Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:32 PM UTC

PDB ID	:	6LY5 / pdb_00006ly5
EMDB ID	:	EMD-30012
Title	:	Organization and energy transfer in a huge diatom PSI-FCPI supercomplex
Authors	:	Xiong, P.; Caizhe, X.
Deposited on	:	2020-02-13
Resolution	:	2.38 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:

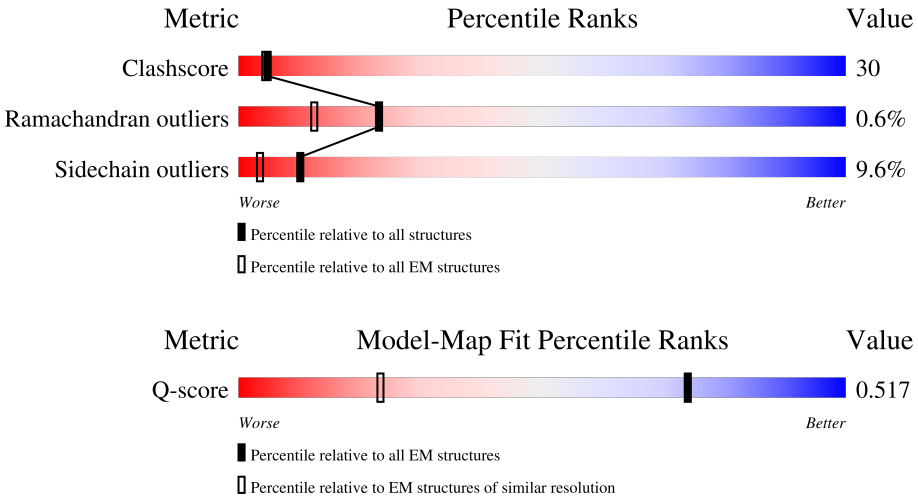
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.38 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.



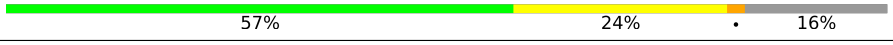
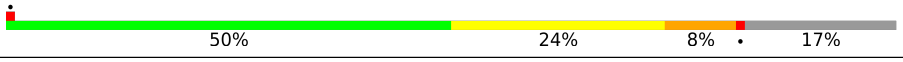
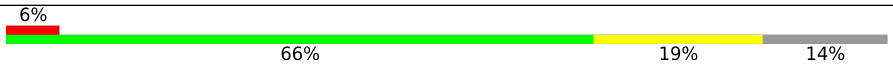
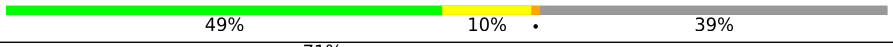
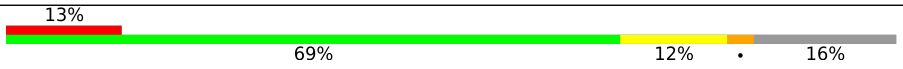
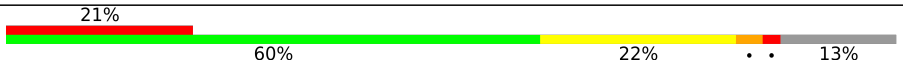
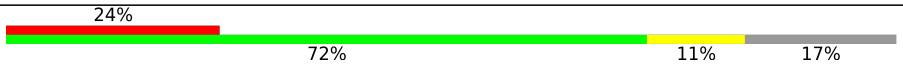
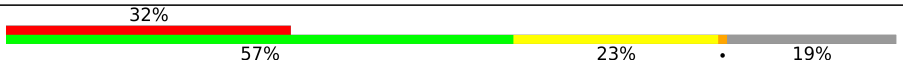
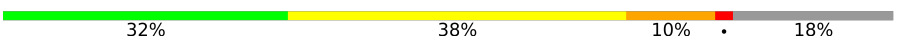
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4811 (1.88 - 2.88)

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	168	65% 31% .
2	B	223	. 38% 17% . 41%
3	C	198	. 58% 20% 5% 18%
4	D	207	56% 20% 7% 17%

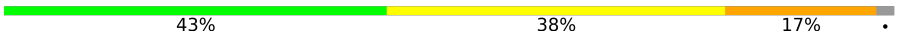
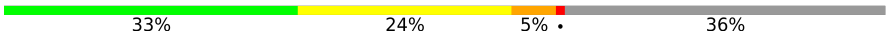
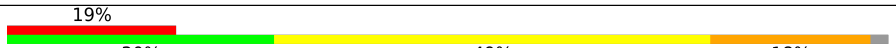
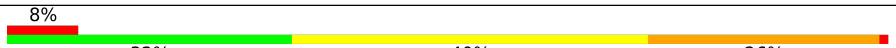
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Mol	Chain	Length	Quality of chain
5	E	222	
6	F	215	
7	G	245	
8	H	203	
9	I	195	
10	J	200	
11	K	207	
12	L	229	
13	M	306	
14	N	219	
15	O	205	
15	P	205	
15	Q	205	
16	R	246	
17	S	254	
18	T	207	
19	W	198	
19	X	198	
20	a	743	
21	b	733	
22	c	80	
23	d	132	
24	e	63	
25	f	162	
26	i	40	

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Mol	Chain	Length	Quality of chain
27	j	42	
28	l	172	
29	m	29	
30	g	134	
31	h	139	
32	U	160	
33	V	179	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	DD6	L	305	-	-	X	-
34	DD6	W	204	-	-	X	-
34	DD6	W	205	-	-	X	-
35	A86	Q	316	-	-	X	-
35	A86	S	304	-	-	X	-
35	A86	V	301	-	-	X	-
35	A86	X	314	-	-	X	-
36	CLA	A	305	X	-	-	-
36	CLA	A	306	X	-	-	-
36	CLA	A	307	X	-	-	-
36	CLA	A	308	X	-	-	-
36	CLA	A	309	X	-	-	-
36	CLA	A	310	X	-	-	-
36	CLA	A	311	X	-	-	-
36	CLA	A	313	X	-	-	-
36	CLA	A	314	X	-	-	-
36	CLA	B	305	X	-	-	-
36	CLA	B	306	X	-	-	-
36	CLA	B	307	X	-	-	-
36	CLA	B	308	X	-	-	-
36	CLA	B	309	X	-	-	-
36	CLA	B	311	X	-	-	-
36	CLA	C	205	X	-	-	-
36	CLA	C	206	X	-	-	-
36	CLA	C	207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	C	208	X	-	-	-
36	CLA	C	209	X	-	-	-
36	CLA	C	210	X	-	-	-
36	CLA	C	211	X	-	-	-
36	CLA	C	212	X	-	-	-
36	CLA	C	214	X	-	-	-
36	CLA	D	306	X	-	-	-
36	CLA	D	307	X	-	-	-
36	CLA	D	308	X	-	-	-
36	CLA	D	309	X	-	-	-
36	CLA	D	310	X	-	-	-
36	CLA	D	312	X	-	-	-
36	CLA	D	313	X	-	-	-
36	CLA	D	315	X	-	-	-
36	CLA	D	316	X	-	-	-
36	CLA	D	317	X	-	-	-
36	CLA	E	308	X	-	-	-
36	CLA	E	311	X	-	-	-
36	CLA	E	312	X	-	-	-
36	CLA	E	313	X	-	-	-
36	CLA	E	314	X	-	-	-
36	CLA	E	315	X	-	X	-
36	CLA	E	316	X	-	-	-
36	CLA	E	317	X	-	-	-
36	CLA	F	309	X	-	-	-
36	CLA	F	310	X	-	-	-
36	CLA	F	311	X	-	-	-
36	CLA	F	312	X	-	-	-
36	CLA	F	313	X	-	-	-
36	CLA	F	314	X	-	-	-
36	CLA	F	316	X	-	-	-
36	CLA	F	317	X	-	X	-
36	CLA	G	309	X	-	-	-
36	CLA	G	310	X	-	-	-
36	CLA	G	311	X	-	-	-
36	CLA	G	312	X	-	-	-
36	CLA	G	313	X	-	-	-
36	CLA	G	314	X	-	-	-
36	CLA	G	315	X	-	X	-
36	CLA	G	316	X	-	-	-
36	CLA	G	319	X	-	-	-
36	CLA	H	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	H	306	X	-	-	-
36	CLA	H	307	X	-	-	-
36	CLA	H	308	X	-	-	-
36	CLA	H	309	X	-	-	-
36	CLA	H	310	X	-	-	-
36	CLA	H	311	X	-	-	-
36	CLA	H	312	X	-	-	-
36	CLA	H	314	X	-	-	-
36	CLA	H	315	X	-	-	-
36	CLA	H	316	X	-	-	-
36	CLA	H	317	X	-	-	-
36	CLA	H	318	X	-	-	-
36	CLA	I	305	X	-	-	-
36	CLA	I	306	X	-	-	-
36	CLA	I	307	X	-	-	-
36	CLA	I	308	X	-	X	-
36	CLA	I	309	X	-	-	-
36	CLA	I	310	X	-	-	-
36	CLA	I	311	X	-	-	-
36	CLA	I	312	X	-	-	-
36	CLA	I	313	X	-	-	-
36	CLA	I	314	X	-	-	-
36	CLA	J	307	X	-	-	-
36	CLA	J	309	X	-	-	-
36	CLA	J	310	X	-	-	-
36	CLA	J	311	X	-	-	-
36	CLA	J	312	X	-	-	-
36	CLA	J	313	X	-	-	-
36	CLA	J	315	X	-	-	-
36	CLA	J	316	X	-	-	-
36	CLA	J	317	X	-	-	-
36	CLA	K	307	X	-	-	-
36	CLA	K	308	X	-	-	-
36	CLA	K	309	X	-	-	-
36	CLA	K	310	X	-	X	-
36	CLA	K	311	X	-	-	-
36	CLA	K	312	X	-	-	-
36	CLA	K	313	X	-	-	-
36	CLA	K	315	X	-	-	-
36	CLA	K	316	X	-	-	-
36	CLA	L	308	X	-	X	-
36	CLA	L	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	L	310	X	-	-	-
36	CLA	L	311	X	-	-	-
36	CLA	L	313	X	-	-	-
36	CLA	L	314	X	-	-	-
36	CLA	L	316	X	-	-	-
36	CLA	L	320	X	-	-	-
36	CLA	M	306	X	-	-	-
36	CLA	M	307	X	-	-	-
36	CLA	M	308	X	-	-	-
36	CLA	M	309	X	-	-	-
36	CLA	M	310	X	-	-	-
36	CLA	M	311	X	-	-	-
36	CLA	M	312	X	-	-	-
36	CLA	M	314	X	-	-	-
36	CLA	M	316	X	-	-	-
36	CLA	N	307	X	-	-	-
36	CLA	N	308	X	-	-	-
36	CLA	N	309	X	-	-	-
36	CLA	N	310	X	-	-	-
36	CLA	N	311	X	-	-	-
36	CLA	N	312	X	-	-	-
36	CLA	N	313	X	-	-	-
36	CLA	N	316	X	-	-	-
36	CLA	N	317	X	-	-	-
36	CLA	N	318	X	-	-	-
36	CLA	N	319	X	-	-	-
36	CLA	O	306	X	-	-	-
36	CLA	O	307	X	-	-	-
36	CLA	O	308	X	-	-	-
36	CLA	O	309	X	-	-	-
36	CLA	O	310	X	-	-	-
36	CLA	O	311	X	-	-	-
36	CLA	O	314	X	-	-	-
36	CLA	O	316	X	-	X	-
36	CLA	P	301	X	-	-	-
36	CLA	P	308	X	-	-	-
36	CLA	P	309	X	-	-	-
36	CLA	P	310	X	-	-	-
36	CLA	P	311	X	-	-	-
36	CLA	P	312	X	-	-	-
36	CLA	P	313	X	-	-	-
36	CLA	P	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	P	318	X	-	-	-
36	CLA	P	319	X	-	-	-
36	CLA	Q	305	X	-	-	-
36	CLA	Q	306	X	-	-	-
36	CLA	Q	307	X	-	-	-
36	CLA	Q	308	X	-	-	-
36	CLA	Q	309	X	-	-	-
36	CLA	Q	312	X	-	-	-
36	CLA	Q	314	X	-	X	-
36	CLA	R	310	X	-	-	-
36	CLA	R	311	X	-	-	-
36	CLA	R	312	X	-	-	-
36	CLA	R	313	X	-	-	-
36	CLA	R	314	X	-	-	-
36	CLA	R	315	X	-	-	-
36	CLA	R	316	X	-	-	-
36	CLA	R	318	X	-	-	-
36	CLA	R	319	X	-	-	-
36	CLA	R	320	X	-	-	-
36	CLA	R	322	X	-	-	-
36	CLA	S	309	X	-	-	-
36	CLA	S	310	X	-	-	-
36	CLA	S	311	X	-	-	-
36	CLA	S	313	X	-	-	-
36	CLA	S	315	X	-	-	-
36	CLA	S	317	X	-	-	-
36	CLA	S	318	X	-	-	-
36	CLA	S	319	X	-	-	-
36	CLA	T	308	X	-	-	-
36	CLA	T	309	X	-	-	-
36	CLA	T	311	X	-	-	-
36	CLA	T	312	X	-	-	-
36	CLA	T	313	X	-	-	-
36	CLA	T	314	X	-	-	-
36	CLA	T	316	X	-	-	-
36	CLA	U	305	X	-	-	-
36	CLA	U	306	X	-	X	-
36	CLA	U	307	X	-	-	-
36	CLA	U	308	X	-	-	-
36	CLA	U	310	X	-	-	-
36	CLA	U	311	X	-	-	-
36	CLA	U	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	V	305	X	-	X	-
36	CLA	V	306	X	-	X	-
36	CLA	V	307	X	-	-	-
36	CLA	V	308	X	-	-	-
36	CLA	V	309	X	-	-	-
36	CLA	V	310	X	-	-	-
36	CLA	V	311	X	-	-	-
36	CLA	V	313	X	-	-	-
36	CLA	V	314	X	-	X	-
36	CLA	W	201	X	-	-	-
36	CLA	W	206	X	-	-	-
36	CLA	W	207	X	-	-	-
36	CLA	W	208	X	-	-	-
36	CLA	W	209	X	-	-	-
36	CLA	W	210	X	-	-	-
36	CLA	W	211	X	-	-	-
36	CLA	W	212	-	-	X	-
36	CLA	W	215	X	-	-	-
36	CLA	W	216	X	-	-	-
36	CLA	W	218	X	-	-	-
36	CLA	X	306	X	-	-	-
36	CLA	X	308	X	-	-	-
36	CLA	X	310	X	-	-	-
36	CLA	X	312	X	-	-	-
36	CLA	X	315	-	-	X	-
36	CLA	a	801	X	-	-	-
36	CLA	a	802	X	-	-	-
36	CLA	a	803	X	-	-	-
36	CLA	a	804	X	-	-	-
36	CLA	a	805	X	-	-	-
36	CLA	a	806	X	-	-	-
36	CLA	a	807	X	-	-	-
36	CLA	a	808	X	-	-	-
36	CLA	a	809	X	-	-	-
36	CLA	a	810	X	-	-	-
36	CLA	a	811	X	-	-	-
36	CLA	a	812	X	-	-	-
36	CLA	a	813	X	-	-	-
36	CLA	a	814	X	-	-	-
36	CLA	a	815	X	-	-	-
36	CLA	a	816	X	-	X	-
36	CLA	a	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	a	818	X	-	-	-
36	CLA	a	819	X	-	-	-
36	CLA	a	820	X	-	-	-
36	CLA	a	821	X	-	-	-
36	CLA	a	822	X	-	-	-
36	CLA	a	823	X	-	-	-
36	CLA	a	824	X	-	-	-
36	CLA	a	825	X	-	-	-
36	CLA	a	826	X	-	-	-
36	CLA	a	827	X	-	-	-
36	CLA	a	828	X	-	-	-
36	CLA	a	829	X	-	-	-
36	CLA	a	831	X	-	-	-
36	CLA	a	832	X	-	-	-
36	CLA	a	833	X	-	-	-
36	CLA	a	834	X	-	-	-
36	CLA	a	835	X	-	-	-
36	CLA	a	836	X	-	-	-
36	CLA	a	837	X	-	-	-
36	CLA	a	838	X	-	-	-
36	CLA	a	839	X	-	-	-
36	CLA	a	841	X	-	-	-
36	CLA	a	848	X	-	-	-
36	CLA	b	801	X	-	-	-
36	CLA	b	802	X	-	-	-
36	CLA	b	805	X	-	-	-
36	CLA	b	806	X	-	-	-
36	CLA	b	807	X	-	-	-
36	CLA	b	808	X	-	-	-
36	CLA	b	809	X	-	-	-
36	CLA	b	810	X	-	-	-
36	CLA	b	811	X	-	-	-
36	CLA	b	812	X	-	-	-
36	CLA	b	813	X	-	-	-
36	CLA	b	814	X	-	-	-
36	CLA	b	815	X	-	-	-
36	CLA	b	816	X	-	-	-
36	CLA	b	817	X	-	-	-
36	CLA	b	819	X	-	-	-
36	CLA	b	820	X	-	-	-
36	CLA	b	821	X	-	-	-
36	CLA	b	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	b	823	X	-	-	-
36	CLA	b	824	X	-	-	-
36	CLA	b	825	X	-	-	-
36	CLA	b	826	X	-	-	-
36	CLA	b	827	X	-	-	-
36	CLA	b	828	X	-	-	-
36	CLA	b	829	X	-	-	-
36	CLA	b	830	X	-	-	-
36	CLA	b	831	X	-	-	-
36	CLA	b	832	X	-	-	-
36	CLA	b	833	X	-	-	-
36	CLA	b	834	X	-	-	-
36	CLA	b	835	X	-	-	-
36	CLA	b	836	X	-	-	-
36	CLA	b	837	X	-	-	-
36	CLA	b	838	X	-	-	-
36	CLA	b	839	X	-	-	-
36	CLA	b	840	X	-	-	-
36	CLA	b	841	X	-	-	-
36	CLA	f	802	X	-	-	-
36	CLA	f	803	X	-	-	-
36	CLA	f	804	X	-	-	-
36	CLA	f	805	X	-	-	-
36	CLA	h	203	X	-	-	-
36	CLA	i	102	X	-	-	-
36	CLA	j	101	X	-	-	-
36	CLA	j	102	X	-	-	-
36	CLA	j	106	X	-	-	-
36	CLA	l	201	X	-	-	-
36	CLA	l	202	X	-	-	-
36	CLA	l	205	X	-	-	-
36	CLA	l	206	X	-	-	-
39	LMT	F	321	-	-	X	-
39	LMT	h	205	-	-	X	-
41	LHG	E	322	-	-	X	-
41	LHG	f	808	-	-	X	-
41	LHG	i	104	-	-	X	-
42	LMG	J	318	-	-	X	-
42	LMG	V	316	-	-	X	-
42	LMG	j	105	-	-	X	-
45	SF4	b	803	-	-	X	-

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 81344 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 FCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	168	1287	825	213	237	12	0	0

- Molecule 2 is a protein called FCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	132	1013	662	166	176	9	0	0

- Molecule 3 is a protein called FCPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	163	1247	796	210	232	9	0	0

- Molecule 4 is a protein called FCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	172	1337	870	214	245	8	0	0

- Molecule 5 is a protein called FCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	188	1411	891	240	265	15	0	0

- Molecule 6 is a protein called FCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	180	1375	880	230	253	12	0	0

- Molecule 7 is a protein called FCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	214	Total	C	N	O	S	0	0
			1668	1079	276	305	8		

- Molecule 8 is a protein called FCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	170	Total	C	N	O	S	0	0
			1291	832	213	236	10		

- Molecule 9 is a protein called FCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	161	Total	C	N	O	S	0	0
			1250	807	208	228	7		

- Molecule 10 is a protein called FCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1301	843	217	236	5		

- Molecule 11 is a protein called FCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	169	Total	C	N	O	S	0	0
			1304	850	214	232	8		

- Molecule 12 is a protein called FCPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	196	Total	C	N	O	S	0	0
			1523	989	250	276	8		

- Molecule 13 is a protein called FCPI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	187	Total	C	N	O	S	0	0
			1423	914	248	255	6		

- Molecule 14 is a protein called FCPI-21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	219	Total	C	N	O	S	0	0
			1716	1119	282	309	6		

- Molecule 15 is a protein called FCPI.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		
15	P	173	Total	C	N	O	S	0	0
			1296	834	213	241	8		
15	Q	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		

- Molecule 16 is a protein called FCPI-24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	211	Total	C	N	O	S	0	0
			1628	1061	266	294	7		

- Molecule 17 is a protein called FCPI-23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	220	Total	C	N	O	S	0	0
			1722	1122	283	311	6		

- Molecule 18 is a protein called FCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	172	Total	C	N	O	S	0	0
			1326	848	226	247	5		

- Molecule 19 is a protein called FCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	160	Total	C	N	O	S	0	0
			1239	799	203	233	4		
19	X	161	Total	C	N	O	S	1	0
			1253	808	207	234	4		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	742	Total	C	N	O	S	0	0
			5858	3826	991	1013	28		

- Molecule 21 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	732	Total	C	N	O	S	1	0
			5820	3828	980	994	18		

- Molecule 22 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	80	Total	C	N	O	S	0	0
			597	368	104	114	11		

- Molecule 23 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	132	Total	C	N	O	S	1	0
			1056	681	186	186	3		

- Molecule 24 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	63	Total	C	N	O	0	0
			507	321	90	96		

- Molecule 25 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	162	Total	C	N	O	S	0	0
			1223	789	211	220	3		

- Molecule 26 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	i	33	Total	C	N	O	S	0	0
			256	176	40	38	2		

- Molecule 27 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	41	Total	C	N	O	S	0	0
			324	219	50	54	1		

- Molecule 28 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	l	144	Total	C	N	O	S	0	0
			1094	726	178	187	3		

- Molecule 29 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	m	28	Total	C	N	O	S	0	0
			198	130	32	34	2		

- Molecule 30 is a protein called PsaS.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	134	Total	C	N	O	0	0
			670	402	134	134		

- Molecule 31 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	89	Total	C	N	O	S	0	0
			676	440	110	120	6		

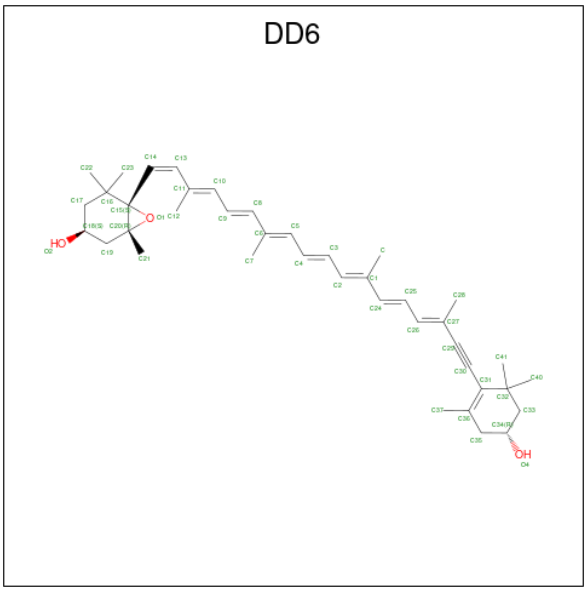
- Molecule 32 is a protein called FCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	156	Total	C	N	O	S	0	0
			1194	766	199	221	8		

- Molecule 33 is a protein called FCPI-19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	179	Total	C	N	O	S	0	0
			1361	871	234	252	4		

- Molecule 34 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: $C_{40}H_{54}O_3$).



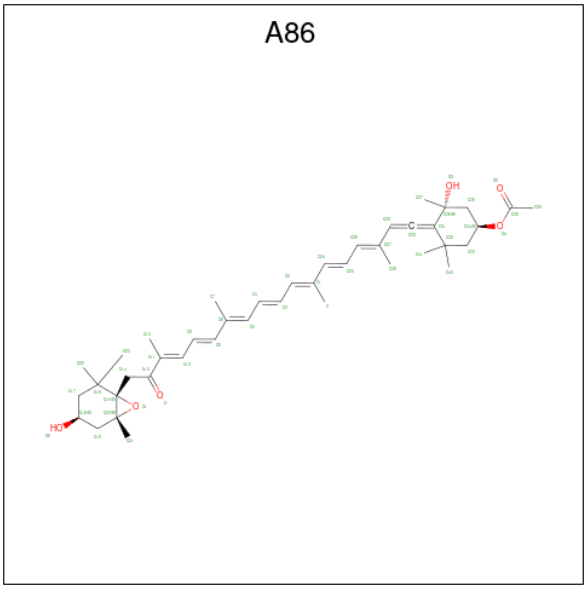
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	C	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
34	F	1	Total	C	O	0
			43	40	3	
34	G	1	Total	C	O	0
			43	40	3	
34	H	1	Total	C	O	0
			43	40	3	
34	H	1	Total	C	O	0
			43	40	3	
34	I	1	Total	C	O	0
			43	40	3	
34	J	1	Total	C	O	0
			43	40	3	
34	K	1	Total	C	O	0
			43	40	3	
34	K	1	Total	C	O	0
			43	40	3	
34	L	1	Total	C	O	0
			43	40	3	
34	M	1	Total	C	O	0
			43	40	3	
34	O	1	Total	C	O	0
			43	40	3	
34	P	1	Total	C	O	0
			43	40	3	
34	Q	1	Total	C	O	0
			43	40	3	
34	R	1	Total	C	O	0
			43	40	3	
34	R	1	Total	C	O	0
			43	40	3	
34	S	1	Total	C	O	0
			43	40	3	
34	S	1	Total	C	O	0
			43	40	3	
34	W	1	Total	C	O	0
			43	40	3	
34	W	1	Total	C	O	0
			43	40	3	
34	a	1	Total	C	O	0
			43	40	3	
34	j	1	Total	C	O	0
			43	40	3	

- Molecule 35 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C O 48 42 6	0
35	A	1	Total C O 48 42 6	0
35	B	1	Total C O 48 42 6	0
35	B	1	Total C O 48 42 6	0
35	C	1	Total C O 48 42 6	0
35	C	1	Total C O 48 42 6	0
35	C	1	Total C O 48 42 6	0
35	D	1	Total C O 48 42 6	0
35	E	1	Total C O 48 42 6	0
35	E	1	Total C O 48 42 6	0
35	E	1	Total C O 48 42 6	0
35	F	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
35	F	1	Total C O 48 42 6	0
35	F	1	Total C O 48 42 6	0
35	F	1	Total C O 48 42 6	0
35	F	1	Total C O 48 42 6	0
35	F	1	Total C O 48 42 6	0
35	G	1	Total C O 48 42 6	0
35	G	1	Total C O 48 42 6	0
35	G	1	Total C O 48 42 6	0
35	G	1	Total C O 48 42 6	0
35	H	1	Total C O 48 42 6	0
35	H	1	Total C O 48 42 6	0
35	I	1	Total C O 48 42 6	0
35	I	1	Total C O 48 42 6	0
35	I	1	Total C O 48 42 6	0
35	J	1	Total C O 48 42 6	0
35	J	1	Total C O 48 42 6	0
35	J	1	Total C O 48 42 6	0
35	J	1	Total C O 48 42 6	0
35	J	1	Total C O 48 42 6	0
35	K	1	Total C O 48 42 6	0
35	K	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms			AltConf
35	K	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	

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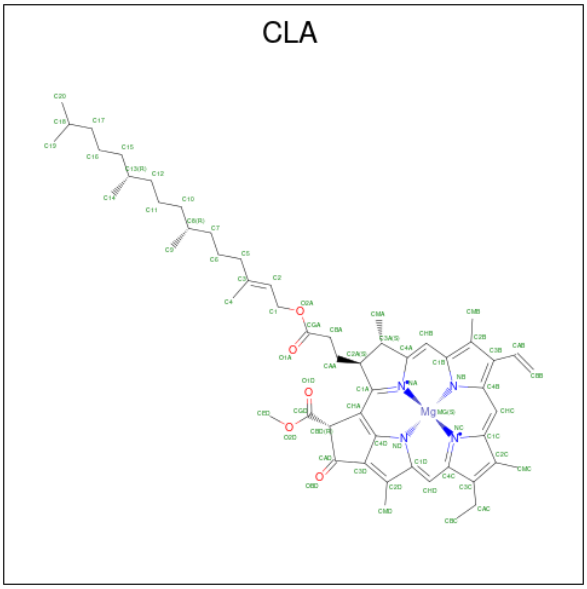
Mol	Chain	Residues	Atoms	AltConf
35	S	1	Total C O 48 42 6	0
35	S	1	Total C O 48 42 6	0
35	T	1	Total C O 48 42 6	0
35	T	1	Total C O 48 42 6	0
35	T	1	Total C O 48 42 6	0
35	T	1	Total C O 48 42 6	0
35	T	1	Total C O 48 42 6	0
35	T	1	Total C O 48 42 6	0
35	T	1	Total C O 48 42 6	0
35	W	1	Total C O 48 42 6	0
35	W	1	Total C O 48 42 6	0
35	X	1	Total C O 48 42 6	0
35	X	1	Total C O 48 42 6	0
35	X	1	Total C O 48 42 6	0
35	X	1	Total C O 48 42 6	0
35	X	1	Total C O 48 42 6	0
35	X	1	Total C O 48 42 6	0
35	h	1	Total C O 48 42 6	0
35	h	1	Total C O 48 42 6	0
35	U	1	Total C O 48 42 6	0
35	U	1	Total C O 48 42 6	0

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Mol	Chain	Residues	Atoms	AltConf
35	U	1	Total C O 48 42 6	0
35	U	1	Total C O 48 42 6	0
35	V	1	Total C O 48 42 6	0
35	V	1	Total C O 48 42 6	0
35	V	1	Total C O 48 42 6	0
35	V	1	Total C O 48 42 6	0

- Molecule 36 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total C Mg N O 49 39 1 4 5	0
36	A	1	Total C Mg N O 61 51 1 4 5	0
36	A	1	Total C Mg N O 60 50 1 4 5	0
36	A	1	Total C Mg N O 65 55 1 4 5	0
36	A	1	Total C Mg N O 46 36 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
36	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	D	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	D	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	F	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
36	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	F	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
36	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	I	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	I	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	J	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	J	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	L	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	L	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
36	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	M	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	M	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
36	N	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
36	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
36	O	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	O	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
36	O	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
36	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
36	P	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
36	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	Q	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	Q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	R	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			45	37	1	4	3	
36	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
36	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	S	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	T	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	W	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	W	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	W	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
36	X	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	X	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
36	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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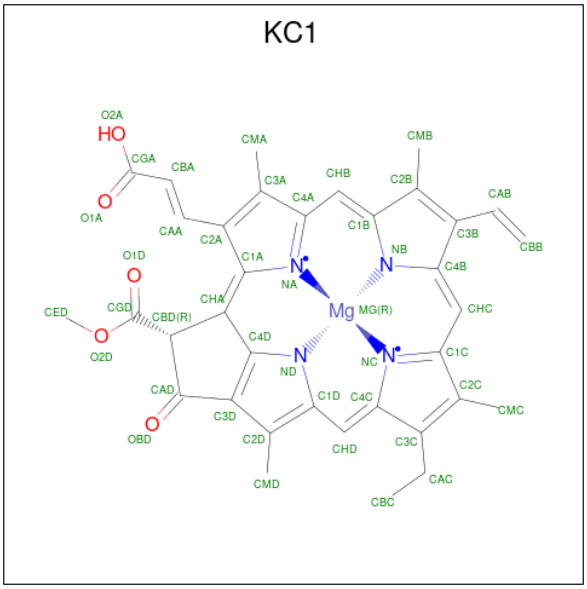
Mol	Chain	Residues	Atoms					AltConf
36	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
36	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	l	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
36	V	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 37 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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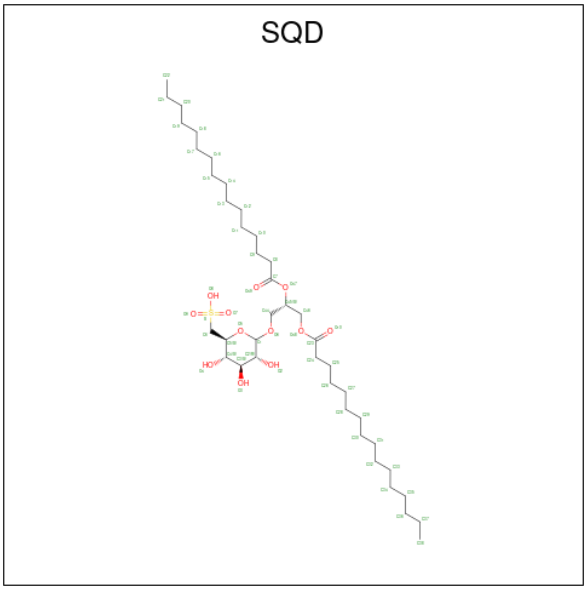
Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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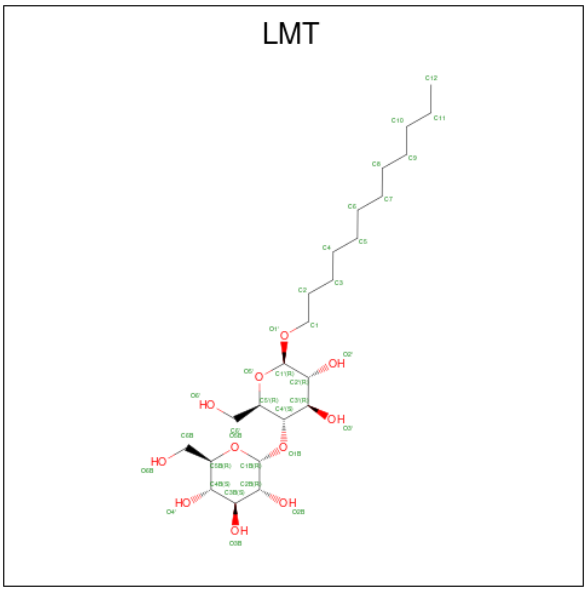
Mol	Chain	Residues	Atoms					AltConf
37	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	O	S	0
			28	15	12	1	
38	b	1	Total	C	O	S	0
			46	33	12	1	

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



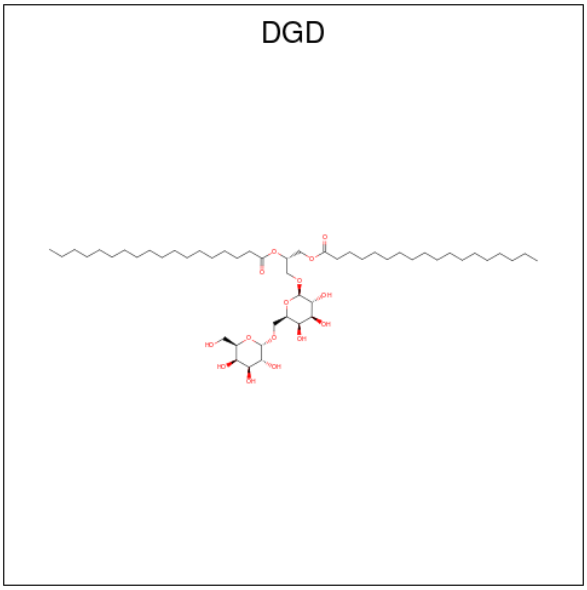
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			35	24	11	
39	B	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			23	17	6	
39	E	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			33	22	11	
39	G	1	Total	C	O	0
			35	24	11	
39	G	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	K	1	Total	C	O	0
			31	20	11	
39	K	1	Total	C	O	0
			35	24	11	
39	L	1	Total	C	O	0
			35	24	11	

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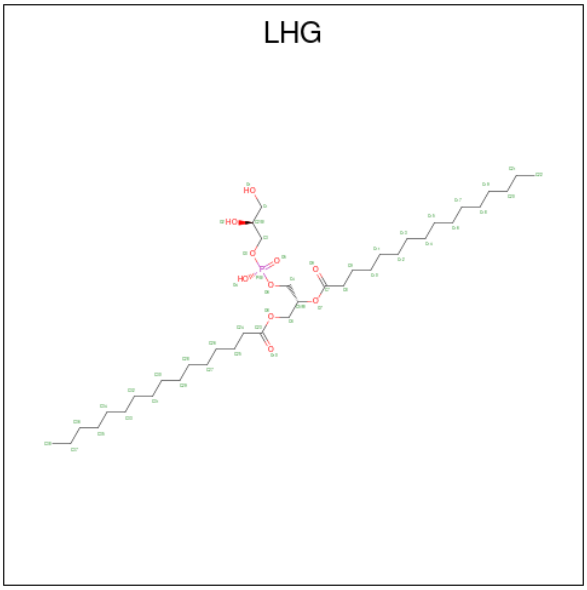
Mol	Chain	Residues	Atoms			AltConf
39	L	1	Total	C	O	0
			31	20	11	
39	P	1	Total	C	O	0
			23	17	6	
39	P	1	Total	C	O	0
			23	17	6	
39	a	1	Total	C	O	0
			35	24	11	
39	a	1	Total	C	O	0
			32	21	11	
39	a	1	Total	C	O	0
			35	24	11	
39	b	1	Total	C	O	0
			35	24	11	
39	b	1	Total	C	O	0
			24	19	5	
39	f	1	Total	C	O	0
			24	18	6	
39	h	1	Total	C	O	0
			35	24	11	
39	U	1	Total	C	O	0
			35	24	11	
39	U	1	Total	C	O	0
			35	24	11	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total 57	C 42	O 15	0
40	L	1	Total 47	C 32	O 15	0
40	b	1	Total 60	C 45	O 15	0

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



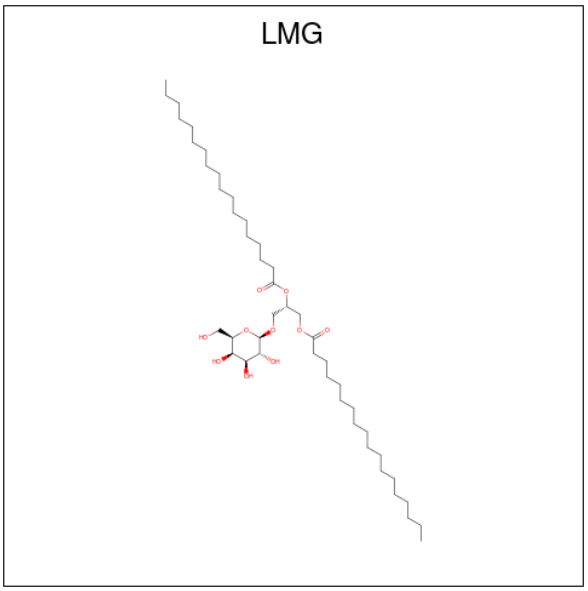
Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total 46	C 35	O 10	P 1	0
41	D	1	Total 49	C 38	O 10	P 1	0
41	E	1	Total 49	C 38	O 10	P 1	0
41	F	1	Total 33	C 24	O 8	P 1	0
41	F	1	Total 41	C 30	O 10	P 1	0
41	G	1	Total 49	C 38	O 10	P 1	0
41	G	1	Total 40	C 29	O 10	P 1	0
41	G	1	Total 47	C 36	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
41	I	1	Total	C	O	P	0
			49	38	10	1	
41	O	1	Total	C	O	P	0
			42	31	10	1	
41	O	1	Total	C	O	P	0
			49	38	10	1	
41	Q	1	Total	C	O	P	0
			49	38	10	1	
41	R	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			48	37	10	1	
41	a	1	Total	C	O	P	0
			27	16	10	1	
41	a	1	Total	C	O	P	0
			47	36	10	1	
41	b	1	Total	C	O	P	0
			49	38	10	1	
41	f	1	Total	C	O	P	0
			49	38	10	1	
41	f	1	Total	C	O	P	0
			42	31	10	1	
41	i	1	Total	C	O	P	0
			46	35	10	1	
41	j	1	Total	C	O	P	0
			49	38	10	1	
41	l	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



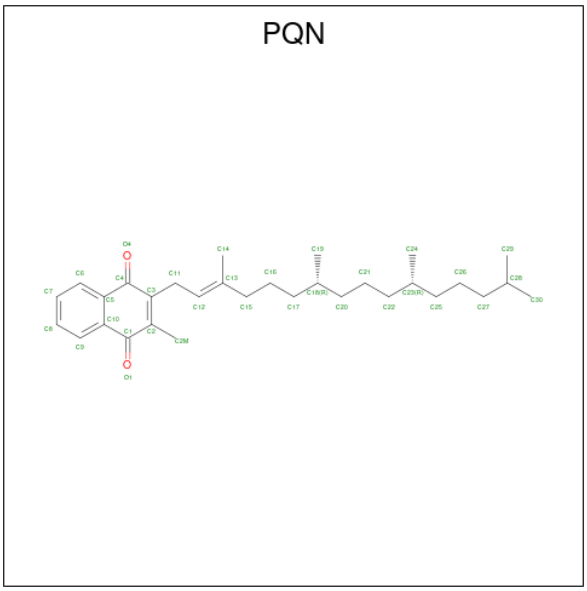
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			46	36	10	
42	D	1	Total	C	O	0
			37	27	10	
42	E	1	Total	C	O	0
			46	36	10	
42	E	1	Total	C	O	0
			40	30	10	
42	G	1	Total	C	O	0
			55	45	10	
42	G	1	Total	C	O	0
			55	45	10	
42	I	1	Total	C	O	0
			55	45	10	
42	J	1	Total	C	O	0
			55	45	10	
42	J	1	Total	C	O	0
			44	34	10	
42	L	1	Total	C	O	0
			33	23	10	
42	a	1	Total	C	O	0
			54	44	10	
42	j	1	Total	C	O	0
			52	42	10	
42	m	1	Total	C	O	0
			37	27	10	
42	h	1	Total	C	O	0
			45	35	10	

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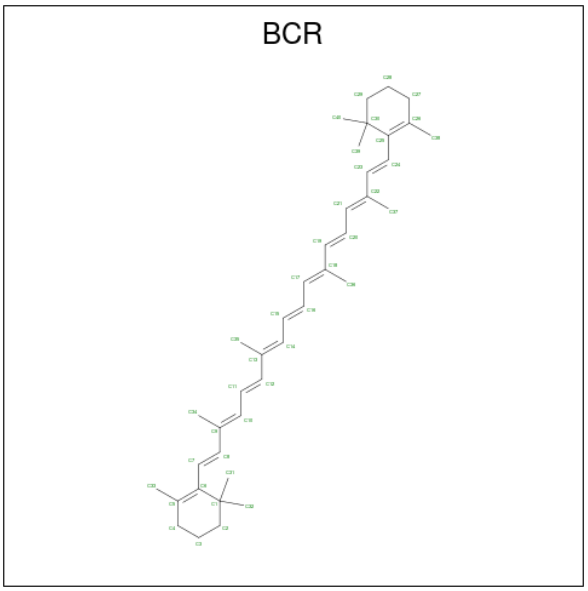
Mol	Chain	Residues	Atoms	AltConf
42	V	1	Total C O 46 36 10	0
42	V	1	Total C O 46 36 10	0

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 44 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



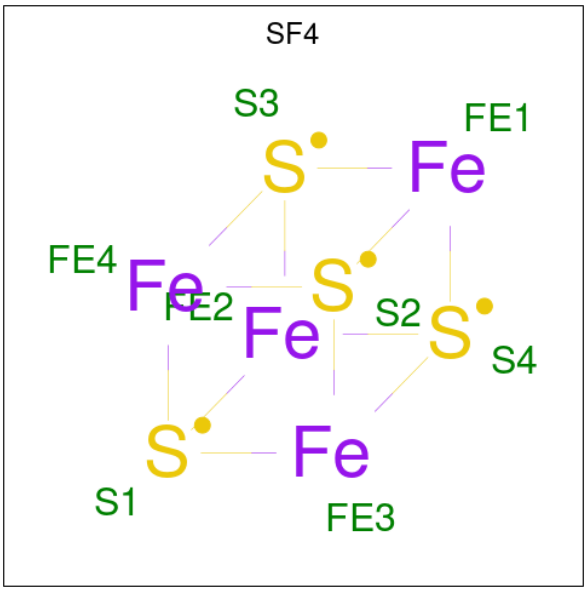
Mol	Chain	Residues	Atoms	AltConf
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	i	1	Total C 40 40	0
44	i	1	Total C 40 40	0
44	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
44	l	1	Total C 40 40	0
44	l	1	Total C 40 40	0
44	m	1	Total C 40 40	0
44	h	1	Total C 40 40	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
45	b	1	Total Fe S 8 4 4	0
45	c	1	Total Fe S 8 4 4	0
45	c	1	Total Fe S 8 4 4	0

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	AltConf
46	a	64	Total O 64 64	0
46	b	72	Total O 72 72	0

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Mol	Chain	Residues	Atoms	AltConf
46	c	7	Total O 7 7	0
46	d	4	Total O 4 4	0
46	f	2	Total O 2 2	0
46	j	1	Total O 1 1	0
46	l	3	Total O 3 3	0

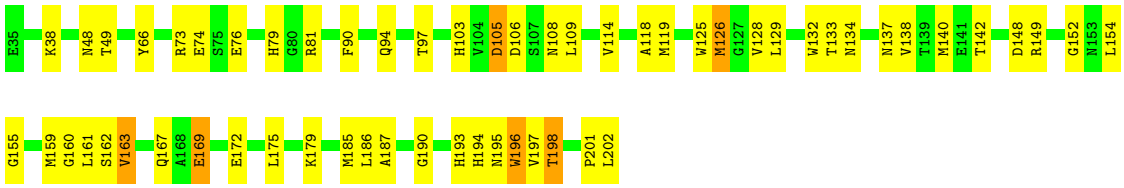
3 Residue-property plots (i)

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

• Molecule 1: FCPI-7

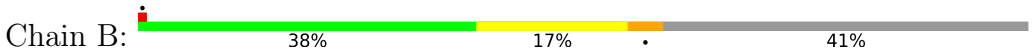
Chain A:

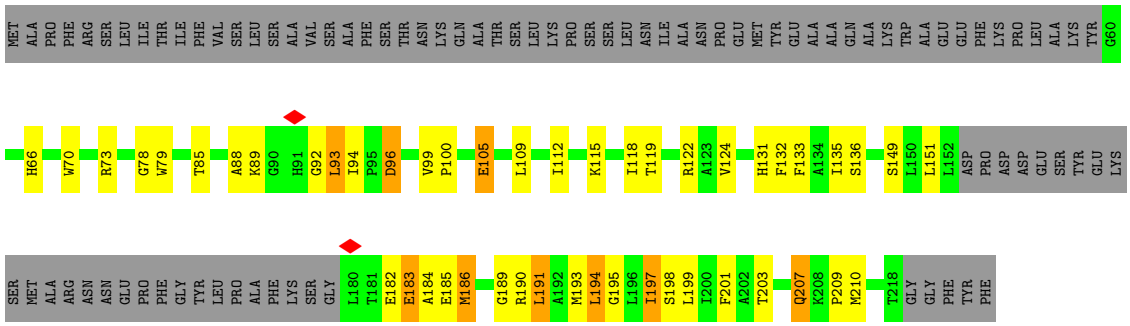




• Molecule 2: FCPI-1

Chain B:

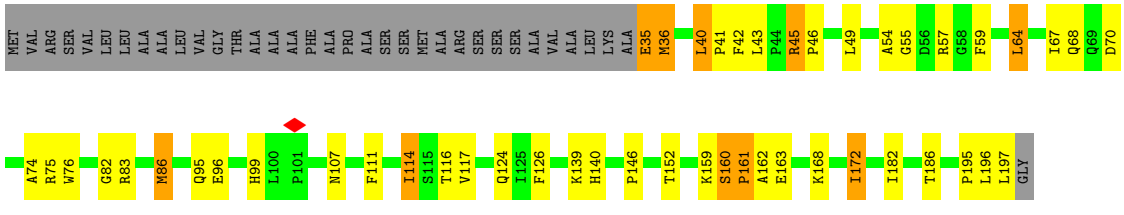




• Molecule 3: FCPI-11

Chain C:

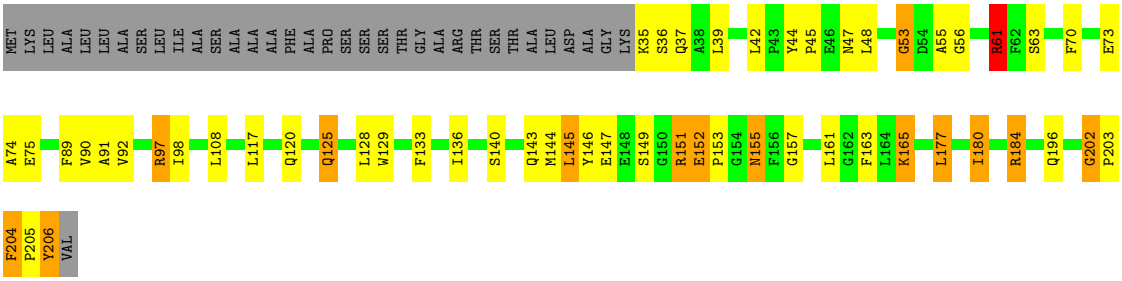




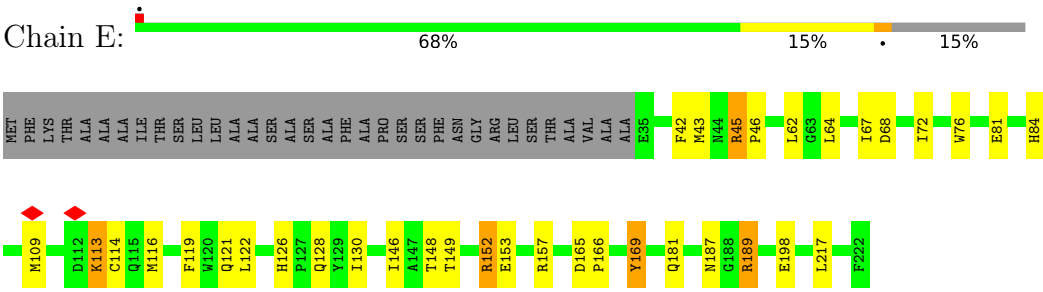
• Molecule 4: FCPI-6

Chain D:

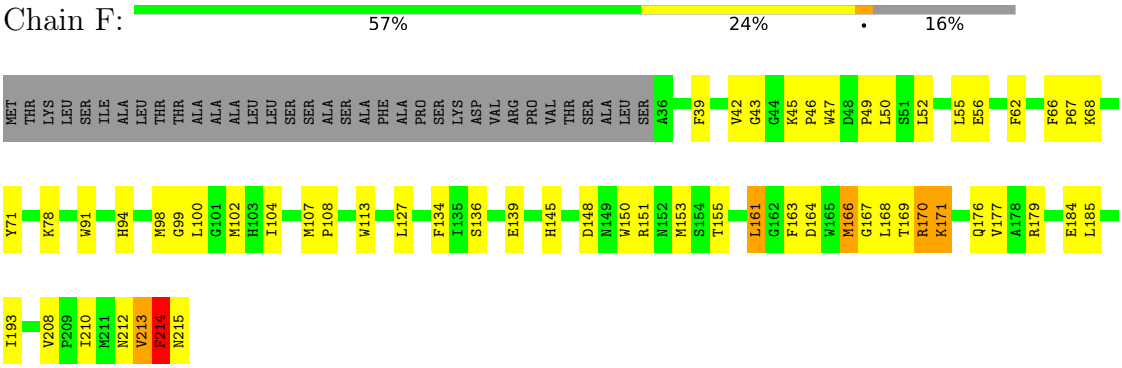




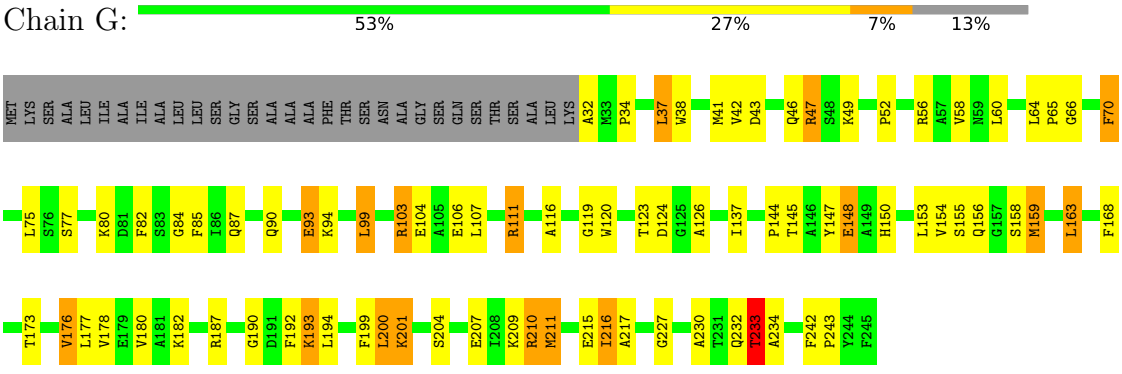
• Molecule 5: FCPI-5



• Molecule 6: FCPI-8

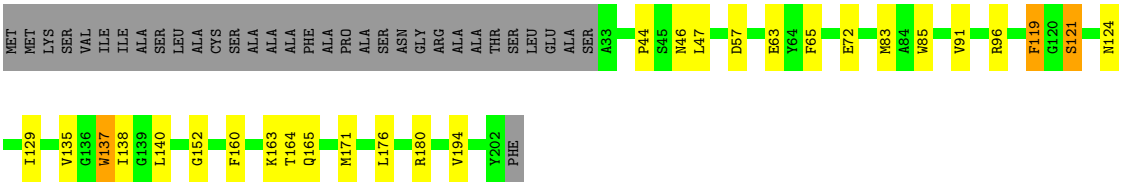


• Molecule 7: FCPI-4



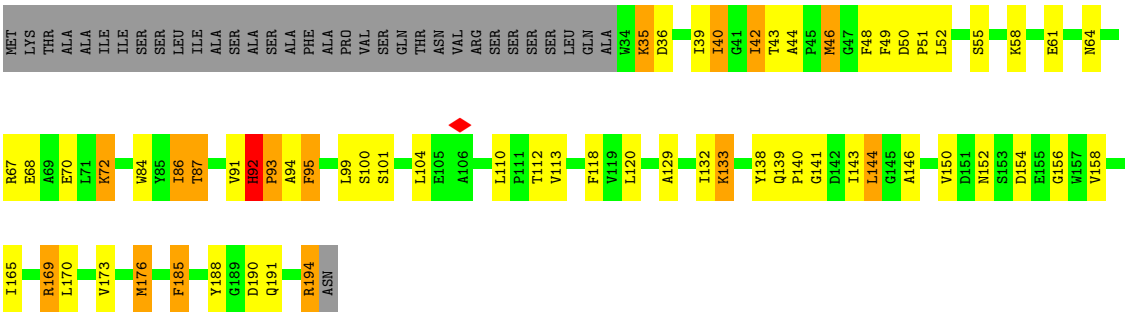
• Molecule 8: FCPI-10





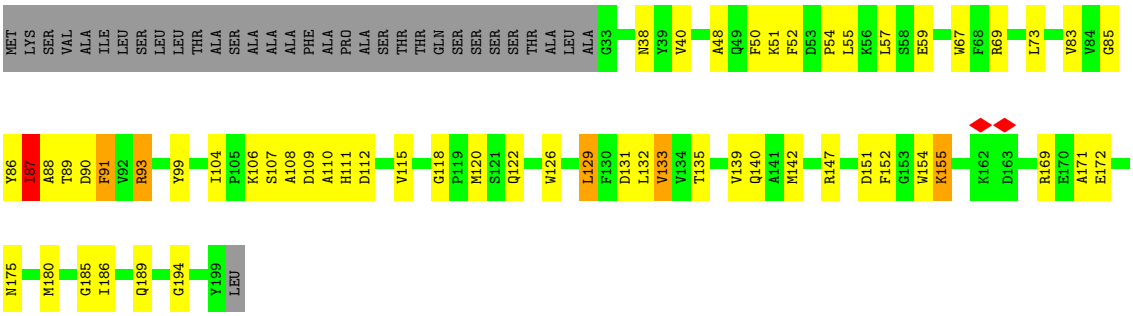
• Molecule 9: FCPI-3





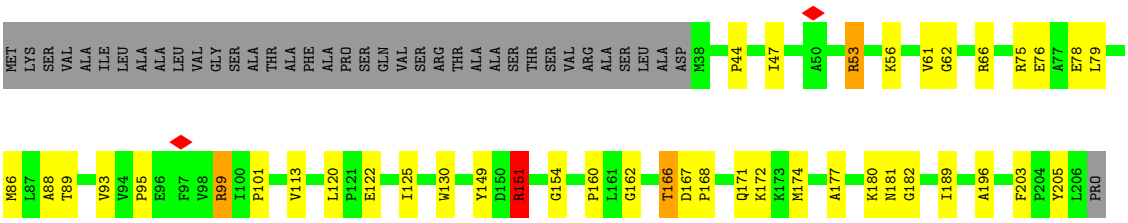
• Molecule 10: FCPI-9





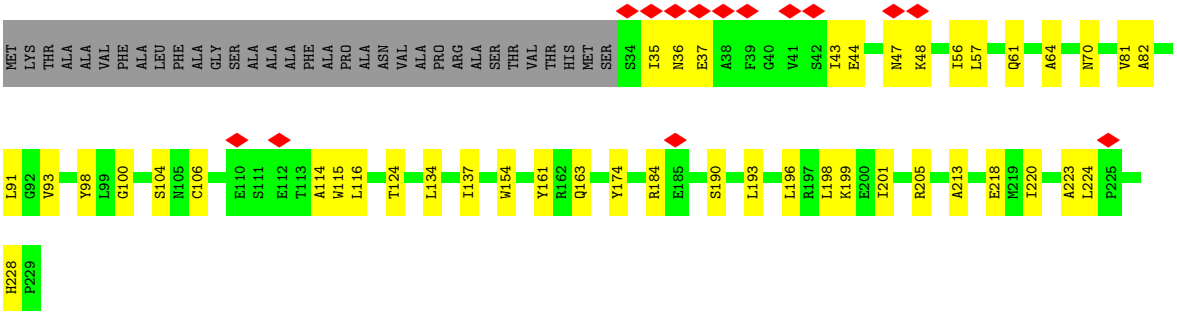
• Molecule 11: FCPI-13

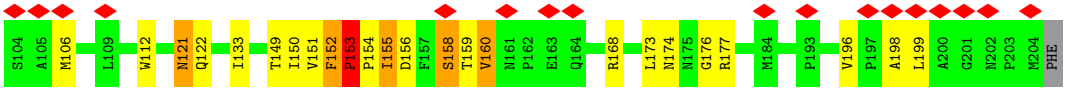




• Molecule 12: FCPI-14



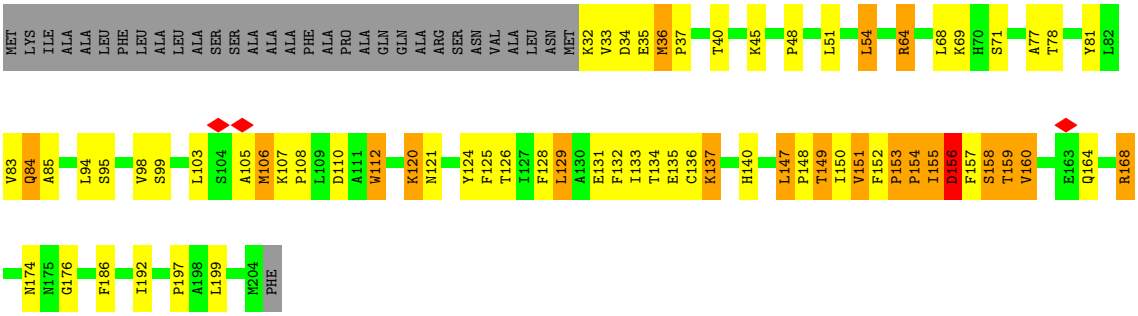




• Molecule 15: FCPI

Chain P:

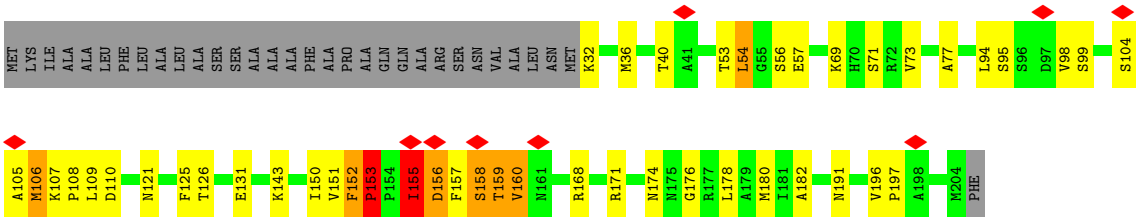




• Molecule 15: FCPI

Chain Q:

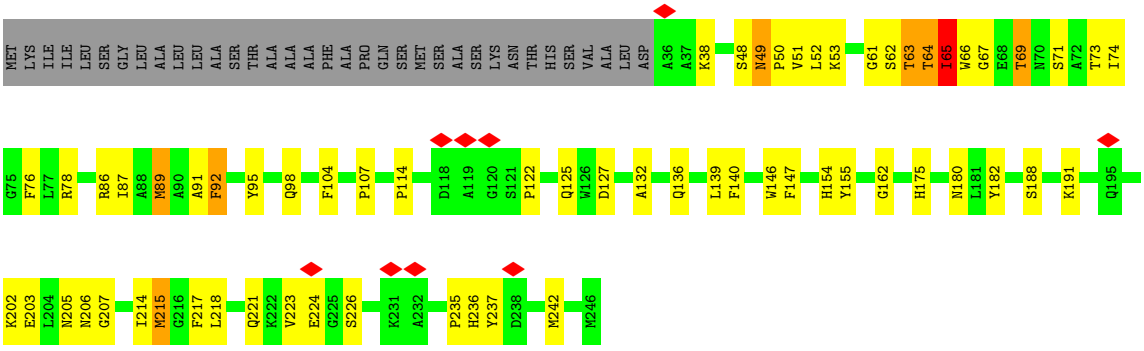




• Molecule 16: FCPI-24

Chain R:

