligand CLA L 316



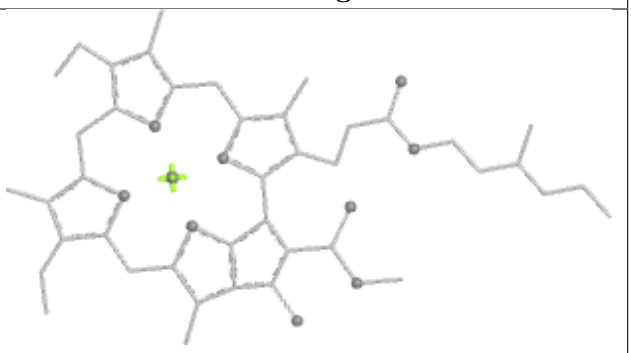
Bond lengths



Bond angles

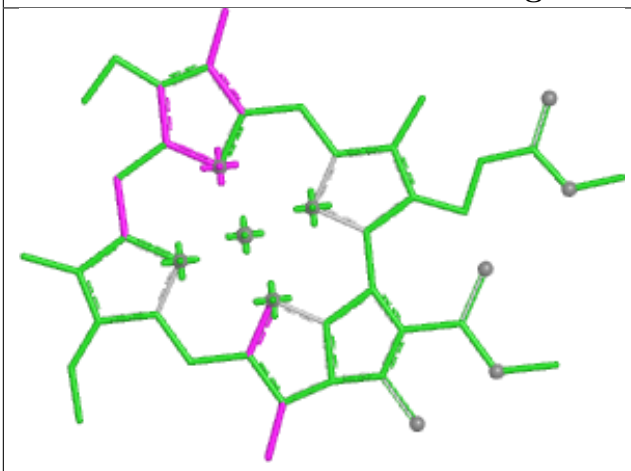


Torsions

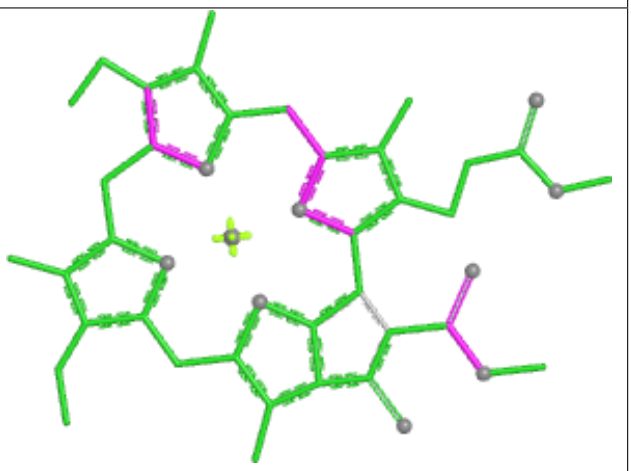


Rings

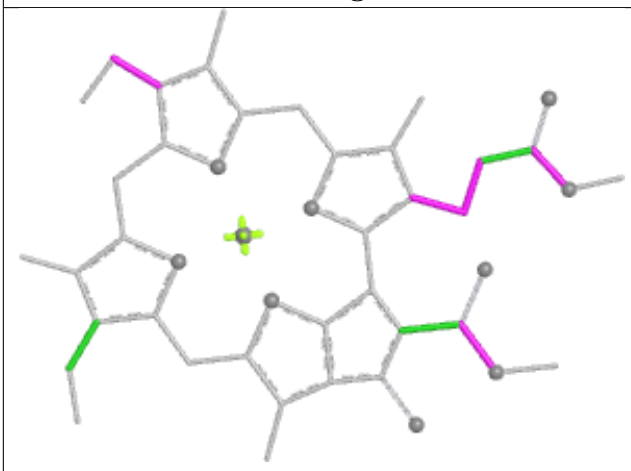
Ligand CLA P 214



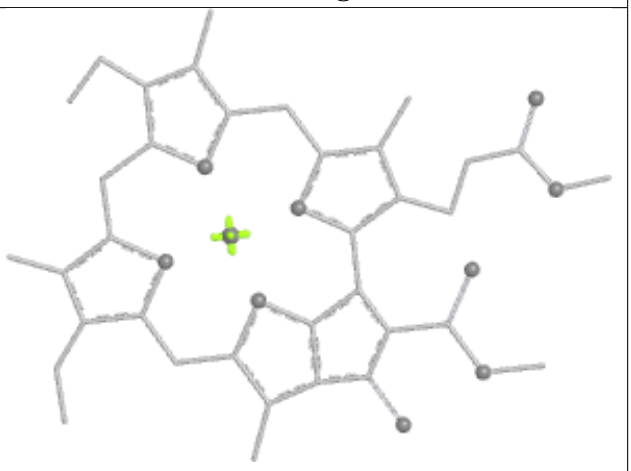
Bond lengths



Bond angles

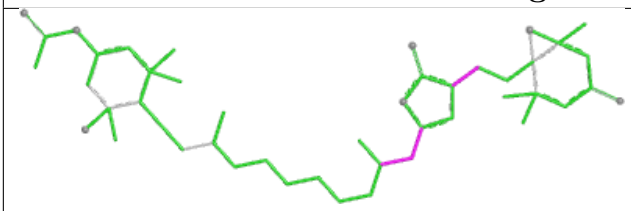


Torsions

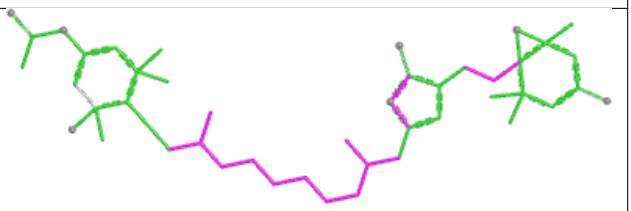


Rings

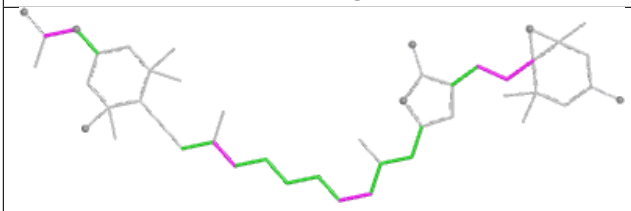
Ligand PID C 305



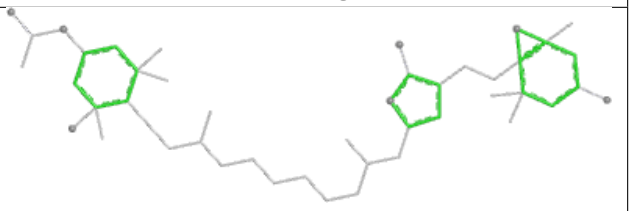
Bond lengths



Bond angles

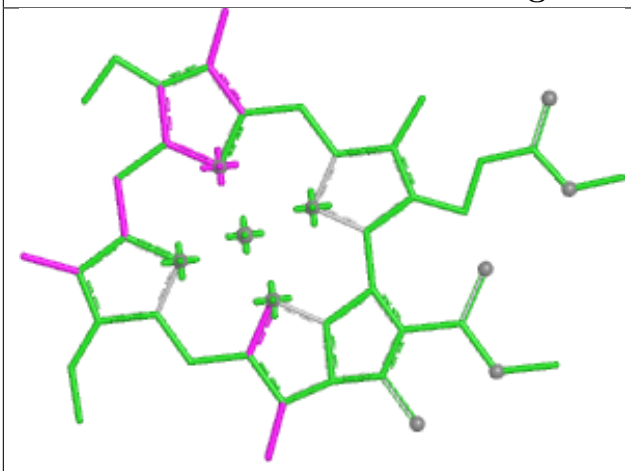


Torsions

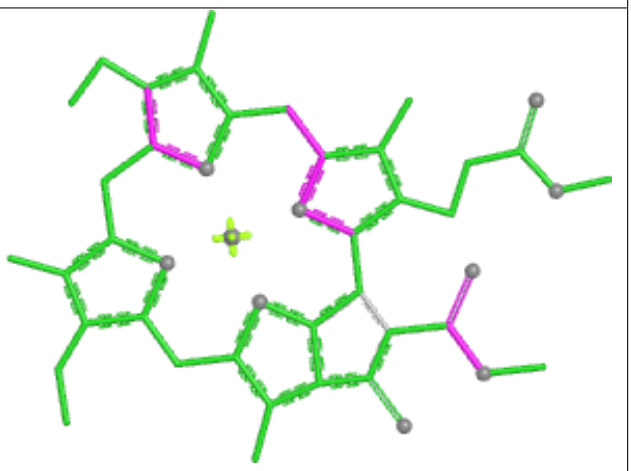


Rings

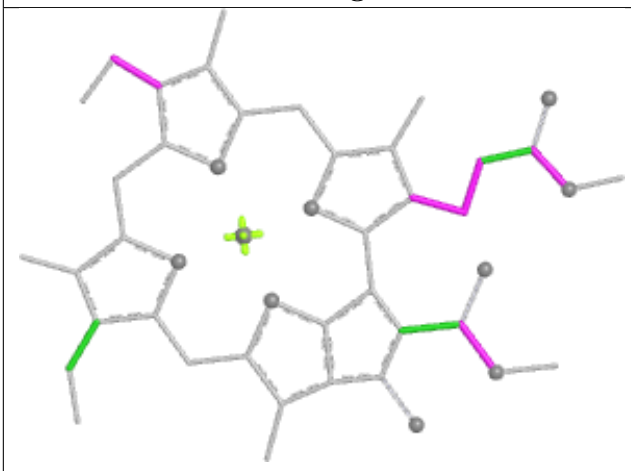
Ligand CLA a 816



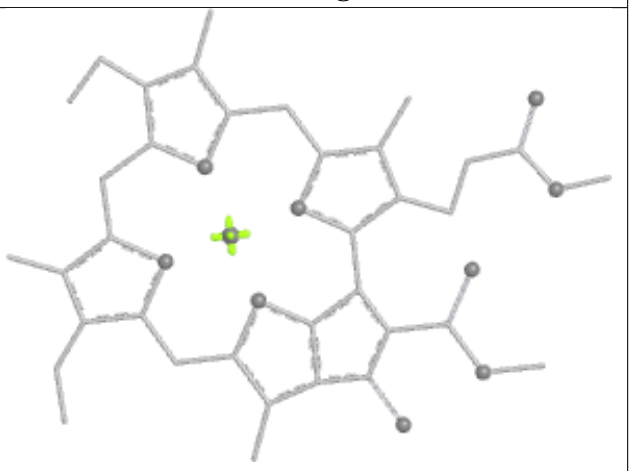
Bond lengths



Bond angles



Torsions

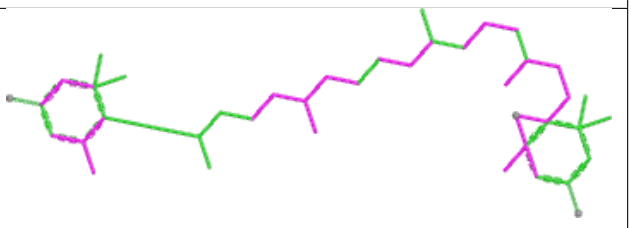


Rings

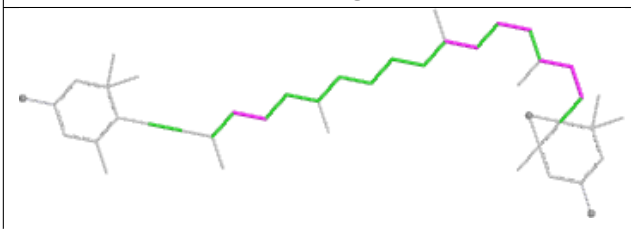
Ligand DD6 D 301



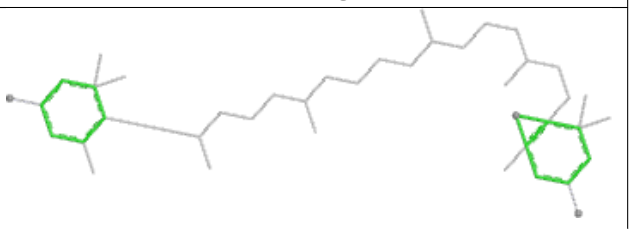
Bond lengths



Bond angles

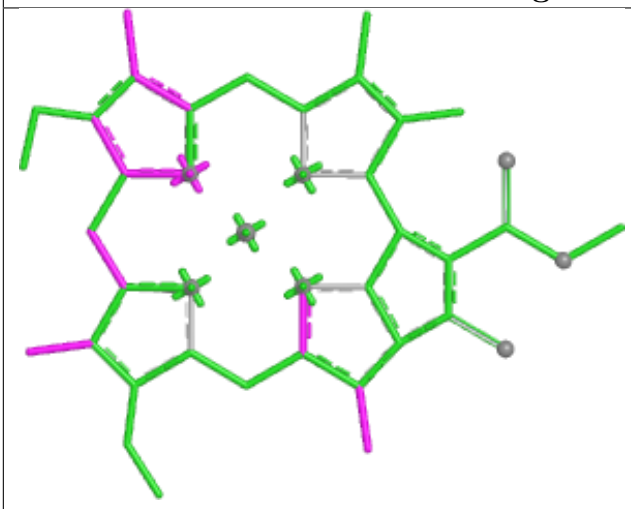


Torsions

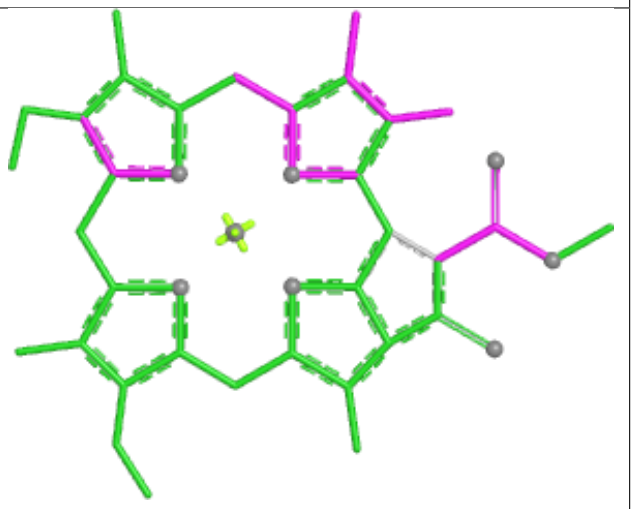


Rings

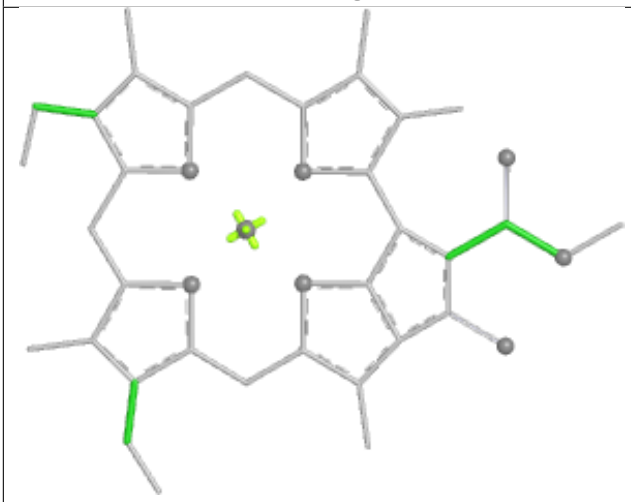
Ligand CLA l 509



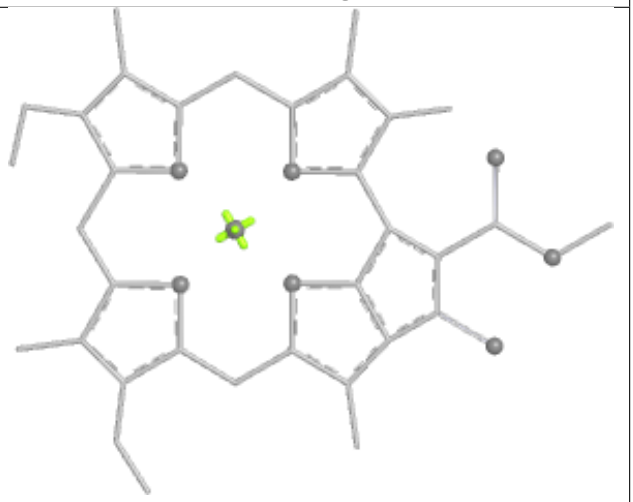
Bond lengths



Bond angles

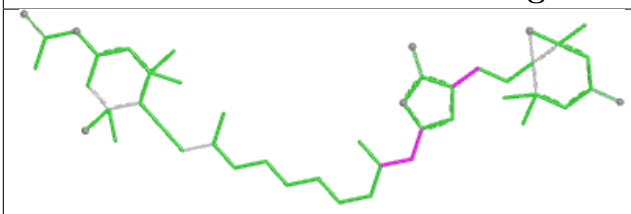


Torsions

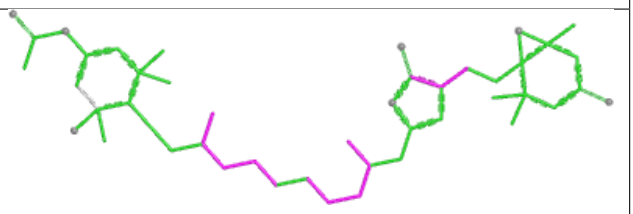


Rings

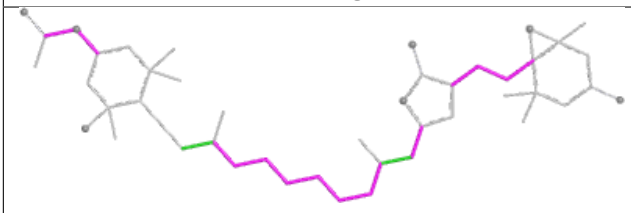
Ligand PID N 305



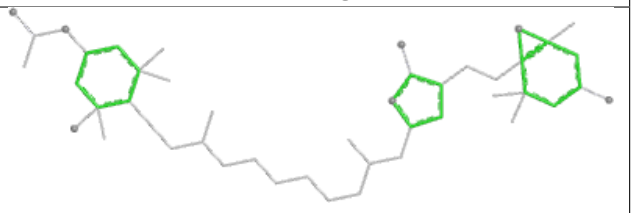
Bond lengths



Bond angles

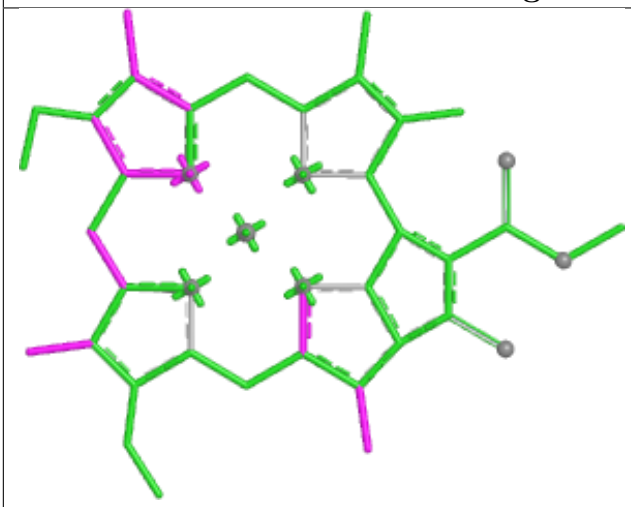


Torsions

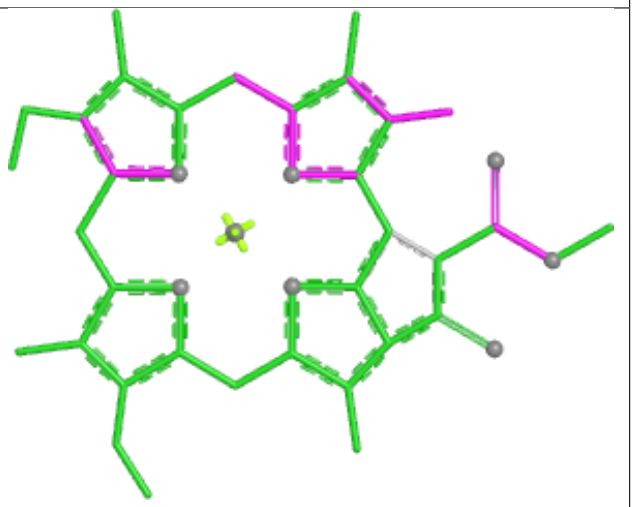


Rings

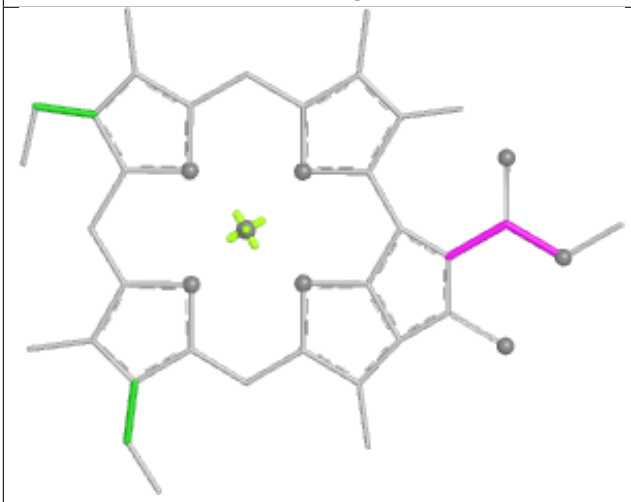
Ligand CLA K 216



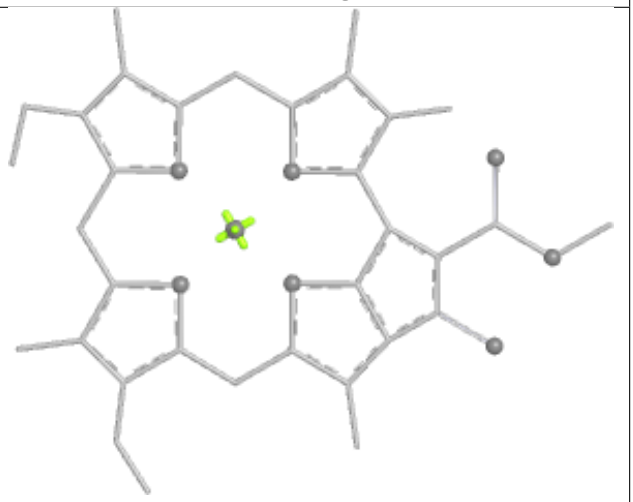
Bond lengths



Bond angles

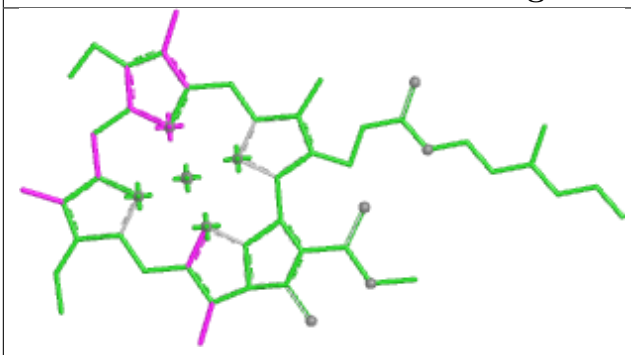


Torsions

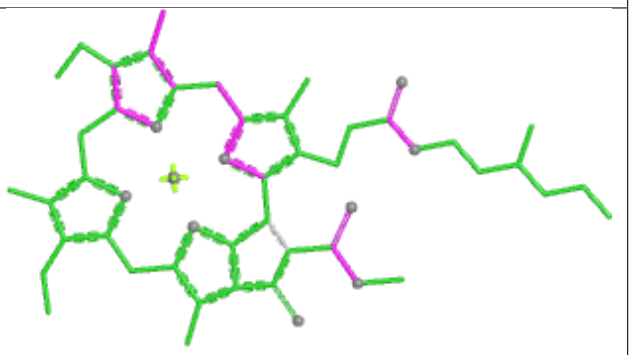


Rings

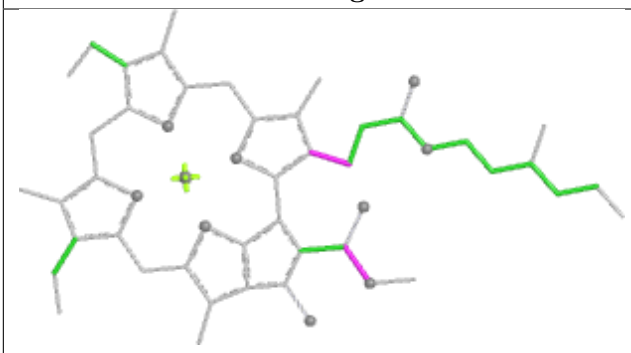
Ligand CLA b 708



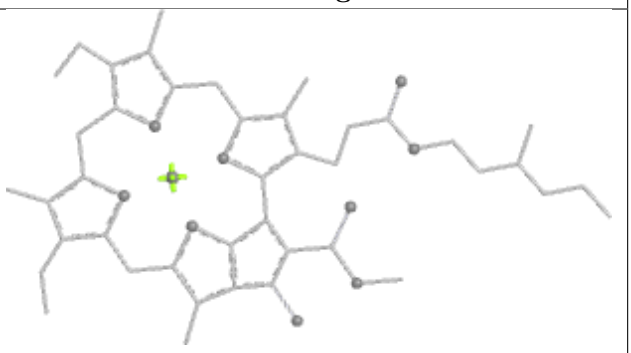
Bond lengths



Bond angles

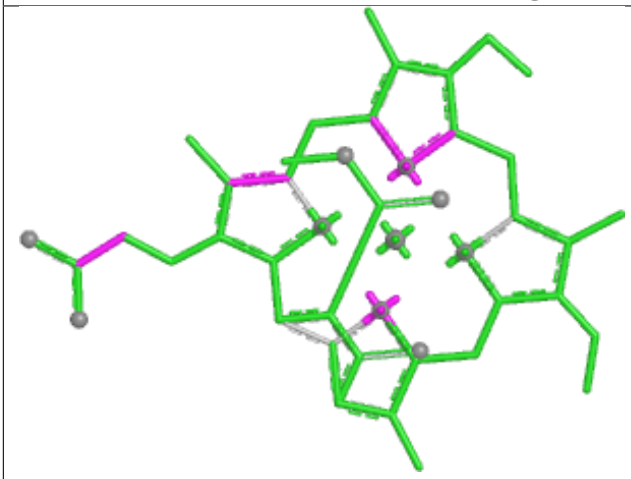


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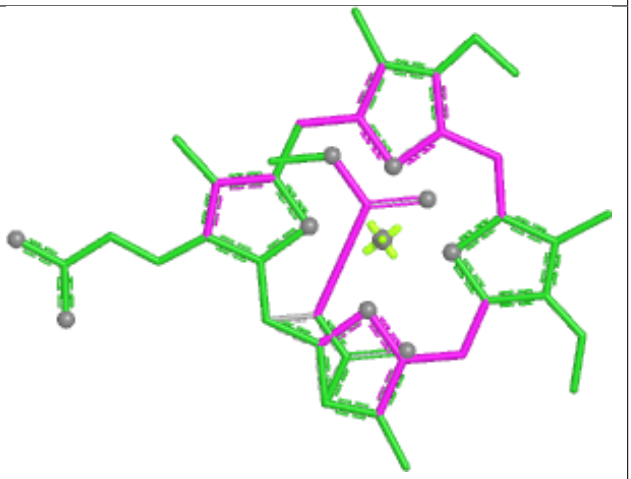


Rings

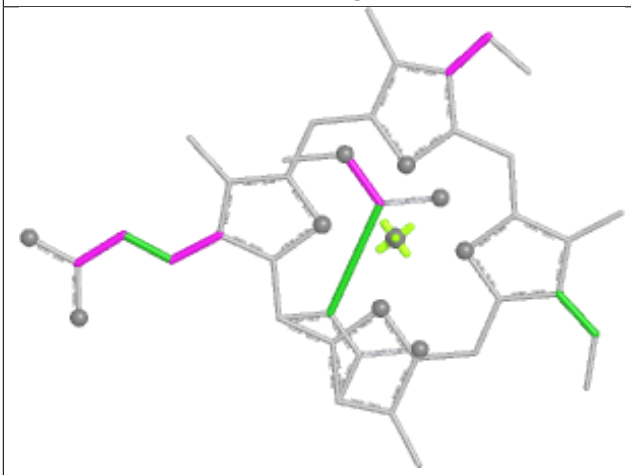
Ligand KC1 C 310



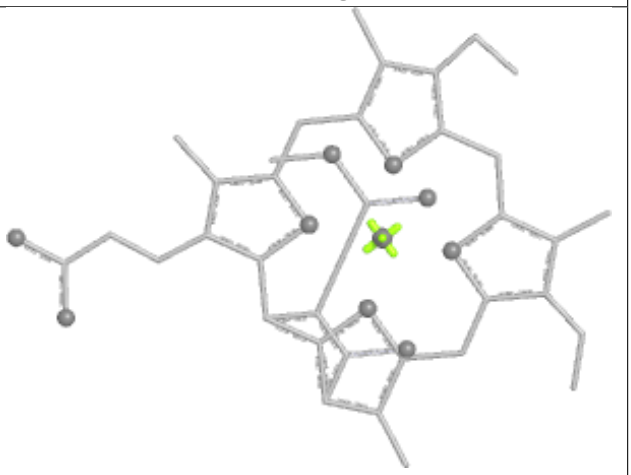
Bond lengths



Bond angles

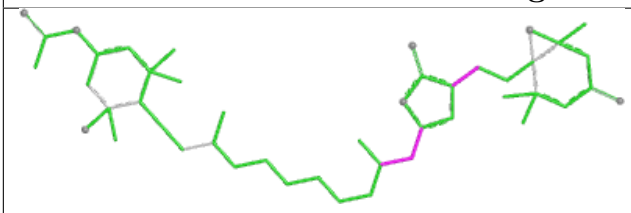


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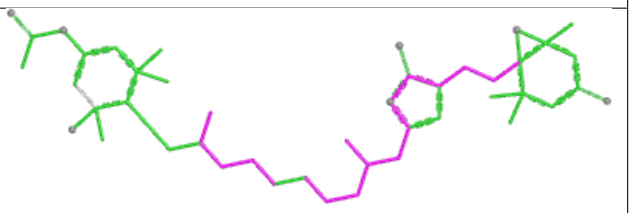


Rings

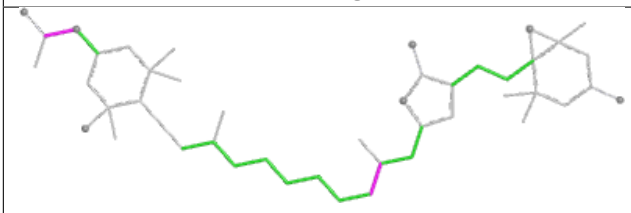
Ligand PID D 306



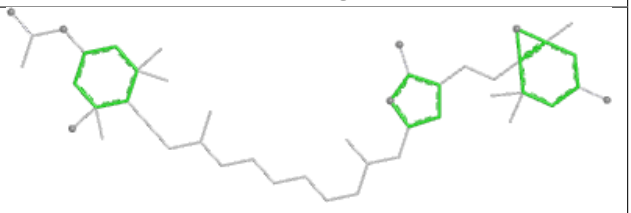
Bond lengths



Bond angles

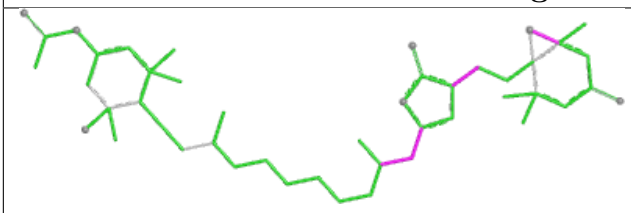


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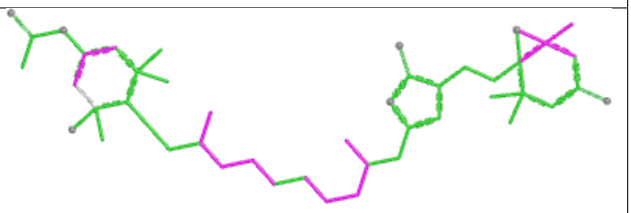


Rings

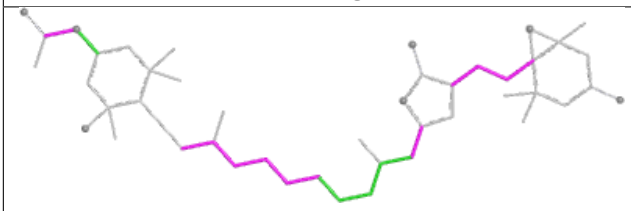
Ligand PID F 304



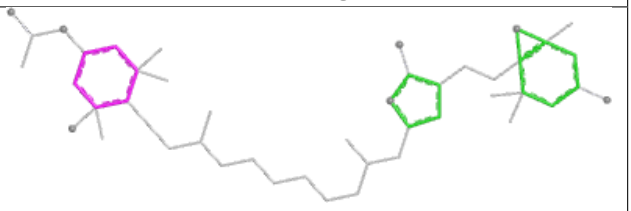
Bond lengths



Bond angles

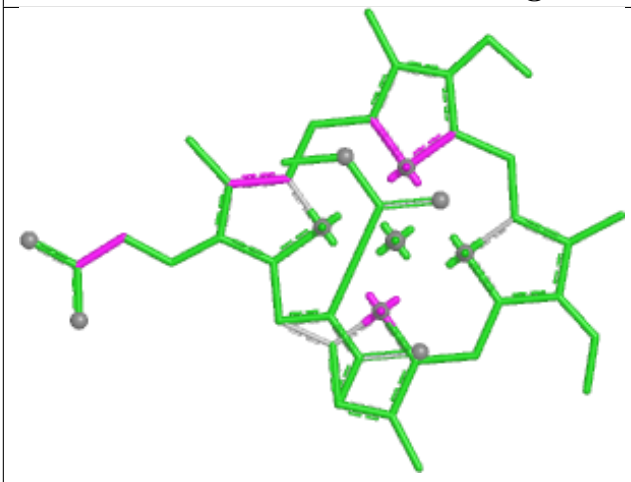


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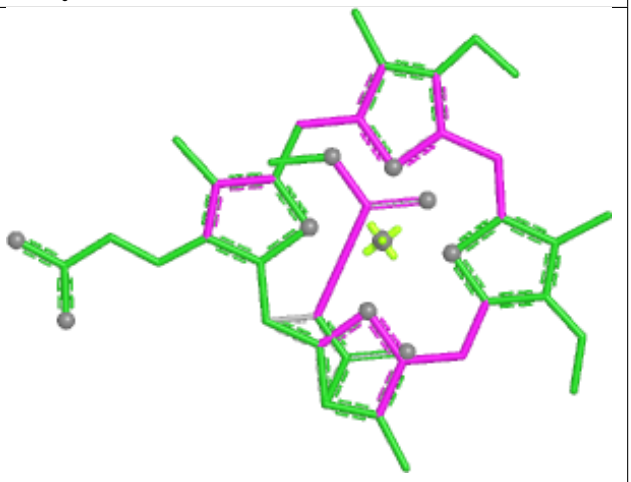


Rings

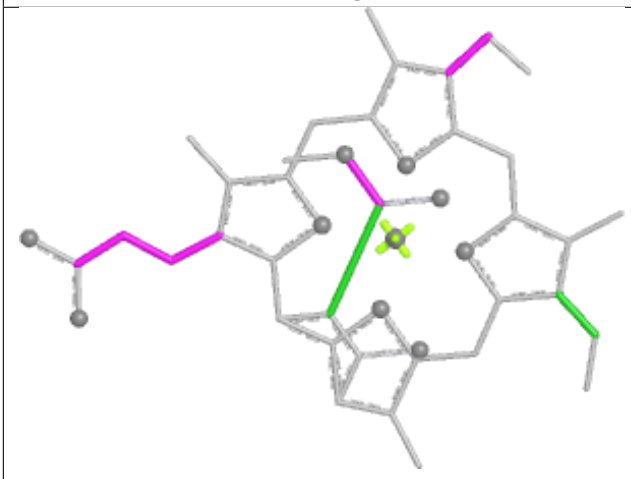
Ligand KC1 Q 314



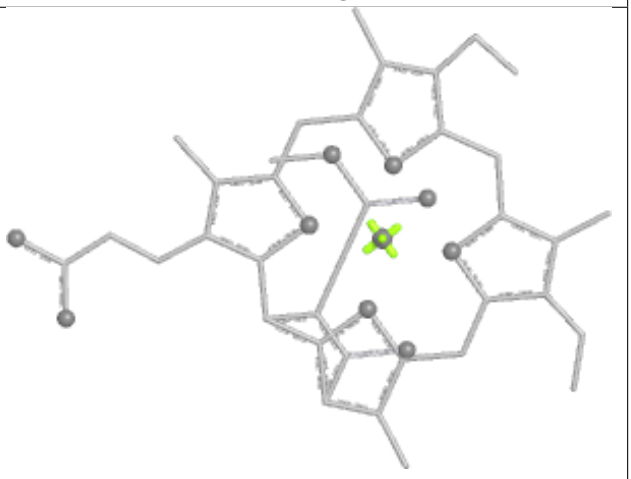
Bond lengths



Bond angles

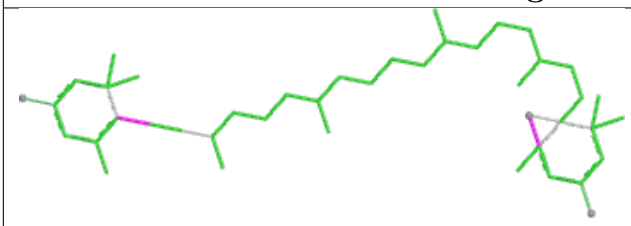


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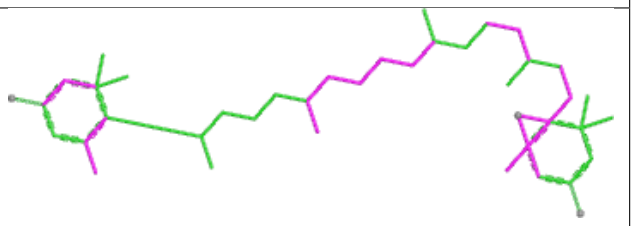


Rings

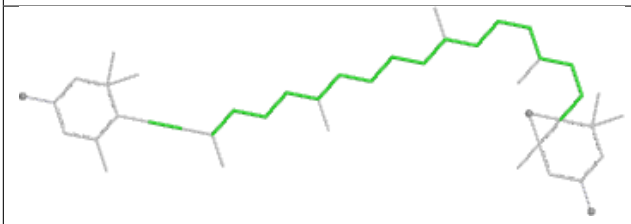
Ligand DD6 F 303



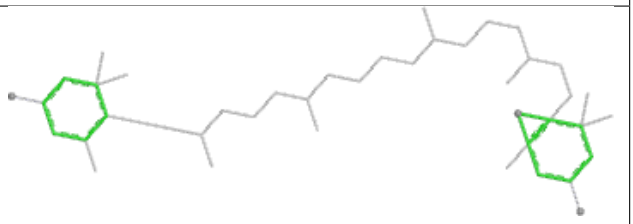
Bond lengths



Bond angles

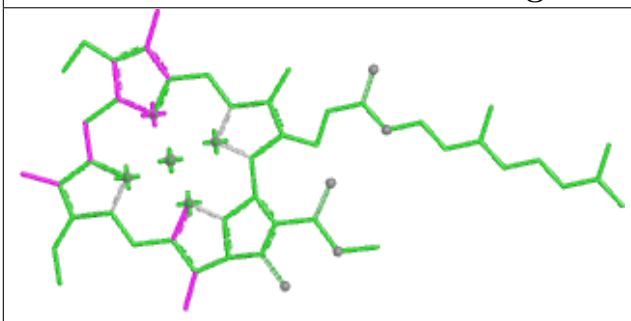


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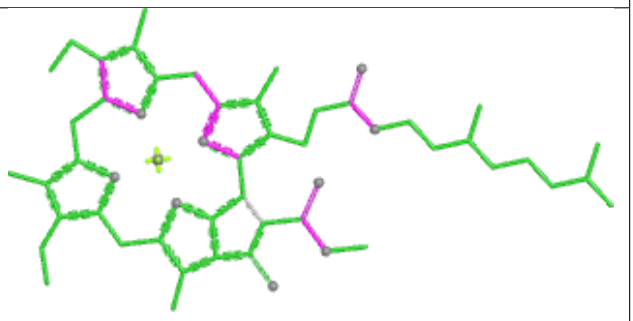


Rings

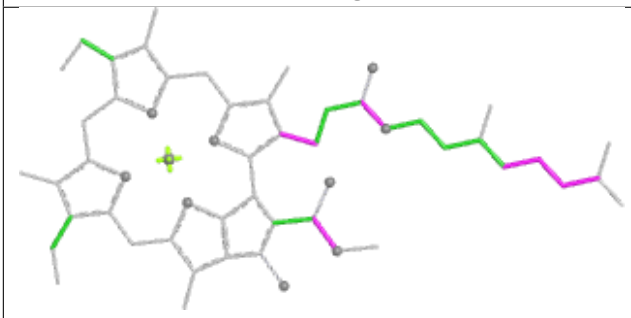
Ligand CLA L 312



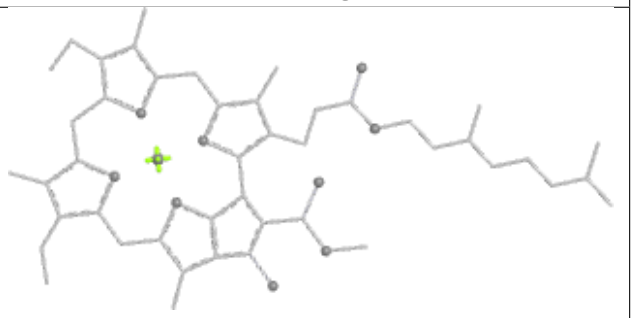
Bond lengths



Bond angles

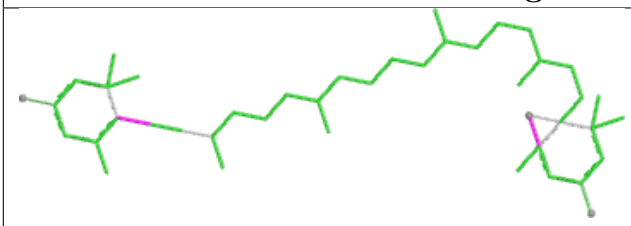


Torsions

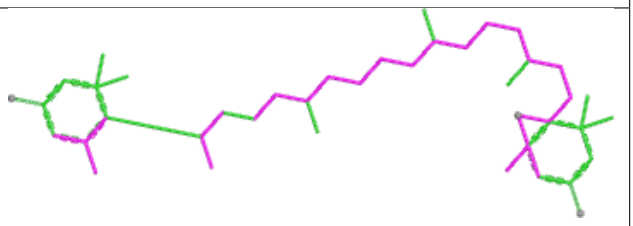


Rings

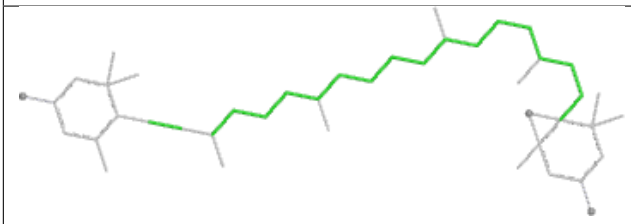
Ligand DD6 C 303



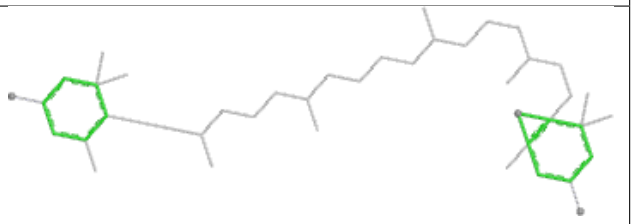
Bond lengths



Bond angles

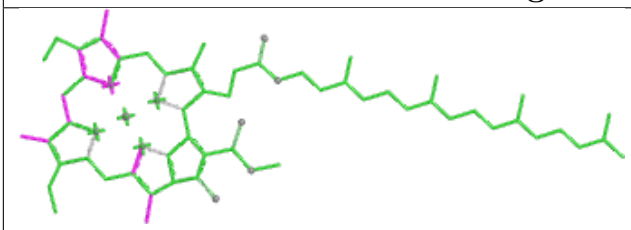


Torsions

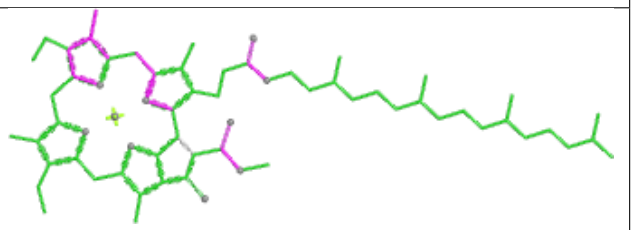


Rings

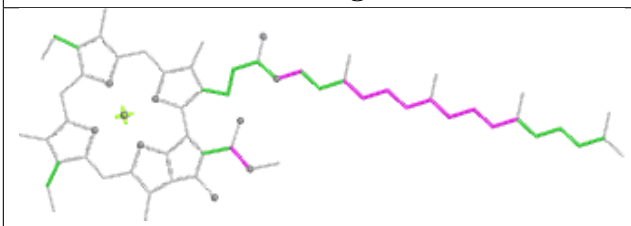
Ligand CLA b 718



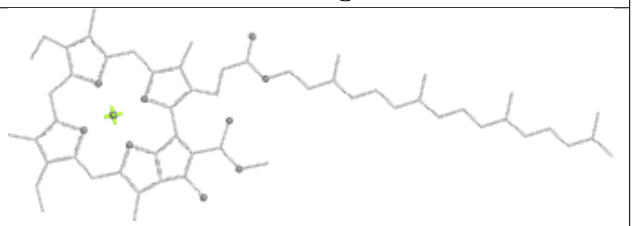
Bond lengths



Bond angles

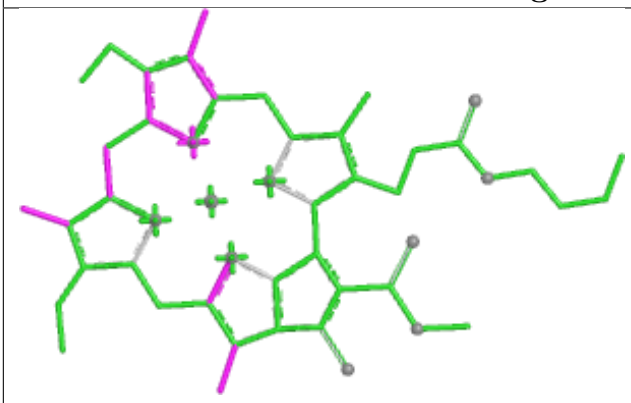


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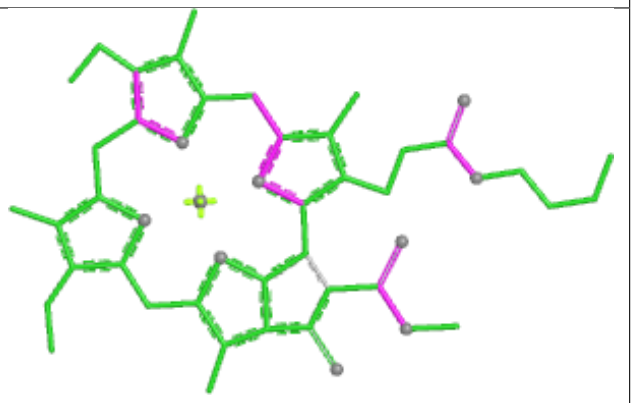


Rings

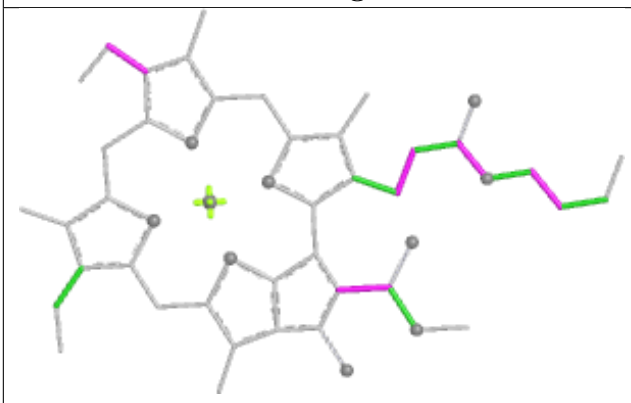
Ligand CLA I 207



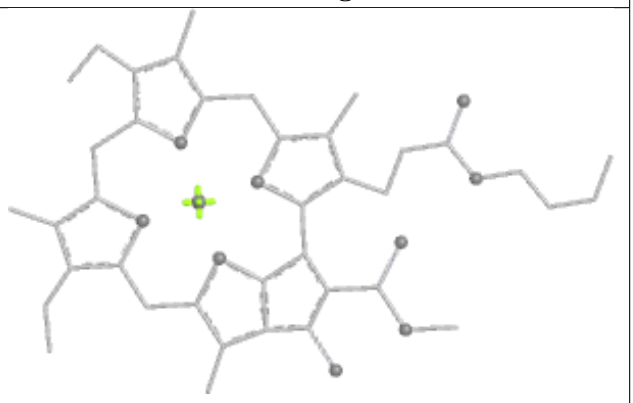
Bond lengths



Bond angles

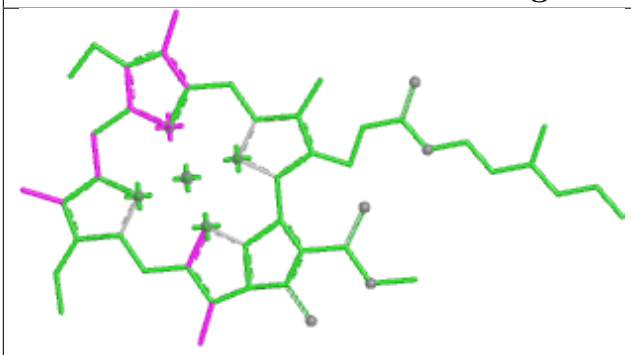


Torsions

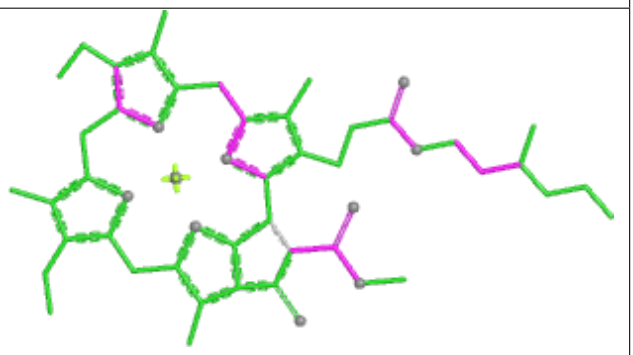


Rings

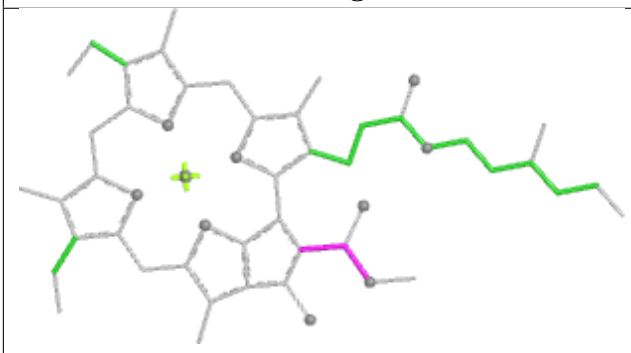
Ligand CLA I 216



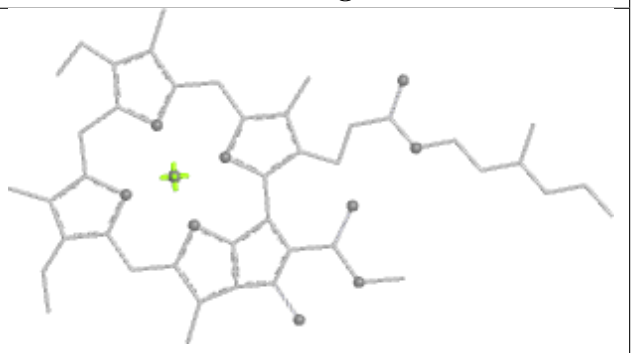
Bond lengths



Bond angles

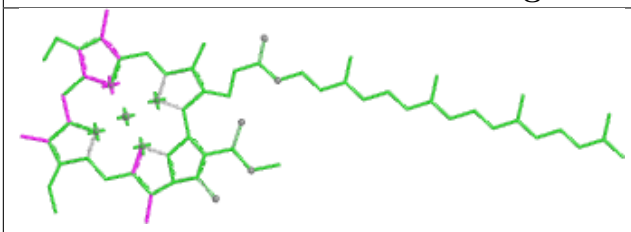


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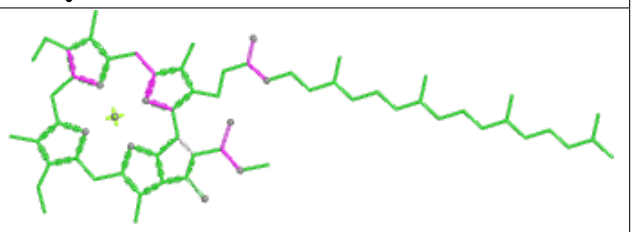


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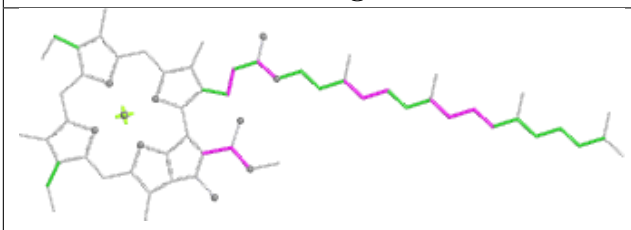
Ligand CLA Q 310



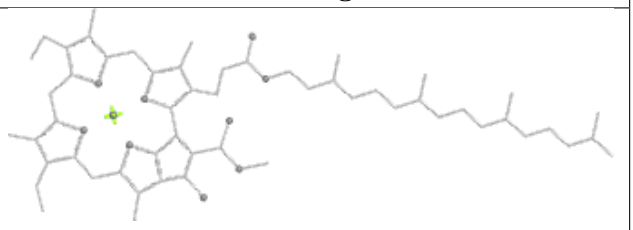
Bond lengths



Bond angles

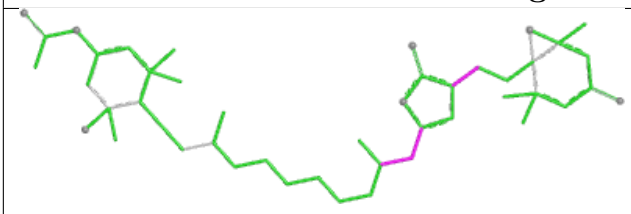


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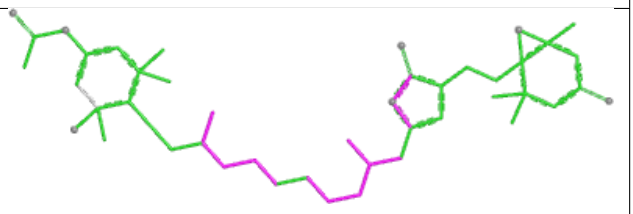


Rings

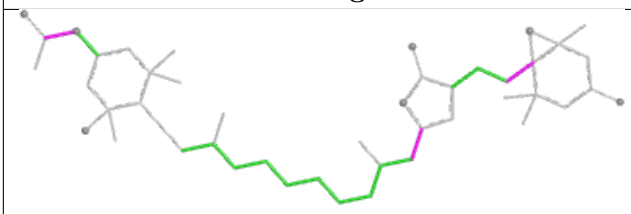
Ligand PID C 301



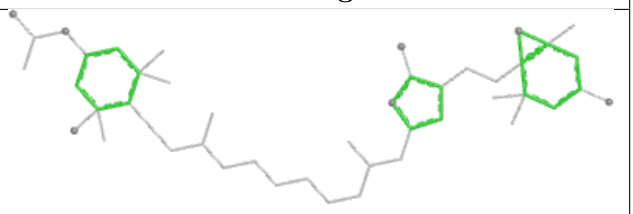
Bond lengths



Bond angles

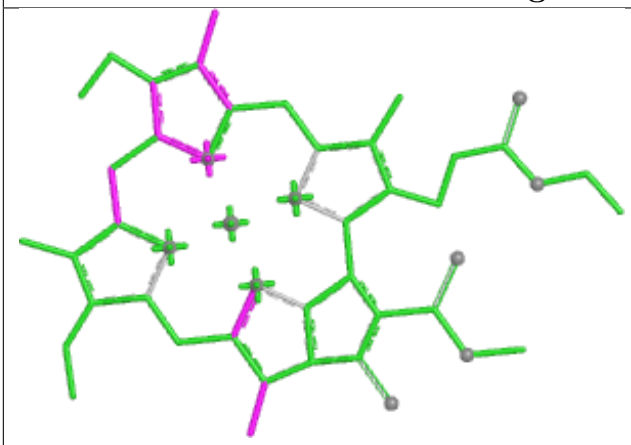


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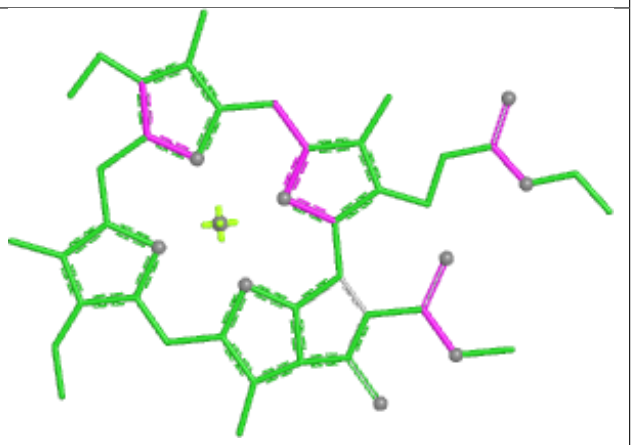