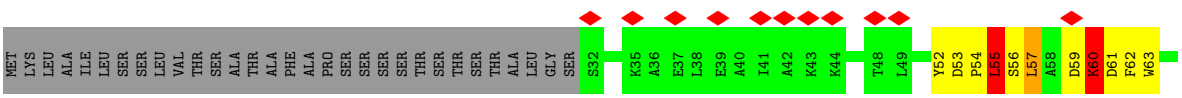


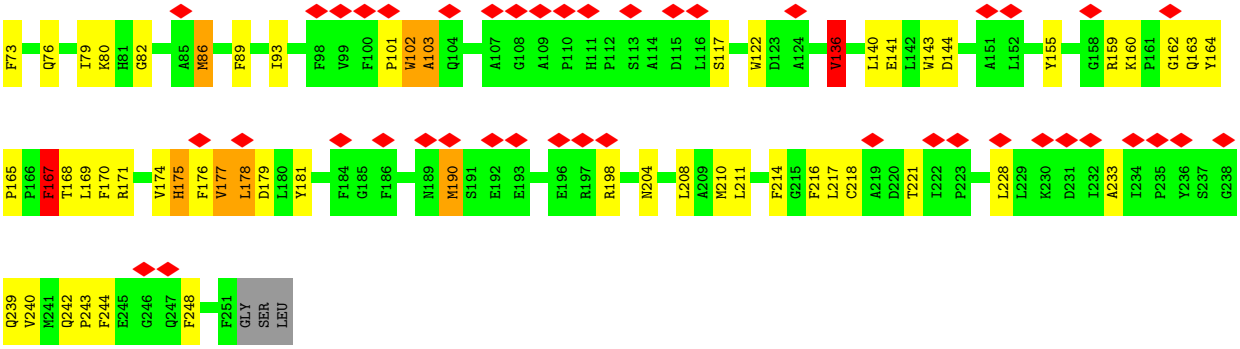


• Molecule 17: FCPI-23

Chain S:

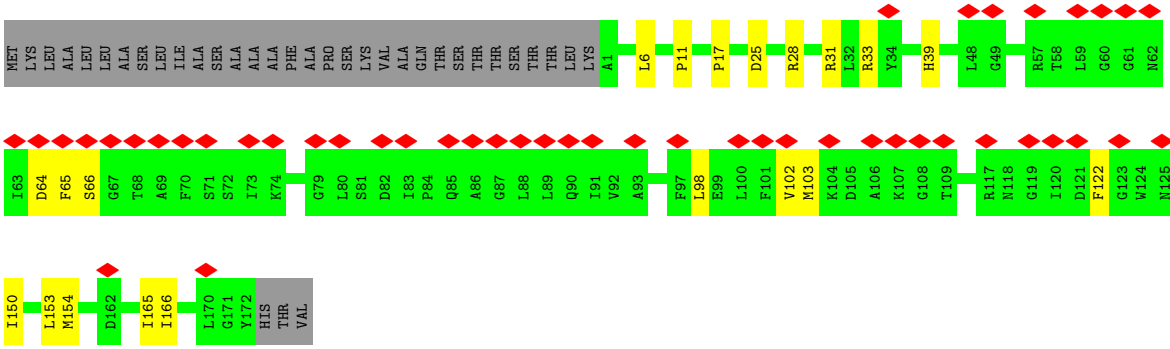






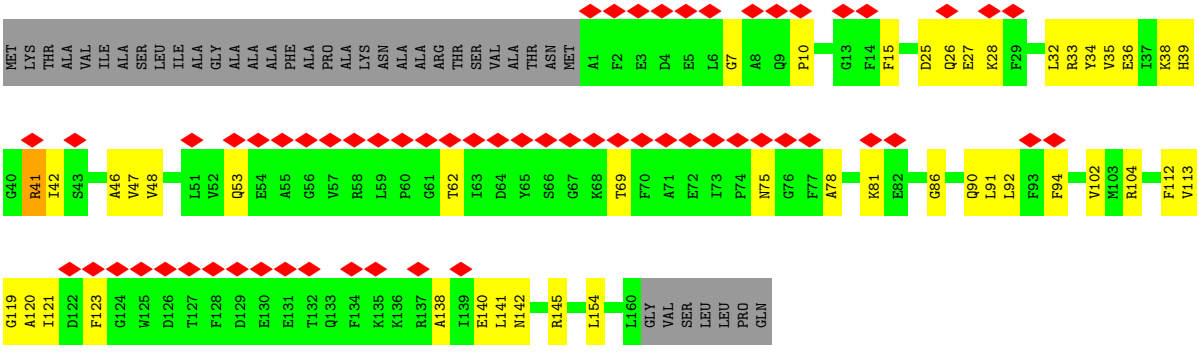
• Molecule 18: FCPI-12



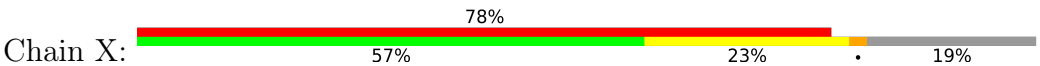


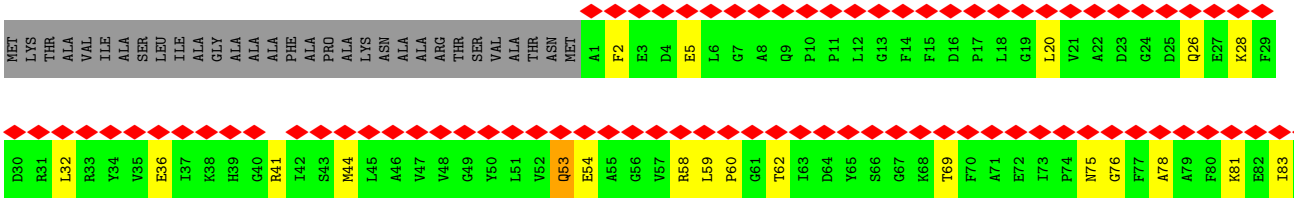
• Molecule 19: FCPI-17

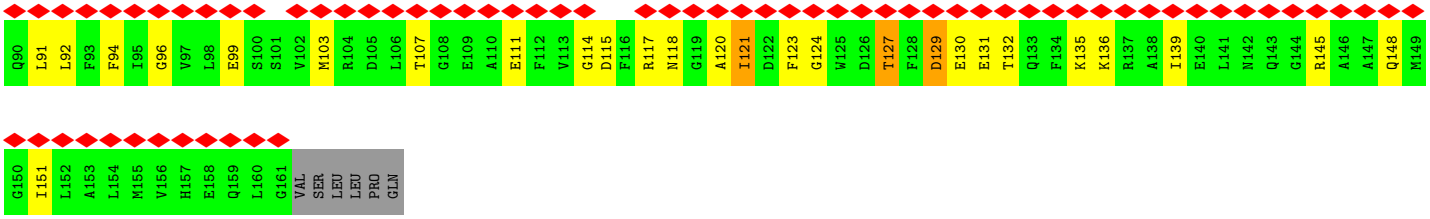




• Molecule 19: FCPI-17



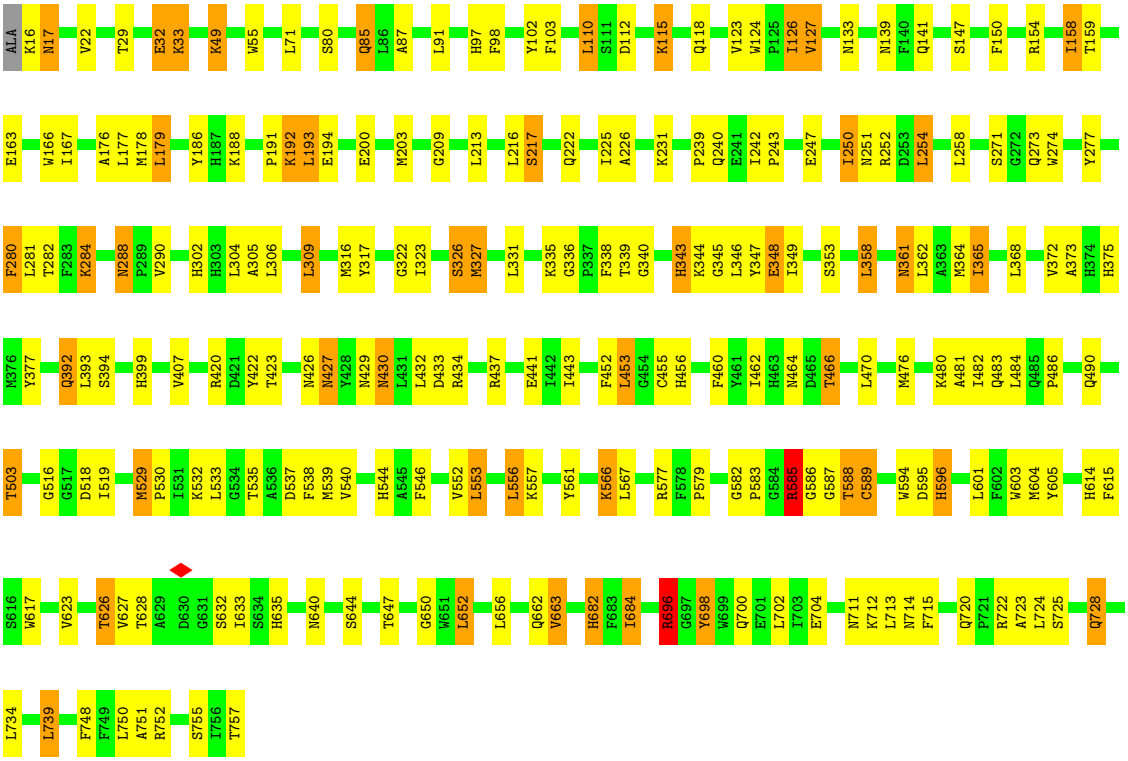




• Molecule 20: PsaA

Chain a:

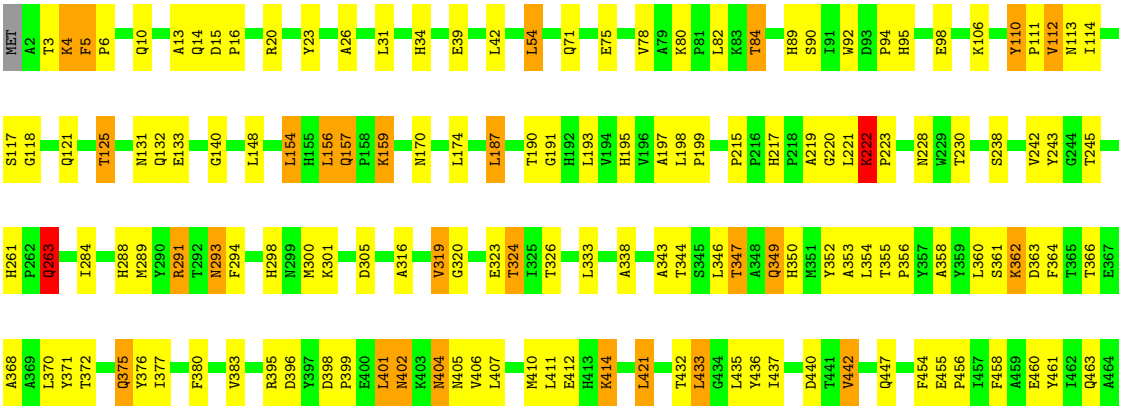


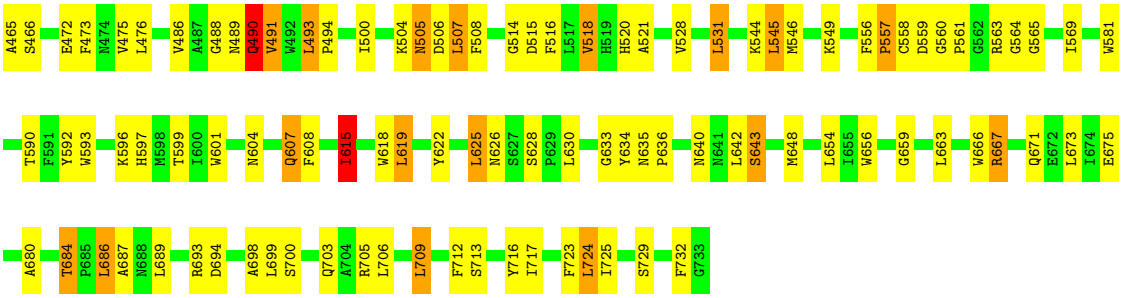


• Molecule 21: PsaB

Chain b:



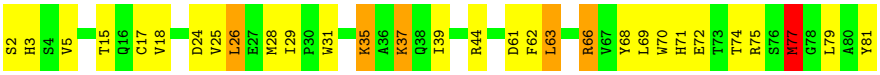




• Molecule 22: PsaC

Chain c:

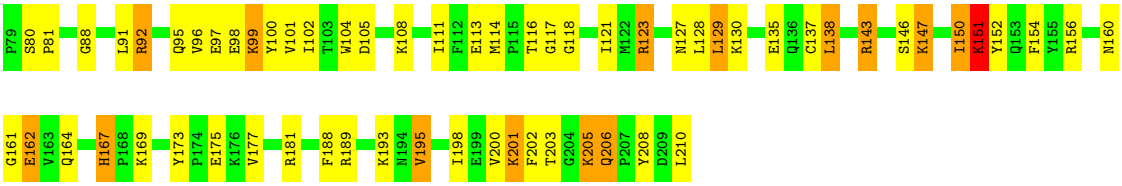




• Molecule 23: PsaD

Chain d:

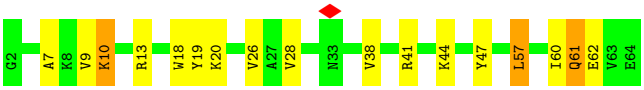




• Molecule 24: PsaE

Chain e:

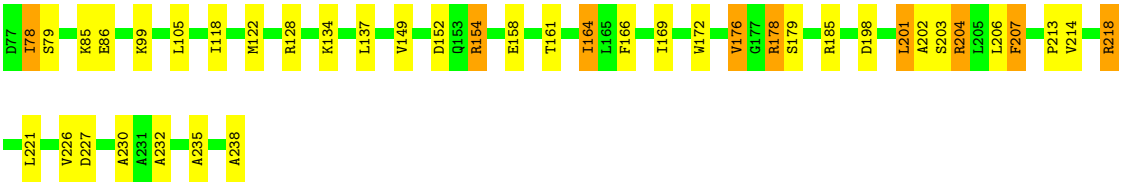




• Molecule 25: PsaF

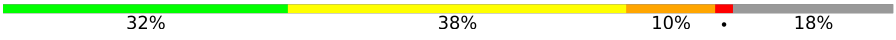
Chain f:

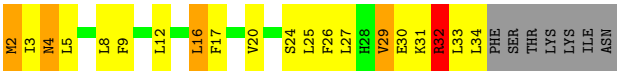




• Molecule 26: PsaI

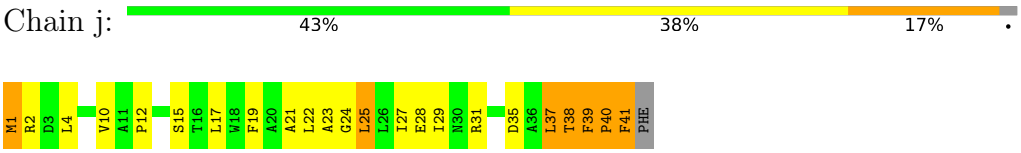
Chain i:





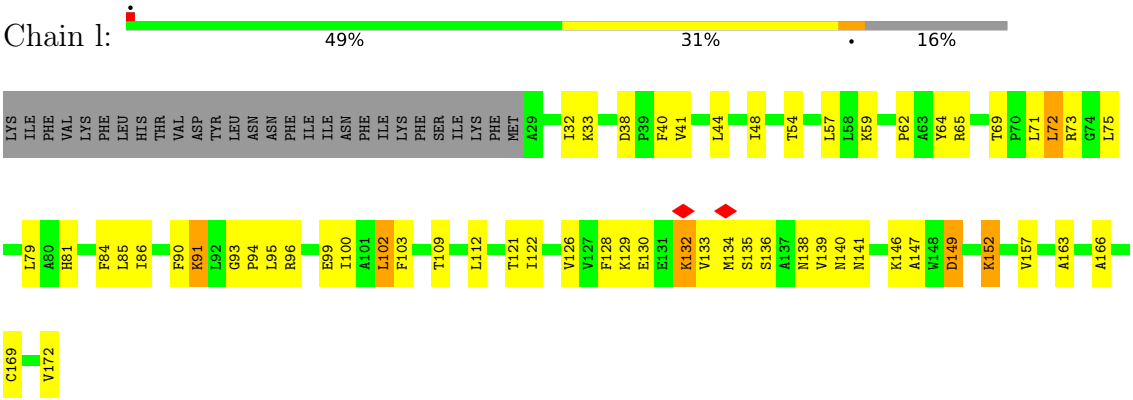
• Molecule 27: PsaJ

Chain j:



• Molecule 28: PsaL

Chain l:



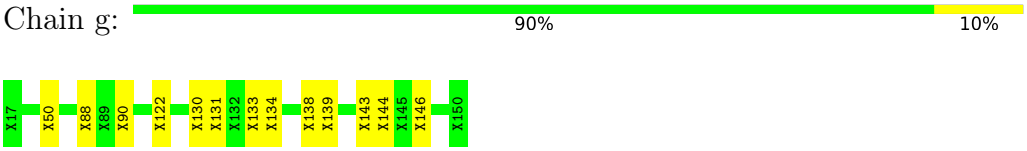
• Molecule 29: PsaM

Chain m:



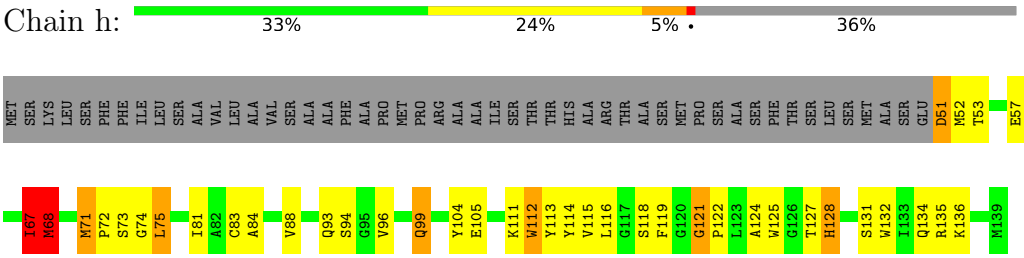
• Molecule 30: PsaS

Chain g:



• Molecule 31: PsaR

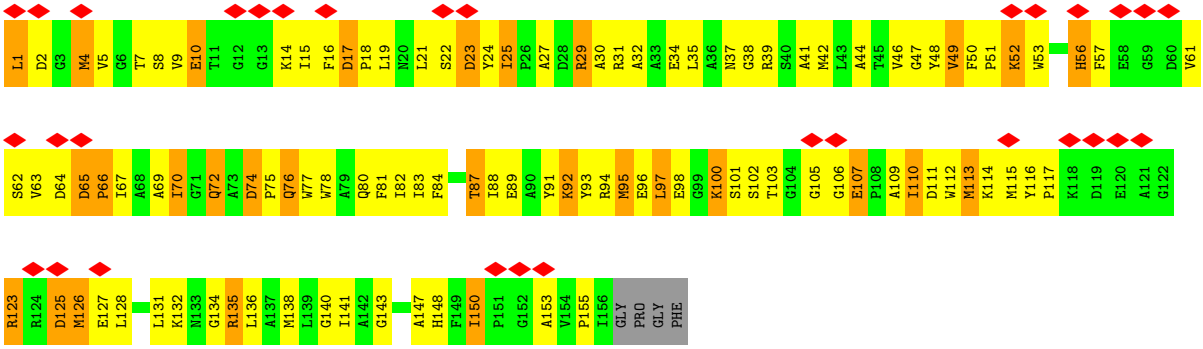
Chain h:



• Molecule 32: FCPI-2

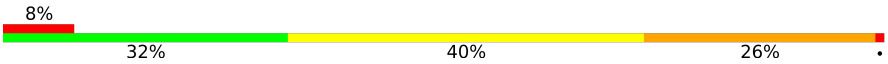
Chain U:



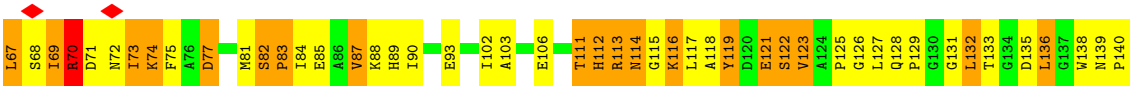


• Molecule 33: FCPI-19

Chain V:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	164480	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	567.32, 567.32, 567.32	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: SQD, DD6, DGD, LMT, KC1, BCR, SF4, PQN, LMG, A86, LHG, CLA

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	0.50	0/1319	0.80	0/1786
2	B	0.87	2/1039 (0.2%)	1.16	11/1412 (0.8%)
3	C	0.41	0/1275	0.77	3/1726 (0.2%)
4	D	0.49	0/1373	0.84	5/1860 (0.3%)
5	E	0.48	0/1439	0.70	1/1944 (0.1%)
6	F	0.43	0/1411	0.84	5/1908 (0.3%)
7	G	0.45	0/1714	0.79	2/2321 (0.1%)
8	H	0.48	0/1326	0.80	1/1798 (0.1%)
9	I	0.44	0/1285	1.00	6/1746 (0.3%)
10	J	0.50	1/1339 (0.1%)	0.94	4/1811 (0.2%)
11	K	0.49	0/1346	0.84	4/1826 (0.2%)
12	L	0.45	0/1571	0.71	0/2141
13	M	0.40	0/1464	0.74	3/1982 (0.2%)
14	N	0.48	0/1770	1.01	7/2405 (0.3%)
15	O	0.47	0/1335	0.92	7/1817 (0.4%)
15	P	0.47	1/1329 (0.1%)	1.31	11/1810 (0.6%)
15	Q	0.48	0/1335	0.92	8/1817 (0.4%)
16	R	0.35	0/1680	0.72	1/2282 (0.0%)
17	S	0.40	0/1776	0.89	3/2413 (0.1%)
18	T	0.34	0/1353	0.62	0/1823
19	W	0.48	1/1265 (0.1%)	0.85	3/1707 (0.2%)
19	X	0.50	2/1282 (0.2%)	0.93	7/1729 (0.4%)
20	a	0.47	0/6053	0.80	19/8238 (0.2%)
21	b	0.48	2/6031 (0.0%)	0.85	20/8231 (0.2%)
22	c	0.45	0/607	0.82	2/822 (0.2%)
23	d	4.08	2/1086 (0.2%)	1.45	9/1461 (0.6%)
24	e	0.40	0/517	0.58	0/701
25	f	0.47	0/1248	0.75	2/1687 (0.1%)
26	i	0.60	0/262	1.24	2/356 (0.6%)
27	j	0.57	0/333	0.82	1/455 (0.2%)
28	l	0.48	0/1121	0.83	2/1520 (0.1%)
29	m	0.57	0/198	0.82	0/269

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	h	0.49	0/698	1.08	10/951 (1.1%)
32	U	0.59	0/1225	2.00	10/1657 (0.6%)
33	V	0.38	0/1393	0.88	5/1894 (0.3%)
All	All	0.76	11/51798 (0.0%)	0.92	174/70306 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	2
14	N	0	7
15	O	0	1
15	P	0	1
15	Q	0	1
17	S	0	2
19	W	0	3
23	d	0	5
30	g	0	1
33	V	0	1
All	All	0	25

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	151[A]	LYS	CA-C	94.74	2.66	1.52
23	d	151[B]	LYS	CA-C	94.74	2.66	1.52
2	B	186	MET	C-N	22.66	1.54	1.33
15	P	156	ASP	C-N	9.60	1.48	1.33
2	B	183	GLU	C-N	-8.62	1.21	1.33
10	J	91	PHE	C-N	-7.53	1.23	1.33
21	b	263[A]	GLN	CA-C	6.41	1.61	1.52
21	b	263[B]	GLN	CA-C	6.41	1.61	1.52
19	X	53	GLN	CD-OE1	5.61	1.34	1.23
19	X	94	PHE	CE2-CZ	5.45	1.55	1.38
19	W	41	ARG	CG-CD	-5.25	1.36	1.52

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	U	65	ASP	CA-C-N	48.07	179.93	119.84
32	U	65	ASP	C-N-CA	48.07	179.93	119.84
23	d	151[A]	LYS	CB-CA-C	-26.47	64.81	109.80
23	d	151[B]	LYS	CB-CA-C	-26.47	64.81	109.80
15	P	156	ASP	O-C-N	-23.88	90.36	123.07
15	P	156	ASP	CA-C-N	19.26	152.33	122.29
15	P	156	ASP	C-N-CA	19.26	152.33	122.29
2	B	183	GLU	O-C-N	16.89	145.06	122.59
9	I	94	ALA	N-CA-C	14.61	127.20	111.28
9	I	93	PRO	N-CA-C	13.91	132.87	113.53
21	b	667	ARG	N-CA-C	13.86	125.89	111.07
23	d	151[A]	LYS	N-CA-C	13.79	133.30	108.48
23	d	151[B]	LYS	N-CA-C	13.79	133.30	108.48
15	P	159	THR	N-CA-C	12.13	124.50	111.28
32	U	65	ASP	C-N-CD	-11.77	76.74	125.00
15	P	85	ALA	N-CA-C	-11.64	98.79	113.23
2	B	183	GLU	CA-C-N	-11.35	101.39	120.68
2	B	183	GLU	C-N-CA	-11.35	101.39	120.68
19	X	53	GLN	CB-CG-CD	11.27	131.75	112.60
23	d	151[A]	LYS	CA-C-O	11.02	135.20	120.11
23	d	151[B]	LYS	CA-C-O	11.02	135.20	120.11
26	i	32	ARG	N-CA-C	11.00	123.27	111.28
15	O	153	PRO	CB-CA-C	10.79	124.09	110.92
11	K	166	THR	N-CA-C	10.66	122.98	111.36
20	a	696	ARG	N-CA-C	10.61	124.17	111.33
21	b	491	VAL	N-CA-C	10.59	120.48	110.53
2	B	186	MET	O-C-N	-10.53	110.20	122.20
15	P	151	VAL	N-CA-C	10.27	121.09	110.72
19	X	53	GLN	CA-CB-CG	-9.87	94.36	114.10
15	Q	153	PRO	N-CA-C	9.85	122.72	110.70
13	M	73	THR	N-CA-C	9.29	121.41	111.28
21	b	263[A]	GLN	CA-C-O	9.07	131.07	120.00
21	b	263[B]	GLN	CA-C-O	9.07	131.07	120.00
10	J	88	ALA	N-CA-C	-8.67	101.70	112.88
19	X	53	GLN	CG-CD-NE2	-8.45	103.73	116.40
2	B	94	ILE	CA-C-N	-8.42	109.31	119.84
2	B	94	ILE	C-N-CA	-8.42	109.31	119.84
6	F	170	ARG	N-CA-C	-8.40	102.80	113.72
8	H	137	TRP	CA-CB-CG	8.37	129.50	113.60
9	I	92	HIS	CA-C-N	8.07	128.01	119.05
9	I	92	HIS	C-N-CA	8.07	128.01	119.05
9	I	156	GLY	N-CA-C	-8.00	103.13	112.73
23	d	118	GLY	N-CA-C	7.80	122.09	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	160	VAL	N-CA-C	7.79	120.84	109.63
31	h	71	MET	CA-C-N	7.54	127.46	119.85
31	h	71	MET	C-N-CA	7.54	127.46	119.85
9	I	154	ASP	N-CA-C	-7.40	96.67	108.73
15	Q	159	THR	CA-C-N	7.33	130.65	122.59
15	Q	159	THR	C-N-CA	7.33	130.65	122.59
15	O	159	THR	CA-C-N	7.30	130.62	122.59
15	O	159	THR	C-N-CA	7.30	130.62	122.59
15	P	105	ALA	N-CA-C	7.28	122.03	112.72
15	Q	105	ALA	N-CA-C	7.25	122.00	112.72
26	i	3	ILE	N-CA-C	-7.25	103.21	113.07
21	b	687	ALA	N-CA-C	-7.19	104.12	114.12
23	d	173	TYR	CA-C-N	7.19	126.89	119.56
23	d	173	TYR	C-N-CA	7.19	126.89	119.56
19	X	94	PHE	CD1-CE1-CZ	7.16	132.89	120.00
7	G	200	LEU	N-CA-C	7.15	121.31	112.59
14	N	177	VAL	N-CA-C	7.11	118.71	107.98
2	B	197	ILE	CA-CB-CG1	-7.09	98.35	110.40
10	J	91	PHE	CA-C-N	-6.99	111.04	122.57
10	J	91	PHE	C-N-CA	-6.99	111.04	122.57
21	b	263[A]	GLN	N-CA-C	6.98	122.16	112.45
21	b	263[B]	GLN	N-CA-C	6.98	122.16	112.45
6	F	213	VAL	N-CA-C	6.96	117.75	110.72
32	U	17	ASP	CA-C-N	6.95	127.10	119.87
32	U	17	ASP	C-N-CA	6.95	127.10	119.87
15	O	153	PRO	CA-N-CD	-6.95	102.28	112.00
32	U	107	GLU	CA-C-N	-6.92	112.52	119.99
32	U	107	GLU	C-N-CA	-6.92	112.52	119.99
6	F	214	PHE	N-CA-C	6.88	118.78	111.28
33	V	61	ILE	N-CA-C	6.86	121.66	113.22
20	a	427	ASN	N-CA-C	6.82	118.89	109.54
21	b	615	ILE	N-CA-C	6.72	117.51	110.72
6	F	212	ASN	N-CA-C	-6.69	103.91	111.07
14	N	185	GLY	N-CA-C	6.60	119.09	111.36
19	W	117	ARG	CB-CG-CD	6.59	126.47	111.30
19	X	53	GLN	CG-CD-OE1	6.57	133.94	120.80
25	f	198	ASP	CA-C-N	6.51	124.34	120.24
25	f	198	ASP	C-N-CA	6.51	124.34	120.24
21	b	490	GLN	N-CA-C	6.48	118.14	111.14
20	a	420	ARG	N-CA-C	6.43	121.30	112.04
33	V	172	ALA	N-CA-C	6.42	118.35	111.36
4	D	61	ARG	N-CA-C	6.41	120.40	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	153	PRO	N-CA-CB	-6.34	96.93	103.08
32	U	66	PRO	CA-N-CD	-6.29	103.19	112.00
20	a	49	LYS	N-CA-C	-6.26	106.28	114.04
14	N	182	ASP	CA-C-N	6.26	127.66	119.84
14	N	182	ASP	C-N-CA	6.26	127.66	119.84
19	X	94	PHE	CE1-CZ-CE2	-6.24	108.77	120.00
20	a	546	PHE	N-CA-C	6.14	118.76	111.33
32	U	65	ASP	N-CA-C	-6.11	101.09	110.32
6	F	62	PHE	N-CA-C	-6.06	97.45	108.85
31	h	121	GLY	CA-C-N	6.01	125.72	119.05
31	h	121	GLY	C-N-CA	6.01	125.72	119.05
2	B	186	MET	CA-C-N	5.99	129.42	122.35
2	B	186	MET	C-N-CA	5.99	129.42	122.35
21	b	261	HIS	N-CA-C	-5.99	102.23	109.83
5	E	169	TYR	N-CA-C	-5.97	100.55	109.15
17	S	190	MET	CB-CG-SD	5.85	130.24	112.70
20	a	566	LYS	N-CA-C	-5.82	105.07	111.82
20	a	585	ARG	N-CA-C	-5.81	103.89	111.74
4	D	53	GLY	N-CA-C	-5.78	100.89	110.95
11	K	151	ARG	N-CA-C	5.77	119.32	110.20
28	l	69	THR	CA-C-N	-5.76	113.68	119.56
28	l	69	THR	C-N-CA	-5.76	113.68	119.56
15	Q	152	PHE	CA-C-N	5.75	126.30	120.38
15	Q	152	PHE	C-N-CA	5.75	126.30	120.38
15	Q	158	SER	CB-CA-C	5.70	121.77	110.42
15	O	158	SER	CB-CA-C	5.70	121.75	110.42
16	R	89	MET	N-CA-C	-5.68	105.17	111.36
31	h	68	MET	N-CA-C	5.68	117.55	111.36
15	P	158	SER	N-CA-C	5.68	117.47	111.28
19	W	41	ARG	CB-CG-CD	-5.66	98.29	111.30
21	b	31	LEU	N-CA-C	5.66	118.22	111.71
22	c	63	LEU	N-CA-C	5.63	117.56	110.24
21	b	112	VAL	N-CA-C	5.63	115.65	107.88
21	b	110	TYR	CA-C-N	5.63	125.56	119.76
21	b	110	TYR	C-N-CA	5.63	125.56	119.76
33	V	67	LEU	N-CA-C	5.62	117.40	111.28
3	C	86	MET	N-CA-C	-5.61	105.08	111.14
31	h	58	TYR	CA-C-N	5.57	126.11	120.38
31	h	58	TYR	C-N-CA	5.57	126.11	120.38
14	N	183	PRO	N-CA-C	-5.55	101.03	112.47
20	a	326	SER	N-CA-C	-5.53	100.69	109.76
13	M	154	GLN	CA-CB-CG	-5.53	103.04	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	127	VAL	CG1-CB-CG2	-5.53	98.63	110.80
31	h	71	MET	N-CA-C	5.51	116.83	109.83
20	a	32	GLU	N-CA-C	5.51	116.97	111.07
20	a	596	HIS	N-CA-C	-5.50	104.93	111.69
4	D	37	GLN	CA-CB-CG	5.49	125.08	114.10
20	a	698	TYR	N-CA-C	-5.49	105.71	112.90
14	N	178	LEU	N-CA-C	-5.49	99.47	109.56
20	a	682	HIS	N-CA-C	-5.46	105.35	112.23
15	P	112	TRP	N-CA-C	-5.45	105.43	112.68
21	b	221	LEU	N-CA-C	5.41	119.71	113.38
20	a	343	HIS	N-CA-C	5.36	119.38	113.21
2	B	151	LEU	CA-CB-CG	5.34	135.00	116.30
7	G	70	PHE	N-CA-C	5.34	117.41	108.23
33	V	119	TYR	N-CA-C	5.34	117.18	111.36
21	b	521	ALA	N-CA-C	-5.30	105.17	111.69
21	b	156	LEU	N-CA-C	-5.29	106.84	113.72
20	a	589	CYS	CA-CB-SG	5.29	126.56	114.40
20	a	361	ASN	N-CA-C	5.28	116.72	111.07
27	j	25	LEU	CA-CB-CG	5.26	134.72	116.30
20	a	126	ILE	N-CA-C	5.26	118.71	113.71
13	M	154	GLN	CB-CG-CD	5.25	121.52	112.60
19	X	121	ILE	N-CA-C	-5.20	107.23	112.17
2	B	197	ILE	CA-CB-CG2	5.19	119.33	110.50
33	V	115	GLY	N-CA-C	5.19	118.95	112.73
22	c	77	MET	N-CA-C	-5.18	106.47	112.89
17	S	167	PHE	CB-CA-C	-5.17	100.13	110.42
19	W	117	ARG	CD-NE-CZ	5.13	131.59	124.40
31	h	112	TRP	N-CA-C	5.13	116.87	111.28
11	K	99	ARG	CA-C-N	5.12	131.60	122.13
11	K	99	ARG	C-N-CA	5.12	131.60	122.13
14	N	246	GLY	N-CA-C	5.12	125.31	113.18
31	h	67	ILE	N-CA-C	5.11	115.34	110.53
21	b	222	LYS	CA-C-N	5.11	124.61	119.19
21	b	222	LYS	C-N-CA	5.11	124.61	119.19
15	O	160	VAL	N-CA-CB	-5.09	106.59	111.89
15	P	36	MET	N-CA-C	5.09	112.71	108.13
15	Q	160	VAL	N-CA-CB	-5.09	106.60	111.89
17	S	167	PHE	CA-CB-CG	5.08	118.88	113.80
3	C	160	SER	CA-C-N	5.07	126.18	119.84
3	C	160	SER	C-N-CA	5.07	126.18	119.84
4	D	202	GLY	CA-C-N	5.07	125.34	119.92
4	D	202	GLY	C-N-CA	5.07	125.34	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	714	ASN	N-CA-C	5.07	119.04	112.86
20	a	192	LYS	N-CA-C	5.04	116.61	110.41
10	J	118	GLY	N-CA-C	5.02	122.59	112.34
32	U	65	ASP	CA-C-O	-5.02	114.28	120.05
21	b	370	LEU	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	91	PHE	Mainchain
12	L	228	HIS	Peptide
12	L	47	ASN	Peptide
14	N	112	PRO	Peptide
14	N	172	ASP	Peptide
14	N	224	GLY	Peptide
14	N	225	SER	Peptide
14	N	231	ASP	Peptide
14	N	233	ALA	Peptide
14	N	246	GLY	Peptide
15	O	156	ASP	Peptide
15	P	156	ASP	Mainchain
15	Q	156	ASP	Peptide
17	S	102	TRP	Mainchain
17	S	136	VAL	Mainchain
33	V	11	GLY	Mainchain
19	W	10	PRO	Peptide
19	W	112	PHE	Peptide
19	W	94	PHE	Peptide
23	d	151[A]	LYS	Peptide,Mainchain
23	d	151[B]	LYS	Peptide,Mainchain
23	d	167	HIS	Peptide
30	g	50	UNK	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1287	0	1265	83	0
2	B	1013	0	1016	100	0
3	C	1247	0	1240	72	0
4	D	1337	0	1310	69	0
5	E	1411	0	1376	46	0
6	F	1375	0	1345	82	0
7	G	1668	0	1631	110	0
8	H	1291	0	1258	47	0
9	I	1250	0	1196	79	0
10	J	1301	0	1256	66	0
11	K	1304	0	1281	48	0
12	L	1523	0	1488	71	0
13	M	1423	0	1397	37	0
14	N	1716	0	1658	139	0
15	O	1302	0	1296	64	0
15	P	1296	0	1291	125	0
15	Q	1302	0	1300	115	0
16	R	1628	0	1588	115	0
17	S	1722	0	1670	149	0
18	T	1326	0	1304	18	0
19	W	1239	0	1208	55	0
19	X	1253	0	1232	91	0
20	a	5858	0	5689	242	0
21	b	5820	0	5647	270	0
22	c	597	0	583	29	0
23	d	1056	0	1074	108	0
24	e	507	0	504	23	0
25	f	1223	0	1238	79	0
26	i	256	0	284	29	0
27	j	324	0	338	48	0
28	l	1094	0	1129	55	0
29	m	198	0	213	27	0
30	g	670	0	143	23	0
31	h	676	0	662	75	0
32	U	1194	0	1160	221	0
33	V	1361	0	1354	361	0
34	A	129	0	0	14	0
34	B	86	0	0	15	0
34	C	43	0	0	4	0
34	D	172	0	0	19	0
34	E	172	0	0	12	0
34	F	43	0	0	3	0
34	G	43	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	86	0	0	6	0
34	I	43	0	0	6	0
34	J	43	0	0	4	0
34	K	86	0	0	8	0
34	L	43	0	0	25	0
34	M	43	0	0	18	0
34	O	43	0	0	6	0
34	P	43	0	0	6	0
34	Q	43	0	0	19	0
34	R	86	0	0	16	0
34	S	86	0	0	3	0
34	W	86	0	0	45	0
34	a	43	0	0	1	0
34	j	43	0	0	4	0
35	A	96	0	0	3	0
35	B	96	0	0	19	0
35	C	144	0	0	16	0
35	D	48	0	0	6	0
35	E	144	0	0	18	0
35	F	288	0	0	12	0
35	G	192	0	0	9	0
35	H	96	0	0	7	0
35	I	144	0	0	21	0
35	J	240	0	0	29	0
35	K	192	0	0	6	0
35	L	240	0	0	14	0
35	M	192	0	0	12	0
35	N	336	0	0	55	0
35	O	240	0	0	27	0
35	P	192	0	0	6	0
35	Q	192	0	0	42	0
35	R	336	0	0	10	0
35	S	288	0	0	27	0
35	T	336	0	0	9	0
35	U	192	0	0	35	0
35	V	192	0	0	46	0
35	W	96	0	0	1	0
35	X	288	0	0	27	0
35	h	96	0	0	9	0
36	A	517	0	509	59	0
36	B	329	0	299	34	0
36	C	516	0	513	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	D	618	0	591	45	0
36	E	550	0	576	54	0
36	F	452	0	431	57	0
36	G	556	0	526	75	0
36	H	760	0	747	60	0
36	I	555	0	520	91	0
36	J	562	0	540	30	0
36	K	529	0	532	61	0
36	L	527	0	523	54	0
36	M	525	0	462	38	0
36	N	601	0	503	65	0
36	O	506	0	492	34	0
36	P	686	0	666	50	0
36	Q	458	0	441	78	0
36	R	661	0	616	25	0
36	S	658	0	611	46	0
36	T	408	0	409	27	0
36	U	449	0	427	96	0
36	V	545	0	565	145	0
36	W	629	0	552	49	0
36	X	368	0	273	36	0
36	a	2437	0	2463	146	0
36	b	2337	0	2371	117	0
36	f	247	0	259	39	0
36	h	65	0	72	11	0
36	i	65	0	71	3	0
36	j	172	0	172	31	0
36	l	294	0	291	24	0
37	A	45	0	0	4	0
37	B	45	0	0	2	0
37	C	45	0	0	1	0
37	D	45	0	0	0	0
37	E	45	0	0	2	0
37	F	90	0	0	20	0
37	G	135	0	0	8	0
37	H	45	0	0	0	0
37	J	45	0	0	0	0
37	K	45	0	0	9	0
37	L	90	0	0	11	0
37	M	135	0	0	7	0
37	N	45	0	0	0	0
37	O	90	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	90	0	0	2	0
37	Q	90	0	0	16	0
37	R	45	0	0	0	0
37	S	45	0	0	4	0
37	T	90	0	0	18	0
37	U	45	0	0	0	0
37	V	45	0	0	1	0
37	W	90	0	0	14	0
37	X	45	0	0	0	0
38	A	28	0	19	7	0
38	b	46	0	56	10	0
39	B	70	0	92	20	0
39	E	93	0	118	25	0
39	F	68	0	85	35	0
39	G	70	0	90	14	0
39	I	70	0	92	22	0
39	K	66	0	81	14	0
39	L	66	0	77	10	0
39	P	46	0	60	8	0
39	U	70	0	92	27	0
39	a	102	0	129	25	0
39	b	59	0	78	25	0
39	f	24	0	35	2	0
39	h	35	0	43	21	0
40	C	57	0	75	19	0
40	L	47	0	52	20	0
40	b	60	0	81	4	0
41	D	95	0	137	28	0
41	E	49	0	74	24	0
41	F	74	0	97	5	0
41	G	136	0	194	27	0
41	I	49	0	74	10	0
41	O	91	0	129	14	0
41	Q	49	0	72	19	0
41	R	49	0	74	14	0
41	a	122	0	160	20	0
41	b	49	0	74	18	0
41	f	91	0	129	41	0
41	i	46	0	65	28	0
41	j	49	0	74	14	0
41	l	48	0	69	17	0
42	D	83	0	109	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	E	86	0	112	25	0
42	G	110	0	172	22	0
42	I	55	0	86	14	0
42	J	99	0	147	36	0
42	L	33	0	36	10	0
42	V	92	0	130	41	0
42	a	54	0	81	20	0
42	h	45	0	63	7	0
42	j	52	0	77	26	0
42	m	37	0	43	9	0
43	a	33	0	46	3	0
43	b	33	0	46	3	0
44	a	160	0	224	13	0
44	b	200	0	280	14	0
44	f	80	0	112	3	0
44	h	40	0	56	4	0
44	i	80	0	112	9	0
44	j	40	0	56	1	0
44	l	80	0	112	5	0
44	m	40	0	56	11	0
45	b	8	0	0	2	0
45	c	16	0	0	0	0
46	a	64	0	0	7	0
46	b	72	0	0	13	0
46	c	7	0	0	0	0
46	d	4	0	0	0	0
46	f	2	0	0	0	0
46	j	1	0	0	0	0
46	l	3	0	0	3	0
All	All	81344	0	72580	4620	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 30.

All (4620) 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)
33:V:140:PRO:CB	35:V:303:A86:C39	1.75	1.63
32:U:42:MET:HB3	35:U:304:A86:C	1.26	1.62
36:Q:314:CLA:HED3	36:Q:314:CLA:C1A	1.29	1.59
33:V:69:ILE:CG2	36:V:309:CLA:CGA	1.75	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:128:GLN:HG3	34:E:301:DD6:C23	1.32	1.56
15:Q:196:VAL:CG2	35:Q:303:A86:C39	1.84	1.55
36:Q:310:CLA:CAA	36:Q:310:CLA:C2A	1.83	1.55
1:A:140:MET:SD	25:f:207:PHE:HZ	1.31	1.53
15:O:54:LEU:CD1	33:V:143:ILE:HG21	1.33	1.53
36:I:312:CLA:C7	42:I:315:LMG:H151	1.35	1.53
12:L:44:GLU:HG2	36:L:308:CLA:C4B	1.35	1.53
33:V:140:PRO:CG	35:V:303:A86:C39	1.86	1.53
2:B:115:LYS:NZ	21:b:98:GLU:CG	1.71	1.52
15:O:54:LEU:HD13	33:V:143:ILE:CG2	1.32	1.52
19:X:60:PRO:HD3	36:X:315:CLA:CED	1.38	1.52
34:D:303:DD6:C1	36:D:309:CLA:HBB1	1.39	1.48
22:c:75:ARG:NH2	30:g:122:UNK:CB	1.77	1.47
37:M:318:KC1:C1A	37:M:318:KC1:NA	1.68	1.47
2:B:115:LYS:CE	21:b:98:GLU:HG3	1.43	1.45
33:V:139:ASN:CG	33:V:142:ASN:HB3	1.42	1.45
34:L:305:DD6:C41	36:L:309:CLA:H11	1.44	1.44
6:F:213:VAL:CG2	33:V:93:GLU:OE1	1.64	1.43
33:V:140:PRO:HB2	35:V:303:A86:C39	1.40	1.43
2:B:78:GLY:HA3	34:B:302:DD6:C22	1.46	1.43
33:V:38:HIS:HB3	33:V:161:MET:CE	1.44	1.43
34:L:305:DD6:C41	36:L:309:CLA:C1	1.97	1.42
41:i:104:LHG:O10	42:m:102:LMG:C11	1.65	1.42
36:b:823:CLA:H42	31:h:68:MET:CE	1.48	1.41
1:A:140:MET:SD	25:f:207:PHE:CZ	2.12	1.40
5:E:153:GLU:OE2	39:E:321:LMT:C6'	1.65	1.39
33:V:69:ILE:HG22	36:V:309:CLA:CGA	1.36	1.39
33:V:8:VAL:HG23	36:V:305:CLA:C2B	1.52	1.39
39:F:321:LMT:H6E	37:O:315:KC1:CED	1.51	1.39
33:V:8:VAL:CG2	36:V:305:CLA:C2B	2.00	1.38
37:F:308:KC1:CBB	39:F:320:LMT:C3	2.01	1.38
33:V:7:PRO:HB3	36:V:305:CLA:CMA	1.53	1.37
2:B:135:ILE:HG22	34:B:304:DD6:C9	1.50	1.37
35:I:302:A86:C4	36:I:308:CLA:C4	1.99	1.36
36:K:310:CLA:C17	42:L:321:LMG:H152	1.52	1.36
16:R:175:HIS:HD2	34:R:307:DD6:C	1.35	1.36
14:N:90:VAL:HG21	35:N:304:A86:C7	1.53	1.35
17:S:176:PHE:CZ	17:S:178:LEU:HD13	1.58	1.35
4:D:204:PHE:O	4:D:206:TYR:CE1	1.77	1.35
2:B:78:GLY:CA	34:B:302:DD6:C22	2.04	1.35
16:R:175:HIS:CD2	34:R:307:DD6:C	2.09	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:PHE:CZ	36:H:310:CLA:OBD	1.78	1.35
2:B:124:VAL:HG22	35:B:301:A86:C37	1.58	1.34
26:i:2:MET:N	26:i:5:LEU:HG	1.38	1.34
33:V:55:GLY:O	33:V:60:ASN:ND2	1.57	1.33
33:V:65:GLU:HA	33:V:75:PHE:CD2	1.64	1.31
6:F:153:MET:CE	31:h:57:GLU:OE2	1.78	1.31
35:I:302:A86:C4	36:I:308:CLA:H43	1.56	1.31
33:V:116:LYS:HB3	36:V:314:CLA:O1D	1.27	1.31
39:F:321:LMT:C4'	37:O:315:KC1:CED	2.08	1.30
33:V:68:SER:HB2	33:V:73:ILE:CG1	1.60	1.30
35:H:304:A86:O3	35:J:301:A86:C8	1.79	1.30
24:e:20:LYS:CE	25:f:232:ALA:O	1.77	1.30
6:F:153:MET:HE1	31:h:57:GLU:OE2	1.16	1.27
37:F:308:KC1:CBB	39:F:320:LMT:H32	1.61	1.27
15:Q:152:PHE:CD2	15:Q:153:PRO:HG2	1.68	1.27
19:X:127:THR:OG1	33:V:9:PHE:HE1	1.07	1.27
21:b:350:HIS:CD2	36:b:819:CLA:OBD	1.86	1.27
33:V:6:GLU:HB3	33:V:9:PHE:O	1.27	1.27
19:X:127:THR:OG1	33:V:9:PHE:CE1	1.73	1.26
39:U:314:LMT:O2'	39:U:315:LMT:H2'	1.30	1.26
36:Q:310:CLA:CAA	36:Q:310:CLA:H2A	1.47	1.26
15:Q:155:ILE:HG22	17:S:60:LYS:NZ	1.47	1.25
39:F:320:LMT:O2B	36:V:314:CLA:CGA	1.81	1.25
36:P:319:CLA:HBA1	39:P:320:LMT:C11	1.64	1.25
15:Q:155:ILE:HG23	17:S:62:PHE:CD1	1.70	1.25
36:I:312:CLA:C7	42:I:315:LMG:C15	2.14	1.25
12:L:44:GLU:HG2	36:L:308:CLA:NB	1.51	1.25
32:U:42:MET:CB	35:U:304:A86:C	2.12	1.25
2:B:96:ASP:OD2	2:B:99:VAL:HG11	1.34	1.24
37:F:308:KC1:O1A	39:F:321:LMT:H1B	1.17	1.24
33:V:8:VAL:HG23	36:V:305:CLA:C1B	1.67	1.24
35:Q:316:A86:C40	17:S:63:TRP:CZ2	2.20	1.24
25:f:218:ARG:HH12	41:f:808:LHG:C5	1.36	1.24
8:H:119:PHE:CE1	8:H:121:SER:HB2	1.72	1.24
9:I:104:LEU:HD21	36:I:308:CLA:O1D	1.36	1.24
19:X:53:GLN:OE1	36:X:308:CLA:NB	1.70	1.24
21:b:350:HIS:HD2	36:b:819:CLA:OBD	1.18	1.23
33:V:81:MET:SD	33:V:89:HIS:HD2	1.61	1.23
27:j:15:SER:O	27:j:19:PHE:HD2	1.16	1.23
39:b:851:LMT:H21	36:f:805:CLA:CBC	1.68	1.23
2:B:115:LYS:NZ	21:b:98:GLU:HG3	1.35	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:GLU:OE2	4:D:184:ARG:NH2	1.72	1.22
34:W:204:DD6:C21	36:W:209:CLA:HBB1	1.70	1.22
34:A:303:DD6:C21	34:D:301:DD6:C37	2.18	1.22
35:Q:316:A86:C19	17:S:221:THR:HG21	1.70	1.22
33:V:139:ASN:OD1	33:V:142:ASN:HB3	1.39	1.22
15:O:199:LEU:HB2	35:O:305:A86:O5	1.35	1.21
35:Q:303:A86:C21	36:Q:310:CLA:H72	1.69	1.21
33:V:8:VAL:CG2	36:V:305:CLA:C3B	2.16	1.21
35:N:304:A86:C41	35:N:306:A86:C12	2.19	1.21
19:W:104:ARG:CB	36:W:215:CLA:OBD	1.87	1.21
35:N:305:A86:C28	36:N:309:CLA:C6	2.17	1.20
15:Q:143:LYS:NZ	37:Q:313:KC1:O1A	1.72	1.20
41:i:104:LHG:HC82	41:l:208:LHG:H171	1.21	1.20
34:W:204:DD6:C21	36:W:209:CLA:CBB	2.19	1.20
5:E:122:LEU:HD11	5:E:126:HIS:CE1	1.77	1.19
39:F:321:LMT:H4'	37:O:315:KC1:CED	1.71	1.19
33:V:138:TRP:CE3	36:V:311:CLA:HMD2	1.76	1.19
16:R:65:ILE:CD1	16:R:73:THR:HG23	1.73	1.19
36:b:841:CLA:CMB	41:b:850:LHG:HC92	1.73	1.19
1:A:196:TRP:CD2	36:A:314:CLA:OBD	1.96	1.18
15:Q:155:ILE:HG23	17:S:62:PHE:CE1	1.78	1.18
36:Q:314:CLA:C1A	36:Q:314:CLA:CED	2.21	1.18
25:f:218:ARG:NH1	41:f:808:LHG:O7	1.75	1.18
32:U:1:LEU:CB	32:U:22:SER:OG	1.91	1.18
39:E:320:LMT:H5B	39:E:320:LMT:H6D	1.24	1.18
2:B:96:ASP:OD2	2:B:99:VAL:CG1	1.90	1.17
33:V:143:ILE:HD13	36:V:311:CLA:H2	1.24	1.17
2:B:115:LYS:NZ	21:b:98:GLU:CD	2.01	1.17
12:L:44:GLU:CG	36:L:308:CLA:C4B	2.22	1.17
42:E:318:LMG:H311	36:a:819:CLA:O2A	1.41	1.17
36:H:308:CLA:H18	31:h:116:LEU:CD1	1.74	1.17
35:U:304:A86:C41	36:U:311:CLA:C4C	2.21	1.17
41:f:809:LHG:H261	42:V:316:LMG:H301	1.26	1.17
33:V:8:VAL:HG21	36:V:305:CLA:C3B	1.70	1.17
8:H:119:PHE:CE1	36:H:310:CLA:OBD	1.98	1.16
39:E:320:LMT:H122	36:a:809:CLA:HBB1	1.25	1.16
36:Q:314:CLA:HED3	36:Q:314:CLA:C2A	1.73	1.16
35:Q:316:A86:O2	17:S:221:THR:CG2	1.91	1.16
33:V:7:PRO:HB3	36:V:305:CLA:HMA1	1.22	1.16
33:V:68:SER:OG	33:V:71:ASP:HB2	1.40	1.16
36:R:320:CLA:CBC	41:R:323:LHG:H151	1.74	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:92:PHE:CZ	35:R:304:A86:C26	2.23	1.16
2:B:135:ILE:HG22	34:B:304:DD6:C8	1.77	1.15
15:O:199:LEU:HB2	35:O:305:A86:C38	1.75	1.15
35:B:303:A86:C28	36:B:309:CLA:HBB2	1.75	1.15
35:U:303:A86:C7	36:U:307:CLA:HBB1	1.77	1.15
15:P:84:GLN:O	15:P:103:LEU:HD11	1.43	1.15
33:V:138:TRP:HH2	35:V:304:A86:C39	1.60	1.15
41:i:104:LHG:H272	29:m:25:ALA:CB	1.75	1.15
33:V:58:LEU:HD12	33:V:75:PHE:CE2	1.79	1.15
36:b:836:CLA:H51	36:b:836:CLA:H101	1.26	1.14
1:A:196:TRP:CG	36:A:314:CLA:OBD	2.00	1.14
35:C:203:A86:O3	29:m:23:LYS:NZ	1.80	1.14
27:j:15:SER:O	27:j:19:PHE:CD2	2.00	1.14
32:U:32:ALA:CB	39:U:314:LMT:O3B	1.95	1.14
2:B:194:LEU:CD1	35:B:303:A86:C23	2.25	1.14
3:C:107:ASN:ND2	3:C:116:THR:OG1	1.80	1.14
16:R:65:ILE:HD12	16:R:73:THR:HG23	1.16	1.14
17:S:76:GLN:O	17:S:79:ILE:HG22	1.44	1.14
21:b:363:ASP:OD2	21:b:366:THR:CG2	1.94	1.14
22:c:2:SER:O	22:c:70:TRP:CB	1.95	1.14
28:l:65:ARG:O	28:l:73:ARG:NH2	1.79	1.14
33:V:111:THR:HB	33:V:117:LEU:CD1	1.76	1.14
39:F:320:LMT:O3'	39:F:321:LMT:H6D	1.45	1.14
36:H:307:CLA:HAC2	35:J:301:A86:C22	1.78	1.14
15:Q:151:VAL:HB	36:Q:314:CLA:CED	1.78	1.14
2:B:115:LYS:HE2	21:b:98:GLU:HG3	1.23	1.13
42:G:324:LMG:C11	42:G:325:LMG:HC2	1.78	1.13
19:X:60:PRO:HD3	36:X:315:CLA:HED1	1.17	1.13
37:F:308:KC1:CBB	39:F:320:LMT:H31	1.66	1.13
15:Q:196:VAL:HG23	35:Q:303:A86:C39	1.71	1.13
33:V:81:MET:SD	33:V:89:HIS:CD2	2.42	1.13
10:J:111:HIS:O	10:J:112:ASP:OD1	1.67	1.13
28:l:126:VAL:O	41:l:208:LHG:HC11	1.47	1.13
39:B:313:LMT:H3'	28:l:149:ASP:OD2	1.48	1.12
36:G:307:CLA:CGA	40:L:302:DGD:HG32	1.79	1.12
15:Q:196:VAL:HG22	35:Q:303:A86:C39	1.61	1.13
32:U:96:GLU:HG2	32:U:102:SER:CB	1.76	1.12
15:P:129:LEU:HD12	36:P:319:CLA:CMA	1.79	1.12
15:Q:152:PHE:CE2	15:Q:153:PRO:HG2	1.82	1.12
24:e:20:LYS:HE3	25:f:232:ALA:O	0.94	1.12
36:Q:314:CLA:HED3	36:Q:314:CLA:CHA	1.79	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:306:CLA:H102	36:A:306:CLA:H142	1.29	1.12
36:K:310:CLA:HHD	36:K:310:CLA:HBC2	1.32	1.11
14:N:183:PRO:HD2	36:N:319:CLA:OBD	1.49	1.11
15:Q:151:VAL:CB	36:Q:314:CLA:HED1	1.79	1.11
15:P:34:ASP:HB3	15:P:45:LYS:CG	1.79	1.11
42:j:105:LMG:H381	42:j:105:LMG:H421	1.23	1.11
33:V:140:PRO:HG3	35:V:303:A86:C39	1.78	1.11
5:E:68:ASP:O	20:a:16:LYS:NZ	1.83	1.11
36:G:307:CLA:HHC	36:G:307:CLA:HBB1	1.27	1.11
17:S:55:LEU:HB3	17:S:57:LEU:HD23	1.28	1.11
37:T:310:KC1:CMD	36:T:313:CLA:C4D	2.28	1.11
32:U:57:PHE:HZ	35:U:302:A86:C26	1.63	1.11
5:E:128:GLN:CG	34:E:301:DD6:C23	2.28	1.11
15:O:199:LEU:CB	35:O:305:A86:O5	1.97	1.11
35:Q:316:A86:O2	17:S:221:THR:HG21	1.46	1.11
41:E:322:LHG:H102	41:E:322:LHG:H252	1.33	1.10
36:R:320:CLA:HBC3	41:R:323:LHG:H151	1.13	1.10
32:U:35:LEU:HD13	32:U:103:THR:HB	1.17	1.10
32:U:76:GLN:HB2	36:U:309:CLA:HED3	1.21	1.10
21:b:375:GLN:HE21	21:b:375:GLN:HA	1.13	1.10
32:U:112:TRP:N	35:U:304:A86:O5	1.84	1.10
2:B:115:LYS:NZ	21:b:98:GLU:OE2	1.85	1.10
34:D:303:DD6:C1	36:D:309:CLA:CBB	2.28	1.10
36:O:309:CLA:H8	36:O:316:CLA:H43	1.33	1.10
36:Q:314:CLA:CED	36:Q:314:CLA:CHA	2.30	1.10
34:L:305:DD6:C41	36:L:309:CLA:H12	1.82	1.10
32:U:95:MET:HB3	32:U:109:ALA:HB1	1.33	1.10
33:V:7:PRO:HB3	36:V:305:CLA:HMA3	1.31	1.10
33:V:68:SER:CB	33:V:73:ILE:HG13	1.81	1.10
33:V:139:ASN:CG	33:V:142:ASN:CB	2.24	1.10
23:d:101:VAL:CG2	23:d:128:LEU:HD11	1.82	1.09
3:C:40:LEU:HD11	3:C:59:PHE:CE1	1.87	1.09
16:R:95:TYR:CE1	16:R:122:PRO:HG2	1.87	1.09
23:d:101:VAL:HG21	23:d:128:LEU:HD11	1.10	1.09
15:O:196:VAL:HG22	35:O:305:A86:C39	1.83	1.09
21:b:412:GLU:HA	25:f:238:ALA:HB1	1.27	1.09
39:F:321:LMT:C6'	37:O:315:KC1:CED	2.29	1.09
14:N:241:MET:HE2	14:N:241:MET:HA	1.26	1.09
21:b:635:ASN:HB2	21:b:636:PRO:HD2	1.32	1.09
32:U:96:GLU:CG	32:U:102:SER:HB2	1.81	1.09
36:F:317:CLA:HBB2	42:J:318:LMG:H152	1.22	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:X:314:A86:C2	33:V:161:MET:HE2	1.83	1.08
21:b:412:GLU:HA	25:f:238:ALA:CB	1.83	1.08
33:V:68:SER:HB2	33:V:73:ILE:HG13	1.14	1.08
36:V:314:CLA:HHC	36:V:314:CLA:HBB1	1.34	1.08
15:O:133:ILE:HD11	35:O:301:A86:C38	1.83	1.08
35:Q:316:A86:C12	17:S:217:LEU:HD21	1.83	1.08
23:d:137:CYS:HB3	23:d:154:PHE:CE2	1.88	1.08
33:V:138:TRP:HE3	36:V:311:CLA:HMD2	0.96	1.08
41:G:321:LHG:H242	41:G:321:LHG:HC92	1.17	1.08
36:G:307:CLA:HBA1	40:L:302:DGD:HG31	1.25	1.08
34:W:205:DD6:C37	36:W:212:CLA:CHD	2.32	1.08
35:U:304:A86:C41	36:U:311:CLA:CHD	2.31	1.08
33:V:119:TYR:O	42:V:315:LMG:O3	1.69	1.08
1:A:106:ASP:HB3	1:A:195:ASN:HD21	1.14	1.08
36:b:823:CLA:C4	31:h:68:MET:HE1	1.83	1.08
39:b:851:LMT:H21	36:f:805:CLA:HBC2	1.09	1.07
35:B:301:A86:C22	36:U:307:CLA:C5	2.32	1.07
15:Q:156:ASP:HB3	17:S:60:LYS:HD2	1.36	1.07
21:b:729:SER:O	21:b:732:PHE:CE1	2.07	1.07
32:U:150:ILE:CG2	32:U:153:ALA:HB2	1.84	1.07
10:J:185:GLY:O	10:J:189:GLN:HG3	1.54	1.07
36:A:309:CLA:HBB2	42:V:315:LMG:H152	1.35	1.07
15:P:121:ASN:O	15:P:125:PHE:HD2	1.37	1.07
32:U:8:SER:OG	36:U:306:CLA:HED2	1.52	1.07
3:C:96:GLU:OE1	3:C:196:LEU:HD23	1.55	1.06
39:F:321:LMT:O1B	37:O:315:KC1:CED	2.02	1.06
12:L:137:ILE:HD11	34:L:305:DD6:C22	1.85	1.06
15:O:54:LEU:HD13	33:V:143:ILE:CB	1.85	1.06
35:Q:316:A86:C12	17:S:217:LEU:CD2	2.33	1.06
19:X:60:PRO:HD3	36:X:315:CLA:HED2	1.32	1.06
36:U:306:CLA:HMB1	36:U:306:CLA:H43	1.34	1.06
8:H:119:PHE:HE1	8:H:121:SER:HB2	0.92	1.06
36:R:320:CLA:HBC3	41:R:323:LHG:C15	1.83	1.06
34:W:205:DD6:C37	36:W:212:CLA:ND	2.18	1.06
32:U:95:MET:HA	32:U:95:MET:HE3	1.37	1.06
6:F:100:LEU:HD12	6:F:102:MET:HE3	1.31	1.06
36:a:806:CLA:H191	42:j:105:LMG:C24	1.84	1.06
35:U:303:A86:C7	36:U:307:CLA:CBB	2.34	1.06
14:N:214:PHE:CD2	35:N:303:A86:C	2.39	1.05
32:U:76:GLN:CB	36:U:309:CLA:HED3	1.86	1.05
39:U:314:LMT:O2'	39:U:315:LMT:C2'	2.04	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:54:LEU:CG	33:V:143:ILE:HG21	1.87	1.05
35:I:302:A86:C4	36:I:308:CLA:H41	1.77	1.05
15:Q:152:PHE:CD2	36:Q:314:CLA:C1C	2.40	1.05
15:Q:168:ARG:NH1	37:Q:311:KC1:O1A	1.88	1.05
36:a:816:CLA:H141	36:a:816:CLA:H193	1.33	1.05
12:L:137:ILE:CD1	34:L:305:DD6:C22	2.34	1.05
15:P:129:LEU:HD12	36:P:319:CLA:HMA1	1.33	1.05
14:N:184:PHE:CE2	36:N:319:CLA:CMD	2.39	1.04
15:Q:152:PHE:CG	15:Q:153:PRO:HD2	1.92	1.04
35:Q:316:A86:C18	17:S:221:THR:HG21	1.87	1.04
1:A:197:VAL:HG23	1:A:198:THR:N	1.70	1.04
14:N:184:PHE:CE2	36:N:319:CLA:HMD3	1.92	1.04
36:a:806:CLA:C19	42:j:105:LMG:C24	2.36	1.04
36:G:315:CLA:C4	41:G:320:LHG:H241	1.87	1.04
42:G:324:LMG:H111	42:G:325:LMG:HC2	1.32	1.04
26:i:2:MET:N	26:i:5:LEU:CG	2.19	1.04
33:V:148:ARG:NH2	36:V:305:CLA:HED1	1.73	1.04
1:A:197:VAL:CG2	1:A:198:THR:H	1.71	1.03
34:A:301:DD6:C37	38:A:315:SQD:H442	1.88	1.03
37:F:308:KC1:O1A	39:F:321:LMT:C1B	2.05	1.03
39:F:320:LMT:O3'	39:F:321:LMT:C6'	2.06	1.03
36:G:307:CLA:CGA	40:L:302:DGD:C3G	2.36	1.03
9:I:118:PHE:HB2	36:I:309:CLA:HBC3	1.34	1.03
13:M:221:LEU:HG	35:M:304:A86:C12	1.87	1.03
15:Q:155:ILE:CG2	17:S:60:LYS:NZ	2.21	1.03
23:d:101:VAL:HG21	23:d:128:LEU:CD1	1.88	1.03
35:D:302:A86:C40	36:D:311:CLA:HAA2	1.87	1.03
15:P:159:THR:HG21	16:R:62:SER:CB	1.88	1.03
41:I:316:LHG:H242	41:I:316:LHG:C8	1.89	1.03
14:N:143:TRP:HZ2	14:N:169:LEU:O	1.42	1.03
35:Q:316:A86:C40	17:S:63:TRP:CE2	2.42	1.03
33:V:38:HIS:HB3	33:V:161:MET:HE3	1.04	1.03
33:V:69:ILE:HG21	36:V:309:CLA:CGA	1.84	1.03
36:H:308:CLA:H18	31:h:116:LEU:HD12	1.38	1.03
14:N:90:VAL:CG2	35:N:304:A86:C7	2.37	1.03
33:V:38:HIS:CB	33:V:161:MET:CE	2.36	1.03
13:M:72:THR:O	13:M:76:GLY:O	1.77	1.03
41:i:104:LHG:C8	41:l:208:LHG:H171	1.88	1.03
33:V:158:ARG:HE	36:V:306:CLA:CHD	1.72	1.03
1:A:175:LEU:CD2	36:A:306:CLA:HED2	1.88	1.02
2:B:135:ILE:CG2	34:B:304:DD6:C9	2.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:P:319:CLA:CBA	39:P:320:LMT:C11	2.37	1.02
19:X:60:PRO:CD	36:X:315:CLA:CED	2.35	1.02
35:X:314:A86:C40	36:V:306:CLA:C2	2.37	1.02
41:i:104:LHG:HC82	41:l:208:LHG:C17	1.89	1.02
39:I:318:LMT:H111	42:a:852:LMG:H272	1.41	1.02
15:P:34:ASP:HB3	15:P:45:LYS:HG3	1.39	1.02
33:V:69:ILE:HG23	36:V:309:CLA:CGA	1.89	1.02
9:I:93:PRO:HD2	36:I:308:CLA:HMD1	1.37	1.02
17:S:55:LEU:HB3	17:S:57:LEU:CD2	1.90	1.02
33:V:119:TYR:OH	36:V:314:CLA:HMD1	1.58	1.02
16:R:65:ILE:CD1	16:R:73:THR:CG2	2.38	1.02
33:V:119:TYR:CD1	42:V:316:LMG:HC72	1.95	1.02
36:K:310:CLA:C17	42:L:321:LMG:C15	2.37	1.01
15:P:121:ASN:O	15:P:125:PHE:CD2	2.11	1.01
34:M:303:DD6:C37	36:M:307:CLA:C1	2.38	1.01
17:S:176:PHE:CZ	17:S:178:LEU:CD1	2.43	1.01
23:d:206:GLN:HE21	30:g:134:UNK:CB	1.71	1.01
41:i:104:LHG:H272	29:m:25:ALA:HB3	1.41	1.01
36:V:314:CLA:CGD	36:V:314:CLA:HBA2	1.90	1.01
1:A:175:LEU:HD23	36:A:306:CLA:HED2	1.02	1.01
35:I:302:A86:C5	36:I:308:CLA:H41	1.91	1.01
19:X:59:LEU:HA	36:X:315:CLA:HED1	1.39	1.01
14:N:214:PHE:HE2	35:N:303:A86:C3	1.71	1.01
15:Q:151:VAL:H	36:Q:314:CLA:CED	1.72	1.01
16:R:66:TRP:HA	35:R:305:A86:O2	1.57	1.01
23:d:101:VAL:CG2	23:d:128:LEU:CD1	2.39	1.01
15:Q:152:PHE:CE2	36:Q:314:CLA:C1C	2.44	1.01
33:V:119:TYR:CZ	42:V:316:LMG:HC71	1.96	1.01
35:I:302:A86:C8	36:I:308:CLA:C7	2.39	1.00
41:I:316:LHG:H242	41:I:316:LHG:HC81	1.40	1.00
21:b:488:GLY:O	21:b:493:LEU:HB2	1.60	1.00
21:b:693:ARG:NH2	26:i:32:ARG:HE	1.59	1.00
33:V:138:TRP:HH2	35:V:304:A86:C38	1.72	1.00
39:B:313:LMT:H31	28:l:121:THR:HG21	1.42	1.00
39:E:320:LMT:H31	41:E:322:LHG:H261	1.38	1.00
36:L:308:CLA:H71	37:L:315:KC1:CMD	1.91	1.00
19:W:47:VAL:HG11	34:W:205:DD6:C8	1.90	1.00
20:a:225:ILE:HD11	36:a:813:CLA:CMD	1.92	1.00
4:D:204:PHE:O	4:D:206:TYR:CD1	2.14	1.00
36:G:307:CLA:CBA	40:L:302:DGD:HG31	1.91	1.00
10:J:142:MET:HE1	42:J:318:LMG:HC61	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:f:808:LHG:H351	42:V:316:LMG:H351	1.43	1.00
35:I:302:A86:C8	36:I:308:CLA:H72	1.91	1.00
41:a:850:LHG:HC61	41:a:850:LHG:HC31	1.37	1.00
36:l:204:CLA:HHC	36:l:204:CLA:HBB1	1.43	1.00
33:V:143:ILE:H	33:V:143:ILE:HD12	1.21	1.00
17:S:79:ILE:HD13	17:S:162:GLY:HA3	1.42	1.00
3:C:96:GLU:OE2	3:C:196:LEU:N	1.94	0.99
36:K:307:CLA:H143	37:K:314:KC1:CHC	1.92	0.99
36:b:836:CLA:H91	36:b:836:CLA:H121	1.41	0.99
9:I:51:PRO:O	34:I:303:DD6:O4	1.79	0.99
16:R:63:THR:CG2	16:R:65:ILE:H	1.74	0.99
15:Q:155:ILE:CG2	17:S:62:PHE:CE1	2.45	0.99
33:V:139:ASN:OD1	33:V:142:ASN:CB	2.09	0.99
36:O:309:CLA:C8	36:O:316:CLA:H43	1.91	0.99
15:Q:156:ASP:O	17:S:60:LYS:HD3	1.60	0.99
10:J:40:VAL:O	10:J:69:ARG:NH2	1.96	0.99
36:D:309:CLA:H71	36:D:309:CLA:H41	1.41	0.99
12:L:137:ILE:HD11	34:L:305:DD6:C17	1.92	0.99
15:Q:155:ILE:HG22	17:S:60:LYS:HZ3	0.83	0.98
33:V:68:SER:OG	33:V:71:ASP:CB	2.10	0.98
33:V:58:LEU:HB2	33:V:75:PHE:CD2	1.98	0.98
7:G:156:GLN:NE2	7:G:158:SER:H	1.62	0.98
9:I:93:PRO:CD	36:I:308:CLA:HMD1	1.93	0.98
14:N:241:MET:HG2	35:N:305:A86:C9	1.94	0.98
32:U:150:ILE:HG21	32:U:153:ALA:HB2	1.01	0.98
15:O:54:LEU:CD1	33:V:143:ILE:HG12	1.93	0.98
20:a:225:ILE:HD11	36:a:813:CLA:HMD3	1.43	0.98
36:K:309:CLA:H111	39:K:318:LMT:H123	1.45	0.98
36:b:841:CLA:HMB2	41:b:850:LHG:HC92	0.99	0.98
33:V:111:THR:HG21	42:V:315:LMG:HC71	1.40	0.98
35:B:303:A86:C28	36:B:309:CLA:CBB	2.42	0.98
15:P:84:GLN:O	15:P:103:LEU:CD1	2.10	0.98
2:B:124:VAL:CG2	35:B:301:A86:C37	2.41	0.98
8:H:119:PHE:CE1	8:H:121:SER:CB	2.46	0.98
33:V:7:PRO:CB	36:V:305:CLA:CMA	2.42	0.98
34:W:205:DD6:C25	36:W:212:CLA:HMC2	1.94	0.98
21:b:363:ASP:CG	21:b:366:THR:HG23	1.88	0.98
22:c:75:ARG:HH22	30:g:122:UNK:CB	1.67	0.98
1:A:197:VAL:HG23	1:A:198:THR:H	1.23	0.97
7:G:199:PHE:CD2	36:G:313:CLA:H2	1.98	0.97
33:V:65:GLU:HA	33:V:75:PHE:HD2	1.06	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:63:THR:HG22	16:R:65:ILE:H	1.27	0.97
19:X:60:PRO:CG	33:V:173:ILE:HG21	1.94	0.97
4:D:73:GLU:OE2	4:D:153:PRO:HA	1.64	0.97
33:V:58:LEU:HD12	33:V:75:PHE:HE2	1.27	0.97
15:O:199:LEU:N	35:O:305:A86:O5	1.96	0.97
39:E:320:LMT:H5B	39:E:320:LMT:C6'	1.94	0.97
21:b:187:LEU:O	21:b:190:THR:HG22	1.65	0.97
36:b:841:CLA:HMB2	41:b:850:LHG:C9	1.93	0.97
41:i:104:LHG:C8	41:l:208:LHG:C17	2.42	0.97
17:S:217:LEU:HD11	17:S:240:VAL:HG11	1.45	0.97
1:A:196:TRP:CG	36:A:314:CLA:CAD	2.48	0.97
32:U:76:GLN:HB2	36:U:309:CLA:CED	1.94	0.97
32:U:95:MET:HE2	32:U:100:LYS:HE3	1.47	0.97
39:I:317:LMT:H12	39:I:317:LMT:C6'	1.95	0.96
33:V:38:HIS:HB3	33:V:161:MET:HE1	1.45	0.96
9:I:118:PHE:HA	36:I:309:CLA:HBC2	1.47	0.96
23:d:195:VAL:HG21	23:d:210:LEU:HD22	1.47	0.96
1:A:175:LEU:HD23	36:A:306:CLA:CED	1.94	0.96
36:b:823:CLA:H42	31:h:68:MET:HE2	1.47	0.96
36:b:823:CLA:H42	31:h:68:MET:HE1	0.97	0.96
1:A:66:TYR:CE2	42:j:105:LMG:HC91	1.99	0.96
33:V:38:HIS:CB	33:V:161:MET:HE3	1.92	0.96
36:X:315:CLA:HMD3	35:V:301:A86:C29	1.96	0.96
32:U:138:MET:O	32:U:141:ILE:HG22	1.66	0.96
6:F:50:LEU:CD2	41:f:809:LHG:H102	1.94	0.96
19:X:60:PRO:HG3	33:V:173:ILE:HG21	1.44	0.96
33:V:119:TYR:CE1	42:V:316:LMG:HC72	2.01	0.96
36:B:309:CLA:HBA1	36:B:309:CLA:HBD	1.48	0.96
35:I:302:A86:C7	36:I:308:CLA:H61	1.94	0.96
34:W:205:DD6:C26	36:W:212:CLA:CHC	2.44	0.96
2:B:78:GLY:HA2	34:B:302:DD6:C22	1.94	0.96
31:h:135:ARG:NH1	36:h:203:CLA:HED1	1.81	0.96
10:J:140:GLN:HG3	42:h:206:LMG:O3	1.65	0.96
15:Q:151:VAL:HB	36:Q:314:CLA:HED1	0.98	0.96
34:W:205:DD6:C37	36:W:212:CLA:C1D	2.44	0.96
33:V:138:TRP:CH2	35:V:304:A86:C39	2.48	0.96
14:N:184:PHE:CZ	36:N:319:CLA:CMD	2.49	0.95
37:T:310:KC1:CMD	36:T:313:CLA:C3D	2.43	0.95
34:W:204:DD6:C21	36:W:209:CLA:C3B	2.43	0.95
15:P:34:ASP:HB3	15:P:45:LYS:CD	1.95	0.95
21:b:363:ASP:OD2	21:b:366:THR:HG23	1.60	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:116:LYS:CB	36:V:314:CLA:O1D	2.14	0.95
2:B:112:ILE:HD12	26:i:4:ASN:ND2	1.81	0.95
41:E:322:LHG:H102	41:E:322:LHG:C25	1.97	0.95
33:V:140:PRO:HG2	35:V:303:A86:C39	1.96	0.95
6:F:100:LEU:HD12	6:F:102:MET:CE	1.95	0.95
35:X:314:A86:C40	36:V:306:CLA:H2	1.96	0.95
15:Q:152:PHE:CD2	15:Q:153:PRO:CG	2.49	0.95
20:a:281:LEU:O	36:a:816:CLA:HED1	1.66	0.95
20:a:587:GLY:N	21:b:667:ARG:HD3	1.81	0.95
7:G:150:HIS:O	7:G:154:VAL:HG23	1.67	0.95
2:B:66:HIS:CE1	2:B:70:TRP:HE1	1.85	0.95
9:I:46:MET:HE2	39:K:318:LMT:H22	1.49	0.95
14:N:178:LEU:HD23	36:N:318:CLA:HED3	1.47	0.95
32:U:1:LEU:HB2	32:U:22:SER:OG	1.10	0.95
8:H:119:PHE:HE1	8:H:121:SER:CB	1.79	0.94
34:W:205:DD6:C37	36:W:212:CLA:C4C	2.45	0.94
36:B:311:CLA:HBA1	39:B:312:LMT:O2'	1.67	0.94
36:a:816:CLA:H141	36:a:816:CLA:C19	1.97	0.94
27:j:15:SER:OG	27:j:19:PHE:HE2	1.47	0.94
31:h:135:ARG:HH12	36:h:203:CLA:CED	1.80	0.94
33:V:139:ASN:ND2	33:V:142:ASN:CB	2.29	0.94
6:F:213:VAL:HG22	33:V:93:GLU:OE1	0.77	0.94
5:E:122:LEU:CD1	5:E:126:HIS:CE1	2.50	0.94
21:b:132:GLN:HE22	29:m:6:GLN:HE22	1.14	0.94
12:L:137:ILE:HD11	34:L:305:DD6:C16	1.96	0.94
20:a:482:ILE:HG23	41:a:850:LHG:HC62	1.45	0.94
41:i:104:LHG:O10	42:m:102:LMG:C12	2.14	0.94
33:V:119:TYR:CE1	42:V:316:LMG:C7	2.49	0.94
16:R:65:ILE:HD13	16:R:73:THR:CG2	1.98	0.94
35:S:304:A86:C21	36:S:315:CLA:C1B	2.46	0.94
22:c:75:ARG:HH21	30:g:122:UNK:CB	1.56	0.94
41:l:208:LHG:HC82	41:l:208:LHG:HC61	1.48	0.94
32:U:35:LEU:CD1	32:U:103:THR:HB	1.97	0.94
33:V:149:ARG:NE	37:V:312:KC1:O1A	2.01	0.94
2:B:194:LEU:HD12	35:B:303:A86:C23	1.96	0.94
42:E:318:LMG:C31	36:a:819:CLA:O2A	2.15	0.94
37:F:308:KC1:CMB	36:V:314:CLA:HAA2	1.96	0.94
36:G:315:CLA:H43	41:G:320:LHG:H252	1.50	0.94
15:P:152:PHE:O	15:P:154:PRO:HD3	1.67	0.94
20:a:126:ILE:HG13	20:a:127:VAL:HG23	1.49	0.94
32:U:39:ARG:HH22	32:U:103:THR:HG22	1.34	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:67:ILE:HD12	32:U:148:HIS:CD2	2.03	0.94
36:A:305:CLA:HED1	38:A:315:SQD:O9	1.66	0.93
9:I:118:PHE:HB2	36:I:309:CLA:CBC	1.98	0.93
21:b:411:LEU:O	25:f:238:ALA:HB3	1.67	0.93
33:V:138:TRP:HE3	36:V:311:CLA:CMD	1.80	0.93
36:H:308:CLA:H18	31:h:116:LEU:HD13	1.47	0.93
36:O:316:CLA:CHC	36:O:316:CLA:H72	1.99	0.93
41:i:104:LHG:O10	42:m:102:LMG:H112	1.69	0.93
34:E:303:DD6:C23	36:M:311:CLA:H192	1.98	0.93
6:F:213:VAL:HG22	33:V:93:GLU:CD	1.91	0.93
15:O:152:PHE:CG	15:O:153:PRO:HD2	2.03	0.93
35:Q:316:A86:O3	17:S:62:PHE:CD2	2.21	0.93
33:V:8:VAL:HG21	36:V:305:CLA:CBB	1.97	0.93
16:R:65:ILE:HD13	16:R:73:THR:OG1	1.69	0.93
44:a:844:BCR:C38	42:a:852:LMG:C44	2.45	0.93
32:U:150:ILE:HG21	32:U:153:ALA:CB	1.95	0.93
33:V:8:VAL:HG21	36:V:305:CLA:HBB1	1.50	0.93
1:A:197:VAL:HG23	1:A:198:THR:HG23	1.50	0.93
4:D:129:TRP:CZ3	34:D:301:DD6:C21	2.52	0.93
36:K:307:CLA:H42	37:K:314:KC1:O1D	1.69	0.93
21:b:693:ARG:HH22	26:i:32:ARG:HE	0.94	0.93
36:O:316:CLA:H72	36:O:316:CLA:HHC	1.49	0.93
2:B:115:LYS:NZ	21:b:98:GLU:HG2	1.84	0.93
28:l:128:PHE:O	41:l:208:LHG:HC32	1.68	0.93
33:V:65:GLU:CA	33:V:75:PHE:CD2	2.52	0.93
33:V:32:ARG:NH2	33:V:35:GLU:OE1	2.01	0.93
34:L:305:DD6:C26	36:L:309:CLA:CHC	2.47	0.92
19:W:48:VAL:HG21	34:W:205:DD6:C	1.98	0.92
19:X:60:PRO:CD	36:X:315:CLA:HED1	1.97	0.92
14:N:178:LEU:HD23	36:N:318:CLA:CED	2.00	0.92
36:b:823:CLA:C4	31:h:68:MET:CE	2.41	0.92
12:L:44:GLU:OE2	36:L:308:CLA:CHB	2.16	0.92
33:V:1:THR:N	33:V:2:PRO:HD3	1.85	0.92
35:Q:316:A86:O2	17:S:221:THR:OG1	1.87	0.92
33:V:68:SER:HB2	33:V:73:ILE:CB	1.98	0.92
39:E:320:LMT:H122	36:a:809:CLA:CBB	2.00	0.92
35:J:306:A86:C23	42:J:319:LMG:H292	2.00	0.92
21:b:363:ASP:OD2	21:b:366:THR:HG21	1.69	0.92
4:D:155:ASN:ND2	4:D:157:GLY:H	1.68	0.92
34:W:204:DD6:C21	36:W:209:CLA:CAB	2.47	0.92
16:R:65:ILE:CD1	16:R:73:THR:OG1	2.18	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:68:SER:CB	33:V:73:ILE:CG1	2.44	0.92
1:A:106:ASP:HB3	1:A:195:ASN:ND2	1.84	0.92
34:E:303:DD6:C23	36:M:311:CLA:H162	1.99	0.92
20:a:587:GLY:CA	21:b:667:ARG:HD3	2.00	0.92
36:L:308:CLA:H2	37:L:315:KC1:OBD	1.70	0.92
16:R:140:PHE:HZ	34:R:308:DD6:C37	1.83	0.91
20:a:358:LEU:HD22	20:a:362:LEU:HG	1.52	0.91
14:N:73:PHE:CZ	36:N:312:CLA:HED1	2.04	0.91
21:b:220:GLY:O	39:b:848:LMT:O3B	1.89	0.91
25:f:218:ARG:HH11	41:f:809:LHG:HC5	1.35	0.91
4:D:129:TRP:HZ3	34:D:301:DD6:C21	1.84	0.91
14:N:241:MET:HA	14:N:241:MET:CE	1.97	0.91
32:U:44:ALA:HB1	35:U:303:A86:C37	2.01	0.91
2:B:66:HIS:CE1	2:B:70:TRP:NE1	2.38	0.91
16:R:175:HIS:CD2	34:R:307:DD6:C1	2.54	0.91
20:a:587:GLY:H	21:b:667:ARG:HH21	1.11	0.91
21:b:368:ALA:HB1	21:b:724:LEU:HD11	1.52	0.91
36:X:315:CLA:HMC1	35:V:301:A86:C7	2.01	0.91
33:V:138:TRP:CH2	35:V:304:A86:C38	2.53	0.91
25:f:218:ARG:NH1	41:f:808:LHG:C5	2.19	0.91
35:M:304:A86:C37	36:M:316:CLA:HED1	2.00	0.91
20:a:713:LEU:O	25:f:178:ARG:NH1	2.03	0.91
27:j:38:THR:C	27:j:40:PRO:HD2	1.95	0.91
15:P:159:THR:OG1	16:R:62:SER:HB3	1.71	0.91
32:U:32:ALA:HB2	39:U:314:LMT:O3B	1.67	0.91
33:V:82:SER:HB2	33:V:83:PRO:CD	2.01	0.91
35:S:304:A86:C21	36:S:315:CLA:CGA	2.48	0.90
21:b:364:PHE:HB3	21:b:601:TRP:CZ3	2.04	0.90
1:A:196:TRP:CD1	36:A:314:CLA:CAD	2.55	0.90
14:N:184:PHE:CZ	36:N:319:CLA:HMD2	2.06	0.90
26:i:25:LEU:HD22	44:i:103:BCR:HC8	1.53	0.90
38:b:804:SQD:H101	44:b:843:BCR:C31	2.02	0.90
6:F:91:TRP:HH2	41:O:318:LHG:H142	1.34	0.90
42:h:206:LMG:HC92	42:h:206:LMG:HC2	1.54	0.90
41:D:318:LHG:HC82	41:D:318:LHG:HC61	1.54	0.90
22:c:24:ASP:OD2	23:d:167:HIS:ND1	2.04	0.90
33:V:177:VAL:HB	33:V:178:PRO:HD2	1.54	0.90
17:S:177:VAL:HG12	36:S:320:CLA:HED3	1.53	0.90
20:a:587:GLY:H	21:b:667:ARG:NH2	1.68	0.90
36:a:803:CLA:H91	36:a:806:CLA:H172	1.53	0.90
33:V:111:THR:HB	33:V:117:LEU:HD13	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:VAL:HG13	35:B:301:A86:C37	2.02	0.90
15:P:159:THR:HG21	16:R:62:SER:HB2	1.53	0.90
19:X:59:LEU:HA	36:X:315:CLA:CED	2.02	0.90
41:D:319:LHG:H212	42:D:320:LMG:H232	1.54	0.90
36:G:315:CLA:H41	41:G:320:LHG:H241	1.52	0.90
41:i:104:LHG:H321	29:m:22:VAL:HG22	1.54	0.90
36:U:306:CLA:H43	36:U:306:CLA:CMB	2.01	0.90
33:V:161:MET:HE1	36:V:306:CLA:HAB	1.50	0.90
32:U:8:SER:OG	36:U:306:CLA:CED	2.19	0.89
4:D:165:LYS:HD3	19:W:26:GLN:NE2	1.86	0.89
34:M:303:DD6:C21	36:M:309:CLA:HBB1	2.01	0.89
21:b:4:LYS:HB2	21:b:13:ALA:HB1	1.51	0.89
32:U:44:ALA:CB	35:U:303:A86:C37	2.50	0.89
1:A:196:TRP:CD1	36:A:314:CLA:C3D	2.56	0.89
21:b:414:LYS:NZ	25:f:235:ALA:HB3	1.87	0.89
33:V:1:THR:N	33:V:2:PRO:CD	2.36	0.89
3:C:40:LEU:HD11	3:C:59:PHE:HE1	1.31	0.89
35:Q:316:A86:C19	17:S:221:THR:CG2	2.50	0.89
39:b:851:LMT:C2	36:f:805:CLA:HBC2	2.00	0.89
33:V:144:LYS:HA	33:V:144:LYS:HE3	1.55	0.89
17:S:181:TYR:OH	35:S:304:A86:C21	2.21	0.89
21:b:133:GLU:CD	36:b:816:CLA:HED1	1.98	0.89
15:Q:152:PHE:CE2	36:Q:314:CLA:CHC	2.54	0.89
20:a:200:GLU:OE2	46:a:902:HOH:O	1.90	0.89
36:a:813:CLA:OBD	46:a:901:HOH:O	1.89	0.89
33:V:111:THR:HB	33:V:117:LEU:HD12	1.54	0.89
33:V:139:ASN:ND2	33:V:142:ASN:HB2	1.88	0.89
17:S:176:PHE:HZ	17:S:178:LEU:HD13	1.36	0.89
21:b:458:PHE:HB3	36:b:836:CLA:H2	1.55	0.89
16:R:89:MET:HE3	16:R:206:ASN:C	1.97	0.89
19:X:53:GLN:OE1	36:X:308:CLA:C1B	2.20	0.89
41:G:321:LHG:HC92	41:G:321:LHG:C24	2.04	0.88
8:H:119:PHE:HZ	36:H:310:CLA:OBD	1.29	0.88
14:N:86:MET:HE1	14:N:202:GLU:HG2	1.55	0.88
33:V:58:LEU:HB3	33:V:64:HIS:O	1.72	0.88
36:D:307:CLA:CBB	42:E:319:LMG:O10	2.21	0.88
36:G:315:CLA:H43	41:G:320:LHG:C25	2.04	0.88
15:O:55:GLY:HA2	33:V:143:ILE:HA	1.55	0.88
41:i:104:LHG:H272	29:m:25:ALA:HB1	1.53	0.88
42:D:320:LMG:HC91	42:D:320:LMG:C11	2.01	0.88
7:G:158:SER:OG	36:G:311:CLA:O1A	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:152:PHE:CE1	36:Q:314:CLA:C3B	2.57	0.88
19:X:127:THR:OG1	33:V:9:PHE:CZ	2.25	0.88
2:B:182:GLU:C	2:B:184:ALA:H	1.80	0.88
7:G:199:PHE:CE2	36:G:313:CLA:H2	2.08	0.88
15:Q:196:VAL:HG21	35:Q:303:A86:C39	2.01	0.88
5:E:122:LEU:HD11	5:E:126:HIS:HE1	1.37	0.88
33:V:8:VAL:HG21	36:V:305:CLA:CAB	2.02	0.88
37:G:317:KC1:CED	39:G:322:LMT:H6E	2.03	0.88
19:X:59:LEU:HD11	35:V:301:A86:C41	2.04	0.88
20:a:225:ILE:CD1	36:a:813:CLA:CMD	2.51	0.88
32:U:67:ILE:HD12	32:U:148:HIS:HD2	1.38	0.88
33:V:82:SER:HB2	33:V:83:PRO:HD2	1.56	0.88
35:I:302:A86:C8	36:I:308:CLA:H71	2.04	0.88
35:I:302:A86:C3	36:I:308:CLA:C4	2.51	0.88
32:U:95:MET:HA	32:U:95:MET:CE	2.02	0.88
35:L:301:A86:O5	36:P:313:CLA:H122	1.72	0.87
35:I:302:A86:C9	36:I:308:CLA:H72	2.02	0.87
37:W:217:KC1:CMD	36:W:218:CLA:CHD	2.52	0.87
4:D:61:ARG:HG3	4:D:61:ARG:HH11	1.37	0.87
11:K:125:ILE:HD11	35:K:301:A86:C33	2.04	0.87
15:O:133:ILE:CD1	35:O:301:A86:C38	2.51	0.87
27:j:38:THR:C	27:j:40:PRO:CD	2.47	0.87
33:V:67:LEU:HB2	33:V:75:PHE:CE1	2.09	0.87
21:b:559:ASP:OD2	21:b:563:ARG:NH2	2.08	0.87
23:d:162:GLU:N	23:d:162:GLU:OE2	2.08	0.87
23:d:208:TYR:OH	30:g:133:UNK:CB	2.22	0.87
41:f:808:LHG:C35	42:V:316:LMG:H351	2.04	0.87
32:U:57:PHE:CZ	35:U:302:A86:C26	2.55	0.87
39:h:205:LMT:O6'	39:h:205:LMT:H6'1	1.75	0.87
4:D:165:LYS:HD3	19:W:26:GLN:HE22	1.39	0.87
41:f:809:LHG:O8	41:f:809:LHG:HC32	1.74	0.87
36:E:311:CLA:C9	42:E:318:LMG:H112	2.04	0.87
36:K:307:CLA:HBB1	36:K:307:CLA:HHC	1.55	0.87
32:U:96:GLU:OE2	32:U:109:ALA:HB3	1.75	0.87
9:I:176:MET:HE3	36:I:307:CLA:HAB	1.57	0.87
15:Q:155:ILE:HG23	17:S:62:PHE:HD1	1.39	0.86
33:V:8:VAL:HG22	36:V:305:CLA:CMB	2.05	0.86
39:b:851:LMT:C2	36:f:805:CLA:CBC	2.52	0.86
1:A:160:GLY:O	1:A:163:VAL:HG13	1.75	0.86
37:E:309:KC1:CMA	39:P:321:LMT:O2'	2.22	0.86
15:Q:155:ILE:CG2	17:S:62:PHE:HE1	1.84	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:G:322:LMT:H1B	39:G:322:LMT:H6D	1.56	0.86
14:N:183:PRO:CD	36:N:319:CLA:CAD	2.52	0.86
19:X:59:LEU:CD1	35:V:301:A86:C41	2.52	0.86
36:a:806:CLA:H102	36:a:808:CLA:H92	1.56	0.86
2:B:115:LYS:CE	21:b:98:GLU:CG	2.35	0.86
32:U:112:TRP:HE1	35:U:304:A86:C40	1.88	0.86
37:F:308:KC1:CMB	39:F:320:LMT:O2'	2.23	0.86
35:I:302:A86:C6	36:I:308:CLA:C7	2.54	0.86
41:i:104:LHG:C27	29:m:25:ALA:HB3	2.05	0.86
32:U:39:ARG:NH2	32:U:103:THR:HG22	1.90	0.86
34:M:303:DD6:C37	36:M:307:CLA:H11	2.06	0.86
16:R:89:MET:HE3	16:R:207:GLY:N	1.90	0.86
32:U:61:VAL:O	32:U:61:VAL:HG12	1.76	0.86
36:L:308:CLA:H102	37:L:315:KC1:CAC	2.06	0.86
33:V:139:ASN:HD21	33:V:142:ASN:HB2	1.40	0.86
41:F:319:LHG:H112	42:J:319:LMG:H181	1.58	0.86
32:U:63:VAL:HG11	32:U:69:ALA:HB1	1.58	0.86
41:i:104:LHG:O9	41:i:104:LHG:H242	1.76	0.86
35:D:302:A86:C40	36:D:311:CLA:CAA	2.53	0.85
17:S:89:PHE:CE2	37:S:316:KC1:CBB	2.59	0.85
41:i:104:LHG:HC81	41:l:208:LHG:H172	1.58	0.85
31:h:84:ALA:HB3	39:h:205:LMT:H112	1.55	0.85
35:E:307:A86:C10	36:E:315:CLA:C2D	2.55	0.85
35:E:307:A86:C9	36:E:315:CLA:C1D	2.55	0.85
36:H:307:CLA:CAC	35:J:301:A86:C22	2.54	0.85
20:a:587:GLY:HA3	21:b:667:ARG:HD3	1.57	0.85
15:O:152:PHE:CD1	15:O:153:PRO:HD2	2.11	0.85
15:Q:152:PHE:CE1	36:Q:314:CLA:C4B	2.59	0.85
24:e:26:VAL:HG21	24:e:41:ARG:CD	2.06	0.85
16:R:175:HIS:HB2	34:R:307:DD6:C25	2.05	0.85
27:j:19:PHE:CZ	36:j:102:CLA:H91	2.11	0.85
32:U:35:LEU:HD13	32:U:103:THR:CB	2.05	0.85
36:L:308:CLA:C10	37:L:315:KC1:CAC	2.53	0.85
33:V:7:PRO:CB	36:V:305:CLA:HMA3	2.04	0.85
5:E:68:ASP:C	20:a:16:LYS:NZ	2.33	0.85
39:F:320:LMT:O2B	36:V:314:CLA:O2A	1.93	0.85
15:O:151:VAL:HG23	36:O:316:CLA:O1D	1.77	0.85
15:P:121:ASN:HD22	36:P:319:CLA:HBC3	1.41	0.85
16:R:242:MET:HG3	35:R:305:A86:C37	2.07	0.85
41:i:104:LHG:H251	42:m:102:LMG:H131	1.57	0.85
35:U:304:A86:C41	36:U:311:CLA:NC	2.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:211:MET:HE1	36:P:301:CLA:O1A	1.76	0.85
15:P:125:PHE:CE1	36:P:319:CLA:C4D	2.60	0.85
15:Q:152:PHE:CZ	36:Q:314:CLA:CHC	2.59	0.85
36:C:205:CLA:HBD	40:C:215:DGD:HG12	1.58	0.85
42:E:318:LMG:C28	36:a:819:CLA:O2A	2.25	0.85
6:F:42:VAL:HG11	6:F:47:TRP:HB2	1.59	0.85
36:J:312:CLA:H42	42:J:318:LMG:H192	1.59	0.85
5:E:217:LEU:HD21	15:P:121:ASN:HD21	1.40	0.84
14:N:73:PHE:CZ	36:N:312:CLA:CED	2.60	0.84
21:b:699:LEU:HD22	21:b:703:GLN:NE2	1.92	0.84
32:U:96:GLU:OE2	32:U:109:ALA:CB	2.25	0.84
36:D:309:CLA:H71	36:D:309:CLA:C4	2.06	0.84
42:G:324:LMG:H291	42:G:324:LMG:O9	1.77	0.84
36:H:308:CLA:C18	31:h:116:LEU:CD1	2.55	0.84
14:N:170:PHE:HZ	36:N:318:CLA:O2A	1.61	0.84
41:O:317:LHG:C31	36:V:313:CLA:H203	2.07	0.84
19:W:121:ILE:HG23	37:W:217:KC1:CED	2.06	0.84
21:b:693:ARG:HH22	26:i:32:ARG:NE	1.73	0.84
27:j:19:PHE:CZ	36:j:102:CLA:C9	2.61	0.84
36:A:306:CLA:H102	36:A:306:CLA:C14	2.00	0.84
34:M:303:DD6:C37	36:M:307:CLA:H12	2.06	0.84
15:Q:73:VAL:CG1	34:Q:302:DD6:C12	2.55	0.84
36:G:315:CLA:H11	36:G:315:CLA:HAA2	1.57	0.84
27:j:19:PHE:HZ	36:j:102:CLA:C9	1.90	0.84
36:O:309:CLA:C10	36:O:316:CLA:H43	2.08	0.84
41:i:104:LHG:O10	42:m:102:LMG:C13	2.25	0.84
33:V:8:VAL:HG22	36:V:305:CLA:C2B	2.08	0.84
13:M:173:ARG:NH1	37:M:318:KC1:O2A	2.11	0.84
36:C:205:CLA:CED	40:C:215:DGD:HD5	2.08	0.83
36:H:308:CLA:C18	31:h:116:LEU:HD13	2.08	0.83
36:O:311:CLA:O1A	37:O:315:KC1:CBB	2.26	0.83
35:Q:316:A86:O2	17:S:221:THR:CB	2.26	0.83
31:h:121:GLY:N	31:h:122:PRO:HD2	1.91	0.83
2:B:135:ILE:CG2	34:B:304:DD6:C8	2.54	0.83
37:E:309:KC1:O2A	39:E:323:LMT:O6B	1.96	0.83
14:N:170:PHE:CE2	14:N:178:LEU:O	2.32	0.83
35:Q:316:A86:C12	17:S:217:LEU:HD23	2.09	0.83
16:R:50:PRO:CB	17:S:169:LEU:HD21	2.08	0.83
34:W:204:DD6:C	36:W:208:CLA:HAB	2.08	0.83
34:W:205:DD6:C25	36:W:212:CLA:CMC	2.56	0.83
23:d:114:MET:HB2	23:d:117:GLY:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:19:THR:HG23	33:V:24:SER:O	1.79	0.83
12:L:44:GLU:CG	36:L:308:CLA:NB	2.34	0.83
15:P:129:LEU:HD12	36:P:319:CLA:HMA2	1.60	0.83
28:l:41:VAL:HG21	30:g:90:UNK:CB	2.08	0.83
36:A:309:CLA:CBB	42:V:315:LMG:H152	2.08	0.83
36:E:315:CLA:C14	36:M:307:CLA:H142	2.09	0.83
35:S:304:A86:C21	36:S:315:CLA:CHB	2.56	0.83
25:f:158:GLU:HA	27:j:38:THR:CG2	2.08	0.83
14:N:183:PRO:HD2	36:N:319:CLA:CAD	2.08	0.83
15:P:64:ARG:HG2	15:P:64:ARG:HH11	1.44	0.83
36:j:101:CLA:H61	42:j:105:LMG:H341	1.60	0.83
33:V:1:THR:H3	33:V:2:PRO:HD3	1.43	0.83
36:O:309:CLA:H101	36:O:316:CLA:C4	2.09	0.83
36:I:312:CLA:C7	42:I:315:LMG:C14	2.56	0.83
33:V:164:ILE:HD13	33:V:164:ILE:O	1.78	0.83
39:I:317:LMT:H12	39:I:317:LMT:H6E	1.61	0.82
19:W:121:ILE:CG2	37:W:217:KC1:CED	2.57	0.82
33:V:113:ARG:HH11	33:V:113:ARG:HG3	1.44	0.82
34:M:303:DD6:C35	36:M:307:CLA:H12	2.09	0.82
23:d:206:GLN:NE2	30:g:134:UNK:CB	2.42	0.82
35:E:307:A86:C10	36:E:315:CLA:C3D	2.57	0.82
39:F:321:LMT:H4'	37:O:315:KC1:O2D	1.79	0.82
15:P:34:ASP:CB	15:P:45:LYS:CG	2.57	0.82
15:Q:155:ILE:CG2	17:S:60:LYS:HZ1	1.92	0.82
33:V:37:LYS:HE2	36:V:310:CLA:C4D	2.09	0.82
14:N:183:PRO:CD	36:N:319:CLA:OBD	2.26	0.82
32:U:50:PHE:N	32:U:51:PRO:CD	2.41	0.82
20:a:429:ASN:HD22	20:a:437:ARG:HH12	1.26	0.82
20:a:452:PHE:O	20:a:456:HIS:HD2	1.62	0.82
36:U:306:CLA:H93	36:U:307:CLA:HMA3	1.61	0.82
6:F:50:LEU:HD21	41:f:809:LHG:H102	1.59	0.82
41:G:320:LHG:H111	41:G:320:LHG:C15	2.10	0.82
42:G:324:LMG:H112	42:G:325:LMG:HC2	1.60	0.82
16:R:215:MET:SD	16:R:218:LEU:HD12	2.20	0.82
37:T:310:KC1:OBD	36:T:313:CLA:HBD	1.79	0.82
20:a:696:ARG:HG3	20:a:724:LEU:O	1.79	0.82
31:h:135:ARG:HH12	36:h:203:CLA:HED1	1.38	0.82
33:V:128:GLN:HB3	33:V:129:PRO:HD2	1.61	0.82
32:U:96:GLU:HG2	32:U:102:SER:HB2	0.88	0.82
38:b:804:SQD:H442	38:b:804:SQD:O10	1.77	0.82
22:c:37:LYS:NZ	22:c:37:LYS:HB2	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V:316:LMG:O2	42:V:316:LMG:HC91	1.80	0.82
36:C:205:CLA:HED1	40:C:215:DGD:HD5	1.62	0.82
36:E:315:CLA:H141	36:M:307:CLA:H142	1.61	0.82
36:O:309:CLA:H101	36:O:316:CLA:H41	1.59	0.82
14:N:118:PRO:O	35:N:303:A86:O2	1.98	0.82
36:a:806:CLA:H102	36:a:808:CLA:C9	2.09	0.82
42:j:105:LMG:H421	42:j:105:LMG:C38	2.06	0.82
7:G:199:PHE:CE2	36:G:313:CLA:C2	2.62	0.81
8:H:65:PHE:CE1	31:h:67:ILE:HG12	2.15	0.81
15:P:125:PHE:CE2	36:P:302:CLA:HED1	2.15	0.81
33:V:65:GLU:N	33:V:65:GLU:OE2	2.12	0.81
1:A:196:TRP:HA	1:A:196:TRP:CE3	2.15	0.81
36:A:305:CLA:CED	38:A:315:SQD:O9	2.28	0.81
2:B:136:SER:HB2	36:B:308:CLA:ND	1.94	0.81
11:K:95:PRO:O	11:K:113:VAL:HG11	1.79	0.81
16:R:50:PRO:HB3	17:S:169:LEU:HD21	1.62	0.81
39:h:205:LMT:H6D	39:h:205:LMT:O5B	1.80	0.81
9:I:40:ILE:O	9:I:67:ARG:NH1	2.12	0.81
9:I:118:PHE:CB	36:I:309:CLA:HBC3	2.10	0.81
15:O:54:LEU:HD12	33:V:143:ILE:HG12	1.62	0.81
36:a:816:CLA:H141	36:a:816:CLA:C18	2.11	0.81
36:B:309:CLA:HBD	36:B:309:CLA:CBA	2.09	0.81
2:B:112:ILE:HD12	26:i:4:ASN:HD21	1.42	0.81
12:L:44:GLU:CG	36:L:308:CLA:C1B	2.58	0.81
17:S:176:PHE:CE2	17:S:178:LEU:HD13	2.16	0.81
35:X:314:A86:C14	33:V:45:ALA:HB1	2.09	0.81
35:U:304:A86:C41	36:U:311:CLA:C1D	2.58	0.81
33:V:140:PRO:HB3	35:V:303:A86:C39	2.06	0.81
2:B:66:HIS:CE1	2:B:70:TRP:CD1	2.68	0.81
36:b:816:CLA:O1A	44:b:845:BCR:H361	1.80	0.81