Rings

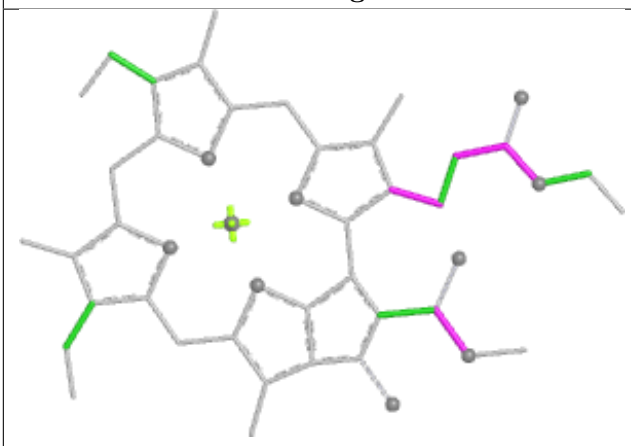
Ligand CLA a 821



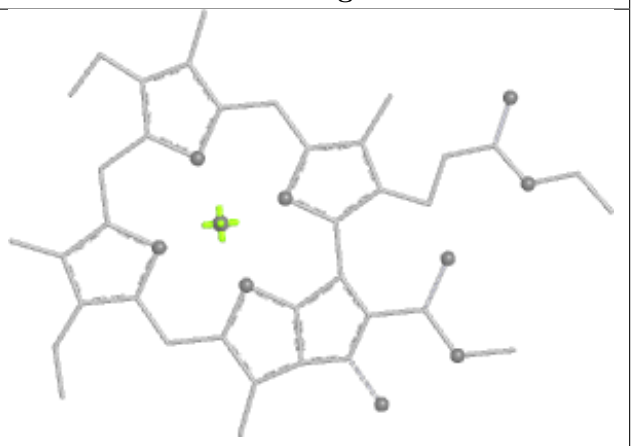
Bond lengths



Bond angles

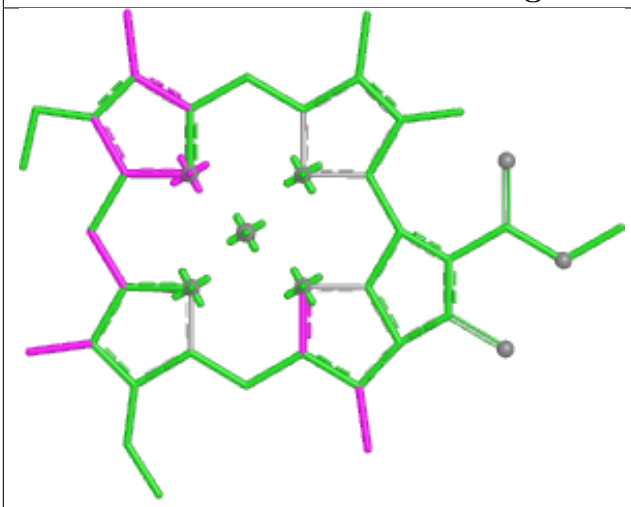


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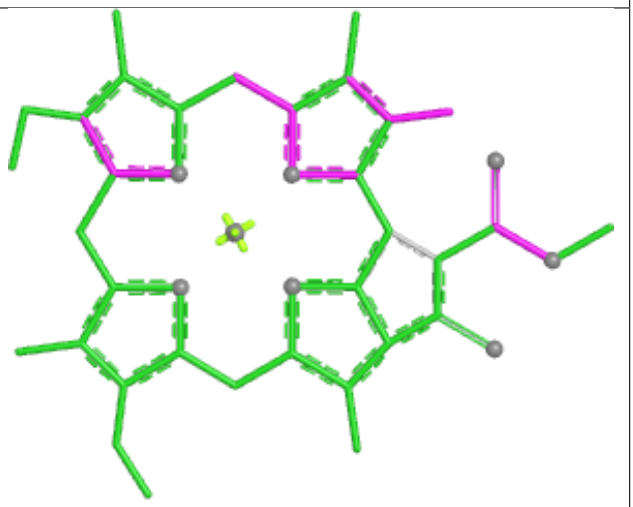


Rings

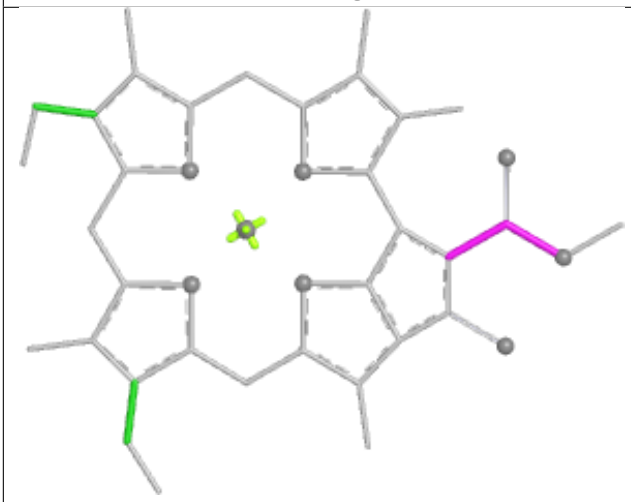
Ligand CLA B 314



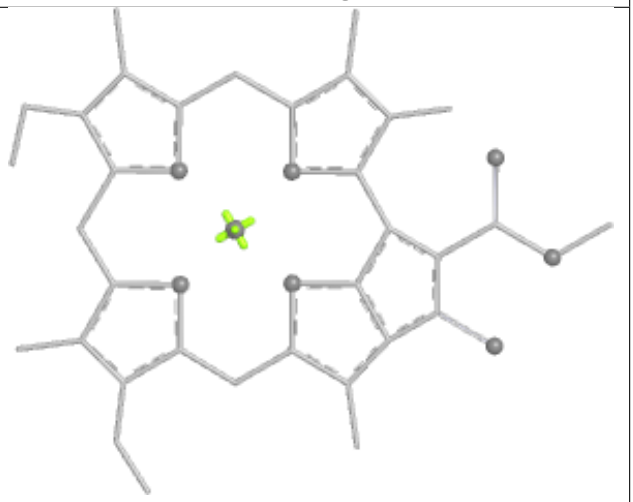
Bond lengths



Bond angles

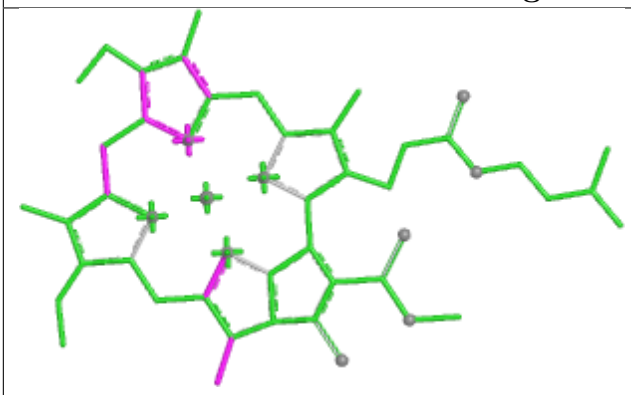


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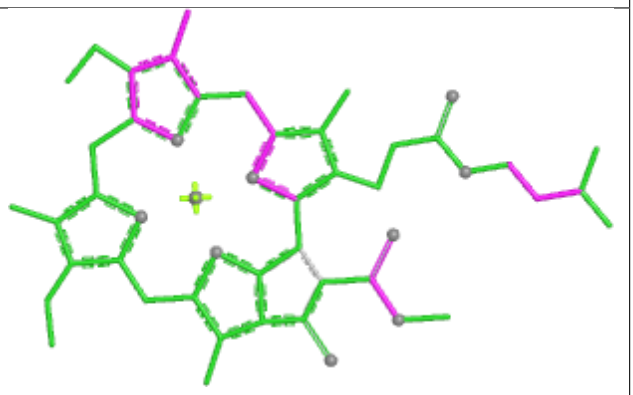


Rings

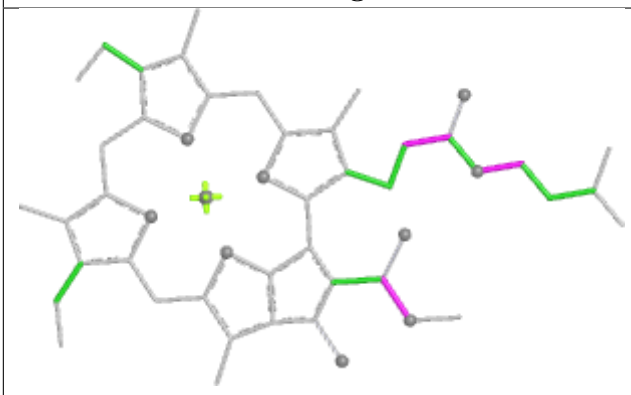
Ligand CLA K 210



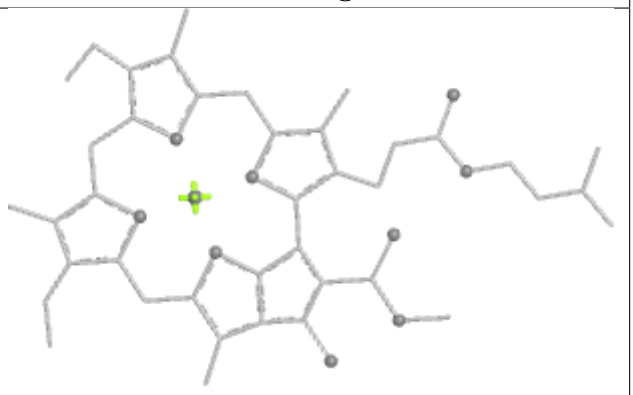
Bond lengths



Bond angles

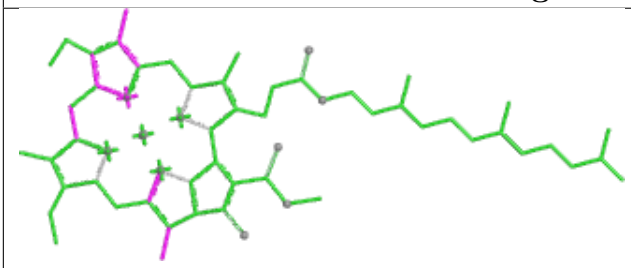


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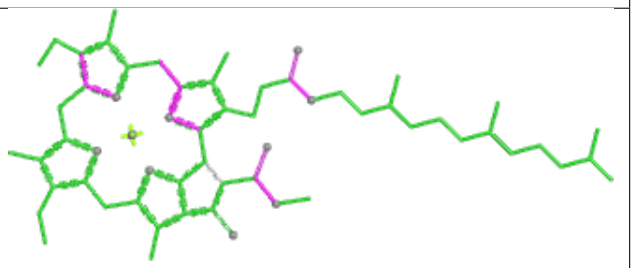


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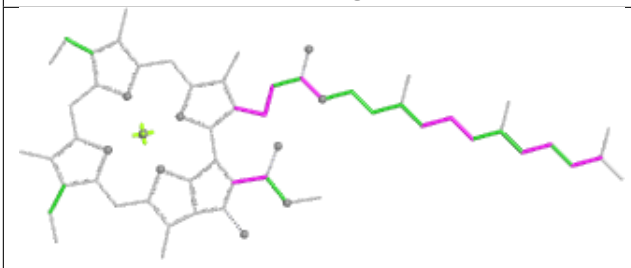
Ligand CLA f 805



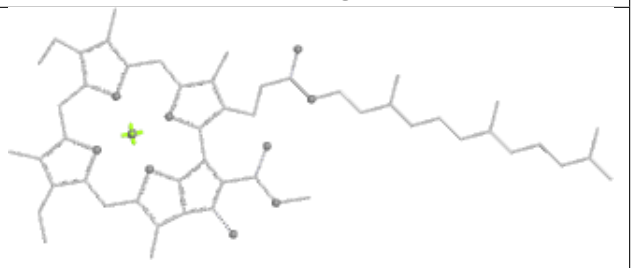
Bond lengths



Bond angles

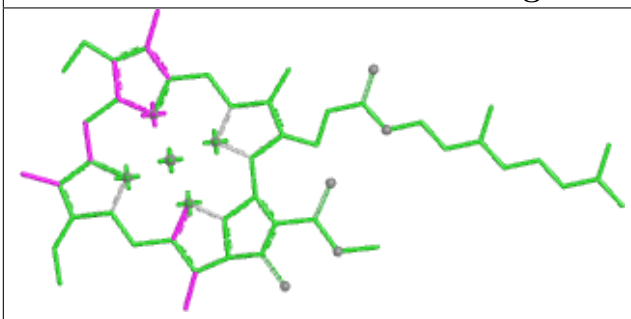


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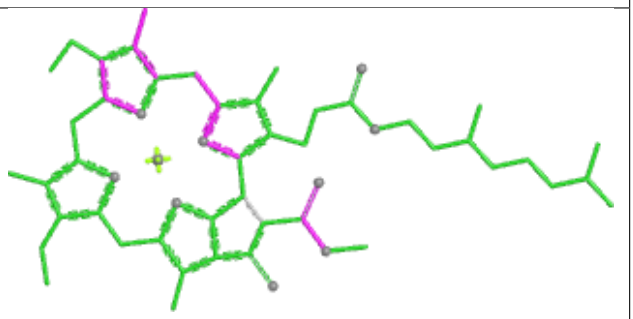


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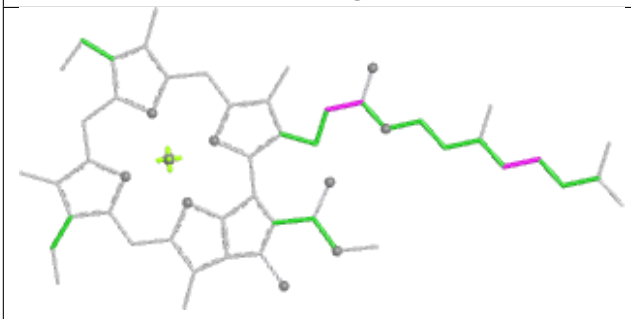
Ligand CLA G 313



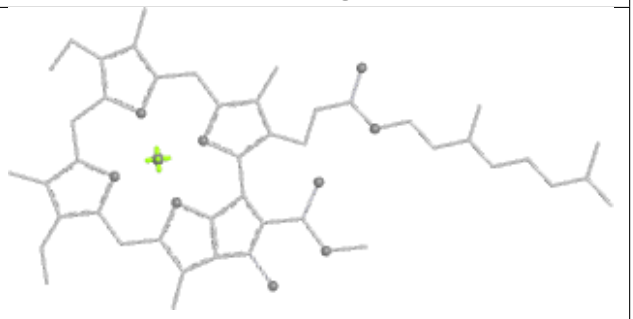
Bond lengths



Bond angles

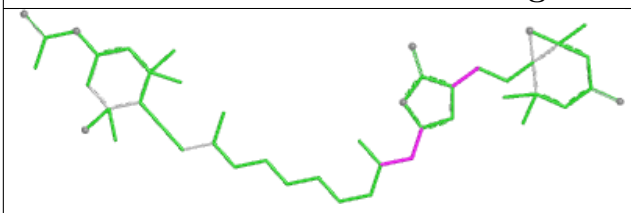


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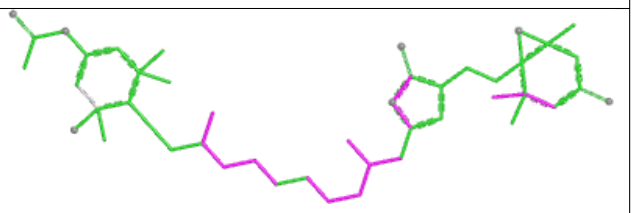


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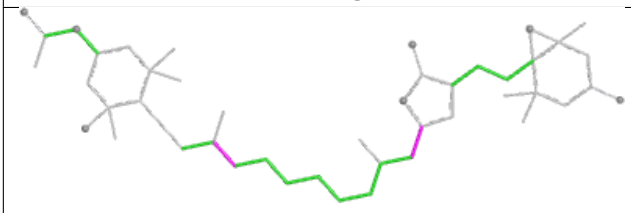
Ligand PID O 304



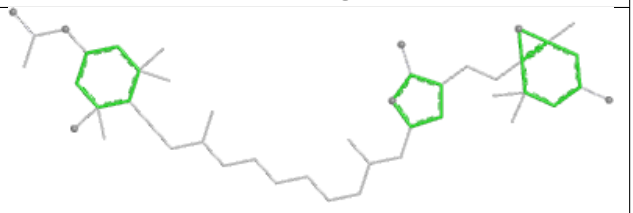
Bond lengths



Bond angles

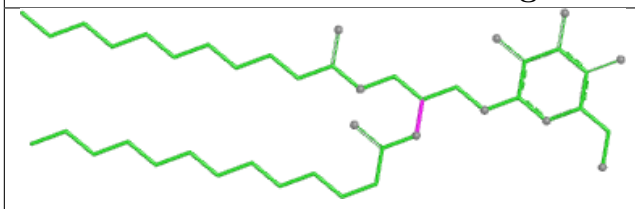


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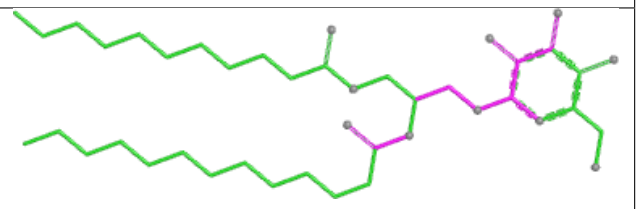


Rings

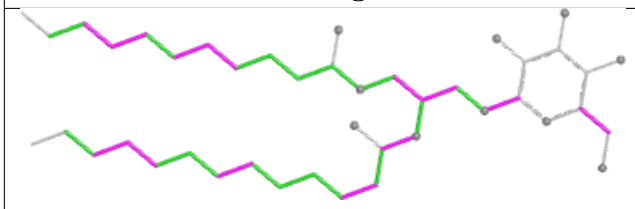
Ligand LMG K 201



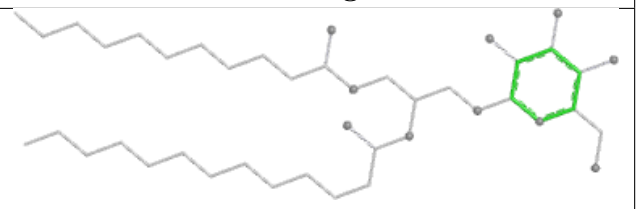
Bond lengths



Bond angles

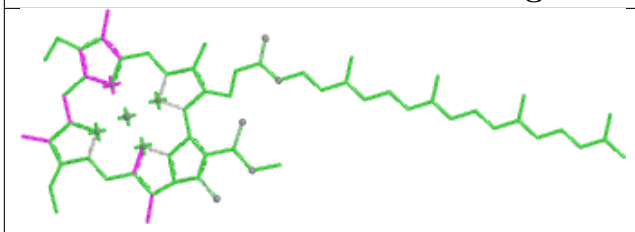


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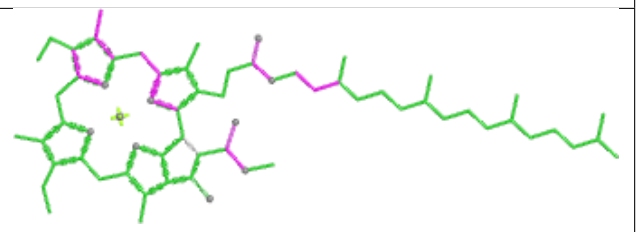


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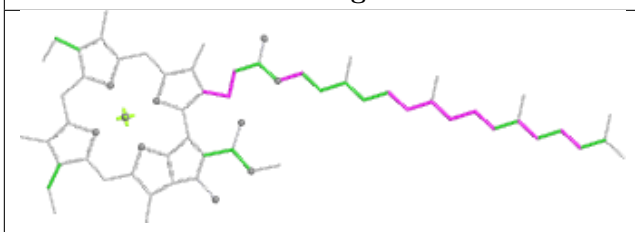
Ligand CLA B 310



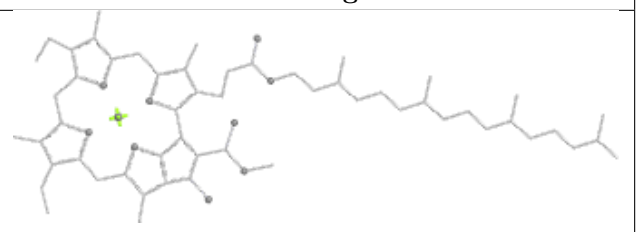
Bond lengths



Bond angles

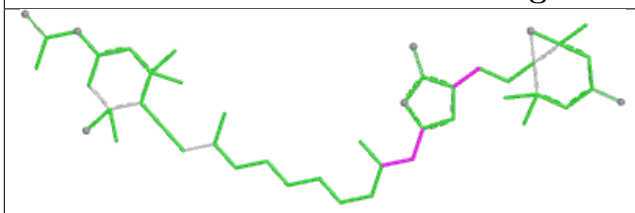


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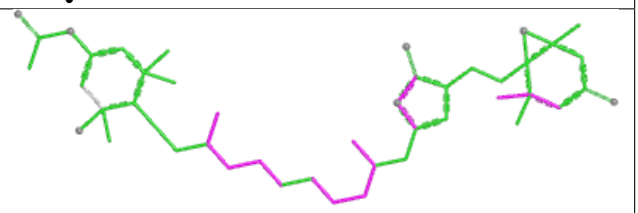


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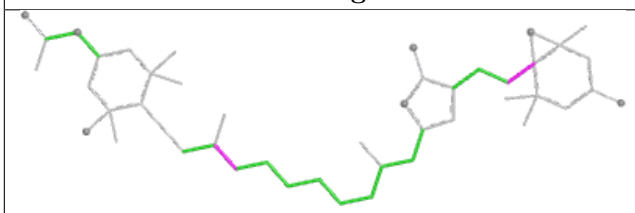
Ligand PID Q 306



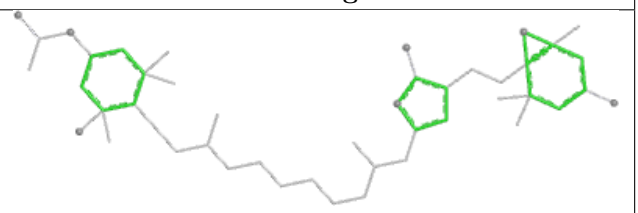
Bond lengths



Bond angles

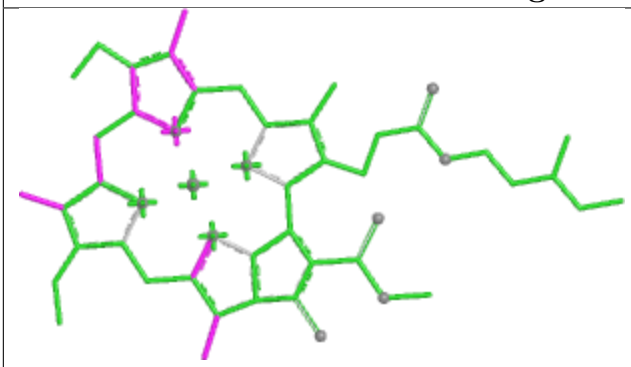


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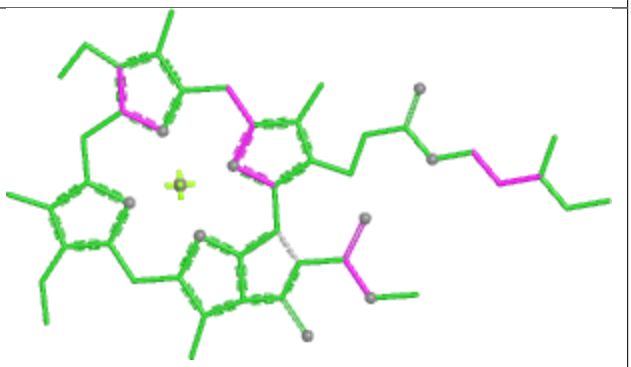


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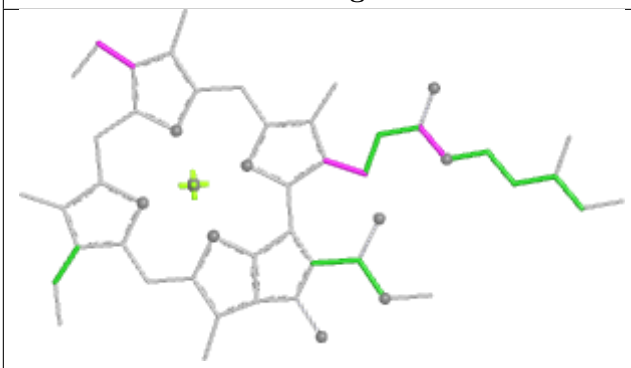
Ligand CLA a 808



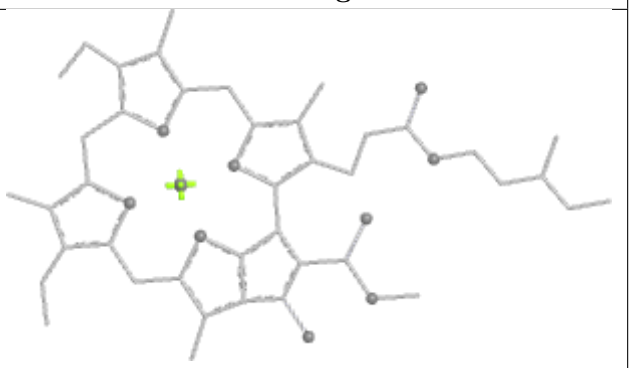
Bond lengths



Bond angles

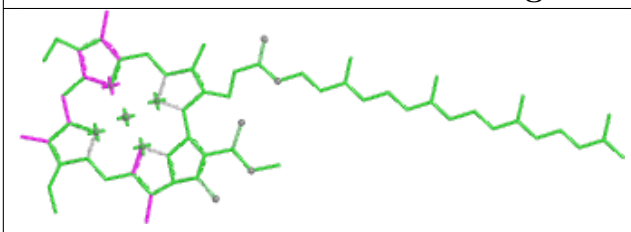


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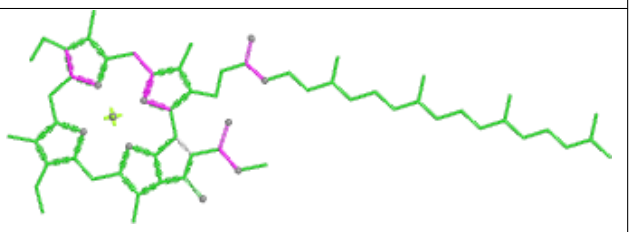


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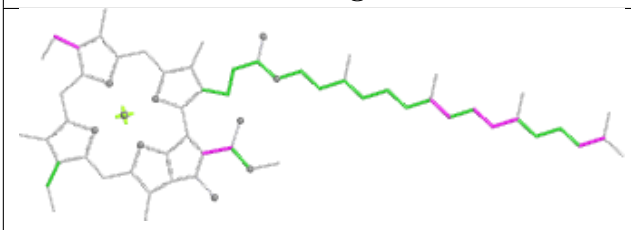
Ligand CLA E 308



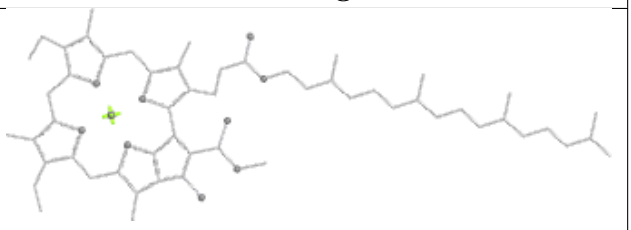
Bond lengths



Bond angles

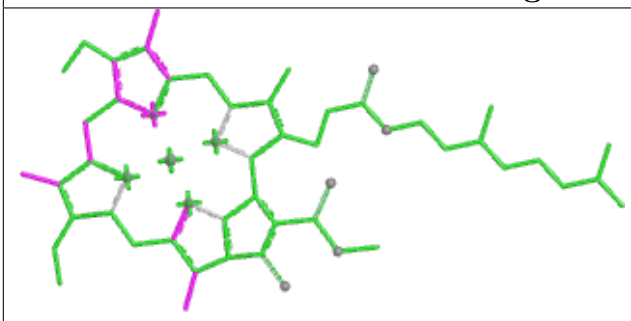


Torsions

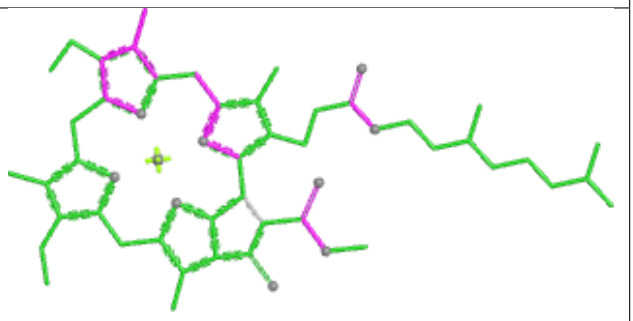


Rings

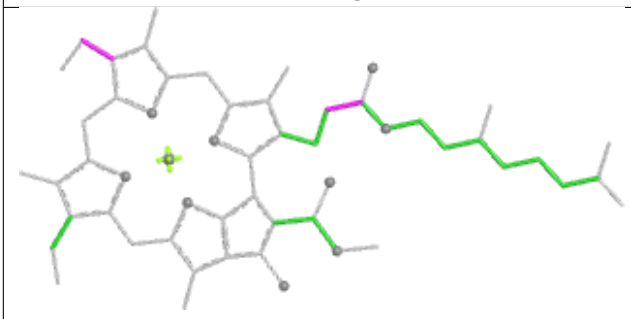
Ligand CLA A 208



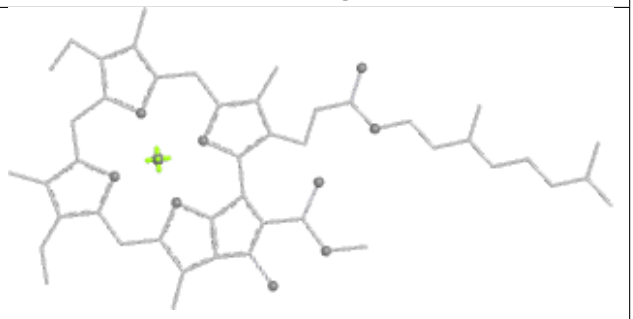
Bond lengths



Bond angles

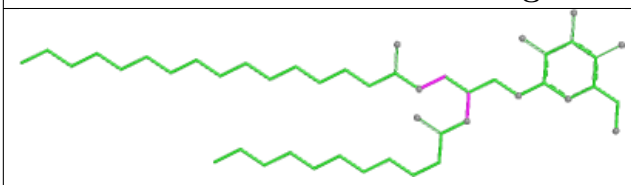


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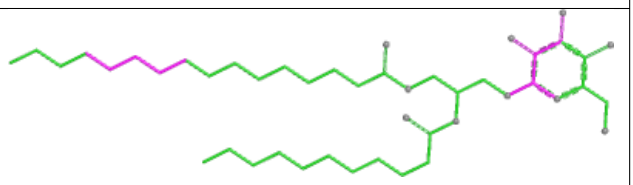


Rings

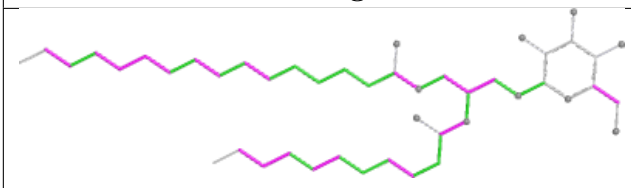
Ligand LMG b 730



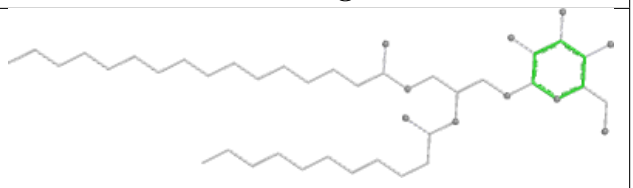
Bond lengths



Bond angles

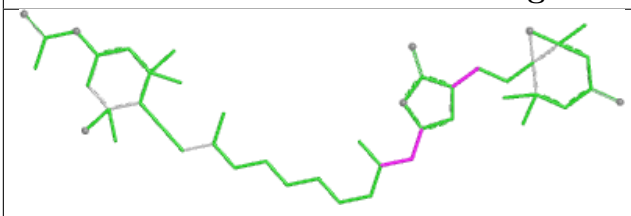


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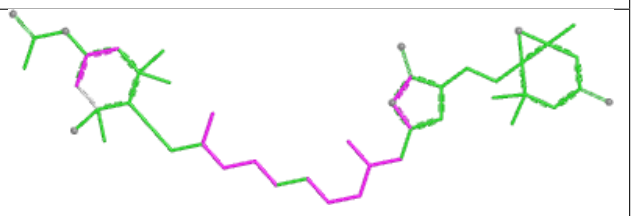


Rings

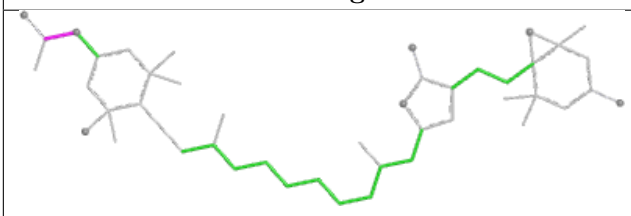
Ligand PID G 310



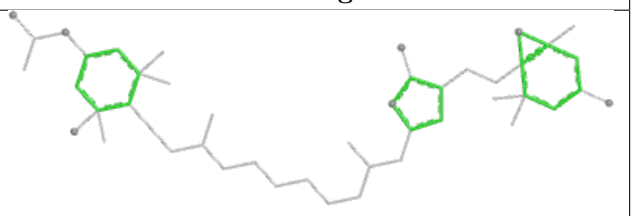
Bond lengths



Bond angles

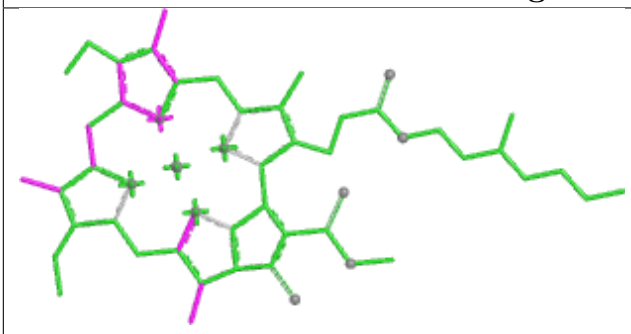


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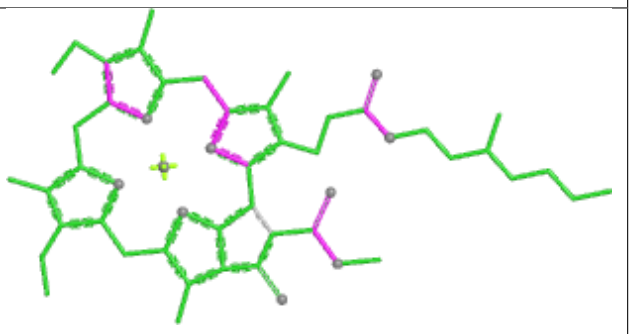


Rings

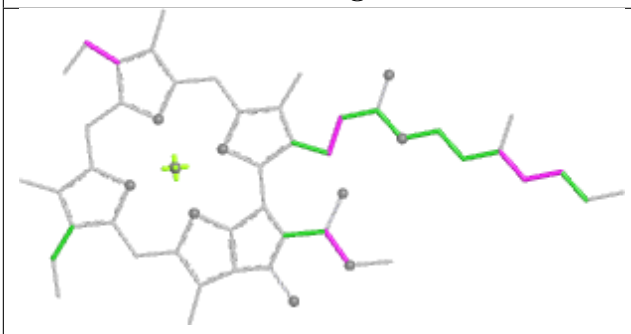
Ligand CLA J 311



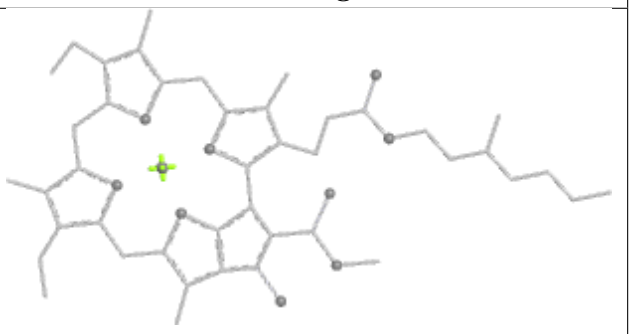
Bond lengths



Bond angles

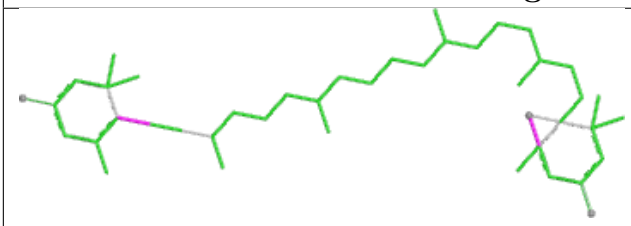


Torsions

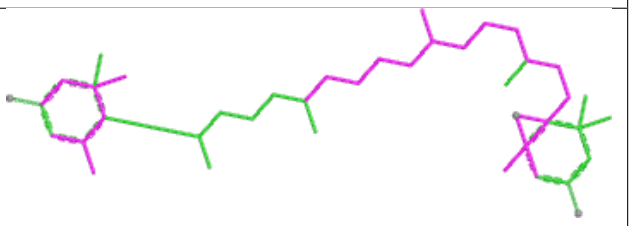


Rings

Ligand DD6 K 205



Bond lengths



Bond angles

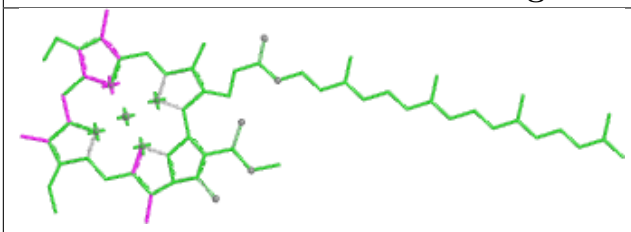


Torsions

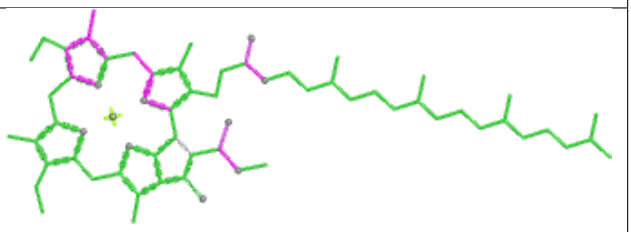


Rings

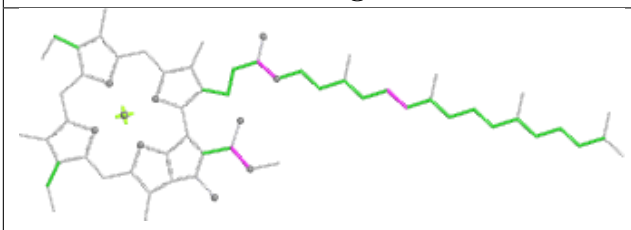
Ligand CLA b 723



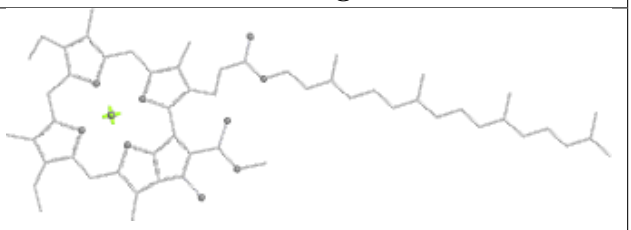
Bond lengths



Bond angles

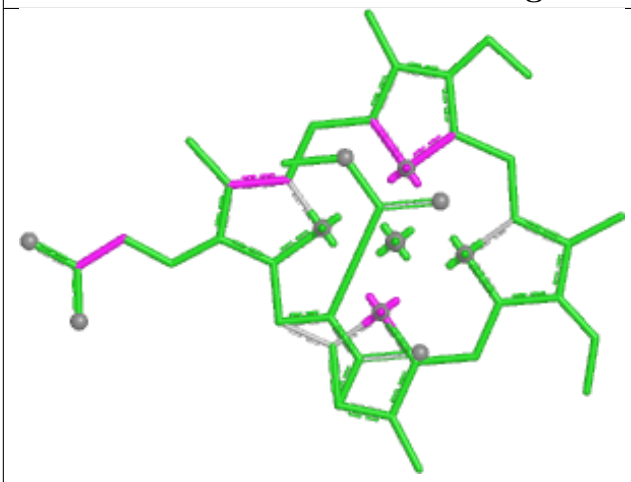


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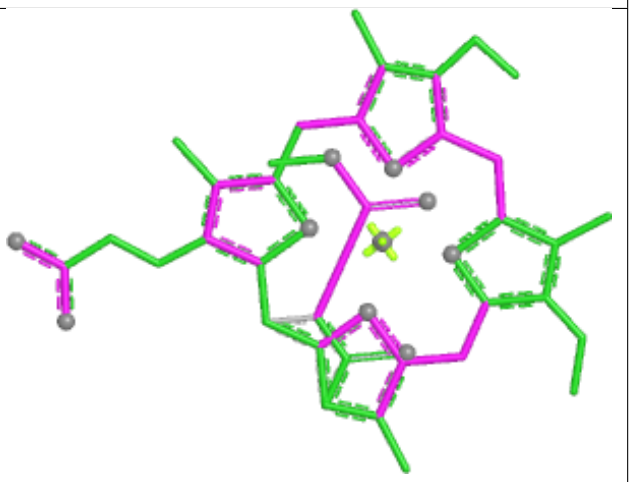


Rings

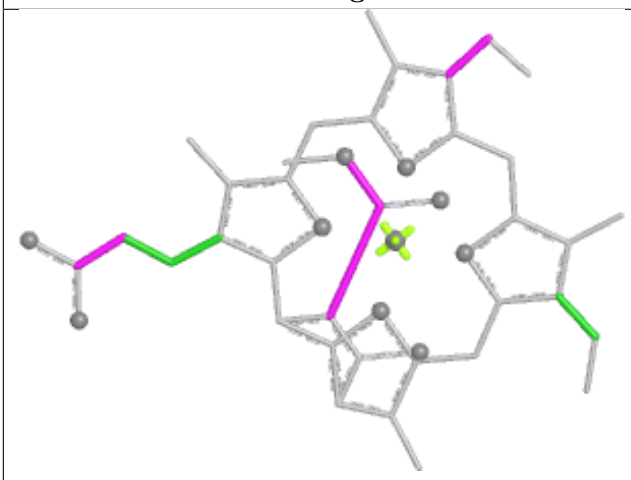
Ligand KC1 A 205



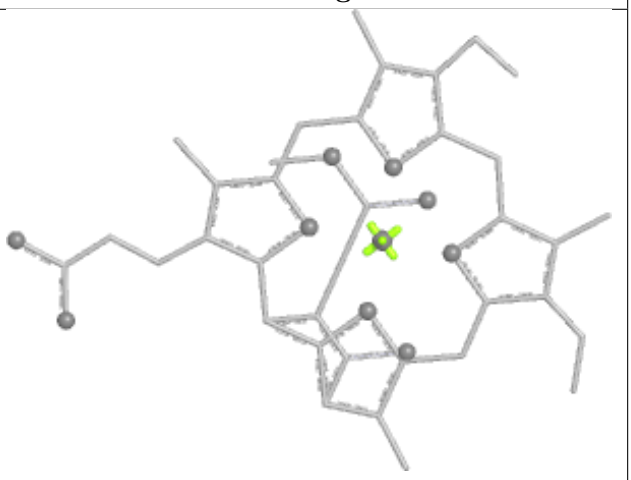
Bond lengths



Bond angles

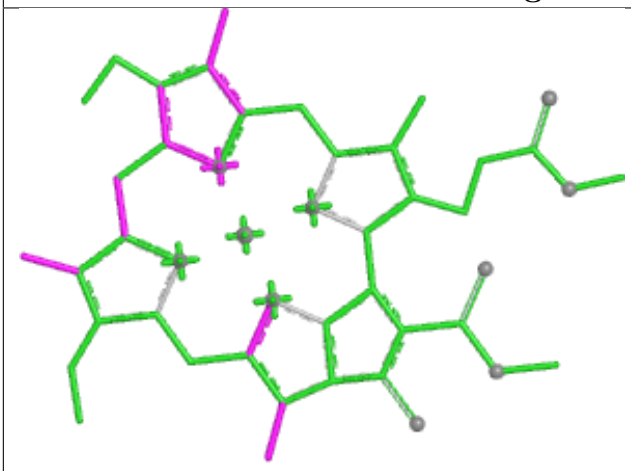


Torsions

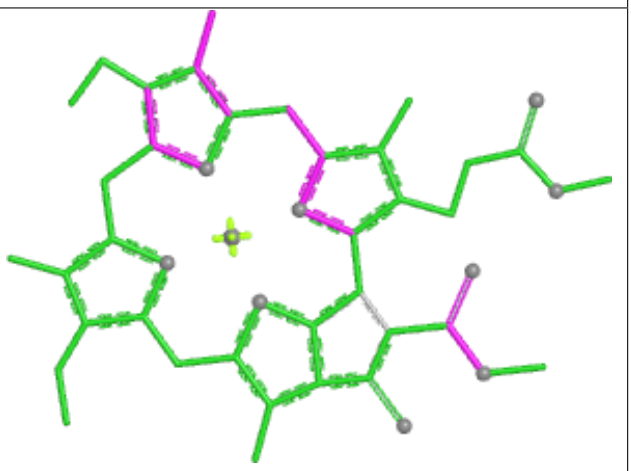


Rings

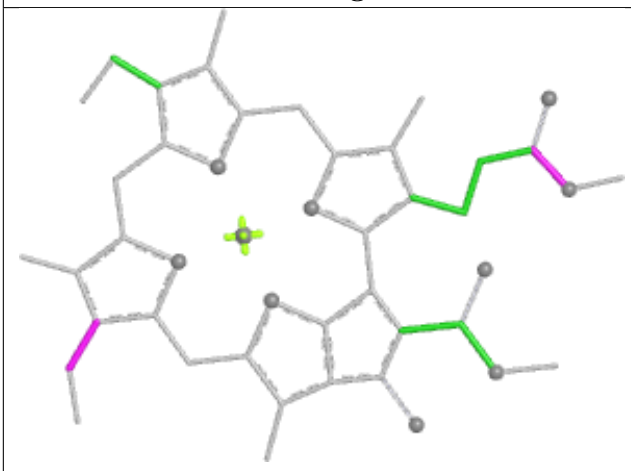
Ligand CLA B 315



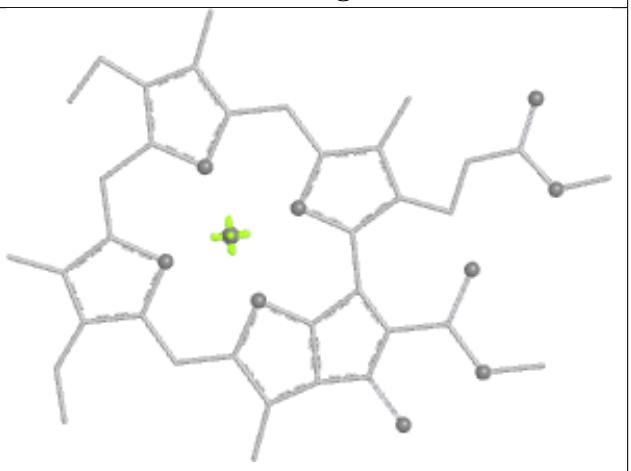
Bond lengths



Bond angles



Torsions

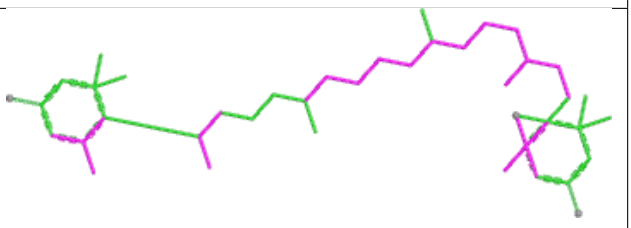


Rings

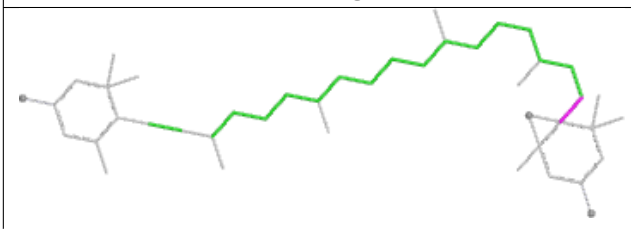
Ligand DD6 G 308



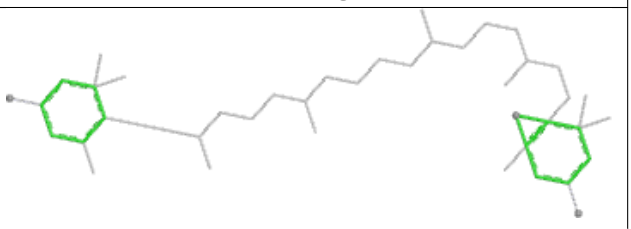
Bond lengths



Bond angles

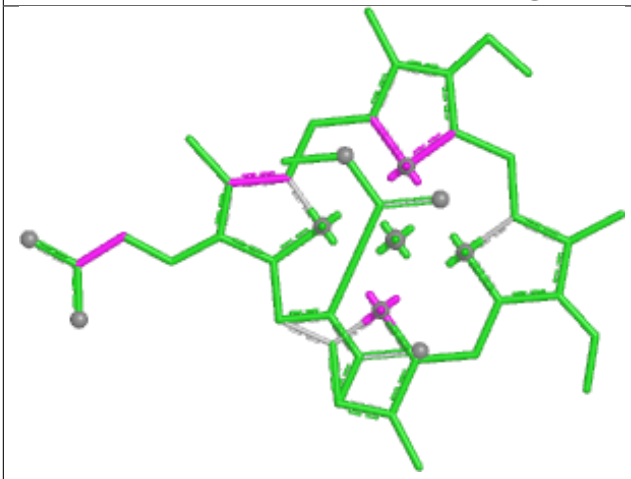


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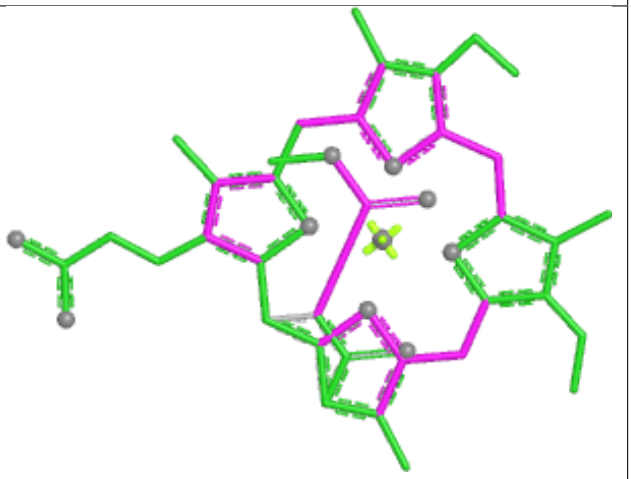


Rings

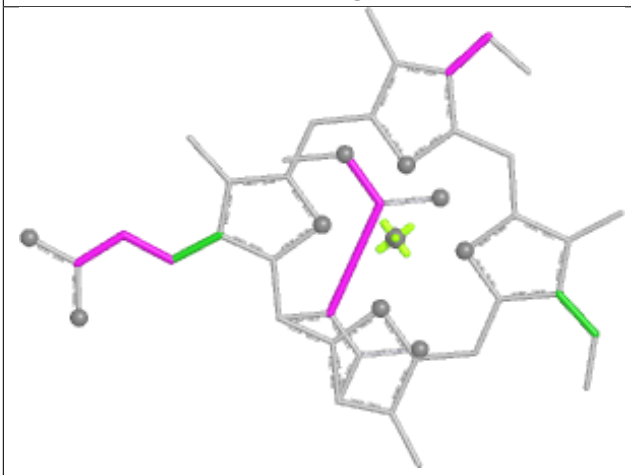
Ligand KC1 C 312



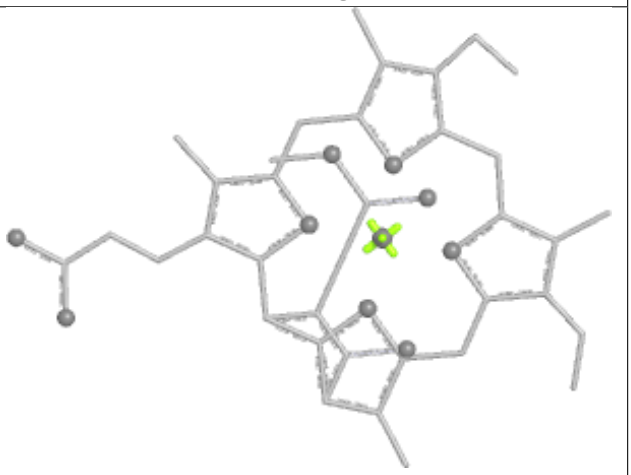
Bond lengths



Bond angles

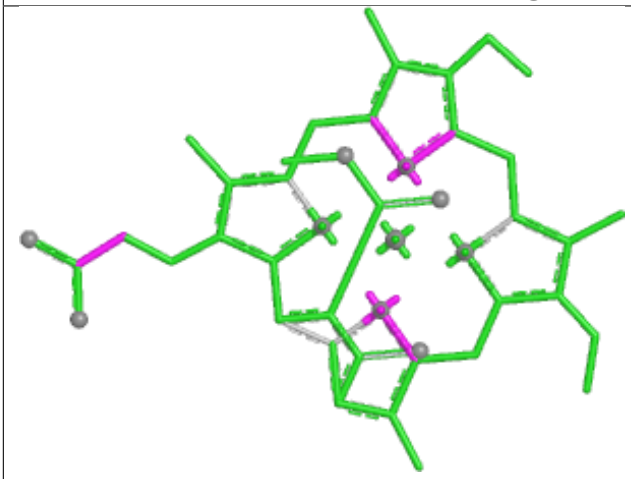


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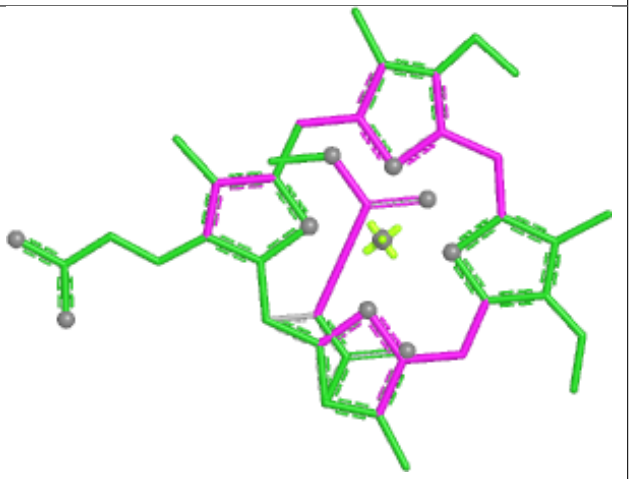


Rings

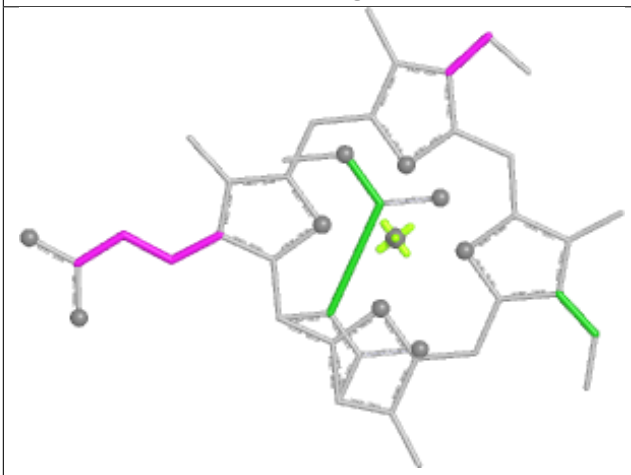
Ligand KC1 G 318



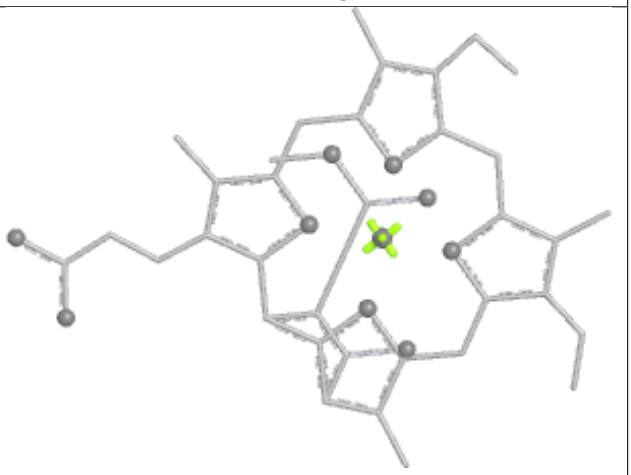
Bond lengths



Bond angles

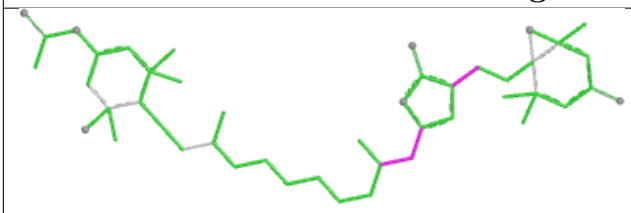


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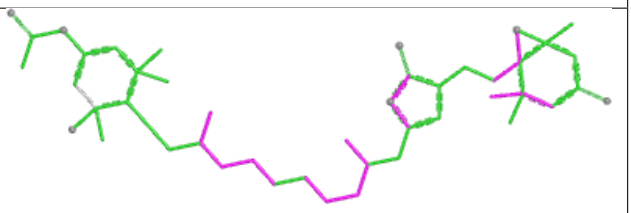


Rings

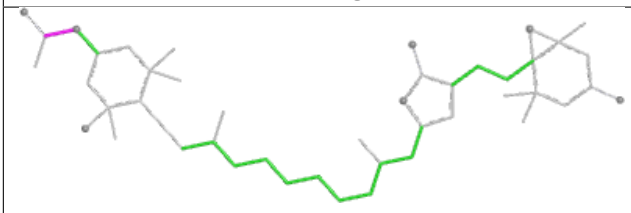
Ligand PID C 307



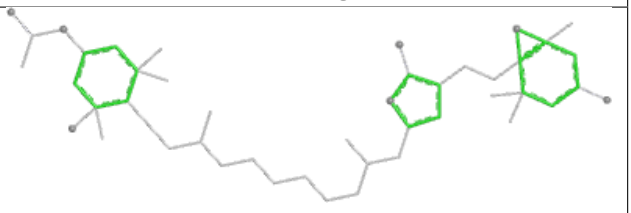
Bond lengths



Bond angles

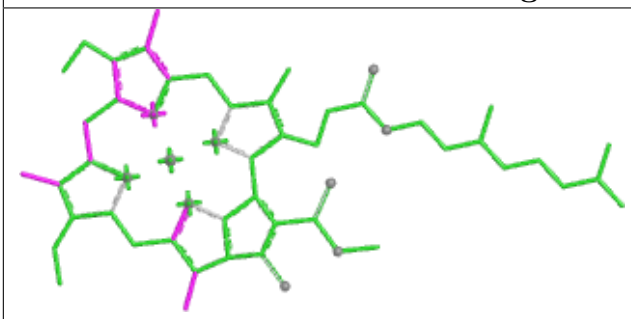


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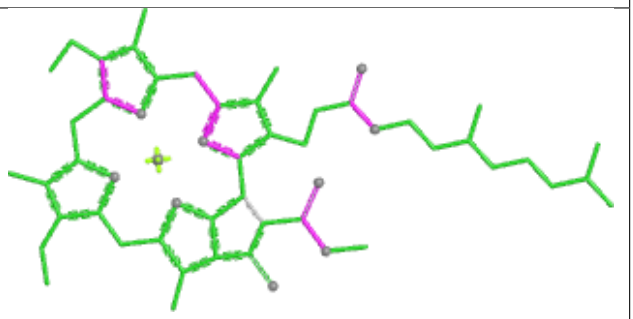


Rings

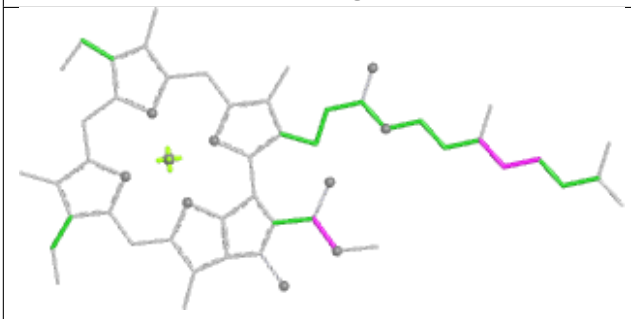
Ligand CLA M 307



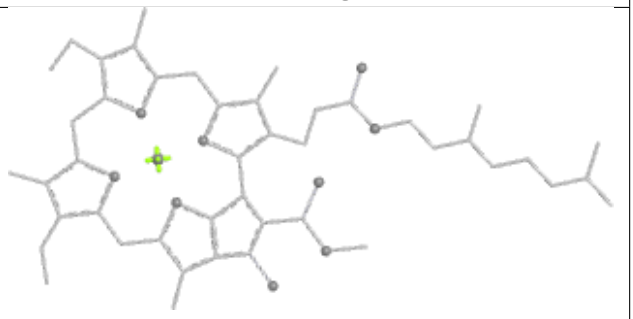
Bond lengths



Bond angles

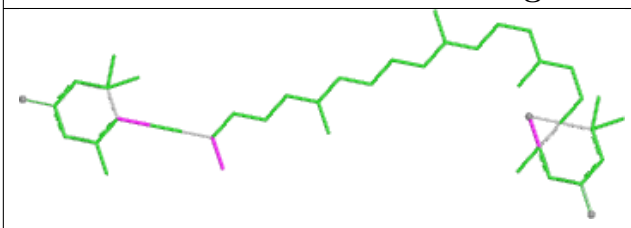


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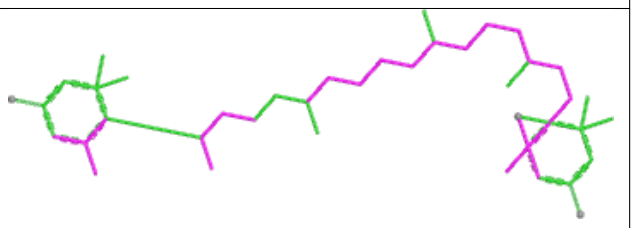


Rings

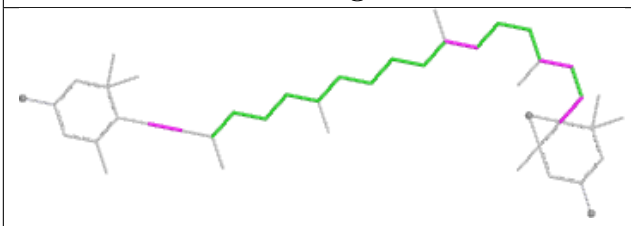
Ligand DD6 K 203



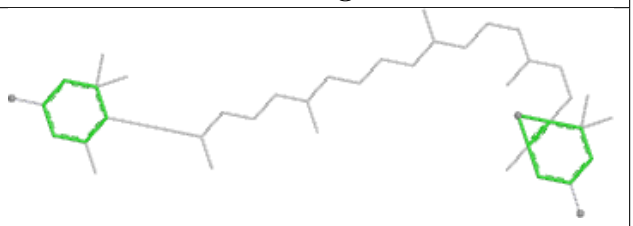
Bond lengths



Bond angles

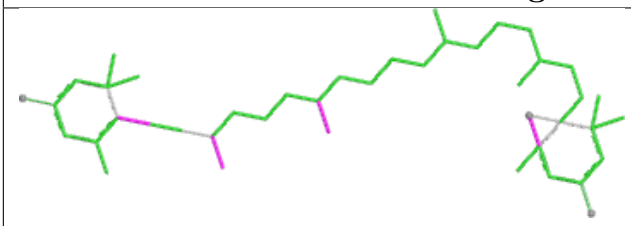


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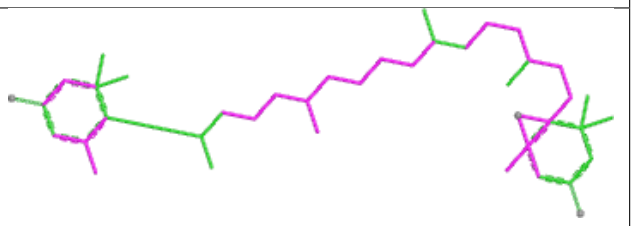


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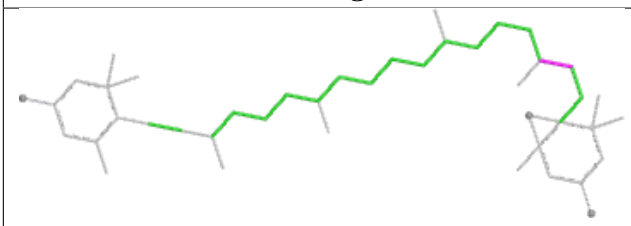
Ligand DD6 h 202



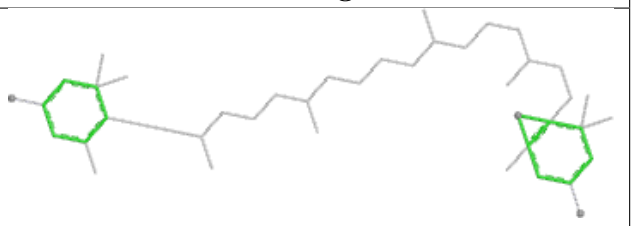
Bond lengths



Bond angles

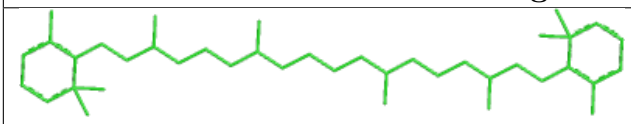


Torsions

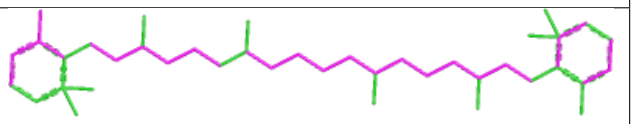


Rings

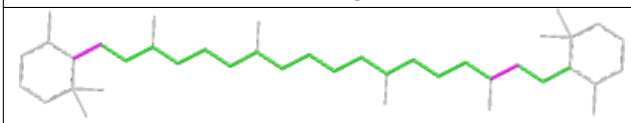
Ligand BCR i 204



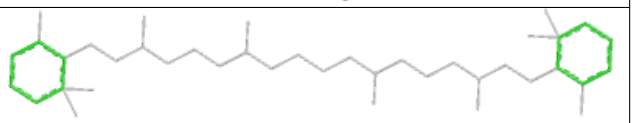
Bond lengths



Bond angles

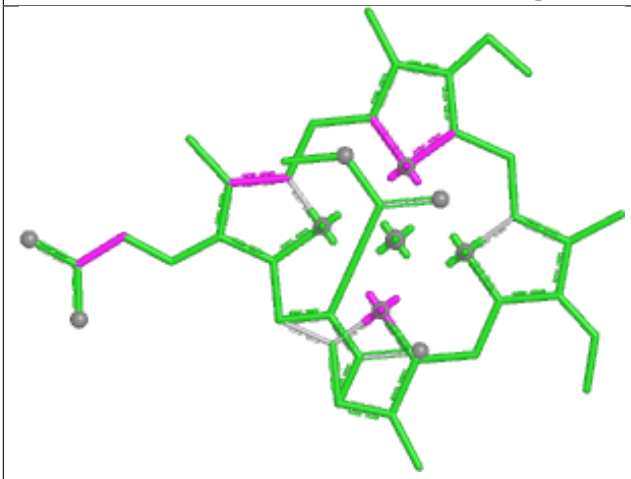


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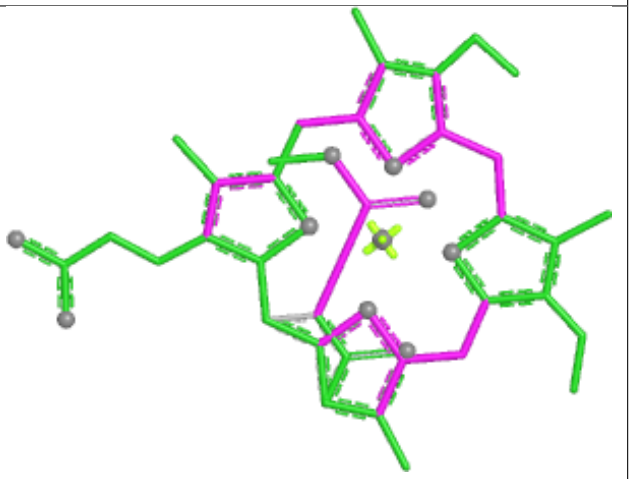


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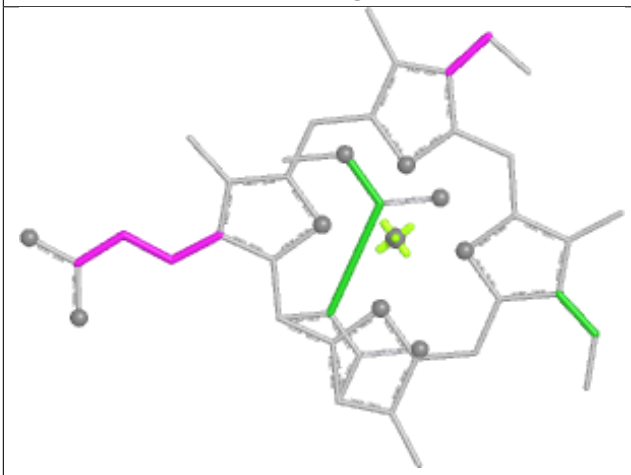
Ligand KC1 J 312



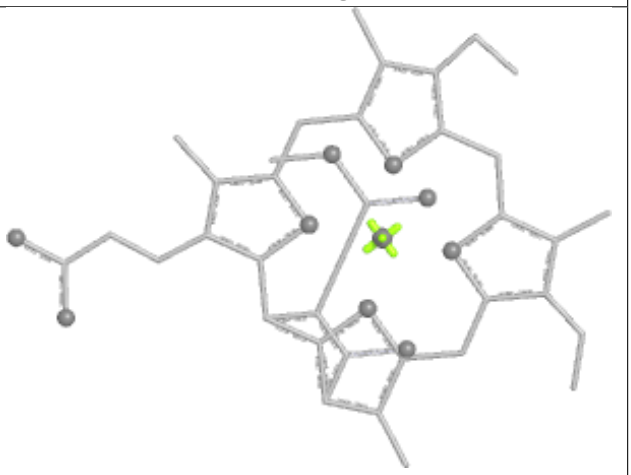
Bond lengths



Bond angles

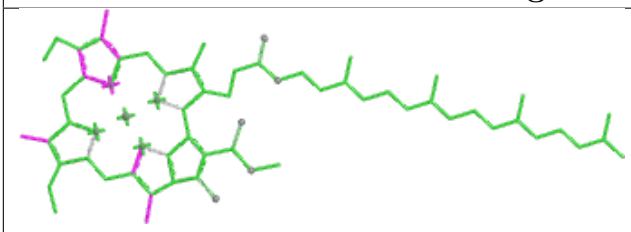


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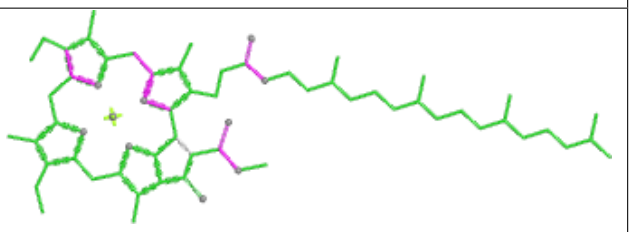


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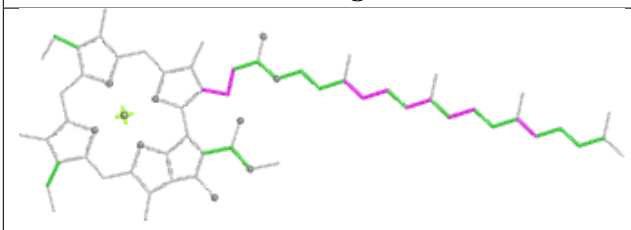
Ligand CLA b 706



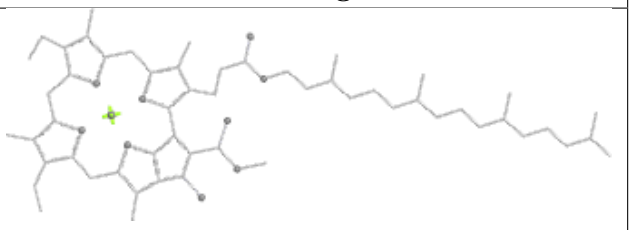
Bond lengths



Bond angles

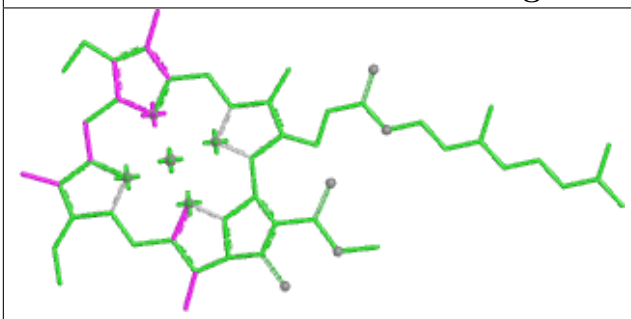


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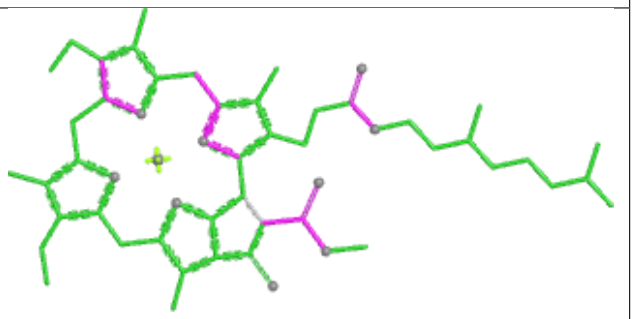


Rings

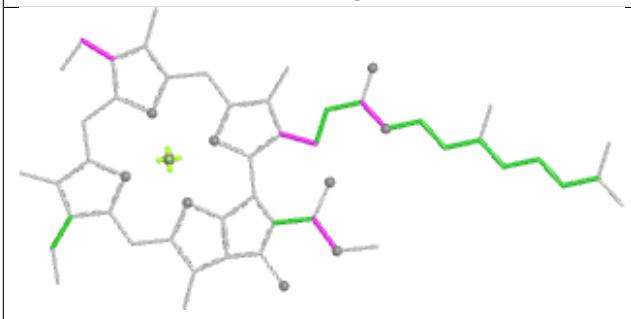
Ligand CLA K 214



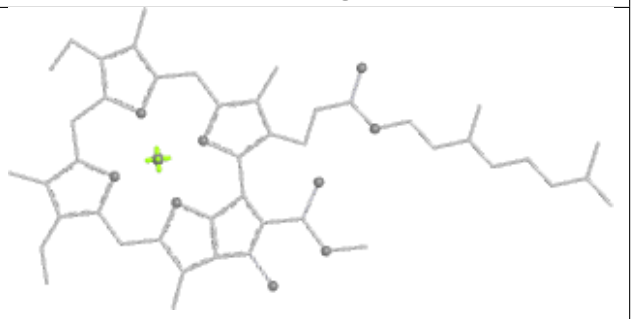
Bond lengths



Bond angles

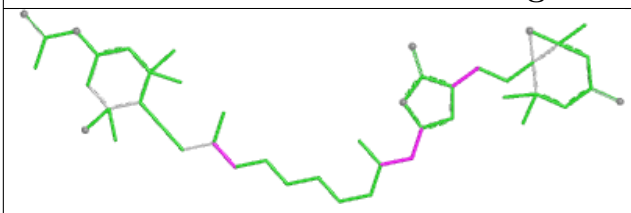


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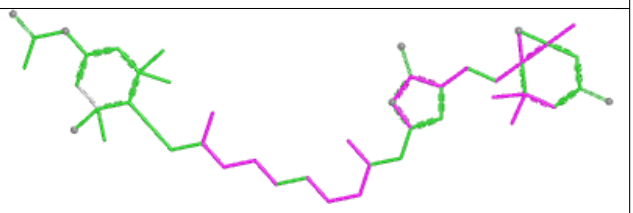


Rings

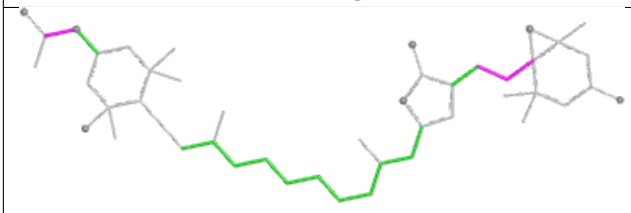
Ligand PID N 307



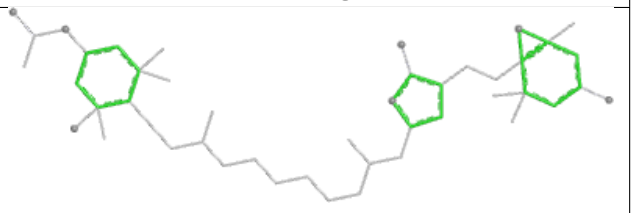
Bond lengths



Bond angles

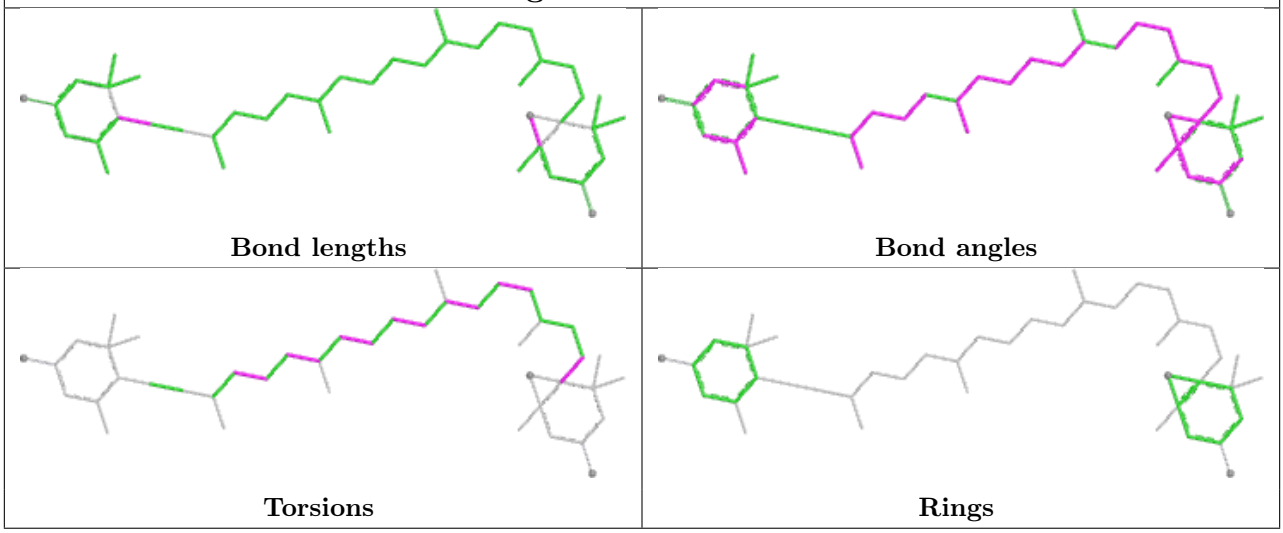


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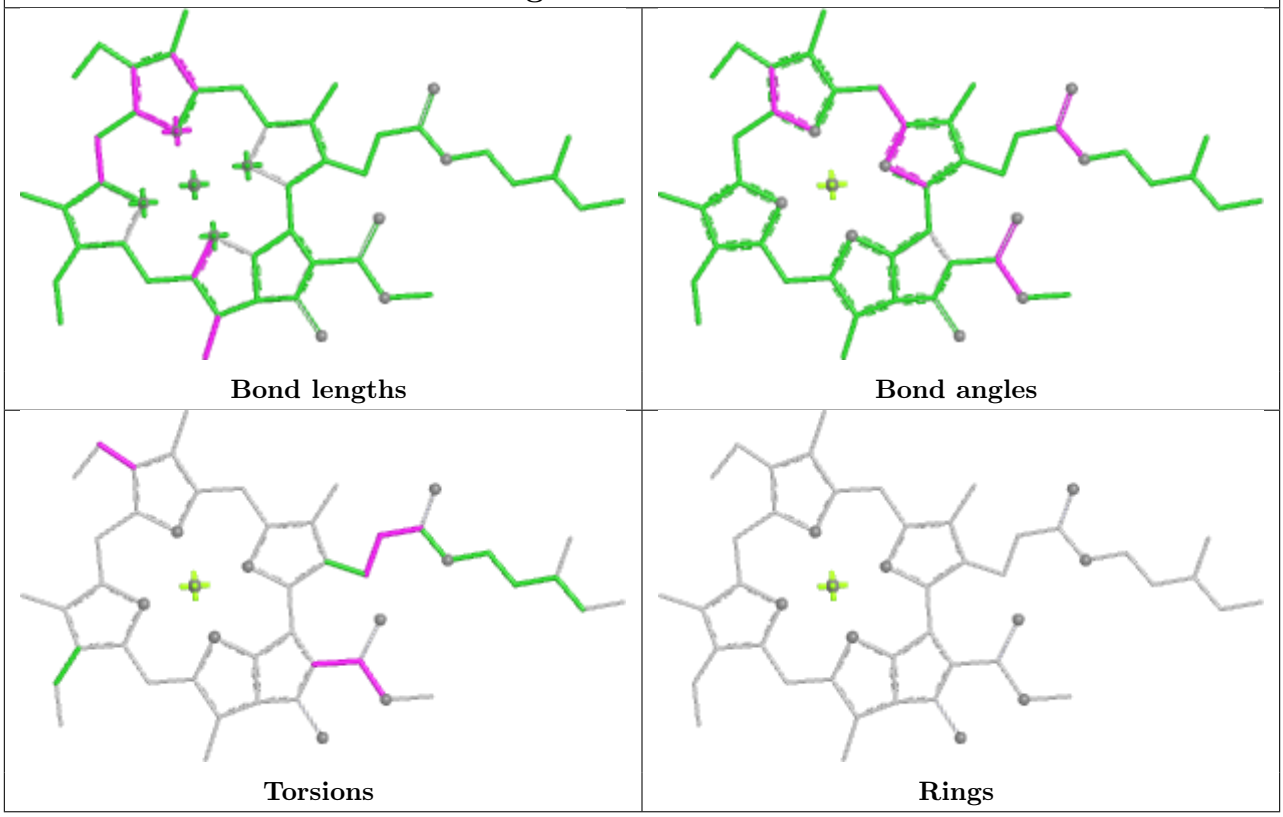


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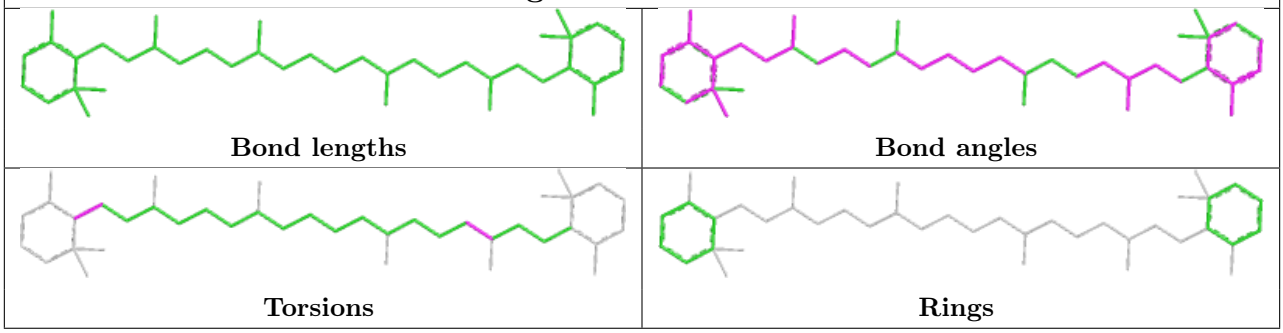
Ligand DD6 B 319



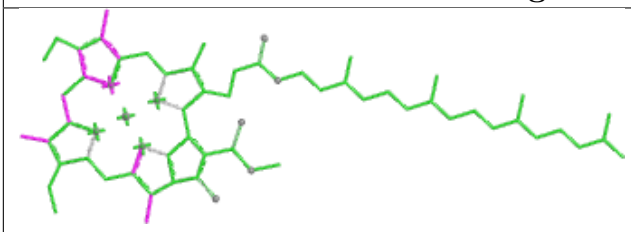
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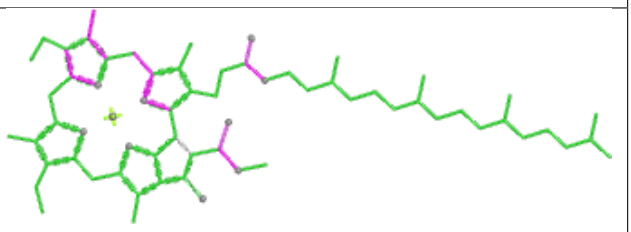
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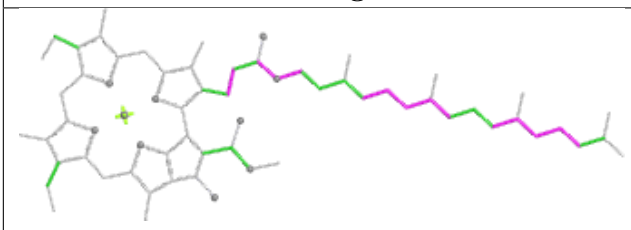
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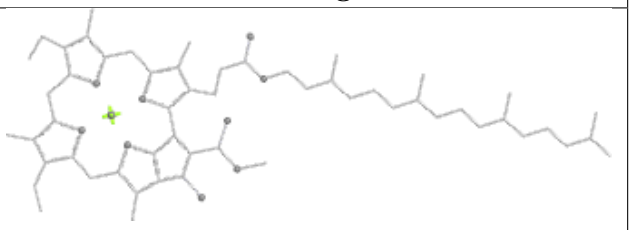
Bond lengths



Bond angles

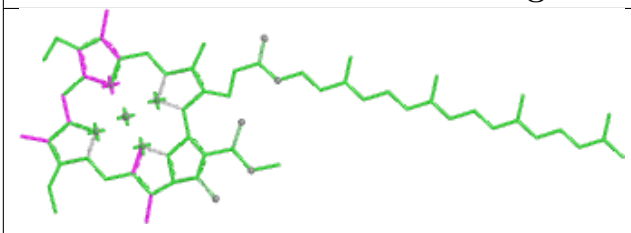


Torsions

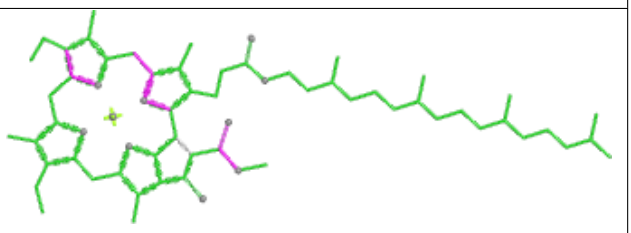


Rings

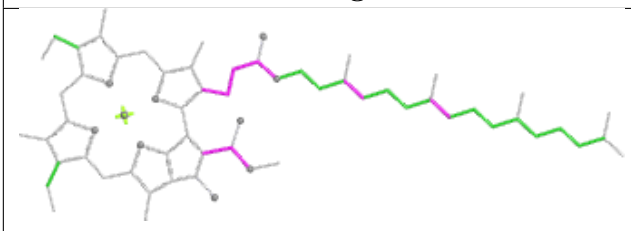
Ligand CLA b 720



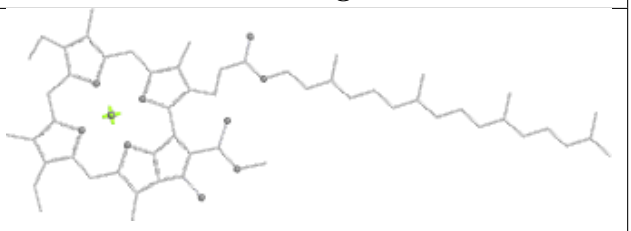
Bond lengths



Bond angles

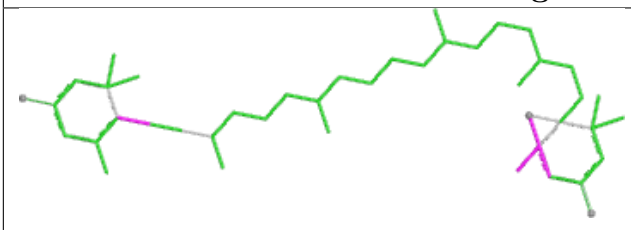


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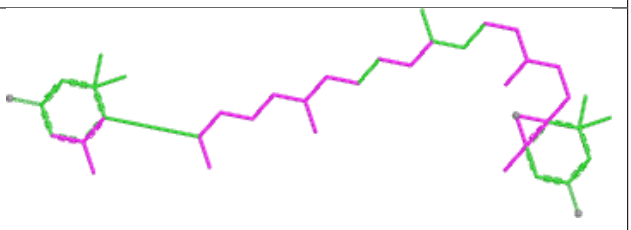


Rings

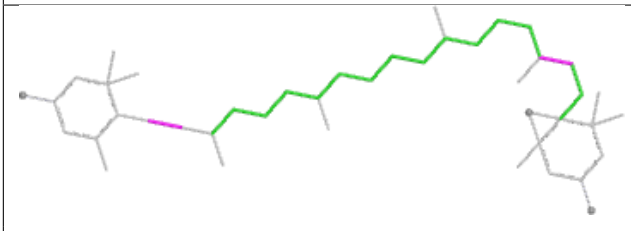
Ligand DD6 I 204



Bond lengths



Bond angles

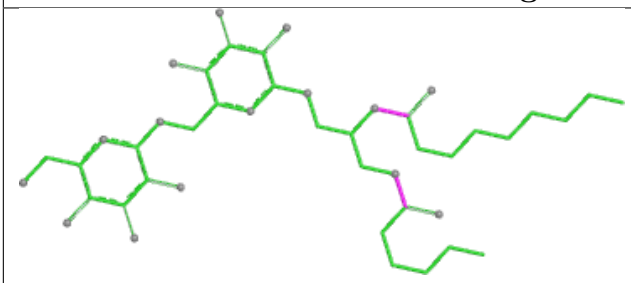


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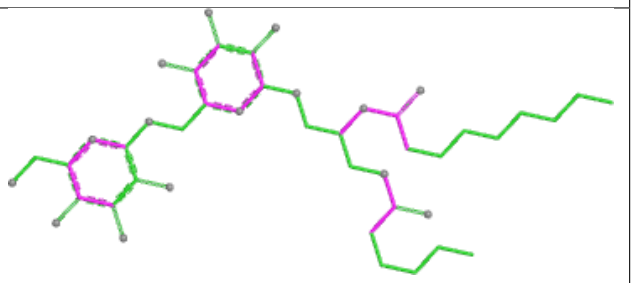


Rings

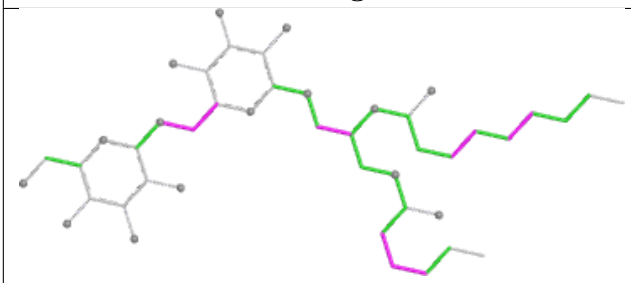
Ligand DGD B 318



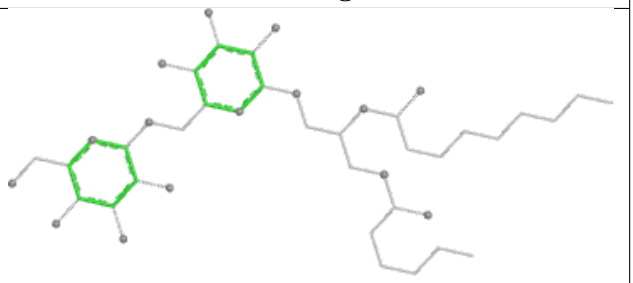
Bond lengths



Bond angles

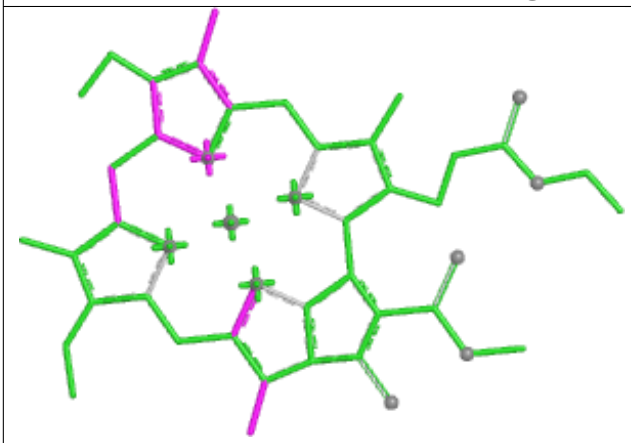


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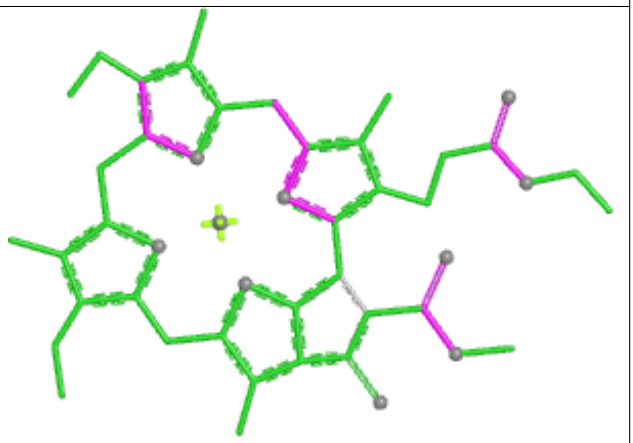


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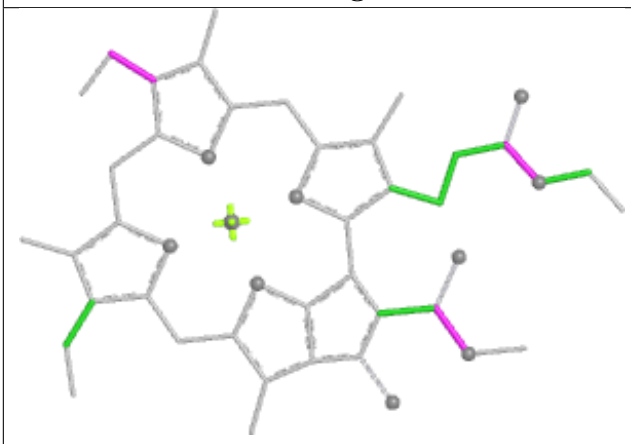
Ligand CLA O 308



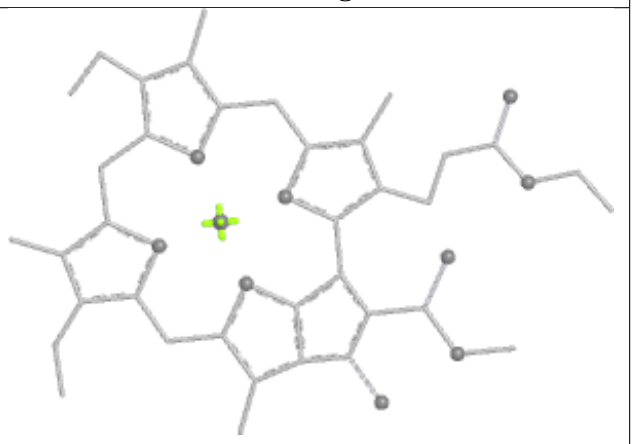
Bond lengths



Bond angles

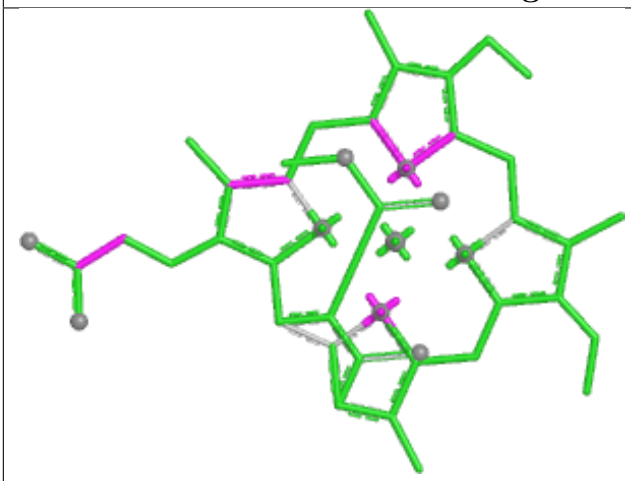


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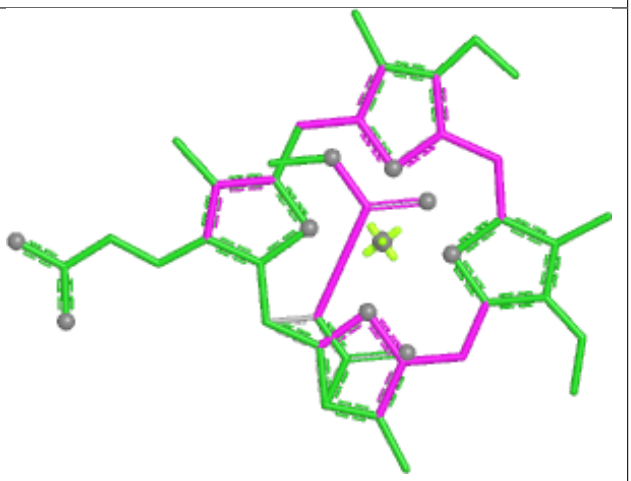


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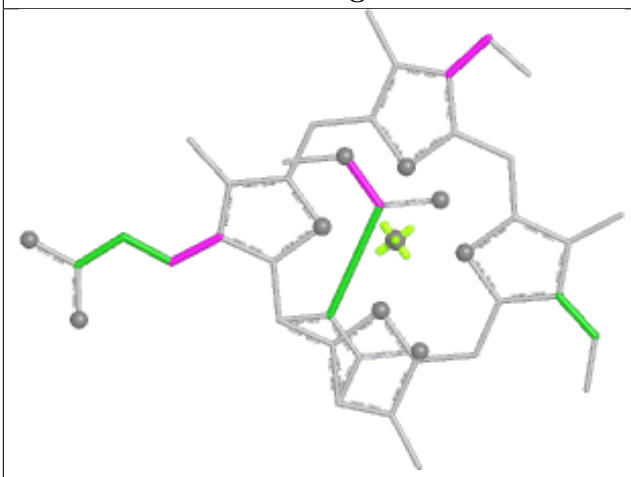
Ligand KC1 M 312



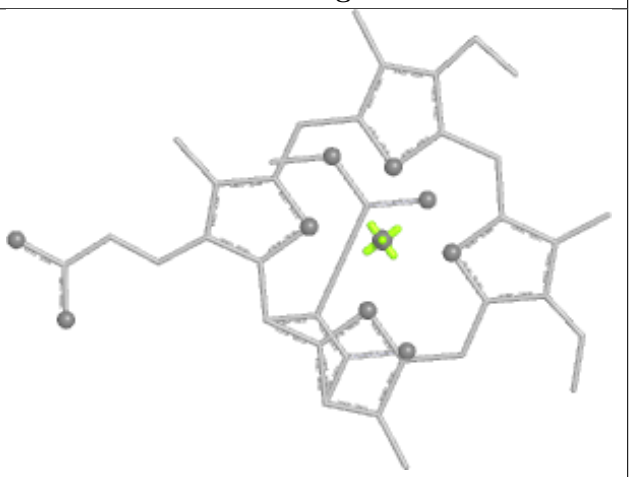
Bond lengths



Bond angles

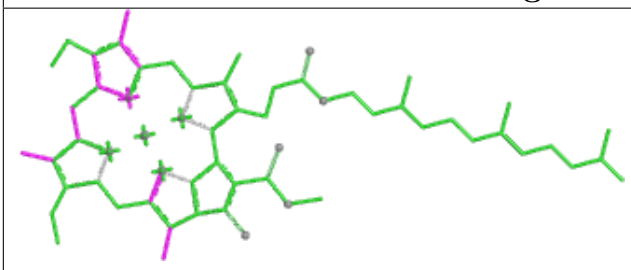


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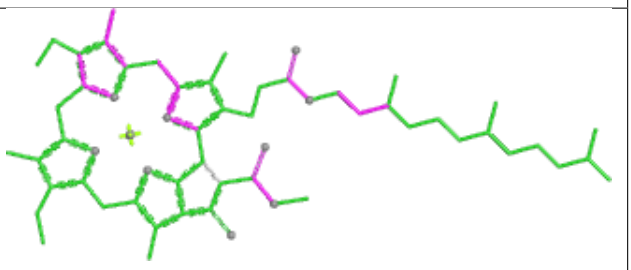


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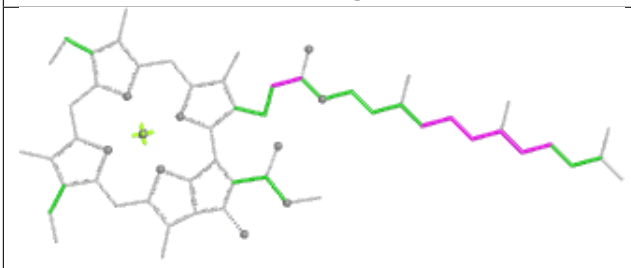
Ligand CLA A 218



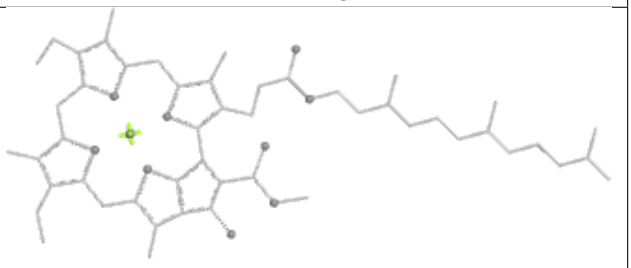
Bond lengths



Bond angles

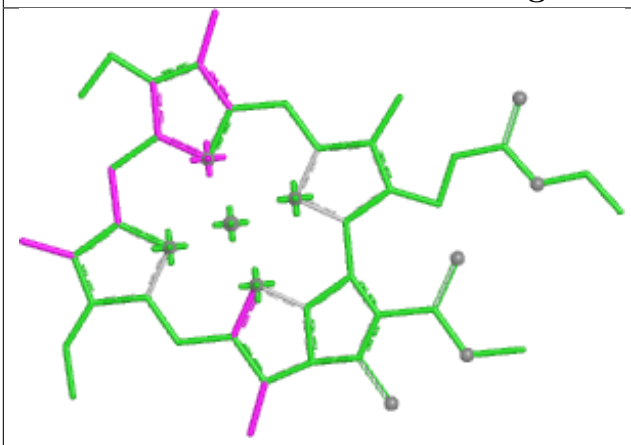


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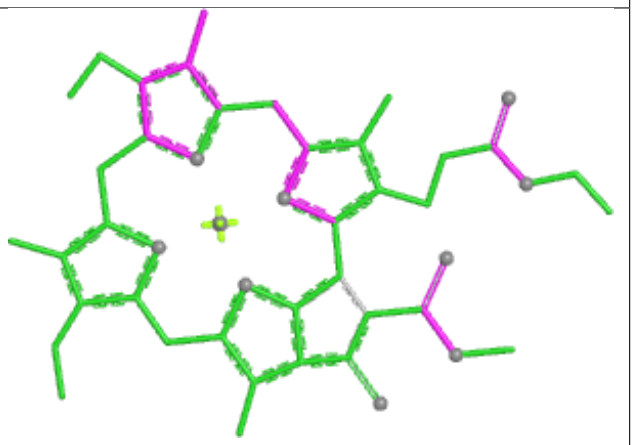


Rings

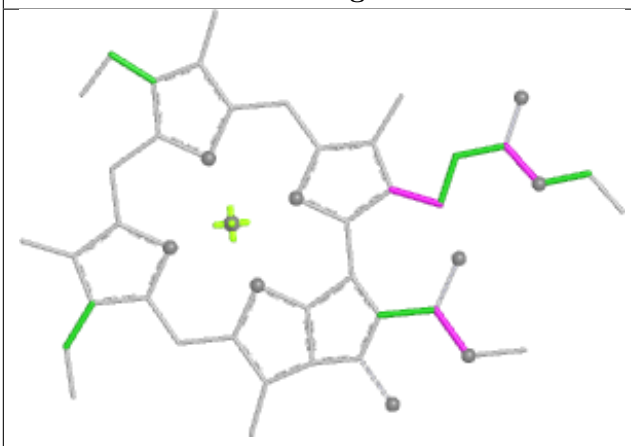
Ligand CLA J 310



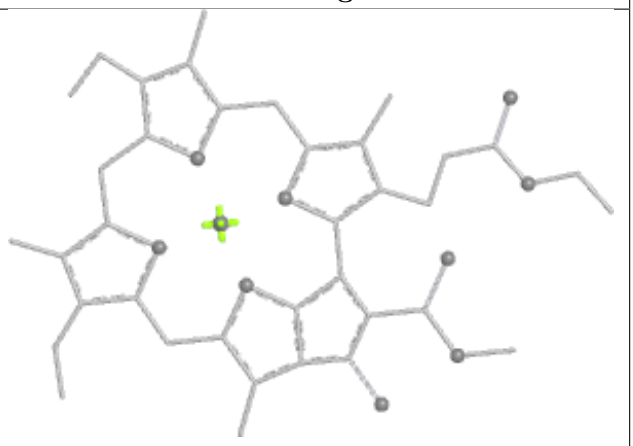
Bond lengths



Bond angles

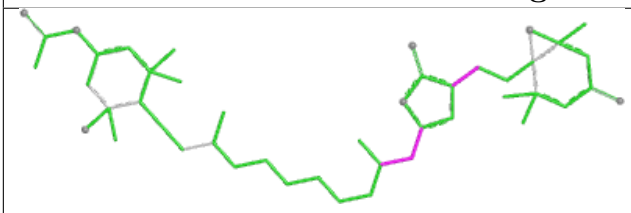


Torsions

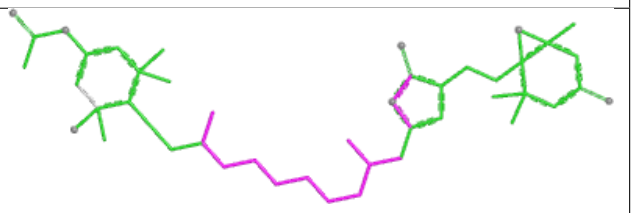


Rings

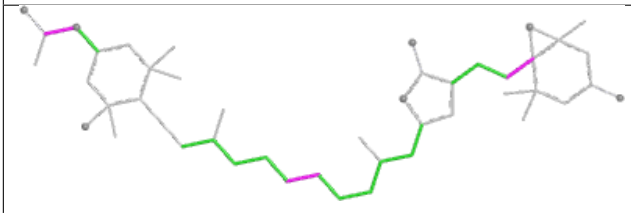
Ligand PID P 202



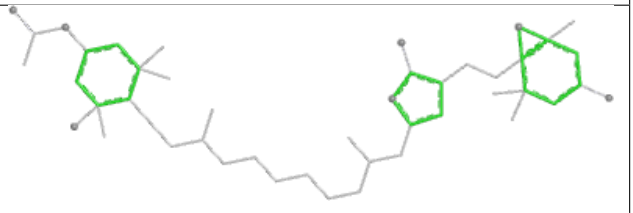
Bond lengths



Bond angles

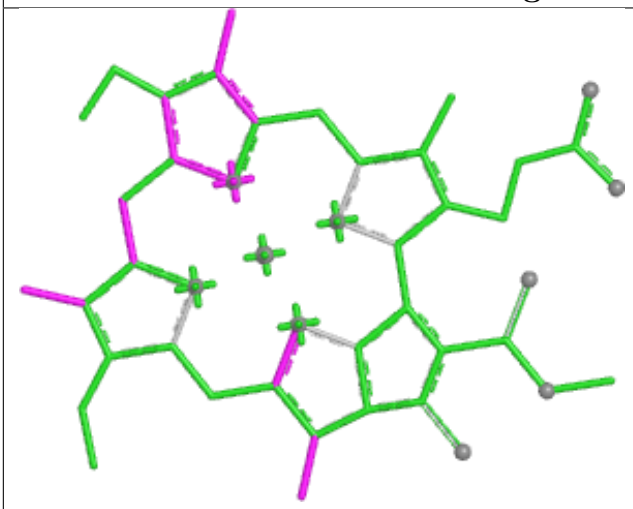


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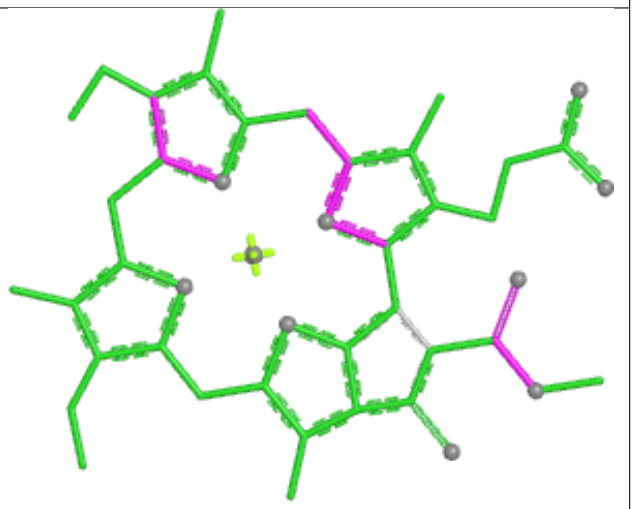


Rings

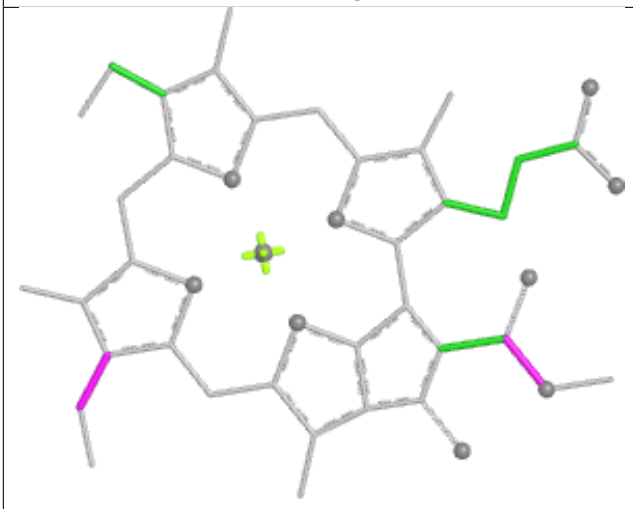
Ligand CLA D 313



Bond lengths



Bond angles

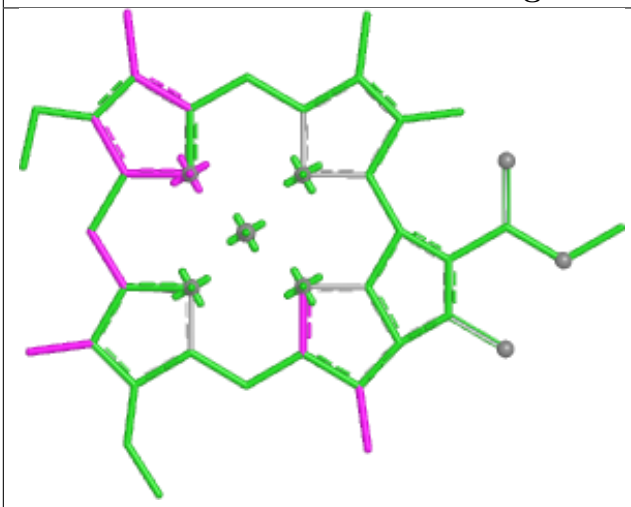


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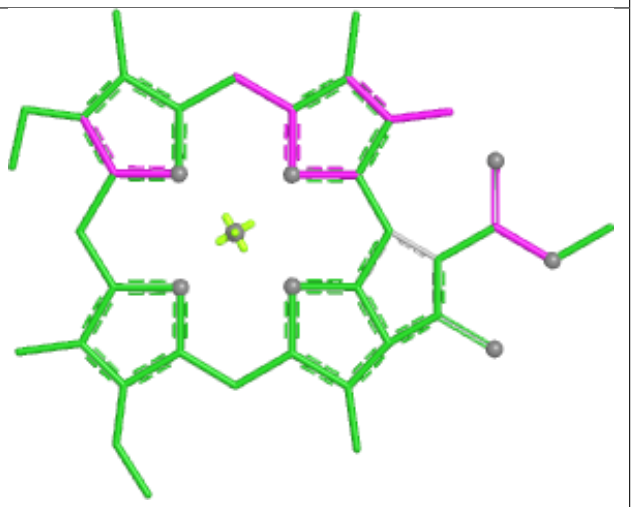


Rings

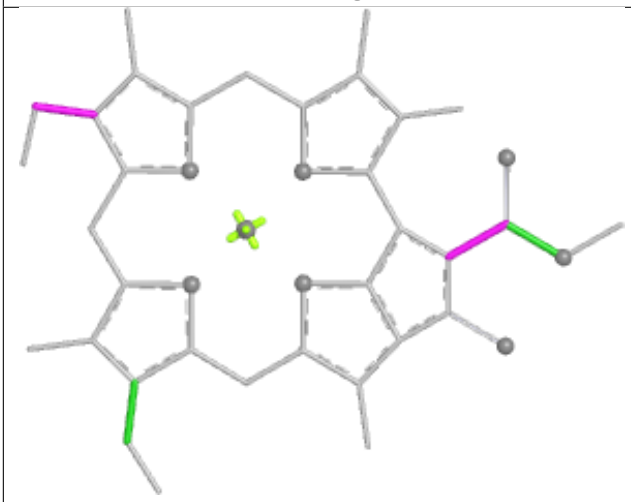
Ligand CLA A 214



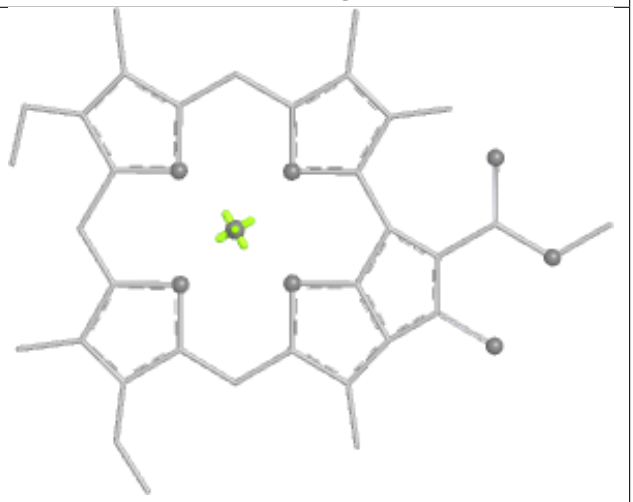
Bond lengths



Bond angles

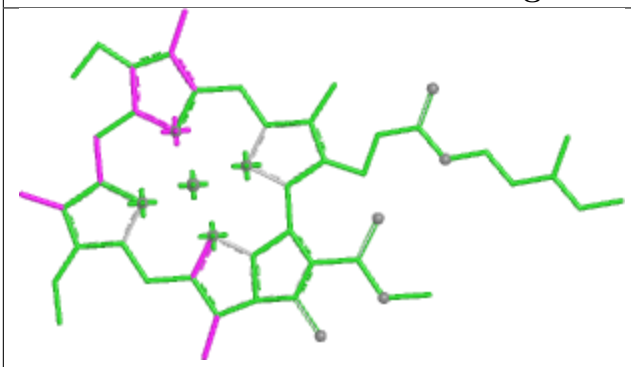


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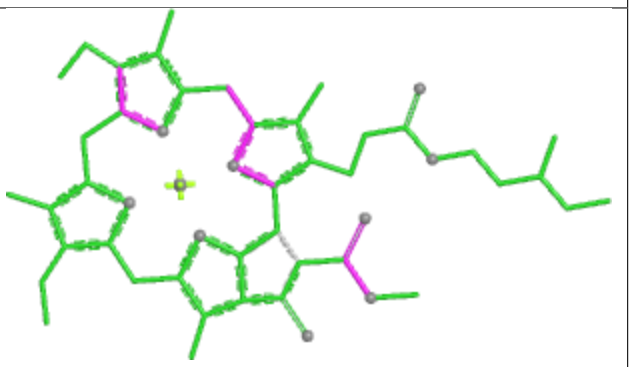