33:V:62:SER:HB2	33:V:63:PRO:HD2	1.63	0.81
9:I:118:PHE:HA	36:I:309:CLA:CBC	2.10	0.81
15:O:196:VAL:CG2	35:O:305:A86:C39	2.58	0.81
35:Q:303:A86:C21	36:Q:310:CLA:C7	2.57	0.81
21:b:133:GLU:OE1	36:b:816:CLA:HED1	1.80	0.81
9:I:104:LEU:CD2	36:I:308:CLA:O1D	2.25	0.81
36:O:309:CLA:C10	36:O:316:CLA:C4	2.59	0.81
15:Q:155:ILE:HG13	35:Q:316:A86:C39	2.08	0.81
2:B:194:LEU:HD11	35:B:303:A86:C23	2.11	0.81
39:B:312:LMT:H52	44:m:101:BCR:C38	2.11	0.81
7:G:70:PHE:HE1	36:G:307:CLA:HBC3	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:460:GLU:OE1	25:f:79:SER:OG	1.97	0.81
33:V:13:ASN:OD1	33:V:14:TYR:N	2.14	0.81
14:N:214:PHE:CE2	35:N:303:A86:C	2.63	0.81
15:Q:152:PHE:CE2	15:Q:153:PRO:CG	2.63	0.81
33:V:58:LEU:CD1	33:V:75:PHE:CE2	2.63	0.81
36:Q:314:CLA:HED3	36:Q:314:CLA:H2A	1.64	0.80
20:a:225:ILE:CD1	36:a:813:CLA:HMD1	2.11	0.80
44:b:843:BCR:H23C	35:h:202:A86:C22	2.11	0.80
10:J:83:VAL:O	10:J:86:TYR:O	1.99	0.80
28:l:126:VAL:O	41:l:208:LHG:C1	2.28	0.80
13:M:77:ARG:CZ	13:M:77:ARG:HB3	2.10	0.80
14:N:184:PHE:CZ	36:N:319:CLA:HMD3	2.13	0.80
34:P:305:DD6:C23	36:P:309:CLA:H2	2.11	0.80
27:j:39:PHE:N	27:j:40:PRO:CD	2.44	0.80
39:E:320:LMT:C3	41:E:322:LHG:H261	2.11	0.80
36:P:319:CLA:HAA2	39:P:320:LMT:C11	2.11	0.80
16:R:175:HIS:HB2	34:R:307:DD6:C26	2.11	0.80
35:X:314:A86:C24	36:V:306:CLA:HHC	2.12	0.80
21:b:706:LEU:HD12	40:b:849:DGD:HB22	1.62	0.80
32:U:126:MET:SD	36:U:311:CLA:H2	2.20	0.80
33:V:158:ARG:HE	36:V:306:CLA:C1D	1.94	0.80
40:C:215:DGD:O4D	40:C:215:DGD:HE4	1.81	0.80
14:N:168:THR:O	14:N:169:LEU:HD13	1.80	0.80
32:U:105:GLY:O	32:U:116:TYR:OH	2.00	0.80
33:V:58:LEU:CB	33:V:75:PHE:CD2	2.64	0.80
15:Q:156:ASP:HB3	17:S:60:LYS:HB2	1.63	0.80
19:W:15:PHE:CE2	34:W:204:DD6:C33	2.65	0.80
23:d:147:LYS:HD2	23:d:147:LYS:N	1.96	0.80
6:F:47:TRP:CZ3	34:F:303:DD6:C22	2.64	0.80
12:L:44:GLU:CG	36:L:308:CLA:C3B	2.59	0.80
14:N:170:PHE:HZ	36:N:318:CLA:C1	1.93	0.80
16:R:218:LEU:HB3	35:R:305:A86:C40	2.12	0.80
32:U:44:ALA:HA	35:U:303:A86:C37	2.11	0.80
33:V:6:GLU:CB	33:V:9:PHE:O	2.20	0.80
19:X:60:PRO:HG3	33:V:173:ILE:CG2	2.12	0.80
20:a:720:GLN:OE1	46:a:903:HOH:O	1.99	0.80
33:V:7:PRO:CB	36:V:305:CLA:HMA1	2.09	0.80
10:J:154:TRP:HB2	36:J:313:CLA:CAD	2.12	0.80
12:L:137:ILE:HD13	34:L:305:DD6:C22	2.10	0.80
20:a:203:MET:HG3	20:a:327:MET:HE1	1.64	0.80
22:c:3:HIS:HA	22:c:70:TRP:CB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:137:CYS:CB	23:d:154:PHE:CE2	2.65	0.80
32:U:97:LEU:O	32:U:97:LEU:HD22	1.82	0.80
15:Q:152:PHE:CD2	36:Q:314:CLA:NC	2.50	0.79
15:Q:152:PHE:CE2	36:Q:314:CLA:C2C	2.66	0.79
27:j:39:PHE:N	27:j:40:PRO:HD3	1.96	0.79
33:V:61:ILE:O	36:V:313:CLA:HBC2	1.80	0.79
36:G:315:CLA:CED	39:a:853:LMT:H5B	2.12	0.79
35:L:307:A86:C33	36:Q:307:CLA:HBC1	2.12	0.79
13:M:144:TRP:CE3	34:M:303:DD6:C23	2.65	0.79
36:I:312:CLA:C7	42:I:315:LMG:H141	2.13	0.79
15:P:34:ASP:CA	15:P:45:LYS:HG2	2.13	0.79
20:a:476:MET:O	20:a:481:ALA:HB3	1.80	0.79
31:h:135:ARG:NH1	36:h:203:CLA:CED	2.41	0.79
32:U:29:ARG:HH22	39:U:315:LMT:H6E	1.48	0.79
33:V:1:THR:H2	33:V:2:PRO:CD	1.95	0.79
33:V:8:VAL:HG23	36:V:305:CLA:C3B	1.95	0.79
3:C:40:LEU:HD11	3:C:59:PHE:CD1	2.16	0.79
41:E:322:LHG:HC61	41:E:322:LHG:HC2	1.62	0.79
37:Q:313:KC1:C1C	41:Q:315:LHG:H291	2.13	0.79
16:R:65:ILE:CD1	16:R:73:THR:CB	2.61	0.79
19:X:120:ALA:HA	33:V:13:ASN:ND2	1.96	0.79
21:b:157:GLN:OE1	29:m:27:GLN:NE2	2.15	0.79
10:J:129:LEU:O	10:J:133:VAL:HG13	1.82	0.79
36:J:312:CLA:C4	42:J:318:LMG:H192	2.13	0.79
15:P:135:GLU:OE1	15:P:140:HIS:HE1	1.65	0.79
20:a:711:ASN:O	25:f:227:ASP:OD1	2.00	0.79
39:B:312:LMT:H52	44:m:101:BCR:H381	1.63	0.79
39:E:320:LMT:O6'	39:E:321:LMT:H12	1.82	0.79
9:I:118:PHE:CB	36:I:309:CLA:CBC	2.61	0.79
36:L:308:CLA:HMC1	36:L:308:CLA:HBC3	1.63	0.79
14:N:184:PHE:CE2	36:N:319:CLA:HMD2	2.18	0.79
41:O:317:LHG:HC62	41:O:317:LHG:HC91	1.65	0.79
16:R:50:PRO:HB2	17:S:169:LEU:HD11	1.62	0.79
21:b:39:GLU:HG3	23:d:202:PHE:CZ	2.17	0.79
39:I:317:LMT:H2B	39:I:317:LMT:H6'2	1.65	0.79
28:l:38:ASP:O	28:l:41:VAL:HG12	1.82	0.79
16:R:63:THR:CG2	16:R:64:THR:N	2.46	0.79
20:a:516:GLY:HA2	20:a:530:PRO:HB3	1.64	0.79
36:a:803:CLA:H91	36:a:806:CLA:C17	2.13	0.79
33:V:8:VAL:CG2	36:V:305:CLA:CMB	2.60	0.79
33:V:138:TRP:CZ3	36:V:308:CLA:C20	2.66	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:113:LYS:HE3	5:E:116:MET:HB2	1.64	0.79
21:b:187:LEU:O	21:b:190:THR:CG2	2.31	0.79
8:H:137:TRP:HE3	36:H:311:CLA:H3A	1.48	0.78
9:I:68:GLU:OE1	9:I:140:PRO:O	2.00	0.78
44:a:844:BCR:H382	42:a:852:LMG:C44	2.13	0.78
27:j:38:THR:HB	27:j:40:PRO:HD3	1.63	0.78
33:V:19:THR:CG2	33:V:24:SER:O	2.31	0.78
33:V:139:ASN:ND2	33:V:142:ASN:HB3	1.95	0.78
20:a:110:LEU:CD1	20:a:159:THR:HA	2.13	0.78
36:B:311:CLA:HED2	36:B:311:CLA:H2A	1.63	0.78
12:L:161:TYR:HE1	40:L:302:DGD:O2E	1.65	0.78
15:Q:152:PHE:CD1	36:Q:314:CLA:C4B	2.66	0.78
36:a:816:CLA:O1A	42:a:852:LMG:O10	2.00	0.78
21:b:461:TYR:CE1	21:b:475:VAL:HG21	2.18	0.78
16:R:92:PHE:HZ	35:R:304:A86:C26	1.95	0.78
36:a:806:CLA:H193	42:j:105:LMG:C24	2.13	0.78
32:U:56:HIS:H	32:U:56:HIS:CD2	2.00	0.78
37:T:310:KC1:C2D	36:T:313:CLA:C3D	2.61	0.78
2:B:85:THR:HG21	36:B:311:CLA:CED	2.13	0.78
17:S:53:ASP:OD2	17:S:56:SER:HA	1.84	0.78
23:d:146:SER:C	23:d:147:LYS:HD2	2.08	0.78
3:C:54:ALA:O	3:C:75:ARG:NH1	2.15	0.78
36:D:307:CLA:HMC1	41:D:318:LHG:C9	2.14	0.78
5:E:72:ILE:HG22	5:E:76:TRP:CD1	2.18	0.78
7:G:210:ARG:NH1	37:G:308:KC1:O1A	2.16	0.78
32:U:25:ILE:HG22	32:U:30:ALA:HB2	1.64	0.78
33:V:139:ASN:CG	36:V:311:CLA:HBA2	2.07	0.78
15:O:198:ALA:C	35:O:305:A86:O5	2.26	0.78
16:R:95:TYR:HE1	16:R:122:PRO:HG2	1.41	0.78
21:b:375:GLN:HA	21:b:375:GLN:NE2	1.94	0.78
41:f:809:LHG:H382	42:V:316:LMG:H321	1.65	0.78
36:a:806:CLA:H71	36:a:808:CLA:H92	1.65	0.78
36:j:102:CLA:H8	36:j:102:CLA:H192	1.64	0.78
4:D:165:LYS:CD	19:W:26:GLN:NE2	2.46	0.78
19:W:154:LEU:HD11	34:W:205:DD6:O1	1.82	0.78
19:X:59:LEU:CA	36:X:315:CLA:HED1	2.13	0.78
36:l:202:CLA:HED1	46:l:303:HOH:O	1.83	0.78
36:B:309:CLA:HBD	36:B:309:CLA:CGA	2.14	0.77
35:I:301:A86:C41	36:K:312:CLA:H171	2.14	0.77
35:X:314:A86:C26	36:V:306:CLA:CHC	2.62	0.77
39:F:320:LMT:H4'	39:F:321:LMT:O6'	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:G:315:CLA:HHC	36:G:315:CLA:HBB1	1.65	0.77
34:W:205:DD6:C26	36:W:212:CLA:C1C	2.62	0.77
4:D:165:LYS:CD	19:W:26:GLN:HE22	1.98	0.77
12:L:161:TYR:HE1	40:L:302:DGD:HO2E	1.29	0.77
35:O:305:A86:C	37:O:313:KC1:CHC	2.62	0.77
15:Q:156:ASP:CB	17:S:60:LYS:HD2	2.13	0.77
20:a:225:ILE:CD1	36:a:813:CLA:HMD3	2.13	0.77
21:b:729:SER:O	21:b:732:PHE:HE1	1.67	0.77
23:d:198:ILE:CD1	23:d:201:LYS:HZ1	1.96	0.77
36:j:102:CLA:H8	36:j:102:CLA:C19	2.13	0.77
32:U:37:ASN:OD1	36:U:310:CLA:HMD1	1.84	0.77
32:U:95:MET:HG3	32:U:109:ALA:O	1.83	0.77
36:A:306:CLA:HHD	36:A:306:CLA:HBC2	1.66	0.77
36:G:315:CLA:HAA2	36:G:315:CLA:C1	2.13	0.77
42:G:324:LMG:C11	42:G:325:LMG:C2	2.62	0.77
17:S:176:PHE:HZ	17:S:178:LEU:CD1	1.91	0.77
20:a:537:ASP:O	20:a:540:VAL:HG12	1.83	0.77
39:K:317:LMT:C2B	39:K:317:LMT:H3'	2.15	0.77
36:a:816:CLA:C5	36:a:816:CLA:H93	2.14	0.77
21:b:3:THR:O	26:i:34:LEU:HG	1.84	0.77
39:E:320:LMT:H2'	39:E:321:LMT:H3'	1.66	0.77
41:G:320:LHG:H111	41:G:320:LHG:H151	1.66	0.77
36:K:307:CLA:H143	37:K:314:KC1:C1C	2.14	0.77
14:N:214:PHE:HD2	35:N:303:A86:C	1.98	0.77
32:U:95:MET:HE3	32:U:95:MET:CA	2.15	0.77
36:V:314:CLA:O1D	36:V:314:CLA:HBA2	1.85	0.77
7:G:41:MET:HB2	7:G:77:SER:HB3	1.66	0.77
36:F:317:CLA:HHC	36:F:317:CLA:HBB1	1.66	0.77
36:I:312:CLA:C1	42:I:315:LMG:H311	2.15	0.77
10:J:87:ILE:HD12	10:J:87:ILE:O	1.85	0.77
19:W:41:ARG:NH2	19:W:140:GLU:OE2	2.16	0.77
33:V:119:TYR:CZ	42:V:316:LMG:C7	2.68	0.77
40:C:215:DGD:HD4	40:C:215:DGD:HE5	1.65	0.77
36:G:307:CLA:CGA	40:L:302:DGD:HG31	2.13	0.77
15:O:199:LEU:CA	35:O:305:A86:O5	2.33	0.77
15:Q:151:VAL:N	36:Q:314:CLA:CED	2.46	0.77
32:U:29:ARG:HH12	39:U:315:LMT:C6'	1.97	0.77
33:V:38:HIS:CB	33:V:161:MET:HE1	2.09	0.77
4:D:61:ARG:HD3	41:E:322:LHG:HC31	1.66	0.76
7:G:32:ALA:HB2	9:I:44:ALA:HA	1.67	0.76
7:G:93:GLU:HA	7:G:93:GLU:OE2	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L:302:DGD:HG2	40:L:302:DGD:O2D	1.85	0.76
36:b:807:CLA:O1A	41:i:104:LHG:C13	2.33	0.76
2:B:112:ILE:CD1	26:i:4:ASN:HD21	1.97	0.76
15:P:159:THR:HG21	16:R:62:SER:HB3	1.66	0.76
21:b:368:ALA:HB1	21:b:724:LEU:CD1	2.14	0.76
3:C:159:LYS:HG2	3:C:163:GLU:HG2	1.66	0.76
21:b:132:GLN:HE22	29:m:6:GLN:NE2	1.83	0.76
21:b:515:ASP:OD1	46:b:901:HOH:O	2.02	0.76
36:M:315:CLA:HBB2	36:M:316:CLA:HBB1	1.66	0.76
37:W:217:KC1:O2D	37:W:217:KC1:CBA	2.34	0.76
36:b:841:CLA:CMB	41:b:850:LHG:C9	2.57	0.76
36:V:308:CLA:H192	36:V:314:CLA:H193	1.67	0.76
11:K:99:ARG:HH21	11:K:113:VAL:CG1	1.98	0.76
15:P:34:ASP:HA	15:P:45:LYS:HG2	1.68	0.76
20:a:336:GLY:HA3	41:a:843:LHG:HC32	1.68	0.76
15:P:159:THR:CG2	16:R:62:SER:CB	2.61	0.76
36:A:314:CLA:HBC3	34:D:301:DD6:C26	2.16	0.76
36:D:307:CLA:HMC1	41:D:318:LHG:HC92	1.67	0.76
36:H:308:CLA:C16	31:h:116:LEU:HD13	2.16	0.76
9:I:50:ASP:OD2	9:I:55:SER:HB3	1.86	0.76
41:Q:315:LHG:O2	41:Q:315:LHG:HC41	1.86	0.76
19:X:117:ARG:HG3	36:X:310:CLA:HED2	1.66	0.76
27:j:15:SER:HG	27:j:19:PHE:HE2	0.78	0.76
20:a:338:PHE:O	20:a:434:ARG:NH1	2.18	0.76
32:U:92:LYS:O	32:U:96:GLU:OE1	2.03	0.76
6:F:99:GLY:O	6:F:100:LEU:HD22	1.86	0.76
23:d:102:ILE:HD12	23:d:154:PHE:CE1	2.21	0.76
1:A:196:TRP:HA	1:A:196:TRP:HE3	1.51	0.76
39:B:312:LMT:H71	44:m:101:BCR:H383	1.66	0.76
10:J:142:MET:HE1	42:J:318:LMG:C6	2.15	0.76
12:L:44:GLU:OE2	36:L:308:CLA:C1B	2.34	0.76
36:Q:314:CLA:CED	36:Q:314:CLA:C2A	2.59	0.76
21:b:156:LEU:HB2	29:m:27:GLN:OE1	1.86	0.76
36:V:314:CLA:HMB2	36:V:314:CLA:H141	1.68	0.76
40:C:215:DGD:HO4E	40:C:215:DGD:HO5E	1.28	0.75
41:D:319:LHG:C21	42:D:320:LMG:H232	2.16	0.75
12:L:44:GLU:HG2	36:L:308:CLA:C1B	2.16	0.75
17:S:210:MET:O	17:S:214:PHE:CD2	2.39	0.75
36:b:836:CLA:H51	36:b:836:CLA:C10	2.14	0.75
14:N:86:MET:HE1	14:N:202:GLU:OE2	1.87	0.75
31:h:118:SER:HB2	35:h:204:A86:O2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:67:PRO:HG3	6:F:150:TRP:CZ3	2.22	0.75
15:P:68:LEU:HG	15:P:147:LEU:CD2	2.17	0.75
15:Q:151:VAL:H	36:Q:314:CLA:HED2	1.51	0.75
33:V:148:ARG:NH2	36:V:305:CLA:CED	2.48	0.75
39:F:321:LMT:C5'	37:O:315:KC1:CED	2.64	0.75
12:L:44:GLU:HG3	36:L:308:CLA:C3B	2.17	0.75
14:N:63:TRP:O	15:O:155:ILE:HG21	1.87	0.75
14:N:169:LEU:HD22	14:N:169:LEU:N	2.01	0.75
14:N:241:MET:HE2	14:N:241:MET:CA	2.13	0.75
15:P:159:THR:CG2	16:R:62:SER:HB3	2.17	0.75
20:a:582:GLY:O	20:a:588:THR:OG1	2.04	0.75
36:V:314:CLA:H122	36:V:314:CLA:C9	2.17	0.75
6:F:166:MET:HB3	6:F:168:LEU:HG	1.68	0.75
34:L:305:DD6:C25	36:L:309:CLA:HHC	2.17	0.75
19:X:60:PRO:HG2	33:V:173:ILE:HD12	1.69	0.75
39:b:851:LMT:O5'	36:f:805:CLA:HBC1	1.86	0.75
28:l:121:THR:HG22	28:l:152:LYS:HZ2	1.50	0.75
36:A:309:CLA:HBB2	42:V:315:LMG:C15	2.14	0.75
36:C:205:CLA:CBD	40:C:215:DGD:HG12	2.16	0.75
39:E:323:LMT:H123	41:G:301:LHG:H151	1.69	0.75
8:H:119:PHE:CZ	36:H:310:CLA:CAD	2.69	0.75
36:K:311:CLA:HBB2	40:L:302:DGD:HB92	1.68	0.75
35:X:314:A86:C2	33:V:161:MET:CE	2.63	0.75
32:U:32:ALA:HB3	39:U:314:LMT:O3B	1.84	0.75
1:A:106:ASP:CB	1:A:195:ASN:HD21	1.98	0.75
3:C:124:GLN:HE22	36:C:210:CLA:C4D	2.00	0.75
14:N:168:THR:OG1	14:N:169:LEU:HD22	1.87	0.75
15:P:168:ARG:NE	37:P:315:KC1:O1A	2.19	0.75
17:S:86:MET:HB3	35:S:304:A86:C7	2.17	0.75
20:a:124:TRP:HE1	39:a:851:LMT:H6E	1.50	0.75
23:d:188:PHE:O	23:d:189:ARG:HG3	1.86	0.75
19:X:60:PRO:CD	36:X:315:CLA:HED2	2.11	0.75
33:V:68:SER:HB3	33:V:73:ILE:H	1.52	0.75
1:A:129:LEU:O	1:A:133:THR:OG1	2.05	0.75
5:E:81:GLU:OE2	5:E:189:ARG:NH2	2.18	0.75
7:G:199:PHE:CD2	36:G:313:CLA:C2	2.69	0.75
36:G:315:CLA:C4	41:G:320:LHG:C24	2.65	0.75
42:G:324:LMG:H112	42:G:325:LMG:C2	2.17	0.75
15:P:159:THR:CB	16:R:62:SER:HB3	2.16	0.75
17:S:89:PHE:CZ	17:S:93:ILE:HD11	2.22	0.74
6:F:213:VAL:CG2	33:V:93:GLU:CD	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:G:321:LHG:O5	41:G:321:LHG:O2	2.05	0.74
39:G:322:LMT:H1B	39:G:322:LMT:C6'	2.10	0.74
36:L:308:CLA:H101	37:L:315:KC1:CAC	2.16	0.74
14:N:214:PHE:CE2	35:N:303:A86:C3	2.64	0.74
20:a:704:GLU:CD	21:b:544:LYS:HB2	2.10	0.74
42:V:315:LMG:H311	42:V:315:LMG:H351	1.69	0.74
1:A:94:GLN:O	1:A:103:HIS:NE2	2.19	0.74
5:E:72:ILE:HG23	39:E:321:LMT:H61	1.68	0.74
12:L:44:GLU:HG2	36:L:308:CLA:C3B	2.16	0.74
12:L:44:GLU:OE2	36:L:308:CLA:C4A	2.34	0.74
21:b:456:PRO:O	21:b:460:GLU:HG3	1.87	0.74
36:P:319:CLA:CAA	39:P:320:LMT:C11	2.65	0.74
23:d:102:ILE:HD12	23:d:154:PHE:CZ	2.22	0.74
36:B:309:CLA:HBA1	36:B:309:CLA:CBD	2.18	0.74
36:D:307:CLA:HBB2	42:E:319:LMG:O10	1.86	0.74
41:Q:315:LHG:O2	41:Q:315:LHG:O9	2.05	0.74
21:b:121:GLN:O	21:b:125:THR:HG23	1.88	0.74
32:U:37:ASN:OD1	36:U:310:CLA:CMD	2.35	0.74
33:V:179:ILE:HD12	33:V:179:ILE:O	1.88	0.74
36:A:314:CLA:HAB	34:D:301:DD6:C7	2.18	0.74
15:P:81:TYR:CZ	15:P:108:PRO:HG2	2.22	0.74
2:B:66:HIS:NE2	2:B:70:TRP:CD1	2.55	0.74
39:h:205:LMT:H6'1	39:h:205:LMT:C6'	2.18	0.74
32:U:96:GLU:CD	32:U:109:ALA:CB	2.60	0.74
9:I:35:LYS:CD	9:I:35:LYS:H	1.98	0.74
9:I:133:LYS:HG3	9:I:138:TYR:CE2	2.23	0.74
35:I:302:A86:C6	36:I:308:CLA:H71	2.15	0.74
36:I:312:CLA:H11	42:I:315:LMG:H311	1.69	0.74
20:a:281:LEU:HB2	36:a:816:CLA:HMA2	1.69	0.74
21:b:398:ASP:O	21:b:402:ASN:ND2	2.20	0.74
36:l:202:CLA:CED	46:l:303:HOH:O	2.35	0.74
36:V:314:CLA:H122	36:V:314:CLA:H91	1.70	0.74
7:G:147:TYR:CD2	7:G:233:THR:HG23	2.22	0.74
17:S:208:LEU:HD21	36:S:309:CLA:HAC2	1.69	0.74
32:U:8:SER:HG	36:U:306:CLA:HED2	1.52	0.74
36:D:307:CLA:H11	37:M:318:KC1:CHB	2.18	0.74
6:F:145:HIS:CG	36:F:317:CLA:HAA2	2.22	0.74
15:P:34:ASP:CB	15:P:45:LYS:HG3	2.16	0.74
20:a:587:GLY:H	21:b:667:ARG:HD3	1.48	0.74
3:C:40:LEU:CD1	3:C:59:PHE:CD1	2.71	0.73
15:P:64:ARG:HG2	15:P:64:ARG:NH1	1.99	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:293:ASN:O	21:b:293:ASN:ND2	2.19	0.73
33:V:18:LEU:HA	33:V:22:TYR:HB2	1.68	0.73
37:G:317:KC1:CBA	39:G:322:LMT:H32	2.18	0.73
35:F:301:A86:C29	36:F:316:CLA:HBD	2.18	0.73
10:J:40:VAL:O	36:J:308:CLA:HED3	1.89	0.73
17:S:52:TYR:CE2	17:S:54:PRO:HG3	2.22	0.73
17:S:76:GLN:O	17:S:79:ILE:CG2	2.33	0.73
36:b:836:CLA:HMB1	36:b:836:CLA:HBB1	1.70	0.73
23:d:205:LYS:C	23:d:206:GLN:HG2	2.11	0.73
41:f:809:LHG:H342	41:f:809:LHG:H291	1.68	0.73
8:H:119:PHE:CD1	8:H:121:SER:HB3	2.24	0.73
14:N:89:PHE:CE2	14:N:93:ILE:HD11	2.24	0.73
21:b:222:LYS:N	21:b:223:PRO:CD	2.51	0.73
25:f:152:ASP:OD1	36:f:805:CLA:CMD	2.36	0.73
33:V:116:LYS:H	33:V:116:LYS:HD2	1.54	0.73
7:G:153:LEU:CD1	36:G:311:CLA:CAA	2.66	0.73
36:K:310:CLA:HHD	36:K:310:CLA:CBC	2.15	0.73
25:f:206:LEU:HD22	36:f:804:CLA:HMD3	1.69	0.73
36:U:306:CLA:O1A	36:U:306:CLA:H3A	1.87	0.73
39:U:314:LMT:C2'	39:U:315:LMT:H2'	2.19	0.73
33:V:140:PRO:C	33:V:141:LEU:HG	2.13	0.73
11:K:95:PRO:HB3	36:K:310:CLA:HED3	1.71	0.73
13:M:108:MET:HE2	35:M:304:A86:C2	2.18	0.73
15:O:55:GLY:CA	33:V:143:ILE:HA	2.19	0.73
39:a:853:LMT:H22	39:a:853:LMT:O2'	1.88	0.73
36:b:817:CLA:H121	36:b:817:CLA:H91	1.70	0.73
9:I:118:PHE:HD1	36:I:309:CLA:HBC1	1.53	0.73
42:J:318:LMG:H351	42:J:318:LMG:H221	1.71	0.73
25:f:206:LEU:HB3	36:f:804:CLA:OBD	1.89	0.73
32:U:67:ILE:HB	32:U:148:HIS:CD2	2.22	0.73
2:B:207:GLN:OE1	2:B:207:GLN:HA	1.87	0.73
3:C:126:PHE:HA	35:C:203:A86:C22	2.19	0.73
36:I:306:CLA:H91	36:I:306:CLA:H121	1.71	0.73
21:b:516:PHE:HA	36:b:837:CLA:HED1	1.69	0.73
38:b:804:SQD:H101	44:b:843:BCR:H313	1.69	0.73
32:U:96:GLU:HG3	32:U:109:ALA:HB2	1.69	0.73
42:G:324:LMG:H292	42:G:325:LMG:O10	1.89	0.73
36:L:308:CLA:C2	37:L:315:KC1:OBD	2.37	0.73
20:a:274:TRP:HB2	36:a:816:CLA:H12	1.71	0.73
14:N:143:TRP:CZ2	14:N:169:LEU:O	2.34	0.72
17:S:76:GLN:C	17:S:79:ILE:HG22	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:831:CLA:HBB1	36:a:832:CLA:H2	1.70	0.72
33:V:132:LEU:CD1	36:V:310:CLA:HED3	2.19	0.72
42:D:320:LMG:HC91	42:D:320:LMG:H111	1.70	0.72
36:F:317:CLA:H12	36:F:317:CLA:H71	1.69	0.72
8:H:137:TRP:CE3	36:H:311:CLA:H3A	2.23	0.72
35:M:304:A86:C37	36:M:316:CLA:CED	2.66	0.72
36:a:830:CLA:HBA2	41:a:843:LHG:HC92	1.70	0.72
34:M:303:DD6:C21	36:M:309:CLA:CMB	2.67	0.72
15:P:152:PHE:HB3	15:P:153:PRO:HD3	1.70	0.72
20:a:247:GLU:O	20:a:251:ASN:OD1	2.06	0.72
3:C:126:PHE:CA	35:C:203:A86:C22	2.68	0.72
5:E:113:LYS:CE	5:E:116:MET:HB2	2.20	0.72
36:H:308:CLA:H201	31:h:112:TRP:HZ3	1.53	0.72
36:X:315:CLA:C2D	35:V:301:A86:C26	2.68	0.72
41:i:104:LHG:HC81	41:l:208:LHG:C17	2.16	0.72
32:U:112:TRP:NE1	35:U:304:A86:C40	2.53	0.72
33:V:65:GLU:HA	33:V:75:PHE:CE2	2.20	0.72
9:I:144:LEU:HD23	9:I:144:LEU:C	2.14	0.72
15:P:33:VAL:O	36:P:309:CLA:HED1	1.88	0.72
16:R:175:HIS:HB2	34:R:307:DD6:C24	2.19	0.72
25:f:158:GLU:HA	27:j:38:THR:HG21	1.70	0.72
31:h:119:PHE:O	31:h:122:PRO:HG2	1.88	0.72
32:U:150:ILE:CG2	32:U:153:ALA:CB	2.63	0.72
6:F:145:HIS:CG	36:F:317:CLA:CAA	2.73	0.72
12:L:198:LEU:HD12	36:L:308:CLA:HED2	1.72	0.72
40:L:302:DGD:O3E	40:L:302:DGD:HE62	1.90	0.72
14:N:170:PHE:CZ	36:N:318:CLA:C1	2.73	0.72
36:j:102:CLA:H192	36:j:102:CLA:H122	1.71	0.72
1:A:197:VAL:CG2	1:A:198:THR:HG23	2.19	0.72
36:C:207:CLA:HBB1	36:C:207:CLA:HMB3	1.71	0.72
14:N:221:THR:HG21	35:N:305:A86:C19	2.19	0.72
15:O:54:LEU:CD1	33:V:143:ILE:CG2	2.19	0.72
15:Q:156:ASP:O	17:S:60:LYS:CD	2.38	0.72
19:X:59:LEU:CD2	35:V:301:A86:C41	2.68	0.72
21:b:421:LEU:HD13	21:b:531:LEU:HA	1.72	0.72
42:V:316:LMG:O2	42:V:316:LMG:O10	2.05	0.72
3:C:124:GLN:OE1	36:C:210:CLA:C4C	2.38	0.72
4:D:73:GLU:OE2	4:D:144:MET:HE1	1.90	0.72
36:F:317:CLA:CBC	42:J:318:LMG:H341	2.19	0.72
14:N:221:THR:HB	35:N:305:A86:C19	2.18	0.72
39:b:851:LMT:C1	36:f:805:CLA:HBC3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:44:ALA:CA	35:U:303:A86:C37	2.67	0.72
33:V:61:ILE:O	36:V:313:CLA:CBC	2.38	0.72
7:G:156:GLN:HE22	7:G:158:SER:CB	2.03	0.72
11:K:180:LYS:NZ	36:K:307:CLA:O1D	2.21	0.72
20:a:704:GLU:OE2	21:b:544:LYS:HB2	1.90	0.72
32:U:77:TRP:CE2	36:U:308:CLA:H3A	2.25	0.72
36:F:317:CLA:HBB2	42:J:318:LMG:C15	2.11	0.71
36:G:315:CLA:H43	41:G:320:LHG:C24	2.19	0.71
35:J:306:A86:C14	42:J:319:LMG:H311	2.19	0.71
17:S:89:PHE:HE2	37:S:316:KC1:CBB	2.03	0.71
35:S:304:A86:C21	36:S:315:CLA:NB	2.53	0.71
41:f:808:LHG:H322	42:V:316:LMG:H312	1.70	0.71
40:L:302:DGD:O6E	40:L:302:DGD:O4D	2.05	0.71
41:f:808:LHG:H331	42:V:316:LMG:H332	1.72	0.71
42:V:315:LMG:H311	42:V:315:LMG:C35	2.20	0.71
35:C:203:A86:C28	29:m:23:LYS:NZ	2.53	0.71
34:M:303:DD6:C21	36:M:309:CLA:HMB1	2.20	0.71
34:M:303:DD6:C36	36:M:307:CLA:H12	2.20	0.71
15:O:54:LEU:CD1	33:V:143:ILE:CG1	2.67	0.71
22:c:3:HIS:O	30:g:131:UNK:CB	2.38	0.71
36:Q:310:CLA:H41	17:S:55:LEU:HA	1.72	0.71
41:b:850:LHG:C7	41:b:850:LHG:H111	2.18	0.71
25:f:176:VAL:HG11	25:f:206:LEU:HD23	1.71	0.71
32:U:112:TRP:CZ2	35:U:304:A86:O3	2.44	0.71
33:V:143:ILE:HD13	36:V:311:CLA:C2	2.14	0.71
10:J:50:PHE:CE2	10:J:52:PHE:HB2	2.26	0.71
19:X:129:ASP:OD1	19:X:131:GLU:HB2	1.90	0.71
20:a:696:ARG:CG	20:a:724:LEU:O	2.38	0.71
36:j:101:CLA:H61	42:j:105:LMG:H361	1.70	0.71
28:l:121:THR:HG22	28:l:152:LYS:NZ	2.04	0.71
36:Q:314:CLA:CED	36:Q:314:CLA:H2A	2.20	0.71
36:a:816:CLA:C3D	42:a:852:LMG:HC91	2.21	0.71
36:b:836:CLA:H121	36:b:836:CLA:C9	2.20	0.71
36:U:306:CLA:H3A	36:U:306:CLA:CGA	2.20	0.71
3:C:159:LYS:HG2	3:C:163:GLU:CG	2.21	0.71
12:L:199:LYS:CG	36:L:308:CLA:HED1	2.20	0.71
15:O:54:LEU:HD13	33:V:143:ILE:CG1	2.21	0.71
35:Q:316:A86:C37	36:S:311:CLA:C1	2.68	0.71
20:a:254:LEU:O	20:a:254:LEU:HD12	1.89	0.71
32:U:63:VAL:HG11	32:U:69:ALA:CB	2.21	0.71
2:B:209:PRO:HA	39:B:312:LMT:H3'	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:173:THR:HG23	7:G:192:PHE:CE1	2.26	0.71
15:Q:196:VAL:HG22	35:Q:303:A86:C38	2.21	0.71
41:Q:315:LHG:HC82	41:Q:315:LHG:HC62	1.73	0.71
36:j:101:CLA:H52	42:j:105:LMG:H362	1.72	0.71
6:F:214:PHE:CE1	36:V:309:CLA:HMB3	2.25	0.71
7:G:107:LEU:O	7:G:111:ARG:HG2	1.91	0.71
41:G:321:LHG:O2	41:G:321:LHG:HC62	1.91	0.71
36:L:308:CLA:HBC3	36:L:308:CLA:CMC	2.20	0.71
35:Q:316:A86:C40	17:S:63:TRP:HZ2	1.99	0.71
16:R:95:TYR:CD1	16:R:122:PRO:HG2	2.24	0.71
36:a:816:CLA:H93	36:a:816:CLA:H51	1.72	0.71
23:d:92:ARG:HD3	23:d:96:VAL:HG21	1.71	0.71
42:E:318:LMG:H382	36:a:811:CLA:HBB2	1.73	0.70
7:G:56:ARG:NH2	7:G:60:LEU:O	2.23	0.70
36:K:307:CLA:H42	37:K:314:KC1:CGD	2.21	0.70
14:N:168:THR:OG1	14:N:169:LEU:CD2	2.38	0.70
14:N:168:THR:C	14:N:169:LEU:HD22	2.15	0.70
16:R:65:ILE:HD13	16:R:73:THR:CB	2.21	0.70
33:V:158:ARG:NE	36:V:306:CLA:C1D	2.54	0.70
36:V:308:CLA:H192	36:V:314:CLA:C19	2.21	0.70
34:E:306:DD6:C9	36:E:311:CLA:HBC1	2.21	0.70
36:X:315:CLA:CMC	35:V:301:A86:C7	2.69	0.70
27:j:19:PHE:HZ	36:j:102:CLA:H93	1.55	0.70
37:F:308:KC1:CBA	39:F:321:LMT:H3'	2.22	0.70
8:H:44:PRO:HG2	8:H:57:ASP:HB3	1.74	0.70
32:U:46:VAL:HG12	36:U:308:CLA:HMC2	1.72	0.70
32:U:63:VAL:HG13	32:U:72:GLN:CB	2.21	0.70
39:E:320:LMT:H31	41:E:322:LHG:C26	2.20	0.70
14:N:86:MET:HE1	14:N:202:GLU:CG	2.20	0.70
41:O:317:LHG:H302	36:V:313:CLA:H121	1.73	0.70
15:Q:155:ILE:HG21	17:S:62:PHE:HE1	1.53	0.70
23:d:198:ILE:CD1	23:d:201:LYS:NZ	2.55	0.70
33:V:111:THR:CB	33:V:117:LEU:CD1	2.65	0.70
33:V:119:TYR:CG	42:V:316:LMG:HC1	2.26	0.70
36:G:315:CLA:HED1	39:a:853:LMT:C6B	2.22	0.70
11:K:53:ARG:HG2	11:K:53:ARG:NH1	2.06	0.70
14:N:52:TYR:HE2	35:N:303:A86:O3	1.75	0.70
36:C:205:CLA:CAD	40:C:215:DGD:HG12	2.20	0.70
6:F:214:PHE:O	6:F:215:ASN:C	2.32	0.70
34:L:305:DD6:C25	36:L:309:CLA:CMC	2.69	0.70
35:Q:316:A86:C26	36:S:311:CLA:O1D	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:564:GLY:O	46:b:903:HOH:O	2.10	0.70
21:b:635:ASN:HB2	21:b:636:PRO:CD	2.16	0.70
33:V:12:GLU:O	33:V:13:ASN:OD1	2.09	0.70
34:D:303:DD6:C2	36:D:309:CLA:HBB1	2.18	0.70
34:L:305:DD6:C26	36:L:309:CLA:HHC	2.21	0.70
19:X:107:THR:HG21	33:V:17:LYS:HG3	1.74	0.70
20:a:336:GLY:CA	41:a:843:LHG:HC32	2.22	0.70
32:U:47:GLY:O	32:U:51:PRO:HD3	1.92	0.70
33:V:116:LYS:HD2	33:V:116:LYS:N	2.06	0.70
42:E:318:LMG:H311	36:a:819:CLA:CGA	2.22	0.70
9:I:144:LEU:HD22	9:I:146:ALA:HB2	1.73	0.70
14:N:63:TRP:CH2	36:N:317:CLA:HMB2	2.27	0.70
14:N:208:LEU:HD22	35:N:304:A86:C	2.21	0.70
35:Q:316:A86:O3	17:S:62:PHE:CG	2.44	0.70
20:a:587:GLY:N	21:b:667:ARG:HH21	1.89	0.70
27:j:24:GLY:O	27:j:28:GLU:HG2	1.91	0.70
33:V:139:ASN:OD1	36:V:311:CLA:HBA2	1.92	0.70
41:a:850:LHG:HC42	46:a:923:HOH:O	1.91	0.70
21:b:371:TYR:CD2	46:b:944:HOH:O	2.44	0.70
32:U:31:ARG:O	32:U:31:ARG:HD3	1.92	0.70
6:F:153:MET:HE2	31:h:57:GLU:OE2	1.87	0.70
36:F:317:CLA:CAB	42:J:318:LMG:HC92	2.21	0.70
11:K:53:ARG:HG2	11:K:53:ARG:HH11	1.56	0.70
19:W:104:ARG:CB	36:W:215:CLA:CAD	2.69	0.70
39:b:851:LMT:C5'	36:f:805:CLA:HBC1	2.22	0.70
39:U:314:LMT:O2'	39:U:315:LMT:C1'	2.40	0.70
39:U:314:LMT:O2'	39:U:315:LMT:O1'	2.10	0.70
4:D:53:GLY:O	36:D:308:CLA:HED2	1.92	0.69
39:G:323:LMT:H41	36:P:301:CLA:HED2	1.73	0.69
37:T:310:KC1:C2D	36:T:313:CLA:CAD	2.70	0.69
24:e:26:VAL:HG21	24:e:41:ARG:HD2	1.73	0.69
3:C:40:LEU:HD21	36:C:205:CLA:C3C	2.22	0.69
16:R:92:PHE:HE1	16:R:217:PHE:CE2	2.10	0.69
41:a:850:LHG:H251	41:a:850:LHG:H121	1.74	0.69
41:E:322:LHG:HC2	41:E:322:LHG:C6	2.23	0.69
35:J:306:A86:C23	42:J:319:LMG:C29	2.70	0.69
12:L:199:LYS:HG2	36:L:308:CLA:HED1	1.72	0.69
15:O:154:PRO:O	15:O:155:ILE:O	2.11	0.69
15:P:34:ASP:HB3	15:P:45:LYS:HD3	1.73	0.69
16:R:38:LYS:NZ	16:R:61:GLY:O	2.26	0.69
36:E:308:CLA:HBC1	7:G:168:PHE:CE2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:165:ILE:O	9:I:169:ARG:HG3	1.92	0.69
19:X:127:THR:CB	33:V:9:PHE:HE1	2.05	0.69
39:b:851:LMT:H21	36:f:805:CLA:HBC3	1.72	0.69
23:d:104:TRP:CD1	23:d:150:ILE:CD1	2.75	0.69
33:V:143:ILE:H	33:V:143:ILE:CD1	2.00	0.69
1:A:179:LYS:HE3	36:A:306:CLA:O1D	1.92	0.69
15:P:34:ASP:CB	15:P:45:LYS:HD3	2.23	0.69
17:S:79:ILE:CD1	17:S:162:GLY:HA3	2.20	0.69
19:W:117:ARG:HB2	19:W:123:PHE:HB2	1.75	0.69
20:a:662:GLN:HE22	20:a:752:ARG:HH11	1.39	0.69
25:f:158:GLU:HA	27:j:38:THR:HG22	1.73	0.69
29:m:24:LEU:O	29:m:24:LEU:HD22	1.92	0.69
31:h:134:GLN:OE1	31:h:134:GLN:HA	1.91	0.69
4:D:152:GLU:OE1	4:D:152:GLU:HA	1.93	0.69
32:U:4:MET:HE1	32:U:27:ALA:HB1	1.72	0.69
9:I:118:PHE:CD1	36:I:309:CLA:HBC1	2.28	0.69
36:a:816:CLA:H193	36:a:816:CLA:C14	2.16	0.69
21:b:414:LYS:HZ1	25:f:235:ALA:HB3	1.53	0.69
2:B:85:THR:HG21	36:B:311:CLA:HED3	1.74	0.69
6:F:50:LEU:HD23	41:f:809:LHG:H102	1.72	0.69
7:G:173:THR:CG2	7:G:192:PHE:CE1	2.75	0.69
9:I:113:VAL:CG1	36:I:309:CLA:O1D	2.41	0.69
39:I:318:LMT:C11	42:a:852:LMG:H272	2.18	0.69
17:S:143:TRP:HD1	17:S:164:TYR:CE1	2.11	0.69
32:U:4:MET:SD	32:U:27:ALA:HB2	2.33	0.69
32:U:101:SER:OG	32:U:105:GLY:HA3	1.92	0.69
33:V:18:LEU:N	33:V:18:LEU:HD23	2.07	0.69
6:F:91:TRP:CH2	41:O:318:LHG:H142	2.23	0.69
6:F:155:THR:HG22	36:F:317:CLA:H93	1.75	0.69
9:I:176:MET:HE3	36:I:307:CLA:CAB	2.23	0.69
36:K:309:CLA:C11	39:K:318:LMT:H123	2.22	0.69
14:N:103:ALA:O	35:N:302:A86:O3	2.10	0.69
35:N:303:A86:C41	36:N:308:CLA:H152	2.22	0.69
15:Q:155:ILE:CG2	17:S:60:LYS:HZ3	1.77	0.69
36:U:310:CLA:HMA2	39:U:314:LMT:H1'	1.73	0.69
36:F:317:CLA:HBC2	42:J:318:LMG:H341	1.73	0.69
7:G:99:LEU:HD22	7:G:99:LEU:O	1.93	0.69
19:W:15:PHE:HE2	34:W:204:DD6:C33	2.05	0.69
21:b:455:GLU:OE2	21:b:460:GLU:OE2	2.11	0.69
30:g:138:UNK:O	30:g:139:UNK:C	2.41	0.69
1:A:160:GLY:O	1:A:163:VAL:CG1	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:204:PHE:O	4:D:206:TYR:CZ	2.45	0.68
42:E:318:LMG:H162	36:G:319:CLA:HAA1	1.74	0.68
12:L:137:ILE:CD1	34:L:305:DD6:C23	2.71	0.68
35:S:304:A86:C12	36:S:321:CLA:O2A	2.41	0.68
23:d:137:CYS:C	23:d:154:PHE:CE2	2.72	0.68
7:G:156:GLN:NE2	7:G:158:SER:N	2.39	0.68
16:R:65:ILE:HD11	16:R:73:THR:OG1	1.93	0.68
21:b:401:LEU:O	21:b:401:LEU:HD22	1.93	0.68
21:b:414:LYS:HZ1	25:f:235:ALA:CB	2.05	0.68
26:i:26:PHE:CE2	28:l:122:ILE:HG22	2.29	0.68
10:J:89:THR:CG2	10:J:107:SER:HB2	2.23	0.68
11:K:162:GLY:O	12:L:61:GLN:NE2	2.25	0.68
15:Q:152:PHE:CD2	15:Q:153:PRO:HD2	2.29	0.68
36:a:825:CLA:HAA2	36:a:826:CLA:OBD	1.94	0.68
41:a:850:LHG:HC61	41:a:850:LHG:C3	2.21	0.68
36:l:204:CLA:HHC	36:l:204:CLA:CBB	2.22	0.68
15:P:159:THR:CG2	16:R:62:SER:HB2	2.22	0.68
15:Q:151:VAL:CA	36:Q:314:CLA:HED1	2.23	0.68
15:Q:156:ASP:HB3	17:S:60:LYS:CD	2.18	0.68
17:S:177:VAL:HG12	36:S:320:CLA:CED	2.24	0.68
36:T:308:CLA:H2A	36:T:308:CLA:HED3	1.76	0.68
19:W:117:ARG:HA	19:W:121:ILE:HG13	1.76	0.68
19:X:53:GLN:OE1	36:X:308:CLA:C4B	2.40	0.68
20:a:336:GLY:N	41:a:843:LHG:HC32	2.08	0.68
36:V:314:CLA:HBC1	42:V:315:LMG:H292	1.75	0.68
1:A:196:TRP:NE1	36:A:314:CLA:C2D	2.56	0.68
12:L:43:ILE:CG2	12:L:44:GLU:OE2	2.42	0.68
36:D:309:CLA:H41	36:D:309:CLA:C7	2.20	0.68
34:L:305:DD6:C25	36:L:309:CLA:HMC2	2.23	0.68
34:M:303:DD6:C21	36:M:309:CLA:C2B	2.71	0.68
16:R:95:TYR:CE1	16:R:122:PRO:CG	2.72	0.68
35:S:304:A86:C9	36:S:315:CLA:HMC2	2.23	0.68
21:b:414:LYS:HZ3	25:f:235:ALA:HB3	1.58	0.68
25:f:218:ARG:HH12	41:f:808:LHG:C6	2.04	0.68
32:U:101:SER:HB3	32:U:107:GLU:O	1.94	0.68
7:G:119:GLY:O	7:G:123:THR:HG23	1.94	0.68
10:J:142:MET:CE	42:J:318:LMG:HC61	2.20	0.68
14:N:241:MET:CG	35:N:305:A86:C9	2.72	0.68
21:b:680:ALA:O	21:b:684:THR:HG23	1.94	0.68
36:b:807:CLA:O1A	41:i:104:LHG:C14	2.42	0.68
36:F:312:CLA:C4	31:h:88:VAL:HG13	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:100:SER:HB2	9:I:188:TYR:CE2	2.28	0.68
35:S:304:A86:C9	36:S:315:CLA:CMC	2.72	0.68
20:a:715:PHE:HA	25:f:185:ARG:HH22	1.59	0.68
39:f:807:LMT:O2'	39:f:807:LMT:H11	1.93	0.68
27:j:19:PHE:CE1	36:j:102:CLA:H91	2.28	0.68
33:V:144:LYS:HG3	33:V:146:THR:HG23	1.75	0.68
36:H:307:CLA:CBC	35:J:301:A86:C22	2.72	0.68
15:O:55:GLY:HA2	33:V:143:ILE:CA	2.24	0.68
21:b:515:ASP:OD2	21:b:596:LYS:NZ	2.25	0.68
26:i:25:LEU:CD2	44:i:103:BCR:HC8	2.23	0.68
9:I:92:HIS:HE1	9:I:99:LEU:HD22	1.58	0.68
9:I:93:PRO:HD3	36:I:308:CLA:HMD1	1.76	0.67
35:I:302:A86:C5	36:I:308:CLA:C4	2.63	0.67
13:M:203:LYS:NZ	35:M:304:A86:C39	2.58	0.67
36:b:817:CLA:H91	36:b:817:CLA:C12	2.23	0.67
25:f:218:ARG:NH1	41:f:809:LHG:HC5	2.06	0.67
28:l:71:LEU:HD21	39:U:315:LMT:H22	1.76	0.67
34:D:303:DD6:C35	36:D:308:CLA:H12	2.24	0.67
7:G:163:LEU:HD13	39:a:853:LMT:H72	1.74	0.67
14:N:170:PHE:CD2	14:N:178:LEU:O	2.48	0.67
16:R:63:THR:HG22	16:R:65:ILE:N	2.07	0.67
42:I:315:LMG:H161	36:a:822:CLA:CHB	2.24	0.67
20:a:110:LEU:HD12	20:a:159:THR:HA	1.76	0.67
32:U:95:MET:HE2	32:U:100:LYS:CE	2.24	0.67
33:V:138:TRP:CH2	35:V:304:A86:O5	2.47	0.67
4:D:161:LEU:HD23	19:W:28:LYS:HE2	1.76	0.67
36:G:315:CLA:H43	41:G:320:LHG:H241	1.72	0.67
39:K:317:LMT:H3'	39:K:317:LMT:H2B	1.77	0.67
15:Q:73:VAL:HG13	34:Q:302:DD6:C12	2.24	0.67
21:b:371:TYR:HD2	46:b:944:HOH:O	1.77	0.67
1:A:105:ASP:O	1:A:201:PRO:HB3	1.94	0.67
8:H:119:PHE:CD1	8:H:121:SER:CB	2.76	0.67
17:S:167:PHE:HB2	17:S:171:ARG:HH21	1.58	0.67
2:B:96:ASP:OD2	2:B:99:VAL:HG12	1.94	0.67
14:N:86:MET:CE	14:N:202:GLU:HG2	2.23	0.67
35:Q:303:A86:C12	36:Q:308:CLA:H193	2.24	0.67
16:R:95:TYR:HE1	16:R:122:PRO:CG	2.07	0.67
20:a:110:LEU:HD11	20:a:159:THR:HA	1.76	0.67
20:a:430:ASN:ND2	20:a:433:ASP:H	1.93	0.67
21:b:320:GLY:O	21:b:324:THR:HG23	1.94	0.67
21:b:680:ALA:O	21:b:684:THR:CG2	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:729:SER:O	21:b:732:PHE:CD1	2.48	0.67
23:d:113:GLU:H	23:d:143:ARG:HE	1.40	0.67
36:A:307:CLA:CBC	34:D:301:DD6:C22	2.72	0.67
35:C:204:A86:C35	40:C:215:DGD:O2E	2.43	0.67
36:K:307:CLA:HHC	36:K:307:CLA:CBB	2.25	0.67
15:Q:152:PHE:CD2	15:Q:153:PRO:CD	2.78	0.67
21:b:706:LEU:CD1	40:b:849:DGD:HB22	2.24	0.67
13:M:108:MET:HE1	36:M:312:CLA:HAB	1.75	0.67
19:X:59:LEU:HD21	35:V:301:A86:C41	2.25	0.67
20:a:553:LEU:O	20:a:553:LEU:HD22	1.95	0.67
34:A:303:DD6:C21	34:D:301:DD6:C36	2.73	0.67
5:E:109:MET:O	5:E:121:GLN:NE2	2.28	0.67
15:P:125:PHE:HE2	36:P:302:CLA:HED1	1.55	0.67
15:P:164:GLN:NE2	15:P:168:ARG:HH22	1.93	0.67
15:Q:155:ILE:CG2	17:S:62:PHE:CD1	2.63	0.67
32:U:140:GLY:HA2	35:U:304:A86:C21	2.25	0.67
33:V:148:ARG:HH21	36:V:305:CLA:HED1	1.59	0.67
1:A:196:TRP:NE1	36:A:314:CLA:C3D	2.58	0.67
41:D:319:LHG:H141	41:D:319:LHG:H182	1.75	0.67
39:K:317:LMT:O2B	39:K:317:LMT:H5'	1.95	0.66
15:P:77:ALA:HB1	34:P:305:DD6:C41	2.25	0.66
15:P:81:TYR:CE1	15:P:108:PRO:HG2	2.30	0.66
15:Q:40:THR:HG21	15:Q:174:ASN:HD21	1.61	0.66
19:X:60:PRO:CG	33:V:173:ILE:CG2	2.71	0.66
32:U:95:MET:O	32:U:100:LYS:HB3	1.95	0.66
33:V:143:ILE:HD12	33:V:143:ILE:N	2.03	0.66
6:F:42:VAL:O	6:F:42:VAL:HG12	1.95	0.66
6:F:179:ARG:HH22	37:F:315:KC1:CED	2.08	0.66
39:F:320:LMT:O3'	39:F:321:LMT:C5'	2.42	0.66
14:N:221:THR:CB	35:N:305:A86:C19	2.73	0.66
34:W:205:DD6:C26	36:W:212:CLA:HHC	2.25	0.66
36:b:833:CLA:H43	41:j:104:LHG:O9	1.96	0.66
2:B:124:VAL:CG1	35:B:301:A86:C37	2.72	0.66
9:I:61:GLU:OE2	41:I:316:LHG:HC11	1.95	0.66
11:K:89:THR:HG21	34:K:305:DD6:C8	2.25	0.66
34:K:304:DD6:C7	36:K:309:CLA:HAB	2.25	0.66
13:M:75:ILE:HG13	41:R:323:LHG:H161	1.77	0.66
15:O:40:THR:HG21	15:O:174:ASN:HD21	1.60	0.66
36:Q:314:CLA:CHA	36:Q:314:CLA:HED2	2.26	0.66
20:a:434:ARG:NH1	36:a:830:CLA:OBD	2.28	0.66
36:a:827:CLA:H151	36:a:848:CLA:H202	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:l:208:LHG:HC61	41:l:208:LHG:C8	2.11	0.66
33:V:57:THR:HG22	36:V:308:CLA:O2D	1.95	0.66
36:A:306:CLA:H142	36:A:306:CLA:C10	2.18	0.66
23:d:101:VAL:CG2	23:d:128:LEU:HD12	2.25	0.66
36:U:306:CLA:HMB1	36:U:306:CLA:C4	2.20	0.66
36:U:306:CLA:H41	36:U:307:CLA:CBA	2.24	0.66
10:J:50:PHE:CD2	10:J:52:PHE:HB2	2.30	0.66
3:C:70:ASP:OD2	21:b:159:LYS:HE2	1.94	0.66
36:G:315:CLA:HHC	36:G:315:CLA:CBB	2.26	0.66
35:O:301:A86:C5	41:O:318:LHG:H161	2.25	0.66
15:Q:77:ALA:HB1	34:Q:302:DD6:C23	2.26	0.66
41:f:808:LHG:H351	42:V:316:LMG:C35	2.21	0.66
36:F:312:CLA:H162	39:h:205:LMT:H111	1.78	0.66
21:b:372:THR:HG23	21:b:590:THR:HG21	1.78	0.66
36:U:306:CLA:H41	36:U:307:CLA:HBA1	1.78	0.66
37:G:317:KC1:CGA	39:G:322:LMT:H32	2.25	0.66
9:I:118:PHE:CA	36:I:309:CLA:CBC	2.73	0.66
14:N:86:MET:SD	36:N:313:CLA:HMC3	2.35	0.66
16:R:175:HIS:HD2	34:R:307:DD6:C1	1.99	0.66
17:S:208:LEU:HD11	36:S:309:CLA:HMD3	1.78	0.66
23:d:114:MET:HB2	23:d:117:GLY:C	2.20	0.66
36:j:102:CLA:H91	36:j:102:CLA:C12	2.25	0.66
33:V:132:LEU:HD13	36:V:310:CLA:HED3	1.77	0.66
42:V:315:LMG:H351	42:V:315:LMG:C31	2.23	0.66
36:A:307:CLA:HBC1	34:D:301:DD6:C22	2.26	0.66
42:D:320:LMG:C22	42:D:320:LMG:H262	2.26	0.66
41:E:322:LHG:H252	41:E:322:LHG:C10	2.19	0.66
15:P:34:ASP:CA	15:P:45:LYS:CG	2.74	0.66
21:b:396:ASP:HA	23:d:198:ILE:HD13	1.77	0.66
1:A:66:TYR:CE2	42:j:105:LMG:C9	2.78	0.66
36:D:306:CLA:O2A	42:E:319:LMG:HC61	1.95	0.66
35:S:304:A86:C28	37:S:316:KC1:CBC	2.74	0.66
21:b:488:GLY:C	21:b:493:LEU:HB2	2.21	0.66
25:f:152:ASP:OD1	36:f:805:CLA:HMD1	1.96	0.66
29:m:23:LYS:HG3	42:m:102:LMG:O3	1.96	0.66
31:h:93:GLN:HE22	39:h:205:LMT:H2'	1.61	0.66
36:V:314:CLA:HBB1	36:V:314:CLA:CHC	2.19	0.66
2:B:186:MET:O	2:B:190:ARG:HG3	1.95	0.65
9:I:67:ARG:NH2	9:I:70:GLU:OE1	2.29	0.65
16:R:180:ASN:O	34:R:308:DD6:O4	2.13	0.65
21:b:558:CYS:SG	45:b:803:SF4:FE4	1.87	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:b:851:LMT:O5'	36:f:805:CLA:CBC	2.43	0.65
33:V:52:HIS:NE2	33:V:82:SER:O	2.29	0.65
7:G:153:LEU:CD1	36:G:311:CLA:HAA2	2.26	0.65
36:I:306:CLA:CGA	36:I:306:CLA:H3A	2.26	0.65
16:R:66:TRP:CD1	35:R:305:A86:C23	2.79	0.65
20:a:348:GLU:CD	20:a:348:GLU:H	2.03	0.65
36:b:836:CLA:H91	36:b:836:CLA:C12	2.22	0.65
10:J:112:ASP:OD1	35:J:306:A86:C39	2.44	0.65
44:a:844:BCR:H271	42:a:852:LMG:C44	2.25	0.65
21:b:39:GLU:HG3	23:d:202:PHE:CE2	2.31	0.65
36:b:836:CLA:H101	36:b:836:CLA:C5	2.12	0.65
28:l:86:ILE:HD11	28:l:163:ALA:HA	1.77	0.65
35:L:307:A86:C40	36:Q:307:CLA:HBC1	2.26	0.65
15:P:40:THR:HG21	15:P:174:ASN:HD21	1.61	0.65
16:R:50:PRO:HB2	17:S:169:LEU:HD21	1.78	0.65
34:W:204:DD6:C26	36:W:207:CLA:CHC	2.75	0.65
19:X:120:ALA:HB1	35:X:314:A86:C39	2.26	0.65
21:b:599:THR:OG1	46:b:902:HOH:O	2.06	0.65
41:D:318:LHG:O9	34:E:301:DD6:C37	2.43	0.65
21:b:402:ASN:HB3	21:b:405:ASN:HD22	1.62	0.65
35:I:302:A86:C7	36:I:308:CLA:C6	2.73	0.65
12:L:100:GLY:HA3	15:Q:109:LEU:HD11	1.79	0.65
36:b:809:CLA:H151	36:b:829:CLA:HBB2	1.79	0.65
15:O:54:LEU:HD13	33:V:143:ILE:HG21	0.67	0.65
21:b:195:HIS:CD2	36:b:816:CLA:CBC	2.80	0.65
7:G:156:GLN:HE22	7:G:158:SER:H	1.39	0.65
16:R:95:TYR:CD2	16:R:217:PHE:CD2	2.84	0.65
21:b:343:ALA:O	21:b:347:THR:HG23	1.97	0.65
39:b:851:LMT:C2	36:f:805:CLA:HBC3	2.25	0.65
32:U:4:MET:HA	32:U:4:MET:HE3	1.79	0.65
32:U:23:ASP:OD1	32:U:23:ASP:N	2.28	0.65
33:V:58:LEU:CD1	33:V:64:HIS:O	2.45	0.65
37:F:308:KC1:O1A	39:F:321:LMT:H3'	1.97	0.65
7:G:47:ARG:HG2	7:G:52:PRO:O	1.97	0.65
39:b:851:LMT:H12	36:f:805:CLA:HBC3	1.79	0.65
23:d:198:ILE:HD12	23:d:201:LYS:HG3	1.78	0.65
41:f:808:LHG:HC61	41:f:808:LHG:O9	1.97	0.65
32:U:25:ILE:HG12	36:U:307:CLA:H11	1.79	0.65
36:U:306:CLA:H11	36:U:306:CLA:CHB	2.27	0.65
36:H:308:CLA:C17	31:h:116:LEU:HD13	2.27	0.65
36:Q:305:CLA:CGA	37:Q:311:KC1:OBD	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD13	34:A:301:DD6:C24	2.26	0.64
36:D:317:CLA:HBA1	42:D:321:LMG:HC91	1.79	0.64
13:M:225:GLY:HA2	35:M:304:A86:C21	2.27	0.64
18:T:135:LYS:HD2	35:T:304:A86:O3	1.98	0.64
22:c:37:LYS:HB2	22:c:37:LYS:HZ1	1.63	0.64
35:U:303:A86:C39	36:U:308:CLA:CHB	2.62	0.64
6:F:161:LEU:N	6:F:161:LEU:HD23	2.12	0.64
10:J:90:ASP:OD1	10:J:107:SER:HB3	1.96	0.64
41:O:317:LHG:C31	36:V:313:CLA:H162	2.28	0.64
36:l:204:CLA:HBA2	39:U:314:LMT:H81	1.79	0.64
39:F:320:LMT:H6D	41:O:317:LHG:HC92	1.79	0.64
11:K:99:ARG:NH2	11:K:113:VAL:HG12	2.11	0.64
15:O:55:GLY:HA2	33:V:143:ILE:O	1.97	0.64
44:a:844:BCR:C26	42:a:852:LMG:C44	2.76	0.64
36:b:807:CLA:O1A	41:i:104:LHG:H132	1.96	0.64
22:c:74:THR:HG21	23:d:97:GLU:OE1	1.96	0.64
27:j:21:ALA:HA	36:j:106:CLA:HBB2	1.78	0.64
1:A:159:MET:O	33:V:27:THR:HA	1.97	0.64
3:C:40:LEU:HD22	8:H:135:VAL:HG11	1.80	0.64
7:G:201:LYS:O	7:G:201:LYS:HG2	1.97	0.64
39:I:317:LMT:H62	36:l:204:CLA:ND	2.11	0.64
19:W:86:GLY:O	19:W:90:GLN:NE2	2.31	0.64
35:X:314:A86:C7	33:V:41:SER:OG	2.46	0.64
36:E:315:CLA:H161	36:M:307:CLA:H142	1.80	0.64
7:G:156:GLN:HE22	7:G:158:SER:N	1.95	0.64
8:H:119:PHE:HE1	36:H:310:CLA:OBD	1.72	0.64
10:J:140:GLN:CG	42:h:206:LMG:O3	2.42	0.64
17:S:208:LEU:CD1	36:S:309:CLA:HMD3	2.28	0.64
23:d:137:CYS:HB3	23:d:154:PHE:CD2	2.32	0.64
32:U:147:ALA:O	32:U:150:ILE:O	2.16	0.64
33:V:119:TYR:CE1	42:V:316:LMG:HC71	2.19	0.64
41:D:319:LHG:H182	41:D:319:LHG:C14	2.27	0.64
5:E:45:ARG:HH21	5:E:45:ARG:HG3	1.61	0.64
15:O:133:ILE:CD1	35:O:301:A86:O5	2.46	0.64
19:X:129:ASP:OD1	19:X:131:GLU:N	2.29	0.64
26:i:34:LEU:C	26:i:34:LEU:HD12	2.23	0.64
41:i:104:LHG:HC2	41:i:104:LHG:O4	1.95	0.64
33:V:62:SER:HA	36:V:313:CLA:HBC3	1.78	0.64
33:V:177:VAL:HB	33:V:178:PRO:CD	2.27	0.64
41:D:319:LHG:O1	42:D:320:LMG:HC72	1.97	0.64
35:P:306:A86:C39	36:P:316:CLA:HMB2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:117:ARG:NH1	36:X:310:CLA:O2D	2.27	0.64
44:a:844:BCR:H381	42:a:852:LMG:C44	2.28	0.64
33:V:68:SER:HB2	33:V:73:ILE:HB	1.79	0.64
33:V:132:LEU:CD1	36:V:310:CLA:CED	2.76	0.64
14:N:178:LEU:CD2	36:N:318:CLA:CED	2.73	0.64
15:P:159:THR:HG1	16:R:62:SER:HB3	1.62	0.64
16:R:89:MET:CE	16:R:206:ASN:CB	2.76	0.64
19:W:25:ASP:OD1	19:W:28:LYS:N	2.30	0.64
20:a:118:GLN:HG3	20:a:150:PHE:CD2	2.32	0.64
38:b:804:SQD:H101	44:b:843:BCR:H311	1.78	0.64
22:c:15:THR:HG22	22:c:28:MET:HG3	1.78	0.64
42:j:105:LMG:HC71	42:j:105:LMG:O2	1.96	0.64
3:C:41:PRO:C	3:C:43:LEU:H	2.04	0.64
35:H:304:A86:O3	35:J:301:A86:C6	2.44	0.64
42:J:318:LMG:H261	42:J:318:LMG:H371	1.80	0.64
14:N:57:LEU:HA	14:N:60:LYS:HE3	1.80	0.64
14:N:221:THR:CG2	35:N:305:A86:C19	2.75	0.64
35:N:301:A86:C25	36:N:315:CLA:HMA3	2.28	0.64
15:O:173:LEU:O	15:O:177:ARG:HG3	1.98	0.64
17:S:159:ARG:NH2	17:S:163:GLN:O	2.31	0.64
27:j:39:PHE:CE1	41:j:104:LHG:HC81	2.33	0.64
32:U:46:VAL:CG1	36:U:308:CLA:HMC2	2.28	0.64
32:U:49:VAL:HG22	32:U:53:TRP:CD2	2.33	0.64
7:G:47:ARG:CZ	11:K:149:TYR:OH	2.45	0.64
10:J:155:LYS:HD3	10:J:155:LYS:N	2.13	0.64
14:N:178:LEU:CD2	36:N:318:CLA:HED3	2.24	0.64
36:R:314:CLA:HAB	36:R:321:CLA:H42	1.79	0.64
17:S:89:PHE:CE2	17:S:93:ILE:HD11	2.33	0.64
21:b:5:PHE:HB2	26:i:29:VAL:HA	1.78	0.64
21:b:154:LEU:O	21:b:154:LEU:HD22	1.98	0.64
24:e:10:LYS:HE2	25:f:230:ALA:O	1.98	0.64
33:V:8:VAL:CG2	36:V:305:CLA:HBB1	2.25	0.64
35:C:203:A86:C28	29:m:23:LYS:HZ1	2.11	0.63
6:F:49:PRO:O	34:F:303:DD6:O2	2.16	0.63
39:I:317:LMT:C6'	39:I:317:LMT:H4O1	2.10	0.63
15:P:168:ARG:HH21	15:P:168:ARG:HG3	1.63	0.63
19:W:46:ALA:HA	34:W:204:DD6:C21	2.28	0.63
19:W:120:ALA:HB1	37:W:217:KC1:O1D	1.98	0.63
21:b:412:GLU:HA	25:f:238:ALA:HB3	1.77	0.63
33:V:18:LEU:O	33:V:23:GLY:N	2.31	0.63
36:H:307:CLA:HHD	35:J:301:A86:C22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:135:ARG:HG2	36:U:306:CLA:C4C	2.28	0.63
33:V:140:PRO:O	33:V:141:LEU:HD12	1.98	0.63
2:B:105:GLU:OE2	28:l:99:GLU:HB2	1.99	0.63
36:I:306:CLA:H91	36:I:306:CLA:C12	2.28	0.63
3:C:126:PHE:N	35:C:203:A86:C22	2.60	0.63
36:F:312:CLA:H43	31:h:88:VAL:HG13	1.80	0.63
11:K:99:ARG:NH2	11:K:113:VAL:CG1	2.61	0.63
14:N:227:PRO:HD2	35:N:304:A86:O5	1.97	0.63
16:R:182:TYR:OH	36:R:316:CLA:HAA2	1.99	0.63
35:X:314:A86:O2	33:V:87:VAL:HG22	1.98	0.63
21:b:193:LEU:HA	21:b:197:ALA:HB3	1.81	0.63
21:b:242:VAL:HB	21:b:245:THR:OG1	1.99	0.63
32:U:112:TRP:CE2	35:U:304:A86:O3	2.50	0.63
33:V:106:GLU:HG3	36:V:310:CLA:C4B	2.27	0.63
9:I:92:HIS:CE1	9:I:99:LEU:HD13	2.33	0.63
39:K:317:LMT:H3'	39:K:317:LMT:O2B	1.99	0.63
19:W:28:LYS:HG3	19:W:32:LEU:HG	1.79	0.63
20:a:280:PHE:C	20:a:281:LEU:HD23	2.24	0.63
31:h:51:ASP:N	31:h:51:ASP:OD1	2.31	0.63
31:h:84:ALA:HB1	39:h:205:LMT:H111	1.80	0.63
16:R:63:THR:HG23	16:R:64:THR:H	1.63	0.63
25:f:202:ALA:O	25:f:206:LEU:HG	1.99	0.63
26:i:27:LEU:HB3	41:l:208:LHG:H101	1.79	0.63
1:A:114:VAL:HG12	1:A:118:ALA:HB3	1.79	0.63
32:U:63:VAL:HG13	32:U:72:GLN:HB2	1.80	0.63
2:B:198:SER:HA	2:B:201:PHE:HD2	1.64	0.63
36:G:315:CLA:CED	39:a:853:LMT:C6B	2.77	0.63
27:j:38:THR:CB	27:j:40:PRO:HD3	2.29	0.63
33:V:82:SER:CB	33:V:83:PRO:CD	2.67	0.63
1:A:197:VAL:CG2	1:A:198:THR:N	2.33	0.63
42:E:318:LMG:C38	36:a:811:CLA:HBB2	2.28	0.63
41:F:319:LHG:H112	42:J:319:LMG:C18	2.27	0.63
12:L:43:ILE:HG23	12:L:44:GLU:CD	2.24	0.63
15:Q:178:LEU:HG	35:Q:303:A86:C25	2.28	0.63
16:R:63:THR:HG22	16:R:64:THR:N	2.13	0.63
21:b:15:ASP:OD1	21:b:16:PRO:HD2	1.99	0.63
23:d:95:GLN:CD	30:g:88:UNK:O	2.42	0.63
3:C:40:LEU:CD1	3:C:59:PHE:CE1	2.75	0.62
3:C:111:PHE:CZ	3:C:186:THR:OG1	2.51	0.62
36:K:310:CLA:C17	42:L:321:LMG:C16	2.77	0.62
16:R:92:PHE:CE1	16:R:217:PHE:CE2	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:171:ARG:NH2	17:S:179:ASP:OD1	2.32	0.62
42:E:318:LMG:C30	36:a:819:CLA:O2A	2.47	0.62
34:J:304:DD6:C40	36:J:308:CLA:H102	2.28	0.62
35:Q:316:A86:C40	17:S:63:TRP:NE1	2.62	0.62
17:S:82:GLY:O	17:S:86:MET:SD	2.57	0.62
27:j:31:ARG:NH1	34:j:103:DD6:C22	2.61	0.62
31:h:84:ALA:CB	39:h:205:LMT:C11	2.77	0.62
36:D:307:CLA:CMC	41:D:318:LHG:HC92	2.29	0.62
42:E:318:LMG:O10	36:a:819:CLA:O2A	2.17	0.62
36:G:315:CLA:CED	39:a:853:LMT:H6'2	2.28	0.62
14:N:60:LYS:H	14:N:70:THR:HG21	1.63	0.62
23:d:102:ILE:CD1	23:d:154:PHE:CE1	2.83	0.62
5:E:149:THR:HB	39:E:321:LMT:H2'	1.80	0.62
7:G:153:LEU:HD13	36:G:311:CLA:HAA2	1.82	0.62
41:G:321:LHG:O3	41:G:321:LHG:HC61	1.98	0.62
36:H:308:CLA:H12	36:H:308:CLA:O1D	2.00	0.62
34:J:304:DD6:C40	36:J:308:CLA:C10	2.77	0.62
12:L:81:VAL:HG12	36:L:311:CLA:HAB	1.81	0.62
15:O:154:PRO:C	15:O:155:ILE:O	2.41	0.62
36:X:315:CLA:CMD	35:V:301:A86:C26	2.77	0.62
36:a:808:CLA:HBB1	44:j:107:BCR:H23C	1.80	0.62
21:b:80:LYS:O	21:b:84:THR:HG22	1.99	0.62
23:d:88:GLY:O	23:d:116:THR:HB	1.98	0.62
32:U:38:GLY:HA2	32:U:138:MET:HE2	1.81	0.62
33:V:14:TYR:O	36:V:306:CLA:O1A	2.17	0.62
4:D:61:ARG:HG3	4:D:61:ARG:NH1	2.11	0.62
7:G:173:THR:CG2	7:G:192:PHE:CZ	2.82	0.62
10:J:89:THR:CG2	10:J:107:SER:CB	2.78	0.62
20:a:529:MET:HE1	20:a:635:HIS:NE2	2.14	0.62
21:b:514:GLY:O	21:b:518:VAL:HG22	2.00	0.62
30:g:143:UNK:O	30:g:146:UNK:N	2.33	0.62
42:E:318:LMG:C29	36:a:819:CLA:O2A	2.47	0.62
41:E:322:LHG:HC2	41:E:322:LHG:C5	2.29	0.62
36:R:320:CLA:HMA3	41:R:323:LHG:O7	1.98	0.62
36:X:315:CLA:C2B	33:V:176:SER:OG	2.48	0.62
28:l:157:VAL:HG11	39:U:315:LMT:H52	1.80	0.62
32:U:50:PHE:H	32:U:51:PRO:HD3	1.64	0.62
1:A:90:PHE:CE1	1:A:108:ASN:OD1	2.53	0.62
36:D:307:CLA:H11	37:M:318:KC1:C4A	2.30	0.62
18:T:102:VAL:HG12	35:T:304:A86:C12	2.30	0.62
21:b:344:THR:HA	21:b:347:THR:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:458:PHE:HB3	36:b:836:CLA:C2	2.28	0.62
32:U:46:VAL:HG12	36:U:308:CLA:CMC	2.29	0.62
6:F:98:MET:HE1	6:F:214:PHE:CD1	2.35	0.62
35:F:301:A86:C22	36:F:309:CLA:CBC	2.77	0.62
7:G:144:PRO:HG2	7:G:148:GLU:OE1	2.00	0.62
17:S:79:ILE:HD13	17:S:162:GLY:CA	2.25	0.62
36:b:833:CLA:C4	41:j:104:LHG:O9	2.47	0.62
39:h:205:LMT:H6D	39:h:205:LMT:C1B	2.29	0.62
33:V:8:VAL:HG23	36:V:305:CLA:C4B	2.29	0.62
36:D:307:CLA:HBB1	42:E:319:LMG:O10	1.98	0.62
8:H:164:THR:OG1	8:H:165:GLN:OE1	2.16	0.62
10:J:99:TYR:OH	36:J:311:CLA:OBD	2.16	0.62
15:P:164:GLN:HE21	15:P:168:ARG:HH22	1.47	0.62
15:P:168:ARG:HD3	36:P:314:CLA:HHB	1.81	0.62
22:c:24:ASP:HB2	23:d:138:LEU:HD21	1.80	0.62
31:h:119:PHE:O	31:h:122:PRO:CG	2.48	0.62
32:U:76:GLN:CG	36:U:309:CLA:HED3	2.30	0.62
35:H:304:A86:O3	35:J:301:A86:C5	2.48	0.62
14:N:227:PRO:HD2	35:N:304:A86:C38	2.29	0.62
15:Q:152:PHE:CD2	36:Q:314:CLA:CHC	2.80	0.62
17:S:143:TRP:HD1	17:S:164:TYR:HE1	1.46	0.62
32:U:70:ILE:HD11	35:U:303:A86:C40	2.29	0.62
2:B:209:PRO:HB3	39:B:312:LMT:O2B	1.99	0.61
3:C:76:TRP:CE3	3:C:140:HIS:CE1	2.87	0.61
41:D:318:LHG:HC82	41:D:318:LHG:C6	2.27	0.61
20:a:225:ILE:HD11	36:a:813:CLA:HMD1	1.72	0.61
21:b:693:ARG:NH2	26:i:32:ARG:NE	2.39	0.61
38:b:804:SQD:H442	38:b:804:SQD:C23	2.30	0.61
41:E:322:LHG:HC5	41:E:322:LHG:C2	2.31	0.61
8:H:119:PHE:HZ	36:H:310:CLA:CAD	2.10	0.61
10:J:89:THR:HG23	10:J:107:SER:HB3	1.82	0.61
19:X:60:PRO:HG2	33:V:173:ILE:HG21	1.79	0.61
20:a:663:VAL:HG21	20:a:748:PHE:HA	1.82	0.61
41:i:104:LHG:H321	29:m:22:VAL:CG2	2.25	0.61
33:V:65:GLU:CA	33:V:75:PHE:HD2	1.95	0.61
4:D:73:GLU:OE1	4:D:153:PRO:O	2.17	0.61
7:G:147:TYR:CE2	7:G:233:THR:HG23	2.35	0.61
36:G:315:CLA:HED3	39:a:853:LMT:H6'2	1.83	0.61
8:H:119:PHE:HD1	8:H:121:SER:HB3	1.64	0.61
36:f:805:CLA:HED3	36:f:805:CLA:H2	1.82	0.61
7:G:193:LYS:HD3	7:G:193:LYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:86:ILE:HG13	9:I:91:VAL:HG23	1.82	0.61
12:L:137:ILE:HG12	34:L:305:DD6:C23	2.30	0.61
15:O:133:ILE:HD11	35:O:301:A86:O5	1.99	0.61
37:T:310:KC1:C3D	36:T:313:CLA:CAD	2.78	0.61
37:T:310:KC1:CHD	36:T:313:CLA:CMD	2.78	0.61
20:a:274:TRP:CH2	36:a:816:CLA:H72	2.35	0.61
32:U:81:PHE:CZ	36:U:310:CLA:HBC2	2.35	0.61
33:V:58:LEU:HD13	33:V:64:HIS:O	2.00	0.61
7:G:200:LEU:HD11	36:G:313:CLA:HMA2	1.82	0.61
10:J:154:TRP:HB2	36:J:313:CLA:OBD	2.00	0.61
36:K:311:CLA:CBB	40:L:302:DGD:HB92	2.29	0.61
12:L:196:LEU:HD23	12:L:199:LYS:HD2	1.81	0.61
16:R:89:MET:HE2	16:R:206:ASN:HB3	1.81	0.61
17:S:89:PHE:CD2	37:S:316:KC1:CBB	2.83	0.61
17:S:102:TRP:O	17:S:103:ALA:CB	2.48	0.61
19:W:35:VAL:O	19:W:39:HIS:ND1	2.30	0.61
39:b:851:LMT:C1'	36:f:805:CLA:HBC3	2.31	0.61
1:A:126:MET:HE2	1:A:126:MET:N	2.16	0.61
36:E:315:CLA:H141	36:M:307:CLA:C14	2.30	0.61
12:L:137:ILE:CD1	34:L:305:DD6:C16	2.72	0.61
31:h:84:ALA:HB3	39:h:205:LMT:C11	2.27	0.61
32:U:63:VAL:HG22	32:U:72:GLN:HB3	1.83	0.61
32:U:91:TYR:HA	32:U:94:ARG:CZ	2.31	0.61
32:U:128:LEU:C	32:U:128:LEU:HD13	2.25	0.61
7:G:37:LEU:N	37:G:317:KC1:O1D	2.32	0.61
35:N:303:A86:C	36:N:309:CLA:CBB	2.79	0.61
15:P:34:ASP:HB3	15:P:45:LYS:HZ3	1.65	0.61
34:Q:302:DD6:O1	36:Q:308:CLA:HMB1	2.00	0.61
21:b:433:LEU:O	21:b:433:LEU:HD22	2.00	0.61
25:f:176:VAL:CG1	25:f:206:LEU:HD23	2.30	0.61
33:V:7:PRO:HB2	36:V:305:CLA:C4A	2.30	0.61
14:N:63:TRP:CH2	36:N:317:CLA:CMB	2.83	0.61
36:O:316:CLA:O1D	36:O:316:CLA:H2A	2.01	0.61
36:R:320:CLA:HBC3	41:R:323:LHG:C14	2.31	0.61
36:a:816:CLA:H141	36:a:816:CLA:C17	2.30	0.61
21:b:301:LYS:HE2	21:b:323:GLU:OE1	2.01	0.61
5:E:67:ILE:HD11	42:E:318:LMG:HC92	1.83	0.61
15:P:68:LEU:HG	15:P:147:LEU:HD22	1.82	0.61
35:X:314:A86:C26	36:V:306:CLA:C4B	2.79	0.61
20:a:503:THR:HG21	36:a:833:CLA:HMD3	1.83	0.61
21:b:195:HIS:O	21:b:199:PRO:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:343:ALA:O	21:b:347:THR:CG2	2.48	0.61
25:f:201:LEU:O	25:f:201:LEU:HD22	2.00	0.61
32:U:38:GLY:CA	32:U:138:MET:HE2	2.30	0.61
32:U:81:PHE:HZ	36:U:310:CLA:HBC2	1.65	0.61
35:U:303:A86:O1	36:U:306:CLA:H2	2.01	0.61
33:V:119:TYR:OH	36:V:314:CLA:CMD	2.41	0.61
39:B:312:LMT:C5	44:m:101:BCR:H383	2.31	0.61
36:H:308:CLA:H162	31:h:116:LEU:HD13	1.81	0.61
10:J:86:TYR:OH	10:J:108:ALA:HA	2.00	0.61
11:K:95:PRO:HG3	36:K:310:CLA:C2D	2.31	0.61
34:Q:302:DD6:C22	36:Q:308:CLA:C3B	2.79	0.61
26:i:2:MET:N	26:i:5:LEU:CD1	2.64	0.61
32:U:147:ALA:HA	32:U:150:ILE:O	2.00	0.61
2:B:135:ILE:CG2	34:B:304:DD6:C7	2.79	0.60
36:F:317:CLA:HHC	36:F:317:CLA:CBB	2.30	0.60
9:I:93:PRO:HD2	36:I:308:CLA:CMD	2.21	0.60
15:Q:152:PHE:CD1	36:Q:314:CLA:NB	2.68	0.60
20:a:302:HIS:NE2	20:a:306:LEU:HD11	2.16	0.60
36:b:823:CLA:H11	31:h:68:MET:HE3	1.82	0.60
33:V:113:ARG:HH11	33:V:113:ARG:CG	2.14	0.60
33:V:162:PHE:HE1	35:V:301:A86:C7	2.13	0.60
33:V:164:ILE:HD13	33:V:164:ILE:C	2.26	0.60
7:G:156:GLN:NE2	7:G:158:SER:HB3	2.15	0.60
41:G:320:LHG:H101	41:G:320:LHG:O9	2.00	0.60
11:K:99:ARG:HH21	11:K:113:VAL:HG12	1.65	0.60
36:K:307:CLA:C4	37:K:314:KC1:O1D	2.44	0.60
15:O:154:PRO:O	15:O:155:ILE:C	2.44	0.60
20:a:652:LEU:HD23	20:a:656:LEU:HD12	1.82	0.60
20:a:663:VAL:HG22	20:a:751:ALA:HB3	1.83	0.60
21:b:291:ARG:HG3	21:b:291:ARG:O	2.00	0.60
3:C:182:ILE:HD11	34:C:201:DD6:C5	2.32	0.60
15:Q:152:PHE:CG	36:Q:314:CLA:NB	2.70	0.60
36:Q:314:CLA:H102	36:Q:314:CLA:HAB	1.82	0.60
34:R:308:DD6:C	36:R:314:CLA:C1C	2.80	0.60
21:b:222:LYS:HB3	21:b:223:PRO:HD3	1.82	0.60
32:U:67:ILE:O	32:U:67:ILE:HG22	2.00	0.60
32:U:111:ASP:OD1	32:U:112:TRP:N	2.33	0.60
2:B:135:ILE:HG22	34:B:304:DD6:C10	2.27	0.60
4:D:165:LYS:CG	19:W:26:GLN:NE2	2.64	0.60
41:G:321:LHG:HC62	41:G:321:LHG:C2	2.31	0.60
10:J:55:LEU:HB2	10:J:57:LEU:CD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:836:CLA:H12	36:b:837:CLA:O1A	2.01	0.60
7:G:233:THR:HG23	7:G:233:THR:O	2.01	0.60
8:H:65:PHE:HE1	31:h:67:ILE:HG12	1.62	0.60
39:I:317:LMT:H2B	39:I:317:LMT:C6B	2.31	0.60
15:O:77:ALA:HB1	34:O:304:DD6:C22	2.31	0.60
16:R:140:PHE:CZ	34:R:308:DD6:C37	2.76	0.60
19:X:2:PHE:HD1	19:X:5:GLU:HG3	1.66	0.60
35:U:301:A86:C21	36:U:305:CLA:HAC2	2.30	0.60
4:D:45:PRO:HA	4:D:61:ARG:NH2	2.16	0.60
5:E:68:ASP:C	20:a:16:LYS:HZ1	2.08	0.60
36:I:306:CLA:HBB1	36:I:306:CLA:HMB3	1.82	0.60
11:K:53:ARG:HH11	11:K:53:ARG:CG	2.14	0.60
13:M:75:ILE:HG23	13:M:75:ILE:O	2.00	0.60
14:N:228:LEU:HD23	35:N:304:A86:C39	2.31	0.60
15:O:54:LEU:CB	33:V:143:ILE:HG21	2.32	0.60
15:Q:150:ILE:HG13	36:Q:314:CLA:C3D	2.31	0.60
16:R:92:PHE:HE1	16:R:217:PHE:CZ	2.20	0.60
18:T:122:PHE:HD2	35:T:304:A86:C	2.15	0.60
19:W:33:ARG:HH12	19:W:145:ARG:HH21	1.49	0.60
20:a:392:GLN:NE2	20:a:392:GLN:HA	2.16	0.60
20:a:452:PHE:O	20:a:456:HIS:CD2	2.50	0.60
21:b:414:LYS:NZ	25:f:235:ALA:CB	2.61	0.60
36:b:841:CLA:HHB	41:b:850:LHG:HC82	1.83	0.60
33:V:111:THR:CG2	42:V:315:LMG:HC71	2.24	0.60
2:B:210:MET:HE3	39:B:312:LMT:O1'	2.02	0.60
42:J:319:LMG:H112	42:J:319:LMG:HC91	1.83	0.60
14:N:52:TYR:CE2	35:N:303:A86:O3	2.54	0.60
23:d:104:TRP:CD1	23:d:150:ILE:HD13	2.37	0.60
24:e:9:VAL:HA	24:e:61:GLN:O	2.01	0.60
32:U:50:PHE:N	32:U:51:PRO:HD3	2.14	0.60
32:U:77:TRP:CE2	36:U:308:CLA:HBA2	2.37	0.60
32:U:77:TRP:HZ2	36:U:308:CLA:CHB	2.14	0.60
36:E:311:CLA:H142	42:E:318:LMG:H182	1.84	0.60
12:L:198:LEU:CD1	36:L:308:CLA:HED2	2.31	0.60
14:N:178:LEU:HD23	36:N:318:CLA:HED1	1.83	0.60
17:S:53:ASP:CG	17:S:56:SER:HA	2.26	0.60
36:X:315:CLA:CMD	35:V:301:A86:C29	2.75	0.60
20:a:579:PRO:HG3	46:b:967:HOH:O	2.01	0.60
41:D:319:LHG:H221	42:D:320:LMG:H231	1.84	0.60
7:G:154:VAL:HA	7:G:159:MET:HB2	1.84	0.60
9:I:42:ILE:HG23	9:I:48:PHE:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:J:318:LMG:O9	42:J:318:LMG:H151	2.02	0.60
16:R:89:MET:CE	16:R:206:ASN:HB2	2.32	0.60
19:X:117:ARG:HA	33:V:14:TYR:CE1	2.37	0.60
23:d:143:ARG:HH21	23:d:143:ARG:CG	2.15	0.60
24:e:26:VAL:HG21	24:e:41:ARG:CG	2.31	0.60
41:f:809:LHG:H242	41:f:809:LHG:H282	1.84	0.60
36:j:101:CLA:C6	42:j:105:LMG:H341	2.31	0.60
28:l:94:PRO:HD2	46:l:303:HOH:O	2.02	0.60
31:h:96:VAL:HG22	39:h:205:LMT:H1B	1.82	0.60
4:D:73:GLU:CD	4:D:153:PRO:O	2.44	0.60
36:G:316:CLA:C4D	41:G:320:LHG:HC92	2.32	0.60
36:H:318:CLA:HED1	21:b:294:PHE:HB2	1.84	0.60
9:I:68:GLU:OE1	9:I:141:GLY:HA2	2.02	0.60
37:W:217:KC1:CMD	36:W:218:CLA:C4C	2.80	0.60
20:a:55:TRP:CG	20:a:728:GLN:HE22	2.20	0.60
25:f:206:LEU:HD22	36:f:804:CLA:CMD	2.32	0.60
30:g:143:UNK:O	30:g:144:UNK:C	2.49	0.60
32:U:61:VAL:O	32:U:61:VAL:CG1	2.49	0.60
33:V:62:SER:HB2	33:V:63:PRO:CD	2.30	0.60
6:F:148:ASP:OD2	6:F:151:ARG:NE	2.25	0.59
7:G:90:GLN:O	20:a:322:GLY:HA3	2.00	0.59
42:G:324:LMG:H112	42:G:325:LMG:O1	2.01	0.59
14:N:241:MET:SD	35:N:305:A86:C7	2.90	0.59
16:R:50:PRO:HB2	17:S:169:LEU:CD1	2.32	0.59
19:W:121:ILE:HG22	37:W:217:KC1:CED	2.32	0.59
32:U:96:GLU:CD	32:U:109:ALA:HB2	2.26	0.59
32:U:112:TRP:O	32:U:113:MET:HG2	2.02	0.59
33:V:102:ILE:HG21	36:V:310:CLA:CMC	2.32	0.59
36:E:308:CLA:HBC1	7:G:168:PHE:HE2	1.65	0.59
36:G:315:CLA:CED	39:a:853:LMT:C5B	2.79	0.59
35:Q:316:A86:C21	17:S:218:CYS:SG	2.90	0.59
23:d:198:ILE:HD11	23:d:201:LYS:HZ1	1.65	0.59
31:h:125:TRP:HB2	35:h:204:A86:C6	2.33	0.59
33:V:81:MET:HE1	33:V:89:HIS:NE2	2.18	0.59
35:E:307:A86:C9	36:E:315:CLA:C2D	2.80	0.59
15:Q:150:ILE:HG13	36:Q:314:CLA:C2D	2.32	0.59
19:X:135:LYS:HE2	19:X:136:LYS:HE2	1.84	0.59
20:a:225:ILE:HD12	36:a:813:CLA:HMD1	1.82	0.59
23:d:104:TRP:HB2	23:d:150:ILE:CD1	2.32	0.59
41:f:808:LHG:C33	42:V:316:LMG:H332	2.31	0.59
36:U:310:CLA:HMB1	39:U:314:LMT:H61	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:ARG:NH2	3:C:46:PRO:O	2.35	0.59
6:F:145:HIS:CG	36:F:317:CLA:HAA1	2.37	0.59
9:I:35:LYS:H	9:I:35:LYS:HD2	1.67	0.59
15:Q:32:LYS:O	15:Q:36:MET:HE2	2.03	0.59
37:Q:313:KC1:NC	41:Q:315:LHG:H272	2.18	0.59
23:d:95:GLN:OE1	30:g:88:UNK:O	2.20	0.59
42:j:105:LMG:H381	42:j:105:LMG:C42	2.16	0.59
32:U:57:PHE:CD2	36:U:308:CLA:CAD	2.85	0.59
35:C:203:A86:C28	29:m:23:LYS:HE2	2.32	0.59
39:G:322:LMT:H6D	39:G:322:LMT:C1B	2.30	0.59
9:I:46:MET:HB3	9:I:49:PHE:HB2	1.84	0.59
35:N:303:A86:O	36:N:310:CLA:HBB1	2.03	0.59
15:P:36:MET:HG2	15:P:37:PRO:HD2	1.84	0.59
16:R:63:THR:HG23	16:R:64:THR:N	2.18	0.59
19:X:62:THR:HA	19:X:69:THR:HA	1.83	0.59
20:a:490:GLN:OE1	39:a:854:LMT:H6E	2.02	0.59
21:b:220:GLY:O	39:b:848:LMT:C3B	2.49	0.59
21:b:293:ASN:HD22	21:b:293:ASN:C	2.08	0.59
3:C:124:GLN:OE1	36:C:210:CLA:CHD	2.51	0.59
14:N:177:VAL:HG13	14:N:177:VAL:O	2.01	0.59
33:V:18:LEU:HD12	33:V:31:LEU:HD11	1.83	0.59
2:B:85:THR:O	2:B:88:ALA:N	2.36	0.59
12:L:184:ARG:NH2	15:Q:53:THR:O	2.36	0.59
19:X:129:ASP:OD1	19:X:131:GLU:CB	2.50	0.59
32:U:29:ARG:NH1	39:U:315:LMT:O6'	2.30	0.59
32:U:96:GLU:CG	32:U:109:ALA:HB2	2.31	0.59
32:U:135:ARG:HG2	36:U:306:CLA:C3C	2.32	0.59
33:V:35:GLU:OE2	36:V:306:CLA:C1B	2.49	0.59
33:V:138:TRP:CE3	36:V:308:CLA:C20	2.86	0.59
36:D:306:CLA:C1B	41:D:318:LHG:H342	2.32	0.59
18:T:122:PHE:CD2	35:T:304:A86:C	2.86	0.59
22:c:81:TYR:HB3	23:d:91:LEU:HD12	1.84	0.59
24:e:26:VAL:HG21	24:e:41:ARG:HG3	1.85	0.59
27:j:28:GLU:OE1	27:j:28:GLU:HA	2.03	0.59
32:U:63:VAL:CG1	32:U:69:ALA:CB	2.80	0.59
42:G:324:LMG:O9	42:G:324:LMG:H131	2.03	0.59
12:L:44:GLU:CD	36:L:308:CLA:C1B	2.75	0.59
14:N:73:PHE:CE2	36:N:312:CLA:HED1	2.37	0.59
14:N:184:PHE:CD2	36:N:319:CLA:HMD3	2.37	0.59
16:R:86:ARG:NH1	16:R:203:GLU:OE2	2.36	0.59
16:R:175:HIS:CD2	34:R:307:DD6:C24	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:144:ASP:OD1	17:S:164:TYR:CD2	2.56	0.59
34:W:205:DD6:C37	36:W:212:CLA:NC	2.65	0.59
24:e:13:ARG:O	24:e:19:TYR:HD1	1.86	0.59
41:f:809:LHG:H342	41:f:809:LHG:C29	2.33	0.59
28:l:172:VAL:HG11	32:U:76:GLN:HE21	1.68	0.59
31:h:99:GLN:OE1	39:h:205:LMT:O4'	2.20	0.59
32:U:138:MET:SD	35:U:303:A86:C5	2.91	0.59
33:V:8:VAL:CG2	36:V:305:CLA:C4B	2.80	0.59
3:C:75:ARG:HG2	3:C:146:PRO:HB2	1.83	0.59
15:Q:156:ASP:HB3	17:S:60:LYS:CB	2.32	0.59
41:b:850:LHG:O5	46:b:904:HOH:O	2.17	0.59
39:b:851:LMT:C6'	36:f:805:CLA:HBC1	2.33	0.59
32:U:77:TRP:CZ2	36:U:308:CLA:CHB	2.86	0.59
14:N:229:LEU:HD13	14:N:232:ILE:HG21	1.85	0.58
15:P:34:ASP:CB	15:P:45:LYS:CD	2.73	0.58
21:b:110:TYR:HB2	21:b:111:PRO:HD2	1.84	0.58
32:U:126:MET:SD	36:U:311:CLA:C2	2.89	0.58
33:V:8:VAL:HG22	36:V:305:CLA:HMB1	1.84	0.58
33:V:68:SER:OG	33:V:73:ILE:HG13	2.03	0.58
3:C:45:ARG:HH21	3:C:45:ARG:CG	2.14	0.58
36:G:307:CLA:HBB1	36:G:307:CLA:CHC	2.13	0.58
23:d:137:CYS:O	23:d:154:PHE:CZ	2.56	0.58
41:i:104:LHG:O9	41:i:104:LHG:HC62	2.03	0.58
32:U:8:SER:HG	36:U:306:CLA:CGD	2.15	0.58
33:V:13:ASN:CG	33:V:14:TYR:H	2.05	0.58
17:S:53:ASP:OD1	17:S:56:SER:N	2.36	0.58
36:a:802:CLA:H92	43:a:840:PQN:H28	1.85	0.58
21:b:5:PHE:HB3	21:b:20:ARG:NH1	2.17	0.58
29:m:11:LEU:HD11	44:m:101:BCR:H382	1.85	0.58
33:V:62:SER:CB	33:V:63:PRO:HD2	2.32	0.58
33:V:112:HIS:H	33:V:112:HIS:CD2	2.21	0.58
35:E:307:A86:C8	36:E:315:CLA:C4D	2.81	0.58
36:G:307:CLA:ND	40:L:302:DGD:HA21	2.19	0.58
9:I:113:VAL:HG11	36:I:309:CLA:O1D	2.03	0.58
13:M:114:TRP:HH2	13:M:140:GLY:HA2	1.67	0.58
35:N:305:A86:C29	36:N:309:CLA:HED2	2.34	0.58
15:O:151:VAL:CG2	36:O:316:CLA:O1D	2.49	0.58
20:a:17:ASN:ND2	20:a:17:ASN:H	2.01	0.58
20:a:483:GLN:HB2	41:a:850:LHG:HC12	1.85	0.58
20:a:601:LEU:HD12	20:a:734:LEU:HD21	1.84	0.58
21:b:170:ASN:HD21	21:b:326:THR:HG22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:F:308:KC1:CMB	36:V:314:CLA:CAA	2.78	0.58
37:G:308:KC1:CMA	40:L:302:DGD:HE4	2.34	0.58
39:G:323:LMT:H3'	15:P:54:LEU:HD23	1.86	0.58
9:I:92:HIS:CE1	9:I:99:LEU:HD22	2.37	0.58
10:J:139:VAL:HA	10:J:147:ARG:HH21	1.68	0.58
10:J:186:ILE:HG12	35:J:305:A86:O1	2.03	0.58
36:L:320:CLA:O1A	37:Q:313:KC1:CBB	2.52	0.58
14:N:57:LEU:HD12	36:N:308:CLA:H2	1.86	0.58
14:N:102:TRP:HD1	35:N:302:A86:O3	1.85	0.58
15:P:168:ARG:HG3	15:P:168:ARG:NH2	2.18	0.58
36:Q:305:CLA:O2A	37:Q:311:KC1:OBD	2.20	0.58
33:V:68:SER:CB	33:V:73:ILE:H	2.15	0.58
36:E:313:CLA:H111	36:E:313:CLA:H161	1.84	0.58
36:G:307:CLA:HHC	36:G:307:CLA:CBB	2.15	0.58
15:O:133:ILE:HD11	35:O:301:A86:C33	2.33	0.58
35:Q:303:A86:C23	37:Q:311:KC1:CMA	2.81	0.58
21:b:132:GLN:NE2	29:m:6:GLN:HE22	1.93	0.58
4:D:70:PHE:HB2	4:D:145:LEU:HD21	1.85	0.58
33:V:136:LEU:N	33:V:136:LEU:HD23	2.19	0.58
36:V:314:CLA:HBA2	36:V:314:CLA:CBD	2.32	0.58
2:B:197:ILE:CD1	34:B:302:DD6:C3	2.82	0.58
3:C:126:PHE:HE1	35:C:203:A86:C8	2.17	0.58
36:C:207:CLA:H3A	36:C:207:CLA:CGA	2.34	0.58
36:F:317:CLA:HAB	42:J:318:LMG:HC92	1.86	0.58
39:F:320:LMT:H3O2	39:F:321:LMT:C5'	2.16	0.58
8:H:160:PHE:HB3	8:H:163:LYS:HD3	1.85	0.58
11:K:61:VAL:O	11:K:66:ARG:NH1	2.31	0.58
12:L:44:GLU:OE1	12:L:44:GLU:N	2.36	0.58
19:X:124:GLY:HA2	33:V:9:PHE:HB3	1.86	0.58
29:m:23:LYS:HD2	42:m:102:LMG:HC2	1.86	0.58
32:U:67:ILE:CD1	32:U:148:HIS:HD2	2.15	0.58
32:U:91:TYR:HA	32:U:94:ARG:NH1	2.19	0.58
33:V:68:SER:OG	33:V:71:ASP:CA	2.51	0.58
33:V:69:ILE:HG23	33:V:69:ILE:O	2.02	0.58
5:E:187:ASN:HD21	36:E:315:CLA:HAA1	1.69	0.58
15:Q:171:ARG:HD2	37:Q:311:KC1:CBA	2.33	0.58
36:a:848:CLA:HAB	21:b:581:TRP:HH2	1.68	0.58
21:b:625:LEU:O	21:b:625:LEU:HD22	2.03	0.58
36:j:102:CLA:H91	36:j:102:CLA:H121	1.86	0.58
3:C:111:PHE:HZ	3:C:186:THR:OG1	1.87	0.58
41:E:322:LHG:HC41	41:E:322:LHG:O9	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:H:302:DD6:C37	36:H:307:CLA:H43	2.34	0.58
10:J:109:ASP:O	10:J:111:HIS:N	2.36	0.58
11:K:149:TYR:CE2	11:K:151:ARG:HB3	2.38	0.58
35:X:314:A86:C11	33:V:45:ALA:HB2	2.33	0.58
36:a:805:CLA:H2	36:a:805:CLA:HED2	1.84	0.58
31:h:132:TRP:CD1	36:h:203:CLA:HAA1	2.38	0.58
2:B:66:HIS:NE2	2:B:70:TRP:NE1	2.51	0.57
42:D:321:LMG:O9	42:D:321:LMG:HC92	1.99	0.57
36:F:312:CLA:O1D	39:h:205:LMT:H6E	2.04	0.57
9:I:46:MET:HE2	39:K:318:LMT:C2	2.30	0.57
9:I:112:THR:HG23	9:I:113:VAL:HG23	1.86	0.57
9:I:133:LYS:NZ	41:I:316:LHG:O5	2.31	0.57
10:J:131:ASP:HA	10:J:135:THR:HG22	1.84	0.57
13:M:108:MET:CE	35:M:304:A86:C2	2.82	0.57
20:a:213:LEU:O	20:a:217:SER:OG	2.21	0.57
20:a:605:TYR:OH	36:a:801:CLA:HED1	2.04	0.57
41:b:850:LHG:H261	41:b:850:LHG:O10	2.02	0.57
23:d:138:LEU:HD13	23:d:154:PHE:CE2	2.39	0.57
36:j:102:CLA:C19	36:j:102:CLA:H122	2.33	0.57
41:j:104:LHG:O5	41:j:104:LHG:O2	2.17	0.57
32:U:138:MET:O	32:U:141:ILE:CG2	2.47	0.57
42:V:315:LMG:H341	42:V:316:LMG:H151	1.86	0.57
1:A:94:GLN:O	1:A:103:HIS:CE1	2.57	0.57
39:E:320:LMT:C12	36:a:809:CLA:HBB1	2.16	0.57
20:a:22:VAL:HA	20:a:191:PRO:HA	1.86	0.57
20:a:339:THR:HG21	41:a:843:LHG:O2	2.05	0.57
24:e:20:LYS:NZ	25:f:232:ALA:O	2.35	0.57
2:B:182:GLU:HG3	2:B:183:GLU:HG2	1.86	0.57
4:D:53:GLY:O	36:D:308:CLA:CED	2.52	0.57
10:J:54:PRO:HB2	42:J:319:LMG:H171	1.87	0.57
15:P:112:TRP:CE2	15:P:120:LYS:HE2	2.39	0.57
19:W:121:ILE:HA	37:W:217:KC1:O1A	2.04	0.57
39:E:320:LMT:C12	36:a:809:CLA:CBB	2.80	0.57
41:E:322:LHG:HC61	41:E:322:LHG:C2	2.31	0.57
6:F:169:THR:HG22	6:F:177:VAL:HG22	1.86	0.57
42:G:324:LMG:H111	42:G:325:LMG:C2	2.21	0.57
36:K:307:CLA:HBB1	36:K:307:CLA:CHC	2.32	0.57
13:M:203:LYS:HZ2	35:M:304:A86:C39	2.17	0.57
15:P:152:PHE:C	15:P:154:PRO:HD3	2.29	0.57
15:P:156:ASP:OD1	16:R:64:THR:OG1	2.23	0.57
20:a:587:GLY:HA3	21:b:667:ARG:CD	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:105:ASP:HB3	23:d:151[B]:LYS:HZ3	1.69	0.57
41:l:208:LHG:O4	41:l:208:LHG:O1	2.22	0.57
39:h:205:LMT:H6D	39:h:205:LMT:C6B	2.35	0.57
36:U:306:CLA:H93	36:U:307:CLA:CMA	2.33	0.57
9:I:95:PHE:N	9:I:95:PHE:CD1	2.73	0.57
12:L:44:GLU:HG3	36:L:308:CLA:C2B	2.35	0.57
13:M:171:THR:HG23	13:M:172:ARG:HG3	1.85	0.57
14:N:86:MET:HB2	36:N:313:CLA:CMC	2.35	0.57
17:S:170:PHE:CZ	17:S:175:HIS:HE1	2.22	0.57
19:X:118:ASN:O	33:V:13:ASN:HA	2.04	0.57
42:D:320:LMG:H162	27:j:4:LEU:HD22	1.85	0.57
21:b:187:LEU:C	21:b:190:THR:HG22	2.29	0.57
31:h:57:GLU:HA	31:h:57:GLU:OE1	2.03	0.57
32:U:49:VAL:O	32:U:49:VAL:HG13	2.02	0.57
4:D:206:TYR:CD1	4:D:206:TYR:N	2.73	0.57
19:X:83:ILE:HD11	36:X:308:CLA:HMD3	1.86	0.57
25:f:204:ARG:O	25:f:207:PHE:CE1	2.57	0.57
42:h:206:LMG:HC71	42:h:206:LMG:O9	2.05	0.57
9:I:46:MET:CE	39:K:318:LMT:H22	2.31	0.57
36:K:310:CLA:HBD	36:K:310:CLA:HAA1	1.87	0.57
15:P:129:LEU:CD1	36:P:319:CLA:HMA1	2.21	0.57
19:W:7:GLY:HA3	19:W:141:LEU:HD23	1.84	0.57
20:a:577:ARG:HG3	20:a:577:ARG:O	2.04	0.57
31:h:121:GLY:N	31:h:122:PRO:CD	2.65	0.57
32:U:8:SER:OG	36:U:306:CLA:CGD	2.52	0.57
15:O:77:ALA:CB	34:O:304:DD6:C22	2.83	0.57
15:P:34:ASP:HB3	15:P:45:LYS:NZ	2.19	0.57
15:P:84:GLN:C	15:P:103:LEU:HD11	2.26	0.57
21:b:156:LEU:CB	29:m:27:GLN:OE1	2.52	0.57
32:U:62:SER:O	32:U:63:VAL:HG23	2.05	0.57
6:F:193:ILE:HD13	35:F:301:A86:C10	2.35	0.57
7:G:124:ASP:OD1	7:G:145:THR:OG1	2.19	0.57
7:G:126:ALA:HB1	7:G:242:PHE:CD1	2.40	0.57
36:G:316:CLA:C3D	41:G:320:LHG:HC92	2.34	0.57
11:K:125:ILE:CD1	35:K:301:A86:C33	2.81	0.57
34:M:303:DD6:C36	36:M:307:CLA:C1	2.81	0.57
15:O:62:TRP:CH2	37:O:315:KC1:C3B	2.88	0.57
41:i:104:LHG:C27	29:m:25:ALA:CB	2.64	0.57
2:B:135:ILE:HD12	35:B:301:A86:C8	2.35	0.56
36:H:308:CLA:C18	31:h:116:LEU:HD12	2.25	0.56
12:L:91:LEU:HD11	12:L:106:CYS:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:113:SER:O	14:N:121:GLN:NE2	2.38	0.56
17:S:198:ARG:HB3	36:S:315:CLA:HHB	1.86	0.56
20:a:358:LEU:HD22	20:a:362:LEU:CG	2.30	0.56
20:a:529:MET:HE3	20:a:623:VAL:HA	1.87	0.56
22:c:29:ILE:HG22	23:d:181:ARG:HB3	1.86	0.56
25:f:213:PRO:HG2	41:f:808:LHG:H191	1.86	0.56
3:C:124:GLN:OE1	36:C:210:CLA:NC	2.38	0.56
40:C:215:DGD:O2D	40:C:215:DGD:HG2	2.05	0.56
6:F:78:LYS:NZ	36:F:313:CLA:O1D	2.36	0.56
36:G:309:CLA:H43	36:G:310:CLA:HBA1	1.85	0.56
8:H:194:VAL:HG21	36:H:316:CLA:HED3	1.87	0.56
9:I:42:ILE:HG23	9:I:48:PHE:N	2.20	0.56
36:K:307:CLA:C14	37:K:314:KC1:CMC	2.82	0.56
35:O:301:A86:C4	41:O:318:LHG:H172	2.36	0.56
16:R:89:MET:HE2	16:R:206:ASN:CB	2.35	0.56
19:X:59:LEU:HD13	35:V:301:A86:C41	2.34	0.56
36:a:848:CLA:HAB	21:b:581:TRP:CH2	2.39	0.56
36:l:204:CLA:HBB1	36:l:204:CLA:CHC	2.25	0.56
33:V:66:TYR:CZ	33:V:74:LYS:HE3	2.40	0.56
4:D:146:TYR:O	4:D:147:GLU:HG2	2.05	0.56
35:E:307:A86:C11	36:E:315:CLA:CMD	2.83	0.56
35:H:304:A86:C37	35:J:301:A86:C5	2.84	0.56
39:I:318:LMT:O6B	39:I:318:LMT:H1B	2.05	0.56
35:L:307:A86:C10	41:Q:315:LHG:H302	2.34	0.56
13:M:203:LYS:NZ	35:M:304:A86:C38	2.68	0.56
14:N:63:TRP:NE1	35:N:305:A86:O3	2.38	0.56
15:P:133:ILE:O	15:P:137:LYS:HE2	2.05	0.56
15:Q:126:THR:HG21	36:Q:314:CLA:H11	1.86	0.56
15:Q:178:LEU:HD23	35:Q:303:A86:C	2.36	0.56
37:T:310:KC1:CMD	36:T:313:CLA:CHA	2.83	0.56
34:W:205:DD6:C26	36:W:212:CLA:C2C	2.83	0.56
35:X:314:A86:C14	33:V:45:ALA:CB	2.83	0.56
20:a:280:PHE:O	20:a:281:LEU:HD23	2.06	0.56
20:a:486:PRO:HB3	36:a:836:CLA:HED3	1.86	0.56
42:a:852:LMG:H112	42:a:852:LMG:C9	2.35	0.56
42:a:852:LMG:H112	42:a:852:LMG:O8	2.05	0.56
23:d:143:ARG:HG3	23:d:143:ARG:NH2	2.19	0.56
32:U:50:PHE:N	32:U:51:PRO:HD2	2.20	0.56
32:U:125:ASP:N	32:U:125:ASP:OD1	2.37	0.56
36:V:314:CLA:O1D	36:V:314:CLA:H2A	2.05	0.56
36:V:314:CLA:H101	36:V:314:CLA:H142	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:H:314:CLA:HBC2	35:J:301:A86:C24	2.35	0.56
15:Q:157:PHE:C	36:Q:310:CLA:HBA1	2.31	0.56
20:a:696:ARG:CD	20:a:724:LEU:O	2.53	0.56
36:a:816:CLA:H51	36:a:816:CLA:C9	2.35	0.56
23:d:137:CYS:O	23:d:154:PHE:HZ	1.88	0.56
36:V:314:CLA:CBC	42:V:315:LMG:H292	2.35	0.56
35:A:316:A86:C6	36:V:310:CLA:HBB1	2.36	0.56
39:B:312:LMT:H52	44:m:101:BCR:H383	1.86	0.56
36:I:307:CLA:H43	18:T:17:PRO:HB2	1.87	0.56
14:N:122:TRP:CZ3	36:N:310:CLA:HHB	2.41	0.56
15:Q:152:PHE:CE1	36:Q:314:CLA:CAB	2.88	0.56
16:R:98:GLN:NE2	16:R:125:GLN:OE1	2.38	0.56
35:X:302:A86:C25	35:V:301:A86:O5	2.53	0.56
39:a:851:LMT:O3'	34:j:103:DD6:C17	2.54	0.56
11:K:189:ILE:HD11	34:K:304:DD6:C40	2.34	0.56
14:N:38:LEU:O	14:N:42:ALA:N	2.39	0.56
36:a:816:CLA:C1D	42:a:852:LMG:H291	2.35	0.56
27:j:17:LEU:HD22	42:j:105:LMG:H201	1.87	0.56
36:j:102:CLA:CMB	36:j:102:CLA:HBB1	2.36	0.56
32:U:95:MET:CG	32:U:109:ALA:O	2.53	0.56
33:V:67:LEU:HB2	33:V:75:PHE:HE1	1.64	0.56
33:V:179:ILE:HD12	33:V:179:ILE:C	2.31	0.56
36:J:312:CLA:H42	42:J:318:LMG:H211	1.86	0.56
12:L:190:SER:HB2	12:L:193:LEU:HD23	1.88	0.56
15:P:112:TRP:O	15:P:120:LYS:HE3	2.05	0.56
35:S:308:A86:C24	36:S:314:CLA:HBB1	2.36	0.56
20:a:663:VAL:HG23	46:a:915:HOH:O	2.06	0.56
41:a:850:LHG:HC31	41:a:850:LHG:C6	2.23	0.56
21:b:80:LYS:O	21:b:84:THR:CG2	2.54	0.56
31:h:96:VAL:CG2	39:h:205:LMT:H1B	2.34	0.56
32:U:95:MET:CE	32:U:100:LYS:HE3	2.27	0.56
33:V:1:THR:H2	33:V:2:PRO:HD2	1.69	0.56
33:V:126:GLY:HA2	33:V:131:GLY:CA	2.35	0.56
1:A:196:TRP:CZ2	36:A:314:CLA:HMD1	2.41	0.56
3:C:40:LEU:CD1	3:C:59:PHE:HD1	2.18	0.56
3:C:45:ARG:NH2	3:C:45:ARG:HG2	2.20	0.56
12:L:43:ILE:CG2	12:L:44:GLU:CD	2.79	0.56
13:M:144:TRP:CZ3	34:M:303:DD6:C23	2.88	0.56
35:N:303:A86:C28	36:N:308:CLA:H172	2.36	0.56
1:A:142:THR:HG21	41:f:808:LHG:HC32	1.87	0.56
1:A:194:HIS:O	1:A:197:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:MET:HG3	3:C:41:PRO:O	2.05	0.56
7:G:200:LEU:CD1	36:G:313:CLA:HAA2	2.36	0.56
14:N:78:GLU:HG3	14:N:79:ILE:HG13	1.88	0.56
23:d:114:MET:O	23:d:117:GLY:O	2.24	0.56
1:A:197:VAL:HG22	1:A:198:THR:H	1.65	0.56
3:C:41:PRO:O	3:C:43:LEU:N	2.39	0.56
36:G:313:CLA:H172	36:P:310:CLA:H122	1.88	0.56
9:I:72:LYS:NZ	36:I:310:CLA:O1D	2.38	0.56
39:I:317:LMT:H12	39:I:317:LMT:C5'	2.36	0.56
12:L:44:GLU:HG2	36:L:308:CLA:CHC	2.29	0.56
17:S:171:ARG:HH22	17:S:179:ASP:CG	2.14	0.56
20:a:696:ARG:HD2	20:a:724:LEU:O	2.05	0.56
21:b:54:LEU:HB3	21:b:148:LEU:HD13	1.88	0.56
36:b:816:CLA:C12	36:b:816:CLA:H91	2.36	0.56
41:b:850:LHG:O10	41:b:850:LHG:HC81	2.05	0.56
24:e:13:ARG:O	24:e:19:TYR:CD1	2.59	0.56
33:V:42:ALA:HB1	33:V:161:MET:HA	1.88	0.56
2:B:122:ARG:HH22	36:B:311:CLA:H11	1.71	0.55
36:I:312:CLA:HED2	39:I:318:LMT:H6D	1.86	0.55
13:M:214:ARG:NH1	37:M:313:KC1:O2A	2.39	0.55
15:O:199:LEU:CB	35:O:305:A86:C38	2.61	0.55
34:W:205:DD6:C26	36:W:212:CLA:CMC	2.84	0.55
21:b:520:HIS:CD2	41:j:104:LHG:H372	2.41	0.55
21:b:546:MET:SD	21:b:549:LYS:HG3	2.46	0.55
32:U:52:LYS:HE3	32:U:65:ASP:OD2	2.06	0.55
33:V:148:ARG:CZ	36:V:305:CLA:CED	2.84	0.55
33:V:158:ARG:HB3	36:V:306:CLA:C3C	2.37	0.55
36:V:314:CLA:H142	36:V:314:CLA:C10	2.34	0.55
6:F:184:GLU:HG3	36:F:314:CLA:NB	2.22	0.55
8:H:163:LYS:HG3	8:H:164:THR:HG23	1.88	0.55
36:K:313:CLA:H2A	36:K:313:CLA:HED3	1.89	0.55
15:O:54:LEU:CB	33:V:143:ILE:CG2	2.84	0.55
37:Q:313:KC1:C2C	41:Q:315:LHG:H291	2.35	0.55
21:b:699:LEU:HD22	21:b:703:GLN:CD	2.31	0.55
36:b:841:CLA:CHB	41:b:850:LHG:HC82	2.36	0.55
23:d:105:ASP:HB3	23:d:151[B]:LYS:NZ	2.21	0.55
33:V:139:ASN:OD1	33:V:142:ASN:CA	2.54	0.55
40:C:215:DGD:O1B	40:C:215:DGD:HG11	2.07	0.55
5:E:45:ARG:HH21	5:E:45:ARG:CG	2.18	0.55
6:F:107:MET:HE3	35:F:302:A86:C29	2.36	0.55
6:F:164:ASP:OD2	6:F:168:LEU:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:93:ARG:HG2	10:J:99:TYR:O	2.06	0.55
36:O:308:CLA:H92	36:O:308:CLA:H41	1.89	0.55
36:R:310:CLA:H92	36:R:310:CLA:H41	1.88	0.55
20:a:423:THR:OG1	20:a:426:ASN:ND2	2.39	0.55
41:l:208:LHG:HC91	41:l:208:LHG:O10	2.06	0.55
33:V:143:ILE:CD1	36:V:311:CLA:H2	2.17	0.55
2:B:194:LEU:HD13	35:B:303:A86:C23	2.34	0.55
2:B:209:PRO:HB3	39:B:312:LMT:H2O1	1.70	0.55
39:P:320:LMT:H22	39:P:320:LMT:O2'	2.06	0.55
20:a:271:SER:O	39:a:853:LMT:O6'	2.20	0.55
20:a:503:THR:HB	36:a:833:CLA:OBD	2.06	0.55
21:b:410:MET:HE2	44:h:201:BCR:H402	1.88	0.55
32:U:100:LYS:HG2	32:U:109:ALA:HA	1.87	0.55
33:V:81:MET:CE	33:V:89:HIS:CD2	2.89	0.55
33:V:82:SER:CB	33:V:83:PRO:HD2	2.30	0.55
33:V:116:LYS:HB3	36:V:314:CLA:CGD	2.25	0.55
36:E:311:CLA:H93	42:E:318:LMG:H112	1.86	0.55
14:N:86:MET:HE1	14:N:202:GLU:CD	2.30	0.55
14:N:89:PHE:CZ	14:N:93:ILE:HD11	2.41	0.55
16:R:95:TYR:HD2	16:R:217:PHE:CD2	2.24	0.55
37:T:310:KC1:CMD	36:T:313:CLA:ND	2.68	0.55
19:X:28:LYS:HD3	19:X:32:LEU:HD11	1.88	0.55
36:b:823:CLA:HAC2	36:b:824:CLA:H72	1.88	0.55
36:b:836:CLA:H8	39:b:851:LMT:H102	1.86	0.55
25:f:206:LEU:CD2	36:f:804:CLA:HMD3	2.35	0.55
36:j:102:CLA:O2A	36:j:102:CLA:H201	2.07	0.55
6:F:56:GLU:HB2	6:F:66:PHE:HB2	1.88	0.55
9:I:185:PHE:N	9:I:185:PHE:CD1	2.73	0.55
21:b:125:THR:HG21	21:b:358:ALA:H	1.70	0.55
21:b:411:LEU:C	25:f:238:ALA:HB3	2.31	0.55
32:U:25:ILE:HG21	36:U:306:CLA:H42	1.88	0.55
33:V:58:LEU:HD12	33:V:75:PHE:CZ	2.39	0.55
33:V:126:GLY:HA2	33:V:131:GLY:HA3	1.88	0.55
4:D:180:ILE:O	4:D:184:ARG:N	2.37	0.55
6:F:145:HIS:CB	36:F:317:CLA:CAA	2.84	0.55
9:I:93:PRO:CD	36:I:308:CLA:CMD	2.79	0.55
10:J:85:GLY:HA2	36:J:310:CLA:C2C	2.36	0.55
36:K:309:CLA:H111	39:K:318:LMT:C12	2.28	0.55
41:O:317:LHG:HC62	41:O:317:LHG:C9	2.36	0.55
15:P:77:ALA:CB	34:P:305:DD6:C41	2.84	0.55
15:P:164:GLN:NE2	15:P:168:ARG:NH2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:155:ILE:CG1	35:Q:316:A86:C39	2.81	0.55
20:a:628:THR:OG1	20:a:632:SER:OG	2.25	0.55
21:b:656:TRP:CZ3	36:b:805:CLA:HHB	2.41	0.55
23:d:137:CYS:C	23:d:154:PHE:HE2	2.15	0.55
31:h:118:SER:CB	35:h:204:A86:O2	2.54	0.55
33:V:77:ASP:N	33:V:77:ASP:OD1	2.38	0.55
39:E:320:LMT:O6'	39:E:321:LMT:C1	2.53	0.55
15:P:51:LEU:HD13	34:P:305:DD6:O2	2.07	0.55
20:a:250:ILE:HD11	36:a:815:CLA:HBC1	1.89	0.55
36:b:806:CLA:H13	44:i:101:BCR:H281	1.89	0.55
36:b:831:CLA:HAB	36:b:838:CLA:HBB2	1.89	0.55
36:b:833:CLA:H43	44:f:801:BCR:HC32	1.89	0.55
36:E:313:CLA:H161	36:E:313:CLA:C11	2.36	0.55
6:F:67:PRO:HG3	6:F:150:TRP:CH2	2.40	0.55
9:I:51:PRO:O	9:I:52:LEU:HB2	2.06	0.55
35:I:301:A86:C40	36:K:312:CLA:H203	2.37	0.55
34:W:204:DD6:C25	36:W:207:CLA:HMC2	2.37	0.55
32:U:29:ARG:NH2	39:U:315:LMT:H6E	2.20	0.55
36:U:310:CLA:C2C	39:U:315:LMT:H121	2.37	0.55
33:V:62:SER:CB	33:V:63:PRO:CD	2.85	0.55
3:C:45:ARG:NH2	3:C:49:LEU:O	2.40	0.55
4:D:47:ASN:ND2	4:D:63:SER:O	2.39	0.55
7:G:38:TRP:CZ2	7:G:42:VAL:HG11	2.42	0.55
7:G:178:VAL:HG21	36:G:319:CLA:HBC2	1.88	0.55
9:I:138:TYR:CE2	9:I:139:GLN:O	2.60	0.55
34:J:304:DD6:C40	36:J:308:CLA:H101	2.37	0.55
13:M:99:SER:O	13:M:103:HIS:ND1	2.33	0.55
35:N:305:A86:C39	35:O:305:A86:C19	2.85	0.55
19:X:120:ALA:CA	33:V:13:ASN:ND2	2.65	0.55
20:a:394:SER:OG	20:a:750:LEU:HD21	2.07	0.55
34:a:849:DD6:C21	34:a:849:DD6:C13	2.86	0.55
21:b:305:ASP:HB3	31:h:53:THR:HG22	1.88	0.55
36:U:306:CLA:CGA	36:U:306:CLA:C3A	2.85	0.55
35:C:204:A86:C19	35:C:204:A86:C23	2.85	0.54
4:D:73:GLU:OE2	4:D:153:PRO:CA	2.47	0.54
36:G:315:CLA:C1	36:G:315:CLA:CAA	2.86	0.54
17:S:122:TRP:HZ3	36:S:312:CLA:HHB	1.73	0.54
35:S:304:A86:C23	35:S:304:A86:C13	2.85	0.54
20:a:583:PRO:HD3	21:b:560:GLY:HA2	1.90	0.54
36:b:802:CLA:CAB	36:f:803:CLA:HMD3	2.37	0.54
39:h:205:LMT:C6'	39:h:205:LMT:C1B	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:h:205:LMT:C6'	39:h:205:LMT:C6B	2.86	0.54
35:U:303:A86:C22	35:U:303:A86:C13	2.85	0.54
36:U:306:CLA:CHB	36:U:306:CLA:C1	2.86	0.54
33:V:163:ALA:CB	35:V:303:A86:C10	2.86	0.54
34:A:303:DD6:C19	34:A:303:DD6:C23	2.86	0.54
3:C:40:LEU:HD12	3:C:59:PHE:HD1	1.72	0.54
3:C:55:GLY:HA3	3:C:172:ILE:HG21	1.88	0.54
36:C:206:CLA:HMA2	40:C:215:DGD:O4D	2.06	0.54
6:F:67:PRO:HB3	6:F:71:TYR:HD2	1.72	0.54
34:G:303:DD6:C21	34:G:303:DD6:C13	2.86	0.54
35:H:304:A86:C33	35:H:304:A86:C39	2.85	0.54
35:L:301:A86:O5	36:P:313:CLA:C12	2.52	0.54
41:Q:315:LHG:O5	41:Q:315:LHG:HC5	2.07	0.54
17:S:242:GLN:NE2	36:S:318:CLA:O1D	2.41	0.54
20:a:429:ASN:ND2	20:a:437:ARG:HH12	2.01	0.54
23:d:137:CYS:C	23:d:154:PHE:CZ	2.85	0.54
23:d:208:TYR:HH	30:g:133:UNK:CB	2.19	0.54
32:U:128:LEU:CD1	36:U:305:CLA:O1D	2.56	0.54
35:V:301:A86:C13	35:V:301:A86:C21	2.86	0.54
1:A:66:TYR:CZ	42:j:105:LMG:HC91	2.42	0.54
35:C:204:A86:C37	35:C:204:A86:C28	2.86	0.54
4:D:196:GLN:HB3	4:D:206:TYR:HB2	1.87	0.54
41:D:318:LHG:H262	41:D:318:LHG:H311	1.89	0.54
6:F:45:LYS:HD2	42:V:316:LMG:HC62	1.89	0.54
36:I:309:CLA:C1	36:l:206:CLA:H2	2.38	0.54
14:N:118:PRO:HA	14:N:121:GLN:HB2	1.90	0.54
15:P:125:PHE:CE2	36:P:302:CLA:CED	2.88	0.54