Rings

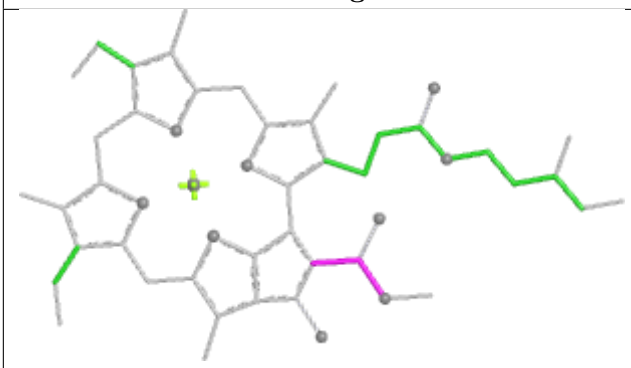
Ligand CLA O 311



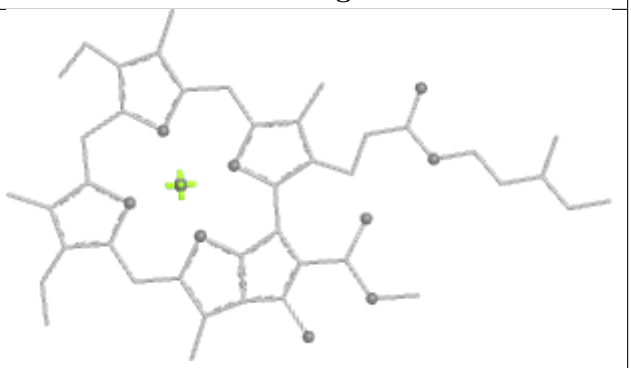
Bond lengths



Bond angles

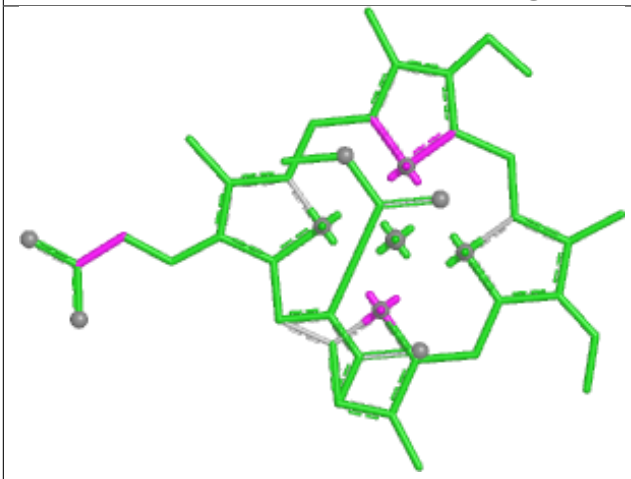


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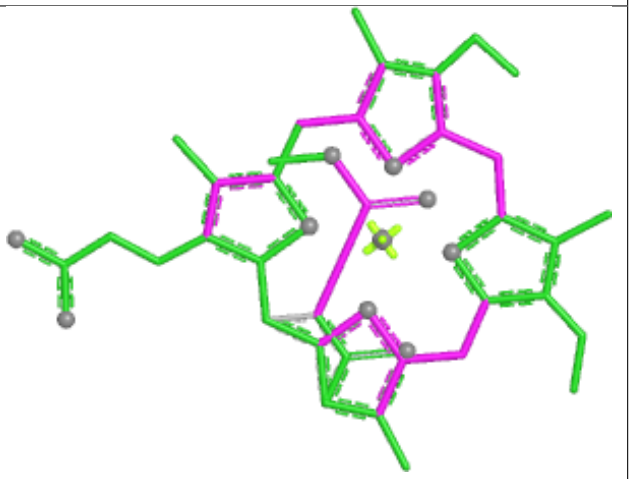


Rings

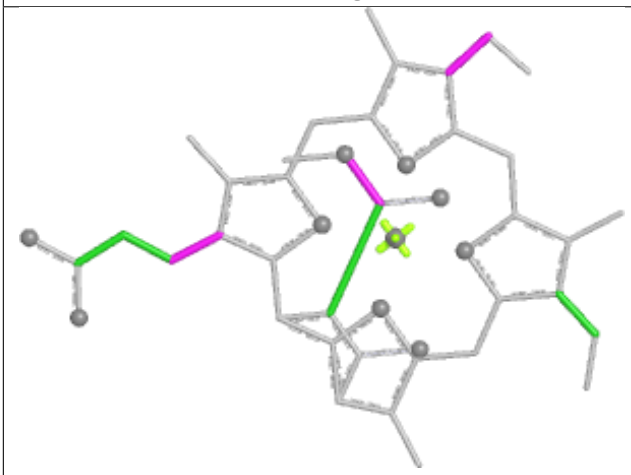
Ligand KC1 H 314



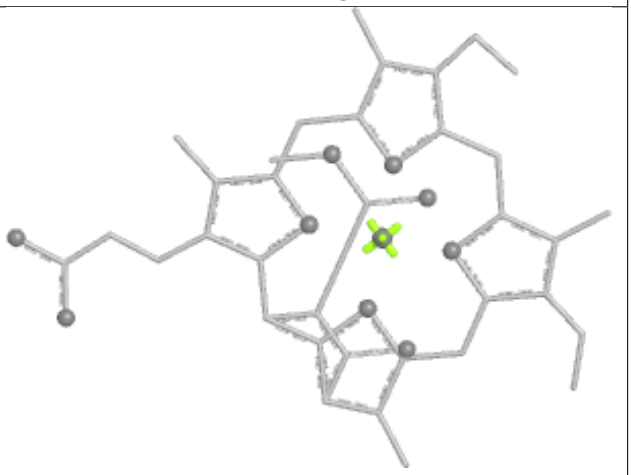
Bond lengths



Bond angles

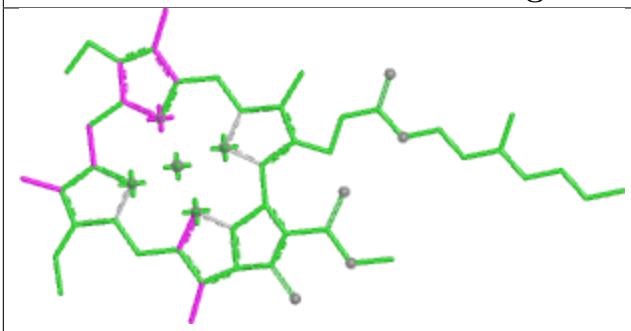


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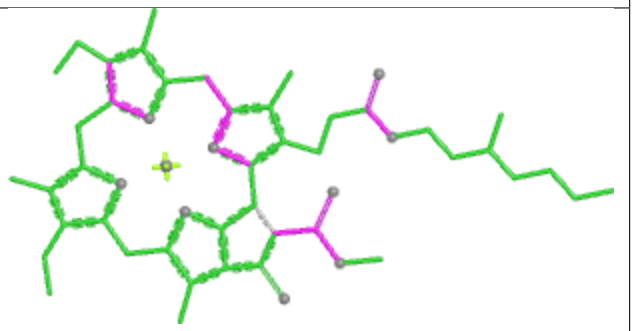


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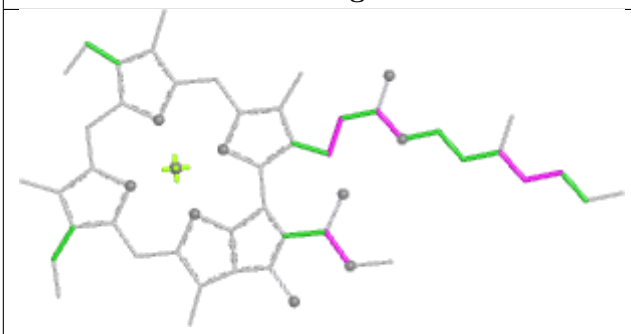
Ligand CLA L 308



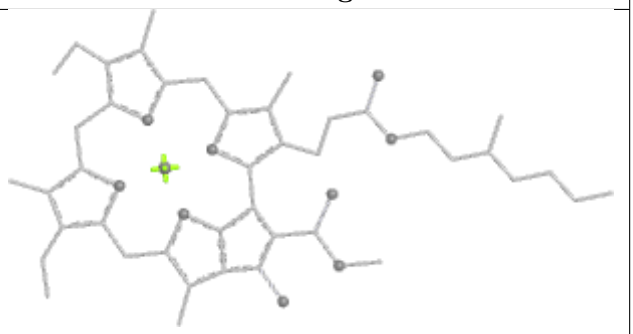
Bond lengths



Bond angles

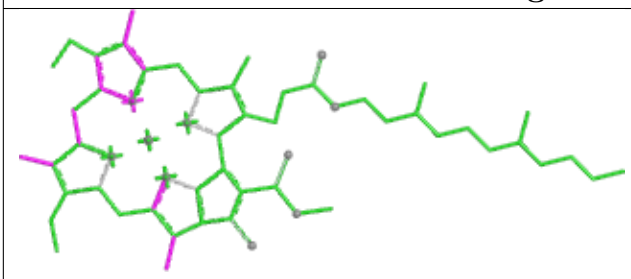


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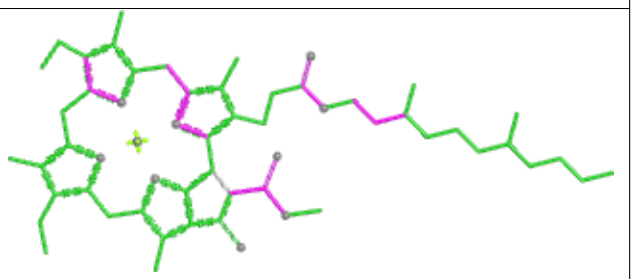


Rings

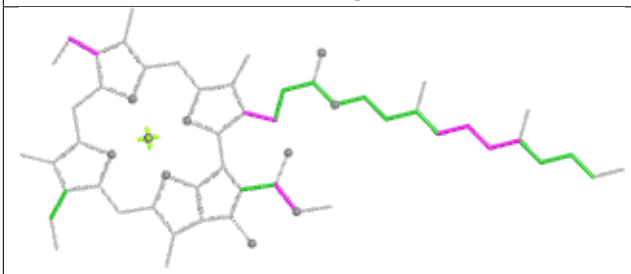
Ligand CLA b 721



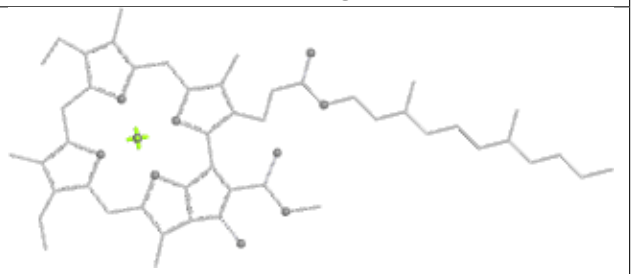
Bond lengths



Bond angles

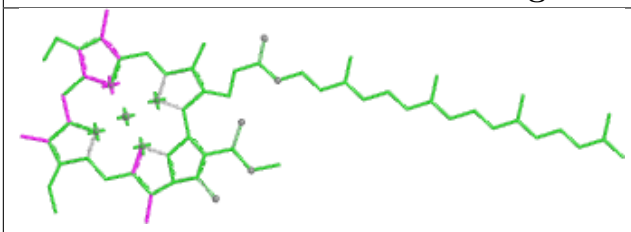


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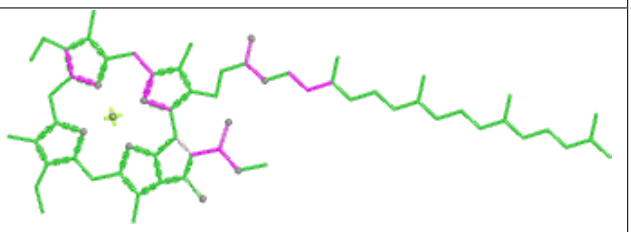


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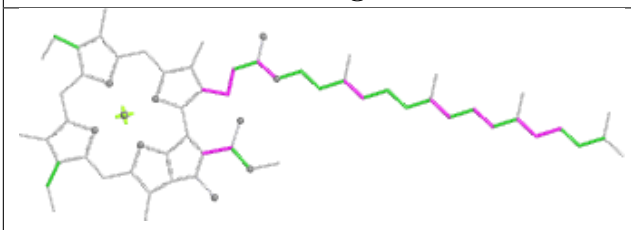
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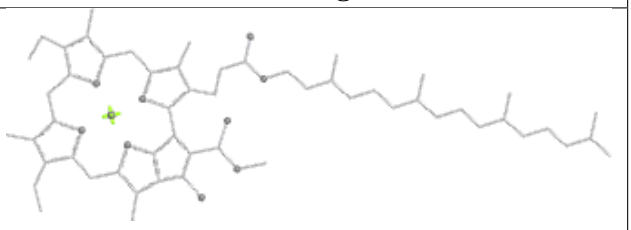
Bond lengths



Bond angles

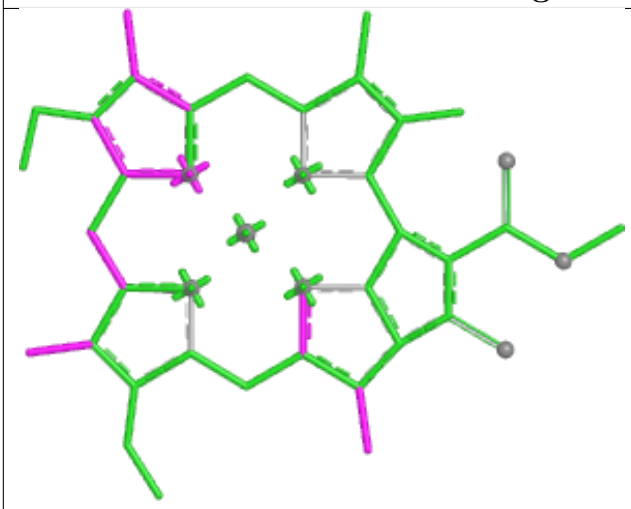


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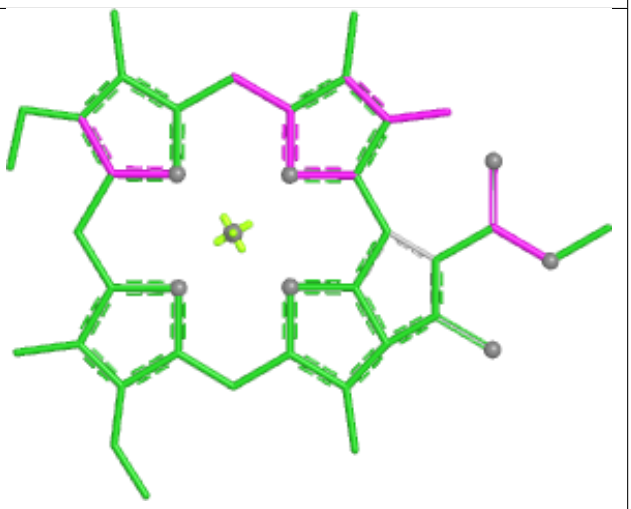


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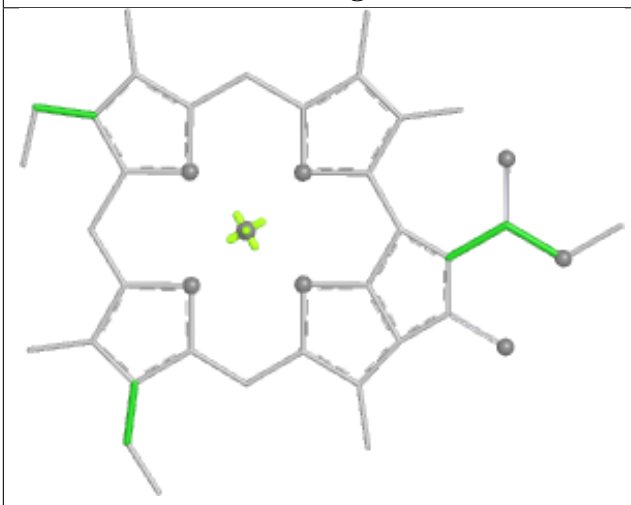
Ligand CLA l 508



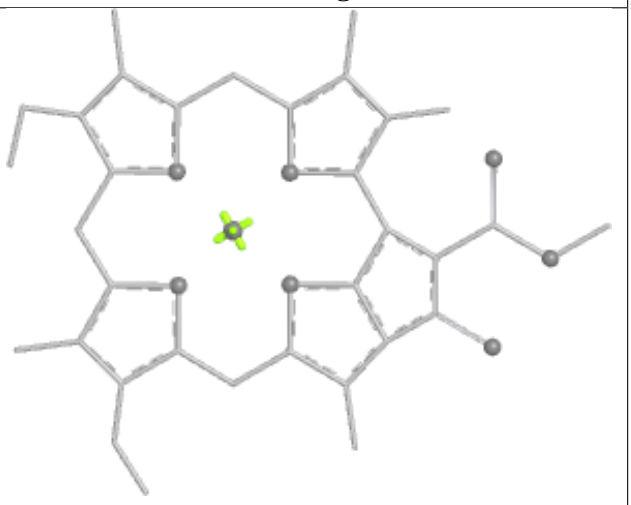
Bond lengths



Bond angles

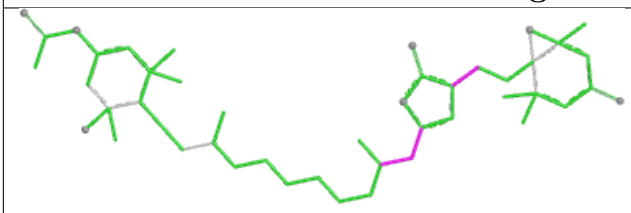


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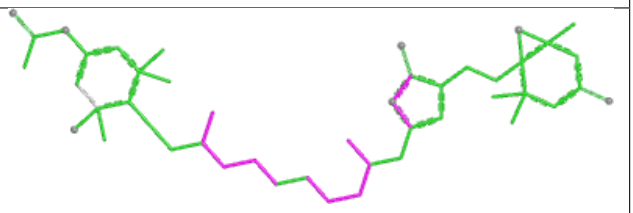


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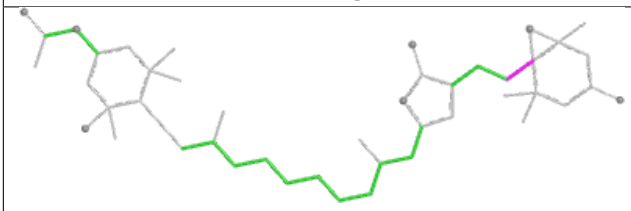
Ligand PID T 304



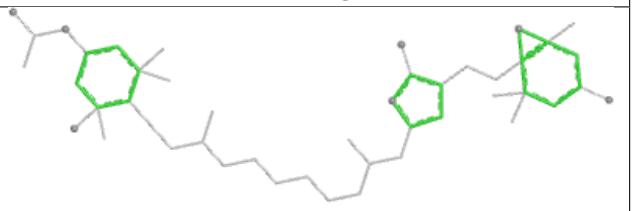
Bond lengths



Bond angles

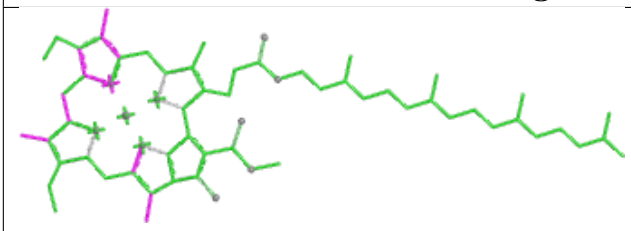


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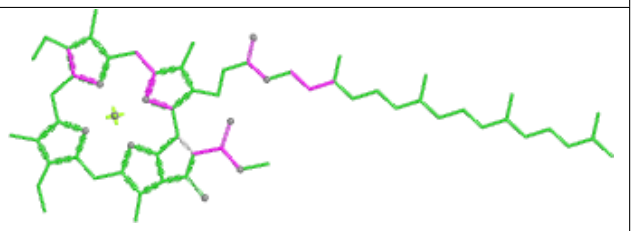


Rings

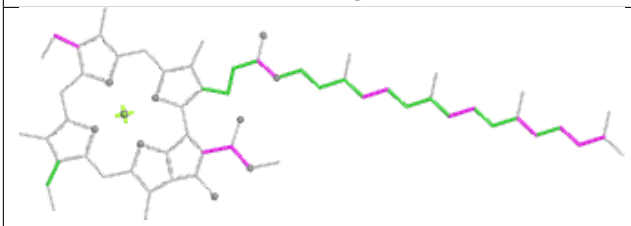
Ligand CLA l 502



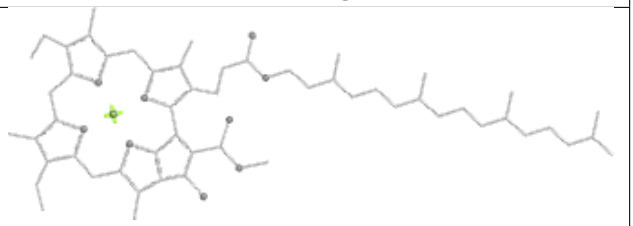
Bond lengths



Bond angles

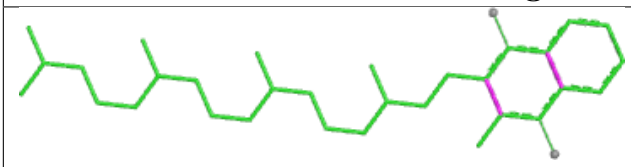


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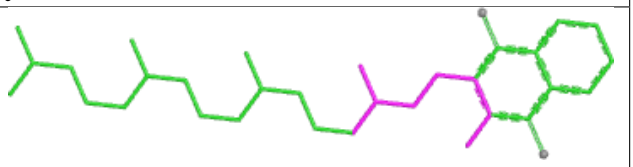


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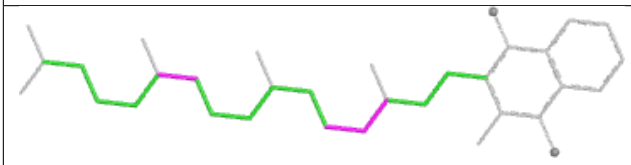
Ligand PQN b 727



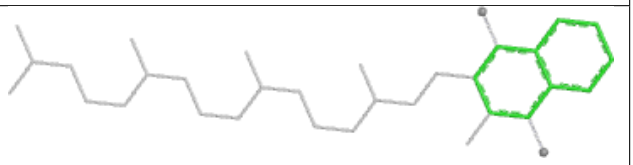
Bond lengths



Bond angles

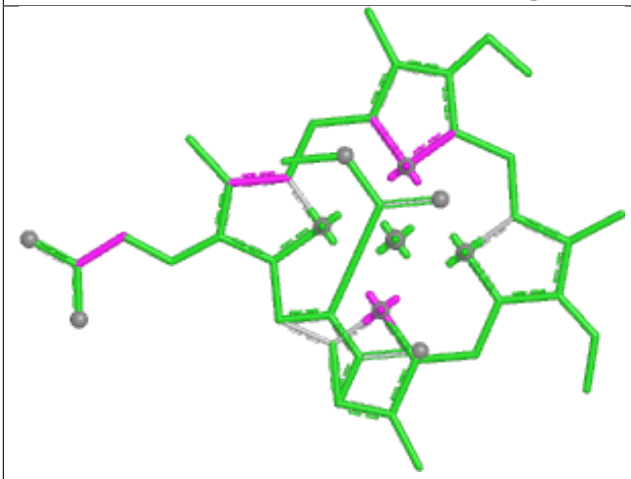


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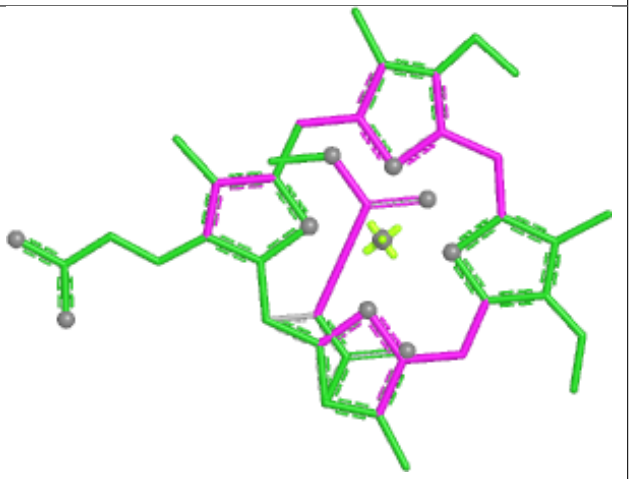


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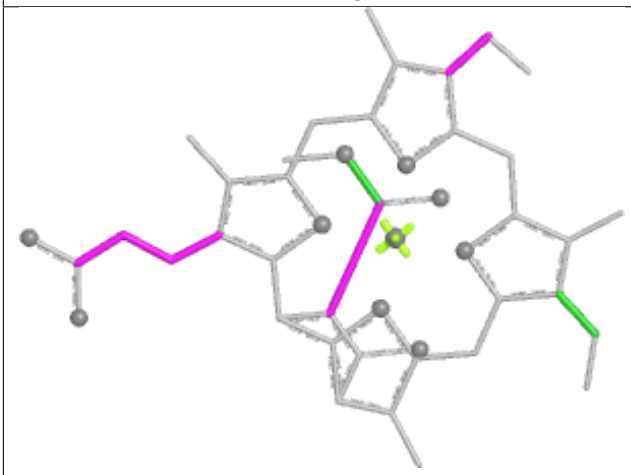
Ligand KC1 N 310



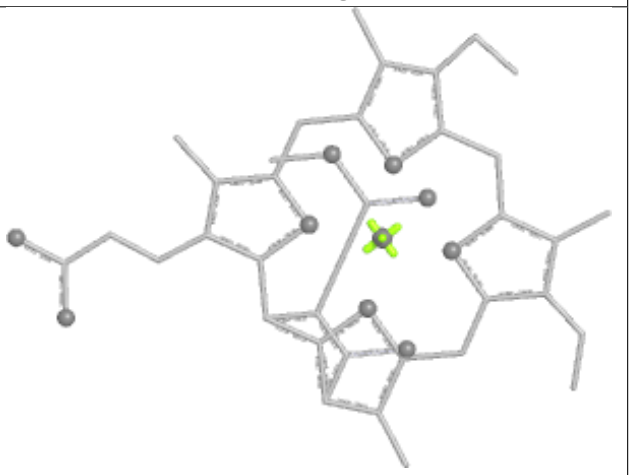
Bond lengths



Bond angles



Torsions

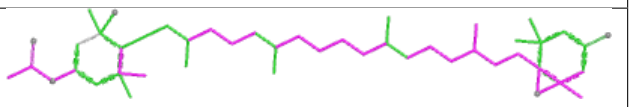


Rings

Ligand UIX E 304



Bond lengths



Bond angles

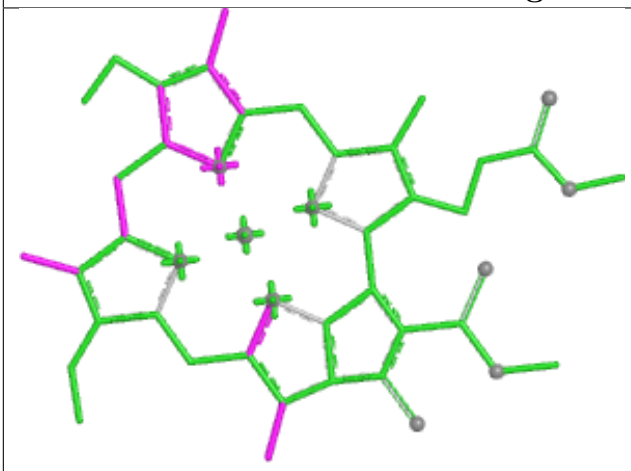


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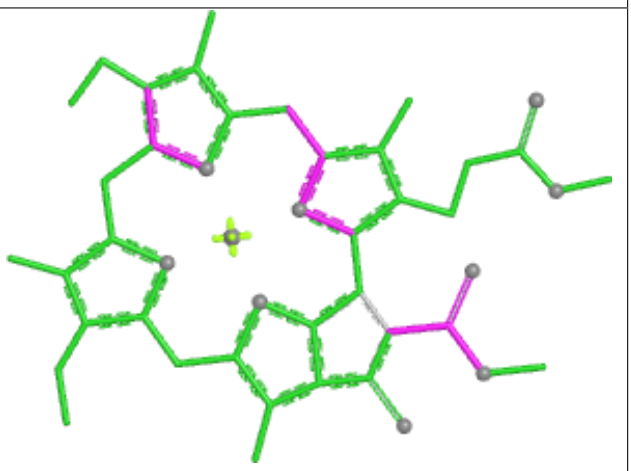


Rings

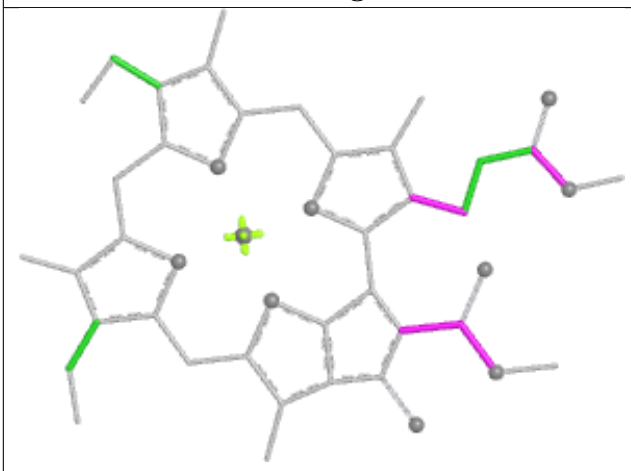
Ligand CLA F 310



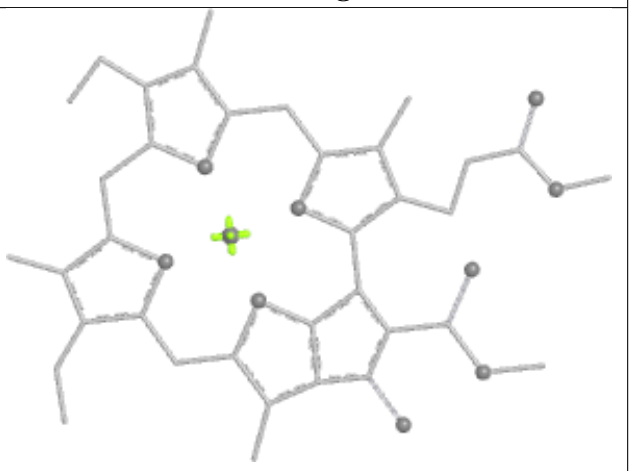
Bond lengths



Bond angles

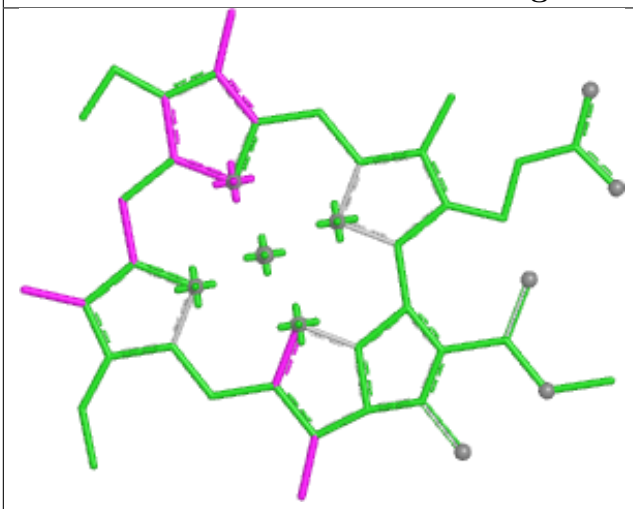


Torsions

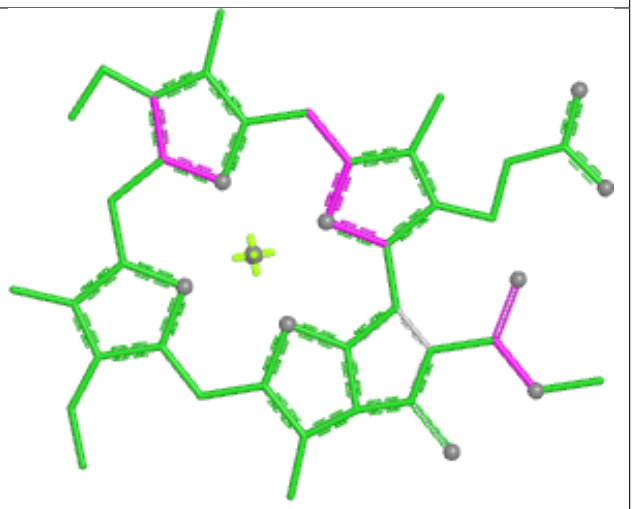


Rings

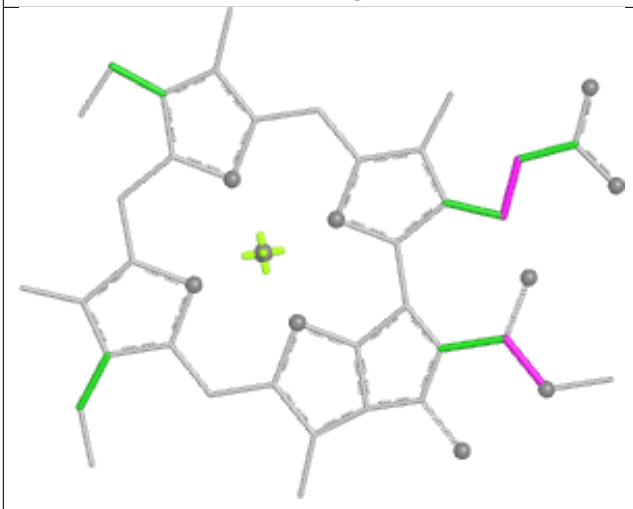
Ligand CLA I 201



Bond lengths



Bond angles

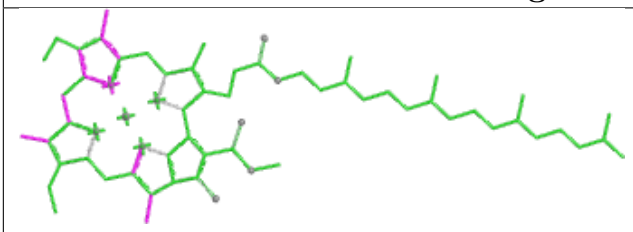


Torsions

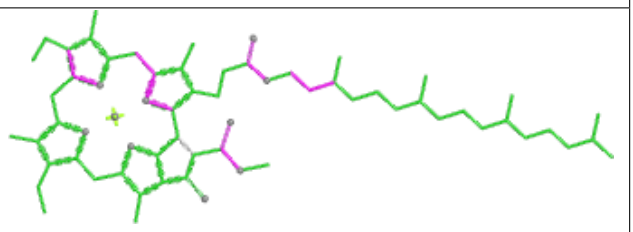


Rings

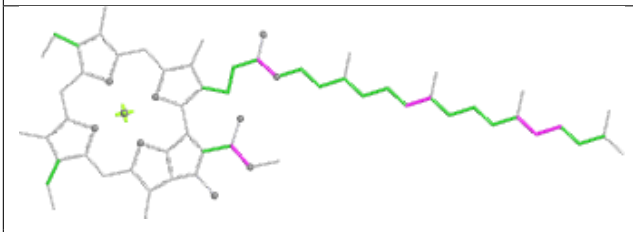
Ligand CLA a 824



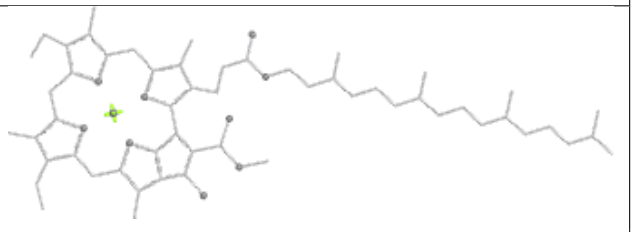
Bond lengths



Bond angles

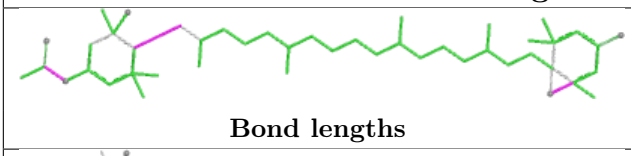


Torsions

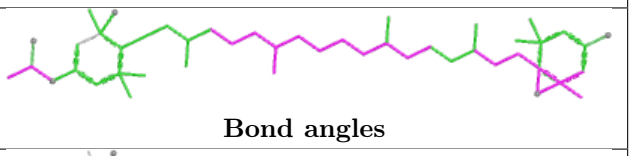


Rings

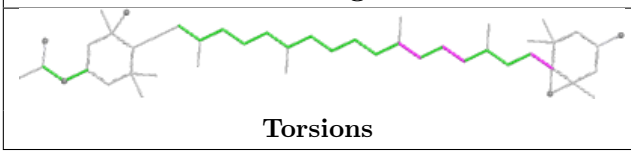
Ligand UIX J 304



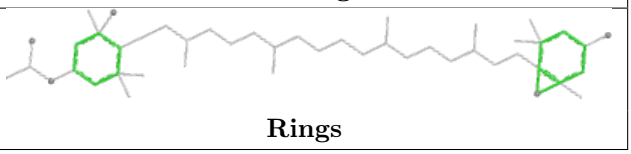
Bond lengths



Bond angles

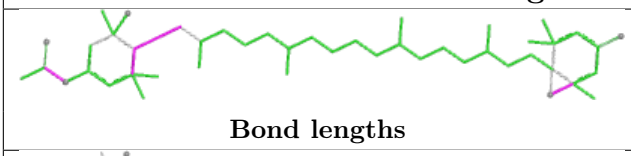


Torsions



Rings

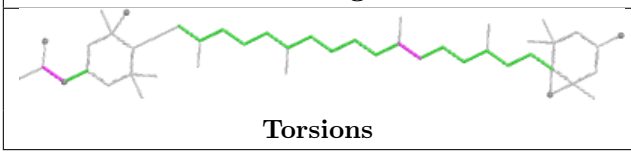
Ligand UIX A 203



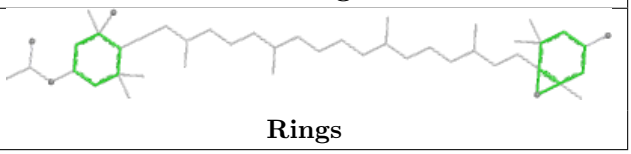
Bond lengths



Bond angles

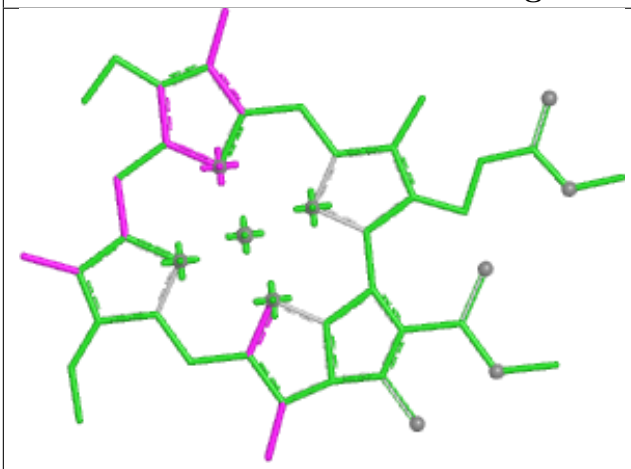


Torsions

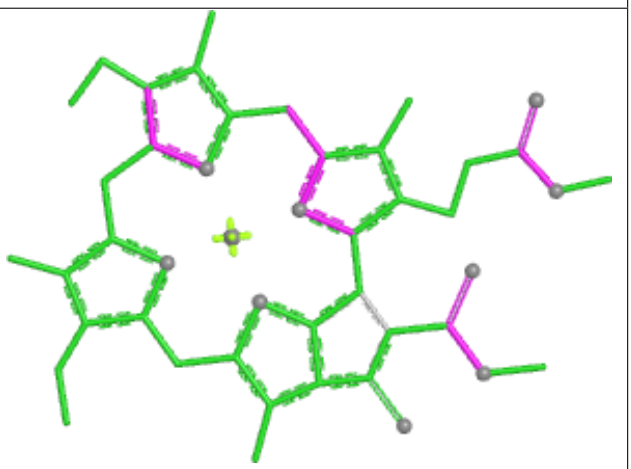


Rings

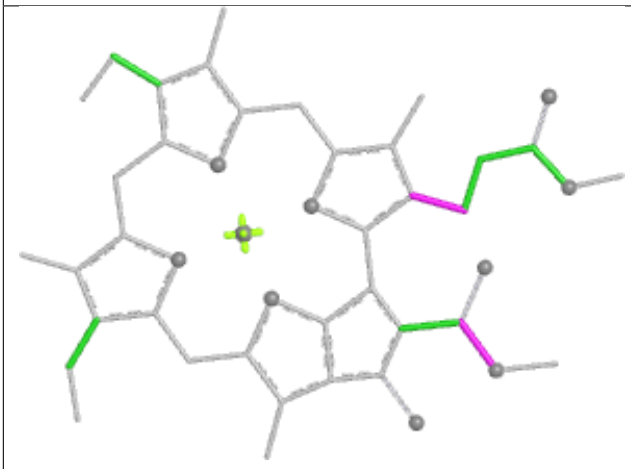
Ligand CLA T 309



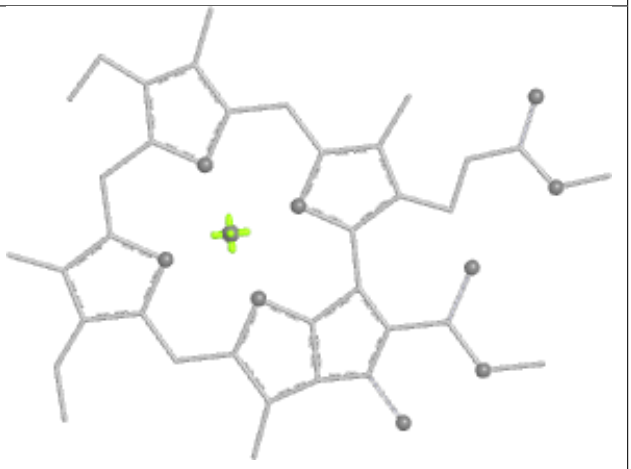
Bond lengths



Bond angles

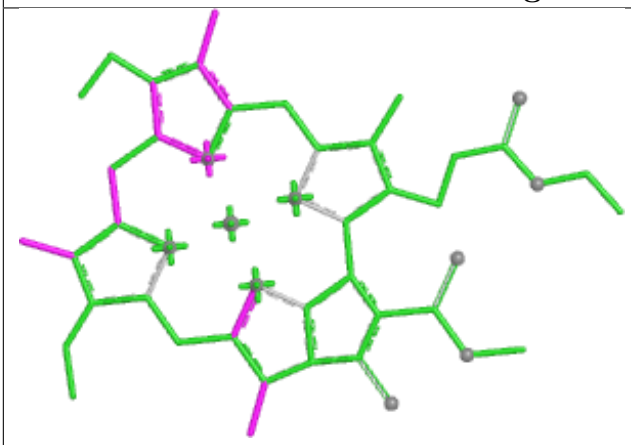


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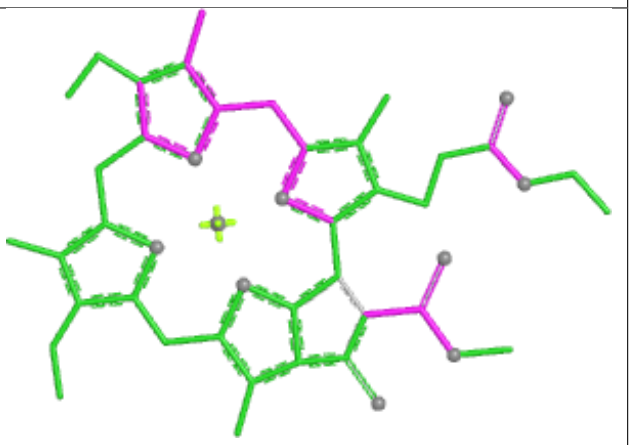


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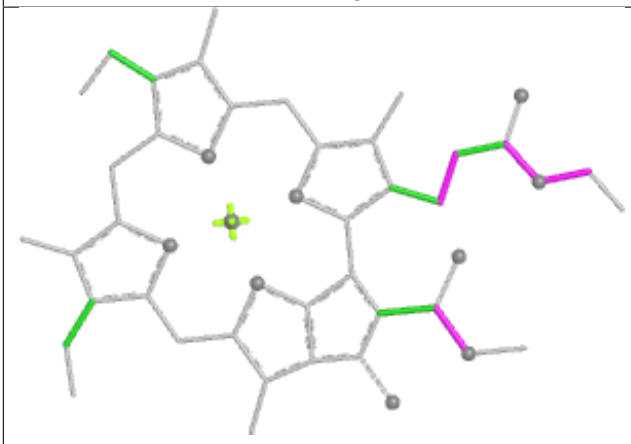
Ligand CLA O 314



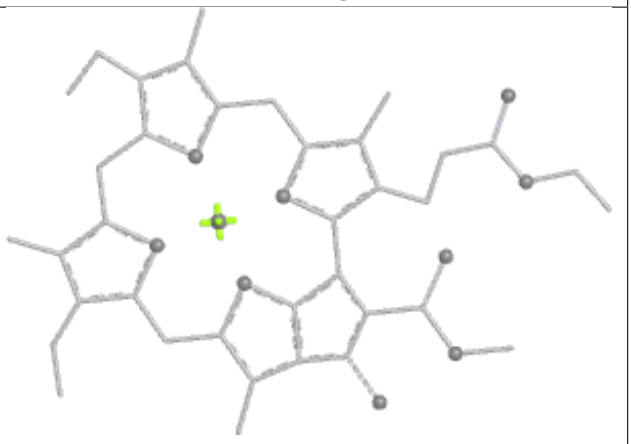
Bond lengths



Bond angles

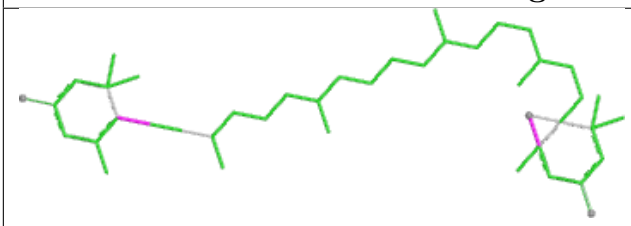


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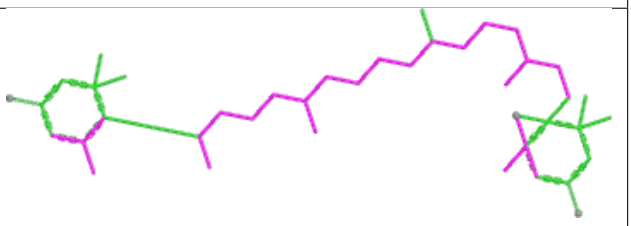


Rings

Ligand DD6 J 301



Bond lengths



Bond angles

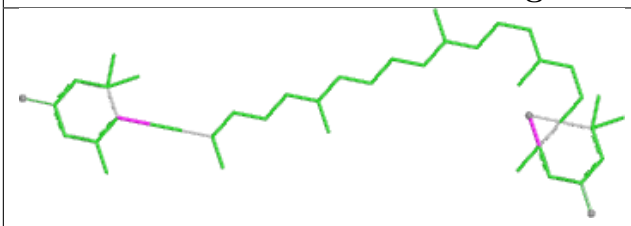


Torsions

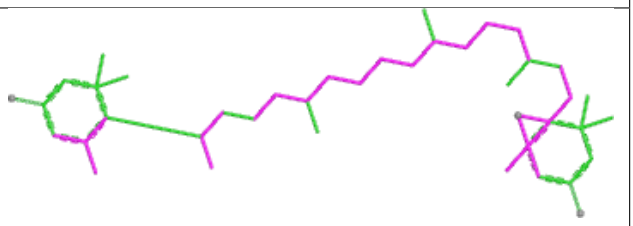


Rings

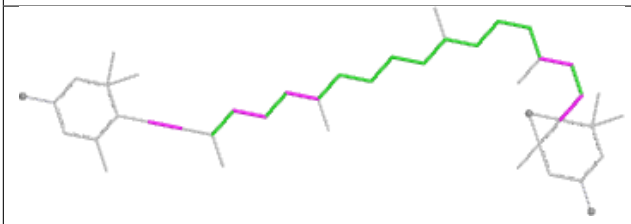
Ligand DD6 T 303



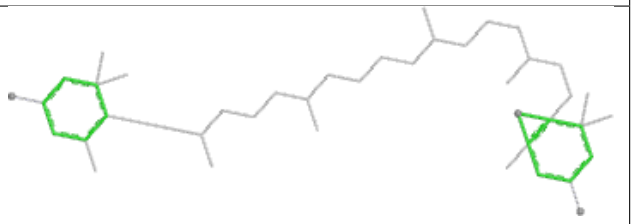
Bond lengths



Bond angles

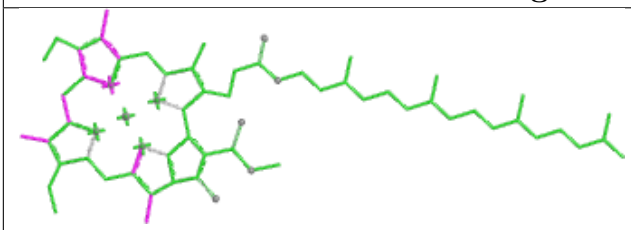


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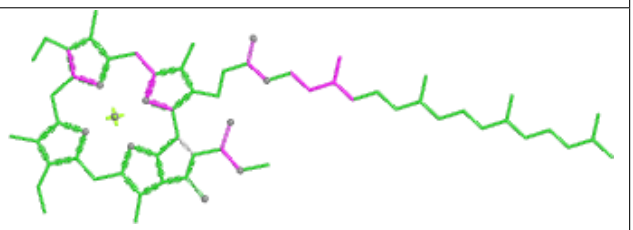


Rings

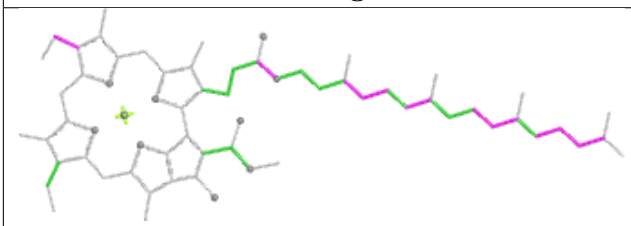
Ligand CLA I 213



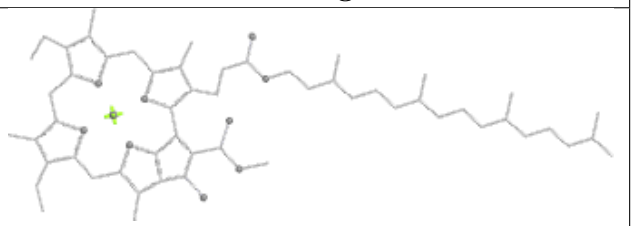
Bond lengths



Bond angles

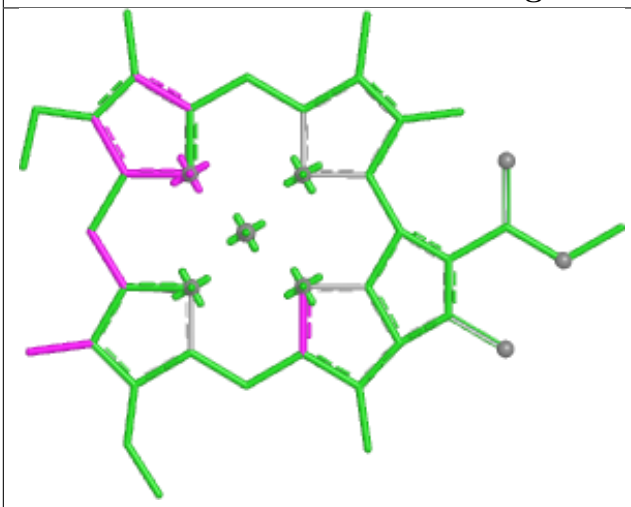


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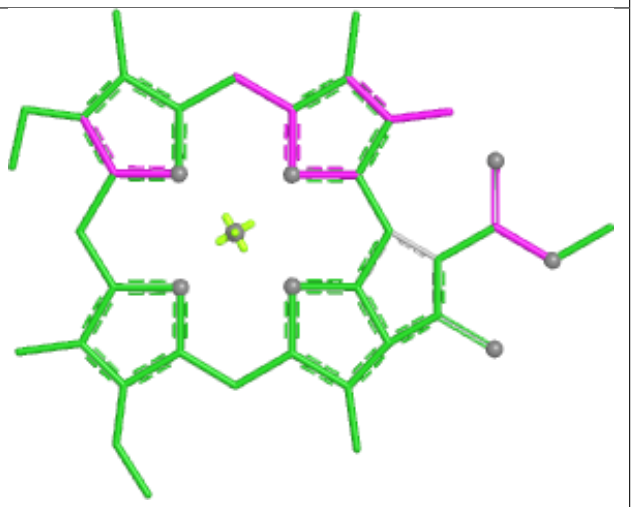


Rings

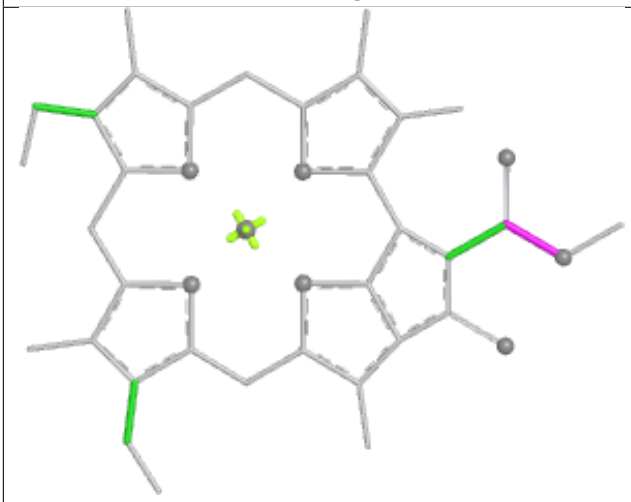
Ligand CLA P 217



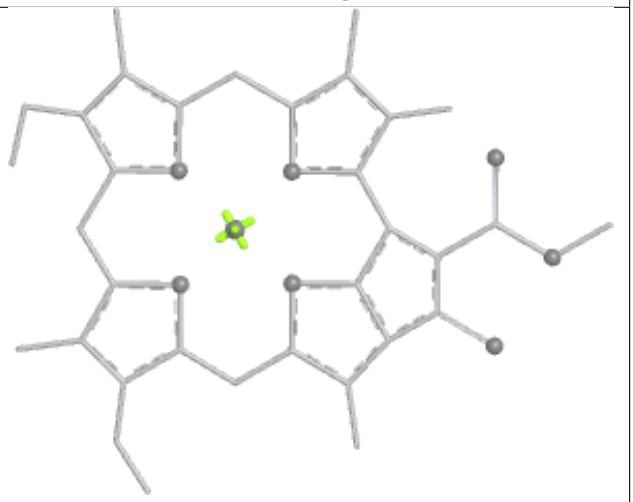
Bond lengths



Bond angles



Torsions

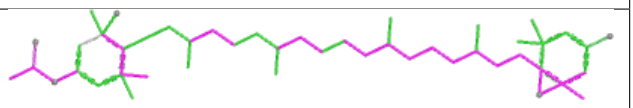


Rings

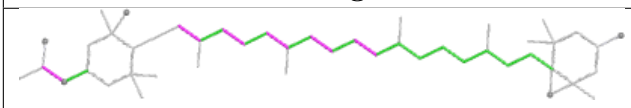
Ligand UIX N 306



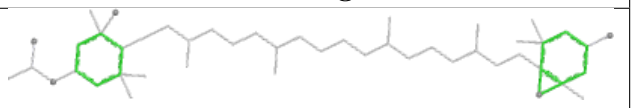
Bond lengths



Bond angles

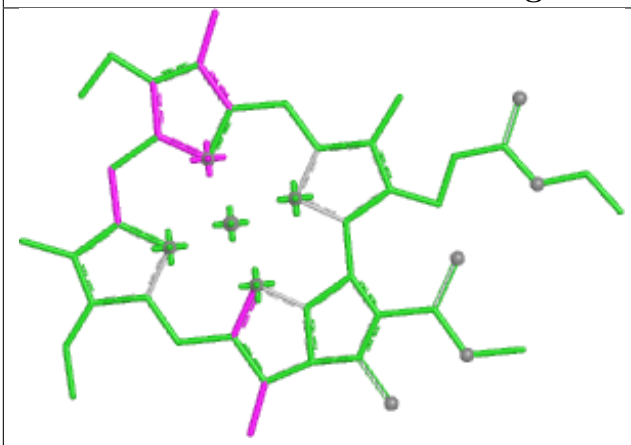


Torsions

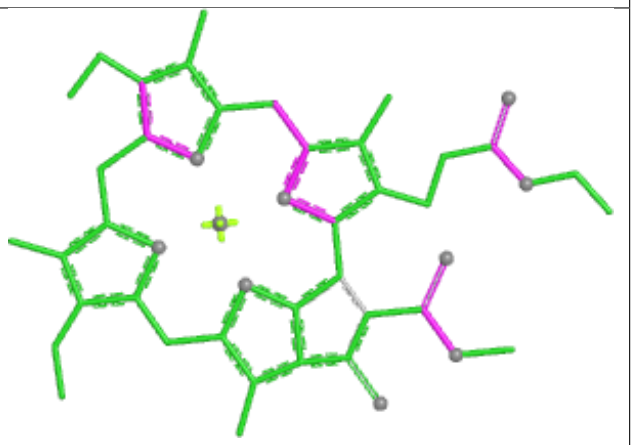


Rings

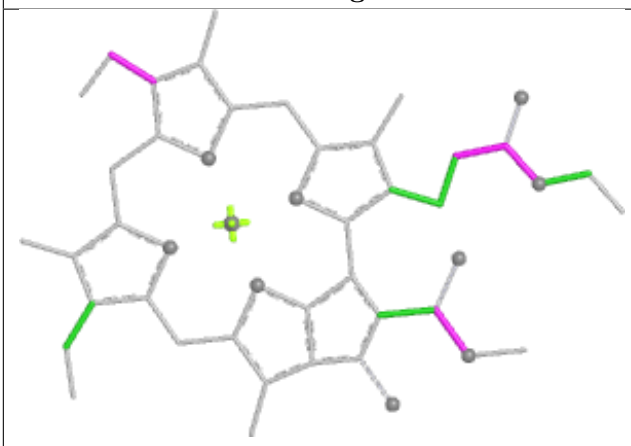
Ligand CLA P 209



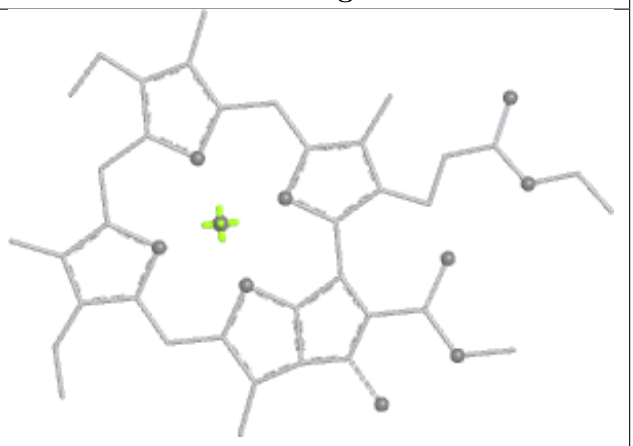
Bond lengths



Bond angles

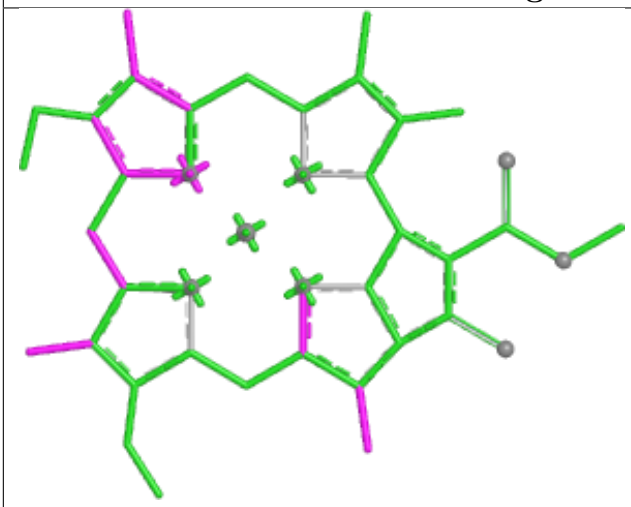


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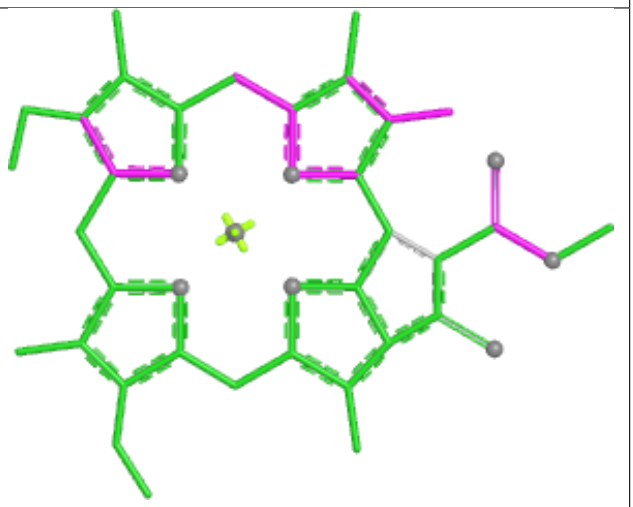


Rings

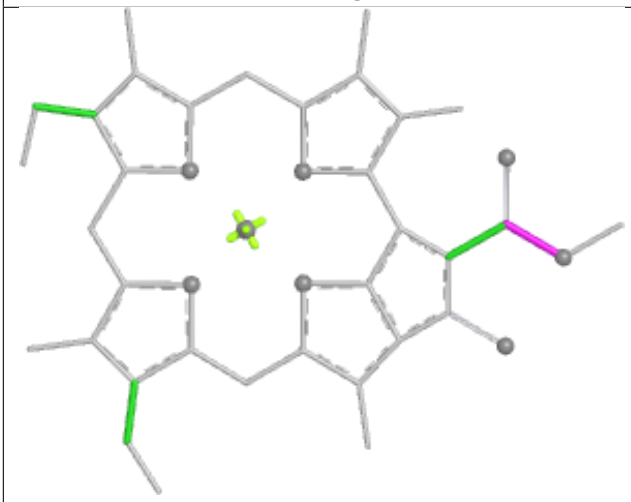
Ligand CLA F 316



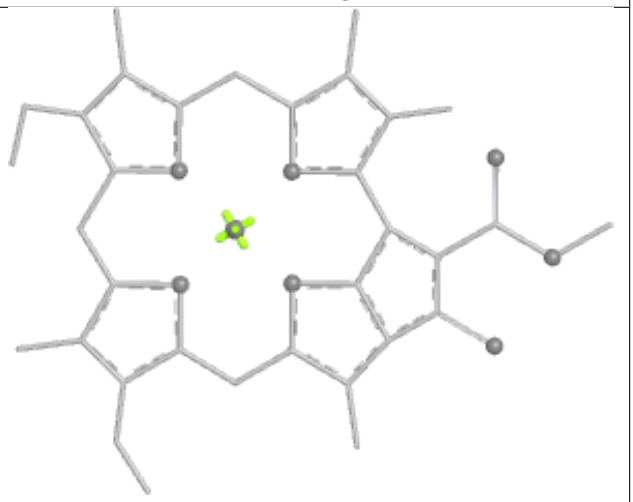
Bond lengths



Bond angles

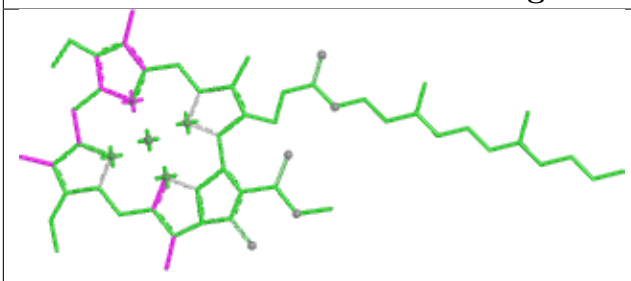


Torsions

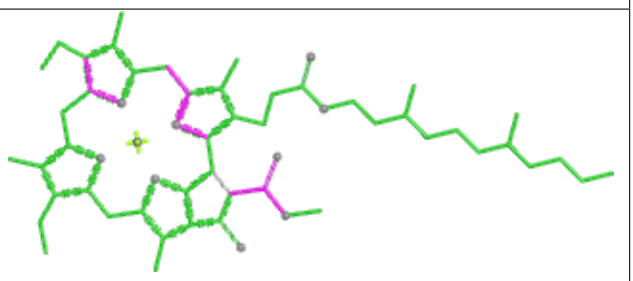


Rings

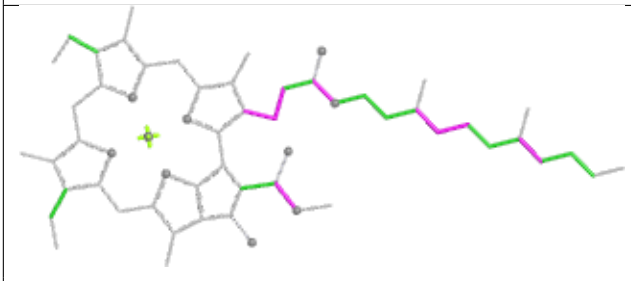
Ligand CLA b 711



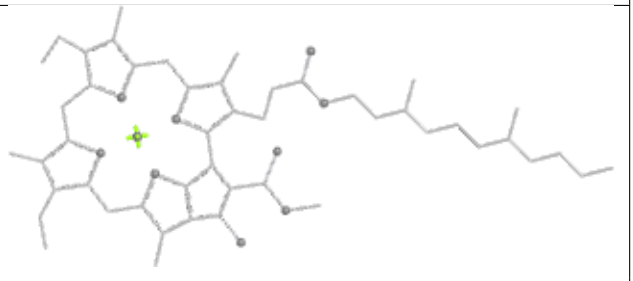
Bond lengths



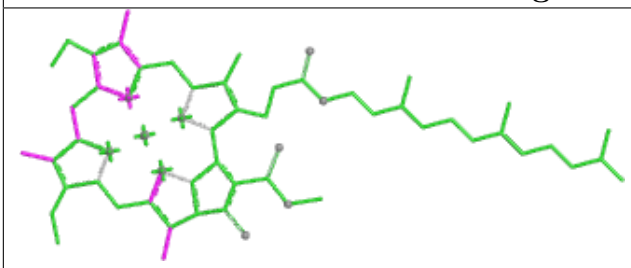
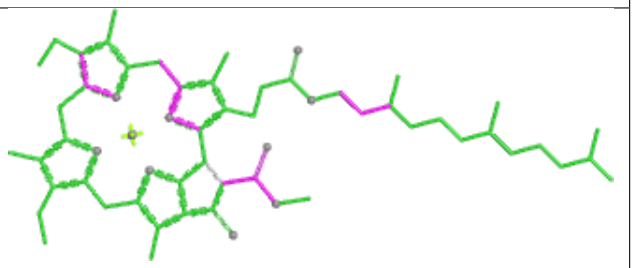
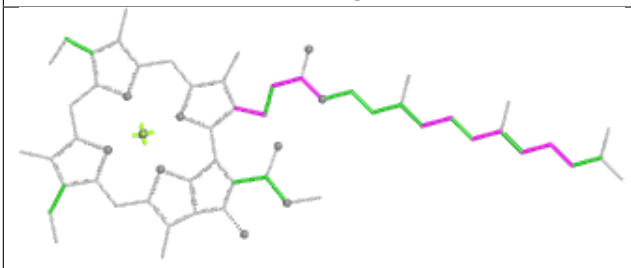
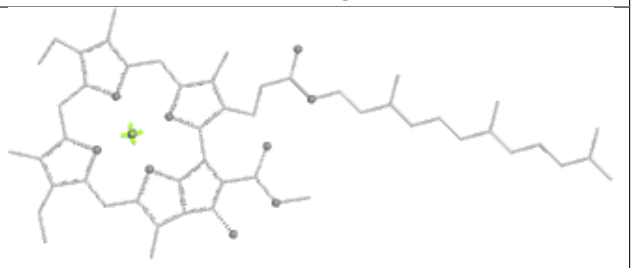
Bond angles

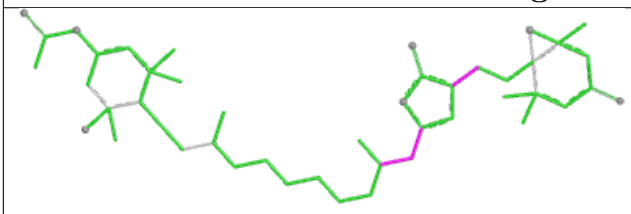
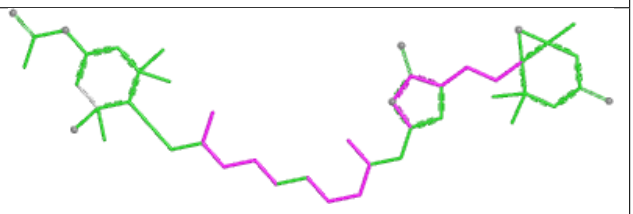
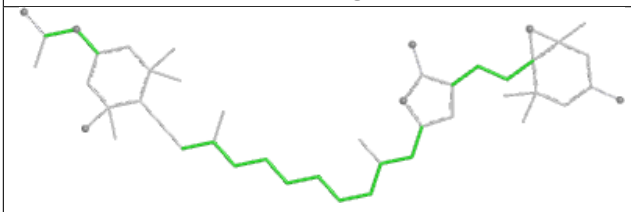
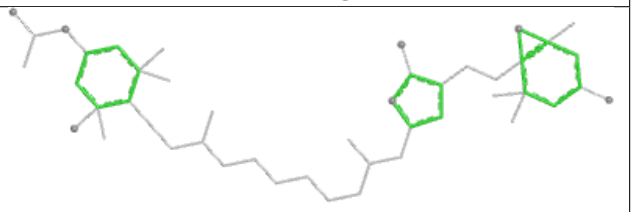


Torsions

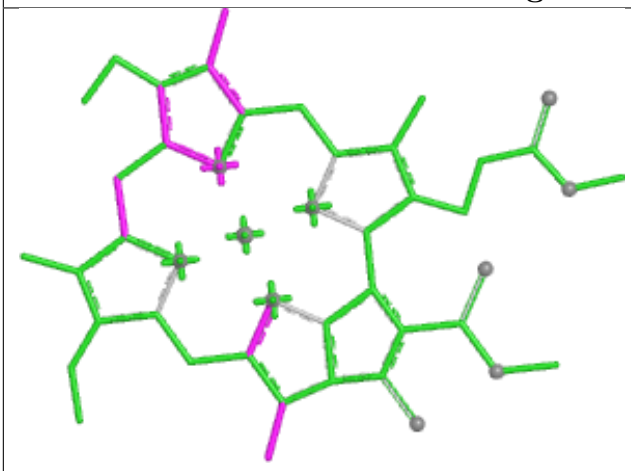


Rings

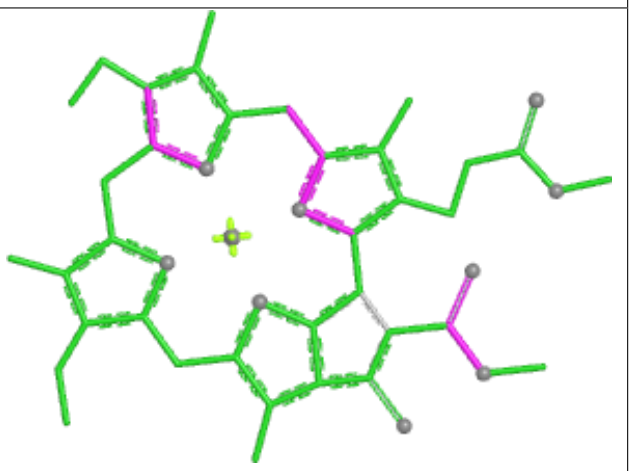
Ligand CLA l 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PID F 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

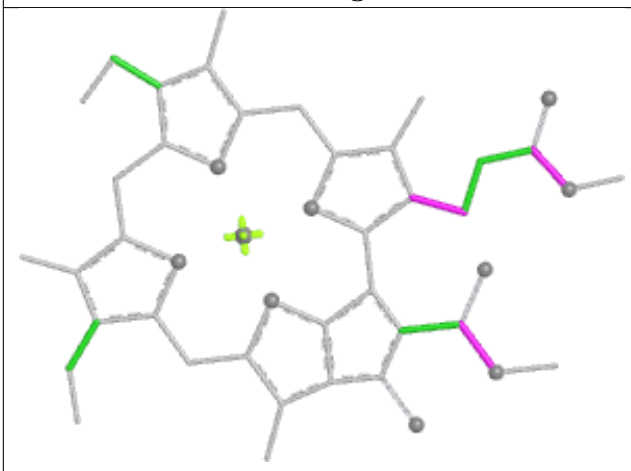
Ligand CLA L 311



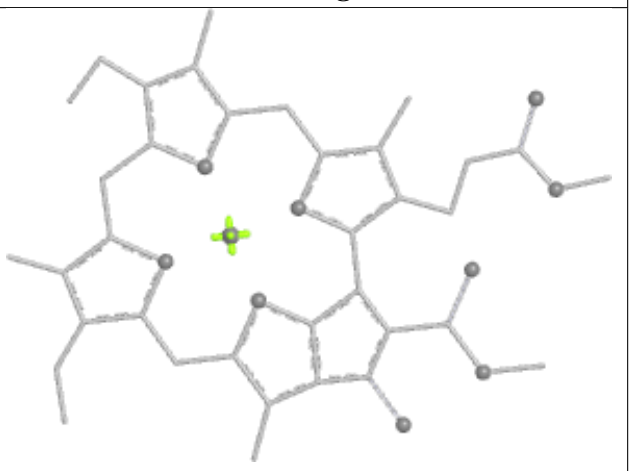
Bond lengths



Bond angles

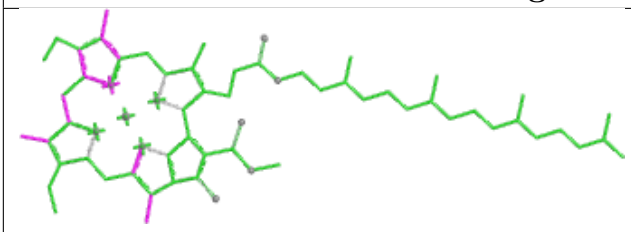


Torsions

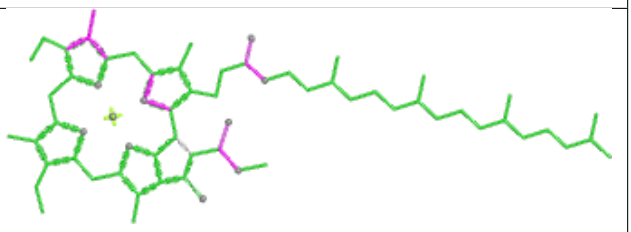


Rings

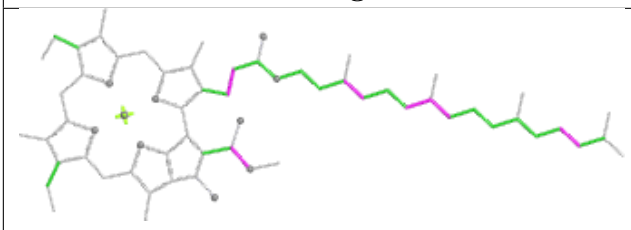
Ligand CLA a 803



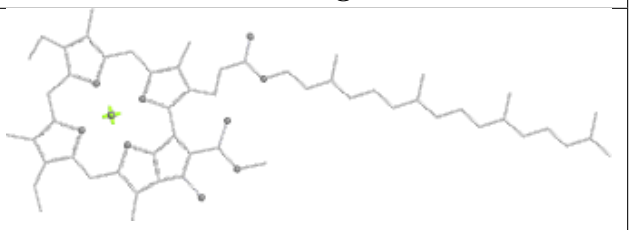
Bond lengths



Bond angles

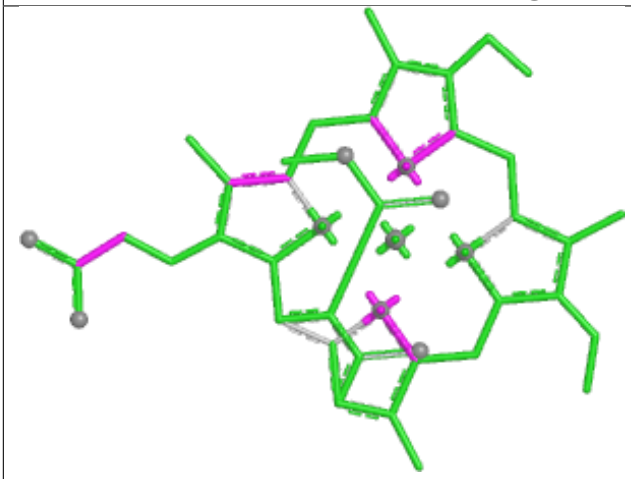


Torsions

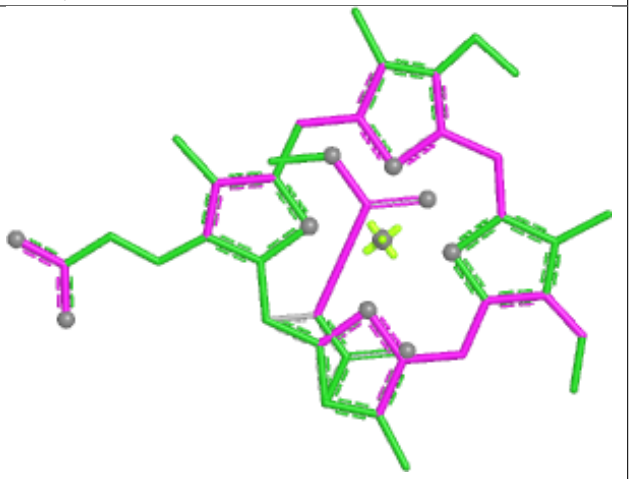


Rings

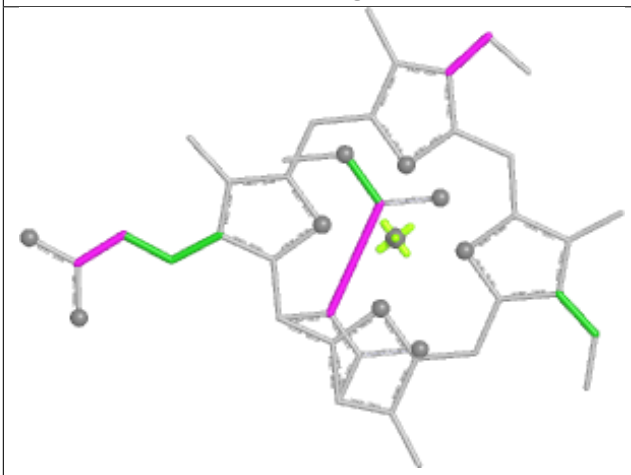
Ligand KC1 Q 311



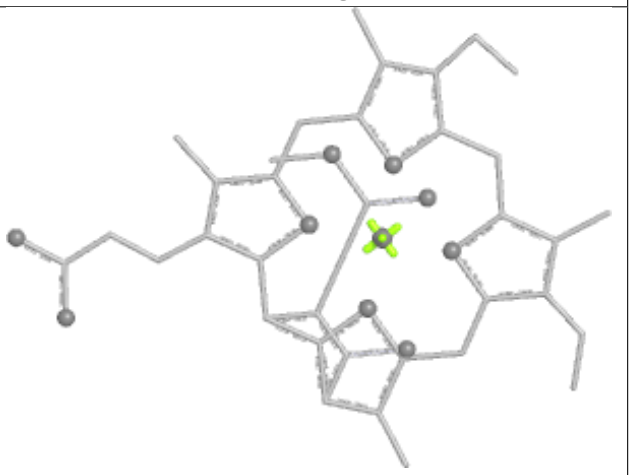
Bond lengths



Bond angles

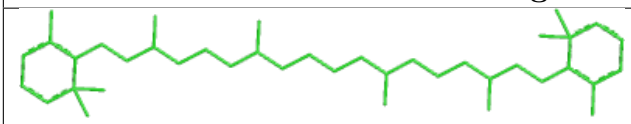


Torsions

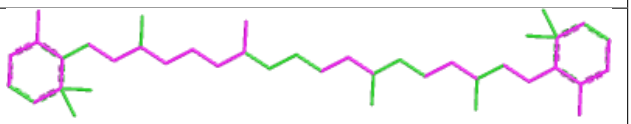


Rings

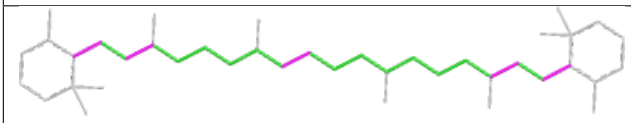
Ligand BCR l 506



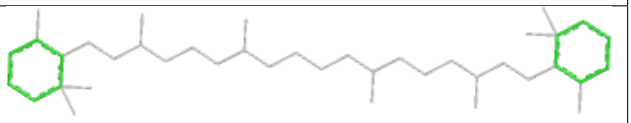
Bond lengths



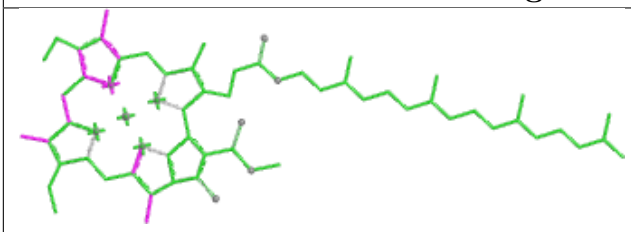
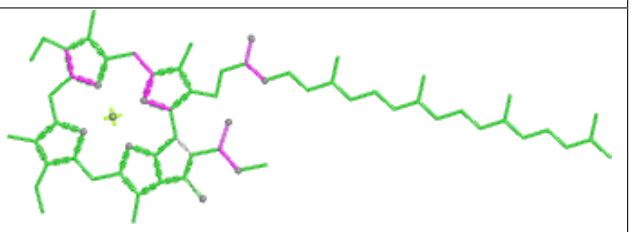
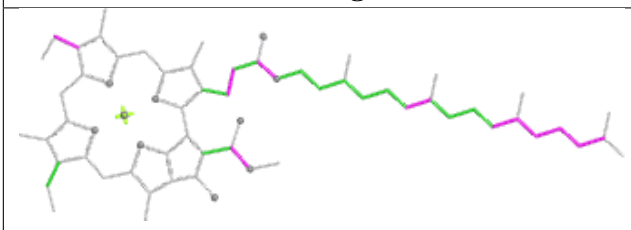
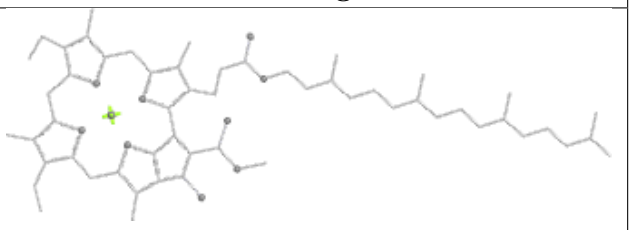
Bond angles

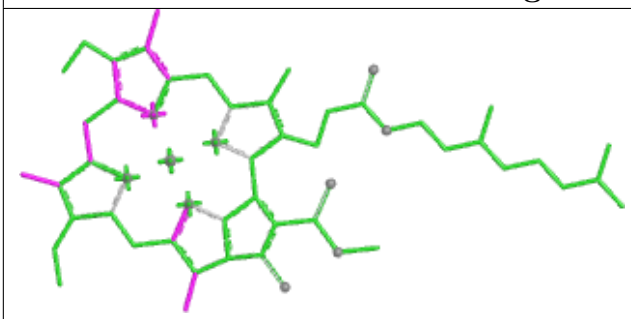
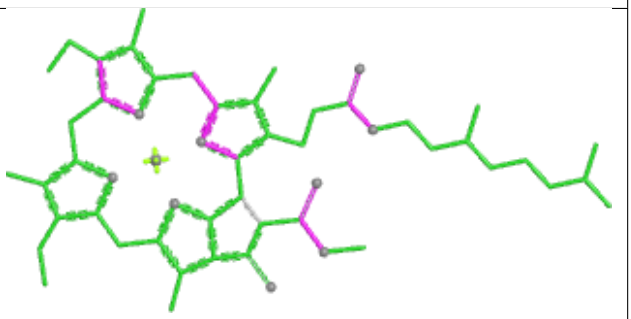
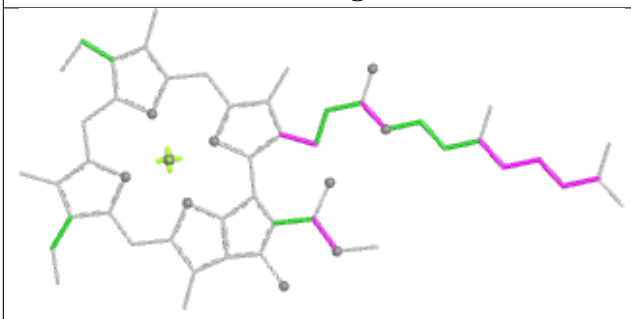
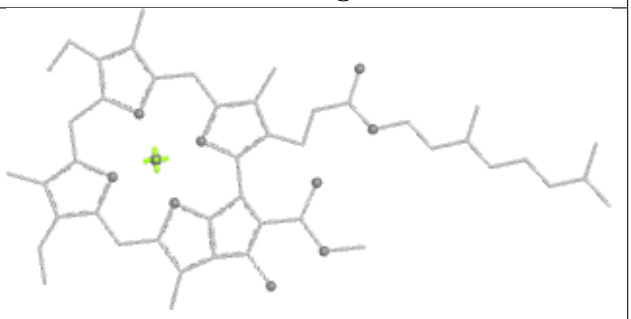


Torsions

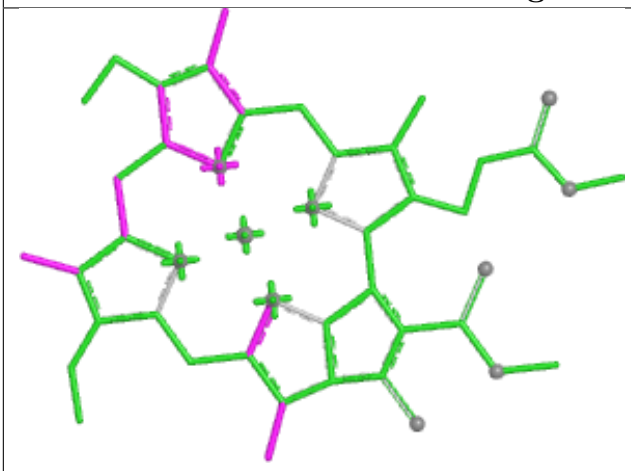


Rings

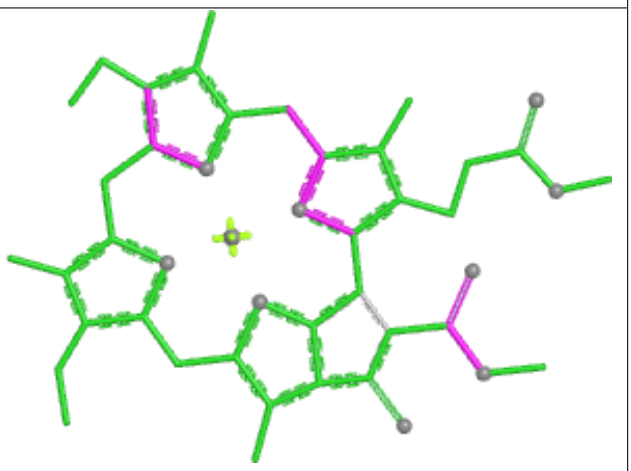
Ligand CLA E 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

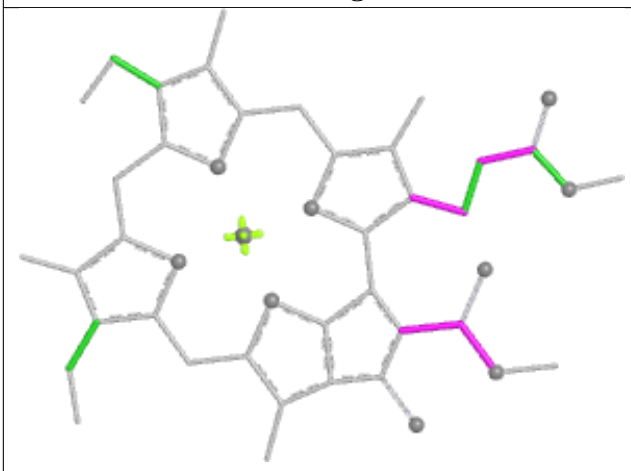
Ligand CLA b 710



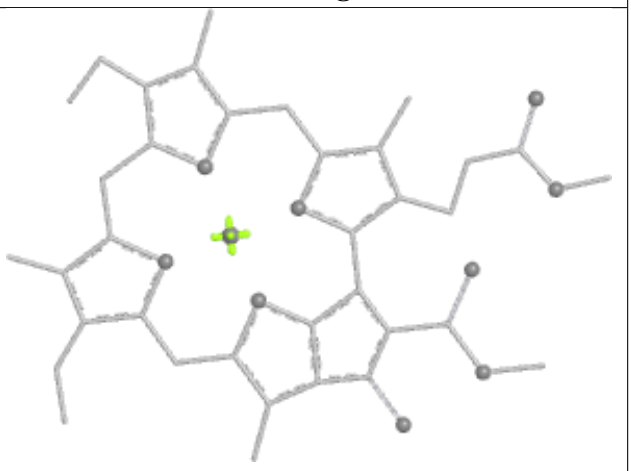
Bond lengths



Bond angles

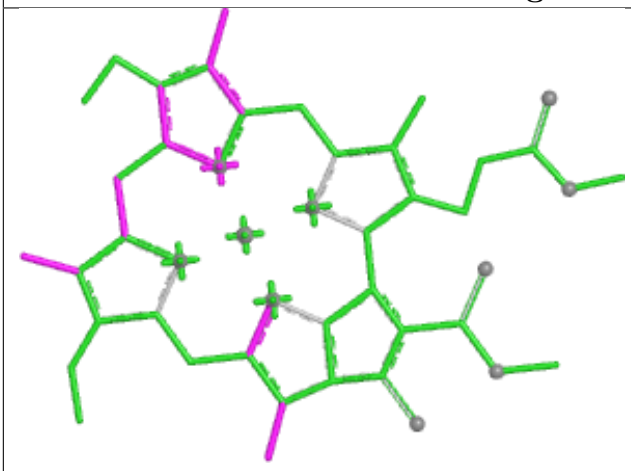


Torsions

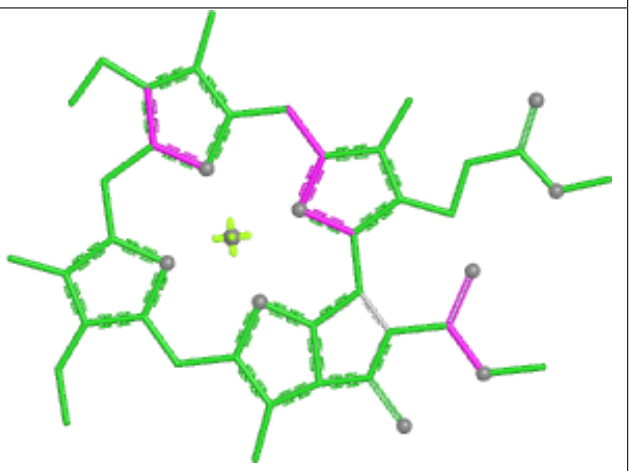


Rings

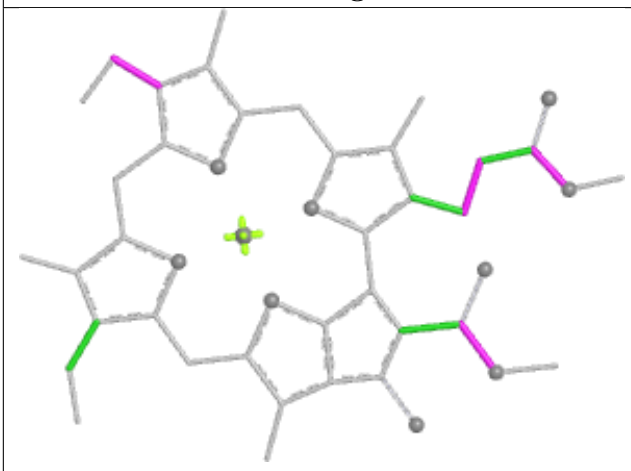
Ligand CLA L 317



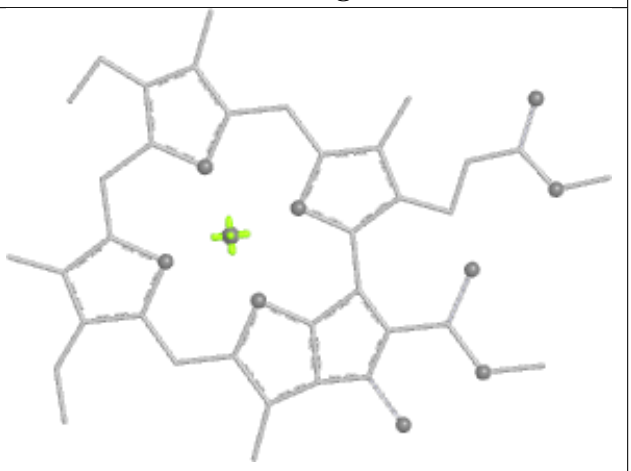
Bond lengths



Bond angles

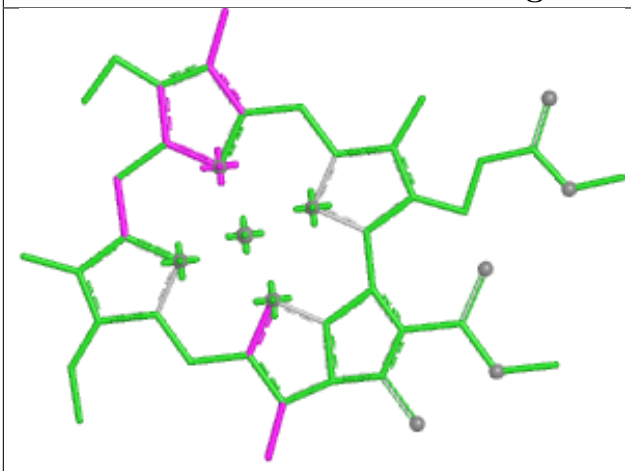


Torsions

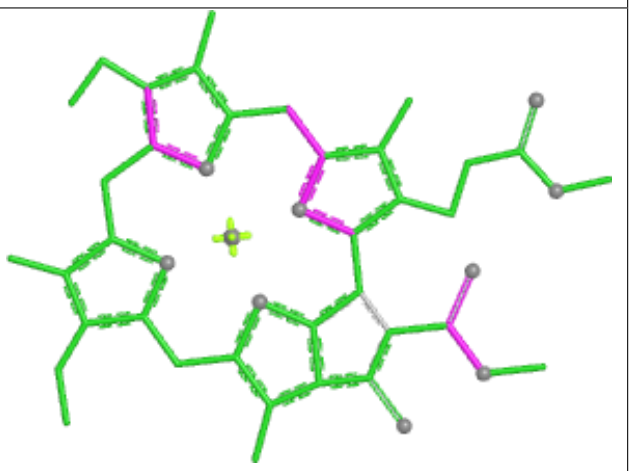


Rings

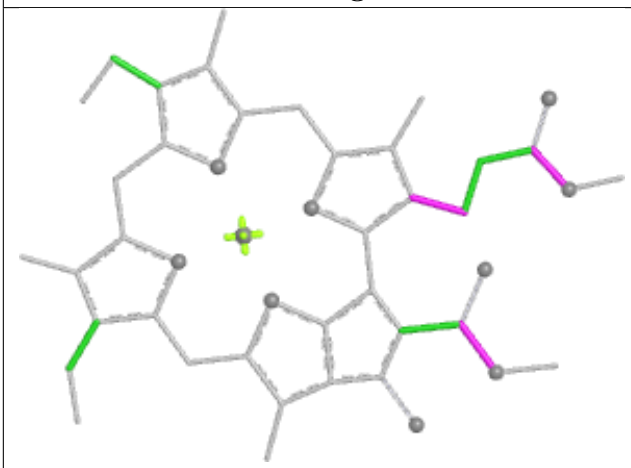
Ligand CLA F 312



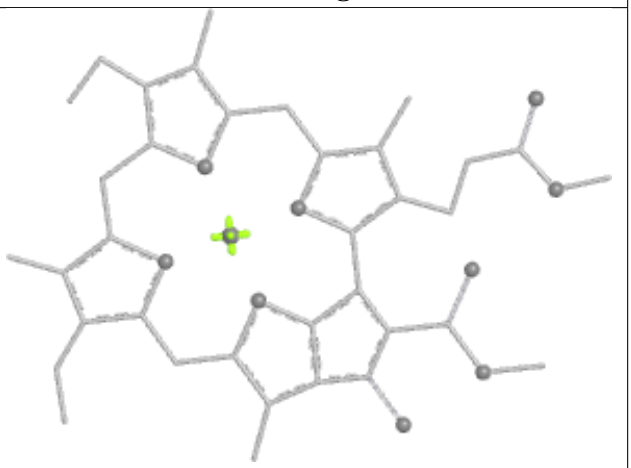
Bond lengths



Bond angles

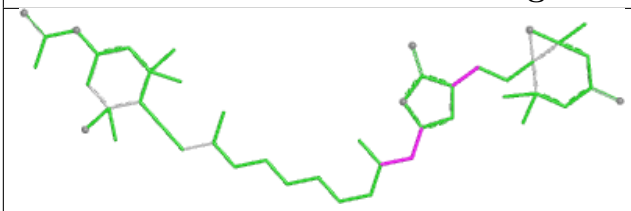


Torsions

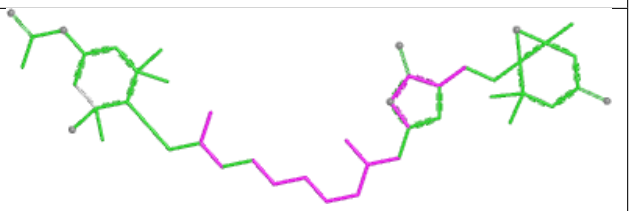


Rings

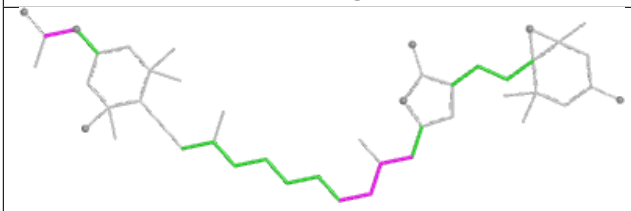
Ligand PID G 303



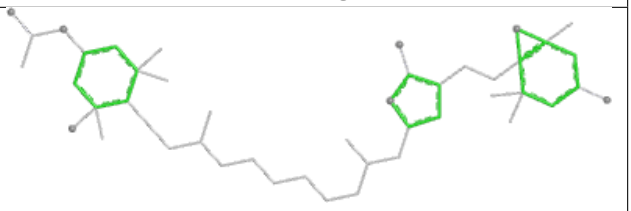
Bond lengths



Bond angles

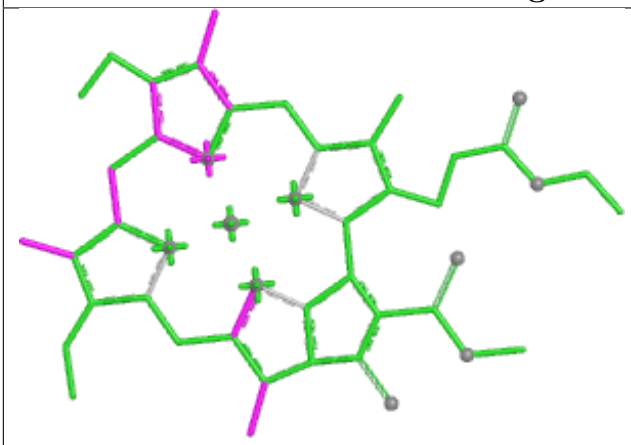


Torsions

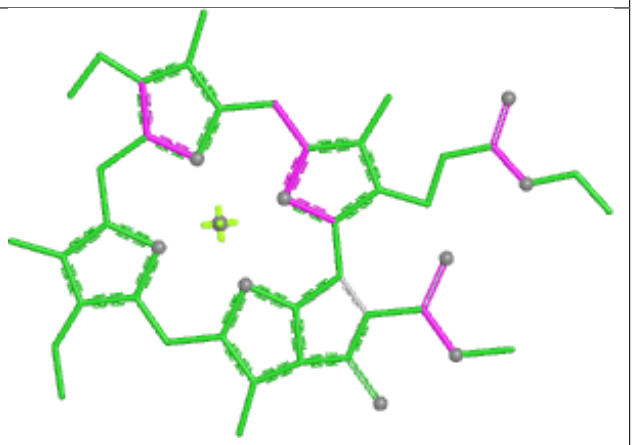


Rings

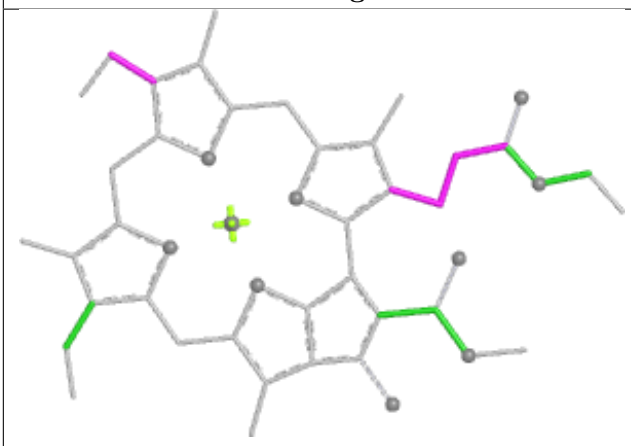
Ligand CLA a 818



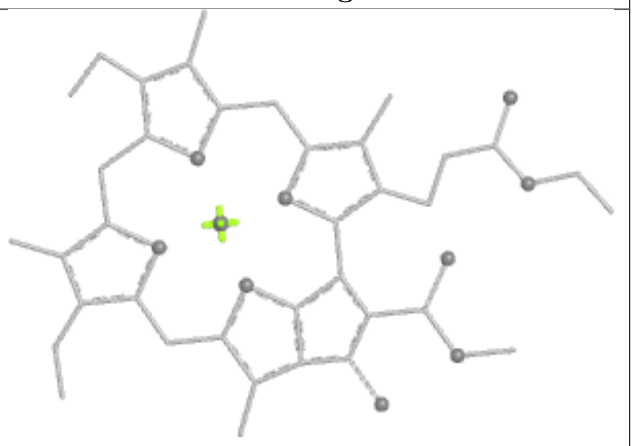
Bond lengths



Bond angles

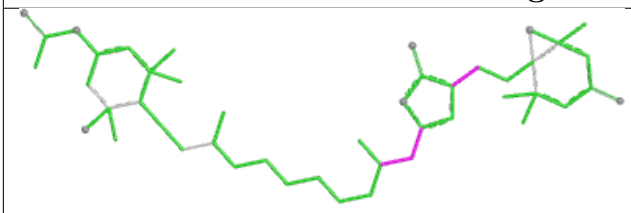


Torsions

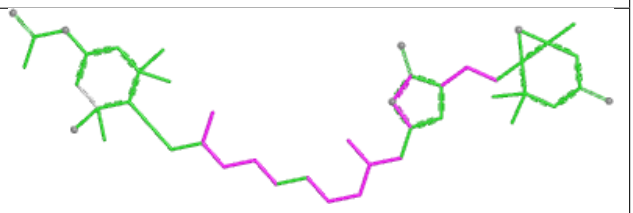


Rings

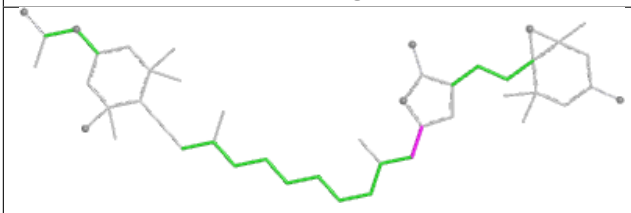
Ligand PID N 304



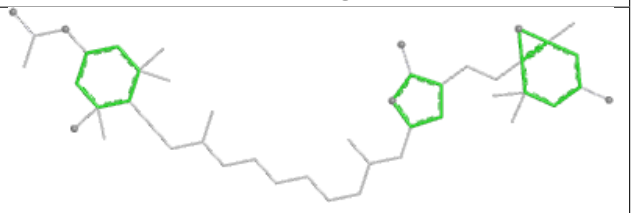
Bond lengths



Bond angles

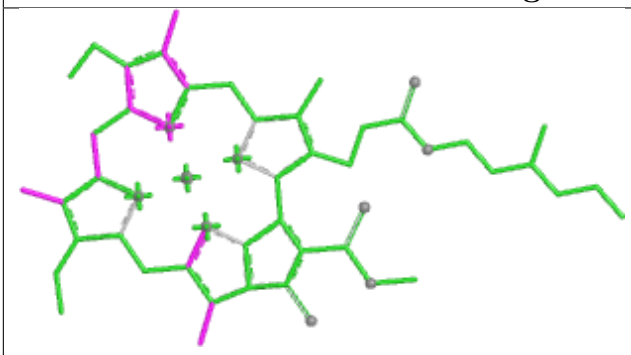


Torsions

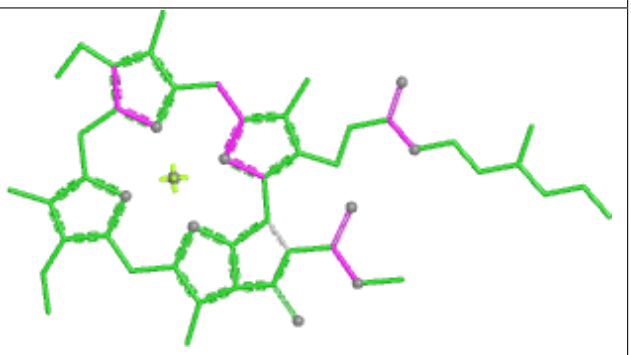


Rings

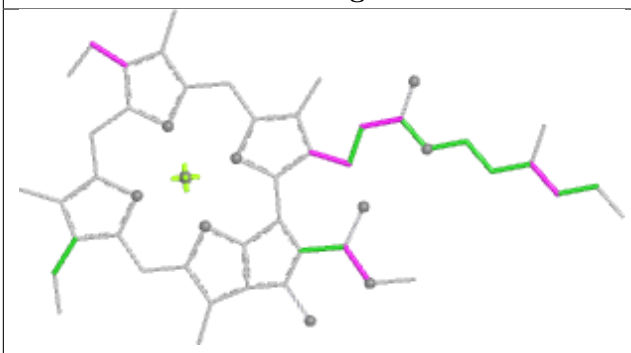
Ligand CLA K 212



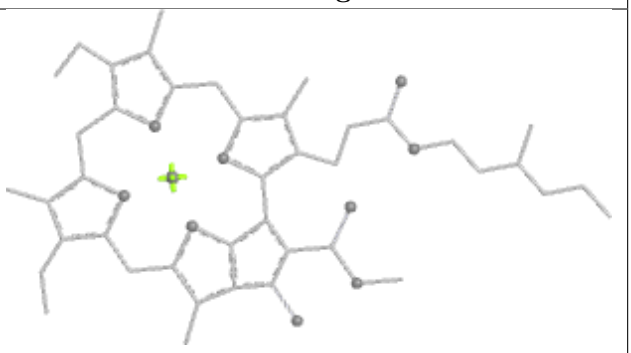
Bond lengths



Bond angles

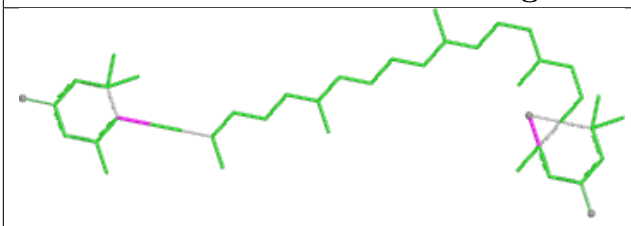


Torsions

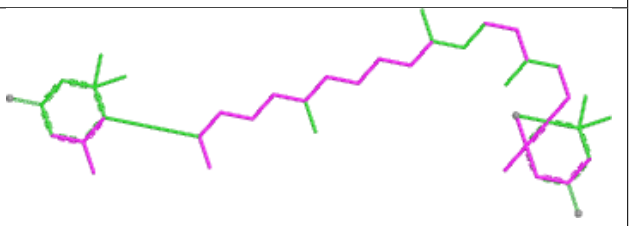


Rings

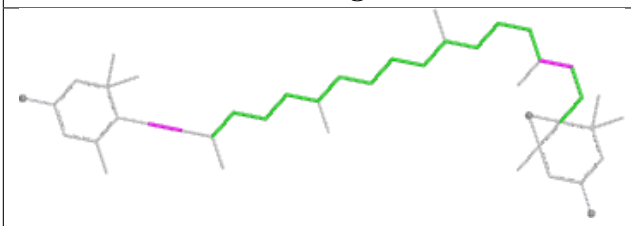
Ligand DD6 M 304



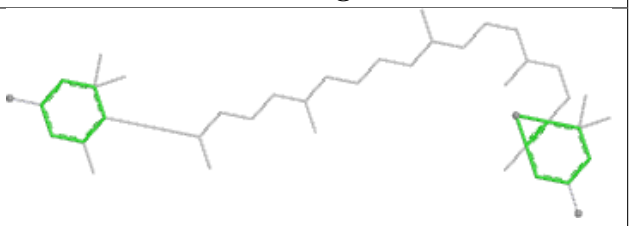
Bond lengths



Bond angles

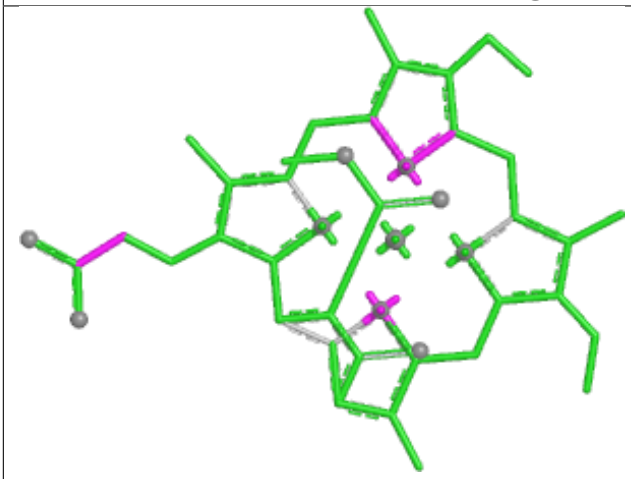


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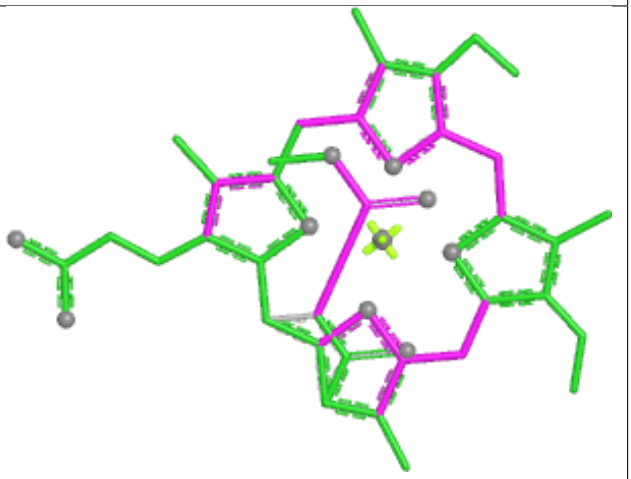


Rings

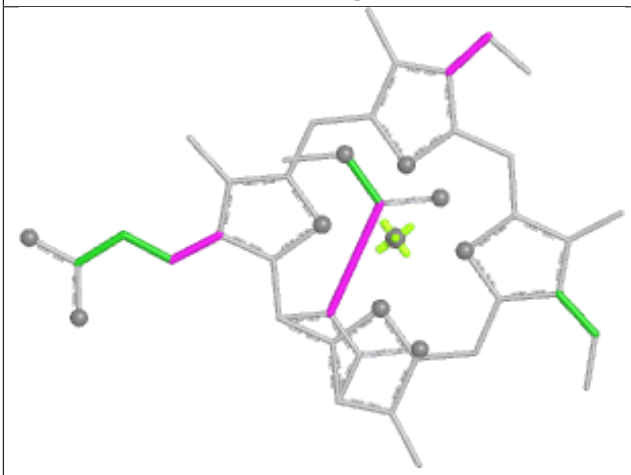
Ligand KC1 T 310



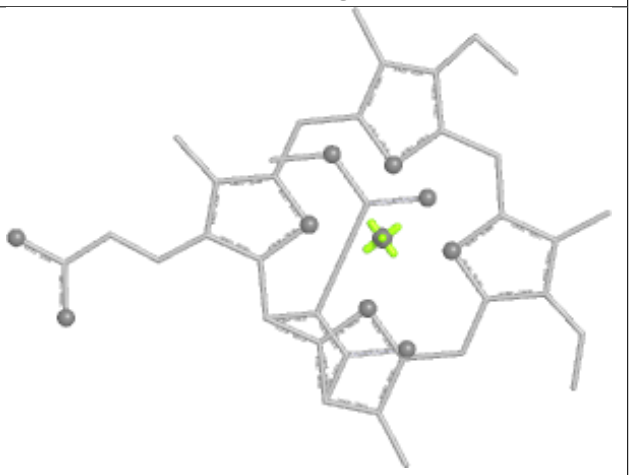
Bond lengths



Bond angles

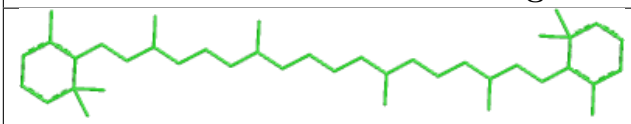


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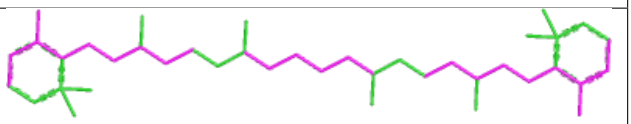