34:R:307:DD6:C21	34:R:307:DD6:C13	2.86	0.54
17:S:228:LEU:HD23	35:S:304:A86:C39	2.36	0.54
35:X:314:A86:C23	35:X:314:A86:C13	2.85	0.54
36:b:818:CLA:HBC2	35:h:202:A86:C26	2.37	0.54
31:h:84:ALA:CB	39:h:205:LMT:H112	2.31	0.54
40:C:215:DGD:O1B	40:C:215:DGD:HB62	2.07	0.54
41:O:317:LHG:H302	36:V:313:CLA:C12	2.38	0.54
34:P:305:DD6:C23	34:P:305:DD6:C13	2.86	0.54
34:W:205:DD6:C21	34:W:205:DD6:C13	2.85	0.54
21:b:402:ASN:O	21:b:405:ASN:HB2	2.07	0.54
36:j:102:CLA:C9	36:j:102:CLA:C12	2.86	0.54
33:V:8:VAL:HG23	36:V:305:CLA:NB	2.21	0.54
34:C:201:DD6:C22	34:C:201:DD6:C13	2.86	0.54
35:F:301:A86:C37	35:F:301:A86:C33	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:242:PHE:N	7:G:243:PRO:HD2	2.22	0.54
35:G:302:A86:C	36:G:311:CLA:HBC2	2.38	0.54
39:I:317:LMT:C6B	39:I:317:LMT:C2B	2.85	0.54
36:K:310:CLA:C1A	36:K:310:CLA:CGA	2.86	0.54
15:P:64:ARG:HH11	15:P:64:ARG:CG	2.14	0.54
15:Q:152:PHE:CG	15:Q:153:PRO:CD	2.78	0.54
17:S:143:TRP:HH2	17:S:169:LEU:HB3	1.73	0.54
35:S:304:A86:C39	35:S:304:A86:C33	2.86	0.54
19:W:154:LEU:CD1	34:W:205:DD6:O1	2.54	0.54
36:X:315:CLA:C1B	33:V:176:SER:OG	2.56	0.54
20:a:126:ILE:HD12	20:a:126:ILE:O	2.08	0.54
39:a:851:LMT:H3'	39:a:851:LMT:O5B	2.05	0.54
27:j:38:THR:CB	27:j:40:PRO:CD	2.85	0.54
35:V:301:A86:C37	35:V:301:A86:C33	2.86	0.54
1:A:196:TRP:CE3	36:A:314:CLA:OBD	2.58	0.54
7:G:120:TRP:CD1	7:G:120:TRP:C	2.85	0.54
7:G:200:LEU:HD21	7:G:211:MET:HG3	1.89	0.54
35:K:301:A86:C35	35:K:301:A86:C41	2.85	0.54
13:M:203:LYS:HZ1	35:M:304:A86:C38	2.21	0.54
16:R:242:MET:CG	35:R:305:A86:C37	2.83	0.54
35:S:304:A86:C9	36:S:315:CLA:HMC3	2.38	0.54
35:V:304:A86:O5	36:V:308:CLA:H202	2.07	0.54
1:A:90:PHE:CZ	1:A:108:ASN:OD1	2.61	0.54
35:C:203:A86:C33	35:C:203:A86:C37	2.86	0.54
41:E:322:LHG:C6	41:E:322:LHG:C2	2.86	0.54
7:G:38:TRP:CE2	7:G:42:VAL:HG11	2.43	0.54
35:G:306:A86:C37	35:G:306:A86:C33	2.86	0.54
35:J:302:A86:C41	35:J:302:A86:C35	2.86	0.54
14:N:62:PHE:HE2	14:N:70:THR:HA	1.72	0.54
14:N:228:LEU:O	35:N:304:A86:C39	2.55	0.54
17:S:144:ASP:OD1	17:S:164:TYR:CE2	2.61	0.54
2:B:136:SER:CB	36:B:308:CLA:C4D	2.86	0.54
34:E:303:DD6:C22	34:E:303:DD6:C13	2.85	0.54
36:G:311:CLA:HBC1	36:G:313:CLA:H202	1.90	0.54
36:G:315:CLA:C4	41:G:320:LHG:H252	2.28	0.54
35:H:304:A86:C	36:H:314:CLA:HBC1	2.37	0.54
35:R:305:A86:C23	35:R:305:A86:C19	2.86	0.54
17:S:228:LEU:CD2	35:S:304:A86:C39	2.86	0.54
34:W:204:DD6:C22	34:W:204:DD6:C13	2.86	0.54
20:a:460:PHE:HB3	20:a:539:MET:HE3	1.88	0.54
36:a:802:CLA:C9	43:a:840:PQN:H28	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:A:301:DD6:C21	34:A:301:DD6:C13	2.86	0.54
34:A:301:DD6:C40	38:A:315:SQD:O2	2.56	0.54
2:B:93:LEU:HG	2:B:93:LEU:O	2.08	0.54
4:D:152:GLU:HB2	4:D:155:ASN:HB3	1.90	0.54
34:F:303:DD6:C23	34:F:303:DD6:C13	2.86	0.54
7:G:47:ARG:HH12	11:K:151:ARG:CB	2.21	0.54
36:G:307:CLA:CBA	40:L:302:DGD:C3G	2.67	0.54
8:H:171:MET:HE2	36:H:312:CLA:H12	1.88	0.54
35:N:305:A86:C8	36:N:316:CLA:CBB	2.85	0.54
16:R:51:VAL:O	16:R:52:LEU:HB3	2.08	0.54
20:a:377:TYR:CD1	20:a:377:TYR:C	2.86	0.54
23:d:195:VAL:CG2	23:d:210:LEU:HD22	2.31	0.54
25:f:214:VAL:O	25:f:218:ARG:HG2	2.08	0.54
41:f:808:LHG:H331	42:V:316:LMG:C33	2.37	0.54
32:U:57:PHE:HD2	36:U:308:CLA:C3D	2.21	0.54
3:C:68:GLN:HE22	3:C:74:ALA:HB2	1.73	0.54
35:C:203:A86:C28	29:m:23:LYS:CE	2.86	0.54
36:D:307:CLA:CMC	41:D:318:LHG:C9	2.85	0.54
36:E:315:CLA:H143	36:M:307:CLA:H142	1.86	0.54
37:F:308:KC1:CMB	39:F:320:LMT:H2O2	2.21	0.54
36:F:317:CLA:HBB1	36:F:317:CLA:CHC	2.36	0.54
35:G:302:A86:C12	36:G:311:CLA:HMB2	2.37	0.54
9:I:84:TRP:C	9:I:84:TRP:CD1	2.86	0.54
34:I:303:DD6:C21	34:I:303:DD6:C13	2.86	0.54
11:K:76:GLU:OE1	11:K:154:GLY:N	2.41	0.54
12:L:114:ALA:O	39:L:318:LMT:O4'	2.21	0.54
34:L:305:DD6:C21	34:L:305:DD6:C13	2.85	0.54
14:N:34:ALA:HB1	14:N:71:ILE:HG12	1.90	0.54
14:N:170:PHE:CZ	36:N:318:CLA:H11	2.43	0.54
20:a:98:PHE:CZ	20:a:102:TYR:CD2	2.96	0.54
36:b:836:CLA:HBB1	36:b:836:CLA:CMB	2.38	0.54
33:V:138:TRP:CE3	36:V:308:CLA:H203	2.42	0.54
35:V:301:A86:C37	35:V:301:A86:C39	2.86	0.54
34:A:304:DD6:C21	34:A:304:DD6:C13	2.85	0.53
34:B:304:DD6:C13	34:B:304:DD6:C23	2.86	0.53
3:C:83:ARG:HB3	36:C:212:CLA:HBC2	1.89	0.53
6:F:208:VAL:HG22	6:F:210:ILE:HG22	1.89	0.53
37:F:315:KC1:OBD	39:F:321:LMT:O2'	2.23	0.53
36:F:317:CLA:CBB	42:J:318:LMG:H152	2.15	0.53
42:J:319:LMG:C11	42:J:319:LMG:C9	2.86	0.53
11:K:44:PRO:HD3	36:K:308:CLA:HED2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:O:305:A86:C39	35:O:305:A86:C35	2.86	0.53
15:P:121:ASN:OD1	36:P:302:CLA:HED2	2.07	0.53
16:R:86:ARG:NH2	16:R:162:GLY:O	2.41	0.53
37:T:310:KC1:CMC	37:T:310:KC1:CBC	2.85	0.53
20:a:91:LEU:HD11	39:a:851:LMT:C12	2.38	0.53
36:a:816:CLA:C18	36:a:816:CLA:C14	2.86	0.53
34:A:303:DD6:C22	34:A:303:DD6:C13	2.85	0.53
6:F:67:PRO:HB3	6:F:71:TYR:CD2	2.43	0.53
36:F:317:CLA:H12	36:F:317:CLA:C7	2.38	0.53
36:F:317:CLA:CGD	36:F:317:CLA:HBA2	2.37	0.53
41:G:320:LHG:H111	41:G:320:LHG:H152	1.87	0.53
41:I:316:LHG:H242	41:I:316:LHG:HC82	1.85	0.53
42:J:319:LMG:HC91	42:J:319:LMG:C11	2.37	0.53
36:N:316:CLA:HED3	36:N:316:CLA:H2	1.90	0.53
15:P:132:PHE:CD2	39:P:320:LMT:H72	2.43	0.53
34:Q:302:DD6:C21	34:Q:302:DD6:C13	2.85	0.53
23:d:138:LEU:N	23:d:154:PHE:HE2	2.06	0.53
34:j:103:DD6:C21	34:j:103:DD6:C13	2.85	0.53
33:V:3:LEU:HD22	33:V:4:GLY:H	1.72	0.53
3:C:82:GLY:O	3:C:86:MET:HG3	2.08	0.53
41:D:318:LHG:H311	41:D:318:LHG:C26	2.39	0.53
7:G:227:GLY:HA2	35:G:305:A86:C	2.38	0.53
35:L:301:A86:C37	35:L:301:A86:C33	2.86	0.53
35:P:307:A86:C13	35:P:307:A86:C23	2.86	0.53
21:b:26:ALA:HA	36:b:830:CLA:H43	1.91	0.53
1:A:94:GLN:HE22	1:A:202:LEU:H	1.55	0.53
2:B:66:HIS:HE1	2:B:70:TRP:HE1	1.47	0.53
36:G:319:CLA:HBC3	36:G:319:CLA:HHD	1.90	0.53
36:K:310:CLA:C17	36:K:310:CLA:C14	2.86	0.53
35:L:307:A86:C41	35:L:307:A86:C35	2.86	0.53
19:X:83:ILE:HG23	36:X:309:CLA:HMA2	1.90	0.53
20:a:33:LYS:HB2	36:a:810:CLA:HAA2	1.90	0.53
20:a:243:PRO:HG3	20:a:254:LEU:HD21	1.90	0.53
33:V:54:LEU:N	33:V:54:LEU:HD23	2.22	0.53
2:B:189:GLY:O	2:B:193:MET:HG3	2.09	0.53
34:H:303:DD6:C13	34:H:303:DD6:C21	2.86	0.53
36:O:312:CLA:HMD3	36:O:316:CLA:OBD	2.09	0.53
34:R:308:DD6:C8	34:R:308:DD6:C12	2.86	0.53
35:S:302:A86:C25	34:S:306:DD6:C17	2.86	0.53
19:X:54:GLU:OE1	19:X:75:ASN:ND2	2.41	0.53
46:a:937:HOH:O	36:l:202:CLA:HED2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:215:PRO:HA	36:b:817:CLA:HED3	1.91	0.53
32:U:4:MET:HA	32:U:4:MET:CE	2.37	0.53
1:A:73:ARG:NH1	1:A:76:GLU:OE1	2.42	0.53
36:C:212:CLA:H2A	36:C:212:CLA:HED3	1.90	0.53
10:J:86:TYR:OH	10:J:108:ALA:CA	2.57	0.53
35:P:306:A86:C19	35:P:306:A86:C22	2.86	0.53
16:R:66:TRP:CZ2	41:R:323:LHG:H241	2.44	0.53
17:S:52:TYR:CZ	17:S:54:PRO:HG3	2.43	0.53
17:S:143:TRP:CD1	17:S:164:TYR:HE1	2.25	0.53
34:W:204:DD6:C26	36:W:207:CLA:HHC	2.39	0.53
19:X:59:LEU:CD2	36:X:315:CLA:OBD	2.57	0.53
20:a:601:LEU:CD1	20:a:734:LEU:HD21	2.39	0.53
36:a:848:CLA:HMA1	36:b:805:CLA:H161	1.90	0.53
21:b:222:LYS:H	21:b:223:PRO:CD	2.22	0.53
23:d:198:ILE:HD12	23:d:201:LYS:NZ	2.22	0.53
25:f:78:ILE:HD11	25:f:154:ARG:NH1	2.23	0.53
35:h:202:A86:C19	35:h:202:A86:C23	2.87	0.53
33:V:113:ARG:HG3	33:V:113:ARG:NH1	2.20	0.53
1:A:196:TRP:CZ2	36:A:314:CLA:CMD	2.91	0.53
3:C:41:PRO:C	3:C:43:LEU:N	2.65	0.53
35:C:203:A86:C33	35:C:203:A86:C39	2.86	0.53
35:E:307:A86:C7	36:E:315:CLA:NC	2.72	0.53
6:F:184:GLU:HG3	36:F:314:CLA:C1B	2.38	0.53
7:G:64:LEU:HD11	7:G:99:LEU:HD11	1.90	0.53
36:K:310:CLA:HBC2	36:K:310:CLA:CHD	2.17	0.53
20:a:124:TRP:HE1	39:a:851:LMT:C6'	2.21	0.53
21:b:5:PHE:CD1	21:b:5:PHE:C	2.85	0.53
21:b:191:GLY:O	21:b:195:HIS:HD2	1.92	0.53
32:U:77:TRP:NE1	36:U:308:CLA:H3A	2.24	0.53
33:V:103:ALA:HA	36:V:310:CLA:HAB	1.90	0.53
3:C:40:LEU:HD21	36:C:205:CLA:CBC	2.38	0.53
4:D:61:ARG:HH11	4:D:61:ARG:CG	2.14	0.53
5:E:146:ILE:CD1	41:E:322:LHG:HC91	2.39	0.53
36:L:308:CLA:C7	37:L:315:KC1:CMD	2.78	0.53
14:N:239:GLN:HG3	14:N:242:GLN:HB2	1.90	0.53
15:P:71:SER:HB2	15:P:176:GLY:HA3	1.91	0.53
18:T:150:ILE:HG22	18:T:154:MET:HE2	1.91	0.53
20:a:281:LEU:HB2	36:a:816:CLA:CMA	2.39	0.53
22:c:77:MET:HB3	22:c:79:LEU:HG	1.91	0.53
25:f:207:PHE:C	25:f:207:PHE:CD1	2.85	0.53
28:l:81:HIS:HA	28:l:84:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:8:SER:OG	36:U:306:CLA:O2D	2.26	0.53
32:U:77:TRP:CZ2	36:U:308:CLA:HBA2	2.43	0.53
32:U:106:GLY:O	32:U:116:TYR:HE2	1.92	0.53
2:B:136:SER:HB2	36:B:308:CLA:C4D	2.39	0.53
3:C:195:PRO:HG2	3:C:197:LEU:HD22	1.91	0.53
7:G:156:GLN:NE2	7:G:158:SER:CB	2.72	0.53
7:G:230:ALA:HB1	35:G:305:A86:C28	2.39	0.53
9:I:92:HIS:HE1	9:I:99:LEU:CD2	2.21	0.53
41:I:316:LHG:O1	41:I:316:LHG:O3	2.26	0.53
36:L:308:CLA:CMC	36:L:308:CLA:CBC	2.85	0.53
14:N:241:MET:CG	35:N:305:A86:C8	2.87	0.53
34:W:204:DD6:C25	36:W:207:CLA:CMC	2.86	0.53
20:a:71:LEU:HD22	20:a:193:LEU:HD21	1.91	0.53
21:b:110:TYR:HB2	21:b:111:PRO:CD	2.39	0.53
32:U:34:GLU:OE2	36:U:306:CLA:C1B	2.36	0.53
32:U:143:GLY:HA2	36:U:313:CLA:HAB	1.91	0.53
33:V:19:THR:HG22	33:V:24:SER:O	2.07	0.53
33:V:64:HIS:HE1	36:V:313:CLA:C4D	2.21	0.53
7:G:43:ASP:HB2	7:G:58:VAL:HG12	1.91	0.53
9:I:46:MET:HE2	39:K:318:LMT:H42	1.91	0.53
12:L:199:LYS:HG3	36:L:308:CLA:HED1	1.88	0.53
14:N:100:PHE:HB3	14:N:102:TRP:CZ3	2.44	0.53
36:N:318:CLA:H2A	36:N:318:CLA:C2	2.39	0.53
19:X:145:ARG:HB3	36:X:307:CLA:HMA2	1.91	0.53
20:a:240:GLN:H	20:a:240:GLN:CD	2.17	0.53
36:b:810:CLA:H71	44:i:101:BCR:HC32	1.91	0.53
25:f:152:ASP:OD1	36:f:805:CLA:HMD3	2.06	0.53
33:V:7:PRO:HB2	36:V:305:CLA:CHB	2.39	0.53
33:V:58:LEU:CB	33:V:75:PHE:CE2	2.92	0.53
33:V:81:MET:HE1	33:V:89:HIS:CD2	2.44	0.53
35:F:301:A86:C22	36:F:309:CLA:HBC1	2.39	0.52
37:F:315:KC1:O1A	35:O:301:A86:O3	2.27	0.52
39:I:317:LMT:H12	39:I:317:LMT:O6'	2.09	0.52
12:L:43:ILE:HG23	12:L:44:GLU:OE2	2.09	0.52
36:O:312:CLA:CMD	36:O:316:CLA:OBD	2.57	0.52
15:P:156:ASP:HB2	16:R:64:THR:H	1.72	0.52
18:T:135:LYS:HZ2	37:T:315:KC1:CGA	2.21	0.52
20:a:628:THR:HG1	20:a:632:SER:HG	1.56	0.52
21:b:217:HIS:HD2	21:b:219:ALA:H	1.57	0.52
34:D:301:DD6:C13	34:D:301:DD6:C23	2.85	0.52
36:G:315:CLA:HED3	39:a:853:LMT:H5B	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:PHE:CE2	36:H:310:CLA:HED2	2.44	0.52
11:K:75:ARG:NH2	11:K:78:GLU:OE1	2.43	0.52
15:Q:152:PHE:CD1	15:Q:153:PRO:HD2	2.42	0.52
19:W:42:ILE:CG2	34:W:204:DD6:C12	2.87	0.52
20:a:112:ASP:OD2	20:a:115:LYS:CG	2.57	0.52
20:a:538:PHE:CD1	20:a:538:PHE:C	2.87	0.52
41:f:808:LHG:H352	42:V:316:LMG:H351	1.90	0.52
31:h:72:PRO:HB2	42:h:206:LMG:HC3	1.91	0.52
32:U:63:VAL:HG12	32:U:64:ASP:N	2.23	0.52
36:A:306:CLA:H51	37:A:312:KC1:C3D	2.39	0.52
7:G:104:GLU:OE1	7:G:190:GLY:N	2.41	0.52
42:G:324:LMG:O7	42:G:324:LMG:HC1	2.09	0.52
36:I:312:CLA:H42	42:I:315:LMG:H351	1.91	0.52
10:J:48:ALA:HA	14:N:151:ALA:HB3	1.92	0.52
12:L:35:ILE:HG13	12:L:37:GLU:H	1.74	0.52
15:O:71:SER:HB2	15:O:176:GLY:HA3	1.91	0.52
37:W:217:KC1:CMC	35:X:305:A86:C7	2.87	0.52
25:f:207:PHE:C	25:f:207:PHE:HD1	2.16	0.52
26:i:4:ASN:O	26:i:8:LEU:HD13	2.10	0.52
4:D:45:PRO:HB2	4:D:48:LEU:HD13	1.91	0.52
6:F:99:GLY:O	6:F:100:LEU:CD2	2.55	0.52
36:F:317:CLA:H71	36:F:317:CLA:C1	2.39	0.52
42:G:325:LMG:H192	36:I:312:CLA:HBC1	1.91	0.52
8:H:46:ASN:HD22	8:H:63:GLU:HA	1.75	0.52
36:I:306:CLA:HBB1	36:I:306:CLA:CMB	2.40	0.52
35:J:302:A86:C24	36:J:315:CLA:HBC2	2.38	0.52
19:X:78:ALA:HA	19:X:81:LYS:HE2	1.92	0.52
21:b:243:TYR:H	21:b:263[A]:GLN:HE21	1.55	0.52
39:b:851:LMT:H31	39:f:807:LMT:H61	1.90	0.52
41:i:104:LHG:O10	42:m:102:LMG:H132	2.08	0.52
33:V:163:ALA:HB2	35:V:303:A86:C10	2.39	0.52
2:B:136:SER:CB	36:B:308:CLA:ND	2.69	0.52
3:C:40:LEU:HD12	3:C:59:PHE:CD1	2.43	0.52
7:G:47:ARG:NE	11:K:149:TYR:OH	2.43	0.52
8:H:137:TRP:HZ2	36:H:318:CLA:H3A	1.74	0.52
9:I:49:PHE:HB3	36:I:306:CLA:HMD3	1.90	0.52
35:I:302:A86:C6	36:I:308:CLA:H72	2.29	0.52
11:K:149:TYR:HE2	11:K:151:ARG:HD3	1.75	0.52
13:M:188:ASN:HD21	13:M:193:LEU:HD23	1.74	0.52
15:P:168:ARG:CZ	37:P:315:KC1:O1A	2.57	0.52
35:S:308:A86:C28	36:S:318:CLA:HBC3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:W:205:DD6:C26	36:W:212:CLA:HMC2	2.39	0.52
36:a:806:CLA:C1D	39:a:851:LMT:H72	2.39	0.52
36:a:806:CLA:C7	36:a:808:CLA:H92	2.37	0.52
36:b:840:CLA:HHC	36:b:840:CLA:HBB1	1.91	0.52
28:l:75:LEU:HD13	28:l:79:LEU:HD12	1.91	0.52
2:B:207:GLN:HE22	29:m:5:ASN:HD21	1.57	0.52
4:D:97:ARG:NH1	4:D:108:LEU:O	2.43	0.52
41:D:318:LHG:H262	41:D:318:LHG:C31	2.40	0.52
5:E:68:ASP:C	20:a:16:LYS:HZ3	2.06	0.52
17:S:190:MET:SD	17:S:198:ARG:NH1	2.83	0.52
20:a:587:GLY:N	21:b:667:ARG:NH2	2.48	0.52
36:a:816:CLA:ND	42:a:852:LMG:H291	2.24	0.52
32:U:126:MET:HG2	36:U:311:CLA:H3A	1.90	0.52
39:U:315:LMT:H2B	39:U:315:LMT:H6'2	1.92	0.52
33:V:140:PRO:C	33:V:141:LEU:CG	2.82	0.52
1:A:140:MET:HB3	25:f:207:PHE:HE1	1.74	0.52
3:C:160:SER:HB2	3:C:161:PRO:HD2	1.91	0.52
10:J:186:ILE:CG1	35:J:305:A86:O1	2.58	0.52
14:N:79:ILE:O	14:N:83:ARG:N	2.40	0.52
15:Q:71:SER:HB2	15:Q:176:GLY:HA3	1.91	0.52
34:Q:302:DD6:C26	36:Q:306:CLA:HHC	2.40	0.52
16:R:49:ASN:ND2	36:R:310:CLA:C1B	2.73	0.52
19:X:99:GLU:HA	19:X:103:MET:HB2	1.91	0.52
19:X:107:THR:CG2	33:V:17:LYS:HG3	2.39	0.52
21:b:546:MET:HE2	21:b:549:LYS:HA	1.92	0.52
24:e:7:ALA:HB1	24:e:62:GLU:OE2	2.10	0.52
27:j:15:SER:OG	27:j:19:PHE:CE2	2.34	0.52
35:U:303:A86:C19	35:U:303:A86:C23	2.87	0.52
33:V:162:PHE:CE1	35:V:301:A86:C7	2.93	0.52
6:F:161:LEU:N	6:F:161:LEU:CD2	2.73	0.52
36:F:317:CLA:C7	36:F:317:CLA:C1	2.88	0.52
36:G:315:CLA:HBB1	36:G:315:CLA:CHC	2.36	0.52
13:M:77:ARG:HH21	13:M:77:ARG:CG	2.23	0.52
36:S:315:CLA:HBC2	36:S:321:CLA:HAA2	1.92	0.52
20:a:594:TRP:CE3	20:a:595:ASP:OD1	2.63	0.52
44:a:844:BCR:C27	42:a:852:LMG:C44	2.87	0.52
36:b:821:CLA:H192	36:b:825:CLA:H141	1.92	0.52
1:A:193:HIS:HD2	36:A:314:CLA:HMA3	1.73	0.52
36:A:306:CLA:HBC1	37:A:312:KC1:CBC	2.40	0.52
7:G:84:GLY:HA2	7:G:87:GLN:O	2.10	0.52
7:G:173:THR:HG22	7:G:173:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:G:314:CLA:HBC1	36:G:316:CLA:HAB	1.91	0.52
12:L:100:GLY:HA2	15:Q:191:ASN:HD21	1.74	0.52
40:L:302:DGD:O1G	40:L:302:DGD:HB21	2.09	0.52
13:M:231:CYS:O	13:M:238:SER:OG	2.24	0.52
15:O:112:TRP:NE1	36:V:313:CLA:OBD	2.29	0.52
15:Q:77:ALA:HA	34:Q:302:DD6:C23	2.40	0.52
20:a:712:LYS:C	25:f:227:ASP:OD1	2.53	0.52
21:b:140:GLY:HA3	36:b:816:CLA:H12	1.92	0.52
36:b:816:CLA:H91	36:b:816:CLA:H121	1.91	0.52
23:d:143:ARG:O	23:d:147:LYS:HB2	2.09	0.52
26:i:16:LEU:HD22	36:l:202:CLA:H193	1.92	0.52
36:A:306:CLA:CMB	36:A:306:CLA:HBB1	2.40	0.52
3:C:40:LEU:N	3:C:41:PRO:HD3	2.24	0.52
35:E:307:A86:C8	36:E:315:CLA:ND	2.73	0.52
6:F:145:HIS:CD2	36:F:317:CLA:HAA2	2.45	0.52
7:G:41:MET:HG3	7:G:41:MET:O	2.09	0.52
9:I:144:LEU:HD23	9:I:144:LEU:O	2.09	0.52
10:J:89:THR:HG23	10:J:107:SER:CB	2.40	0.52
15:P:128:PHE:C	15:P:128:PHE:CD1	2.88	0.52
15:Q:77:ALA:CA	34:Q:302:DD6:C23	2.87	0.52
19:X:117:ARG:CB	33:V:14:TYR:CZ	2.93	0.52
21:b:14:GLN:HE22	30:g:139:UNK:CB	2.22	0.52
35:G:306:A86:C7	42:G:324:LMG:H192	2.39	0.51
10:J:89:THR:HG21	10:J:107:SER:HB2	1.91	0.51
15:Q:77:ALA:CB	34:Q:302:DD6:C23	2.88	0.51
21:b:324:THR:HG21	21:b:402:ASN:OD1	2.10	0.51
32:U:46:VAL:CG1	36:U:308:CLA:CMC	2.89	0.51
3:C:40:LEU:CD2	36:C:205:CLA:C2C	2.88	0.51
5:E:45:ARG:NH2	5:E:46:PRO:O	2.43	0.51
5:E:62:LEU:HD12	5:E:64:LEU:HD11	1.92	0.51
12:L:82:ALA:HB1	34:L:305:DD6:C13	2.40	0.51
12:L:98:TYR:OH	15:Q:109:LEU:O	2.26	0.51
34:M:303:DD6:C36	36:M:307:CLA:H2	2.40	0.51
35:N:305:A86:C7	36:N:309:CLA:C2C	2.87	0.51
35:N:305:A86:C29	36:N:309:CLA:CED	2.88	0.51
15:P:159:THR:HG21	16:R:62:SER:C	2.35	0.51
19:X:117:ARG:HE	19:X:121:ILE:H	1.57	0.51
20:a:483:GLN:H	41:a:850:LHG:HC2	1.76	0.51
23:d:104:TRP:HB2	23:d:150:ILE:HD11	1.92	0.51
26:i:26:PHE:CD2	28:l:122:ILE:CG2	2.93	0.51
31:h:125:TRP:HB2	35:h:204:A86:C5	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:96:GLU:HG2	32:U:102:SER:CA	2.38	0.51
4:D:143:GLN:O	4:D:149:SER:N	2.44	0.51
36:E:316:CLA:H112	36:P:313:CLA:HBB1	1.91	0.51
8:H:72:GLU:HG2	8:H:140:LEU:HD13	1.92	0.51
8:H:137:TRP:CZ2	36:H:318:CLA:H3A	2.45	0.51
36:I:312:CLA:CED	39:I:318:LMT:H6D	2.40	0.51
12:L:134:LEU:HD23	12:L:218:GLU:HG2	1.92	0.51
35:O:305:A86:C19	35:O:305:A86:C22	2.88	0.51
16:R:107:PRO:HA	16:R:114:PRO:HA	1.92	0.51
20:a:340:GLY:HA2	46:a:945:HOH:O	2.09	0.51
20:a:430:ASN:C	20:a:430:ASN:HD22	2.19	0.51
21:b:305:ASP:HB3	31:h:53:THR:CG2	2.41	0.51
32:U:9:VAL:HG21	32:U:15:ILE:HG13	1.92	0.51
32:U:77:TRP:HZ2	36:U:308:CLA:HHB	1.76	0.51
2:B:185:GLU:HG3	36:B:309:CLA:C1B	2.40	0.51
4:D:155:ASN:HD21	4:D:157:GLY:H	1.54	0.51
34:D:303:DD6:C22	34:D:303:DD6:C13	2.88	0.51
35:E:307:A86:C13	36:E:315:CLA:HMD1	2.40	0.51
7:G:242:PHE:CD1	7:G:242:PHE:C	2.86	0.51
9:I:87:THR:HB	9:I:101:SER:OG	2.09	0.51
15:O:133:ILE:HD11	35:O:301:A86:C34	2.40	0.51
16:R:87:ILE:O	16:R:91:ALA:N	2.42	0.51
21:b:490:GLN:HB3	31:h:104:TYR:CD1	2.45	0.51
36:b:817:CLA:C12	36:b:817:CLA:C9	2.86	0.51
23:d:95:GLN:NE2	30:g:88:UNK:O	2.43	0.51
28:l:75:LEU:HD13	28:l:79:LEU:CD1	2.41	0.51
31:h:67:ILE:HG23	31:h:71:MET:HE3	1.93	0.51
32:U:62:SER:O	32:U:63:VAL:CG2	2.59	0.51
32:U:92:LYS:O	32:U:95:MET:N	2.43	0.51
2:B:122:ARG:NH1	36:i:102:CLA:OBD	2.42	0.51
3:C:182:ILE:CD1	34:C:201:DD6:C8	2.89	0.51
36:E:315:CLA:H161	36:M:307:CLA:C14	2.41	0.51
7:G:34:PRO:HD3	39:G:322:LMT:H2B	1.92	0.51
36:H:314:CLA:HBC3	35:J:301:A86:C	2.40	0.51
36:O:308:CLA:H72	36:V:311:CLA:H152	1.93	0.51
19:X:127:THR:CB	33:V:9:PHE:CE1	2.87	0.51
20:a:698:TYR:C	20:a:698:TYR:CD1	2.88	0.51
36:a:801:CLA:HMB3	36:a:848:CLA:OBD	2.09	0.51
36:a:816:CLA:H141	36:a:816:CLA:H172	1.91	0.51
39:a:854:LMT:O3'	39:a:854:LMT:H1B	2.11	0.51
41:b:850:LHG:HC91	36:h:203:CLA:H143	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:84:ALA:CB	39:h:205:LMT:H111	2.40	0.51
31:h:128:HIS:NE2	36:h:203:CLA:NA	2.59	0.51
32:U:17:ASP:N	32:U:18:PRO:HD3	2.25	0.51
33:V:106:GLU:HG3	36:V:310:CLA:NB	2.26	0.51
1:A:196:TRP:CE2	36:A:314:CLA:CMD	2.93	0.51
35:A:302:A86:O3	36:A:309:CLA:O1A	2.29	0.51
2:B:112:ILE:CD1	26:i:4:ASN:ND2	2.59	0.51
39:B:312:LMT:C5	44:m:101:BCR:C38	2.83	0.51
5:E:116:MET:HE1	34:E:306:DD6:C23	2.40	0.51
5:E:198:GLU:OE2	35:E:305:A86:O1	2.29	0.51
6:F:55:LEU:HD13	25:f:221:LEU:HD21	1.93	0.51
9:I:194:ARG:NH1	36:I:314:CLA:HED2	2.25	0.51
35:N:305:A86:C4	36:N:316:CLA:HMC3	2.41	0.51
20:a:158:ILE:O	20:a:163:GLU:OE1	2.29	0.51
20:a:222:GLN:HA	20:a:226:ALA:HB3	1.92	0.51
23:d:99:LYS:HG3	23:d:100:TYR:N	2.26	0.51
33:V:112:HIS:HA	33:V:117:LEU:HA	1.93	0.51
1:A:197:VAL:HG23	1:A:198:THR:CG2	2.34	0.51
2:B:136:SER:HB2	36:B:308:CLA:C1D	2.41	0.51
6:F:98:MET:HE1	6:F:214:PHE:CE1	2.45	0.51
12:L:196:LEU:HD21	15:Q:54:LEU:HD21	1.93	0.51
13:M:150:TRP:HB2	36:M:310:CLA:HED2	1.91	0.51
14:N:73:PHE:HZ	36:N:312:CLA:CED	2.20	0.51
14:N:89:PHE:CD2	35:N:304:A86:C2	2.94	0.51
15:Q:152:PHE:CD1	36:Q:314:CLA:C1B	2.94	0.51
17:S:140:LEU:O	17:S:164:TYR:OH	2.29	0.51
19:W:138:ALA:O	19:W:142:ASN:ND2	2.43	0.51
20:a:17:ASN:HD22	20:a:17:ASN:N	2.09	0.51
21:b:174:LEU:HD12	21:b:300:MET:HE1	1.92	0.51
35:U:303:A86:O1	36:U:306:CLA:C2	2.59	0.51
33:V:57:THR:O	33:V:61:ILE:HG22	2.10	0.51
2:B:135:ILE:CG2	34:B:304:DD6:C6	2.89	0.51
2:B:184:ALA:HB3	36:B:309:CLA:CMB	2.40	0.51
35:C:204:A86:C7	37:C:213:KC1:CAC	2.89	0.51
4:D:125:GLN:O	4:D:128:LEU:N	2.43	0.51
6:F:68:LYS:HG3	6:F:151:ARG:HA	1.93	0.51
7:G:80:LYS:HE3	42:G:324:LMG:H121	1.92	0.51
7:G:153:LEU:HD13	36:G:311:CLA:CAA	2.39	0.51
36:G:315:CLA:HBD	36:G:315:CLA:HAA1	1.93	0.51
39:G:322:LMT:H72	42:G:324:LMG:H211	1.93	0.51
34:K:304:DD6:C9	36:K:308:CLA:HMC1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L:318:LMT:O2B	39:L:318:LMT:H5'	2.09	0.51
36:O:316:CLA:HAB	36:O:316:CLA:H71	1.93	0.51
15:P:34:ASP:N	15:P:45:LYS:HG2	2.25	0.51
15:P:121:ASN:HB3	15:P:125:PHE:HE2	1.75	0.51
16:R:66:TRP:CZ2	41:R:323:LHG:H252	2.46	0.51
19:X:148:GLN:HA	19:X:151:ILE:HG22	1.91	0.51
20:a:552:VAL:O	20:a:556:LEU:HB2	2.11	0.51
21:b:486:VAL:CG1	31:h:99:GLN:HE21	2.24	0.51
46:b:930:HOH:O	25:f:149:VAL:HG22	2.09	0.51
31:h:75:LEU:CD2	42:h:206:LMG:H342	2.41	0.51
34:A:301:DD6:C7	36:A:313:CLA:HBC3	2.41	0.51
16:R:221:GLN:NE2	16:R:236:HIS:O	2.44	0.51
19:W:78:ALA:HA	19:W:81:LYS:HE3	1.93	0.51
20:a:203:MET:HG3	20:a:327:MET:CE	2.37	0.51
20:a:490:GLN:HG2	39:a:854:LMT:H6'2	1.93	0.51
42:a:852:LMG:HC92	42:a:852:LMG:C11	2.41	0.51
21:b:516:PHE:C	21:b:516:PHE:CD1	2.89	0.51
27:j:2:ARG:O	42:j:105:LMG:HC61	2.11	0.51
27:j:10:VAL:HG22	27:j:12:PRO:HD2	1.92	0.51
32:U:138:MET:C	32:U:141:ILE:HG22	2.35	0.51
33:V:58:LEU:CG	33:V:75:PHE:CE2	2.94	0.51
4:D:61:ARG:NH1	4:D:61:ARG:CG	2.73	0.51
6:F:43:GLY:HA2	36:V:314:CLA:CED	2.41	0.51
6:F:145:HIS:CB	36:F:317:CLA:HAA2	2.41	0.51
36:I:305:CLA:H143	36:I:312:CLA:C4B	2.40	0.51
35:J:302:A86:C1	36:J:315:CLA:HBC2	2.41	0.51
14:N:136:VAL:HG13	36:N:318:CLA:HBA2	1.93	0.51
15:P:125:PHE:CZ	36:P:302:CLA:CED	2.93	0.51
17:S:210:MET:O	17:S:214:PHE:CE2	2.63	0.51
20:a:118:GLN:HG3	20:a:150:PHE:CE2	2.45	0.51
36:a:801:CLA:HMB3	36:a:848:CLA:HMD1	1.92	0.51
23:d:164:GLN:NE2	30:g:144:UNK:O	2.43	0.51
27:j:39:PHE:HE1	41:j:104:LHG:HC81	1.76	0.51
33:V:38:HIS:C	33:V:161:MET:HE3	2.36	0.51
33:V:68:SER:OG	33:V:71:ASP:N	2.43	0.51
36:H:305:CLA:HBB1	36:H:305:CLA:HHC	1.92	0.50
9:I:118:PHE:CA	36:I:309:CLA:HBC3	2.38	0.50
10:J:112:ASP:H	10:J:115:VAL:HG23	1.75	0.50
10:J:151:ASP:O	36:J:313:CLA:OBD	2.29	0.50
40:L:302:DGD:HA31	42:L:321:LMG:H291	1.92	0.50
36:P:301:CLA:H201	41:Q:315:LHG:H202	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S:304:A86:C19	35:S:304:A86:C22	2.89	0.50
20:a:85:GLN:HE21	20:a:85:GLN:C	2.17	0.50
20:a:724:LEU:HB3	20:a:728:GLN:HG2	1.92	0.50
23:d:188:PHE:C	23:d:189:ARG:HG3	2.35	0.50
25:f:172:TRP:CD1	25:f:172:TRP:C	2.89	0.50
32:U:37:ASN:OD1	36:U:310:CLA:HMD2	2.11	0.50
34:D:301:DD6:C3	36:j:101:CLA:HBB2	2.41	0.50
7:G:147:TYR:HD2	7:G:233:THR:HG23	1.71	0.50
11:K:75:ARG:HD2	11:K:79:LEU:HD11	1.94	0.50
14:N:102:TRP:CD1	35:N:302:A86:O3	2.64	0.50
15:P:150:ILE:HG12	15:P:153:PRO:HD2	1.91	0.50
35:X:314:A86:C4	33:V:161:MET:HG2	2.42	0.50
20:a:482:ILE:HA	41:a:850:LHG:HC32	1.91	0.50
20:a:533:LEU:HA	20:a:537:ASP:OD2	2.10	0.50
36:a:803:CLA:HAB	36:a:810:CLA:H142	1.93	0.50
21:b:489:ASN:HA	21:b:493:LEU:HB2	1.92	0.50
32:U:136:LEU:HD23	32:U:136:LEU:C	2.36	0.50
3:C:45:ARG:NH2	3:C:45:ARG:CG	2.73	0.50
3:C:160:SER:C	3:C:162:ALA:H	2.19	0.50
36:E:315:CLA:H172	36:M:307:CLA:H141	1.93	0.50
36:F:313:CLA:H42	36:h:203:CLA:H101	1.91	0.50
8:H:72:GLU:OE1	8:H:152:GLY:N	2.39	0.50
42:J:318:LMG:H221	42:J:318:LMG:C35	2.41	0.50
36:K:313:CLA:H92	36:K:313:CLA:H41	1.93	0.50
34:Q:302:DD6:C22	36:Q:308:CLA:C2B	2.89	0.50
34:W:205:DD6:C19	34:W:205:DD6:C23	2.89	0.50
20:a:373:ALA:HB2	20:a:399:HIS:HB2	1.93	0.50
36:a:816:CLA:OBD	36:a:834:CLA:HED2	2.11	0.50
21:b:556:PHE:HB2	21:b:557:PRO:HD2	1.92	0.50
32:U:62:SER:C	32:U:63:VAL:HG23	2.37	0.50
2:B:184:ALA:HB3	36:B:309:CLA:HMB1	1.94	0.50
36:K:307:CLA:H141	37:K:314:KC1:CMC	2.40	0.50
12:L:43:ILE:HG22	12:L:44:GLU:OE2	2.11	0.50
34:L:305:DD6:C26	36:L:309:CLA:C1C	2.90	0.50
35:Q:316:A86:C4	36:S:311:CLA:C4B	2.89	0.50
35:Q:316:A86:C6	36:S:311:CLA:HBB1	2.41	0.50
17:S:56:SER:O	17:S:56:SER:OG	2.24	0.50
17:S:181:TYR:HD1	36:S:321:CLA:H2A	1.75	0.50
20:a:85:GLN:O	20:a:85:GLN:NE2	2.35	0.50
21:b:640:ASN:ND2	46:b:919:HOH:O	2.44	0.50
4:D:92:VAL:O	4:D:92:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:130:TRP:HB2	36:K:311:CLA:HBC2	1.94	0.50
20:a:462:ILE:O	20:a:466:THR:CG2	2.60	0.50
21:b:219:ALA:HB1	21:b:223:PRO:CG	2.42	0.50
23:d:143:ARG:CG	23:d:143:ARG:NH2	2.73	0.50
33:V:144:LYS:CG	33:V:146:THR:HG23	2.40	0.50
41:D:319:LHG:C14	41:D:319:LHG:C18	2.86	0.50
34:E:303:DD6:C23	34:E:303:DD6:C19	2.89	0.50
39:G:323:LMT:H1'	15:P:54:LEU:HD23	1.94	0.50
14:N:187:ASN:HD21	36:N:319:CLA:HED1	1.76	0.50
15:Q:152:PHE:CD1	36:Q:314:CLA:C3B	2.94	0.50
19:X:58:ARG:O	36:X:315:CLA:CED	2.59	0.50
19:X:120:ALA:CB	35:X:314:A86:C39	2.88	0.50
42:a:852:LMG:H131	42:a:852:LMG:H292	1.94	0.50
21:b:700:SER:HB3	46:b:969:HOH:O	2.11	0.50
36:b:802:CLA:H192	25:f:206:LEU:CD2	2.42	0.50
39:U:314:LMT:O3'	39:U:314:LMT:H1B	2.12	0.50
33:V:140:PRO:O	33:V:141:LEU:C	2.53	0.50
2:B:124:VAL:CB	35:B:301:A86:C37	2.89	0.50
4:D:74:ALA:HB2	36:D:312:CLA:HED2	1.93	0.50
5:E:72:ILE:CG2	39:E:321:LMT:H61	2.41	0.50
15:O:150:ILE:CG2	15:O:154:PRO:HA	2.42	0.50
19:X:111:GLU:N	19:X:115:ASP:OD2	2.44	0.50
20:a:739:LEU:O	20:a:739:LEU:HD22	2.12	0.50
21:b:5:PHE:HB3	21:b:20:ARG:HH12	1.75	0.50
32:U:61:VAL:O	32:U:63:VAL:HG23	2.11	0.50
33:V:65:GLU:C	33:V:75:PHE:CD2	2.90	0.50
33:V:151:LEU:O	33:V:151:LEU:HD22	2.12	0.50
1:A:74:GLU:OE1	1:A:152:GLY:N	2.39	0.50
35:C:203:A86:C12	36:C:208:CLA:HBC1	2.42	0.50
37:F:308:KC1:CGA	39:F:321:LMT:H3'	2.42	0.50
9:I:110:LEU:HD21	36:I:309:CLA:HED2	1.93	0.50
35:O:319:A86:O	35:V:303:A86:O2	2.29	0.50
15:Q:180:MET:SD	34:Q:302:DD6:C2	3.00	0.50
17:S:181:TYR:CD1	36:S:321:CLA:H2A	2.47	0.50
19:W:33:ARG:NH1	19:W:36:GLU:OE1	2.45	0.50
20:a:331:LEU:O	20:a:343:HIS:HB2	2.12	0.50
20:a:476:MET:O	20:a:481:ALA:CB	2.54	0.50
36:a:838:CLA:H172	27:j:23:ALA:HB2	1.92	0.50
21:b:34:HIS:HE1	36:b:807:CLA:HED1	1.77	0.50
33:V:35:GLU:OE2	36:V:306:CLA:C4A	2.57	0.50
33:V:162:PHE:CZ	35:V:301:A86:C12	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:E:322:LHG:HC2	41:E:322:LHG:O6	2.11	0.50
6:F:134:PHE:CE1	36:F:317:CLA:HBC1	2.47	0.50
42:G:324:LMG:H112	42:G:325:LMG:C1	2.42	0.50
10:J:111:HIS:O	35:J:306:A86:C39	2.59	0.50
42:L:321:LMG:HC71	42:L:321:LMG:O9	2.12	0.50
13:M:188:ASN:ND2	13:M:193:LEU:HD23	2.27	0.50
20:a:98:PHE:CE1	20:a:102:TYR:HD2	2.30	0.50
21:b:121:GLN:O	21:b:125:THR:CG2	2.58	0.50
21:b:528:VAL:HG11	21:b:581:TRP:CE2	2.47	0.50
36:b:824:CLA:HBA1	44:h:201:BCR:H16C	1.93	0.50
36:b:836:CLA:C9	36:b:836:CLA:C12	2.86	0.50
36:D:307:CLA:H2	37:M:318:KC1:CED	2.41	0.49
9:I:92:HIS:HE1	9:I:99:LEU:HD13	1.77	0.49
11:K:168:PRO:HB3	11:K:172:LYS:NZ	2.27	0.49
40:L:302:DGD:C3A	42:L:321:LMG:H291	2.42	0.49
35:M:304:A86:C39	36:M:312:CLA:H11	2.42	0.49
14:N:202:GLU:HA	14:N:205:ASN:HB2	1.94	0.49
37:W:217:KC1:CMD	36:W:218:CLA:C1D	2.90	0.49
20:a:594:TRP:HE3	20:a:595:ASP:OD1	1.94	0.49
41:a:850:LHG:H242	41:a:850:LHG:H111	1.94	0.49
31:h:64:LEU:HB3	31:h:68:MET:HB2	1.94	0.49
5:E:217:LEU:HD21	15:P:121:ASN:ND2	2.19	0.49
35:F:301:A86:C7	36:F:316:CLA:HMC1	2.41	0.49
39:F:320:LMT:C4'	39:F:321:LMT:O6'	2.59	0.49
7:G:107:LEU:O	7:G:111:ARG:CG	2.58	0.49
15:Q:182:ALA:HB2	35:Q:303:A86:C29	2.42	0.49
20:a:17:ASN:ND2	20:a:17:ASN:N	2.60	0.49
20:a:626:THR:OG1	20:a:627:VAL:N	2.45	0.49
20:a:662:GLN:NE2	20:a:752:ARG:HH11	2.09	0.49
21:b:593:TRP:HA	36:b:836:CLA:HBC3	1.94	0.49
36:b:824:CLA:H2A	36:b:824:CLA:HED3	1.93	0.49
36:f:804:CLA:CHC	27:j:22:LEU:HD21	2.42	0.49
28:l:126:VAL:O	41:l:208:LHG:C2	2.61	0.49
32:U:31:ARG:HD3	32:U:31:ARG:C	2.36	0.49
32:U:32:ALA:CB	39:U:314:LMT:C3B	2.90	0.49
32:U:112:TRP:O	32:U:113:MET:CG	2.60	0.49
33:V:162:PHE:CE2	35:V:301:A86:C12	2.96	0.49
35:E:305:A86:C3	36:E:315:CLA:HMB3	2.42	0.49
35:G:306:A86:C41	42:G:324:LMG:HC72	2.42	0.49
35:I:302:A86:C7	36:I:308:CLA:C7	2.90	0.49
39:I:317:LMT:O6'	39:I:317:LMT:O4'	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:111:HIS:HB3	35:J:306:A86:C39	2.42	0.49
14:N:44:LYS:HG3	14:N:200:VAL:HG11	1.95	0.49
14:N:171:ARG:O	14:N:171:ARG:HG2	2.10	0.49
15:P:48:PRO:HB2	41:Q:315:LHG:H131	1.93	0.49
20:a:700:GLN:HE22	20:a:722:ARG:HA	1.77	0.49
21:b:619:LEU:O	21:b:619:LEU:HD22	2.12	0.49
22:c:66:ARG:HG2	22:c:68:TYR:CZ	2.47	0.49
36:j:101:CLA:H52	42:j:105:LMG:C36	2.42	0.49
2:B:88:ALA:HA	2:B:92:GLY:HA3	1.95	0.49
6:F:42:VAL:O	6:F:42:VAL:CG1	2.60	0.49
7:G:47:ARG:HH12	11:K:151:ARG:HB2	1.78	0.49
15:P:150:ILE:HG21	15:P:153:PRO:O	2.13	0.49
15:Q:150:ILE:HD11	36:Q:314:CLA:C1D	2.42	0.49
19:W:62:THR:HA	19:W:69:THR:HA	1.95	0.49
34:W:204:DD6:C25	36:W:207:CLA:HHC	2.42	0.49
21:b:14:GLN:NE2	30:g:139:UNK:CB	2.75	0.49
21:b:489:ASN:O	21:b:494:PRO:HD3	2.11	0.49
26:i:34:LEU:C	26:i:34:LEU:CD1	2.86	0.49
28:l:133:VAL:C	28:l:135:SER:H	2.20	0.49
33:V:162:PHE:CE1	35:V:301:A86:C12	2.95	0.49
36:A:306:CLA:HBB1	36:A:306:CLA:HMB3	1.92	0.49
34:C:201:DD6:C19	34:C:201:DD6:C23	2.91	0.49
36:F:313:CLA:H61	41:b:850:LHG:H151	1.94	0.49
7:G:66:GLY:HA3	7:G:216:ILE:HG21	1.94	0.49
36:H:308:CLA:H43	38:b:804:SQD:C28	2.42	0.49
9:I:194:ARG:C	9:I:194:ARG:CD	2.86	0.49
10:J:86:TYR:OH	10:J:108:ALA:HB2	2.11	0.49
35:J:305:A86:C40	35:J:305:A86:C35	2.91	0.49
12:L:70:ASN:HD21	12:L:163:GLN:HE22	1.59	0.49
14:N:170:PHE:HE2	14:N:178:LEU:HB3	1.76	0.49
14:N:241:MET:HG2	35:N:305:A86:C10	2.40	0.49
36:Q:310:CLA:H93	17:S:55:LEU:HD11	1.93	0.49
16:R:188:SER:HA	16:R:191:LYS:HD3	1.92	0.49
17:S:204:ASN:O	17:S:208:LEU:HG	2.13	0.49
17:S:242:GLN:HE22	36:S:318:CLA:HED3	1.76	0.49
35:X:314:A86:C21	33:V:45:ALA:HA	2.42	0.49
36:X:315:CLA:CMD	35:V:301:A86:C27	2.90	0.49
36:b:816:CLA:C12	36:b:816:CLA:C9	2.89	0.49
36:b:834:CLA:H2	44:b:846:BCR:HC42	1.94	0.49
33:V:62:SER:HA	36:V:313:CLA:CBC	2.43	0.49
1:A:140:MET:CB	25:f:207:PHE:CE1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:O	1:A:190:GLY:N	2.46	0.49
41:D:318:LHG:O9	41:D:318:LHG:H102	2.11	0.49
11:K:101:PRO:O	35:K:303:A86:O3	2.30	0.49
15:O:133:ILE:HD13	35:O:301:A86:O5	2.13	0.49
20:a:17:ASN:H	20:a:17:ASN:HD22	1.60	0.49
21:b:640:ASN:OD1	21:b:642:LEU:HB2	2.13	0.49
25:f:164:ILE:HG22	41:j:104:LHG:H161	1.94	0.49
26:i:16:LEU:HD22	36:l:202:CLA:C19	2.42	0.49
28:l:141:ASN:O	28:l:147:ALA:CB	2.61	0.49
32:U:110:ILE:HG23	36:U:311:CLA:HMD1	1.95	0.49
36:U:310:CLA:C1C	39:U:315:LMT:H121	2.43	0.49
33:V:113:ARG:CG	33:V:113:ARG:NH1	2.73	0.49
4:D:180:ILE:O	4:D:184:ARG:HG3	2.13	0.49
4:D:203:PRO:HB2	4:D:205:PRO:HD2	1.94	0.49
5:E:42:PHE:HE2	7:G:176:VAL:CG2	2.26	0.49
39:E:323:LMT:H22	39:E:323:LMT:O2'	2.13	0.49
6:F:136:SER:HA	36:F:313:CLA:HAB	1.94	0.49
7:G:147:TYR:HD2	7:G:233:THR:CG2	2.25	0.49
35:G:306:A86:C13	35:G:306:A86:C23	2.91	0.49
12:L:199:LYS:HG2	36:L:308:CLA:CED	2.43	0.49
36:a:818:CLA:H8	36:a:818:CLA:HAB	1.94	0.49
21:b:622:TYR:O	21:b:626:ASN:HB2	2.13	0.49
23:d:188:PHE:O	23:d:189:ARG:CG	2.60	0.49
32:U:27:ALA:O	32:U:31:ARG:HB3	2.12	0.49
33:V:61:ILE:O	33:V:61:ILE:HG12	2.12	0.49
2:B:78:GLY:C	34:B:302:DD6:C22	2.82	0.49
2:B:135:ILE:CD1	35:B:301:A86:C8	2.90	0.49
41:I:316:LHG:C32	41:I:316:LHG:H151	2.42	0.49
36:K:307:CLA:C14	37:K:314:KC1:C2C	2.91	0.49
34:L:305:DD6:C25	36:L:309:CLA:HMC3	2.41	0.49
16:R:146:TRP:CE3	16:R:147:PHE:HA	2.47	0.49
35:T:301:A86:C41	35:T:301:A86:C35	2.90	0.49
19:X:20:LEU:HD23	36:X:307:CLA:HBC2	1.94	0.49
20:a:585:ARG:NH1	23:d:135:GLU:OE2	2.46	0.49
36:b:828:CLA:HBC3	40:b:849:DGD:HBV2	1.94	0.49
32:U:98:GLU:HG3	32:U:98:GLU:O	2.12	0.49
36:B:309:CLA:CBA	36:B:309:CLA:CBD	2.85	0.49
36:G:313:CLA:HMB3	36:P:301:CLA:HBA2	1.94	0.49
9:I:176:MET:HB3	36:I:313:CLA:HMC1	1.94	0.49
36:K:313:CLA:H2A	36:K:313:CLA:CED	2.43	0.49
36:K:313:CLA:H52	36:K:313:CLA:H8	1.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:L:318:LMT:H6E	39:L:318:LMT:H2'	1.95	0.49
20:a:239:PRO:HA	20:a:242:ILE:HD12	1.94	0.49
20:a:557:LYS:NZ	20:a:596:HIS:HE1	2.10	0.49
41:a:850:LHG:HC31	41:a:850:LHG:C4	2.43	0.49
21:b:465:ALA:HB1	21:b:476:LEU:HD12	1.94	0.49
42:j:105:LMG:C38	42:j:105:LMG:C42	2.86	0.49
33:V:145:VAL:O	33:V:145:VAL:HG12	2.12	0.49
41:E:322:LHG:H102	41:E:322:LHG:H251	1.90	0.49
42:I:315:LMG:H161	36:a:822:CLA:C1B	2.43	0.49
35:L:301:A86:C38	36:P:313:CLA:H162	2.43	0.49
21:b:353:ALA:HA	21:b:506:ASP:HB3	1.95	0.49
22:c:24:ASP:OD2	23:d:167:HIS:CE1	2.66	0.49
23:d:143:ARG:HH21	23:d:143:ARG:HG3	1.77	0.49
32:U:42:MET:HB2	35:U:304:A86:C	2.29	0.49
33:V:69:ILE:O	33:V:70:ARG:HB2	2.12	0.49
33:V:149:ARG:HH11	33:V:149:ARG:CG	2.26	0.49
1:A:90:PHE:HE1	1:A:108:ASN:OD1	1.94	0.48
35:A:316:A86:C39	33:V:87:VAL:HG21	2.43	0.48
4:D:140:SER:OG	4:D:151:ARG:HD3	2.12	0.48
37:G:317:KC1:O1A	42:G:325:LMG:HC61	2.13	0.48
35:T:304:A86:C26	36:T:314:CLA:HAA2	2.43	0.48
20:a:282:THR:HB	20:a:284:LYS:HG2	1.95	0.48
20:a:317:TYR:CE1	20:a:327:MET:SD	3.06	0.48
20:a:345:GLY:O	20:a:348:GLU:HG2	2.13	0.48
36:a:802:CLA:H141	36:a:802:CLA:H162	1.58	0.48
21:b:463:GLN:HG2	21:b:508:PHE:CD1	2.47	0.48
23:d:206:GLN:NE2	30:g:133:UNK:O	2.46	0.48
41:f:809:LHG:H242	41:f:809:LHG:C28	2.40	0.48
31:h:74:GLY:HA3	42:h:206:LMG:O2	2.13	0.48
7:G:173:THR:HG21	7:G:192:PHE:CZ	2.47	0.48
36:G:313:CLA:HED3	36:G:313:CLA:H2A	1.95	0.48
42:J:318:LMG:H221	42:J:318:LMG:H342	1.94	0.48
36:K:307:CLA:H2	36:K:307:CLA:O1A	2.12	0.48
14:N:178:LEU:CD2	36:N:318:CLA:HED1	2.40	0.48
15:Q:158:SER:C	15:Q:160:VAL:H	2.21	0.48
36:R:310:CLA:H12	17:S:174:VAL:HG23	1.93	0.48
20:a:422:TYR:CD1	20:a:422:TYR:C	2.90	0.48
21:b:659:GLY:O	21:b:663:LEU:HG	2.13	0.48
32:U:42:MET:HE2	32:U:134:GLY:HA2	1.95	0.48
33:V:37:LYS:HE2	36:V:310:CLA:CHA	2.42	0.48
41:D:319:LHG:H221	42:D:320:LMG:C23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:E:322:LHG:C5	41:E:322:LHG:C2	2.90	0.48
6:F:193:ILE:CD1	35:F:301:A86:C14	2.91	0.48
7:G:65:PRO:O	7:G:103:ARG:NH2	2.46	0.48
36:H:314:CLA:HBC3	35:J:301:A86:C1	2.43	0.48
36:K:309:CLA:H142	36:K:312:CLA:H71	1.96	0.48
15:O:133:ILE:HG12	35:O:301:A86:C40	2.43	0.48
15:Q:151:VAL:CA	36:Q:314:CLA:CED	2.88	0.48
36:Q:310:CLA:HBD	36:Q:310:CLA:CGA	2.43	0.48
17:S:208:LEU:HD12	35:S:304:A86:C	2.43	0.48
35:S:304:A86:C10	36:S:315:CLA:HHC	2.43	0.48
37:T:310:KC1:CMD	36:T:313:CLA:C2D	2.90	0.48
21:b:376:TYR:O	21:b:380:PHE:HD1	1.96	0.48
22:c:31:TRP:O	22:c:37:LYS:HA	2.12	0.48
32:U:8:SER:HG	36:U:306:CLA:CED	2.17	0.48
36:V:308:CLA:H43	36:V:313:CLA:HBB2	1.95	0.48
36:B:309:CLA:CGA	36:B:309:CLA:CBD	2.87	0.48
3:C:40:LEU:HD23	36:C:205:CLA:C1C	2.43	0.48
7:G:193:LYS:N	7:G:193:LYS:CD	2.76	0.48
36:K:309:CLA:HBC2	36:K:316:CLA:HBC2	1.96	0.48
18:T:39:HIS:HE1	37:T:310:KC1:NC	2.11	0.48
35:X:314:A86:C3	33:V:161:MET:HG2	2.44	0.48
21:b:654:LEU:HD23	36:b:801:CLA:HAA1	1.95	0.48
33:V:57:THR:CG2	36:V:308:CLA:O2D	2.61	0.48
3:C:40:LEU:HD23	36:C:205:CLA:C2C	2.44	0.48
6:F:113:TRP:HZ3	41:F:318:LHG:HC92	1.78	0.48
9:I:194:ARG:HB2	36:I:314:CLA:C2D	2.43	0.48
36:Q:305:CLA:HBD	37:Q:311:KC1:CAD	2.44	0.48
19:W:91:LEU:HD22	19:W:92:LEU:HD22	1.95	0.48
19:X:136:LYS:HA	19:X:139:ILE:HB	1.94	0.48
21:b:454:PHE:CE1	25:f:149:VAL:HG11	2.48	0.48
32:U:131:LEU:O	32:U:135:ARG:HD2	2.13	0.48
3:C:172:ILE:HA	3:C:172:ILE:HD13	1.65	0.48
36:C:207:CLA:H51	36:C:208:CLA:H3A	1.94	0.48
10:J:40:VAL:C	36:J:308:CLA:CED	2.87	0.48
14:N:213:ILE:HD13	35:N:303:A86:C8	2.44	0.48
15:O:158:SER:C	15:O:160:VAL:H	2.21	0.48
35:Q:303:A86:C22	35:Q:303:A86:C19	2.90	0.48
16:R:127:ASP:OD2	16:R:237:TYR:OH	2.30	0.48
17:S:167:PHE:HB2	17:S:171:ARG:NH2	2.27	0.48
19:X:117:ARG:HH21	19:X:121:ILE:HB	1.78	0.48
20:a:346:LEU:HA	20:a:349:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:198:ILE:HD11	23:d:201:LYS:NZ	2.24	0.48
28:l:93:GLY:O	28:l:96:ARG:HD3	2.14	0.48
32:U:57:PHE:CZ	35:U:302:A86:C29	2.96	0.48
32:U:138:MET:HG2	35:U:303:A86:C5	2.44	0.48
36:U:310:CLA:CMB	39:U:314:LMT:H61	2.43	0.48
33:V:128:GLN:HB3	33:V:129:PRO:CD	2.38	0.48
4:D:39:LEU:HB3	4:D:42:LEU:HD23	1.94	0.48
41:G:321:LHG:H112	41:G:321:LHG:HC81	1.45	0.48
10:J:109:ASP:O	10:J:111:HIS:O	2.31	0.48
14:N:63:TRP:CZ2	36:N:317:CLA:HMB1	2.49	0.48
16:R:50:PRO:O	16:R:53:LYS:HD2	2.12	0.48
34:W:205:DD6:C27	36:W:212:CLA:C2C	2.92	0.48
20:a:193:LEU:O	20:a:193:LEU:HD22	2.13	0.48
42:a:852:LMG:C9	42:a:852:LMG:C11	2.91	0.48
23:d:95:GLN:OE1	30:g:88:UNK:N	2.47	0.48
27:j:38:THR:C	27:j:40:PRO:HD3	2.29	0.48
36:j:101:CLA:H61	42:j:105:LMG:C36	2.40	0.48
32:U:84:PHE:HA	32:U:87:THR:OG1	2.14	0.48
33:V:138:TRP:CZ3	36:V:308:CLA:H201	2.46	0.48
4:D:61:ARG:CD	41:E:322:LHG:HC31	2.41	0.48
36:D:306:CLA:C2C	41:D:318:LHG:H281	2.43	0.48
37:F:315:KC1:C4C	41:O:317:LHG:H211	2.44	0.48
9:I:190:ASP:HB3	9:I:194:ARG:HB3	1.96	0.48
35:L:307:A86:C33	35:L:307:A86:C39	2.89	0.48
34:M:303:DD6:C37	36:M:307:CLA:C2	2.91	0.48
35:N:304:A86:C22	35:N:304:A86:C19	2.86	0.48
34:R:307:DD6:C19	34:R:307:DD6:C23	2.91	0.48
17:S:167:PHE:HB2	17:S:171:ARG:HE	1.79	0.48