Rings

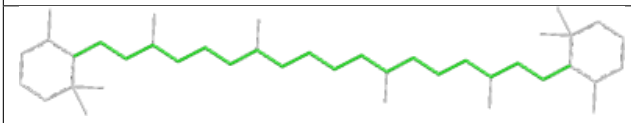
Ligand BCR a 834



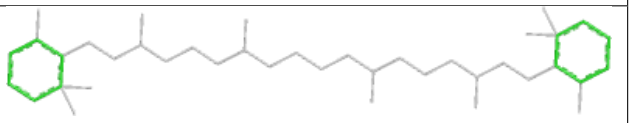
Bond lengths



Bond angles

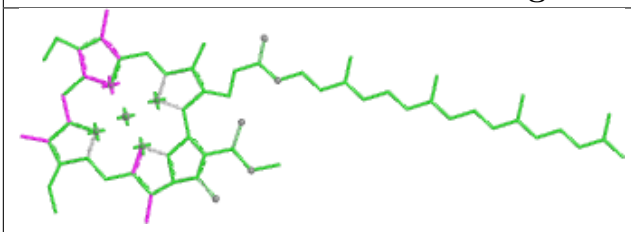


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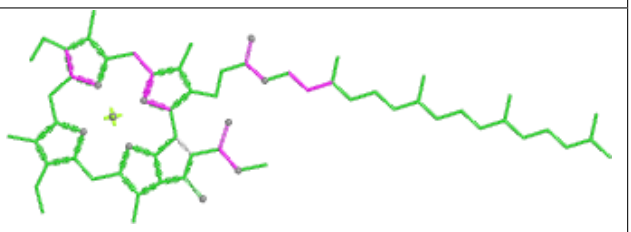


Rings

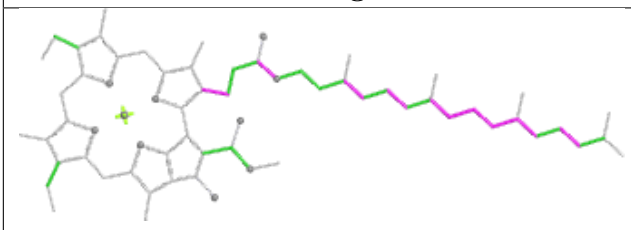
Ligand CLA a 807



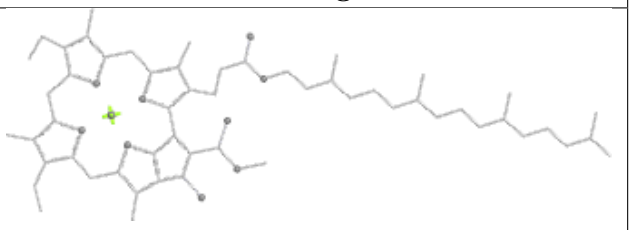
Bond lengths



Bond angles

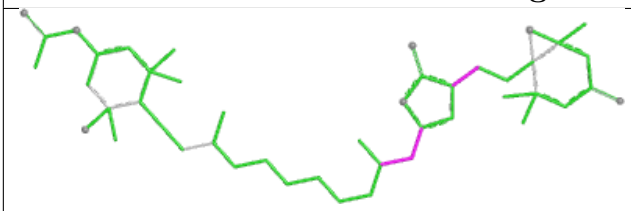


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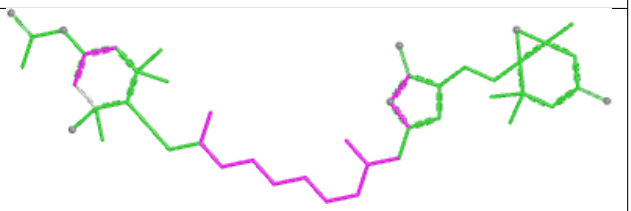


Rings

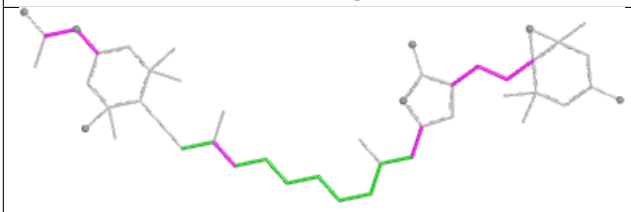
Ligand PID T 317



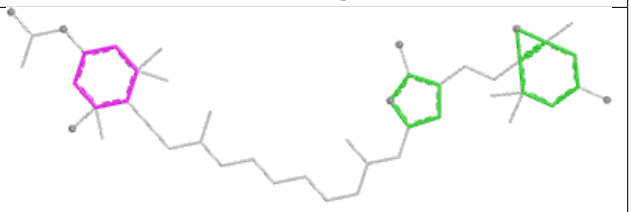
Bond lengths



Bond angles

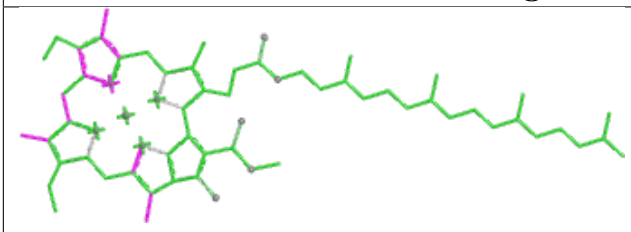


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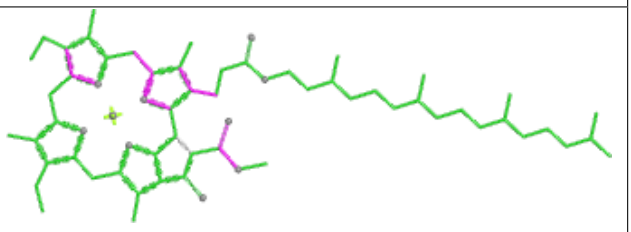


Rings

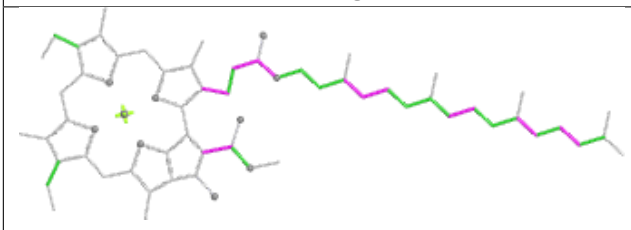
Ligand CLA G 302



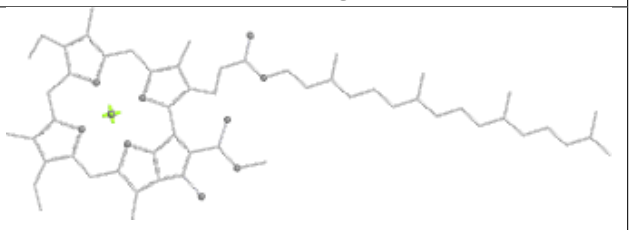
Bond lengths



Bond angles

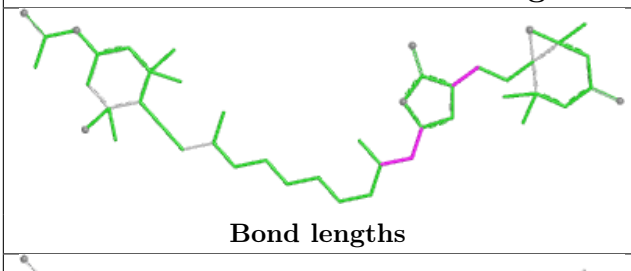


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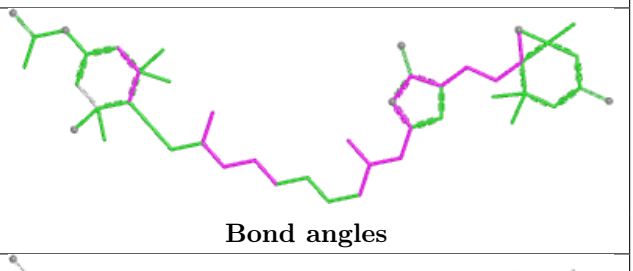


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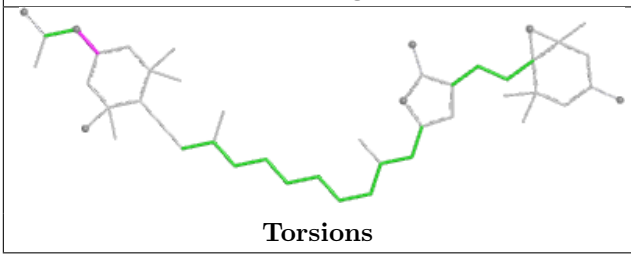
Ligand PID D 303



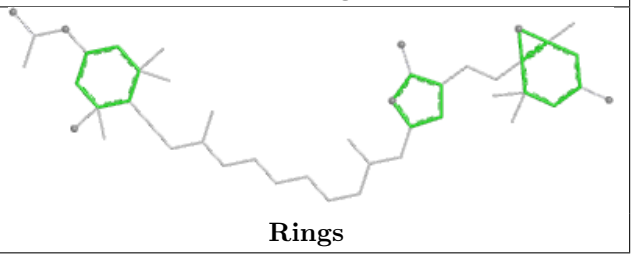
Bond lengths



Bond angles

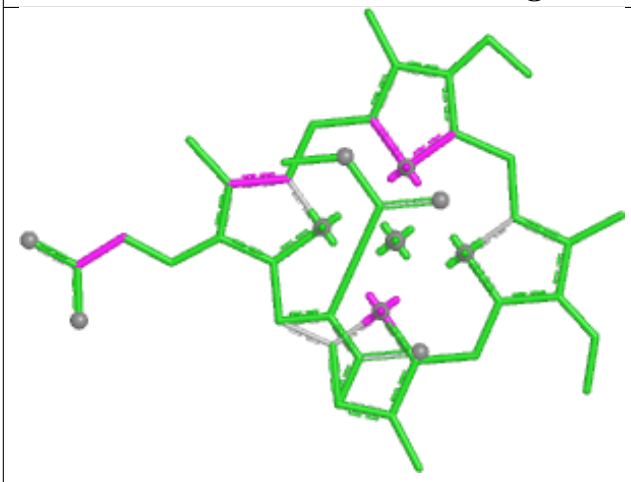


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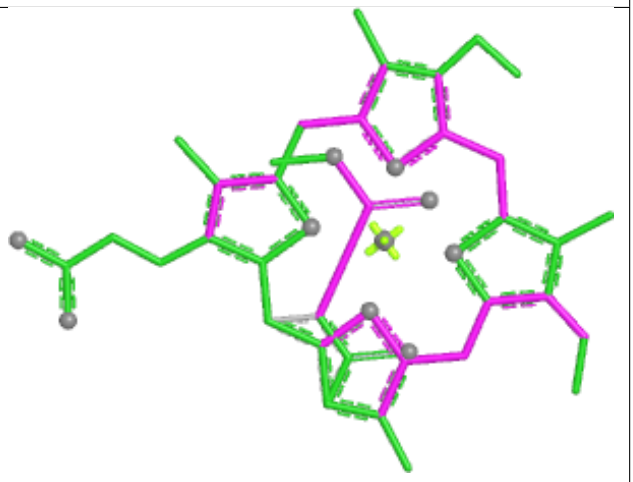


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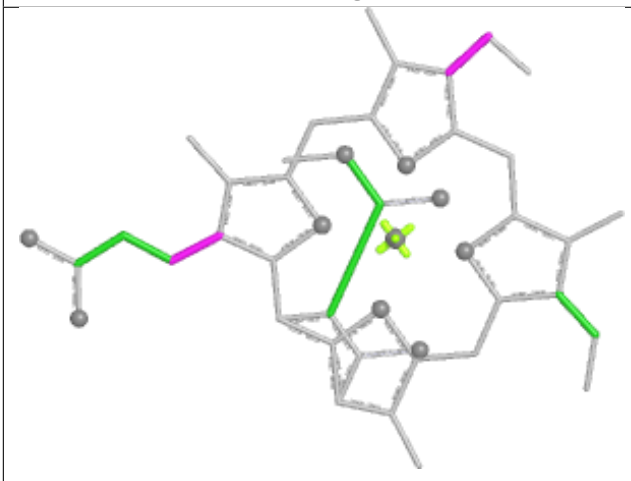
Ligand KC1 O 312



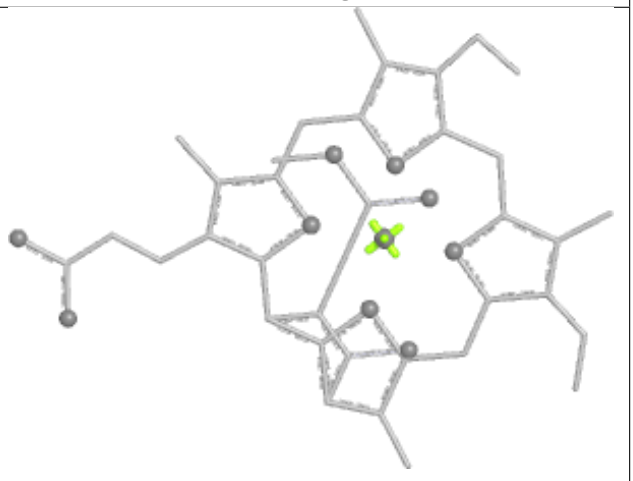
Bond lengths



Bond angles

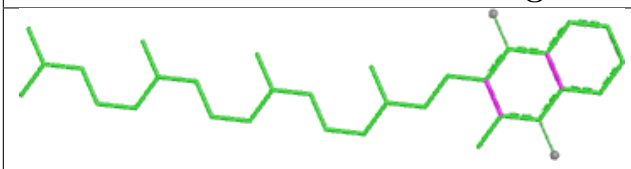


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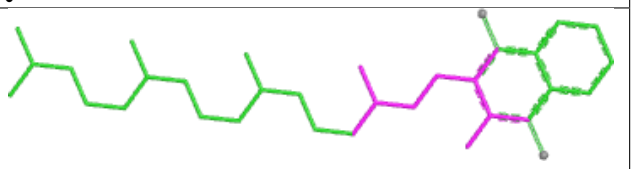


Rings

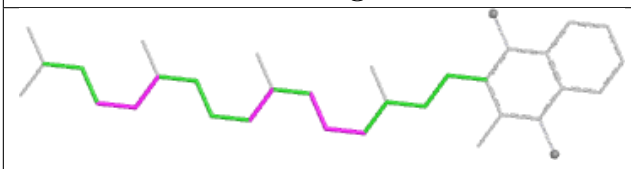
Ligand PQN a 832



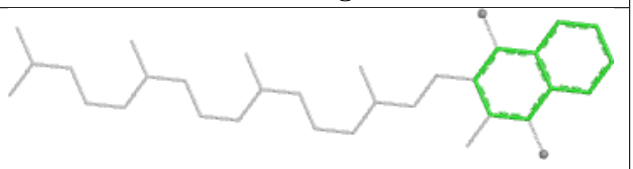
Bond lengths



Bond angles

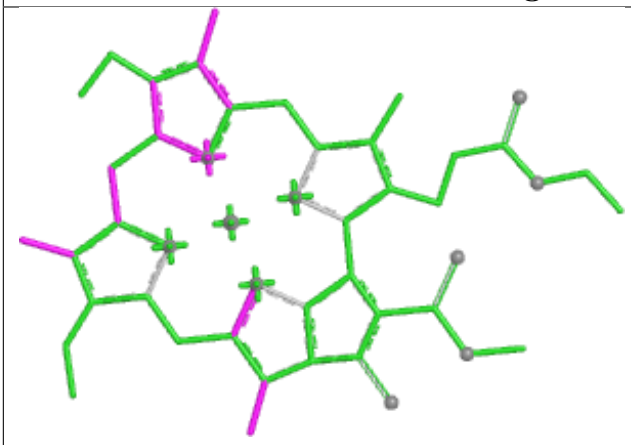


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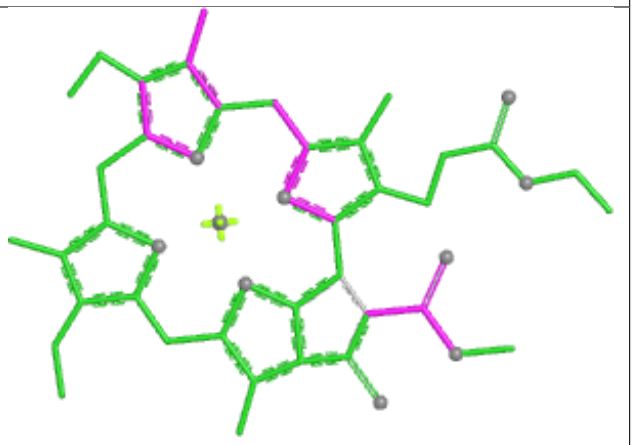


Rings

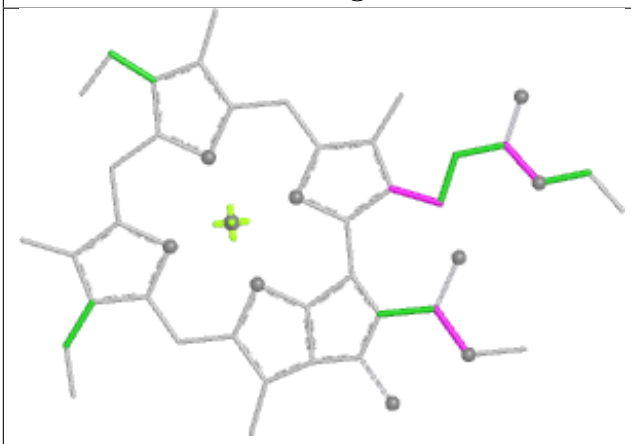
Ligand CLA D 314



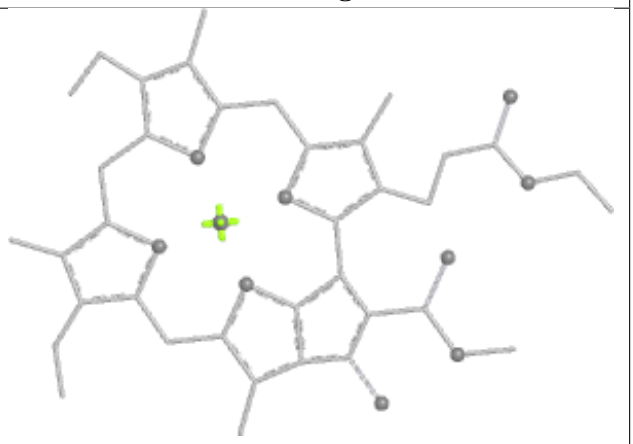
Bond lengths



Bond angles

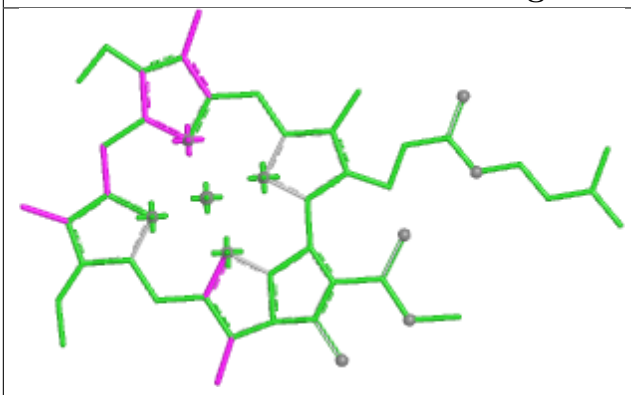


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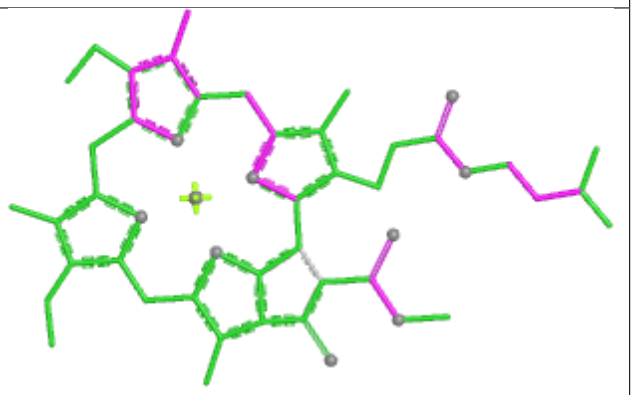


Rings

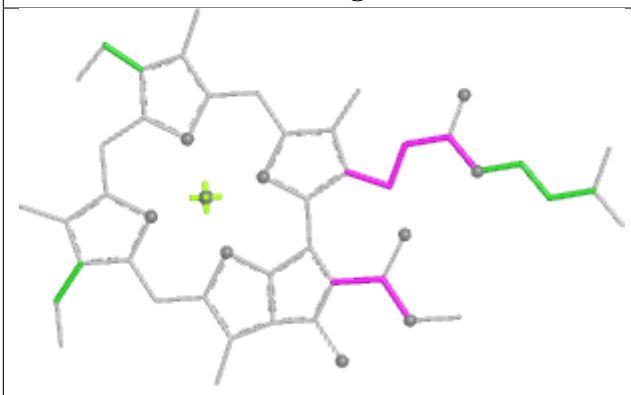
Ligand CLA b 719



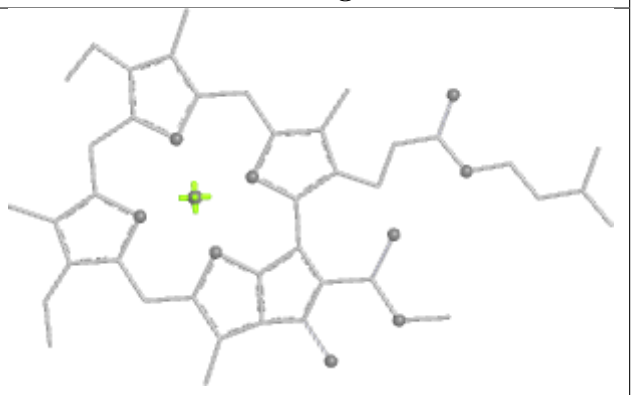
Bond lengths



Bond angles

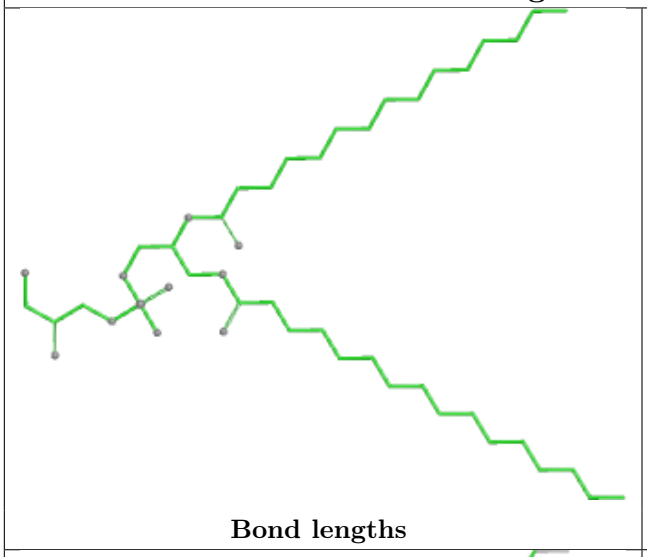


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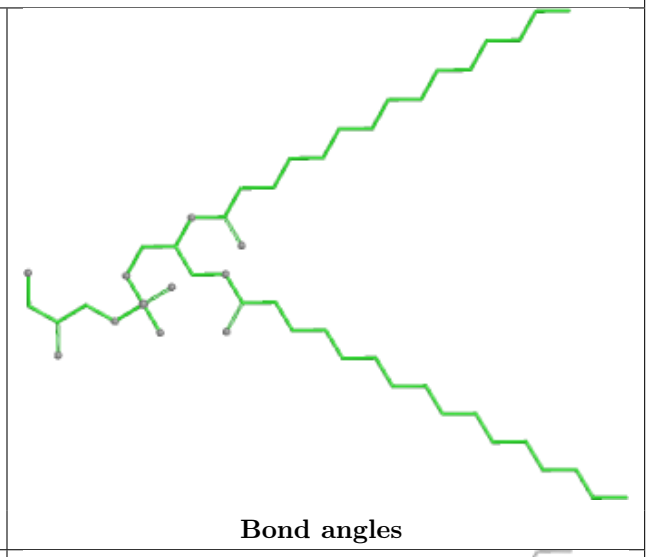


Rings

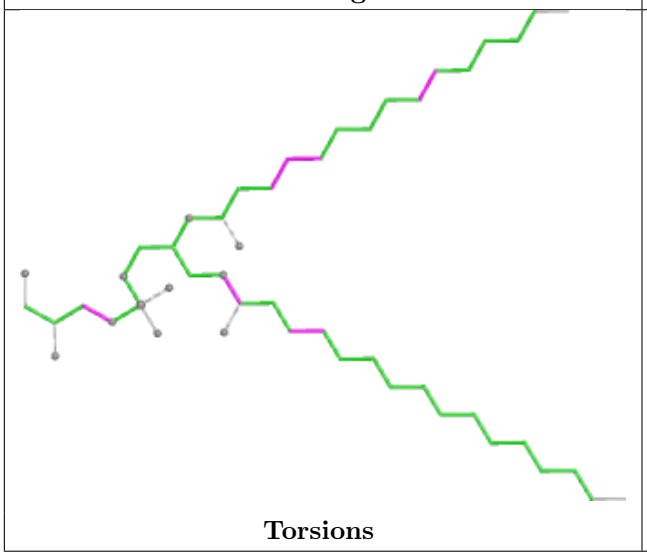
Ligand LHG a 833



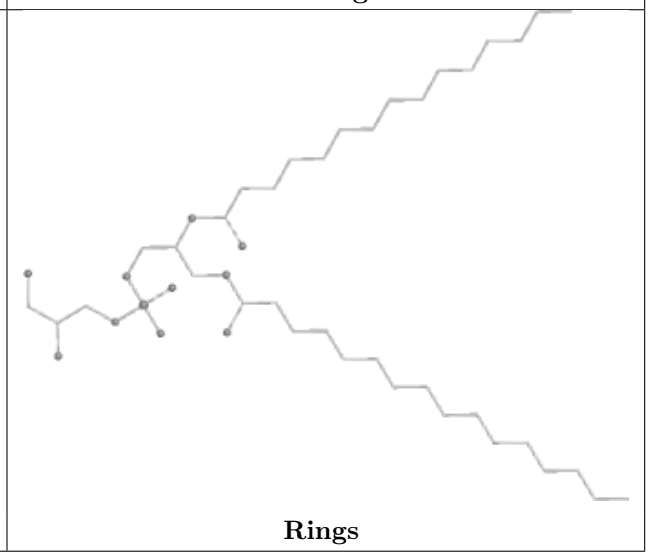
Bond lengths



Bond angles

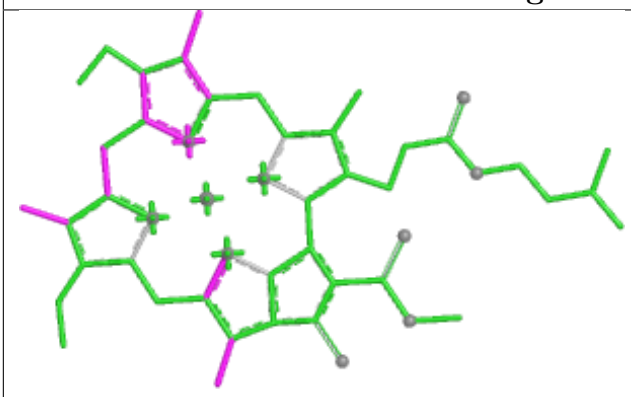


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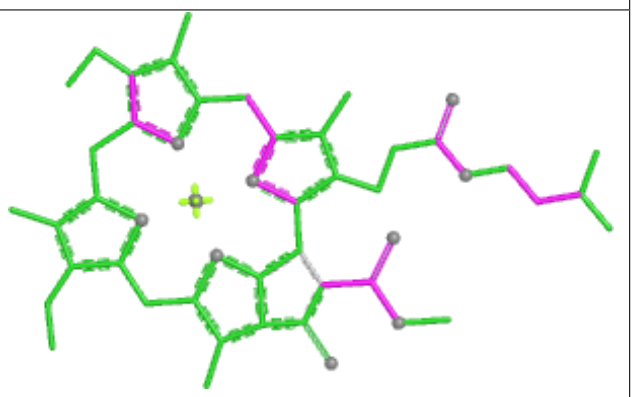


Rings

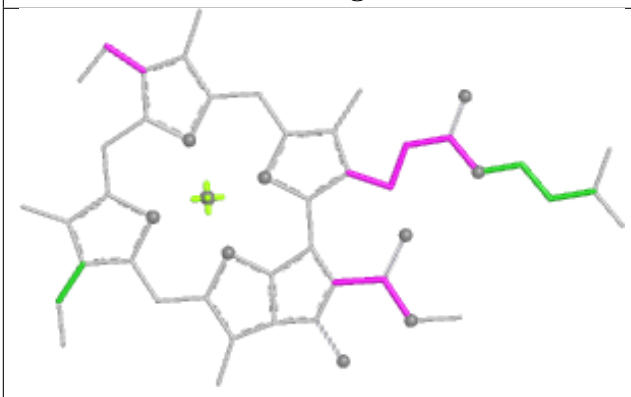
Ligand CLA L 307



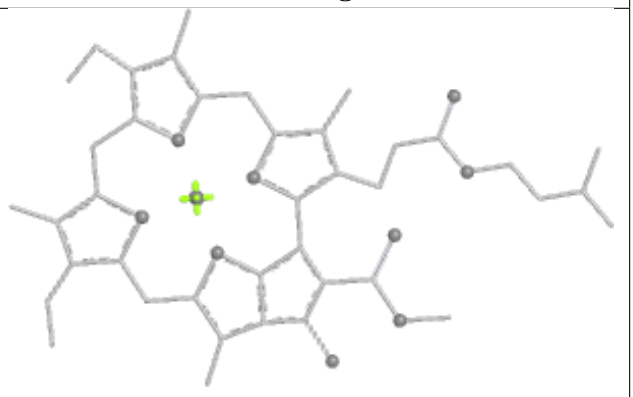
Bond lengths



Bond angles



Torsions



Rings

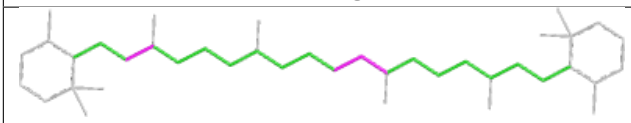
Ligand BCR f 801



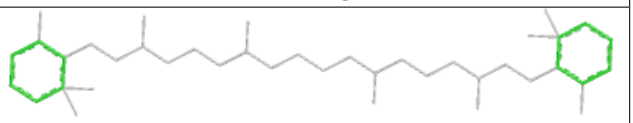
Bond lengths



Bond angles

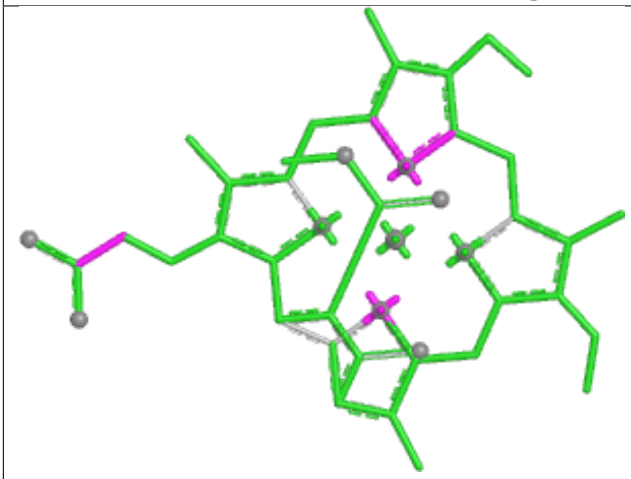


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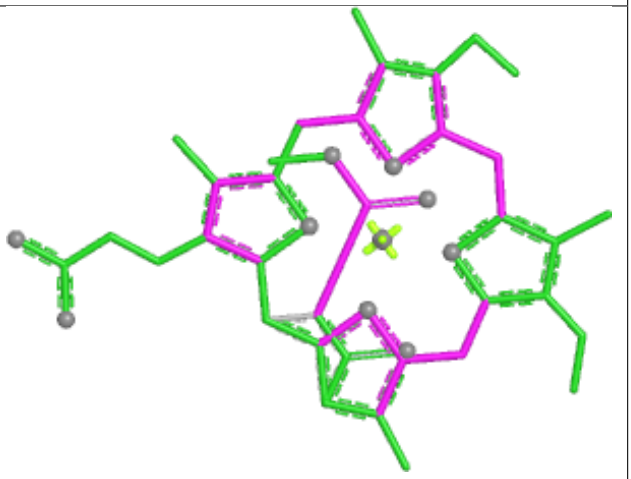


Rings

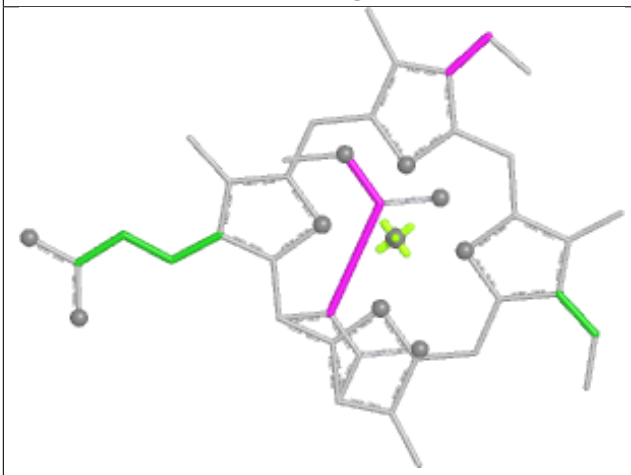
Ligand KC1 N 312



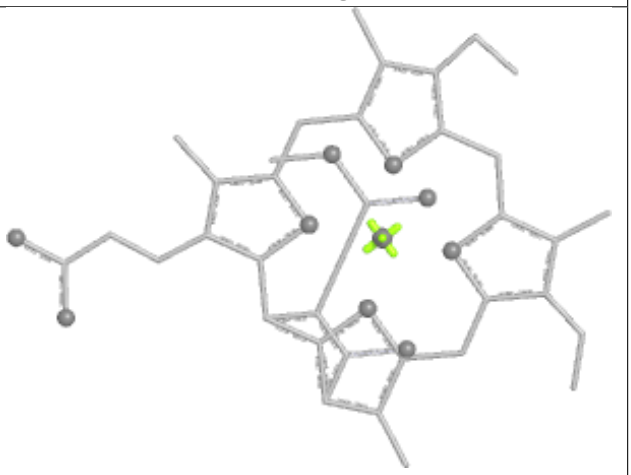
Bond lengths



Bond angles

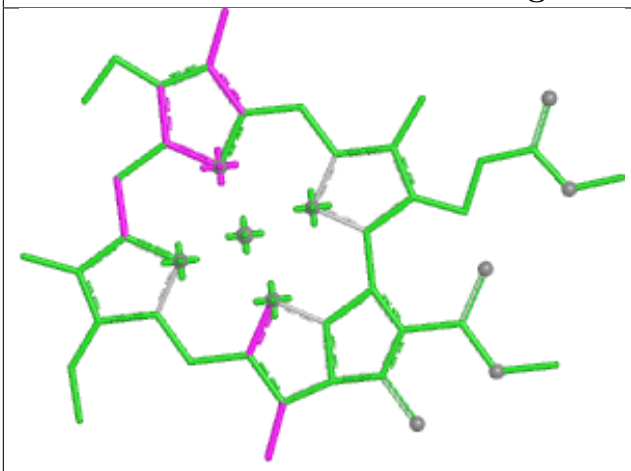


Torsions

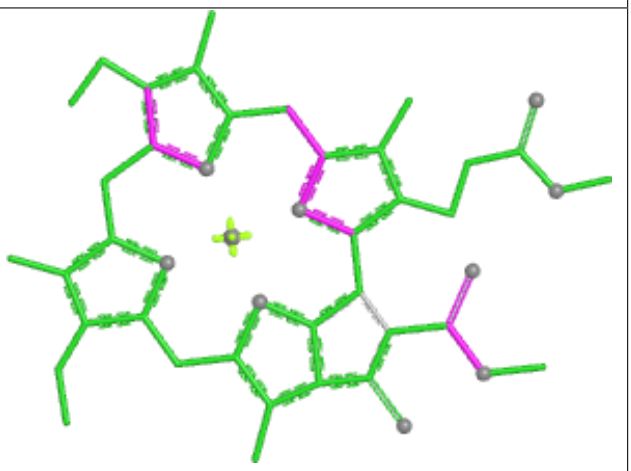


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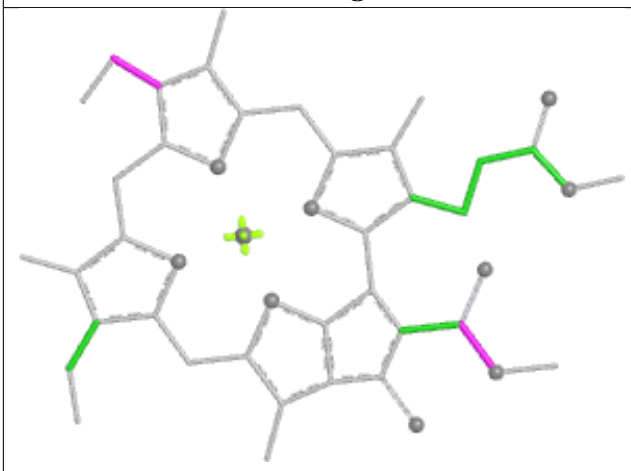
Ligand CLA J 305



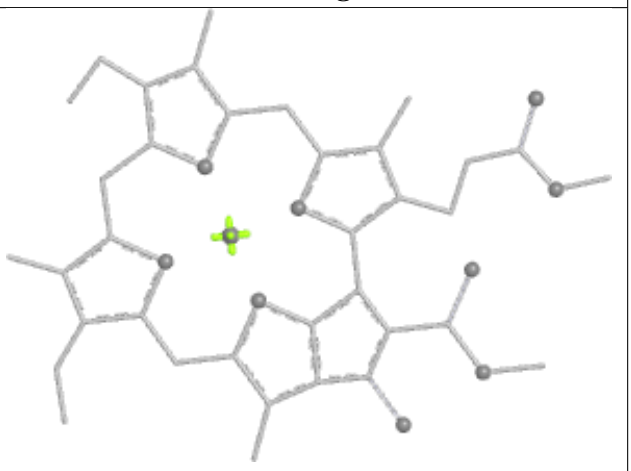
Bond lengths



Bond angles

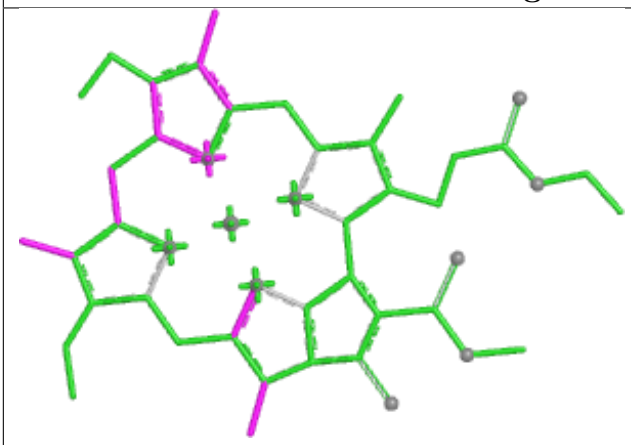


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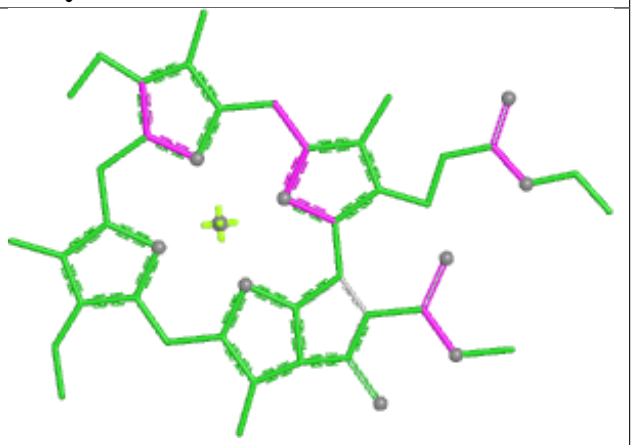


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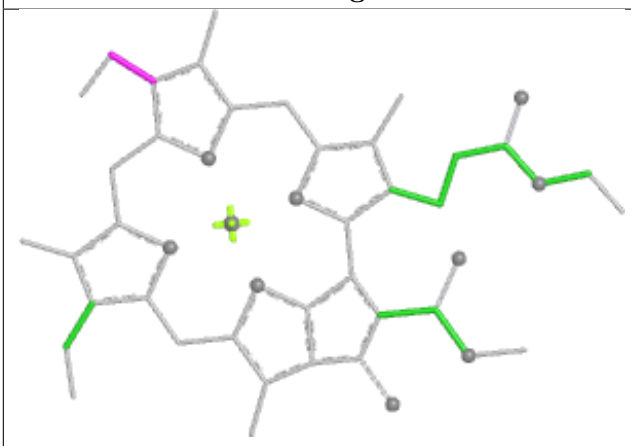
Ligand CLA Q 307



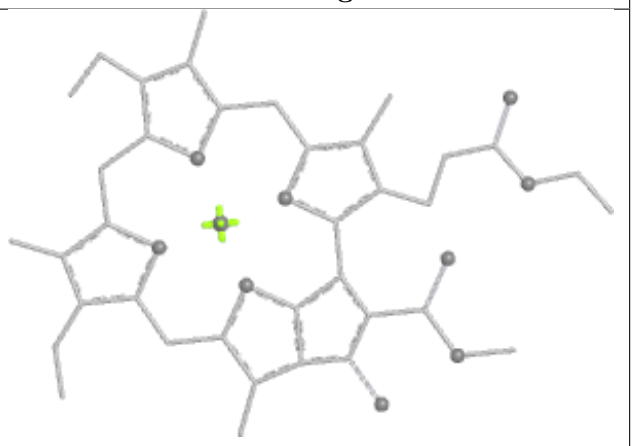
Bond lengths



Bond angles

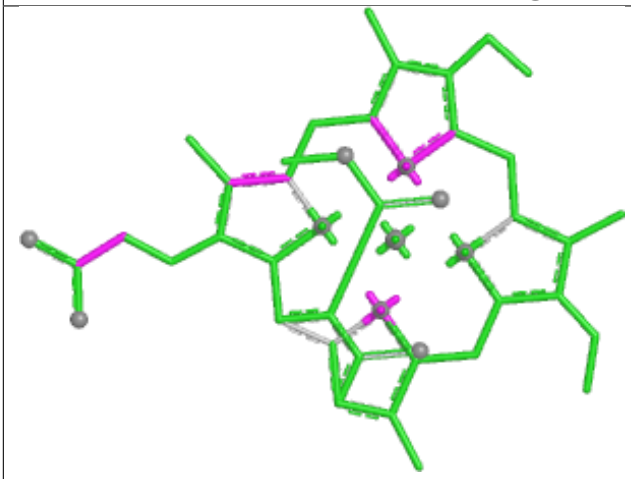


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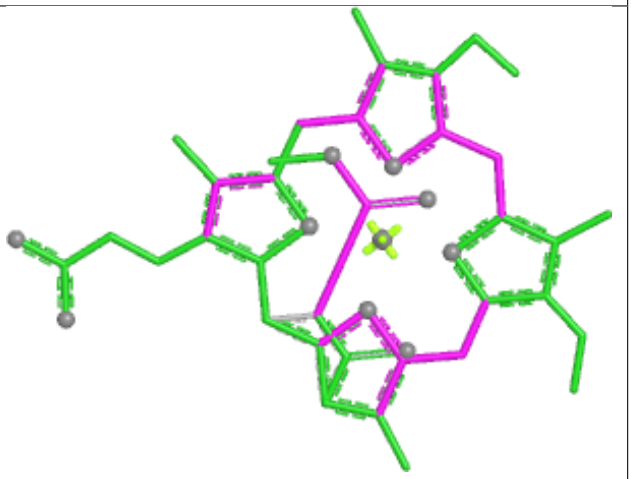


Rings

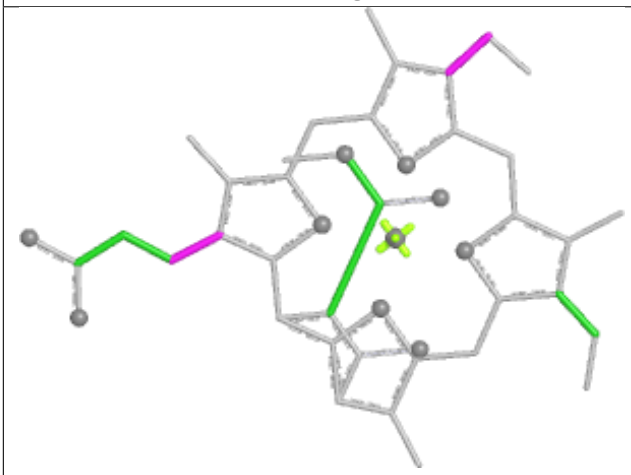
Ligand KC1 T 312



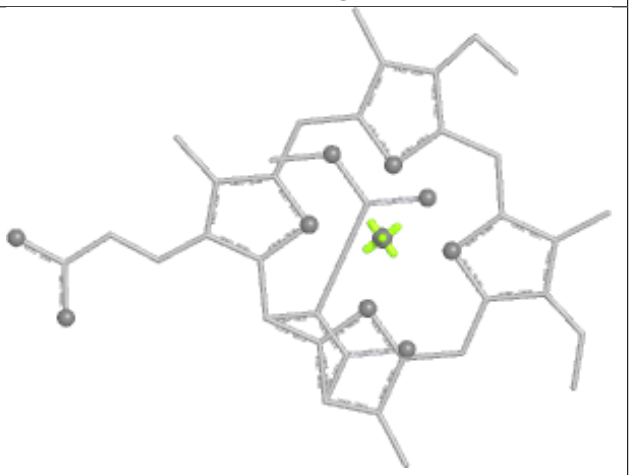
Bond lengths



Bond angles

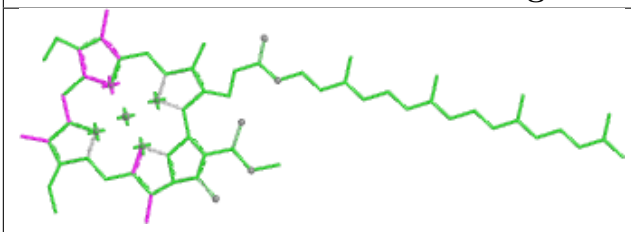


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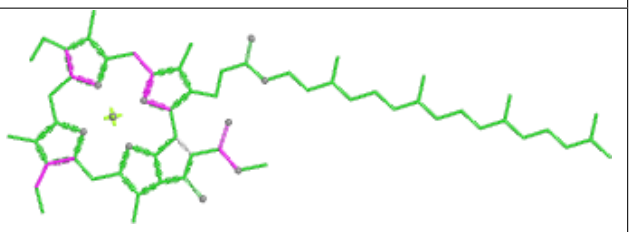


Rings

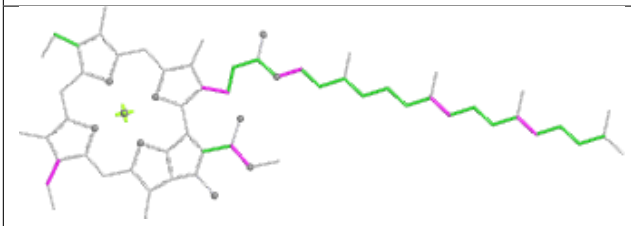
Ligand CLA b 705



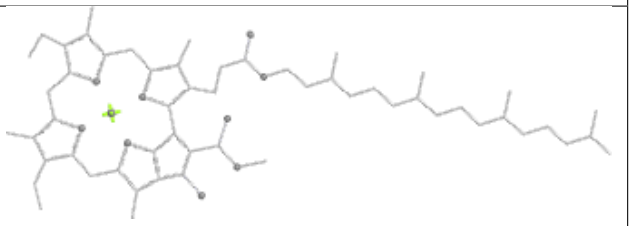
Bond lengths



Bond angles

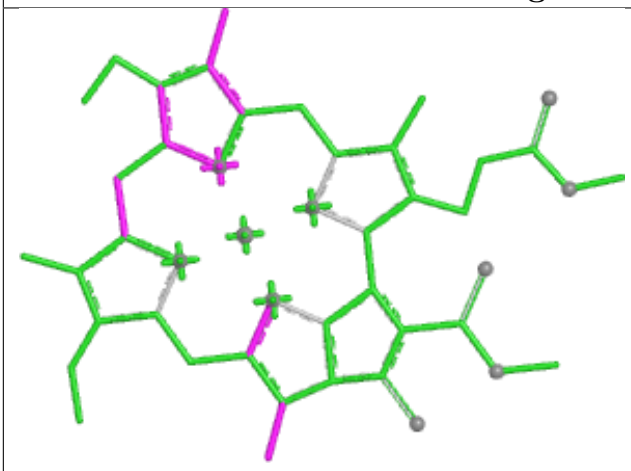


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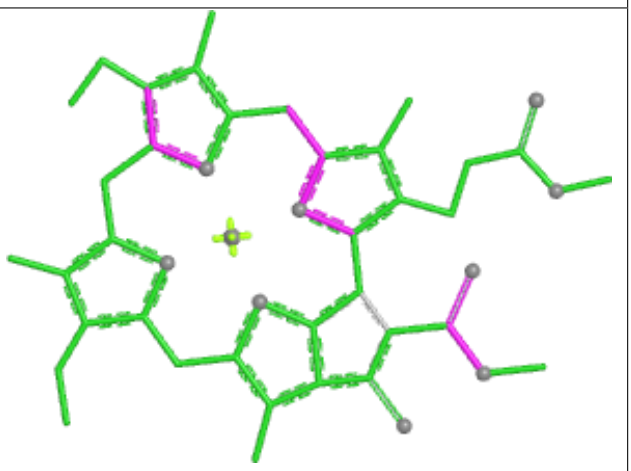


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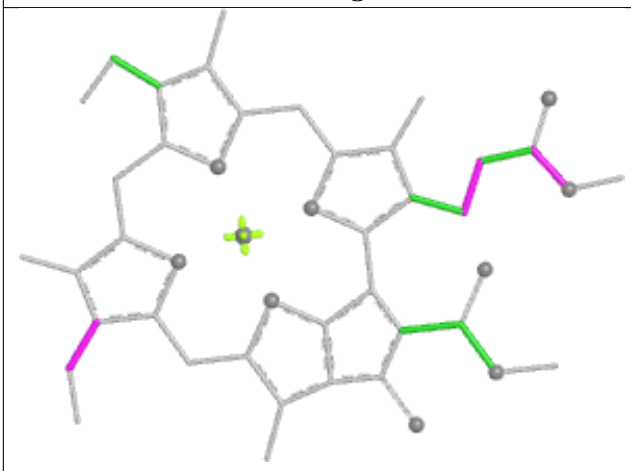
Ligand CLA J 309



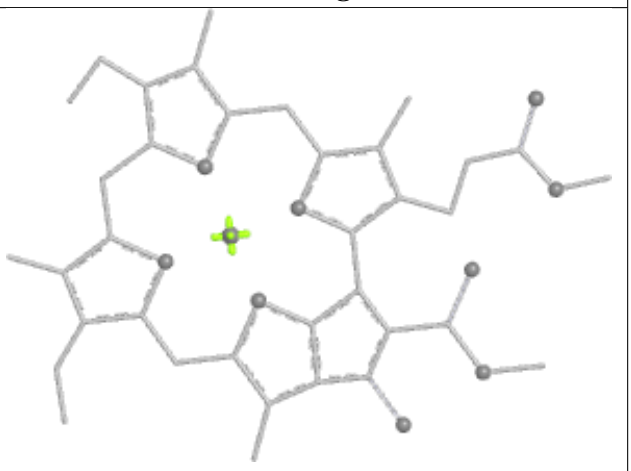
Bond lengths



Bond angles

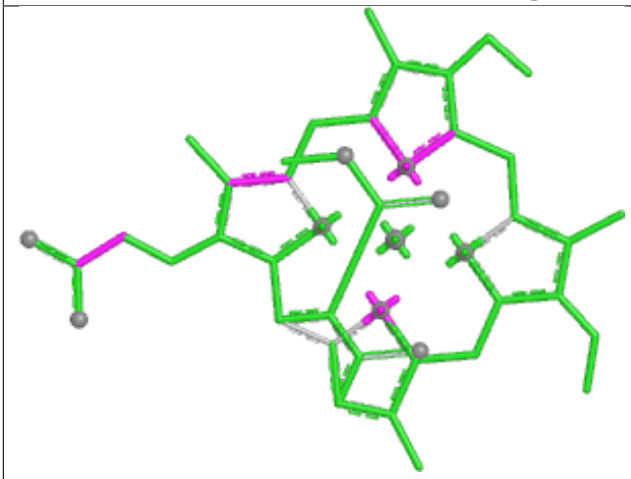


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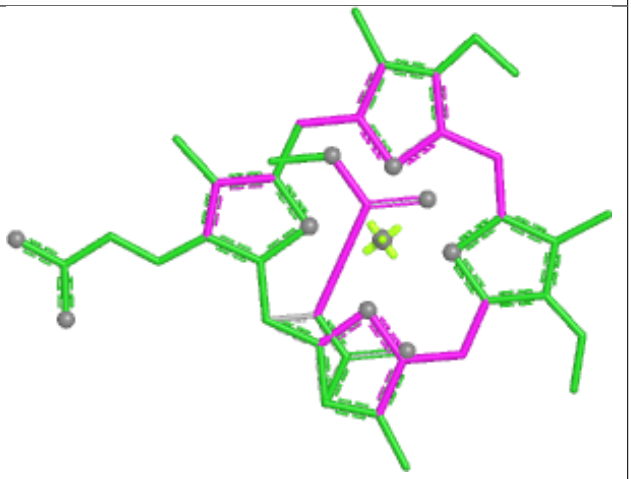


Rings

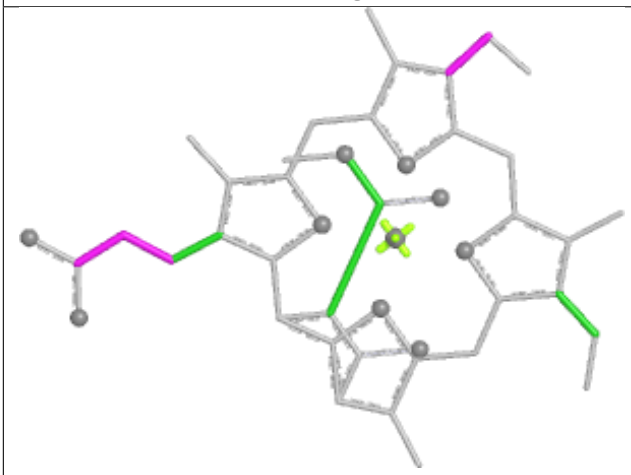
Ligand KC1 A 213



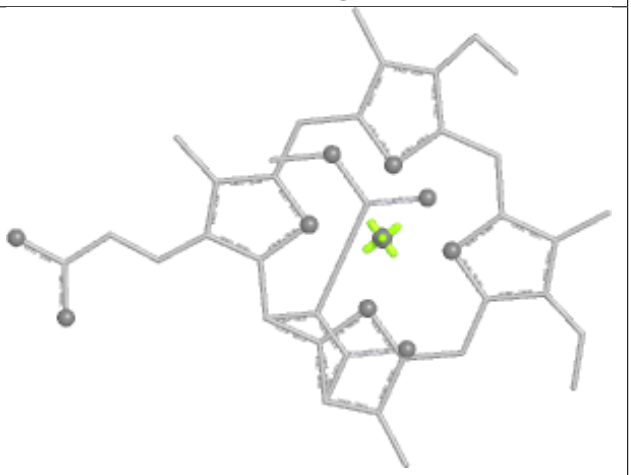
Bond lengths



Bond angles

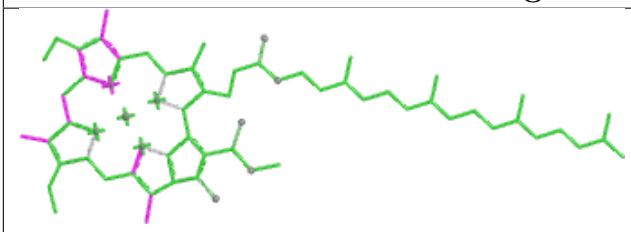


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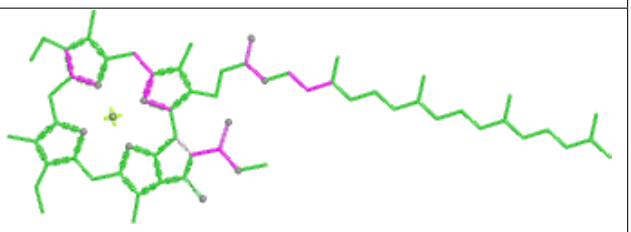


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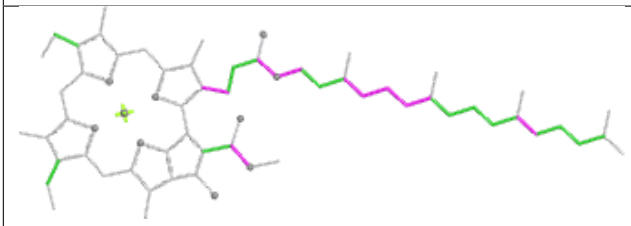
Ligand CLA B 308



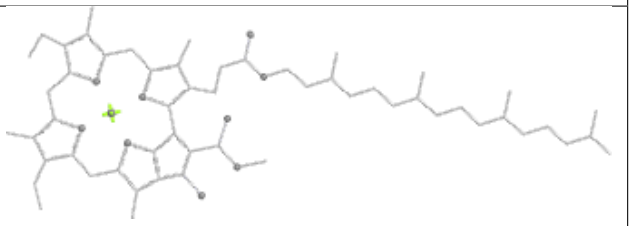
Bond lengths



Bond angles

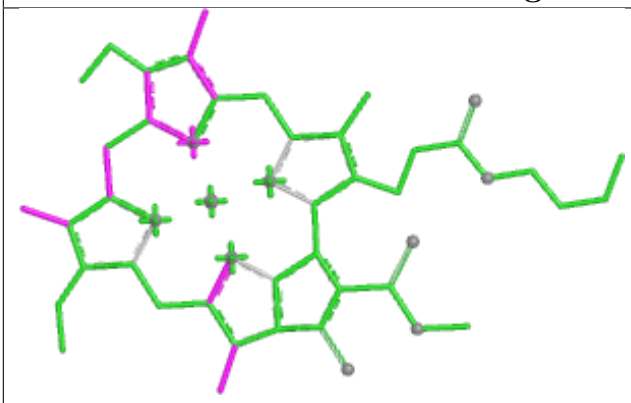


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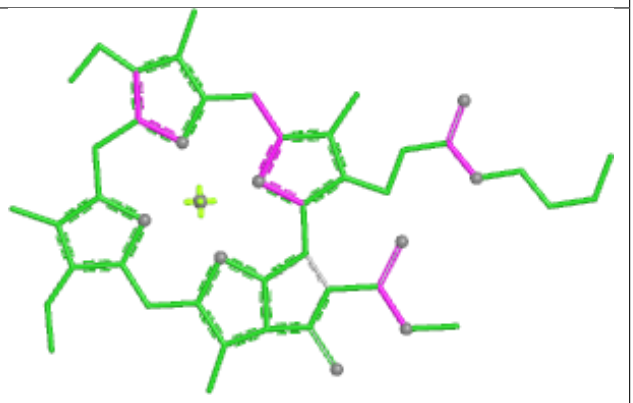


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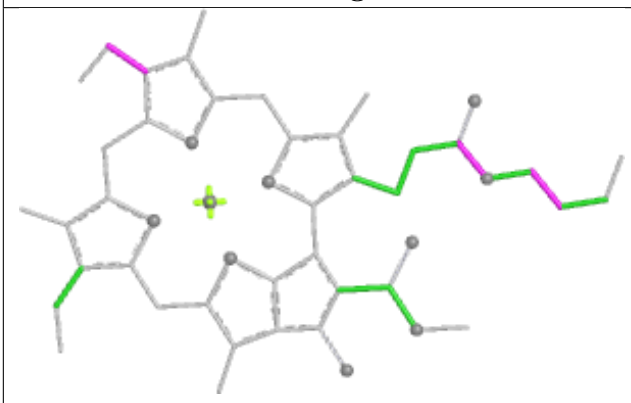
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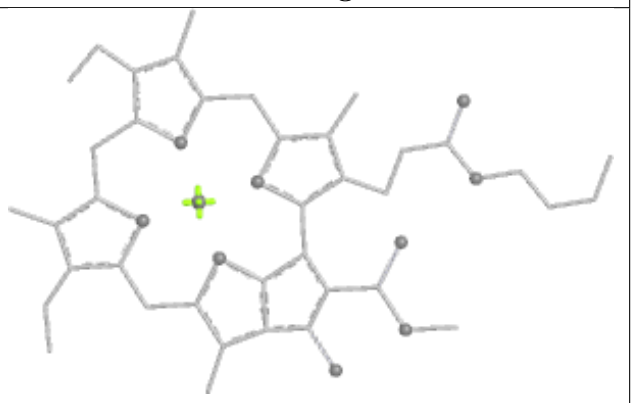
Bond lengths



Bond angles

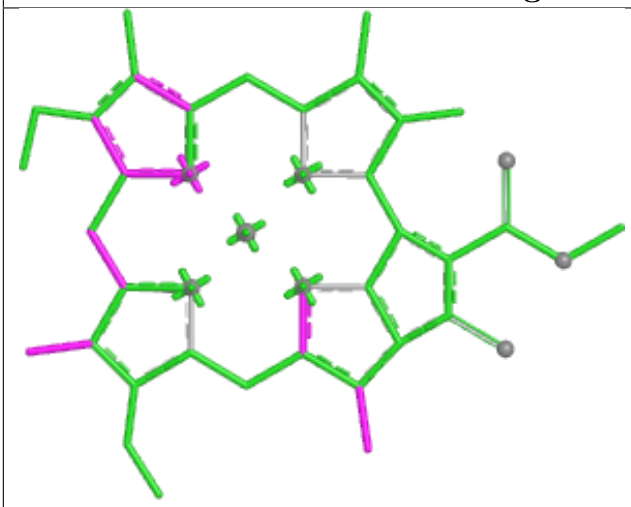


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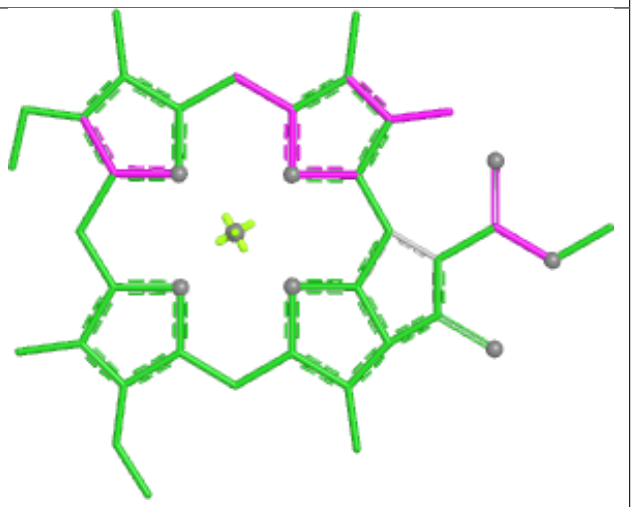


Rings

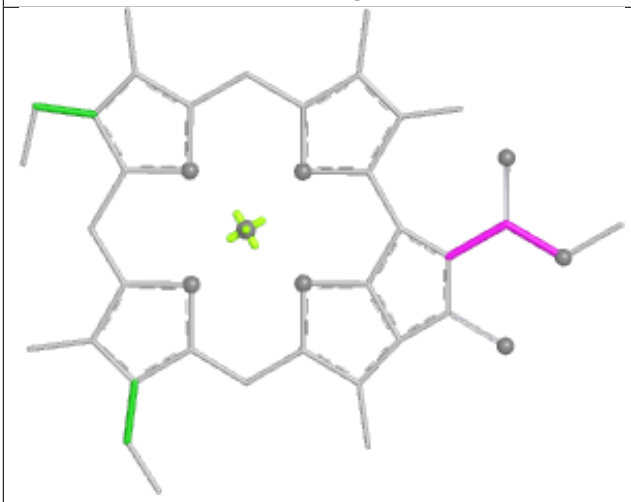
Ligand CLA O 316



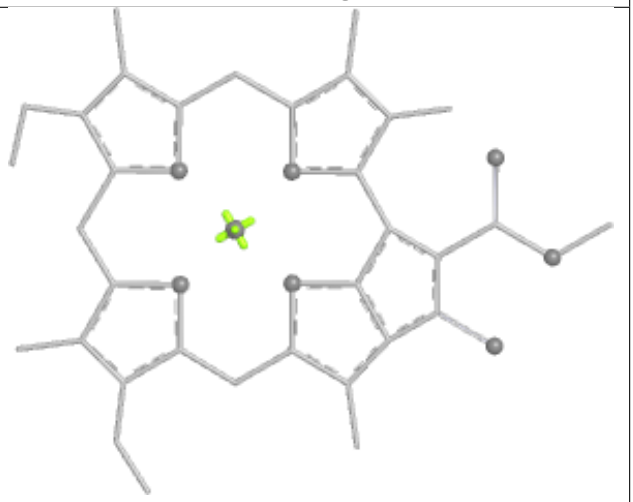
Bond lengths



Bond angles

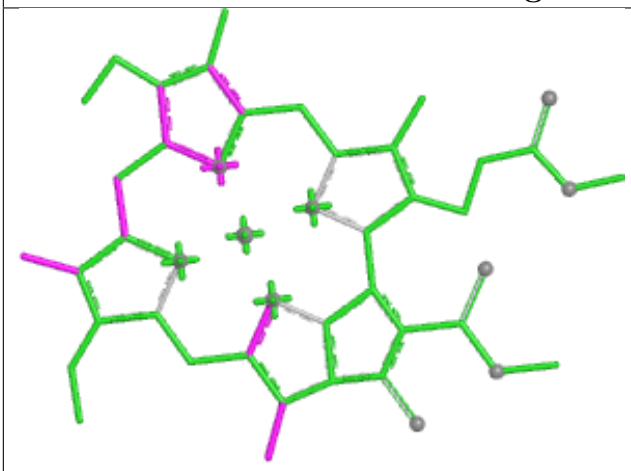


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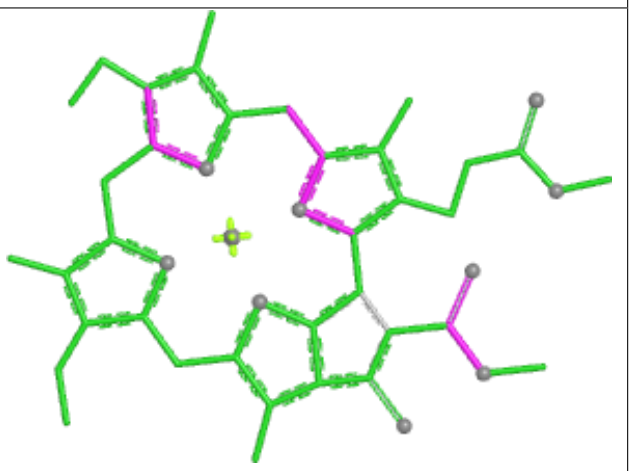


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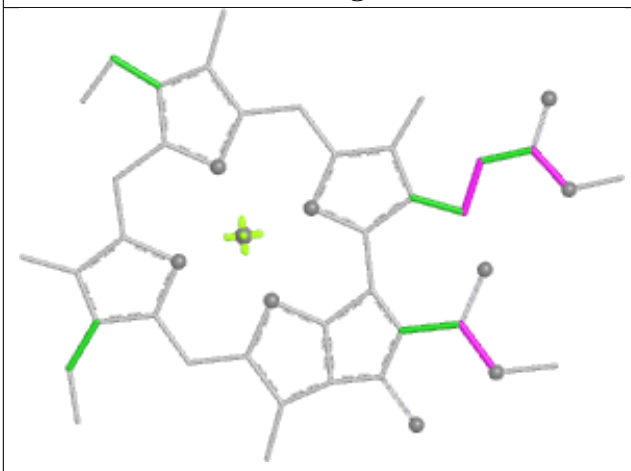
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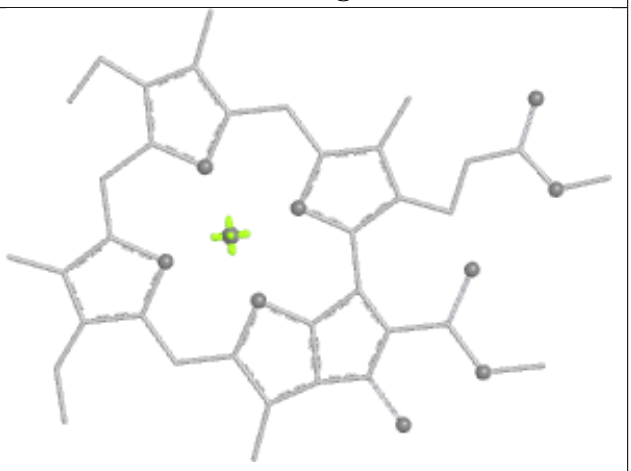
Bond lengths



Bond angles

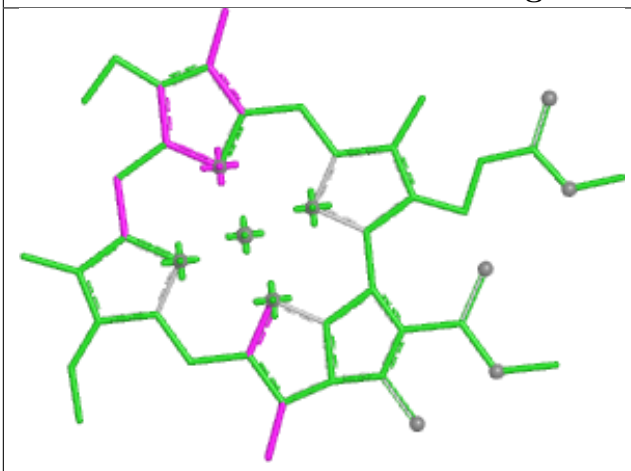


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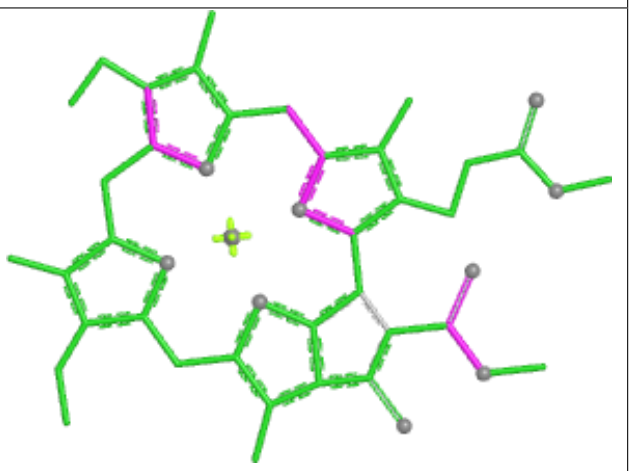


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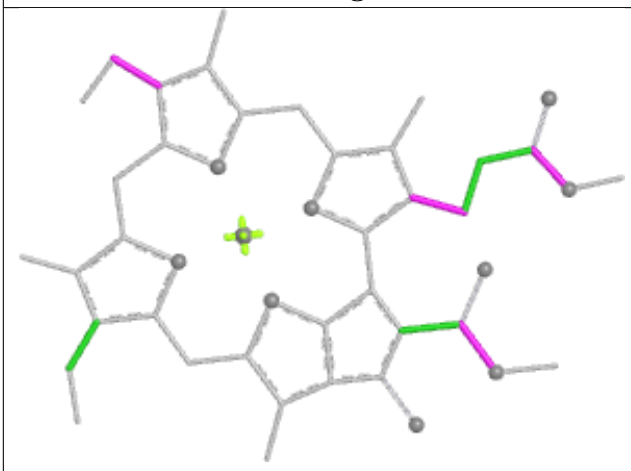
Ligand CLA E 309



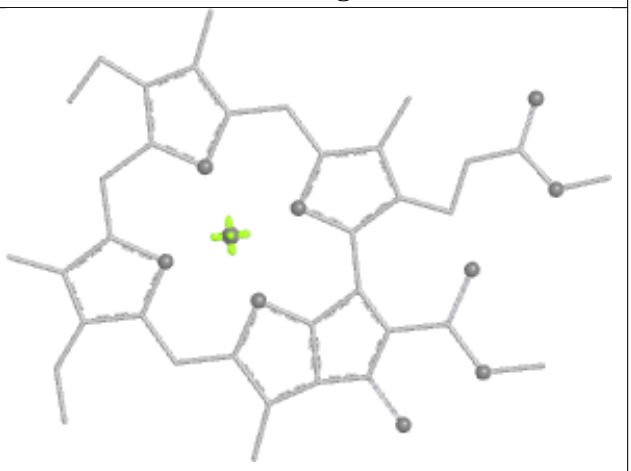
Bond lengths



Bond angles



Torsions

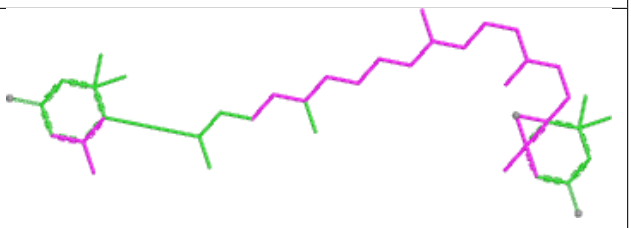


Rings

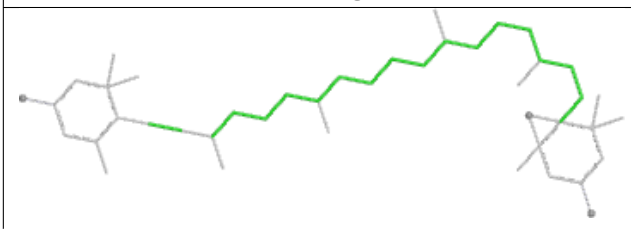
Ligand DD6 m 101



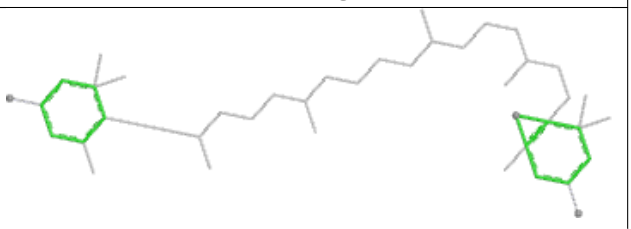
Bond lengths



Bond angles

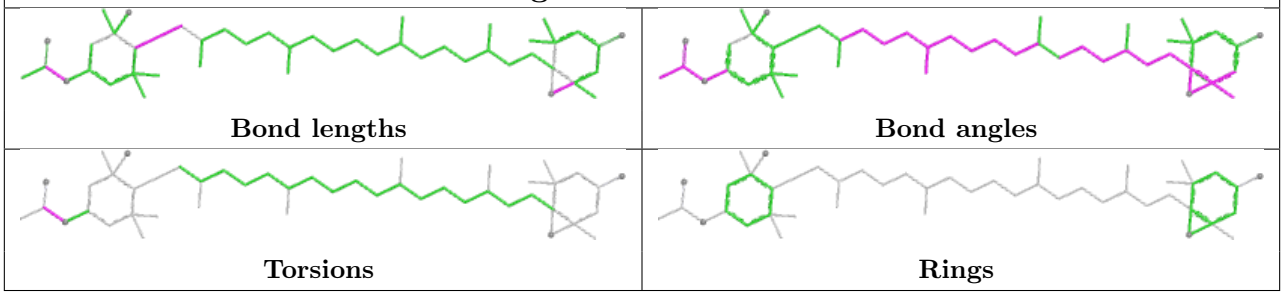


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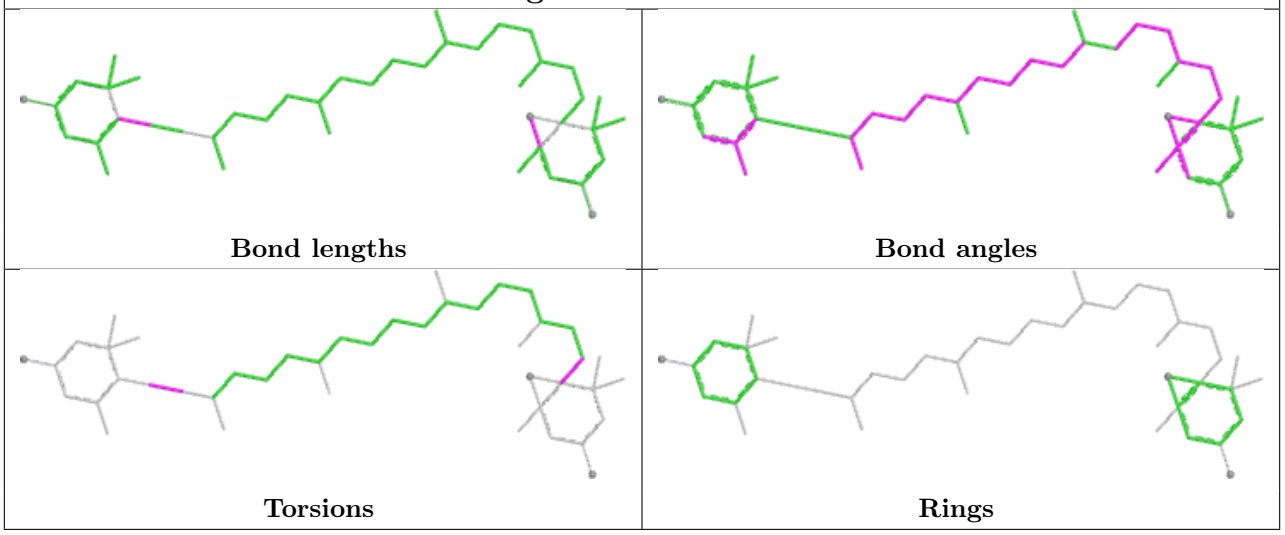


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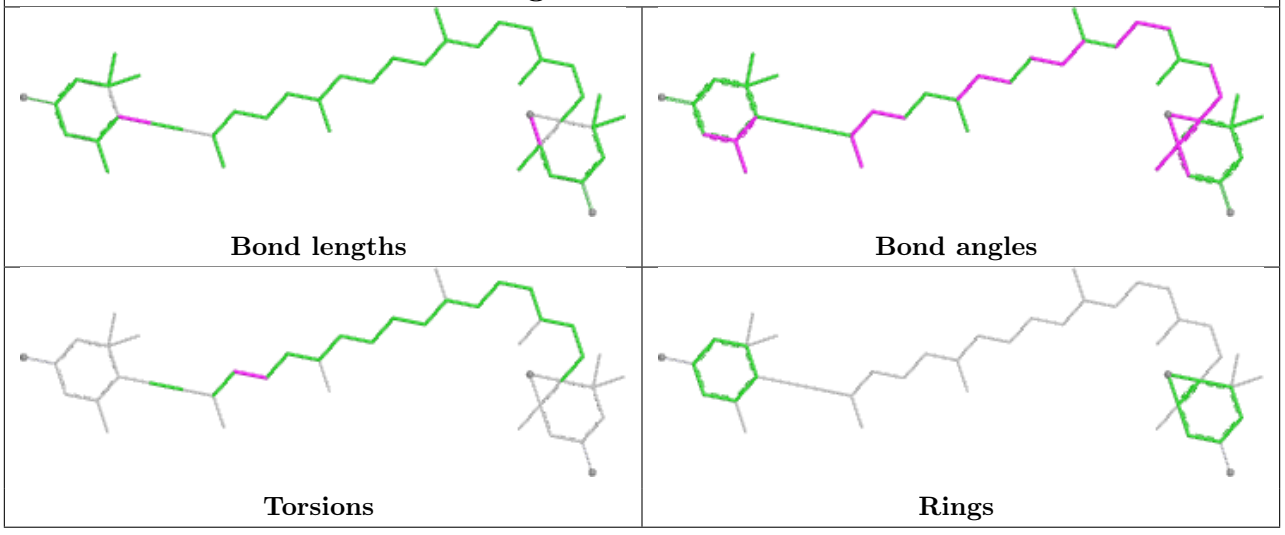
Ligand UIX L 302



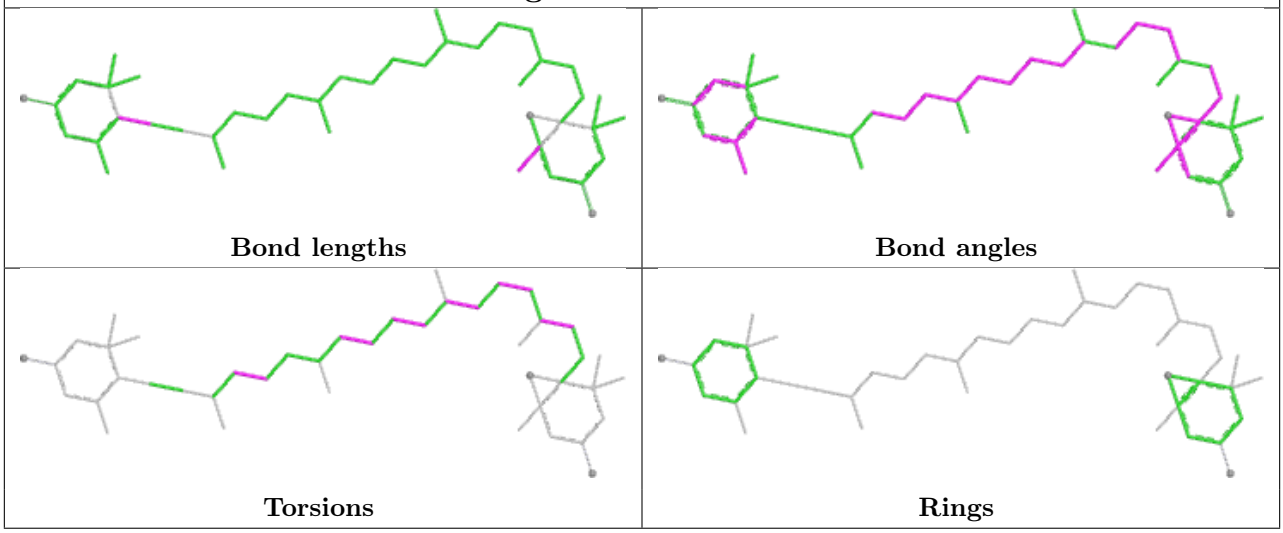
Ligand DD6 B 305



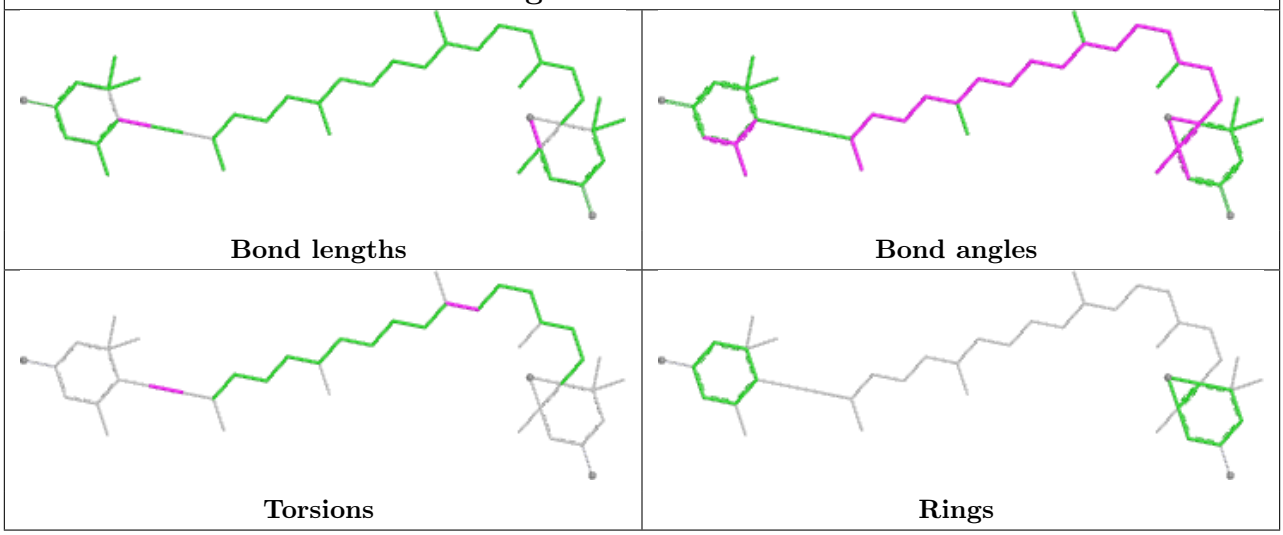
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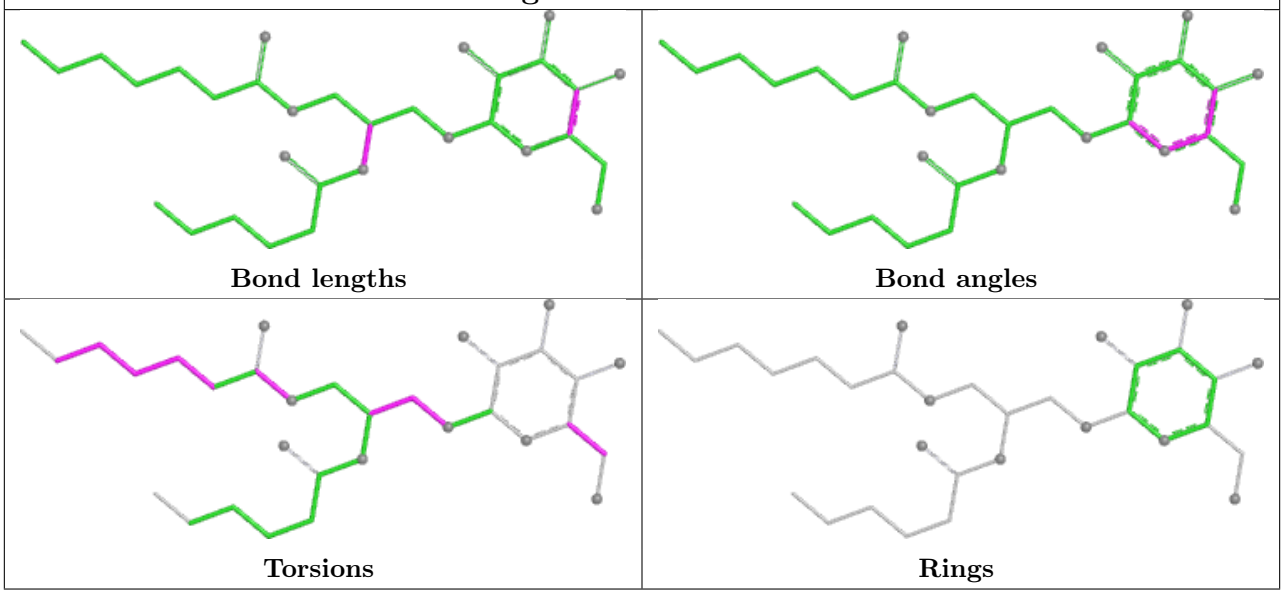
Ligand DD6 K 202



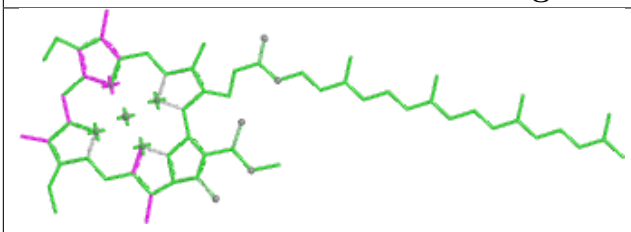
Ligand DD6 A 201



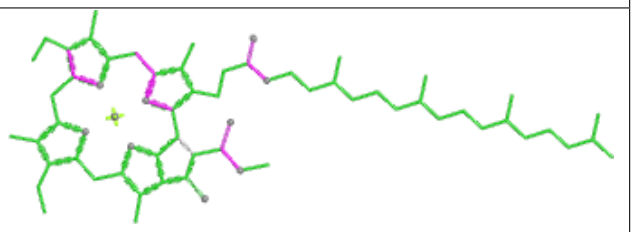
Ligand LMG E 316



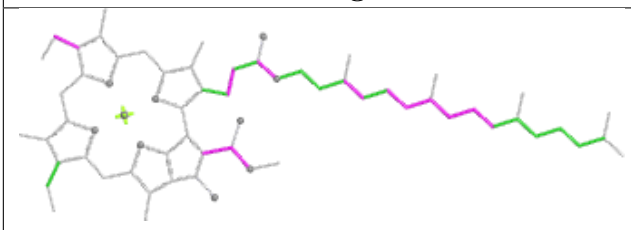
Ligand CLA l 503



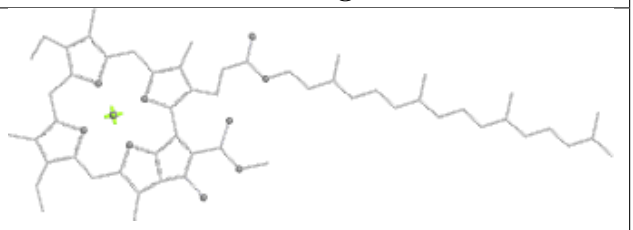
Bond lengths



Bond angles

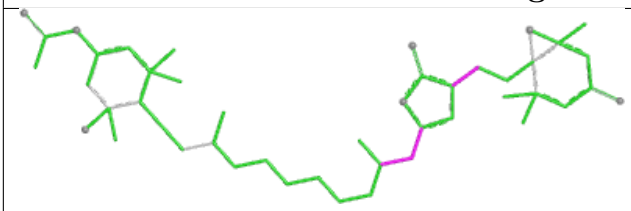


Torsions

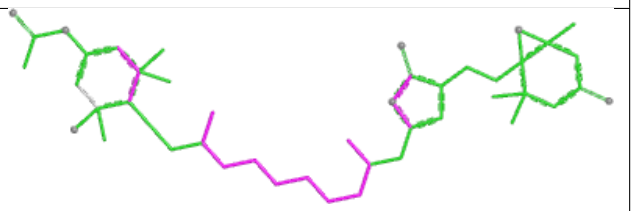


Rings

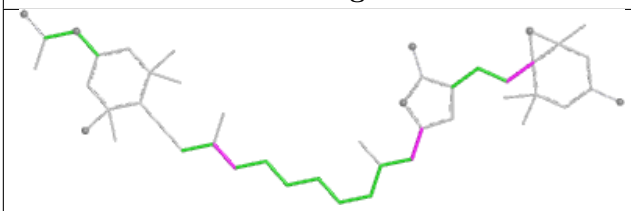
Ligand PID D 307



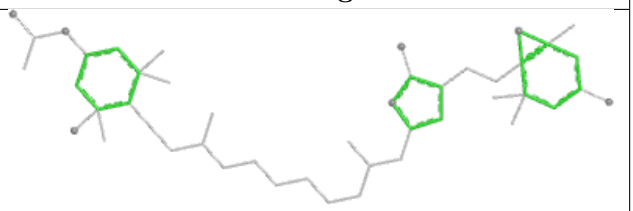
Bond lengths



Bond angles

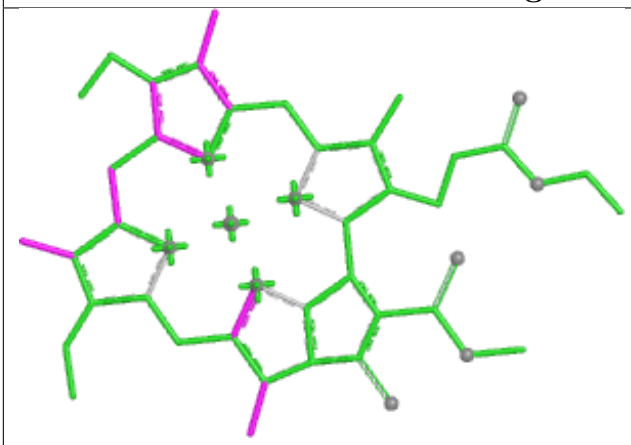


Torsions

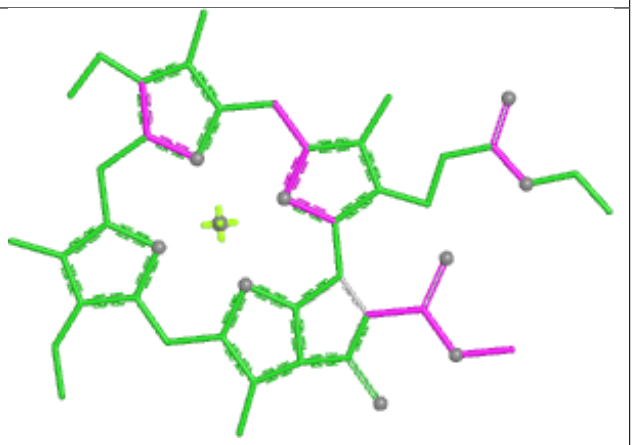


Rings

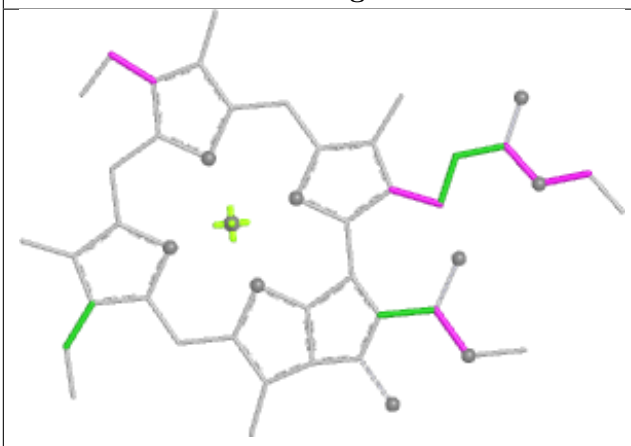
Ligand CLA P 215



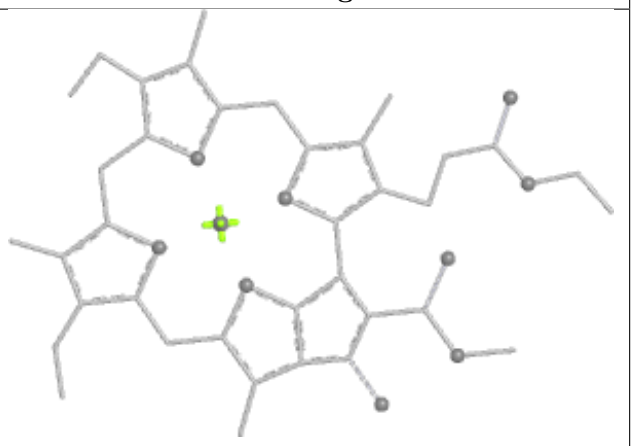
Bond lengths



Bond angles

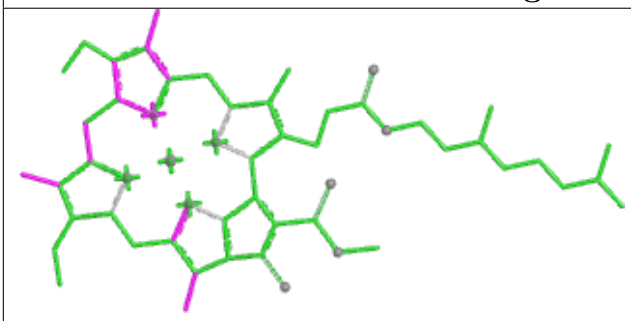


Torsions

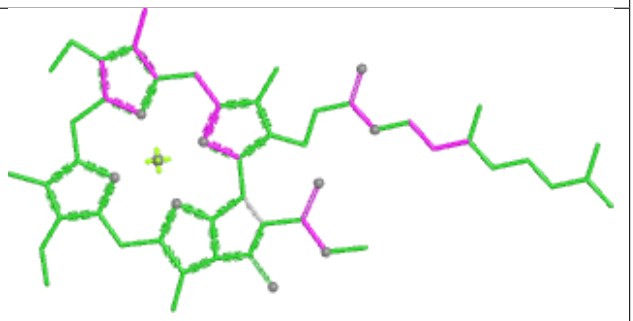


Rings

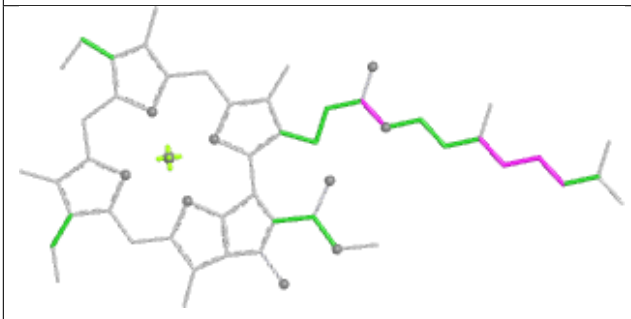
Ligand CLA A 211



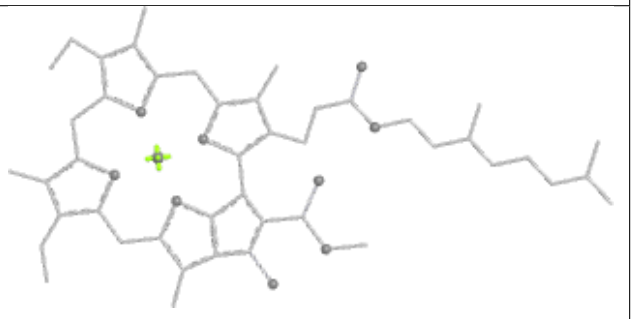
Bond lengths



Bond angles

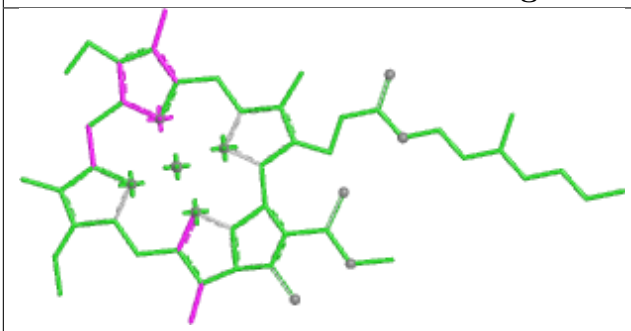


Torsions

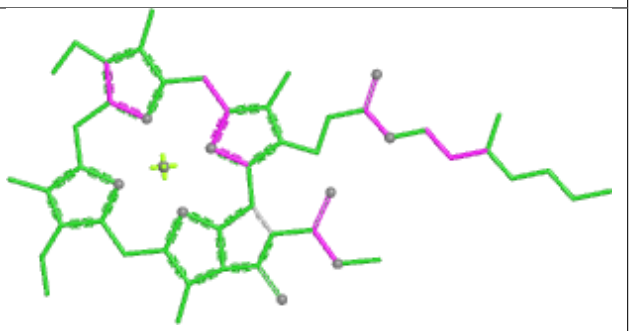


Rings

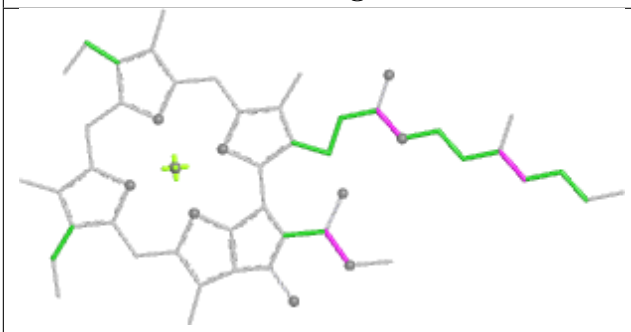
Ligand CLA M 306



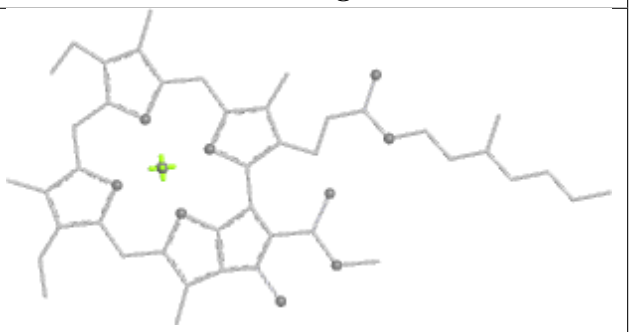
Bond lengths



Bond angles

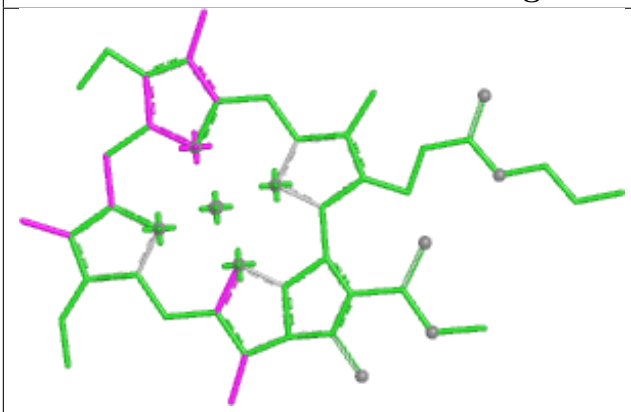


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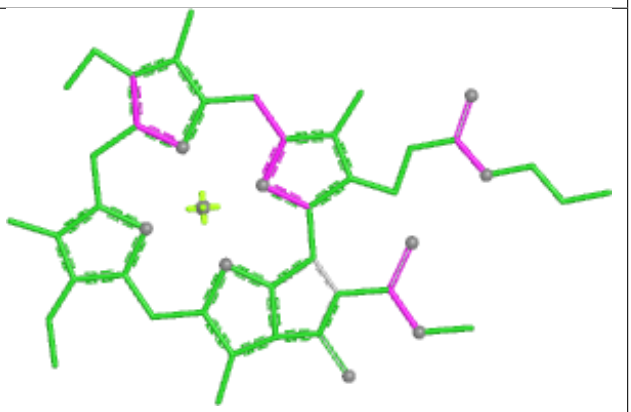


Rings

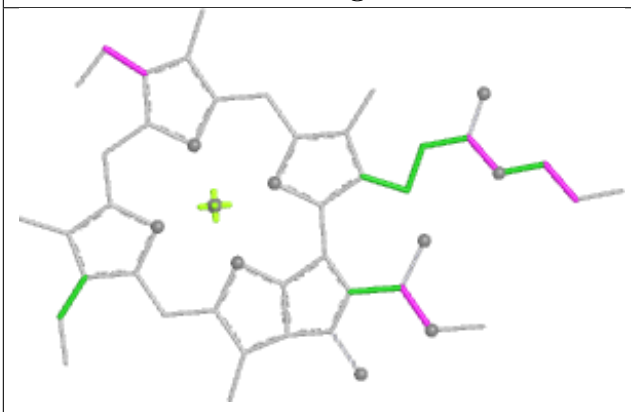
Ligand CLA K 213



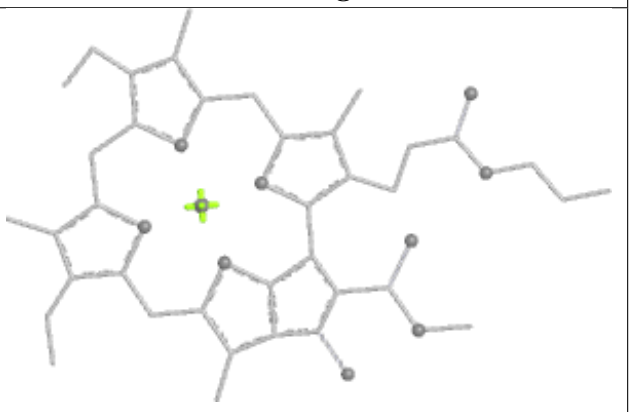
Bond lengths



Bond angles

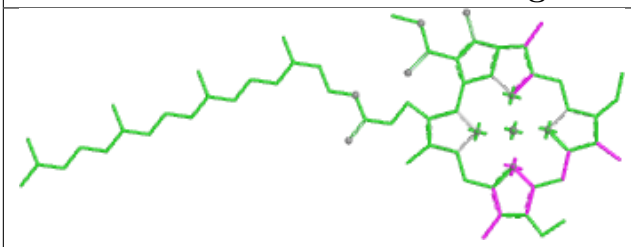


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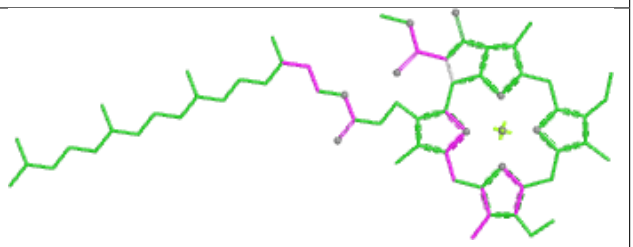


Rings

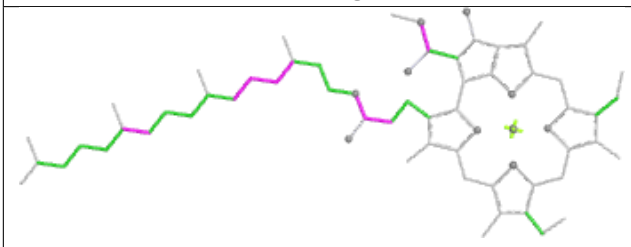
Ligand CLA a 831



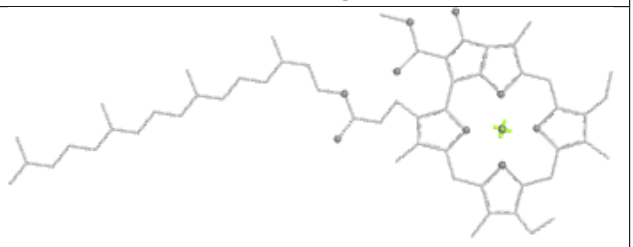
Bond lengths



Bond angles

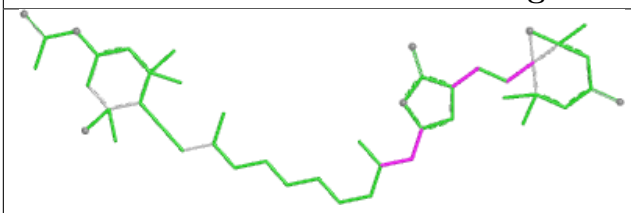


Torsions

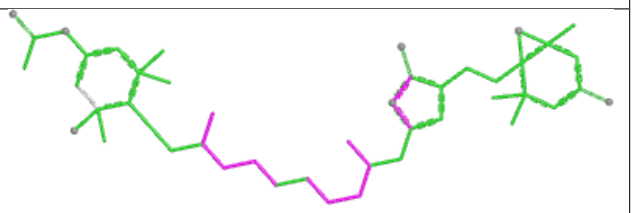


Rings

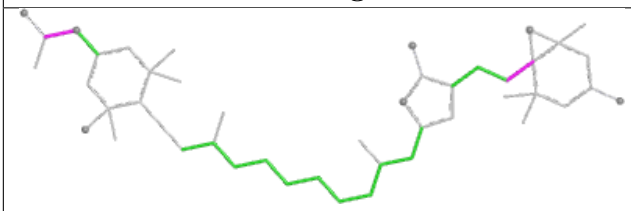
Ligand PID H 306



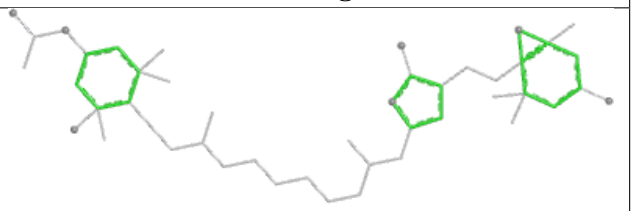
Bond lengths



Bond angles

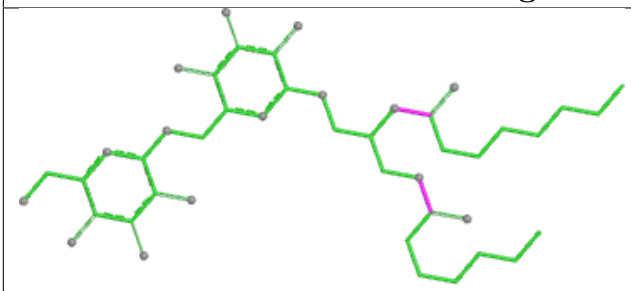


Torsions

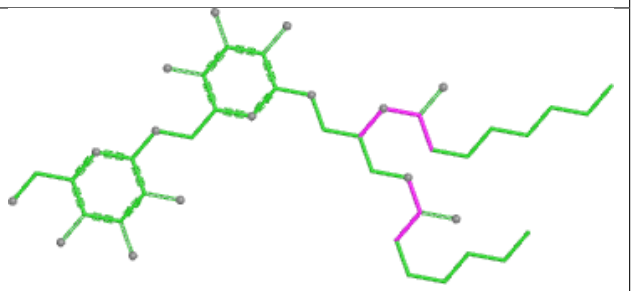


Rings

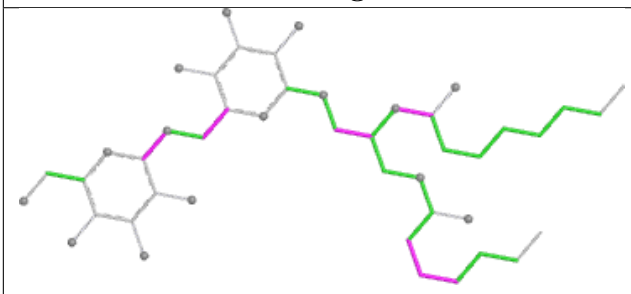
Ligand DGD G 320



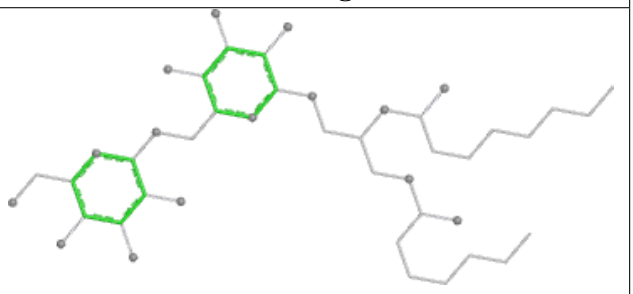
Bond lengths



Bond angles

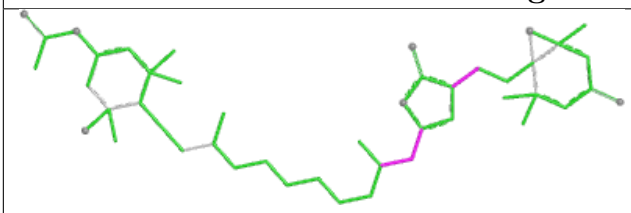


Torsions

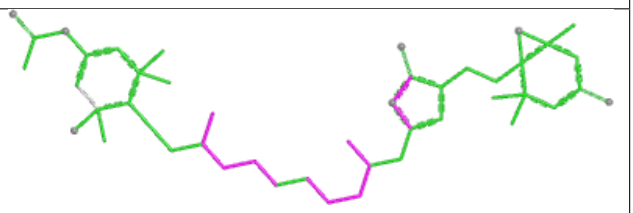


Rings

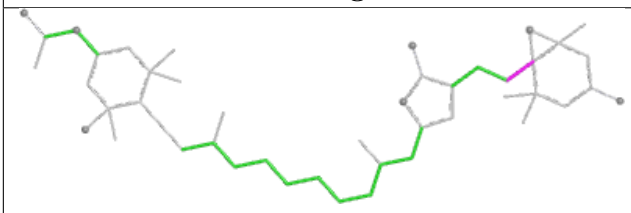
Ligand PID D 302



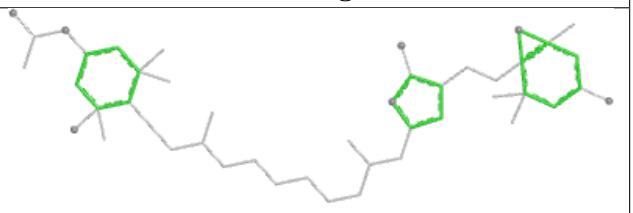
Bond lengths



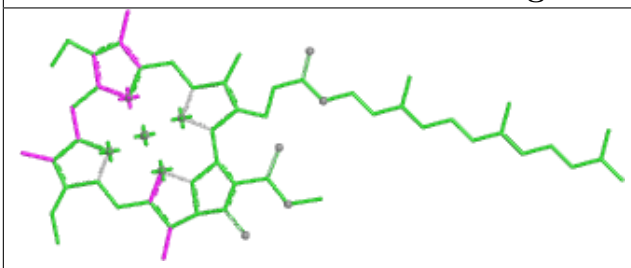
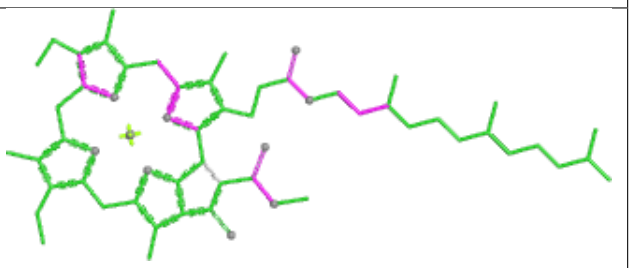
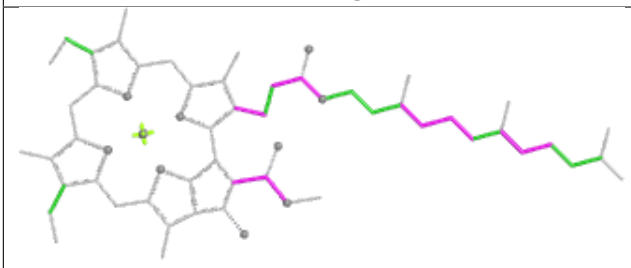
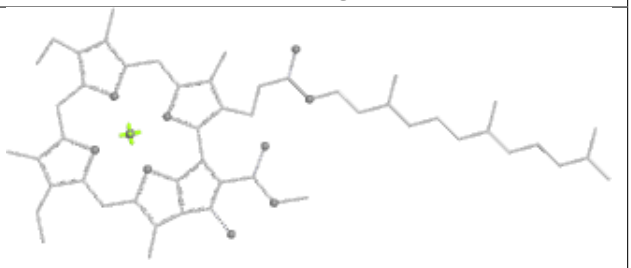
Bond angles

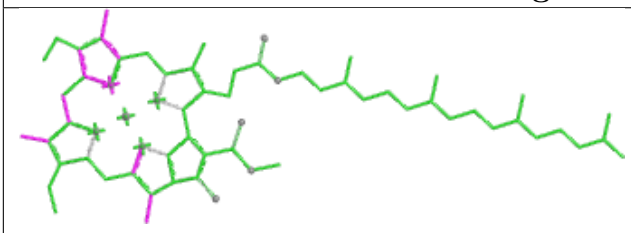
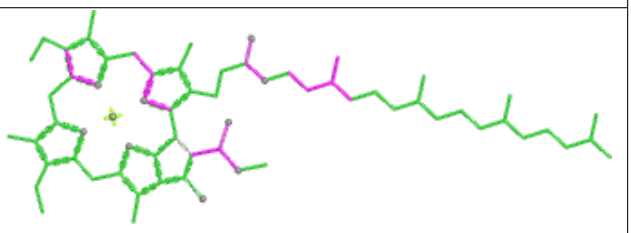
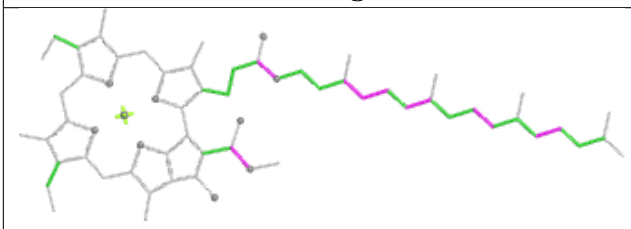
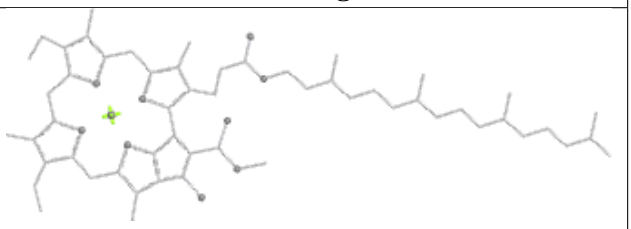