21:b:14:GLN:HE22	30:g:138:UNK:C	2.27	0.48
23:d:81:PRO:HD2	28:l:40:PHE:HZ	1.78	0.48
4:D:155:ASN:HD22	4:D:157:GLY:H	1.55	0.48
4:D:163:PHE:HA	19:W:25:ASP:HB3	1.94	0.48
7:G:199:PHE:CG	36:G:313:CLA:H2	2.45	0.48
11:K:86:MET:SD	36:K:313:CLA:HAB	2.54	0.48
11:K:167:ASP:O	11:K:171:GLN:HG3	2.13	0.48
34:M:303:DD6:C36	36:M:307:CLA:C2	2.92	0.48
36:M:309:CLA:H61	36:M:309:CLA:H101	1.71	0.48
15:Q:178:LEU:HG	35:Q:303:A86:C26	2.44	0.48
16:R:66:TRP:NE1	35:R:305:A86:C23	2.77	0.48
19:X:36:GLU:OE2	19:X:145:ARG:NE	2.45	0.48
19:X:59:LEU:HD22	36:X:315:CLA:OBD	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:327:MET:HB2	20:a:347:TYR:HE1	1.77	0.48
21:b:421:LEU:HD13	21:b:531:LEU:CA	2.42	0.48
36:b:815:CLA:H13	36:b:820:CLA:HAB	1.95	0.48
32:U:128:LEU:HD11	32:U:132:LYS:NZ	2.28	0.48
36:U:310:CLA:HBA1	39:U:315:LMT:H62	1.95	0.48
33:V:102:ILE:HG21	36:V:310:CLA:C2C	2.43	0.48
7:G:34:PRO:HG3	39:G:322:LMT:H6D	1.94	0.48
36:K:316:CLA:H43	36:K:316:CLA:H152	1.94	0.48
14:N:170:PHE:CZ	36:N:318:CLA:O2A	2.53	0.48
15:O:62:TRP:CZ2	37:O:315:KC1:CAB	2.96	0.48
15:O:149:THR:O	36:O:316:CLA:CED	2.62	0.48
35:Q:316:A86:C8	36:S:311:CLA:HBB1	2.43	0.48
19:X:117:ARG:HB2	33:V:14:TYR:CZ	2.49	0.48
36:b:841:CLA:HMB3	41:b:850:LHG:C9	2.42	0.48
4:D:92:VAL:O	4:D:97:ARG:NH2	2.47	0.47
36:D:307:CLA:CMC	41:D:318:LHG:HC81	2.44	0.47
9:I:113:VAL:HG12	36:I:309:CLA:O1D	2.12	0.47
36:I:310:CLA:H192	36:T:316:CLA:HBD	1.95	0.47
39:I:317:LMT:O6'	39:I:317:LMT:O5B	2.32	0.47
12:L:116:LEU:O	35:L:304:A86:O3	2.32	0.47
20:a:327:MET:HB2	20:a:347:TYR:CE1	2.49	0.47
20:a:538:PHE:HA	36:a:836:CLA:HED1	1.95	0.47
36:a:808:CLA:H143	36:a:810:CLA:H151	1.95	0.47
41:a:850:LHG:H111	41:a:850:LHG:C24	2.43	0.47
2:B:149:SER:HB2	39:B:313:LMT:H6'2	1.95	0.47
35:F:301:A86:C22	36:F:309:CLA:HAC2	2.44	0.47
8:H:65:PHE:CD1	31:h:67:ILE:HG12	2.48	0.47
13:M:77:ARG:HH21	13:M:77:ARG:HG3	1.78	0.47
14:N:169:LEU:N	14:N:169:LEU:CD2	2.73	0.47
15:P:121:ASN:OD1	36:P:302:CLA:CED	2.62	0.47
17:S:59:ASP:C	17:S:60:LYS:CG	2.86	0.47
20:a:696:ARG:HD2	20:a:725:SER:HA	1.97	0.47
36:a:816:CLA:CHD	42:a:852:LMG:H291	2.43	0.47
36:a:817:CLA:HBA2	36:a:817:CLA:H3A	1.60	0.47
21:b:706:LEU:HD23	21:b:706:LEU:C	2.39	0.47
23:d:104:TRP:HB2	23:d:150:ILE:HD12	1.96	0.47
24:e:26:VAL:HG21	24:e:41:ARG:NE	2.28	0.47
26:i:17:PHE:O	26:i:20:VAL:HG12	2.15	0.47
32:U:63:VAL:CG1	32:U:69:ALA:HB1	2.36	0.47
32:U:96:GLU:HA	32:U:100:LYS:O	2.14	0.47
32:U:112:TRP:H	35:U:304:A86:C38	2.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:162:PHE:CD2	35:V:301:A86:C12	2.98	0.47
33:V:163:ALA:HB2	35:V:303:A86:C13	2.45	0.47
36:D:309:CLA:CBC	36:D:316:CLA:HAB	2.44	0.47
14:N:241:MET:HG2	35:N:305:A86:C8	2.40	0.47
17:S:89:PHE:HE1	17:S:216:PHE:CE2	2.32	0.47
19:W:118:ASN:OD1	19:W:119:GLY:N	2.48	0.47
36:a:802:CLA:H111	36:a:802:CLA:H151	1.50	0.47
36:a:816:CLA:HBA2	36:a:816:CLA:H3A	1.47	0.47
21:b:461:TYR:CZ	21:b:475:VAL:HG11	2.49	0.47
21:b:473:PHE:CD1	39:b:851:LMT:C6'	2.97	0.47
23:d:104:TRP:HD1	23:d:150:ILE:HD13	1.78	0.47
23:d:206:GLN:O	23:d:210:LEU:HD12	2.14	0.47
26:i:32:ARG:HG2	26:i:32:ARG:HH11	1.79	0.47
3:C:160:SER:C	3:C:162:ALA:N	2.68	0.47
6:F:179:ARG:NH2	37:F:315:KC1:CED	2.76	0.47
15:Q:152:PHE:CG	36:Q:314:CLA:C4B	2.97	0.47
20:a:544:HIS:HB3	36:a:835:CLA:HAB	1.96	0.47
22:c:31:TRP:O	22:c:37:LYS:CA	2.62	0.47
33:V:139:ASN:CG	36:V:311:CLA:CBA	2.85	0.47
33:V:161:MET:CE	36:V:306:CLA:HAB	2.35	0.47
36:B:311:CLA:HHC	36:B:311:CLA:HBB1	1.95	0.47
3:C:45:ARG:HH21	3:C:45:ARG:HG2	1.77	0.47
36:C:205:CLA:HED1	40:C:215:DGD:C5D	2.40	0.47
5:E:148:THR:O	5:E:152:ARG:HG2	2.14	0.47
35:E:305:A86:C2	36:E:315:CLA:HMB1	2.44	0.47
37:G:317:KC1:O1A	42:G:325:LMG:C6	2.61	0.47
10:J:122:GLN:OE1	10:J:126:TRP:NE1	2.45	0.47
12:L:44:GLU:CG	36:L:308:CLA:C2B	2.90	0.47
12:L:56:ILE:HG23	12:L:57:LEU:HG	1.95	0.47
36:O:308:CLA:H71	36:V:311:CLA:H93	1.96	0.47
15:P:174:ASN:ND2	36:P:308:CLA:O1D	2.45	0.47
16:R:136:GLN:HA	16:R:139:LEU:HB2	1.97	0.47
36:b:823:CLA:C1	31:h:68:MET:HE3	2.44	0.47
28:l:48:ILE:HG12	36:l:201:CLA:C2D	2.43	0.47
33:V:138:TRP:CE3	36:V:311:CLA:CMD	2.68	0.47
36:A:306:CLA:CBC	37:A:312:KC1:CBC	2.92	0.47
7:G:147:TYR:CE2	7:G:233:THR:O	2.68	0.47
7:G:204:SER:O	7:G:207:GLU:N	2.47	0.47
36:P:314:CLA:H91	36:P:314:CLA:H111	1.77	0.47
15:Q:152:PHE:CE1	36:Q:314:CLA:CHC	2.86	0.47
36:R:310:CLA:HAB	17:S:170:PHE:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:225:ILE:CG1	36:a:813:CLA:HMD3	2.44	0.47
20:a:682:HIS:CD2	36:a:848:CLA:HED3	2.48	0.47
36:a:812:CLA:H62	36:a:812:CLA:H101	1.77	0.47
25:f:105:LEU:HD22	25:f:122:MET:HE1	1.97	0.47
41:f:809:LHG:HC12	41:f:809:LHG:O10	2.15	0.47
28:l:85:LEU:HD13	28:l:112:LEU:HD12	1.96	0.47
36:h:203:CLA:H41	36:h:203:CLA:H61	1.55	0.47
32:U:63:VAL:HG13	32:U:72:GLN:HB3	1.97	0.47
32:U:78:TRP:CE3	32:U:78:TRP:HA	2.48	0.47
33:V:111:THR:CB	33:V:117:LEU:HD13	2.35	0.47
33:V:162:PHE:CD1	35:V:301:A86:C12	2.97	0.47
4:D:98:ILE:HG21	36:W:201:CLA:HBB1	1.96	0.47
42:D:320:LMG:H132	27:j:1:MET:HB3	1.95	0.47
41:E:322:LHG:HC81	41:E:322:LHG:H112	1.58	0.47
36:F:312:CLA:H162	31:h:84:ALA:HB1	1.96	0.47
36:H:307:CLA:H3A	36:H:307:CLA:CGA	2.44	0.47
10:J:89:THR:CG2	10:J:107:SER:HB3	2.45	0.47
10:J:171:ALA:O	10:J:175:ASN:ND2	2.48	0.47
42:J:318:LMG:H351	42:J:318:LMG:H242	1.95	0.47
42:J:318:LMG:O9	42:J:318:LMG:H132	2.14	0.47
12:L:137:ILE:HD11	34:L:305:DD6:C23	2.37	0.47
34:L:305:DD6:C23	34:L:305:DD6:C19	2.93	0.47
36:L:308:CLA:H72	37:L:315:KC1:CHD	2.44	0.47
15:O:62:TRP:CH2	37:O:315:KC1:CAB	2.97	0.47
16:R:49:ASN:HD21	36:R:310:CLA:C4B	2.27	0.47
17:S:168:THR:HA	17:S:171:ARG:HG2	1.95	0.47
18:T:150:ILE:HD13	18:T:153:LEU:HD12	1.96	0.47
34:W:204:DD6:C21	36:W:209:CLA:C2B	2.92	0.47
35:X:314:A86:C10	33:V:45:ALA:HB2	2.44	0.47
36:a:816:CLA:HBC3	36:a:816:CLA:HHD	1.97	0.47
21:b:4:LYS:HB3	21:b:6:PRO:HD2	1.96	0.47
21:b:14:GLN:NE2	30:g:138:UNK:O	2.46	0.47
21:b:486:VAL:HG11	31:h:99:GLN:HE21	1.80	0.47
21:b:705:ARG:O	21:b:709:LEU:HB2	2.14	0.47
41:b:850:LHG:HC91	36:h:203:CLA:C14	2.45	0.47
23:d:80:SER:HB3	28:l:40:PHE:HE2	1.79	0.47
23:d:137:CYS:CB	23:d:154:PHE:HE2	2.24	0.47
24:e:10:LYS:N	24:e:61:GLN:O	2.46	0.47
24:e:18:TRP:HE1	24:e:44:LYS:HG3	1.80	0.47
25:f:201:LEU:HD22	25:f:201:LEU:C	2.40	0.47
27:j:41:PHE:CD1	27:j:41:PHE:C	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:U:315:LMT:O1B	39:U:315:LMT:O4'	2.27	0.47
33:V:65:GLU:O	33:V:75:PHE:N	2.47	0.47
7:G:116:ALA:HB1	34:G:303:DD6:C13	2.44	0.47
8:H:47:LEU:HB2	36:H:307:CLA:HED1	1.97	0.47
8:H:85:TRP:CE3	34:H:303:DD6:C8	2.97	0.47
36:L:308:CLA:C7	36:L:308:CLA:H41	2.45	0.47
13:M:101:VAL:HG12	13:M:105:ARG:HH12	1.80	0.47
14:N:122:TRP:HZ3	36:N:310:CLA:HHB	1.77	0.47
15:P:34:ASP:H	15:P:45:LYS:HD3	1.80	0.47
35:Q:316:A86:O2	17:S:221:THR:HG23	2.02	0.47
17:S:208:LEU:CD1	36:S:309:CLA:CMD	2.93	0.47
20:a:519:ILE:HD12	20:a:633:ILE:HD11	1.97	0.47
36:a:816:CLA:H93	36:a:816:CLA:H52	1.93	0.47
41:a:850:LHG:H301	41:a:850:LHG:H331	1.58	0.47
21:b:219:ALA:HB1	21:b:223:PRO:HG2	1.97	0.47
21:b:349:GLN:HG3	36:b:826:CLA:HED3	1.19	0.47
26:i:26:PHE:CD2	28:l:122:ILE:HG22	2.50	0.47
28:l:91:LYS:O	28:l:96:ARG:HD2	2.15	0.47
36:U:311:CLA:H3A	36:U:311:CLA:HBA2	1.66	0.47
36:V:311:CLA:H91	36:V:311:CLA:H112	1.75	0.47
36:D:309:CLA:HBA1	36:D:309:CLA:H3A	1.64	0.47
5:E:187:ASN:ND2	36:E:315:CLA:HAA1	2.30	0.47
36:G:319:CLA:H12	36:G:319:CLA:HED3	1.96	0.47
36:H:315:CLA:C2D	39:b:848:LMT:H52	2.44	0.47
39:I:317:LMT:O6'	39:I:317:LMT:H32	2.14	0.47
36:K:307:CLA:C14	37:K:314:KC1:C1C	2.91	0.47
13:M:77:ARG:NH2	13:M:77:ARG:CB	2.78	0.47
14:N:86:MET:HB2	36:N:313:CLA:HMC3	1.96	0.47
17:S:79:ILE:CG2	17:S:80:LYS:N	2.78	0.47
17:S:117:SER:HB3	17:S:233:ALA:HB3	1.97	0.47
35:S:308:A86:C5	36:S:319:CLA:CMC	2.92	0.47
20:a:118:GLN:CD	20:a:150:PHE:HB2	2.39	0.47
20:a:281:LEU:CB	36:a:816:CLA:HMA2	2.41	0.47
21:b:92:TRP:CZ3	21:b:94:PRO:HD3	2.50	0.47
21:b:222:LYS:N	21:b:223:PRO:HD2	2.29	0.47
21:b:412:GLU:CA	25:f:238:ALA:CB	2.74	0.47
21:b:686:LEU:HD23	28:l:64:TYR:CE2	2.50	0.47
22:c:2:SER:N	22:c:71:HIS:O	2.48	0.47
22:c:81:TYR:HB3	23:d:91:LEU:CD1	2.45	0.47
41:f:809:LHG:H291	41:f:809:LHG:C34	2.43	0.47
27:j:38:THR:O	27:j:40:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:U:306:CLA:CMB	36:U:306:CLA:C4	2.86	0.47
1:A:81:ARG:HH12	1:A:154:LEU:HD23	1.80	0.47
1:A:105:ASP:OD1	1:A:201:PRO:HG3	2.15	0.47
2:B:133:PHE:O	2:B:136:SER:OG	2.27	0.47
3:C:95:GLN:O	3:C:99:HIS:CD2	2.68	0.47
35:D:302:A86:C3	36:D:311:CLA:HAC1	2.45	0.47
42:E:318:LMG:H372	36:a:819:CLA:HBB1	1.97	0.47
6:F:104:ILE:HD11	36:F:311:CLA:H43	1.96	0.47
39:F:321:LMT:C6B	39:F:321:LMT:H2B	2.45	0.47
7:G:111:ARG:NH2	7:G:190:GLY:O	2.48	0.47
41:G:321:LHG:HC61	41:G:321:LHG:P	2.55	0.47
42:I:315:LMG:H302	36:a:841:CLA:C1D	2.45	0.47
39:K:318:LMT:O6'	39:K:318:LMT:H5B	2.14	0.47
15:P:150:ILE:CG2	15:P:153:PRO:O	2.63	0.47
15:P:168:ARG:HB3	36:P:314:CLA:HMA3	1.97	0.47
36:Q:314:CLA:HAB	36:Q:314:CLA:H72	1.97	0.47
17:S:122:TRP:HE3	36:S:312:CLA:HMA1	1.80	0.47
17:S:136:VAL:HG21	36:S:313:CLA:HBC2	1.96	0.47
20:a:720:GLN:NE2	24:e:44:LYS:HE3	2.29	0.47
36:b:811:CLA:H62	36:b:811:CLA:H102	1.74	0.47
39:b:851:LMT:C5'	36:f:805:CLA:CBC	2.93	0.47
41:f:809:LHG:H382	42:V:316:LMG:C32	2.39	0.47
32:U:77:TRP:CE3	36:U:308:CLA:HBA1	2.49	0.47
32:U:92:LYS:C	32:U:96:GLU:OE1	2.58	0.47
36:A:314:CLA:H202	36:A:314:CLA:H161	1.81	0.46
5:E:42:PHE:CD2	7:G:176:VAL:HG11	2.50	0.46
7:G:38:TRP:O	7:G:42:VAL:HB	2.15	0.46
36:H:305:CLA:HBB2	10:J:154:TRP:HE1	1.80	0.46
34:I:303:DD6:C19	34:I:303:DD6:C23	2.93	0.46
35:J:301:A86:C41	36:J:311:CLA:HMA1	2.45	0.46
34:K:305:DD6:C23	36:K:315:CLA:HMB1	2.45	0.46
14:N:73:PHE:CZ	36:N:312:CLA:HED2	2.46	0.46
34:O:304:DD6:C22	36:O:309:CLA:HBB1	2.45	0.46
15:P:156:ASP:CG	16:R:64:THR:OG1	2.58	0.46
15:P:157:PHE:CE1	36:P:314:CLA:HBA2	2.50	0.46
20:a:194:GLU:CD	20:a:194:GLU:N	2.73	0.46
21:b:437:ILE:HG22	36:b:833:CLA:HAC1	1.97	0.46
23:d:206:GLN:O	23:d:210:LEU:CD1	2.64	0.46
28:l:48:ILE:HG12	36:l:201:CLA:CMD	2.45	0.46
32:U:67:ILE:HB	32:U:148:HIS:NE2	2.30	0.46
33:V:118:ALA:HB1	33:V:121:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:OE1	1:A:167:GLN:HA	2.16	0.46
2:B:203:THR:HG21	2:B:210:MET:HG2	1.96	0.46
4:D:129:TRP:CH2	34:D:301:DD6:C21	2.98	0.46
6:F:78:LYS:NZ	6:F:139:GLU:OE2	2.30	0.46
10:J:67:TRP:CH2	42:J:318:LMG:H112	2.49	0.46
10:J:169:ARG:NH2	10:J:172:GLU:OE1	2.48	0.46
12:L:220:ILE:HG13	12:L:223:ALA:HB2	1.97	0.46
13:M:214:ARG:O	13:M:218:ASN:ND2	2.48	0.46
15:P:68:LEU:HD12	15:P:147:LEU:HD23	1.97	0.46
15:Q:77:ALA:O	34:Q:302:DD6:C23	2.64	0.46
18:T:25:ASP:OD1	18:T:28:ARG:N	2.43	0.46
34:W:204:DD6:C19	34:W:204:DD6:C23	2.92	0.46
20:a:277:TYR:CD1	20:a:280:PHE:CZ	3.03	0.46
21:b:634:TYR:HB3	21:b:643:SER:OG	2.15	0.46
44:b:846:BCR:H15C	44:b:846:BCR:H351	1.77	0.46
41:b:850:LHG:H111	41:b:850:LHG:O9	2.16	0.46
25:f:161:THR:HG23	41:j:104:LHG:H132	1.97	0.46
28:l:100:ILE:CG2	28:l:103:PHE:HB2	2.45	0.46
32:U:92:LYS:O	32:U:93:TYR:C	2.58	0.46
32:U:116:TYR:CZ	32:U:123:ARG:HD3	2.49	0.46
2:B:132:PHE:CE2	35:B:301:A86:C	2.98	0.46
2:B:132:PHE:HD1	36:B:308:CLA:HBA2	1.80	0.46
36:B:309:CLA:H2A	36:B:309:CLA:O1D	2.15	0.46
4:D:155:ASN:ND2	4:D:155:ASN:C	2.73	0.46
36:E:311:CLA:H92	42:E:318:LMG:H112	1.95	0.46
36:E:315:CLA:CMB	36:E:315:CLA:HBB1	2.45	0.46
8:H:91:VAL:O	8:H:96:ARG:NH1	2.36	0.46
35:H:304:A86:C40	36:H:307:CLA:CBC	2.93	0.46
10:J:115:VAL:HA	10:J:120:MET:HB2	1.96	0.46
10:J:151:ASP:OD1	10:J:155:LYS:HE2	2.15	0.46
10:J:154:TRP:CH2	36:J:310:CLA:H171	2.50	0.46
36:J:307:CLA:H61	36:J:307:CLA:H41	1.68	0.46
12:L:115:TRP:CD1	39:L:318:LMT:H6E	2.50	0.46
34:M:303:DD6:C21	36:M:309:CLA:CBB	2.85	0.46
15:O:133:ILE:CD1	35:O:301:A86:C39	2.93	0.46
35:S:304:A86:C12	36:S:321:CLA:HBA2	2.45	0.46
34:S:306:DD6:C19	34:S:306:DD6:C23	2.93	0.46
19:W:32:LEU:HD22	36:W:207:CLA:H42	1.97	0.46
20:a:98:PHE:CZ	20:a:102:TYR:HD2	2.32	0.46
36:a:816:CLA:C14	36:a:816:CLA:H18	2.45	0.46
36:b:823:CLA:C4	31:h:68:MET:HE2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:137:LEU:HD23	25:f:158:GLU:OE2	2.15	0.46
25:f:166:PHE:HB2	44:f:801:BCR:H321	1.97	0.46
41:f:808:LHG:HC62	41:f:809:LHG:HC61	1.97	0.46
1:A:132:TRP:CE3	42:V:315:LMG:HC5	2.51	0.46
39:B:312:LMT:H71	44:m:101:BCR:C38	2.42	0.46
36:C:211:CLA:H111	36:C:211:CLA:H72	1.77	0.46
39:F:320:LMT:O3'	39:F:321:LMT:O5'	2.33	0.46
7:G:153:LEU:CD1	36:G:311:CLA:HAA1	2.42	0.46
7:G:192:PHE:O	36:G:313:CLA:OBD	2.33	0.46
34:I:303:DD6:C24	36:I:306:CLA:HAB	2.45	0.46
39:I:317:LMT:H52	39:I:317:LMT:H22	1.40	0.46
10:J:86:TYR:OH	10:J:108:ALA:CB	2.64	0.46
34:O:304:DD6:C19	34:O:304:DD6:C23	2.93	0.46
19:W:116:PHE:HB3	36:W:212:CLA:HMD2	1.98	0.46
19:X:117:ARG:NE	19:X:120:ALA:H	2.14	0.46
20:a:177:LEU:HD23	20:a:177:LEU:HA	1.85	0.46
36:b:820:CLA:H8	36:b:820:CLA:H51	1.45	0.46
23:d:138:LEU:N	23:d:154:PHE:CE2	2.84	0.46
33:V:7:PRO:CG	36:V:305:CLA:HMA3	2.44	0.46
33:V:132:LEU:HD12	36:V:310:CLA:CED	2.45	0.46
33:V:149:ARG:HH11	33:V:149:ARG:HG3	1.80	0.46
2:B:79:TRP:HH2	2:B:199:LEU:HD21	1.81	0.46
36:C:212:CLA:H72	36:C:212:CLA:H111	1.64	0.46
40:C:215:DGD:HB31	40:C:215:DGD:HB71	1.96	0.46
36:D:313:CLA:H91	36:D:313:CLA:H111	1.79	0.46
39:E:320:LMT:C3	41:E:322:LHG:C26	2.88	0.46
39:E:323:LMT:O1B	39:E:323:LMT:O6'	2.33	0.46
36:J:308:CLA:H101	36:J:308:CLA:H62	1.83	0.46
12:L:137:ILE:CG1	34:L:305:DD6:C23	2.93	0.46
14:N:63:TRP:CD1	35:N:305:A86:O3	2.69	0.46
15:O:55:GLY:HA2	33:V:143:ILE:C	2.39	0.46
34:Q:302:DD6:C28	36:Q:306:CLA:H152	2.44	0.46
16:R:66:TRP:CH2	41:R:323:LHG:H241	2.50	0.46
17:S:59:ASP:C	17:S:60:LYS:HG3	2.39	0.46
21:b:402:ASN:HB3	21:b:405:ASN:CB	2.46	0.46
29:m:12:ILE:HG12	44:m:101:BCR:H403	1.97	0.46
35:U:303:A86:C7	36:U:307:CLA:CAB	2.89	0.46
4:D:89:PHE:CD1	4:D:89:PHE:C	2.93	0.46
39:E:320:LMT:O6'	39:E:321:LMT:H1'	2.16	0.46
35:F:301:A86:C13	35:F:301:A86:C23	2.93	0.46
39:F:320:LMT:C3'	39:F:321:LMT:C6'	2.91	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:I:317:LMT:H4'	39:I:317:LMT:O1'	2.15	0.46
36:J:309:CLA:C14	42:J:319:LMG:H261	2.46	0.46
14:N:78:GLU:OE1	14:N:207:ARG:NH1	2.49	0.46
15:P:150:ILE:O	15:P:150:ILE:HG23	2.15	0.46
41:Q:315:LHG:H251	41:Q:315:LHG:H281	1.49	0.46
16:R:175:HIS:NE2	34:R:307:DD6:C	2.73	0.46
20:a:166:TRP:CD1	36:a:815:CLA:HAA2	2.50	0.46
20:a:490:GLN:NE2	20:a:533:LEU:O	2.45	0.46
20:a:712:LYS:O	25:f:227:ASP:OD1	2.34	0.46
41:f:809:LHG:HC32	41:f:809:LHG:C23	2.45	0.46
41:j:104:LHG:H352	41:j:104:LHG:H383	1.57	0.46
28:l:57:LEU:HD12	28:l:57:LEU:O	2.16	0.46
1:A:161:LEU:HD13	36:A:311:CLA:H11	1.98	0.46
2:B:135:ILE:HD13	35:B:301:A86:C6	2.46	0.46
36:C:206:CLA:H41	36:C:206:CLA:H61	1.66	0.46
6:F:68:LYS:HG2	6:F:150:TRP:O	2.14	0.46
9:I:173:VAL:HG11	35:I:301:A86:C9	2.46	0.46
10:J:83:VAL:HG11	35:J:305:A86:C8	2.45	0.46
14:N:73:PHE:O	14:N:76:GLN:HB3	2.16	0.46
15:Q:156:ASP:C	17:S:60:LYS:HD3	2.39	0.46
36:R:320:CLA:HBC3	41:R:323:LHG:H142	1.97	0.46
35:T:303:A86:C1	37:T:310:KC1:CBB	2.94	0.46
19:W:42:ILE:HG22	34:W:204:DD6:C12	2.46	0.46
20:a:274:TRP:CZ3	36:a:816:CLA:H72	2.51	0.46
21:b:544:LYS:HD2	21:b:544:LYS:HA	1.68	0.46
36:b:828:CLA:H93	36:b:828:CLA:H111	1.80	0.46
46:b:924:HOH:O	31:h:53:THR:HA	2.15	0.46
32:U:31:ARG:C	32:U:31:ARG:CD	2.88	0.46
40:C:215:DGD:HB52	40:C:215:DGD:HB22	1.40	0.46
4:D:145:LEU:HD12	4:D:145:LEU:HA	1.75	0.46
34:D:304:DD6:C41	36:D:310:CLA:H18	2.46	0.46
5:E:42:PHE:HD2	7:G:176:VAL:HG11	1.80	0.46
5:E:217:LEU:CD2	15:P:121:ASN:HD21	2.20	0.46
7:G:156:GLN:O	41:G:301:LHG:O5	2.34	0.46
7:G:173:THR:HG23	7:G:192:PHE:HE1	1.78	0.46
7:G:215:GLU:HG3	36:G:313:CLA:NB	2.31	0.46
7:G:242:PHE:N	7:G:243:PRO:CD	2.78	0.46
35:L:307:A86:C40	36:Q:307:CLA:CBC	2.94	0.46
14:N:76:GLN:HA	14:N:164:TYR:CD1	2.51	0.46
36:O:316:CLA:H151	36:O:316:CLA:H18	1.32	0.46
15:P:34:ASP:N	15:P:45:LYS:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:149:THR:CG2	15:P:150:ILE:N	2.79	0.46
16:R:50:PRO:HB2	17:S:169:LEU:CD2	2.46	0.46
17:S:80:LYS:NZ	17:S:141:GLU:OE2	2.42	0.46
19:W:102:VAL:HG13	19:W:114:GLY:HA3	1.97	0.46
19:X:124:GLY:HA2	33:V:9:PHE:CG	2.51	0.46
36:X:315:CLA:HMD1	35:V:301:A86:C26	2.45	0.46
20:a:302:HIS:O	20:a:306:LEU:HG	2.16	0.46
20:a:529:MET:HG2	20:a:530:PRO:HD2	1.97	0.46
21:b:528:VAL:HG11	21:b:581:TRP:CZ2	2.50	0.46
36:b:818:CLA:HAB	35:h:202:A86:C5	2.46	0.46
36:b:840:CLA:H12	44:b:847:BCR:H353	1.97	0.46
22:c:17:CYS:SG	22:c:18:VAL:N	2.88	0.46
32:U:4:MET:HE1	32:U:27:ALA:CB	2.42	0.46
1:A:162:SER:HB2	36:A:311:CLA:HBA1	1.98	0.46
1:A:163:VAL:HG22	1:A:163:VAL:O	2.15	0.46
2:B:193:MET:HE1	36:B:305:CLA:HAB	1.97	0.46
8:H:85:TRP:CD2	34:H:303:DD6:C8	2.99	0.46
34:I:303:DD6:C25	36:I:306:CLA:HMC1	2.46	0.46
42:I:315:LMG:HC8	42:I:315:LMG:O6	2.15	0.46
14:N:170:PHE:CZ	36:N:318:CLA:C2	2.99	0.46
36:P:314:CLA:CGA	36:P:314:CLA:H3A	2.44	0.46
15:Q:156:ASP:CA	17:S:60:LYS:HD2	2.46	0.46
18:T:6:LEU:HB2	18:T:133:MET:HE1	1.97	0.46
19:X:124:GLY:CA	33:V:9:PHE:CG	2.99	0.46
20:a:209:GLY:HA2	36:a:819:CLA:HBC1	1.98	0.46
20:a:483:GLN:H	41:a:850:LHG:C2	2.29	0.46
20:a:704:GLU:OE2	24:e:47:TYR:OH	2.30	0.46
36:a:818:CLA:H3A	36:a:818:CLA:HBA2	1.66	0.46
36:b:819:CLA:HBA2	36:b:819:CLA:H3A	1.42	0.46
23:d:101:VAL:HG22	23:d:102:ILE:N	2.31	0.46
32:U:77:TRP:CD2	36:U:308:CLA:HBA1	2.50	0.46
32:U:81:PHE:CD1	32:U:81:PHE:C	2.93	0.46
36:U:306:CLA:H151	36:U:306:CLA:H112	1.55	0.46
33:V:37:LYS:HD2	36:V:310:CLA:C3D	2.46	0.46
33:V:128:GLN:CB	33:V:129:PRO:HD2	2.38	0.46
33:V:139:ASN:ND2	36:V:311:CLA:HBA2	2.29	0.46
1:A:140:MET:CB	25:f:207:PHE:HE1	2.29	0.46
36:E:314:CLA:H41	36:E:314:CLA:H61	1.76	0.46
36:E:314:CLA:H193	36:E:314:CLA:H161	1.79	0.46
42:E:318:LMG:H232	42:E:318:LMG:H201	1.26	0.46
9:I:64:ASN:HD22	9:I:140:PRO:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:154:TRP:HD1	39:L:303:LMT:H101	1.81	0.46
15:P:133:ILE:HG23	15:P:137:LYS:HZ3	1.80	0.46
35:P:306:A86:C39	36:P:316:CLA:CMB	2.93	0.46
21:b:320:GLY:O	21:b:324:THR:CG2	2.61	0.46
21:b:558:CYS:HG	45:b:803:SF4:FE4	1.30	0.46
39:b:851:LMT:H1'	36:f:805:CLA:HBC3	1.98	0.46
23:d:114:MET:CB	23:d:117:GLY:O	2.57	0.46
36:l:201:CLA:H101	36:l:201:CLA:H62	1.74	0.46
35:h:202:A86:C41	35:h:202:A86:C35	2.94	0.46
36:A:310:CLA:H203	36:A:310:CLA:H161	1.86	0.45
36:D:306:CLA:C1D	41:D:318:LHG:H252	2.47	0.45
41:E:322:LHG:HC5	41:E:322:LHG:O2	2.15	0.45
11:K:62:GLY:O	11:K:66:ARG:HG2	2.16	0.45
36:L:320:CLA:H61	36:L:320:CLA:H92	1.81	0.45
36:O:308:CLA:H52	36:O:308:CLA:H8	1.70	0.45
36:O:316:CLA:HBA2	36:O:316:CLA:H3A	1.52	0.45
15:P:32:LYS:HD2	15:P:32:LYS:N	2.30	0.45
41:Q:315:LHG:HC62	41:Q:315:LHG:C8	2.45	0.45
17:S:160:LYS:HD2	36:S:315:CLA:HED2	1.98	0.45
36:W:207:CLA:H93	36:W:207:CLA:H61	1.84	0.45
19:X:124:GLY:O	33:V:9:PHE:CE1	2.69	0.45
20:a:470:LEU:HD13	21:b:95:HIS:O	2.15	0.45
36:a:806:CLA:H43	34:j:103:DD6:C5	2.46	0.45
44:a:846:BCR:H20C	44:a:846:BCR:H361	1.82	0.45
21:b:442:VAL:HG13	21:b:447:GLN:O	2.16	0.45
21:b:604:ASN:ND2	21:b:607:GLN:HG3	2.31	0.45
36:b:802:CLA:H192	25:f:206:LEU:HD21	1.97	0.45
41:f:808:LHG:HC62	41:f:809:LHG:C6	2.46	0.45
28:l:133:VAL:C	28:l:135:SER:N	2.69	0.45
36:V:314:CLA:H2	36:V:314:CLA:HMA2	1.99	0.45
3:C:124:GLN:OE1	36:C:210:CLA:C1D	2.63	0.45
7:G:104:GLU:HG2	7:G:177:LEU:HD21	1.98	0.45
36:H:317:CLA:H112	36:H:317:CLA:H72	1.62	0.45
9:I:152:ASN:OD1	9:I:158:VAL:HG22	2.15	0.45
36:I:312:CLA:C7	39:I:318:LMT:H12	2.46	0.45
34:K:305:DD6:C23	36:K:315:CLA:CMB	2.95	0.45
36:P:301:CLA:H3A	36:P:301:CLA:HBA1	1.58	0.45
36:P:319:CLA:H3A	36:P:319:CLA:HBA2	1.53	0.45
15:Q:152:PHE:HE2	36:Q:314:CLA:C2C	2.27	0.45
16:R:202:LYS:O	16:R:206:ASN:ND2	2.49	0.45
17:S:79:ILE:HG23	17:S:80:LYS:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:86:MET:HB2	36:S:315:CLA:HMC1	1.97	0.45
35:X:314:A86:C24	36:V:306:CLA:CHC	2.90	0.45
36:a:801:CLA:CMB	36:a:848:CLA:OBD	2.65	0.45
36:a:806:CLA:ND	39:a:851:LMT:H72	2.31	0.45
21:b:371:TYR:CE2	46:b:944:HOH:O	2.68	0.45
21:b:593:TRP:O	21:b:597:HIS:HD2	2.00	0.45
36:b:822:CLA:HBB1	36:b:823:CLA:H93	1.97	0.45
23:d:161:GLY:C	23:d:162:GLU:OE2	2.59	0.45
36:l:201:CLA:H152	36:l:201:CLA:H112	1.74	0.45
32:U:37:ASN:HD22	36:U:306:CLA:HBB2	1.80	0.45
32:U:101:SER:O	32:U:109:ALA:N	2.49	0.45
33:V:112:HIS:H	33:V:112:HIS:HD2	1.63	0.45
33:V:162:PHE:CG	35:V:301:A86:C12	3.00	0.45
41:G:321:LHG:HC62	41:G:321:LHG:HC2	1.97	0.45
39:G:322:LMT:C6'	39:G:322:LMT:C1B	2.88	0.45
9:I:100:SER:CB	9:I:188:TYR:CE2	2.99	0.45
36:I:305:CLA:H143	36:I:312:CLA:C3B	2.46	0.45
36:L:312:CLA:HBA1	36:L:312:CLA:HED2	1.97	0.45
13:M:101:VAL:HG12	13:M:105:ARG:NH1	2.32	0.45
14:N:86:MET:SD	36:N:313:CLA:CMC	3.03	0.45
36:O:308:CLA:H12	36:O:308:CLA:H51	1.73	0.45
36:T:309:CLA:H41	36:T:309:CLA:H62	1.75	0.45
36:T:311:CLA:HMC2	36:T:311:CLA:H71	1.98	0.45
19:X:117:ARG:HA	33:V:14:TYR:HE1	1.78	0.45
20:a:280:PHE:N	20:a:280:PHE:CD1	2.84	0.45
36:a:836:CLA:H62	36:a:836:CLA:H41	1.63	0.45
36:b:817:CLA:H8	36:b:817:CLA:H122	1.65	0.45
41:f:808:LHG:HC2	41:f:808:LHG:O5	2.16	0.45
32:U:10:GLU:OE2	32:U:10:GLU:HA	2.16	0.45
32:U:110:ILE:HG23	36:U:311:CLA:CMD	2.47	0.45
36:U:311:CLA:H91	36:U:311:CLA:H142	1.99	0.45
6:F:43:GLY:HA2	36:V:314:CLA:HED3	1.98	0.45
36:H:308:CLA:C20	31:h:116:LEU:CD1	2.95	0.45
36:I:310:CLA:H62	36:I:310:CLA:H41	1.75	0.45
11:K:88:ALA:HB2	36:K:310:CLA:CBB	2.47	0.45
12:L:115:TRP:O	12:L:124:THR:OG1	2.33	0.45
12:L:201:ILE:O	12:L:205:ARG:N	2.46	0.45
35:S:308:A86:C34	36:S:311:CLA:HBC1	2.47	0.45
19:X:129:ASP:O	19:X:132:THR:N	2.44	0.45
35:X:314:A86:C10	33:V:45:ALA:CB	2.95	0.45
21:b:368:ALA:CB	21:b:724:LEU:HD11	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:489:ASN:HA	21:b:493:LEU:CB	2.45	0.45
21:b:505:ASN:HD22	21:b:505:ASN:HA	1.54	0.45
28:l:90:PHE:CE2	28:l:91:LYS:HE2	2.51	0.45
29:m:23:LYS:CG	42:m:102:LMG:O3	2.64	0.45
32:U:52:LYS:HE3	32:U:65:ASP:CB	2.47	0.45
32:U:147:ALA:O	32:U:148:HIS:C	2.59	0.45
33:V:71:ASP:N	33:V:71:ASP:OD1	2.49	0.45
2:B:136:SER:HB3	36:B:308:CLA:C4D	2.47	0.45
36:E:313:CLA:C11	36:E:313:CLA:C16	2.94	0.45
6:F:169:THR:CG2	36:F:314:CLA:O1A	2.64	0.45
15:P:159:THR:OG1	16:R:62:SER:CB	2.56	0.45
15:Q:150:ILE:HD11	36:Q:314:CLA:C2D	2.46	0.45
34:Q:302:DD6:O1	36:Q:308:CLA:CMB	2.63	0.45
17:S:89:PHE:CE2	17:S:93:ILE:CD1	3.00	0.45
37:T:310:KC1:CHD	36:T:313:CLA:HMD1	2.45	0.45
20:a:112:ASP:OD1	20:a:115:LYS:HG2	2.15	0.45
20:a:288:ASN:HD22	20:a:290:VAL:H	1.64	0.45
20:a:484:LEU:HB2	20:a:535:THR:OG1	2.16	0.45
21:b:465:ALA:HB1	21:b:476:LEU:CD1	2.47	0.45
23:d:198:ILE:HD12	23:d:201:LYS:HZ2	1.82	0.45
42:j:105:LMG:H292	42:j:105:LMG:HC92	1.82	0.45
31:h:93:GLN:HB3	31:h:114:TYR:CZ	2.52	0.45
32:U:63:VAL:CG1	32:U:64:ASP:N	2.80	0.45
33:V:82:SER:HB2	33:V:83:PRO:HD3	1.89	0.45
2:B:182:GLU:C	2:B:184:ALA:N	2.56	0.45
3:C:159:LYS:CG	3:C:163:GLU:HG2	2.42	0.45
35:E:307:A86:C9	36:E:315:CLA:ND	2.79	0.45
36:G:311:CLA:H62	36:G:311:CLA:H41	1.64	0.45
36:G:315:CLA:HED1	39:a:853:LMT:C5B	2.45	0.45
9:I:118:PHE:CD1	36:I:309:CLA:CBC	2.98	0.45
10:J:40:VAL:O	36:J:308:CLA:CED	2.61	0.45
10:J:109:ASP:C	10:J:111:HIS:H	2.23	0.45
36:J:315:CLA:HBC1	36:J:317:CLA:HAB	1.98	0.45
14:N:170:PHE:HE2	14:N:178:LEU:O	1.93	0.45
16:R:49:ASN:HD21	36:R:310:CLA:C1B	2.30	0.45
16:R:50:PRO:O	16:R:53:LYS:CD	2.64	0.45
16:R:154:HIS:CG	36:R:320:CLA:HAA1	2.52	0.45
35:S:304:A86:C21	36:S:315:CLA:C4A	2.94	0.45
20:a:490:GLN:HG2	39:a:854:LMT:C6B	2.46	0.45
36:a:818:CLA:H203	36:a:826:CLA:H3A	1.98	0.45
21:b:372:THR:HG23	21:b:590:THR:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:592:TYR:CZ	36:b:836:CLA:HBC2	2.52	0.45
22:c:25:VAL:HG13	22:c:44:ARG:O	2.17	0.45
36:f:803:CLA:HBC3	36:f:803:CLA:HHD	1.99	0.45
41:f:809:LHG:H351	42:V:316:LMG:H211	1.99	0.45
44:i:101:BCR:H20C	44:i:101:BCR:H361	1.80	0.45
33:V:112:HIS:CD2	33:V:112:HIS:N	2.84	0.45
36:V:313:CLA:H3A	36:V:313:CLA:HBA2	1.66	0.45
36:V:314:CLA:H141	36:V:314:CLA:CMB	2.44	0.45
34:A:304:DD6:C19	34:A:304:DD6:C23	2.94	0.45
36:D:306:CLA:CHD	41:D:318:LHG:H252	2.47	0.45
35:E:305:A86:C3	36:E:315:CLA:CMB	2.95	0.45
6:F:166:MET:HE3	6:F:168:LEU:HD11	1.99	0.45
36:F:314:CLA:CGA	36:F:314:CLA:H3A	2.45	0.45
36:F:317:CLA:CGD	36:F:317:CLA:CBA	2.94	0.45
36:G:309:CLA:H61	36:G:309:CLA:H102	1.65	0.45
36:J:313:CLA:H143	36:J:313:CLA:H161	1.89	0.45
11:K:95:PRO:HG3	36:K:310:CLA:C1D	2.46	0.45
12:L:93:VAL:HG23	12:L:104:SER:HB3	1.99	0.45
13:M:75:ILE:HG13	41:R:323:LHG:C16	2.46	0.45
15:O:54:LEU:CD2	33:V:143:ILE:HG21	2.43	0.45
16:R:48:SER:HB2	16:R:205:ASN:HD21	1.82	0.45
37:T:310:KC1:CHD	36:T:313:CLA:HMD3	2.46	0.45
34:W:205:DD6:C25	36:W:212:CLA:HHC	2.47	0.45
19:X:60:PRO:HG2	33:V:173:ILE:CG2	2.43	0.45
20:a:349:ILE:HD11	20:a:427:ASN:HD21	1.82	0.45
20:a:443:ILE:HG13	20:a:561:TYR:HE2	1.81	0.45
21:b:356:PRO:HG3	36:b:820:CLA:HBA1	1.99	0.45
21:b:712:PHE:O	21:b:716:TYR:HB2	2.16	0.45
36:b:833:CLA:HMA1	41:j:104:LHG:H261	1.98	0.45
28:l:62:PRO:HG3	36:l:205:CLA:HED2	1.99	0.45
31:h:125:TRP:HE1	36:h:203:CLA:C3B	2.30	0.45
32:U:95:MET:CE	32:U:95:MET:CA	2.86	0.45
33:V:177:VAL:CB	33:V:178:PRO:HD2	2.36	0.45
36:V:306:CLA:H192	36:V:306:CLA:H161	1.83	0.45
3:C:160:SER:O	3:C:162:ALA:N	2.50	0.45
35:E:307:A86:C9	36:E:315:CLA:C4D	2.94	0.45
36:E:313:CLA:H41	36:E:313:CLA:H61	1.48	0.45
36:H:315:CLA:C3D	39:b:848:LMT:H52	2.46	0.45
34:L:305:DD6:C1	36:L:310:CLA:HAB	2.46	0.45
35:L:307:A86:C8	41:Q:315:LHG:H302	2.46	0.45
14:N:52:TYR:OH	35:N:303:A86:C34	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:81:TYR:CE1	15:P:108:PRO:CG	2.99	0.45
15:Q:152:PHE:CZ	36:Q:314:CLA:HHC	2.49	0.45
36:Q:307:CLA:H51	36:Q:307:CLA:H12	1.73	0.45
41:R:323:LHG:H301	41:R:323:LHG:H332	1.52	0.45
36:W:216:CLA:HBB1	37:W:217:KC1:O1D	2.17	0.45
36:a:839:CLA:H152	44:i:103:BCR:H17C	1.99	0.45
21:b:608:PHE:CD1	21:b:608:PHE:C	2.95	0.45
36:b:814:CLA:H3A	36:b:814:CLA:HBA2	1.72	0.45
32:U:81:PHE:HZ	36:U:310:CLA:CBC	2.28	0.45
33:V:46:VAL:HG23	33:V:164:ILE:HB	1.99	0.45
4:D:44:TYR:HA	4:D:45:PRO:HD3	1.84	0.45
7:G:232:GLN:C	7:G:234:ALA:H	2.24	0.45
39:G:323:LMT:H41	36:P:301:CLA:CED	2.43	0.45
15:P:34:ASP:CG	15:P:45:LYS:HD3	2.42	0.45
15:P:106:MET:HE2	15:P:106:MET:HB3	1.75	0.45
15:P:133:ILE:CG2	15:P:137:LYS:NZ	2.80	0.45
20:a:644:SER:O	20:a:650:GLY:HA3	2.17	0.45
20:a:700:GLN:NE2	20:a:723:ALA:H	2.15	0.45
36:a:825:CLA:H143	36:a:825:CLA:H111	1.67	0.45
21:b:6:PRO:HG2	21:b:13:ALA:HB2	1.99	0.45
21:b:361:SER:O	21:b:362:LYS:HD3	2.16	0.45
36:f:802:CLA:HMC2	41:j:104:LHG:H292	1.99	0.45
33:V:158:ARG:HB3	36:V:306:CLA:CAC	2.47	0.45
2:B:194:LEU:HD22	2:B:194:LEU:HA	1.82	0.45
39:E:320:LMT:H11	36:a:809:CLA:HBD	1.99	0.45
41:F:319:LHG:H161	41:F:319:LHG:H132	1.82	0.45
36:H:308:CLA:O1D	36:H:308:CLA:H2A	2.17	0.45
13:M:77:ARG:CZ	13:M:77:ARG:CB	2.86	0.45
36:M:306:CLA:H62	36:M:306:CLA:H41	1.55	0.45
14:N:184:PHE:O	14:N:184:PHE:CD1	2.70	0.45
15:Q:152:PHE:CE2	36:Q:314:CLA:CMC	3.00	0.45
15:Q:196:VAL:HA	15:Q:197:PRO:HD3	1.88	0.45
20:a:696:ARG:CD	20:a:725:SER:HA	2.47	0.45
36:a:806:CLA:H193	42:j:105:LMG:C23	2.47	0.45
38:b:804:SQD:H141	44:b:843:BCR:H343	1.98	0.45
36:b:818:CLA:H41	36:b:818:CLA:H62	1.73	0.45
36:b:822:CLA:HHB	36:b:823:CLA:H2	1.98	0.45
44:b:846:BCR:H20C	44:b:846:BCR:H361	1.86	0.45
36:f:804:CLA:H61	36:f:804:CLA:H101	1.70	0.45
32:U:16:PHE:CD1	32:U:16:PHE:O	2.70	0.45
32:U:57:PHE:CE1	35:U:302:A86:C29	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:77:TRP:CD2	36:U:308:CLA:CBA	3.00	0.45
32:U:89:GLU:OE2	36:U:310:CLA:HMA3	2.17	0.45
33:V:114:ASN:HD22	33:V:114:ASN:HA	1.67	0.45
33:V:138:TRP:HE3	36:V:311:CLA:C2D	2.29	0.45
2:B:194:LEU:HD11	35:B:303:A86:C17	2.46	0.44
35:E:307:A86:C14	36:E:315:CLA:OBD	2.65	0.44
39:F:321:LMT:H1B	39:F:321:LMT:H3'	1.78	0.44
8:H:119:PHE:CD2	36:H:310:CLA:HED2	2.52	0.44
8:H:119:PHE:O	8:H:119:PHE:CG	2.70	0.44
8:H:176:LEU:O	8:H:180:ARG:N	2.47	0.44
10:J:106:LYS:NZ	10:J:194:GLY:O	2.50	0.44
36:S:319:CLA:H112	36:S:319:CLA:H72	1.74	0.44
18:T:64:ASP:OD2	18:T:66:SER:OG	2.31	0.44
19:W:41:ARG:HH12	36:W:212:CLA:HMD3	1.82	0.44
20:a:110:LEU:HD23	20:a:110:LEU:HA	1.80	0.44
20:a:585:ARG:HE	20:a:585:ARG:HB2	1.64	0.44
36:a:807:CLA:HBA2	36:a:807:CLA:H3A	1.48	0.44
36:a:817:CLA:H102	36:a:834:CLA:HBA1	2.00	0.44
21:b:648:MET:HE1	36:b:828:CLA:C4	2.46	0.44
23:d:104:TRP:HD1	23:d:150:ILE:CD1	2.27	0.44
41:i:104:LHG:H122	41:i:104:LHG:H152	1.58	0.44
27:j:41:PHE:CD1	27:j:41:PHE:O	2.70	0.44
36:j:102:CLA:H2	36:j:102:CLA:H62	1.47	0.44
1:A:159:MET:CE	36:V:307:CLA:HED1	2.48	0.44
36:A:311:CLA:H3A	36:A:311:CLA:HBA2	1.61	0.44
5:E:45:ARG:CG	5:E:45:ARG:NH2	2.76	0.44
6:F:107:MET:HB3	6:F:108:PRO:HD2	1.99	0.44
6:F:127:LEU:HD21	35:F:302:A86:C24	2.48	0.44
36:F:311:CLA:H62	36:F:311:CLA:H2	1.70	0.44
7:G:120:TRP:CD1	7:G:120:TRP:O	2.70	0.44
36:I:312:CLA:HHC	36:I:312:CLA:HBB1	2.00	0.44
12:L:82:ALA:CB	34:L:305:DD6:C10	2.94	0.44
36:O:316:CLA:H41	36:O:316:CLA:H61	1.73	0.44
15:P:199:LEU:HD22	35:P:306:A86:C41	2.47	0.44
20:a:464:ASN:HB3	20:a:647:THR:HG22	1.98	0.44
27:j:37:LEU:HD12	27:j:37:LEU:O	2.18	0.44
41:j:104:LHG:H142	41:j:104:LHG:H112	1.33	0.44
1:A:196:TRP:NE1	36:A:314:CLA:CMD	2.80	0.44
3:C:64:LEU:HD11	36:b:814:CLA:H12	1.99	0.44
3:C:114:ILE:H	3:C:114:ILE:HG13	1.45	0.44
4:D:204:PHE:N	4:D:205:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:I:315:LMG:H362	42:I:315:LMG:H392	1.57	0.44
14:N:90:VAL:HG12	36:N:310:CLA:HBC2	2.00	0.44
14:N:209:ALA:HB2	35:N:304:A86:C	2.47	0.44
35:Q:304:A86:C37	37:Q:311:KC1:CMA	2.95	0.44
17:S:243:PRO:HD3	35:S:308:A86:C41	2.48	0.44
36:W:212:CLA:HBD	36:W:212:CLA:HBA1	1.99	0.44
19:X:117:ARG:HB3	33:V:14:TYR:OH	2.17	0.44
20:a:519:ILE:CD1	20:a:633:ILE:HD11	2.47	0.44
42:a:852:LMG:H112	42:a:852:LMG:HC92	1.98	0.44
21:b:675:GLU:HG2	22:c:81:TYR:HE2	1.83	0.44
36:b:829:CLA:H3A	36:b:829:CLA:HBA2	1.81	0.44
36:b:833:CLA:H112	36:b:833:CLA:H91	1.78	0.44
36:b:834:CLA:HBB1	36:b:836:CLA:H112	1.99	0.44
23:d:101:VAL:HG23	23:d:129:LEU:O	2.18	0.44
23:d:138:LEU:HD13	23:d:154:PHE:CZ	2.52	0.44
25:f:85:LYS:HG3	25:f:86:GLU:HG3	1.98	0.44
42:j:105:LMG:H152	42:j:105:LMG:H181	1.39	0.44
32:U:50:PHE:O	32:U:50:PHE:CD1	2.70	0.44
32:U:72:GLN:N	32:U:72:GLN:HE21	2.15	0.44
35:B:301:A86:C23	36:U:307:CLA:C5	2.96	0.44
42:D:321:LMG:H131	42:D:321:LMG:H162	1.53	0.44
36:E:315:CLA:HMB3	36:E:315:CLA:HBB1	1.99	0.44
6:F:214:PHE:CE1	36:V:309:CLA:CMB	2.97	0.44
7:G:242:PHE:CD1	7:G:242:PHE:O	2.70	0.44
42:G:324:LMG:H182	42:G:324:LMG:H151	1.66	0.44
36:H:308:CLA:H92	36:H:308:CLA:H61	1.79	0.44
10:J:50:PHE:HE2	10:J:52:PHE:HB2	1.77	0.44
39:K:317:LMT:O2B	39:K:317:LMT:H5B	2.17	0.44
14:N:227:PRO:CD	35:N:304:A86:O5	2.66	0.44
35:N:303:A86:C3	36:N:309:CLA:CBB	2.95	0.44
35:N:304:A86:C20	36:N:319:CLA:O2D	2.65	0.44
15:Q:150:ILE:HD11	36:Q:314:CLA:CHD	2.48	0.44
15:Q:171:ARG:HD2	37:Q:311:KC1:CAA	2.47	0.44
16:R:73:THR:O	16:R:76:PHE:N	2.48	0.44
17:S:53:ASP:OD1	17:S:56:SER:HA	2.18	0.44
17:S:143:TRP:NE1	17:S:165:PRO:O	2.44	0.44
19:W:38:LYS:NZ	35:W:203:A86:O2	2.49	0.44
19:W:117:ARG:HH11	19:X:26:GLN:HE21	1.65	0.44
21:b:319:VAL:CG1	31:h:53:THR:HG21	2.47	0.44
21:b:324:THR:HG22	21:b:401:LEU:HD13	1.98	0.44
28:l:72:LEU:HD12	28:l:72:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:U:306:CLA:HBB1	36:U:306:CLA:HMB3	1.99	0.44
33:V:53:LYS:HA	33:V:53:LYS:HD2	1.51	0.44
36:V:311:CLA:H92	36:V:311:CLA:H61	1.77	0.44
36:A:306:CLA:HBC2	36:A:306:CLA:CHD	2.43	0.44
41:D:319:LHG:H291	20:a:179:LEU:HB3	1.99	0.44
36:F:312:CLA:O1D	39:h:205:LMT:C6'	2.65	0.44
9:I:49:PHE:CD2	9:I:49:PHE:O	2.70	0.44
10:J:73:LEU:HD23	10:J:73:LEU:HA	1.83	0.44
10:J:142:MET:HB2	10:J:147:ARG:NH2	2.33	0.44
36:K:310:CLA:C17	42:L:321:LMG:H161	2.46	0.44
36:W:212:CLA:H202	36:W:212:CLA:H161	1.85	0.44
43:a:840:PQN:H193	36:f:803:CLA:CAB	2.48	0.44
21:b:507:LEU:HD23	21:b:507:LEU:HA	1.79	0.44
22:c:31:TRP:CE3	22:c:39:ILE:HB	2.52	0.44
23:d:80:SER:HB3	28:l:40:PHE:CE2	2.52	0.44
25:f:218:ARG:NH2	41:f:808:LHG:O3	2.50	0.44
33:V:167:TRP:HE1	35:V:303:A86:C21	2.31	0.44
36:B:309:CLA:H2	36:B:309:CLA:H62	1.55	0.44
36:E:310:CLA:H91	36:E:310:CLA:H112	1.82	0.44
36:E:316:CLA:H3A	36:E:316:CLA:HBA2	1.51	0.44
6:F:213:VAL:HG23	33:V:93:GLU:OE1	1.95	0.44
6:F:214:PHE:CZ	36:V:309:CLA:CMB	3.00	0.44
11:K:174:MET:HE3	36:K:313:CLA:HHB	1.99	0.44
15:P:128:PHE:CD1	15:P:128:PHE:O	2.71	0.44
19:W:62:THR:HG22	19:W:69:THR:HG22	2.00	0.44
41:a:850:LHG:HC61	41:a:850:LHG:C1	2.48	0.44
21:b:89:HIS:CE1	21:b:113:ASN:HD22	2.35	0.44
21:b:372:THR:O	21:b:372:THR:HG22	2.17	0.44
28:l:48:ILE:HG21	36:l:201:CLA:C4D	2.48	0.44
2:B:73:ARG:HD3	36:B:309:CLA:CHD	2.48	0.44
3:C:159:LYS:HG2	3:C:163:GLU:HG3	1.98	0.44
5:E:146:ILE:HG12	41:E:322:LHG:HC91	2.00	0.44
36:F:317:CLA:O1A	36:F:317:CLA:H2	2.18	0.44
7:G:99:LEU:HD22	7:G:99:LEU:C	2.42	0.44
7:G:150:HIS:O	7:G:154:VAL:CG2	2.52	0.44
9:I:48:PHE:CD2	9:I:48:PHE:O	2.70	0.44
41:I:316:LHG:HC81	41:I:316:LHG:C24	2.28	0.44
12:L:36:ASN:N	12:L:48:LYS:HB2	2.33	0.44
42:L:321:LMG:O2	42:L:321:LMG:HC92	2.17	0.44
14:N:62:PHE:HZ	14:N:74:LEU:HG	1.82	0.44
14:N:146:CYS:HB3	14:N:155:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:P:307:A86:C37	35:P:307:A86:C28	2.96	0.44
36:R:313:CLA:H202	36:R:313:CLA:H162	1.88	0.44
17:S:170:PHE:CZ	17:S:175:HIS:CE1	3.04	0.44
19:W:15:PHE:CD2	34:W:204:DD6:C33	3.00	0.44
19:X:132:THR:HG23	19:X:135:LYS:NZ	2.33	0.44
20:a:365:ILE:HD13	36:a:824:CLA:CGA	2.47	0.44
27:j:39:PHE:O	27:j:40:PRO:C	2.60	0.44
32:U:57:PHE:HD2	36:U:308:CLA:CAD	2.30	0.44
1:A:196:TRP:HB3	36:A:314:CLA:CGD	2.47	0.44
42:D:321:LMG:HC2	42:D:321:LMG:HC71	1.33	0.44
36:I:306:CLA:H8	36:I:306:CLA:H122	1.72	0.44
36:K:310:CLA:CBC	36:K:310:CLA:CHD	2.86	0.44
15:P:34:ASP:HA	15:P:45:LYS:CG	2.42	0.44
36:R:310:CLA:H2A	36:R:310:CLA:HED3	1.98	0.44
17:S:60:LYS:HB2	17:S:61:ASP:H	1.47	0.44
18:T:165:ILE:HG23	18:T:166:ILE:HG13	2.00	0.44
20:a:466:THR:HG21	36:a:832:CLA:HAC2	2.00	0.44
20:a:704:GLU:OE1	21:b:544:LYS:HB2	2.17	0.44
36:a:806:CLA:H102	36:a:808:CLA:H91	1.98	0.44
36:b:834:CLA:H2	36:b:834:CLA:H61	1.76	0.44
23:d:111:ILE:HG12	23:d:121:ILE:HG12	2.00	0.44
41:f:808:LHG:H271	41:f:808:LHG:H241	1.25	0.44
36:j:102:CLA:HBB1	36:j:102:CLA:HMB3	1.99	0.44
28:l:44:LEU:HD23	28:l:44:LEU:HA	1.86	0.44
28:l:126:VAL:O	41:l:208:LHG:HC2	2.18	0.44
32:U:101:SER:O	32:U:109:ALA:HB2	2.18	0.44
32:U:112:TRP:O	32:U:113:MET:SD	2.76	0.44
33:V:143:ILE:CD1	33:V:143:ILE:N	2.73	0.44
2:B:85:THR:CG2	36:B:311:CLA:HED3	2.45	0.44
34:B:304:DD6:C7	36:B:307:CLA:HBB1	2.48	0.44
36:B:309:CLA:CGA	36:B:309:CLA:CHA	2.96	0.44
4:D:165:LYS:CE	19:W:26:GLN:HE22	2.30	0.44
35:D:302:A86:C28	36:D:311:CLA:C4D	2.96	0.44
7:G:82:PHE:HD1	7:G:85:PHE:HE2	1.65	0.44
9:I:84:TRP:CD1	9:I:84:TRP:O	2.71	0.44
36:I:307:CLA:HBC2	36:I:310:CLA:H143	1.99	0.44
35:J:305:A86:C25	36:J:313:CLA:H152	2.48	0.44
35:K:301:A86:C2	36:K:311:CLA:HAB	2.48	0.44
14:N:117:SER:O	14:N:121:GLN:N	2.46	0.44
14:N:216:PHE:HD2	14:N:217:LEU:HD22	1.83	0.44
15:P:77:ALA:HA	34:P:305:DD6:C41	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:125:PHE:CE1	36:P:319:CLA:CHA	3.00	0.44
16:R:76:PHE:HA	16:R:155:TYR:HE2	1.83	0.44
34:W:204:DD6:C19	36:W:209:CLA:C1B	2.95	0.44
19:X:58:ARG:O	36:X:315:CLA:HED1	2.18	0.44
35:X:314:A86:C25	36:V:306:CLA:CHC	2.96	0.44
20:a:375:HIS:ND1	36:a:817:CLA:OBD	2.49	0.44
36:a:810:CLA:H143	36:a:810:CLA:H161	1.81	0.44
44:a:847:BCR:H20C	44:a:847:BCR:H361	1.77	0.44
21:b:493:LEU:HD23	21:b:493:LEU:HA	1.82	0.44
36:b:815:CLA:H112	36:b:820:CLA:H93	1.99	0.44
23:d:104:TRP:CD1	23:d:150:ILE:HD11	2.51	0.44
36:i:102:CLA:H3A	36:i:102:CLA:HBA1	1.54	0.44
35:U:304:A86:C41	36:U:311:CLA:ND	2.81	0.44
36:U:306:CLA:H2A	36:U:306:CLA:O1D	2.18	0.44
33:V:132:LEU:HD13	36:V:310:CLA:CED	2.46	0.44
33:V:163:ALA:HB2	35:V:303:A86:C11	2.48	0.44
1:A:79:HIS:HB3	1:A:185:MET:HE2	2.00	0.43
36:C:209:CLA:H112	36:C:209:CLA:H152	1.71	0.43
36:L:314:CLA:CHB	36:L:314:CLA:H2	2.48	0.43
14:N:102:TRP:CD1	35:N:302:A86:C37	3.01	0.43
17:S:244:PHE:HB3	17:S:248:PHE:HB3	2.00	0.43
18:T:98:LEU:HD22	18:T:103:MET:HE1	2.00	0.43
19:X:59:LEU:HD13	35:V:301:A86:C34	2.48	0.43
20:a:273:GLN:NE2	39:a:853:LMT:H1B	2.32	0.43