Torsions

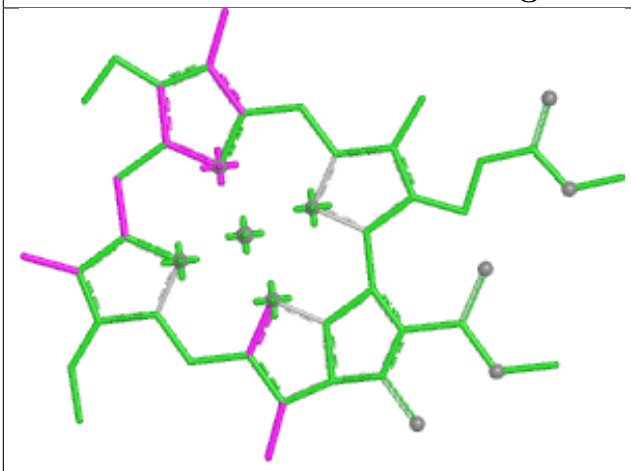


Rings

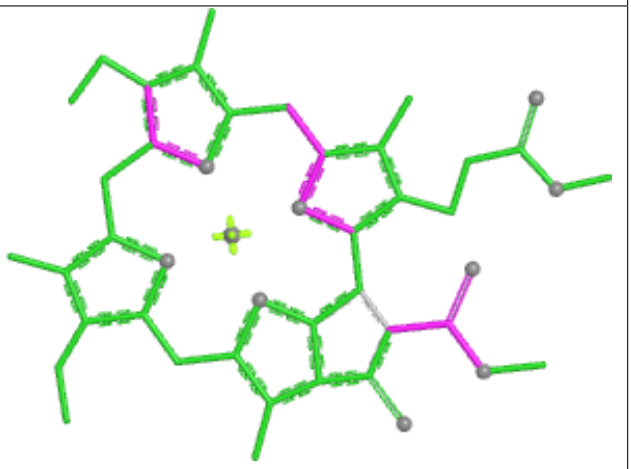
Ligand CLA b 709	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

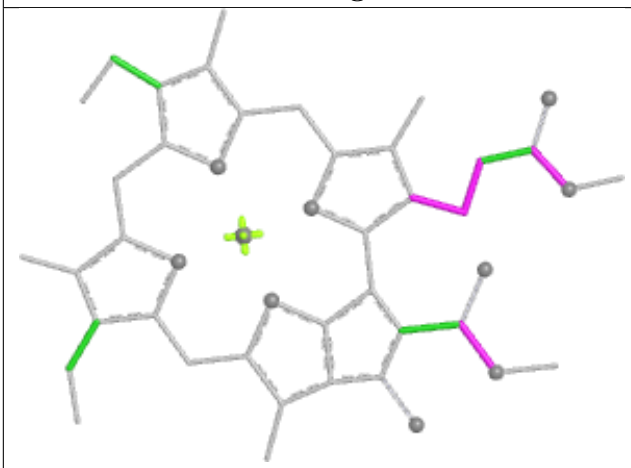
Ligand CLA M 311



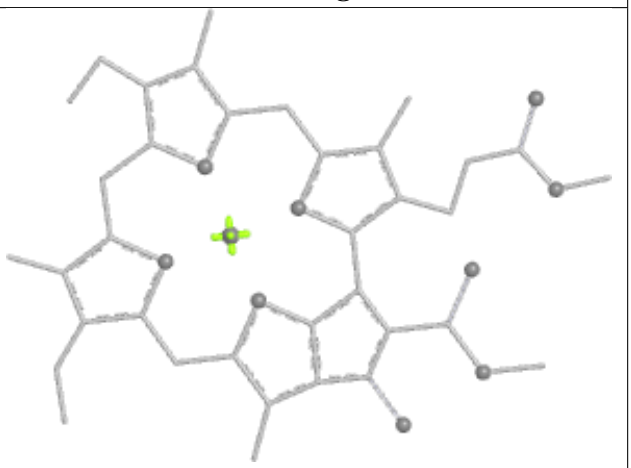
Bond lengths



Bond angles

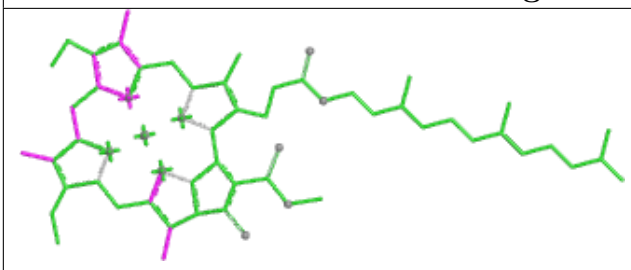


Torsions

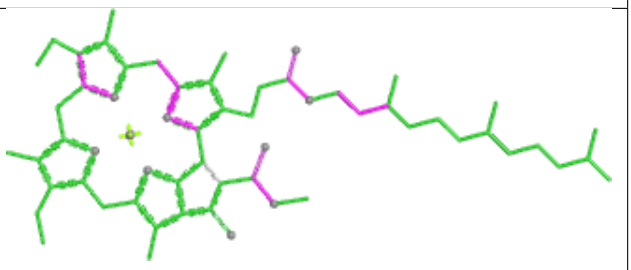


Rings

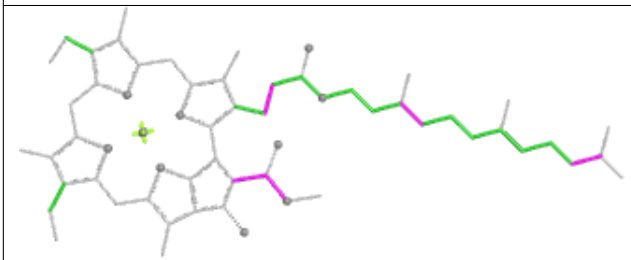
Ligand CLA G 314



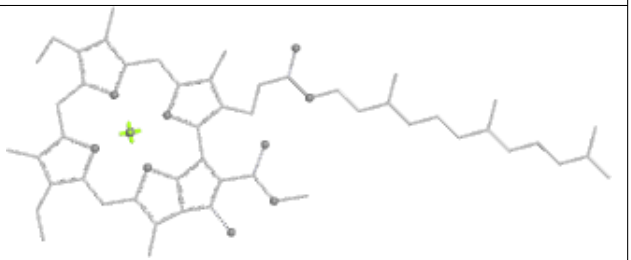
Bond lengths



Bond angles

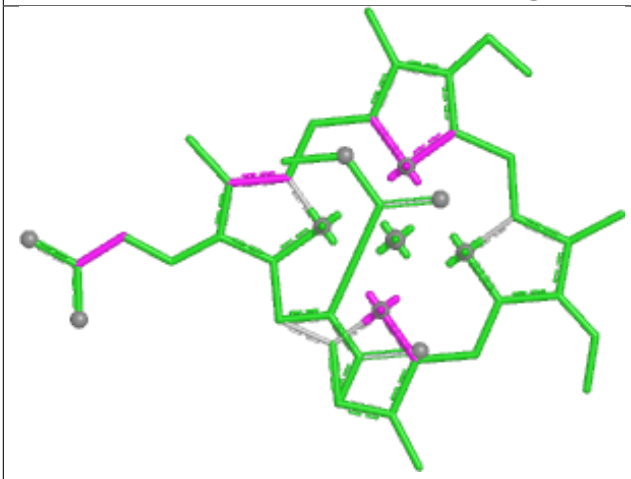


Torsions

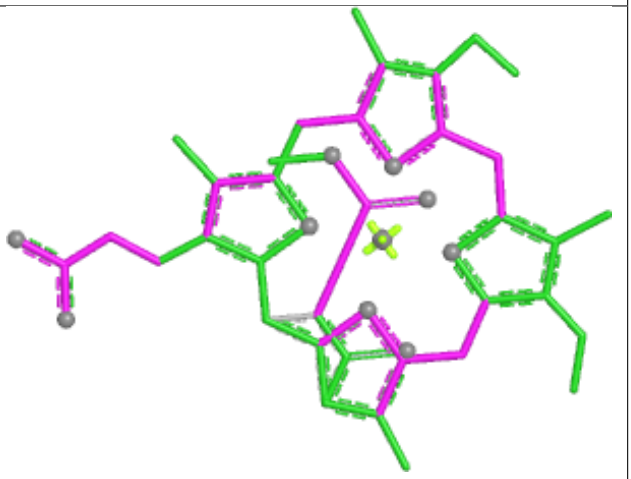


Rings

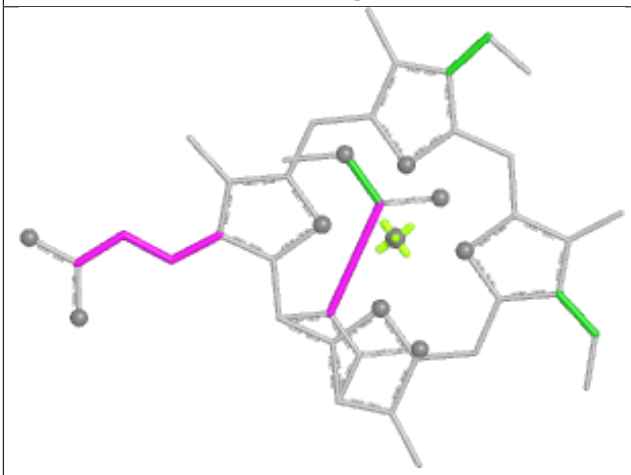
Ligand KC1 K 215



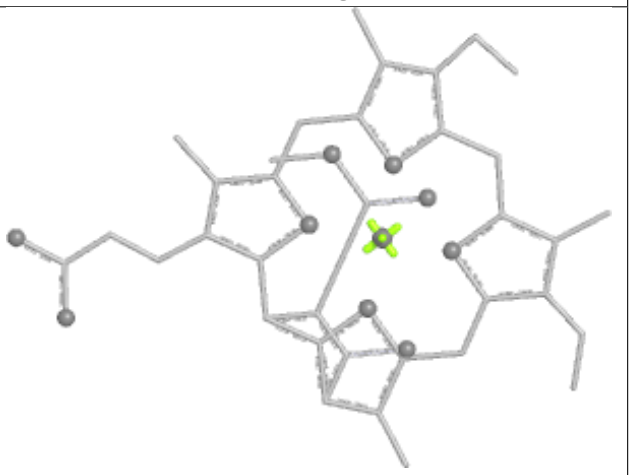
Bond lengths



Bond angles

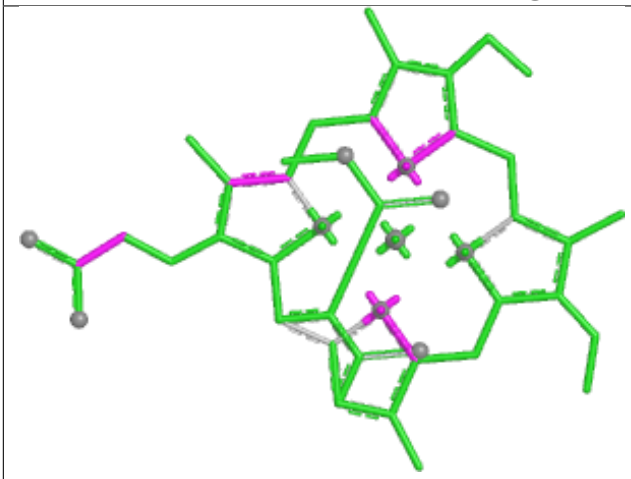


Torsions

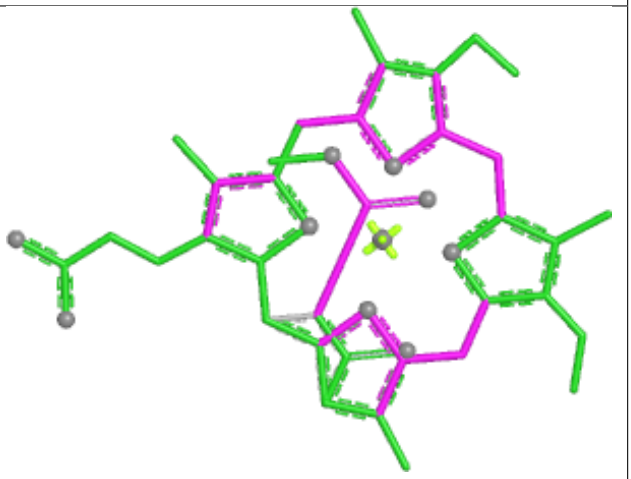


Rings

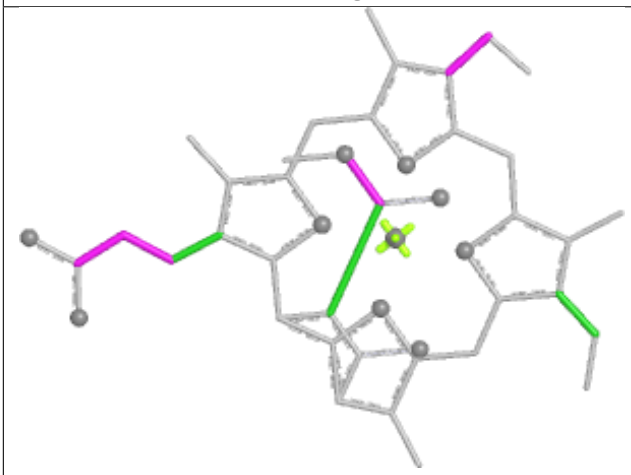
Ligand KC1 B 313



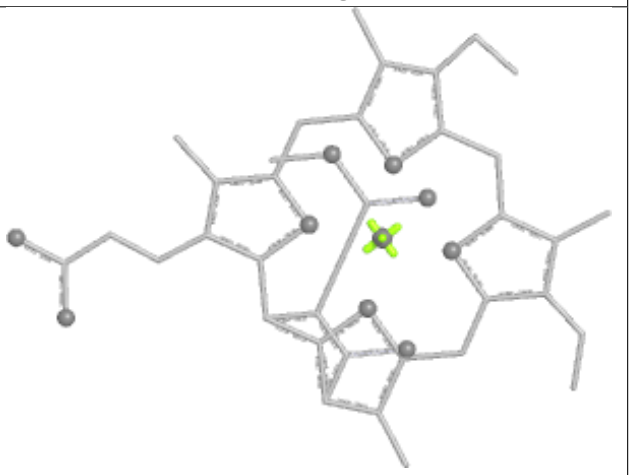
Bond lengths



Bond angles

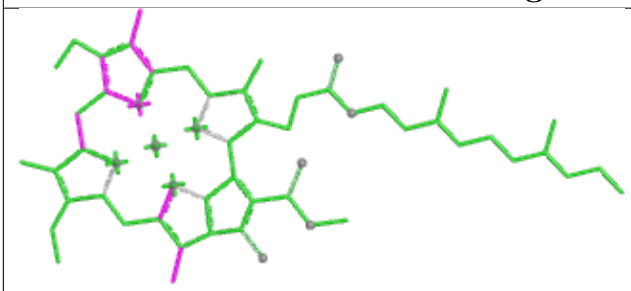


Torsions

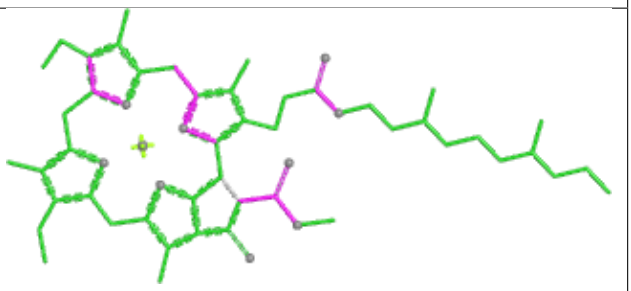


Rings

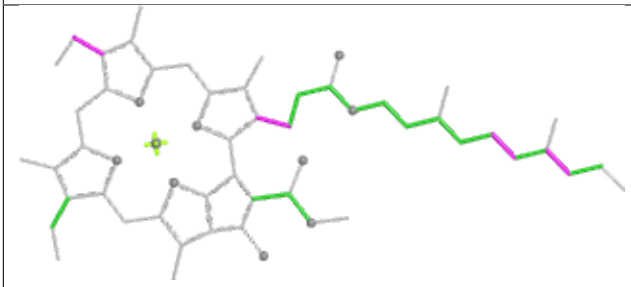
Ligand CLA E 315



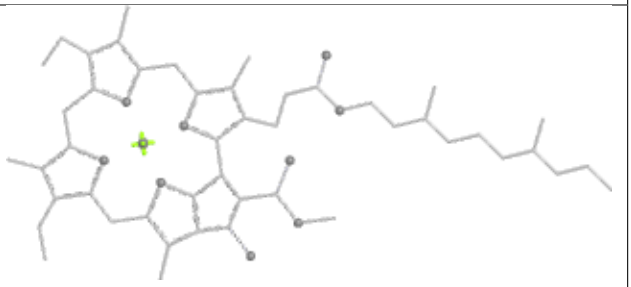
Bond lengths



Bond angles

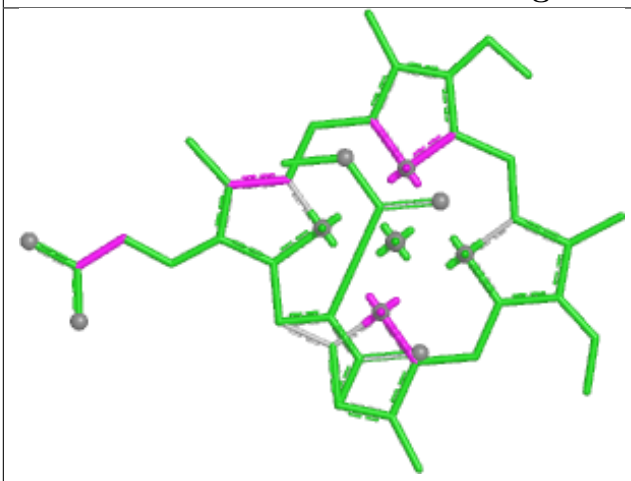


Torsions

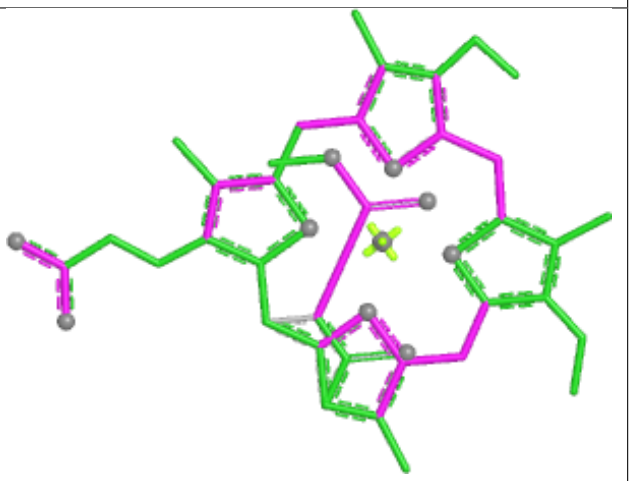


Rings

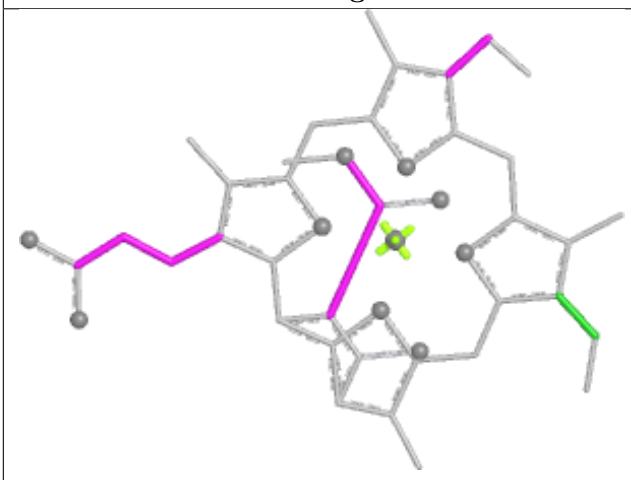
Ligand KC1 I 215



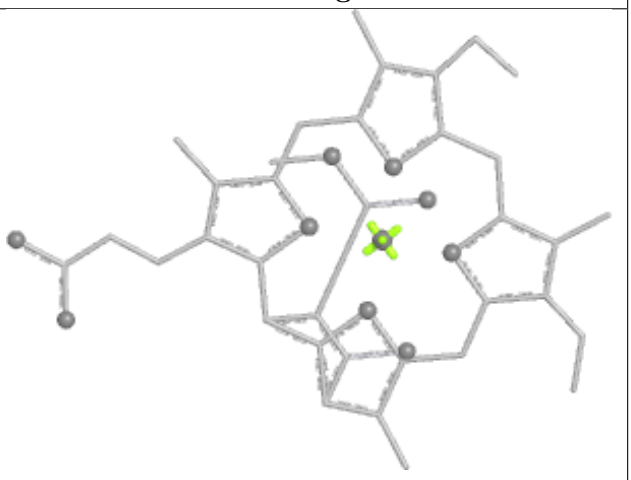
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

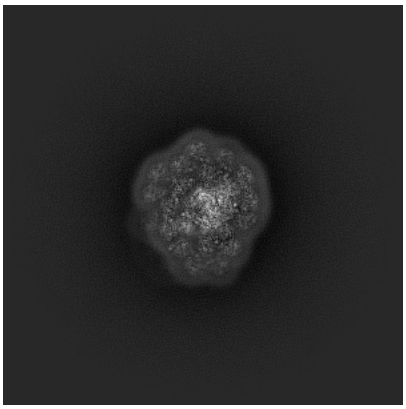
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36678. These allow visual inspection of the internal detail of the map and identification of artifacts.

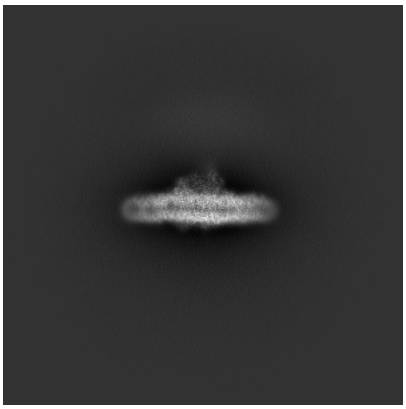
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

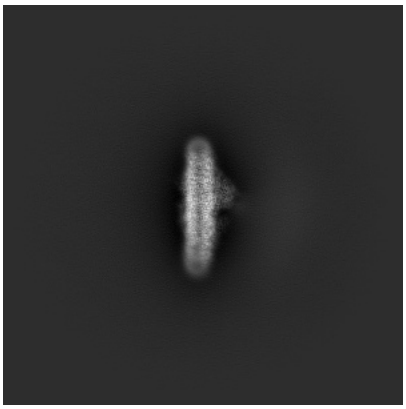
6.1.1 Primary map



X

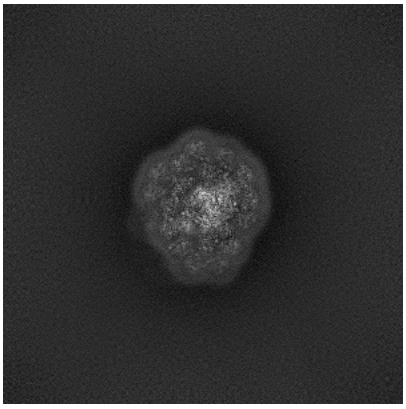


Y

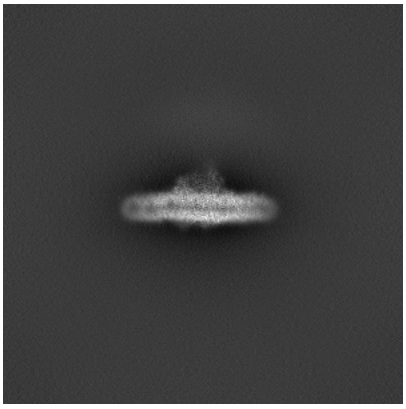


Z

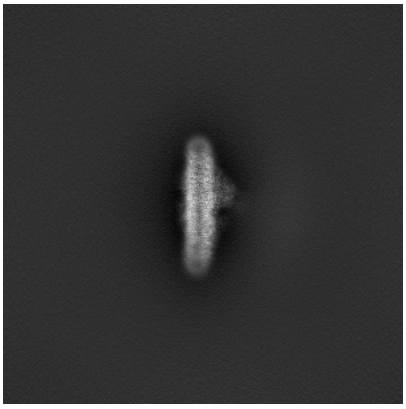
6.1.2 Raw map



X



Y

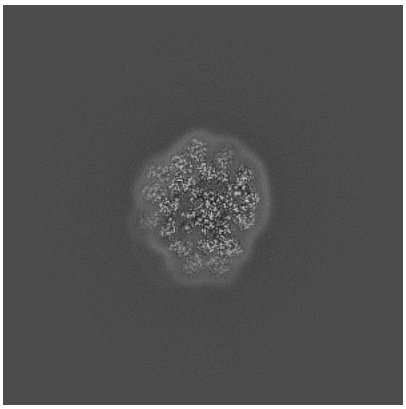


Z

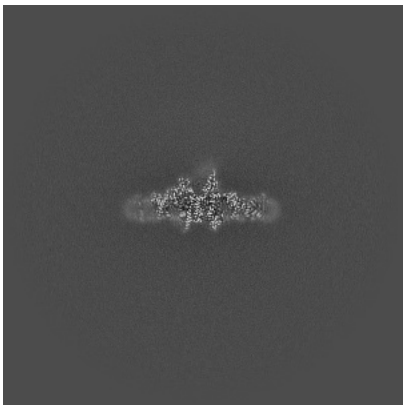
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

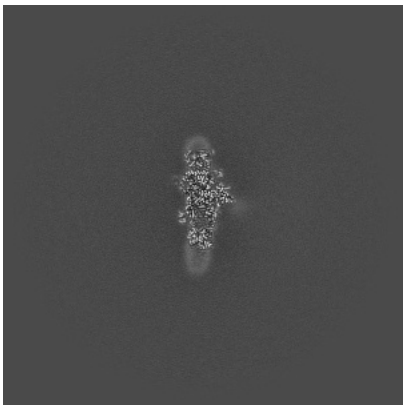
6.2.1 Primary map



X Index: 256

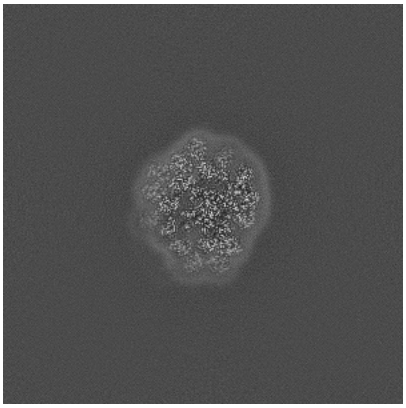


Y Index: 256

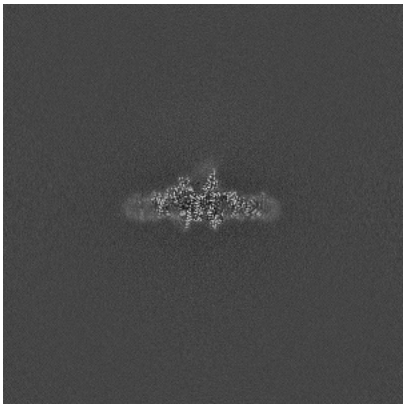


Z Index: 256

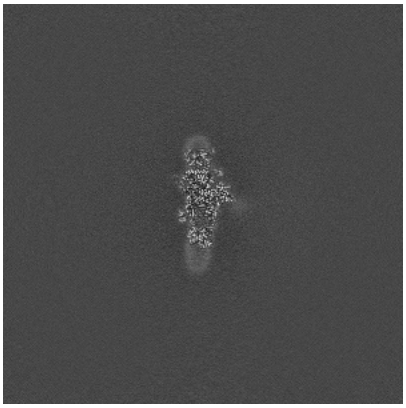
6.2.2 Raw map



X Index: 256



Y Index: 256

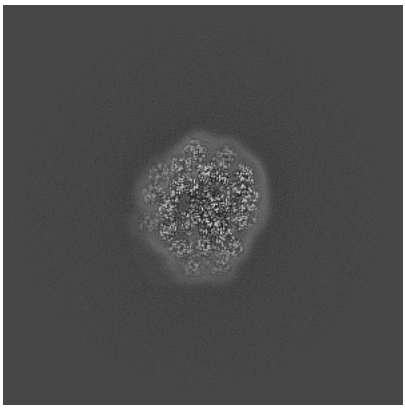


Z Index: 256

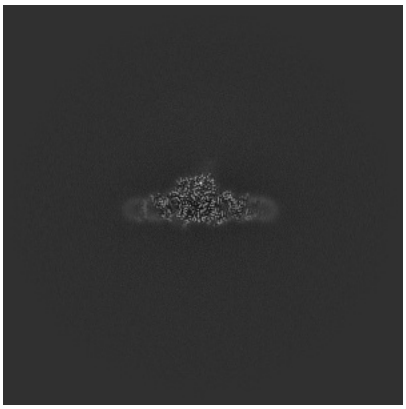
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 259

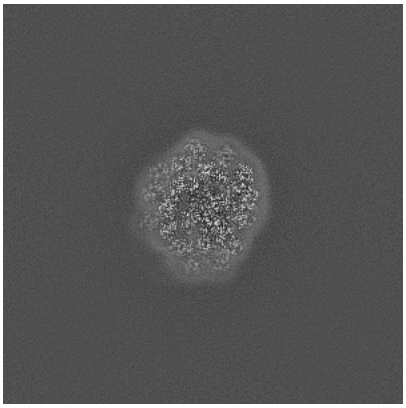


Y Index: 262

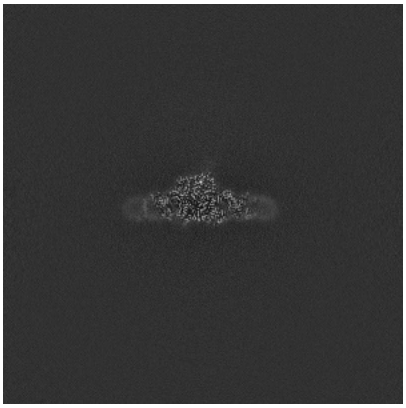


Z Index: 262

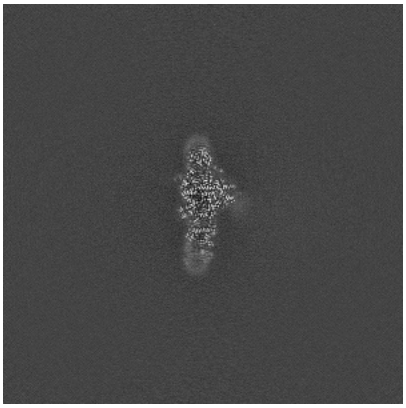
6.3.2 Raw map



X Index: 259



Y Index: 262

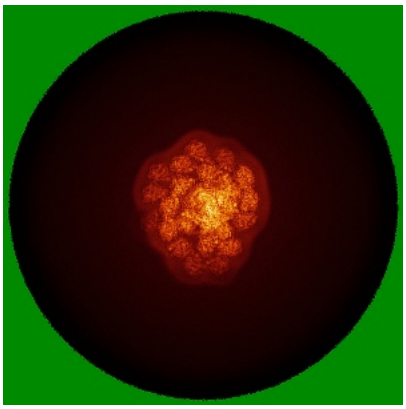


Z Index: 262

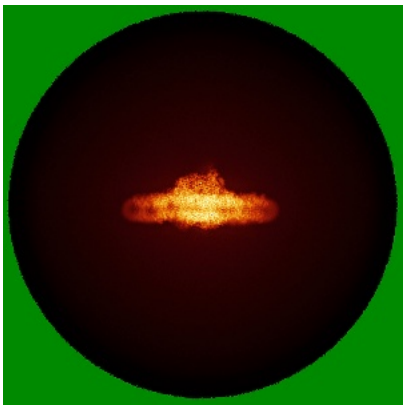
The images above show the largest variance slices of the map in three orthogonal directions.

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

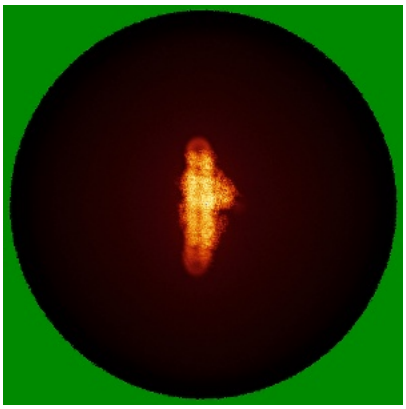
6.4.1 Primary map



X

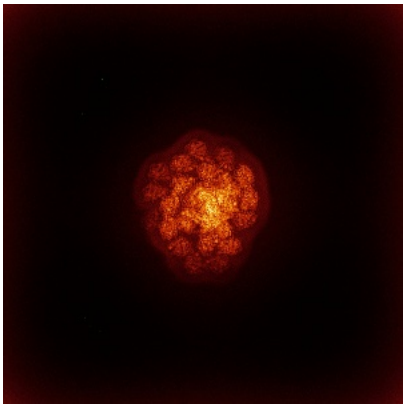


Y

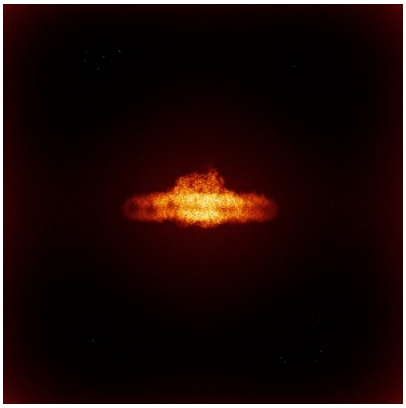


Z

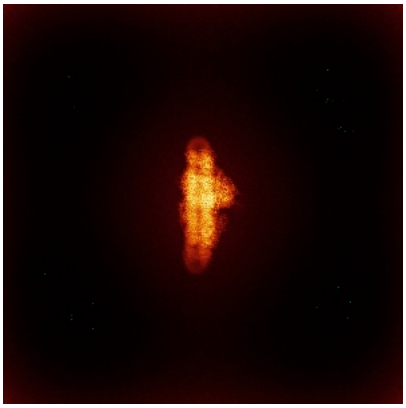
6.4.2 Raw map



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 0.22. 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.

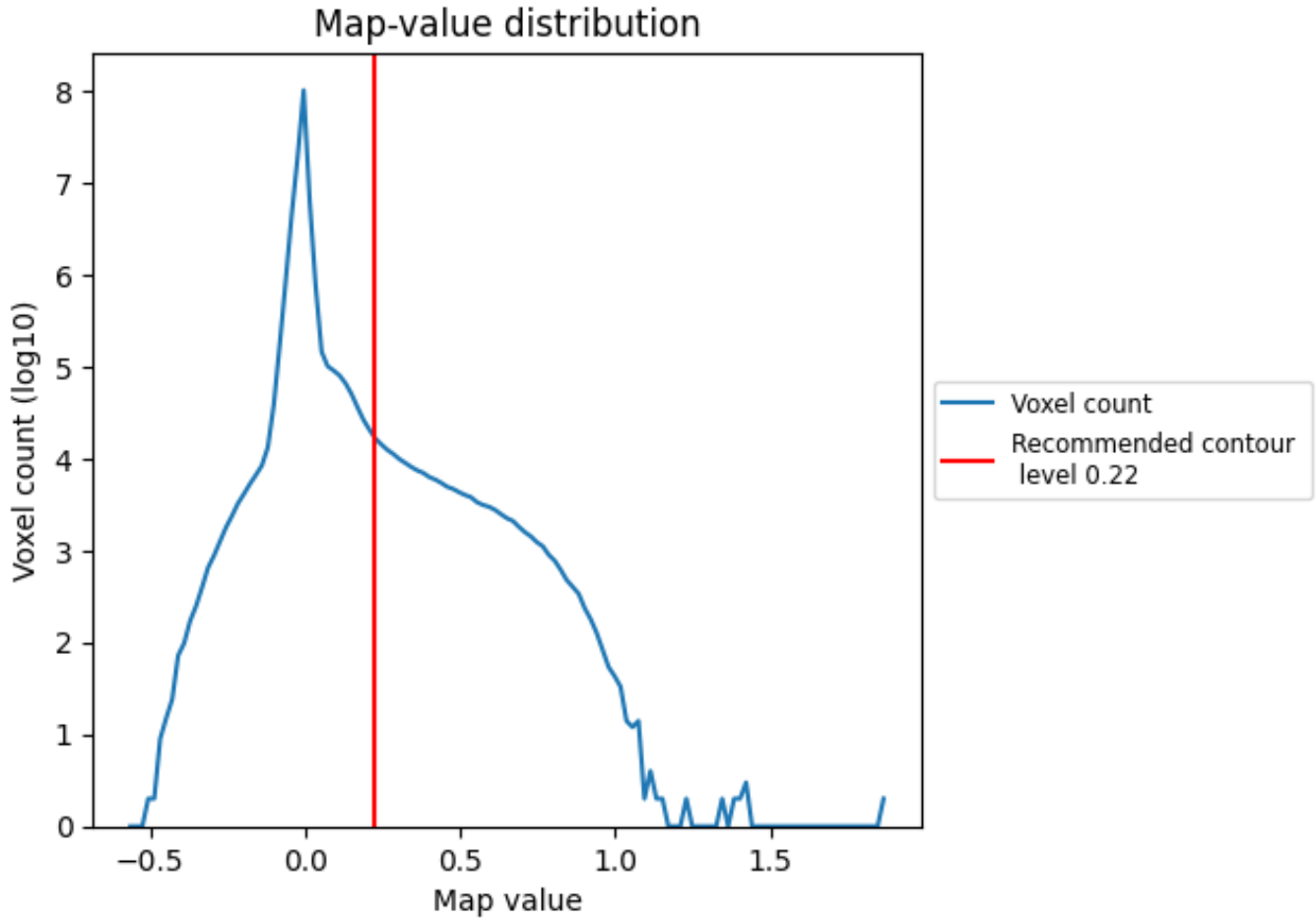
6.6 Mask visualisation (i)

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

7 Map analysis

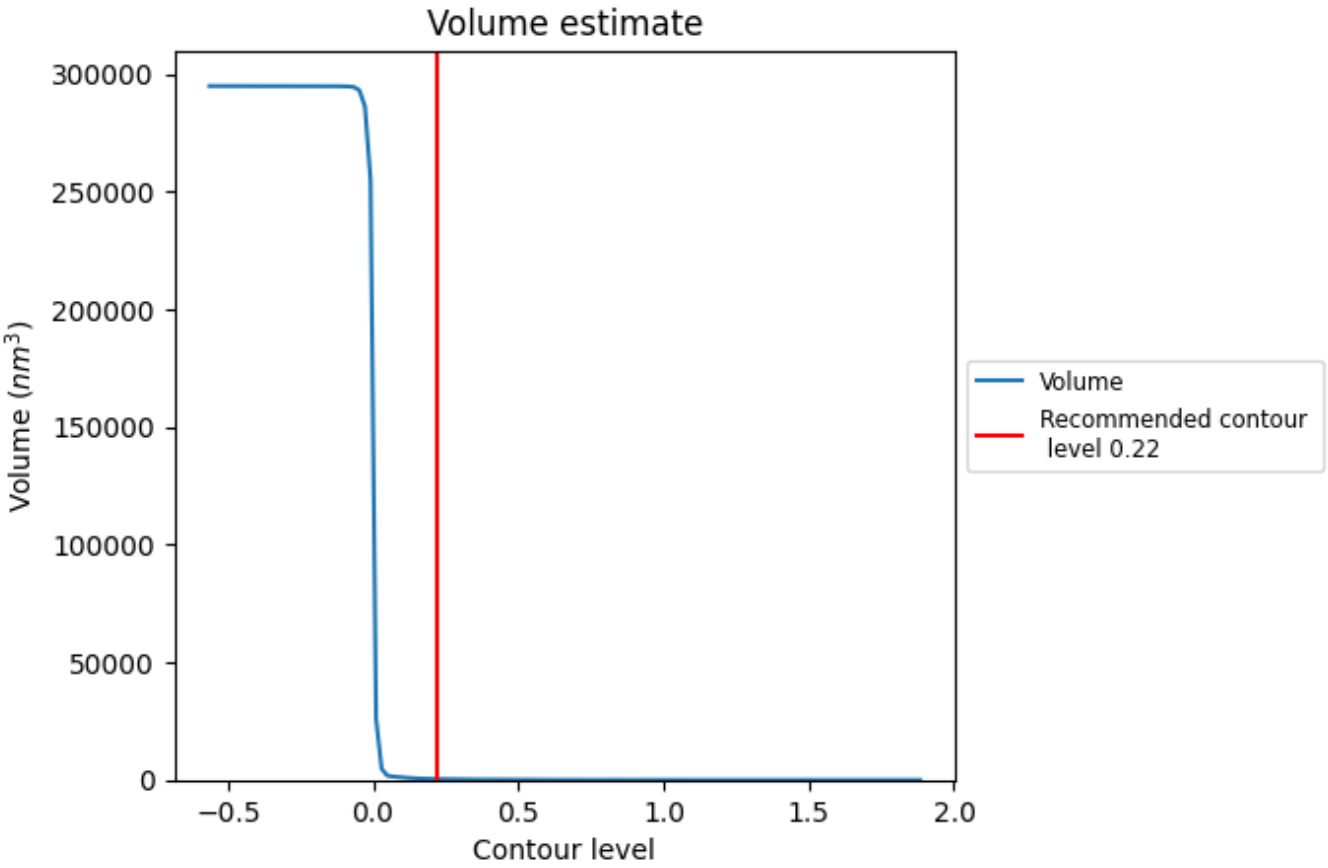
This section contains the results of statistical analysis of the map.

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.

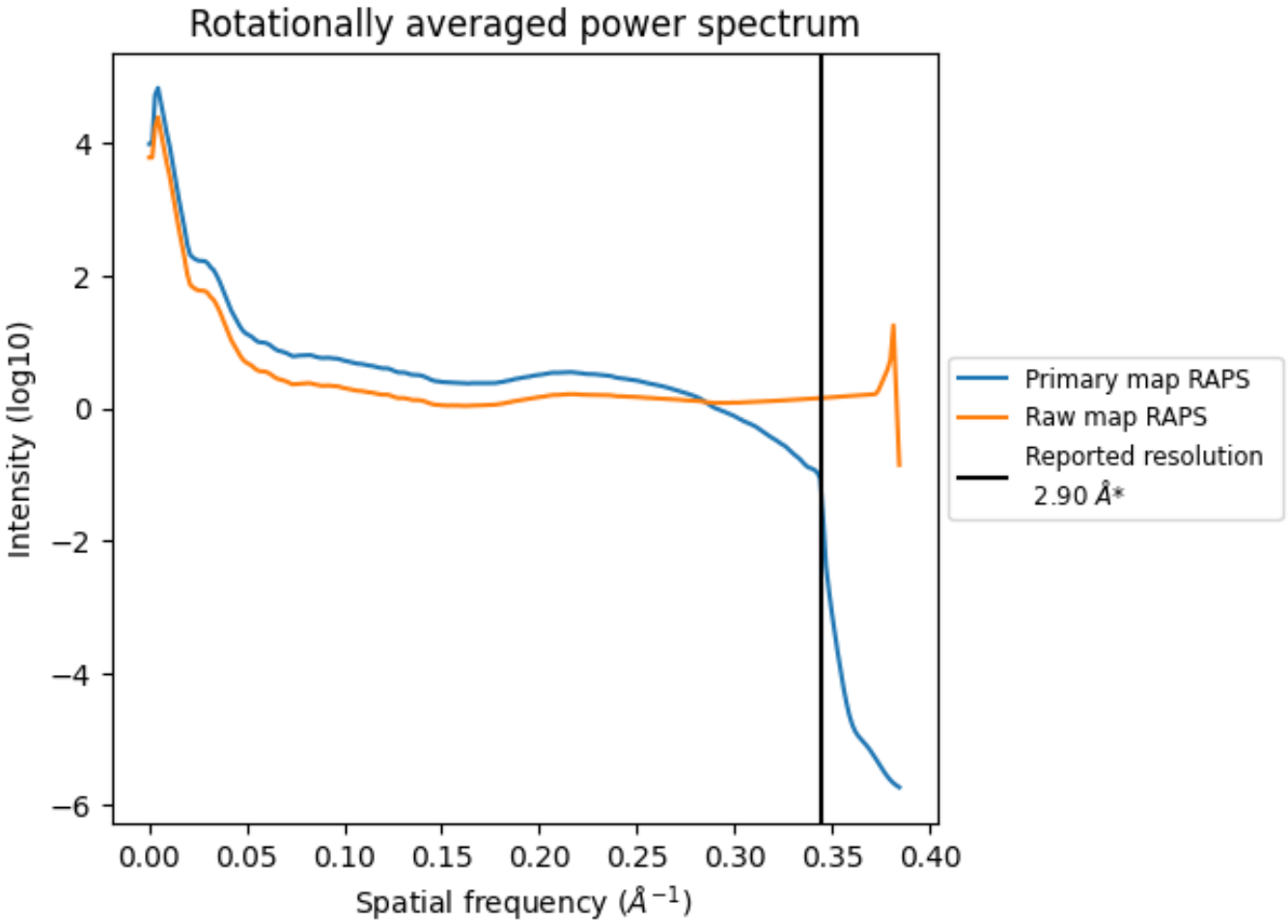
7.2 Volume estimate



The volume at the recommended contour level is 378 nm^3; this corresponds to an approximate mass of 342 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)

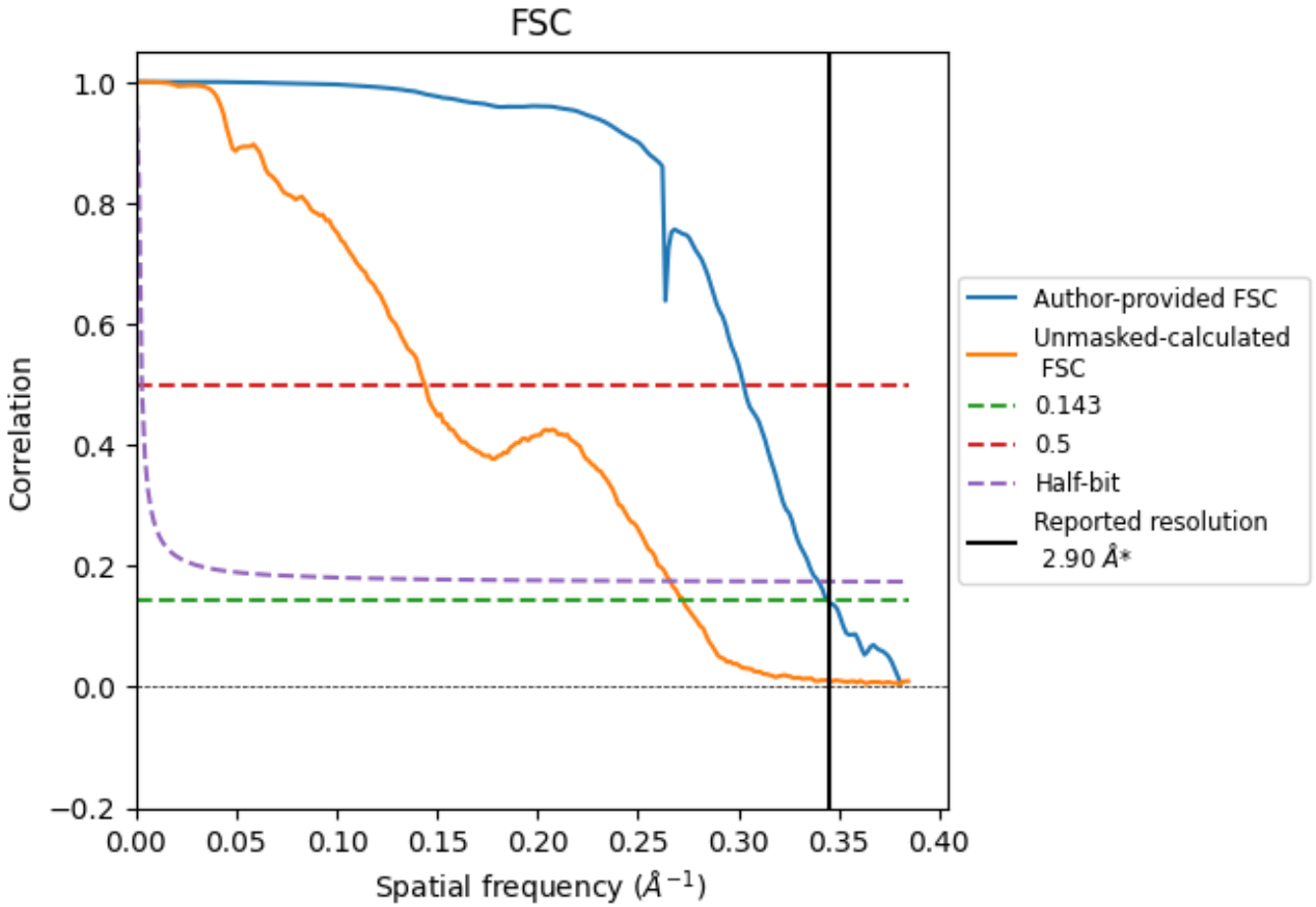


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

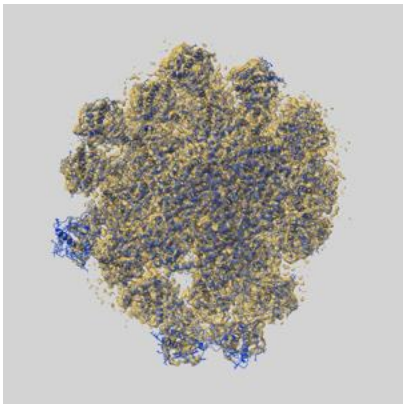
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.31	2.94
Unmasked-calculated*	3.67	6.95	3.76

*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 3.67 differs from the reported value 2.9 by more than 10 %

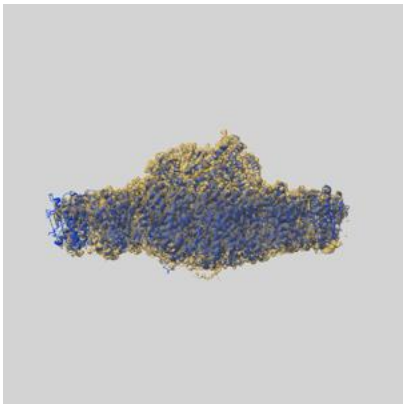
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36678 and PDB model 8JW0. Per-residue inclusion information can be found in section 3 on page 40.

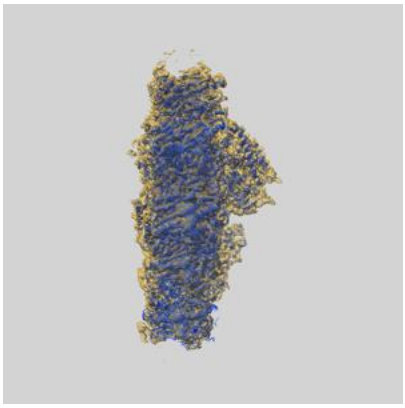
9.1 Map-model overlay



X



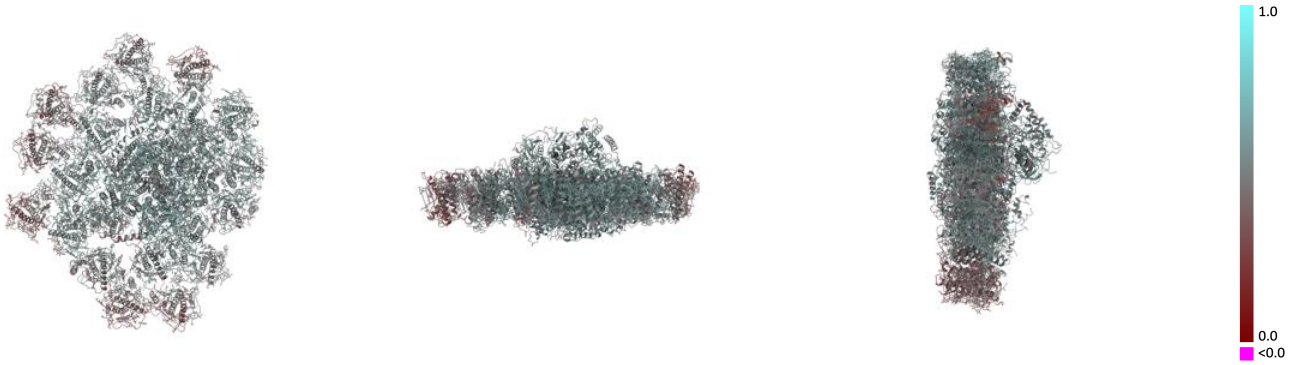
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22 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.

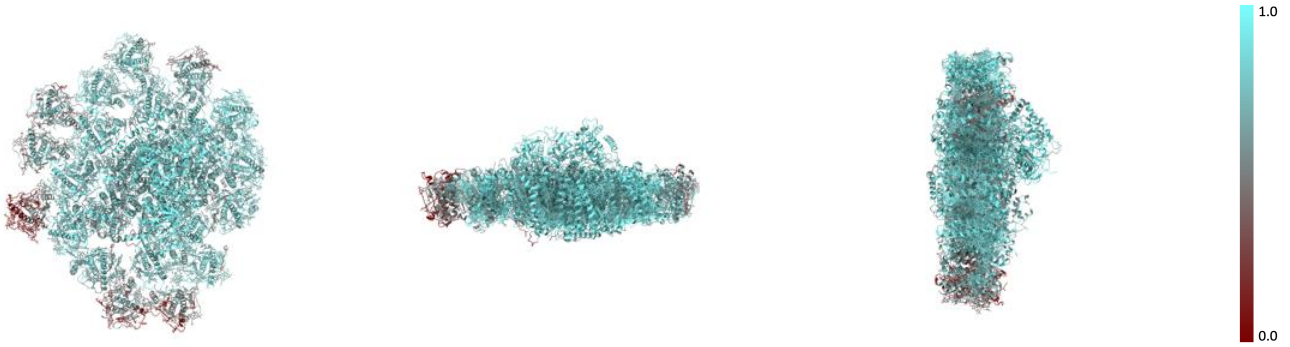
9.2 Q-score mapped to coordinate model (i)



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.

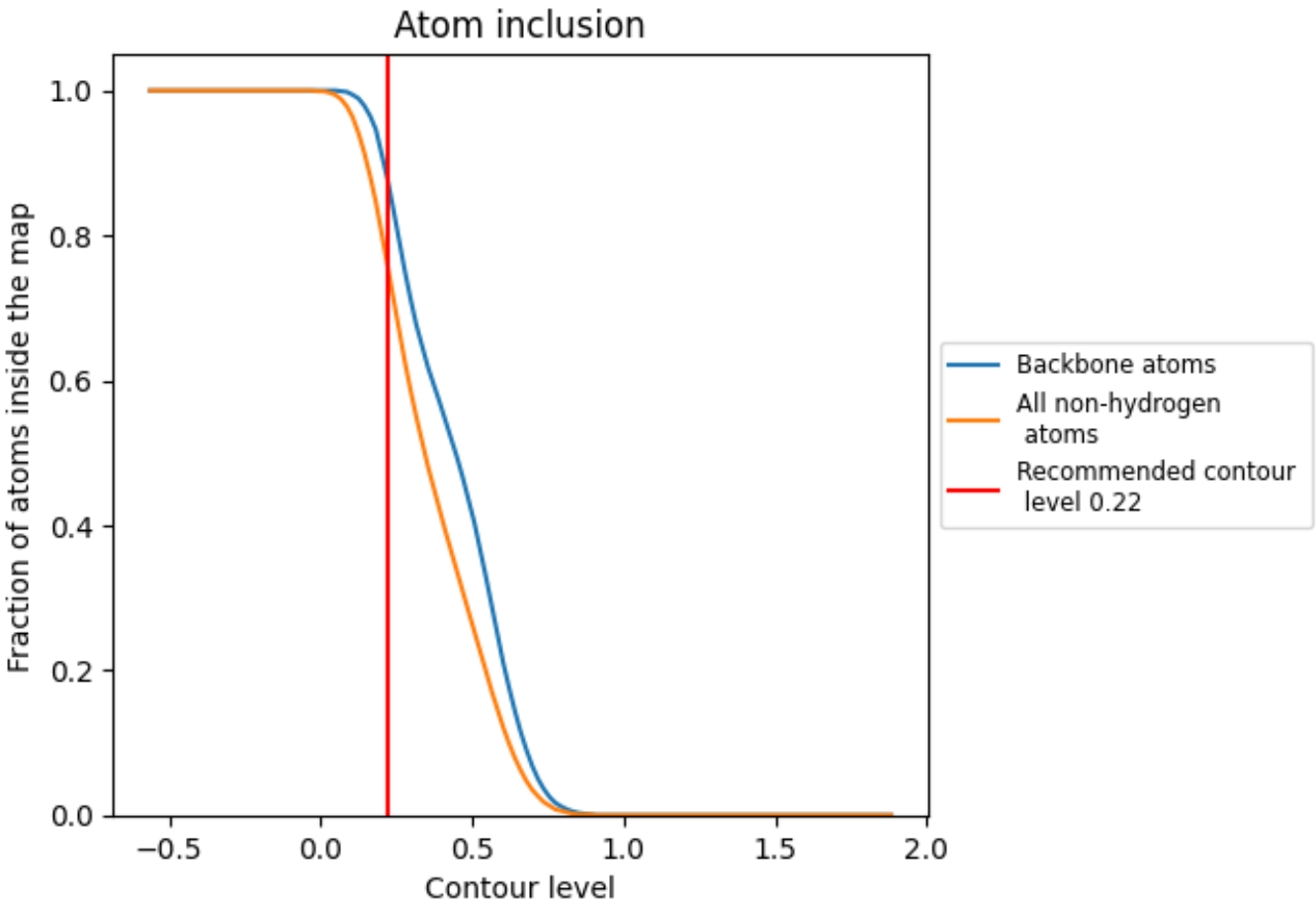
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.22).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.5100
A	0.8530	0.5420
B	0.8250	0.5400
C	0.7340	0.4710
D	0.6420	0.4360
E	0.7510	0.5040
F	0.7860	0.5010
G	0.8350	0.5470
H	0.3850	0.3860
I	0.8550	0.5520
J	0.8020	0.5160
K	0.8480	0.5520
L	0.8120	0.5330
M	0.7040	0.4660
N	0.4320	0.3830
O	0.5950	0.4070
P	0.2580	0.3780
Q	0.8000	0.5110
T	0.5580	0.3790
a	0.8120	0.5450
b	0.8740	0.5690
c	0.9430	0.5590
d	0.8890	0.5480
e	0.9090	0.5690
f	0.8360	0.5440
h	0.8700	0.5530
i	0.8300	0.5450
j	0.8020	0.5450
l	0.8340	0.5370
m	0.7750	0.5380