20:a:566:LYS:HB2	21:b:675:GLU:OE1	2.19	0.43
20:a:640:ASN:O	20:a:644:SER:HB3	2.17	0.43
36:a:803:CLA:H91	36:a:806:CLA:H171	1.98	0.43
21:b:118:GLY:HA2	46:b:931:HOH:O	2.18	0.43
21:b:412:GLU:CA	25:f:238:ALA:HB1	2.19	0.43
21:b:593:TRP:HB2	36:b:836:CLA:HMC1	1.99	0.43
41:b:850:LHG:H131	41:b:850:LHG:H101	1.59	0.43
24:e:28:VAL:HG22	24:e:38:VAL:HG22	1.99	0.43
41:f:809:LHG:C38	42:V:316:LMG:H321	2.41	0.43
36:l:204:CLA:HBA2	36:l:204:CLA:H3A	1.45	0.43
33:V:59:ASN:ND2	33:V:59:ASN:H	2.15	0.43
1:A:137:ASN:HD22	1:A:142:THR:HB	1.82	0.43
1:A:148:ASP:O	1:A:149:ARG:HB3	2.17	0.43
36:C:206:CLA:H71	36:C:206:CLA:H112	1.73	0.43
5:E:72:ILE:CG2	5:E:76:TRP:CD1	2.95	0.43
36:E:308:CLA:HBC1	7:G:168:PHE:CD2	2.53	0.43
36:E:315:CLA:H143	36:M:307:CLA:H112	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:VAL:HG13	42:V:316:LMG:O9	2.18	0.43
36:I:312:CLA:H61	36:I:312:CLA:H2	1.80	0.43
11:K:177:ALA:O	11:K:181:ASN:ND2	2.51	0.43
14:N:170:PHE:CE2	36:N:318:CLA:H11	2.53	0.43
36:P:313:CLA:H142	36:P:313:CLA:H111	1.81	0.43
36:Q:310:CLA:C9	17:S:55:LEU:HD11	2.48	0.43
16:R:89:MET:CE	16:R:206:ASN:HB3	2.45	0.43
36:R:322:CLA:HED2	36:R:322:CLA:HBD	1.70	0.43
17:S:208:LEU:CD1	35:S:304:A86:C	2.96	0.43
17:S:240:VAL:O	17:S:240:VAL:HG12	2.16	0.43
19:W:117:ARG:HH11	19:X:26:GLN:NE2	2.15	0.43
20:a:368:LEU:O	20:a:372:VAL:HG23	2.17	0.43
36:a:816:CLA:H18	36:a:816:CLA:H151	1.78	0.43
21:b:402:ASN:ND2	21:b:402:ASN:N	2.66	0.43
21:b:561:PRO:HA	21:b:565:GLY:HA2	2.00	0.43
27:j:22:LEU:HD12	27:j:25:LEU:HD13	1.99	0.43
32:U:84:PHE:HE2	36:U:308:CLA:C11	2.31	0.43
34:A:301:DD6:C34	38:A:315:SQD:O2	2.67	0.43
4:D:89:PHE:CD1	4:D:89:PHE:O	2.70	0.43
6:F:98:MET:CE	6:F:214:PHE:CD1	3.00	0.43
6:F:151:ARG:O	6:F:153:MET:N	2.51	0.43
36:G:307:CLA:CHA	40:L:302:DGD:HG11	2.48	0.43
36:H:308:CLA:H111	36:H:308:CLA:H152	1.74	0.43
17:S:208:LEU:HD11	36:S:309:CLA:CMD	2.45	0.43
36:a:801:CLA:H161	36:a:801:CLA:H122	1.79	0.43
36:b:820:CLA:HBA2	36:b:820:CLA:H3A	1.46	0.43
22:c:5:VAL:HG11	22:c:26:LEU:HD21	1.99	0.43
23:d:138:LEU:HD12	23:d:138:LEU:HA	1.81	0.43
32:U:39:ARG:HG2	36:U:311:CLA:C3C	2.49	0.43
33:V:18:LEU:O	33:V:23:GLY:CA	2.67	0.43
33:V:46:VAL:CG2	33:V:164:ILE:HB	2.48	0.43
33:V:154:LEU:HD23	33:V:154:LEU:HA	1.89	0.43
6:F:167:GLY:O	6:F:171:LYS:HG2	2.18	0.43
11:K:93:VAL:HG22	11:K:203:PHE:CZ	2.54	0.43
13:M:174:ALA:HB2	13:M:189:MET:HE2	2.01	0.43
36:N:313:CLA:HBC2	36:N:319:CLA:H3A	1.99	0.43
35:T:301:A86:C22	36:T:309:CLA:HMD1	2.49	0.43
20:a:87:ALA:HB2	20:a:178:MET:HB2	2.01	0.43
20:a:225:ILE:HG13	36:a:813:CLA:C2D	2.48	0.43
21:b:5:PHE:CD1	21:b:5:PHE:O	2.71	0.43
21:b:289:MET:HG3	21:b:298:HIS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:432:THR:OG1	41:j:104:LHG:H381	2.18	0.43
22:c:31:TRP:O	22:c:37:LYS:C	2.62	0.43
25:f:214:VAL:O	25:f:218:ARG:CG	2.67	0.43
32:U:39:ARG:CZ	32:U:103:THR:HG22	2.45	0.43
32:U:126:MET:HE3	32:U:126:MET:HB2	1.65	0.43
2:B:191:LEU:CD2	37:B:310:KC1:CBC	2.96	0.43
36:G:313:CLA:H143	36:G:313:CLA:H111	1.87	0.43
41:I:316:LHG:H151	41:I:316:LHG:H322	2.01	0.43
12:L:213:ALA:HB1	12:L:224:LEU:HD22	2.00	0.43
36:M:315:CLA:HMD3	37:M:318:KC1:OBD	2.18	0.43
15:P:133:ILE:HG23	15:P:137:LYS:NZ	2.33	0.43
15:P:137:LYS:HD3	15:P:137:LYS:HA	1.43	0.43
16:R:66:TRP:CE2	41:R:323:LHG:H241	2.53	0.43
36:T:311:CLA:HHD	36:T:311:CLA:HAC2	1.59	0.43
19:W:116:PHE:HD1	36:W:212:CLA:C2D	2.31	0.43
20:a:586:GLY:HA3	21:b:667:ARG:NH2	2.33	0.43
44:a:846:BCR:H15C	44:a:846:BCR:H351	1.93	0.43
36:a:848:CLA:H41	36:a:848:CLA:H61	1.65	0.43
21:b:198:LEU:HB2	21:b:199:PRO:HD3	1.99	0.43
2:B:210:MET:HE3	39:B:312:LMT:C1'	2.49	0.43
36:C:207:CLA:H111	36:C:207:CLA:H92	1.78	0.43
6:F:166:MET:HE2	6:F:166:MET:HB2	1.75	0.43
36:I:306:CLA:CGA	36:I:306:CLA:C3A	2.95	0.43
11:K:120:LEU:HD22	36:K:310:CLA:HAA2	2.01	0.43
14:N:38:LEU:HD13	14:N:42:ALA:HB2	2.01	0.43
14:N:45:ALA:HB1	14:N:204:ASN:HD21	1.82	0.43
17:S:55:LEU:O	17:S:56:SER:C	2.60	0.43
20:a:348:GLU:CD	20:a:348:GLU:N	2.73	0.43
36:a:830:CLA:HBA1	36:a:830:CLA:H3A	1.42	0.43
24:e:26:VAL:HG11	24:e:41:ARG:HE	1.83	0.43
36:l:201:CLA:H41	36:l:201:CLA:H61	1.62	0.43
33:V:56:LEU:H	33:V:56:LEU:HG	1.58	0.43
33:V:127:LEU:HD23	33:V:127:LEU:HA	1.82	0.43
35:E:307:A86:C9	36:E:315:CLA:C3D	2.96	0.43
36:G:309:CLA:H142	36:G:309:CLA:H111	1.83	0.43
36:I:308:CLA:H18	36:I:308:CLA:H152	1.87	0.43
42:I:315:LMG:H251	36:a:821:CLA:HBB2	2.00	0.43
36:J:310:CLA:H111	36:J:310:CLA:H91	1.78	0.43
34:M:303:DD6:C23	34:M:303:DD6:C19	2.96	0.43
14:N:60:LYS:HB2	15:O:168:ARG:NH2	2.33	0.43
14:N:209:ALA:HB2	35:N:304:A86:C1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:174:ASN:ND2	36:O:306:CLA:O1D	2.45	0.43
15:Q:73:VAL:HG12	34:Q:302:DD6:C12	2.44	0.43
16:R:69:THR:HG23	16:R:71:SER:H	1.84	0.43
34:W:205:DD6:C27	36:W:212:CLA:C1C	2.96	0.43
20:a:179:LEU:HD23	20:a:179:LEU:HA	1.77	0.43
20:a:316:MET:O	20:a:316:MET:HG2	2.19	0.43
20:a:427:ASN:HB3	20:a:430:ASN:OD1	2.19	0.43
21:b:686:LEU:HD23	28:l:64:TYR:HE2	1.84	0.43
25:f:161:THR:HG21	27:j:39:PHE:CE2	2.54	0.43
36:f:802:CLA:H18	44:f:806:BCR:H17C	2.00	0.43
36:j:102:CLA:H8	36:j:102:CLA:H122	1.52	0.43
28:l:139:VAL:O	28:l:139:VAL:HG12	2.17	0.43
30:g:130:UNK:O	30:g:131:UNK:C	2.63	0.43
31:h:121:GLY:H	31:h:122:PRO:HD2	1.80	0.43
33:V:46:VAL:HG11	35:V:303:A86:C8	2.49	0.43
1:A:128:VAL:HG21	41:f:808:LHG:H371	2.01	0.43
42:D:320:LMG:H232	42:D:320:LMG:H262	1.62	0.43
36:E:317:CLA:HBA2	36:E:317:CLA:H3A	1.83	0.43
36:F:314:CLA:H62	36:F:314:CLA:H41	1.79	0.43
39:F:320:LMT:C3'	39:F:321:LMT:O6'	2.67	0.43
36:N:316:CLA:H13	36:N:316:CLA:H171	1.74	0.43
37:Q:313:KC1:NC	41:Q:315:LHG:H291	2.33	0.43
37:W:217:KC1:OBD	36:W:218:CLA:C4D	2.67	0.43
19:X:121:ILE:HA	19:X:123:PHE:CE1	2.53	0.43
20:a:251:ASN:OD1	20:a:251:ASN:N	2.52	0.43
20:a:587:GLY:H	21:b:667:ARG:CD	2.25	0.43
21:b:490:GLN:HB3	21:b:490:GLN:HE21	1.64	0.43
27:j:29:ILE:HD11	36:j:101:CLA:H201	2.00	0.43
36:j:102:CLA:HBA1	36:j:102:CLA:H202	2.01	0.43
1:A:169:GLU:H	1:A:169:GLU:HG2	1.32	0.43
1:A:196:TRP:CE2	36:A:314:CLA:HMD1	2.53	0.43
2:B:191:LEU:HD22	37:B:310:KC1:CBC	2.49	0.43
36:D:313:CLA:HED3	36:D:313:CLA:H2A	2.00	0.43
36:E:312:CLA:HBC3	36:E:314:CLA:H192	2.01	0.43
39:E:323:LMT:O6'	39:E:323:LMT:O5B	2.36	0.43
36:I:308:CLA:H92	36:I:308:CLA:H111	1.61	0.43
36:I:311:CLA:H102	36:I:311:CLA:H61	1.84	0.43
36:J:312:CLA:H202	36:J:312:CLA:H161	1.88	0.43
11:K:95:PRO:HG3	36:K:310:CLA:C3D	2.48	0.43
36:T:308:CLA:H52	36:T:308:CLA:H12	1.81	0.43
19:X:75:ASN:OD1	19:X:76:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:80:SER:OG	20:a:186:TYR:HB2	2.18	0.43
20:a:309:LEU:HD23	20:a:309:LEU:HA	1.75	0.43
20:a:462:ILE:O	20:a:466:THR:HG22	2.19	0.43
20:a:728:GLN:O	20:a:728:GLN:HG3	2.18	0.43
42:a:852:LMG:H182	42:a:852:LMG:H152	1.31	0.43
23:d:205:LYS:HB2	23:d:206:GLN:H	1.51	0.43
36:j:101:CLA:H62	36:j:101:CLA:H41	1.56	0.43
41:G:301:LHG:H311	36:G:311:CLA:H52	2.00	0.43
36:H:308:CLA:H41	38:b:804:SQD:H311	2.01	0.43
36:H:311:CLA:H202	36:H:311:CLA:H161	1.85	0.43
34:I:303:DD6:C21	36:I:308:CLA:HBB1	2.48	0.43
36:I:306:CLA:C15	36:I:306:CLA:H203	2.48	0.43
40:L:302:DGD:HB21	40:L:302:DGD:C1A	2.49	0.43
36:L:314:CLA:H61	36:L:314:CLA:H93	1.79	0.43
15:P:112:TRP:HZ2	15:P:124:TYR:OH	2.01	0.43
15:P:133:ILE:HD12	15:P:151:VAL:HG13	2.00	0.43
19:X:117:ARG:NE	19:X:121:ILE:H	2.16	0.43
35:X:314:A86:C2	33:V:161:MET:SD	3.07	0.43
36:a:801:CLA:CMB	36:a:848:CLA:HMD1	2.49	0.43
36:a:803:CLA:C9	36:a:806:CLA:C17	2.91	0.43
21:b:671:GLN:NE2	21:b:698:ALA:H	2.17	0.43
36:b:829:CLA:H12	44:b:844:BCR:H393	2.01	0.43
36:l:205:CLA:H162	36:l:205:CLA:H193	1.60	0.43
31:h:96:VAL:HG22	39:h:205:LMT:H4B	2.01	0.43
31:h:104:TYR:CD1	31:h:104:TYR:C	2.97	0.43
33:V:31:LEU:HD23	33:V:31:LEU:HA	1.92	0.43
36:A:308:CLA:H111	36:A:308:CLA:H91	1.78	0.42
36:D:308:CLA:H62	36:D:308:CLA:H41	1.80	0.42
41:D:319:LHG:H152	41:D:319:LHG:H122	1.83	0.42
6:F:184:GLU:HG3	36:F:314:CLA:C4B	2.49	0.42
36:F:317:CLA:HBC2	42:J:318:LMG:C34	2.46	0.42
34:Q:302:DD6:C14	36:Q:308:CLA:HBB1	2.49	0.42
16:R:63:THR:HG23	16:R:65:ILE:H	1.75	0.42
16:R:214:ILE:O	16:R:218:LEU:HG	2.19	0.42
34:S:307:DD6:C23	34:S:307:DD6:C19	2.97	0.42
35:T:306:A86:C29	37:T:310:KC1:CAA	2.97	0.42
36:b:820:CLA:H72	36:b:820:CLA:H112	1.79	0.42
36:b:825:CLA:H12	36:b:825:CLA:H52	1.83	0.42
43:b:842:PQN:H292	44:i:103:BCR:C12	2.49	0.42
22:c:35:LYS:HE2	22:c:35:LYS:HB3	1.25	0.42
3:C:124:GLN:NE2	36:C:210:CLA:ND	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:SER:OG	4:D:56:GLY:O	2.35	0.42
36:D:308:CLA:H93	36:D:308:CLA:H61	1.91	0.42
5:E:98:VAL:HG23	5:E:114:CYS:HB2	2.00	0.42
35:K:303:A86:C8	36:K:310:CLA:C9	2.97	0.42
15:O:95:SER:HB3	15:O:98:VAL:HG12	2.00	0.42
15:O:121:ASN:HD22	15:O:121:ASN:HA	1.62	0.42
15:O:150:ILE:HG21	15:O:154:PRO:HA	2.01	0.42
36:O:308:CLA:H141	36:O:308:CLA:H161	1.80	0.42
36:O:316:CLA:HAB	36:O:316:CLA:H102	2.00	0.42
36:O:316:CLA:O2A	36:O:316:CLA:H42	2.18	0.42
15:P:69:LYS:NZ	15:P:131:GLU:OE1	2.52	0.42
15:P:95:SER:HB3	15:P:98:VAL:HG12	2.00	0.42
36:P:310:CLA:H12	36:P:310:CLA:H51	1.73	0.42
15:Q:151:VAL:N	36:Q:314:CLA:O2D	2.47	0.42
19:X:26:GLN:HB3	19:X:28:LYS:HE3	2.00	0.42
20:a:305:ALA:HA	36:a:816:CLA:HMC2	2.00	0.42
20:a:617:TRP:O	20:a:617:TRP:CD1	2.73	0.42
21:b:473:PHE:CE1	39:b:851:LMT:C6'	3.02	0.42
36:b:839:CLA:HAB	43:b:842:PQN:H172	2.01	0.42
25:f:221:LEU:HA	25:f:221:LEU:HD23	1.72	0.42
44:l:203:BCR:H20C	44:l:203:BCR:H361	1.85	0.42
31:h:119:PHE:O	31:h:122:PRO:HD2	2.19	0.42
1:A:140:MET:HB2	25:f:207:PHE:CE1	2.55	0.42
36:A:305:CLA:HBC2	4:D:136:ILE:HG13	2.02	0.42
36:A:306:CLA:H71	37:A:312:KC1:ND	2.34	0.42
36:C:207:CLA:H102	36:C:208:CLA:CMB	2.49	0.42
36:D:309:CLA:HED2	36:D:309:CLA:H2	2.01	0.42
11:K:44:PRO:HB2	11:K:56:LYS:O	2.19	0.42
15:P:155:ILE:H	15:P:155:ILE:HG12	1.33	0.42
15:Q:159:THR:HG21	17:S:60:LYS:HG2	2.01	0.42
36:R:311:CLA:H41	36:R:311:CLA:H62	1.66	0.42
18:T:11:PRO:HB3	36:T:308:CLA:HAB	2.00	0.42
36:a:836:CLA:H161	36:a:836:CLA:H141	1.82	0.42
21:b:635:ASN:CB	21:b:636:PRO:HD2	2.21	0.42
36:b:808:CLA:H3A	36:b:808:CLA:HBA1	1.60	0.42
36:b:831:CLA:HBA2	36:b:831:CLA:H3A	1.50	0.42
44:b:843:BCR:H20C	44:b:843:BCR:H361	1.79	0.42
23:d:104:TRP:CG	23:d:150:ILE:HD11	2.54	0.42
24:e:38:VAL:HG21	24:e:57:LEU:CD2	2.49	0.42
27:j:17:LEU:CD2	42:j:105:LMG:H201	2.49	0.42
33:V:119:TYR:CG	42:V:316:LMG:HC72	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:C:212:CLA:H102	36:C:212:CLA:H13	1.73	0.42
6:F:145:HIS:HB2	36:F:317:CLA:HAA2	2.00	0.42
36:K:310:CLA:HAA1	36:K:310:CLA:CBD	2.50	0.42
14:N:242:GLN:NE2	14:N:244:PHE:O	2.52	0.42
36:O:316:CLA:CHC	36:O:316:CLA:C7	2.85	0.42
36:O:316:CLA:H91	36:O:316:CLA:H111	1.74	0.42
41:O:318:LHG:H172	41:O:318:LHG:H201	1.79	0.42
17:S:102:TRP:O	17:S:103:ALA:HB2	2.17	0.42
36:W:211:CLA:H3A	36:W:215:CLA:CMC	2.49	0.42
21:b:125:THR:CG2	21:b:358:ALA:H	2.33	0.42
21:b:396:ASP:OD1	23:d:201:LYS:HE3	2.20	0.42
21:b:630:LEU:HD22	21:b:723:PHE:HA	2.00	0.42
21:b:633:GLY:HA2	21:b:640:ASN:HD21	1.83	0.42
26:i:16:LEU:CD2	36:l:202:CLA:H193	2.49	0.42
44:l:207:BCR:H20C	44:l:207:BCR:H361	1.81	0.42
32:U:100:LYS:HE2	32:U:100:LYS:HB2	1.74	0.42
2:B:85:THR:O	2:B:89:LYS:N	2.46	0.42
3:C:114:ILE:O	3:C:117:VAL:HG12	2.19	0.42
34:E:306:DD6:C7	36:E:313:CLA:C3C	2.97	0.42
42:E:319:LMG:HC91	42:E:319:LMG:C12	2.50	0.42
39:E:320:LMT:C5B	39:E:320:LMT:H6'	2.28	0.42
6:F:52:LEU:HD13	36:F:309:CLA:H42	2.00	0.42
36:F:317:CLA:HBC3	42:J:318:LMG:H332	2.01	0.42
8:H:171:MET:HE3	36:H:312:CLA:HHB	2.00	0.42
36:I:312:CLA:H11	42:I:315:LMG:H351	2.00	0.42
35:L:301:A86:O5	36:P:313:CLA:H162	2.20	0.42
34:M:303:DD6:C21	36:M:309:CLA:C3B	2.97	0.42
35:Q:316:A86:C37	17:S:62:PHE:CE2	3.03	0.42
16:R:65:ILE:HD12	16:R:73:THR:CG2	2.07	0.42
17:S:55:LEU:HA	17:S:55:LEU:HD23	1.76	0.42
17:S:210:MET:O	17:S:214:PHE:HD2	1.96	0.42
19:W:120:ALA:O	37:W:217:KC1:CED	2.67	0.42
19:X:129:ASP:O	19:X:131:GLU:N	2.52	0.42
35:X:314:A86:C24	36:V:306:CLA:CAB	2.97	0.42
20:a:217:SER:HB2	36:a:813:CLA:HAB	2.01	0.42
20:a:603:TRP:O	20:a:604:MET:C	2.63	0.42
44:a:845:BCR:H15C	44:a:845:BCR:H351	1.89	0.42
41:i:104:LHG:H271	29:m:25:ALA:HB3	1.95	0.42
28:l:79:LEU:HD21	44:l:207:BCR:H331	2.02	0.42
32:U:16:PHE:CD1	32:U:16:PHE:C	2.97	0.42
32:U:34:GLU:CD	36:U:306:CLA:C1B	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:U:310:CLA:H142	36:U:310:CLA:H111	1.92	0.42
33:V:111:THR:O	33:V:125:PRO:HG2	2.20	0.42
34:A:301:DD6:C7	36:A:313:CLA:CBC	2.98	0.42
36:C:212:CLA:H41	36:C:212:CLA:H62	1.57	0.42
42:E:318:LMG:H181	42:E:318:LMG:H152	1.36	0.42
42:E:318:LMG:H381	36:a:819:CLA:CHC	2.49	0.42
6:F:145:HIS:CB	36:F:317:CLA:HAA1	2.48	0.42
35:F:301:A86:C24	36:F:316:CLA:C4D	2.98	0.42
7:G:173:THR:O	7:G:176:VAL:HG23	2.19	0.42
8:H:83:MET:HE1	34:H:303:DD6:C28	2.49	0.42
34:H:303:DD6:C22	34:H:303:DD6:C19	2.97	0.42
36:I:308:CLA:H193	36:I:308:CLA:C15	2.49	0.42
12:L:115:TRP:CZ2	39:L:318:LMT:H21	2.54	0.42
15:O:133:ILE:HD12	15:O:151:VAL:HG13	2.02	0.42
15:P:126:THR:HG22	36:P:318:CLA:H3A	2.00	0.42
15:Q:152:PHE:HE1	36:Q:314:CLA:CBB	2.33	0.42
36:W:212:CLA:H141	36:W:212:CLA:H162	1.83	0.42
36:a:804:CLA:H72	44:a:845:BCR:HC8	2.01	0.42
36:a:806:CLA:H193	42:j:105:LMG:H232	2.00	0.42
24:e:26:VAL:CG2	24:e:41:ARG:HG3	2.48	0.42
36:f:804:CLA:H141	36:j:101:CLA:CBC	2.50	0.42
28:l:86:ILE:HA	28:l:109:THR:HG21	2.02	0.42
32:U:52:LYS:HE3	32:U:65:ASP:CG	2.44	0.42
33:V:39:GLY:O	33:V:43:MET:HG3	2.18	0.42
36:V:314:CLA:HBD	36:V:314:CLA:CBA	2.49	0.42
34:B:304:DD6:C41	34:B:304:DD6:C35	2.97	0.42
3:C:40:LEU:HD21	36:C:205:CLA:HBC3	2.01	0.42
4:D:73:GLU:OE2	4:D:153:PRO:O	2.36	0.42
36:H:308:CLA:HBC1	39:b:848:LMT:H123	2.02	0.42
42:J:318:LMG:H231	42:J:318:LMG:H262	1.22	0.42
11:K:162:GLY:O	12:L:64:ALA:HB2	2.20	0.42
39:L:318:LMT:H6'	39:L:318:LMT:H2O1	1.66	0.42
13:M:167:GLU:HA	13:M:170:HIS:HD2	1.84	0.42
14:N:80:LYS:NZ	36:N:312:CLA:O1D	2.37	0.42
15:Q:56:SER:OG	15:Q:57:GLU:N	2.53	0.42
19:X:92:LEU:O	19:X:96:GLY:N	2.51	0.42
20:a:200:GLU:HB3	20:a:317:TYR:HB3	2.00	0.42
21:b:198:LEU:N	21:b:199:PRO:CD	2.82	0.42
21:b:671:GLN:NE2	21:b:671:GLN:HA	2.34	0.42
36:f:804:CLA:HHC	36:f:804:CLA:HBB1	2.02	0.42
32:U:52:LYS:CE	32:U:65:ASP:OD2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:8:VAL:CG2	36:V:305:CLA:CBB	2.85	0.42
36:V:305:CLA:H72	36:V:305:CLA:H111	1.63	0.42
36:A:306:CLA:HBA2	36:A:306:CLA:CHA	2.50	0.42
4:D:204:PHE:HA	4:D:206:TYR:CZ	2.54	0.42
7:G:199:PHE:CD2	36:G:313:CLA:O2A	2.72	0.42
36:K:310:CLA:H141	42:L:321:LMG:H172	2.01	0.42
13:M:101:VAL:HG22	13:M:216:ILE:HG12	2.01	0.42
35:M:304:A86:C24	36:M:312:CLA:HMC2	2.50	0.42
15:Q:95:SER:HB3	15:Q:98:VAL:HG12	2.00	0.42
36:T:311:CLA:H91	36:T:311:CLA:H111	1.83	0.42
36:T:311:CLA:H141	36:T:311:CLA:H162	1.90	0.42
36:a:827:CLA:H13	36:a:829:CLA:H203	2.01	0.42
21:b:71:GLN:NE2	21:b:90:SER:OG	2.52	0.42
36:f:804:CLA:H62	41:j:104:LHG:H223	2.01	0.42
44:h:201:BCR:H24C	44:h:201:BCR:H371	1.90	0.42
32:U:41:ALA:HB1	32:U:138:MET:HA	2.01	0.42
32:U:132:LYS:HB3	36:U:305:CLA:HMD2	2.00	0.42
33:V:37:LYS:HE2	36:V:310:CLA:C3D	2.50	0.42
33:V:42:ALA:CB	33:V:161:MET:HG3	2.50	0.42
33:V:119:TYR:CD2	42:V:316:LMG:HC1	2.54	0.42
34:A:301:DD6:C6	36:A:313:CLA:CBC	2.98	0.42
2:B:100:PRO:HA	2:B:119:THR:HA	2.02	0.42
5:E:166:PRO:HB3	42:E:319:LMG:H111	2.02	0.42
41:E:322:LHG:H341	41:E:322:LHG:H371	1.89	0.42
36:K:307:CLA:H41	36:K:307:CLA:H61	1.39	0.42
14:N:84:ILE:O	14:N:88:ALA:N	2.52	0.42
14:N:168:THR:OG1	14:N:169:LEU:HD21	2.20	0.42
14:N:240:VAL:O	14:N:241:MET:HE2	2.19	0.42
15:P:125:PHE:CD1	36:P:319:CLA:C1A	3.02	0.42
15:Q:150:ILE:CD1	36:Q:314:CLA:CMD	2.98	0.42
17:S:86:MET:HE2	36:S:315:CLA:HMC3	2.01	0.42
18:T:28:ARG:O	18:T:28:ARG:HD2	2.20	0.42
19:W:34:TYR:CE1	19:W:113:VAL:HA	2.55	0.42
20:a:368:LEU:HD23	20:a:368:LEU:HA	1.93	0.42
36:a:822:CLA:CAB	36:a:841:CLA:HBB1	2.49	0.42
44:a:845:BCR:H20C	44:a:845:BCR:H361	1.80	0.42
23:d:200:VAL:O	23:d:203:THR:OG1	2.26	0.42
23:d:201:LYS:HG3	23:d:201:LYS:HZ2	1.60	0.42
25:f:176:VAL:HG21	25:f:206:LEU:O	2.19	0.42
41:i:104:LHG:HC82	41:l:208:LHG:C18	2.48	0.42
32:U:49:VAL:C	32:U:51:PRO:HD2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:116:LYS:CB	36:V:314:CLA:CGD	2.93	0.42
33:V:149:ARG:CG	33:V:149:ARG:NH1	2.82	0.42
2:B:201:PHE:HE2	36:B:305:CLA:H171	1.85	0.42
3:C:35:GLU:O	3:C:35:GLU:HG2	2.20	0.42
4:D:133:PHE:HD2	35:D:302:A86:C22	2.33	0.42
5:E:84:HIS:CE1	36:E:313:CLA:HMD1	2.55	0.42
9:I:118:PHE:HD1	36:I:309:CLA:CBC	2.26	0.42
35:I:301:A86:O	36:I:305:CLA:HAC1	2.20	0.42
16:R:224:GLU:OE2	16:R:236:HIS:ND1	2.52	0.42
36:S:312:CLA:H62	36:S:321:CLA:HBB1	2.01	0.42
36:W:206:CLA:H41	36:W:206:CLA:H62	1.73	0.42
19:X:44:MET:HE3	36:X:310:CLA:HBB1	2.01	0.42
19:X:59:LEU:C	36:X:315:CLA:HED1	2.45	0.42
20:a:240:GLN:CD	20:a:240:GLN:N	2.77	0.42
20:a:462:ILE:O	20:a:466:THR:HG23	2.19	0.42
36:a:815:CLA:HHC	36:a:815:CLA:HBB1	2.00	0.42
21:b:352:TYR:CD1	21:b:352:TYR:C	2.97	0.42
27:j:19:PHE:CZ	36:j:102:CLA:H93	2.40	0.42
42:j:105:LMG:H192	42:j:105:LMG:H222	1.27	0.42
44:m:101:BCR:H15C	44:m:101:BCR:H351	1.81	0.42
36:U:311:CLA:H12	36:U:311:CLA:H51	1.57	0.42
1:A:134:ASN:HD21	1:A:138:VAL:HA	1.84	0.41
4:D:120:GLN:NE2	36:D:311:CLA:O2D	2.49	0.41
4:D:202:GLY:HA3	4:D:203:PRO:HD2	1.83	0.41
36:D:309:CLA:HBC3	36:D:312:CLA:H143	2.02	0.41
5:E:165:ASP:OD2	5:E:169:TYR:O	2.38	0.41
39:I:317:LMT:H4O1	39:I:317:LMT:H6D	1.83	0.41
34:K:305:DD6:C23	34:K:305:DD6:C19	2.98	0.41
12:L:115:TRP:HA	39:L:318:LMT:O3'	2.20	0.41
39:L:318:LMT:H3B	39:L:318:LMT:H4'	2.02	0.41
36:O:311:CLA:HAA2	37:O:315:KC1:CHC	2.50	0.41
15:P:135:GLU:OE1	15:P:140:HIS:CE1	2.57	0.41
15:Q:108:PRO:O	34:Q:302:DD6:O2	2.38	0.41
15:Q:150:ILE:CD1	36:Q:314:CLA:C2D	2.97	0.41
15:Q:155:ILE:HG22	15:Q:156:ASP:H	1.85	0.41
36:S:311:CLA:HBA1	36:S:311:CLA:H3A	1.85	0.41
19:W:46:ALA:HB2	34:W:204:DD6:C14	2.49	0.41
21:b:222:LYS:N	21:b:223:PRO:HD3	2.34	0.41
21:b:545:LEU:HD23	24:e:47:TYR:HD2	1.85	0.41
44:i:101:BCR:H24C	44:i:101:BCR:H371	1.84	0.41
31:h:83:CYS:HB3	31:h:124:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:41:ALA:CB	32:U:138:MET:HG3	2.50	0.41
36:A:305:CLA:HED3	38:A:315:SQD:O9	2.18	0.41
2:B:115:LYS:HE2	21:b:98:GLU:CG	2.17	0.41
36:C:208:CLA:H143	36:C:208:CLA:H111	1.95	0.41
5:E:86:ARG:HG2	36:E:314:CLA:C3C	2.49	0.41
36:F:313:CLA:H11	41:b:850:LHG:H132	2.02	0.41
7:G:41:MET:C	7:G:42:VAL:HG23	2.45	0.41
7:G:192:PHE:O	7:G:194:LEU:N	2.47	0.41
36:I:305:CLA:H42	39:I:318:LMT:O1'	2.20	0.41
10:J:93:ARG:NH2	10:J:104:ILE:HG22	2.35	0.41
10:J:180:MET:HB3	34:J:304:DD6:C	2.49	0.41
36:M:307:CLA:H141	36:M:307:CLA:H161	1.85	0.41
15:P:112:TRP:CZ2	15:P:120:LYS:HE2	2.56	0.41
37:Q:313:KC1:C4C	41:Q:315:LHG:H291	2.50	0.41
16:R:95:TYR:HD2	16:R:217:PHE:CE2	2.37	0.41
36:R:310:CLA:H41	36:R:310:CLA:H61	1.67	0.41
17:S:211:LEU:HA	17:S:214:PHE:HD2	1.85	0.41
20:a:126:ILE:HG12	27:j:27:ILE:HG23	2.02	0.41
36:a:824:CLA:HBA1	36:a:828:CLA:H202	2.02	0.41
44:a:844:BCR:H361	44:a:844:BCR:H20C	1.80	0.41
44:b:844:BCR:H15C	44:b:844:BCR:H351	1.93	0.41
39:b:851:LMT:C1'	36:f:805:CLA:CBC	2.98	0.41
23:d:156:ARG:HB3	23:d:164:GLN:HB2	2.02	0.41
36:f:802:CLA:HHC	36:f:802:CLA:HBB1	2.02	0.41
28:l:132:LYS:H	28:l:132:LYS:HG2	1.46	0.41
33:V:65:GLU:O	33:V:74:LYS:HA	2.20	0.41
33:V:69:ILE:O	33:V:70:ARG:HD3	2.20	0.41
1:A:125:TRP:HB3	36:A:309:CLA:HBC2	2.01	0.41
36:A:306:CLA:H62	36:A:306:CLA:H41	1.43	0.41
39:B:313:LMT:O3'	39:B:313:LMT:H1B	2.21	0.41
3:C:107:ASN:ND2	3:C:116:THR:CB	2.78	0.41
36:C:208:CLA:H41	36:C:208:CLA:H62	1.66	0.41
36:F:309:CLA:H93	36:F:309:CLA:H111	1.93	0.41
8:H:137:TRP:HE1	36:H:318:CLA:HAA1	1.84	0.41
11:K:86:MET:HE2	11:K:182:GLY:CA	2.51	0.41
11:K:88:ALA:HB1	34:K:304:DD6:C40	2.50	0.41
12:L:196:LEU:HA	12:L:199:LYS:HB2	2.02	0.41
35:N:305:A86:C5	36:N:316:CLA:CBB	2.98	0.41
17:S:239:GLN:HG3	17:S:242:GLN:HB2	2.02	0.41
36:W:207:CLA:H161	36:W:207:CLA:H141	1.83	0.41
19:X:87:GLY:HA3	36:X:309:CLA:HMA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:55:TRP:CB	20:a:728:GLN:HE22	2.33	0.41
20:a:627:VAL:HG12	20:a:633:ILE:HA	2.02	0.41
21:b:195:HIS:CD2	36:b:816:CLA:HBC1	2.55	0.41
21:b:219:ALA:CB	21:b:223:PRO:HG2	2.51	0.41
21:b:593:TRP:CE3	21:b:593:TRP:C	2.98	0.41
36:b:812:CLA:H91	36:b:840:CLA:H11	2.01	0.41
36:j:101:CLA:C6	42:j:105:LMG:H361	2.44	0.41
28:l:102:LEU:HD23	28:l:102:LEU:HA	1.86	0.41
44:l:207:BCR:H15C	44:l:207:BCR:H351	1.85	0.41
33:V:90:ILE:HD11	36:V:308:CLA:H3A	2.01	0.41
33:V:158:ARG:NE	36:V:306:CLA:CHD	2.57	0.41
1:A:97:THR:HG23	36:A:308:CLA:HED3	2.02	0.41
2:B:209:PRO:CB	39:B:312:LMT:H2O1	2.33	0.41
36:C:207:CLA:CGA	36:C:207:CLA:C3A	2.99	0.41
5:E:119:PHE:CE1	5:E:130:ILE:HD11	2.55	0.41
37:F:308:KC1:C2B	39:F:320:LMT:O2'	2.68	0.41
7:G:211:MET:HB3	36:G:313:CLA:HMA2	2.01	0.41
9:I:129:ALA:HA	9:I:132:ILE:HD12	2.03	0.41
10:J:186:ILE:HD11	35:J:305:A86:C14	2.49	0.41
11:K:122:GLU:HB3	36:K:311:CLA:HED2	2.02	0.41
36:L:311:CLA:H62	36:L:311:CLA:H92	1.86	0.41
14:N:225:SER:HB2	14:N:229:LEU:HB3	2.01	0.41
36:O:309:CLA:H192	36:O:309:CLA:H162	1.90	0.41
36:O:311:CLA:H92	36:O:311:CLA:H61	1.81	0.41
36:P:301:CLA:H93	36:P:301:CLA:H62	1.88	0.41
16:R:74:ILE:O	16:R:78:ARG:HG3	2.20	0.41
16:R:215:MET:HE3	35:R:303:A86:C5	2.50	0.41
19:X:41:ARG:HH22	19:X:114:GLY:HA3	1.85	0.41
19:X:127:THR:CG2	33:V:9:PHE:HE1	2.34	0.41
20:a:589:CYS:HB2	21:b:666:TRP:HB3	2.02	0.41
21:b:398:ASP:HA	21:b:399:PRO:HD2	1.88	0.41
21:b:531:LEU:O	21:b:531:LEU:HD22	2.20	0.41
23:d:123:ARG:O	23:d:127:ASN:ND2	2.50	0.41
23:d:151[A]:LYS:CA	23:d:152:TYR:N	2.83	0.41
32:U:32:ALA:HB1	39:U:314:LMT:O3B	2.08	0.41
1:A:193:HIS:CD2	36:A:314:CLA:HMA3	2.53	0.41
39:B:313:LMT:H31	28:l:121:THR:CG2	2.30	0.41
40:C:215:DGD:O2D	40:C:215:DGD:HB21	2.21	0.41
41:G:321:LHG:H241	41:G:321:LHG:C7	2.50	0.41
36:I:306:CLA:H141	36:I:306:CLA:H161	1.74	0.41
35:J:301:A86:C41	36:J:311:CLA:CMA	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:L:317:KC1:O1A	41:Q:315:LHG:O8	2.38	0.41
34:O:304:DD6:C22	34:O:304:DD6:C13	2.98	0.41
36:P:316:CLA:HMB1	15:Q:125:PHE:HE2	1.85	0.41
36:Q:306:CLA:H62	36:Q:306:CLA:H41	1.92	0.41
37:T:310:KC1:C3D	36:T:313:CLA:OBD	2.69	0.41
20:a:124:TRP:NE1	39:a:851:LMT:H6E	2.28	0.41
20:a:430:ASN:ND2	20:a:430:ASN:C	2.78	0.41
36:a:811:CLA:H61	36:a:811:CLA:H41	1.76	0.41
36:a:821:CLA:HBA2	36:a:821:CLA:H3A	1.67	0.41
36:a:836:CLA:H43	39:a:854:LMT:H123	2.02	0.41
21:b:75:GLU:HG3	21:b:131:ASN:ND2	2.35	0.41
21:b:404:ASN:HD22	21:b:404:ASN:HA	1.68	0.41
21:b:618:TRP:O	21:b:622:TYR:HB3	2.21	0.41
21:b:694:ASP:OD2	26:i:30:GLU:OE2	2.38	0.41
38:b:804:SQD:H111	38:b:804:SQD:H81	1.74	0.41
36:f:802:CLA:H2	36:f:802:CLA:H62	1.69	0.41
36:f:804:CLA:HHC	36:f:804:CLA:CBB	2.51	0.41
41:f:808:LHG:H301	42:V:316:LMG:H312	2.03	0.41
27:j:41:PHE:O	27:j:41:PHE:CG	2.70	0.41
28:l:100:ILE:HG23	28:l:103:PHE:HB2	2.01	0.41
1:A:155:GLY:C	33:V:123:VAL:HG21	2.45	0.41
1:A:160:GLY:C	1:A:163:VAL:CG1	2.93	0.41
38:A:315:SQD:O49	38:A:315:SQD:H441	2.19	0.41
2:B:197:ILE:HD13	36:B:305:CLA:H151	2.03	0.41
3:C:40:LEU:HD21	36:C:205:CLA:C2C	2.49	0.41
5:E:42:PHE:HE2	7:G:176:VAL:HG21	1.85	0.41
41:I:316:LHG:O1	41:I:316:LHG:P	2.79	0.41
39:L:318:LMT:O6B	39:L:318:LMT:H1B	2.19	0.41
15:O:77:ALA:HA	34:O:304:DD6:C22	2.50	0.41
17:S:73:PHE:HA	17:S:155:TYR:CE2	2.55	0.41
17:S:80:LYS:HD2	36:S:314:CLA:C3D	2.50	0.41
20:a:615:PHE:CD1	20:a:615:PHE:C	2.98	0.41
36:b:817:CLA:CMB	36:b:817:CLA:HBB1	2.51	0.41
36:b:825:CLA:H92	36:b:825:CLA:H61	1.83	0.41
32:U:10:GLU:HB2	32:U:132:LYS:HE3	1.36	0.41
33:V:18:LEU:N	33:V:18:LEU:CD2	2.77	0.41
2:B:191:LEU:HD21	35:B:303:A86:C5	2.50	0.41
2:B:209:PRO:HA	39:B:312:LMT:C3'	2.48	0.41
36:D:313:CLA:H12	36:D:313:CLA:H52	1.81	0.41
6:F:39:PHE:CE1	6:F:46:PRO:HA	2.55	0.41
36:I:308:CLA:O1D	36:I:308:CLA:H2A	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:196:ALA:HB2	11:K:205:TYR:HE1	1.86	0.41
12:L:163:GLN:HB2	12:L:174:TYR:HE1	1.85	0.41
15:Q:94:LEU:H	15:Q:99:SER:HA	1.86	0.41
15:Q:174:ASN:ND2	36:Q:305:CLA:O1D	2.45	0.41
34:Q:302:DD6:C22	36:Q:308:CLA:HBB1	2.50	0.41
18:T:65:PHE:HD2	36:T:312:CLA:HAA1	1.85	0.41
20:a:85:GLN:HG2	36:a:804:CLA:H3A	2.02	0.41
20:a:103:PHE:CE1	36:a:806:CLA:HED2	2.56	0.41
20:a:225:ILE:CG1	36:a:813:CLA:CMD	2.98	0.41
21:b:82:LEU:HD23	21:b:82:LEU:HA	1.87	0.41
36:b:824:CLA:H41	36:b:824:CLA:H62	1.72	0.41
36:i:102:CLA:H18	36:l:202:CLA:H13	2.02	0.41
44:h:201:BCR:H20C	44:h:201:BCR:H361	1.84	0.41
36:V:306:CLA:H161	36:V:306:CLA:H141	1.85	0.41
2:B:184:ALA:CB	36:B:309:CLA:HMB1	2.51	0.41
4:D:90:VAL:O	4:D:91:ALA:C	2.63	0.41
36:E:311:CLA:H142	36:E:311:CLA:H112	1.89	0.41
36:F:313:CLA:C6	41:b:850:LHG:H151	2.51	0.41
42:G:325:LMG:O10	42:G:325:LMG:H311	2.21	0.41
11:K:47:ILE:HD11	11:K:180:LYS:NZ	2.36	0.41
37:L:317:KC1:CAA	41:Q:315:LHG:H242	2.50	0.41
15:P:48:PRO:HA	37:Q:313:KC1:CED	2.51	0.41
36:R:321:CLA:H3A	36:R:321:CLA:HBA2	1.88	0.41
17:S:167:PHE:CD2	17:S:179:ASP:HA	2.56	0.41
17:S:242:GLN:NE2	17:S:244:PHE:O	2.51	0.41
20:a:453:LEU:HD21	36:a:836:CLA:HMB2	2.02	0.41
21:b:222:LYS:H	21:b:223:PRO:HD3	1.85	0.41
36:b:836:CLA:H52	36:b:836:CLA:H11	1.84	0.41
22:c:61:ASP:HA	22:c:62:PHE:HA	1.91	0.41
26:i:5:LEU:HB3	26:i:9:PHE:HE2	1.85	0.41
31:h:111:LYS:O	31:h:115:VAL:HG23	2.21	0.41
36:U:310:CLA:H72	36:U:310:CLA:H112	1.89	0.41
39:U:315:LMT:H2B	39:U:315:LMT:C6B	2.50	0.41
2:B:112:ILE:HD11	2:B:118:ILE:HG22	2.01	0.41
4:D:177:LEU:C	4:D:177:LEU:CD2	2.94	0.41
36:D:308:CLA:H202	36:D:308:CLA:H162	1.91	0.41
36:E:316:CLA:H202	36:E:316:CLA:H162	1.92	0.41
7:G:103:ARG:NH1	7:G:106:GLU:OE1	2.54	0.41
36:G:315:CLA:HAA1	36:G:315:CLA:CBD	2.51	0.41
8:H:121:SER:HB2	36:H:310:CLA:OBD	2.21	0.41
8:H:124:ASN:O	8:H:124:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:H:308:CLA:C4	38:b:804:SQD:H282	2.51	0.41
9:I:92:HIS:HE1	9:I:99:LEU:CD1	2.34	0.41
35:I:302:A86:C3	36:I:308:CLA:H42	2.46	0.41
11:K:160:PRO:HB3	42:L:321:LMG:O7	2.21	0.41
36:M:309:CLA:H93	36:M:309:CLA:H111	1.89	0.41
15:P:68:LEU:CD1	15:P:147:LEU:HD23	2.51	0.41
15:P:134:THR:HG23	15:P:148:PRO:HG3	2.03	0.41
15:P:136:CYS:SG	39:P:321:LMT:H21	2.61	0.41
15:Q:106:MET:HB3	15:Q:106:MET:HE3	1.65	0.41
16:R:221:GLN:NE2	16:R:235:PRO:O	2.54	0.41
16:R:223:VAL:HB	16:R:226:SER:HB3	2.02	0.41
36:R:310:CLA:H112	36:R:310:CLA:H71	1.81	0.41
18:T:33:ARG:NH1	18:T:140:LEU:HD11	2.35	0.41
36:T:309:CLA:H192	36:T:309:CLA:H161	1.85	0.41
34:W:204:DD6:C19	36:W:209:CLA:C2B	2.99	0.41
37:W:217:KC1:CMA	35:X:305:A86:C29	2.99	0.41
20:a:133:ASN:HB3	20:a:141:GLN:HB3	2.02	0.41
20:a:361:ASN:ND2	36:a:804:CLA:OBD	2.48	0.41
20:a:614:HIS:CD2	20:a:614:HIS:O	2.73	0.41
36:a:816:CLA:C5	36:a:816:CLA:C9	2.86	0.41
36:b:809:CLA:H111	36:b:809:CLA:H71	1.89	0.41
36:b:833:CLA:H111	25:f:169:ILE:HD11	2.02	0.41
43:b:842:PQN:H262	43:b:842:PQN:H243	1.67	0.41
23:d:143:ARG:HH21	23:d:143:ARG:CB	2.34	0.41
25:f:105:LEU:HD13	25:f:118:ILE:HB	2.03	0.41
25:f:218:ARG:HH21	41:f:808:LHG:HC2	1.85	0.41
36:f:804:CLA:HBA1	36:f:804:CLA:H3A	1.85	0.41
28:l:54:THR:CG2	36:l:205:CLA:H191	2.51	0.41
44:l:207:BCR:H24C	44:l:207:BCR:H371	1.81	0.41
32:U:112:TRP:C	32:U:113:MET:HG2	2.46	0.41
36:U:311:CLA:H162	36:U:311:CLA:H141	1.86	0.41
33:V:38:HIS:ND1	36:V:306:CLA:HBB2	2.35	0.41
33:V:142:ASN:N	33:V:142:ASN:HD22	2.19	0.41
1:A:49:THR:HB	36:A:307:CLA:HED1	2.02	0.41
36:A:309:CLA:CBB	42:V:315:LMG:C15	2.86	0.41
3:C:67:ILE:HD13	36:b:813:CLA:HAA2	2.02	0.41
7:G:216:ILE:CG2	7:G:217:ALA:N	2.83	0.41
36:I:306:CLA:C9	36:I:307:CLA:HMB3	2.51	0.41
36:L:308:CLA:HBA2	36:L:308:CLA:H3A	1.70	0.41
36:M:311:CLA:H11	36:M:311:CLA:H52	1.93	0.41
14:N:143:TRP:HE1	14:N:167:PHE:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:69:LYS:NZ	15:Q:131:GLU:OE1	2.52	0.41
15:Q:152:PHE:CE2	36:Q:314:CLA:HMC3	2.56	0.41
16:R:132:ALA:HB3	36:R:314:CLA:HED2	2.03	0.41
19:X:91:LEU:HA	19:X:91:LEU:HD23	1.86	0.41
20:a:231:LYS:HD3	20:a:258:LEU:HD22	2.03	0.41
20:a:441:GLU:OE2	36:a:830:CLA:HMA3	2.21	0.41
20:a:652:LEU:HD22	20:a:652:LEU:O	2.20	0.41
36:a:823:CLA:H61	36:a:823:CLA:H41	1.85	0.41
21:b:110:TYR:CB	21:b:111:PRO:CD	2.99	0.41
44:i:103:BCR:H15C	44:i:103:BCR:H351	1.85	0.41
32:U:48:TYR:OH	32:U:67:ILE:HG13	2.21	0.41
32:U:74:ASP:OD1	32:U:74:ASP:N	2.52	0.41
32:U:95:MET:HE1	32:U:98:GLU:CD	2.46	0.41
1:A:73:ARG:HA	1:A:73:ARG:HD3	1.78	0.40
41:D:319:LHG:C22	42:D:320:LMG:C23	2.99	0.40
37:F:308:KC1:CBB	39:F:320:LMT:H52	2.51	0.40
37:F:308:KC1:O1A	39:F:321:LMT:C3'	2.67	0.40
35:G:305:A86:C21	36:G:309:CLA:HBC2	2.51	0.40
42:G:325:LMG:H422	42:G:325:LMG:H453	1.73	0.40
8:H:57:ASP:OD1	36:H:307:CLA:HBA2	2.22	0.40
8:H:129:ILE:HD13	8:H:129:ILE:HG21	1.84	0.40
36:J:308:CLA:H51	36:J:309:CLA:H3A	2.03	0.40
36:J:312:CLA:H142	36:J:312:CLA:H111	1.94	0.40
42:J:319:LMG:C11	42:J:319:LMG:H161	2.51	0.40
36:K:310:CLA:H102	36:K:310:CLA:H13	1.94	0.40
36:K:316:CLA:H72	36:K:316:CLA:H112	1.85	0.40
39:K:317:LMT:H5'	39:K:317:LMT:O5B	2.19	0.40
14:N:100:PHE:CZ	36:N:310:CLA:HMD2	2.56	0.40
35:N:301:A86:C5	36:N:308:CLA:H202	2.51	0.40
15:O:122:GLN:NE2	41:O:318:LHG:O10	2.53	0.40
15:Q:107:LYS:HG3	15:Q:110:ASP:H	1.86	0.40
35:Q:316:A86:C5	36:S:311:CLA:HBB1	2.51	0.40
19:W:25:ASP:CG	19:W:27:GLU:H	2.27	0.40
19:X:148:GLN:HE22	36:X:307:CLA:HED3	1.85	0.40
20:a:97:HIS:CD2	20:a:167:ILE:HG21	2.57	0.40
25:f:206:LEU:HD22	36:f:804:CLA:OBD	2.21	0.40
32:U:49:VAL:HG22	32:U:53:TRP:CE2	2.56	0.40
32:U:95:MET:HE3	32:U:95:MET:O	2.21	0.40
32:U:116:TYR:HB2	36:U:311:CLA:HBA1	2.03	0.40
33:V:142:ASN:N	33:V:142:ASN:ND2	2.68	0.40
33:V:144:LYS:HA	33:V:144:LYS:CE	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:GLY:O	2:B:199:LEU:N	2.54	0.40
3:C:43:LEU:HD11	8:H:138:ILE:HD11	2.03	0.40
3:C:152:THR:HG23	36:C:212:CLA:HBA2	2.03	0.40
36:C:205:CLA:HED3	40:C:215:DGD:HD5	1.98	0.40
34:D:304:DD6:C13	34:D:304:DD6:C21	2.99	0.40
42:D:321:LMG:H341	42:D:321:LMG:H312	1.78	0.40
5:E:43:MET:HB3	7:G:176:VAL:HG13	2.03	0.40
34:E:306:DD6:C7	36:E:313:CLA:C2C	2.98	0.40
41:F:319:LHG:HC91	42:J:319:LMG:H162	2.03	0.40
36:G:313:CLA:H43	36:P:301:CLA:H42	2.02	0.40
36:H:314:CLA:HBC1	36:H:316:CLA:HAB	2.03	0.40
9:I:191:GLN:HE22	36:I:313:CLA:HED2	1.87	0.40
36:I:306:CLA:H93	36:I:307:CLA:HMB3	2.01	0.40
36:J:310:CLA:H202	36:J:310:CLA:H162	1.93	0.40
13:M:188:ASN:OD1	13:M:189:MET:N	2.47	0.40
15:P:36:MET:CB	15:P:37:PRO:HD2	2.52	0.40
15:P:197:PRO:HD2	36:P:316:CLA:HMB2	2.04	0.40
17:S:73:PHE:HA	17:S:155:TYR:HE2	1.86	0.40
17:S:89:PHE:CE1	17:S:216:PHE:CE2	3.09	0.40
34:W:205:DD6:C25	36:W:212:CLA:HMC3	2.45	0.40
19:X:59:LEU:HD22	35:V:301:A86:C41	2.48	0.40
20:a:203:MET:CG	20:a:327:MET:HE1	2.44	0.40
36:a:806:CLA:H193	36:a:806:CLA:H161	1.79	0.40
36:a:841:CLA:H61	36:a:841:CLA:H2	1.85	0.40
21:b:54:LEU:HD12	21:b:54:LEU:HA	1.77	0.40
21:b:191:GLY:O	21:b:195:HIS:CD2	2.72	0.40
36:b:833:CLA:H61	36:b:833:CLA:H41	1.65	0.40
36:b:836:CLA:H41	36:b:836:CLA:H62	1.73	0.40
23:d:162:GLU:N	23:d:162:GLU:CD	2.73	0.40
32:U:25:ILE:HG12	36:U:307:CLA:C1	2.49	0.40
33:V:6:GLU:HA	33:V:7:PRO:HD3	1.90	0.40
1:A:154:LEU:O	33:V:122:SER:HB2	2.21	0.40
41:D:319:LHG:H311	20:a:176:ALA:HB1	2.02	0.40
7:G:156:GLN:HE22	7:G:158:SER:CA	2.34	0.40
7:G:199:PHE:CD2	36:G:313:CLA:C1	3.03	0.40
8:H:180:ARG:HD3	36:H:307:CLA:C4C	2.51	0.40
10:J:129:LEU:HD12	10:J:129:LEU:HA	1.81	0.40
35:L:307:A86:C33	36:Q:307:CLA:CBC	2.93	0.40
36:N:316:CLA:H112	36:N:316:CLA:H152	1.84	0.40
15:P:94:LEU:H	15:P:99:SER:HA	1.86	0.40
15:P:107:LYS:HG3	15:P:110:ASP:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:P:301:CLA:C20	41:Q:315:LHG:H191	2.51	0.40
36:P:313:CLA:H61	36:P:313:CLA:H92	1.81	0.40
36:T:309:CLA:H161	36:T:309:CLA:H141	1.83	0.40
20:a:684:ILE:HD13	20:a:684:ILE:HA	1.80	0.40
21:b:316:ALA:O	21:b:319:VAL:HG23	2.21	0.40
21:b:436:TYR:HB3	21:b:615:ILE:HD12	2.03	0.40
21:b:493:LEU:N	21:b:494:PRO:HD2	2.36	0.40
36:b:836:CLA:C10	36:b:836:CLA:C5	2.86	0.40
23:d:101:VAL:HG22	23:d:128:LEU:HD12	2.01	0.40
25:f:172:TRP:O	25:f:172:TRP:HD1	2.04	0.40
1:A:160:GLY:HA3	33:V:26:ALA:HB3	2.03	0.40
2:B:109:LEU:HD12	2:B:109:LEU:HA	1.73	0.40
4:D:133:PHE:CD2	35:D:302:A86:C22	3.04	0.40
36:D:307:CLA:H101	36:D:307:CLA:H62	1.75	0.40
35:E:307:A86:C10	36:E:315:CLA:CMD	2.99	0.40
36:L:308:CLA:H72	37:L:315:KC1:C1D	2.50	0.40
15:P:78:THR:HG23	15:P:186:PHE:HE2	1.87	0.40
41:Q:315:LHG:O10	41:Q:315:LHG:H262	2.21	0.40
16:R:92:PHE:CE1	16:R:217:PHE:HE2	2.36	0.40
36:S:315:CLA:HBC2	36:S:321:CLA:H3A	2.02	0.40
19:W:53:GLN:HB3	19:W:75:ASN:ND2	2.35	0.40
20:a:194:GLU:N	20:a:194:GLU:OE1	2.51	0.40
21:b:23:TYR:CE2	40:b:849:DGD:HG32	2.57	0.40
36:b:812:CLA:H121	36:b:828:CLA:H193	2.02	0.40
27:j:39:PHE:O	27:j:41:PHE:CD1	2.74	0.40
28:l:95:LEU:HD12	36:l:202:CLA:H43	2.04	0.40
28:l:166:ALA:HA	28:l:169:CYS:HB2	2.03	0.40
29:m:12:ILE:HD11	44:m:101:BCR:H281	2.03	0.40
36:A:314:CLA:CBC	34:D:301:DD6:C26	2.96	0.40
3:C:57:ARG:HB2	36:C:207:CLA:HMD1	2.03	0.40
40:C:215:DGD:HE4	40:C:215:DGD:HO4D	1.81	0.40
4:D:165:LYS:HG2	19:W:26:GLN:NE2	2.36	0.40
36:D:315:CLA:HBC2	34:E:301:DD6:C7	2.52	0.40
6:F:94:HIS:CD2	35:O:301:A86:C22	3.05	0.40
6:F:170:ARG:NH2	10:J:59:GLU:HB3	2.36	0.40
36:H:314:CLA:CBC	35:J:301:A86:C1	3.00	0.40
36:H:315:CLA:H111	36:H:315:CLA:H142	1.88	0.40
36:I:305:CLA:H61	36:I:305:CLA:H41	1.77	0.40
13:M:114:TRP:CH2	13:M:140:GLY:HA2	2.52	0.40
14:N:100:PHE:CE1	36:N:310:CLA:HMD2	2.56	0.40
16:R:104:PHE:HE2	36:R:313:CLA:H11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:215:MET:N	16:R:215:MET:HE2	2.36	0.40
41:R:323:LHG:H362	41:R:323:LHG:H331	1.84	0.40
36:S:314:CLA:H92	36:S:314:CLA:H62	1.89	0.40
20:a:112:ASP:OD2	20:a:115:LYS:HG2	2.20	0.40
20:a:455:CYS:O	36:a:832:CLA:HBB2	2.21	0.40
21:b:284:ILE:O	21:b:288:HIS:HD2	2.05	0.40
21:b:338:ALA:HB2	44:b:846:BCR:H372	2.04	0.40
21:b:435:LEU:HD23	21:b:435:LEU:HA	1.89	0.40
36:b:806:CLA:H121	36:b:806:CLA:H8	1.89	0.40
36:b:810:CLA:H111	36:b:810:CLA:HBB1	2.02	0.40
24:e:9:VAL:CA	24:e:61:GLN:O	2.67	0.40
25:f:128:ARG:HD3	27:j:35:ASP:CG	2.46	0.40
25:f:204:ARG:HA	25:f:207:PHE:CZ	2.56	0.40
28:l:172:VAL:HG22	32:U:75:PRO:HB2	2.03	0.40
33:V:69:ILE:O	33:V:70:ARG:CB	2.69	0.40
33:V:138:TRP:CZ3	36:V:308:CLA:H203	2.52	0.40
33:V:144:LYS:HB3	33:V:149:ARG:HH11	1.87	0.40
36:V:314:CLA:C9	36:V:314:CLA:C12	2.86	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	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	10 14
2	B	128/223 (57%)	121 (94%)	7 (6%)	0	100 100
3	C	161/198 (81%)	150 (93%)	9 (6%)	2 (1%)	10 14
4	D	170/207 (82%)	160 (94%)	9 (5%)	1 (1%)	21 30
5	E	186/222 (84%)	178 (96%)	8 (4%)	0	100 100
6	F	178/215 (83%)	165 (93%)	13 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	212/245 (86%)	197 (93%)	14 (7%)	1 (0%)	24 34
8	H	168/203 (83%)	151 (90%)	17 (10%)	0	100 100
9	I	159/195 (82%)	146 (92%)	13 (8%)	0	100 100
10	J	165/200 (82%)	145 (88%)	17 (10%)	3 (2%)	6 8
11	K	167/207 (81%)	152 (91%)	15 (9%)	0	100 100
12	L	194/229 (85%)	176 (91%)	18 (9%)	0	100 100
13	M	185/306 (60%)	169 (91%)	15 (8%)	1 (0%)	24 34
14	N	217/219 (99%)	174 (80%)	40 (18%)	3 (1%)	9 11
15	O	171/205 (83%)	147 (86%)	21 (12%)	3 (2%)	6 8
15	P	171/205 (83%)	153 (90%)	16 (9%)	2 (1%)	10 14
15	Q	171/205 (83%)	150 (88%)	19 (11%)	2 (1%)	10 14
16	R	209/246 (85%)	182 (87%)	25 (12%)	2 (1%)	12 17
17	S	218/254 (86%)	184 (84%)	29 (13%)	5 (2%)	5 5
18	T	170/207 (82%)	164 (96%)	6 (4%)	0	100 100
19	W	158/198 (80%)	133 (84%)	25 (16%)	0	100 100
19	X	160/198 (81%)	146 (91%)	13 (8%)	1 (1%)	21 30
20	a	740/743 (100%)	713 (96%)	26 (4%)	1 (0%)	48 62
21	b	731/733 (100%)	699 (96%)	31 (4%)	1 (0%)	48 62
22	c	78/80 (98%)	74 (95%)	4 (5%)	0	100 100
23	d	131/132 (99%)	125 (95%)	6 (5%)	0	100 100
24	e	61/63 (97%)	60 (98%)	1 (2%)	0	100 100
25	f	160/162 (99%)	152 (95%)	8 (5%)	0	100 100
26	i	31/40 (78%)	31 (100%)	0	0	100 100
27	j	39/42 (93%)	37 (95%)	1 (3%)	1 (3%)	4 4
28	l	142/172 (83%)	131 (92%)	11 (8%)	0	100 100
29	m	26/29 (90%)	26 (100%)	0	0	100 100
31	h	87/139 (63%)	87 (100%)	0	0	100 100
32	U	154/160 (96%)	123 (80%)	26 (17%)	5 (3%)	3 2
33	V	177/179 (99%)	152 (86%)	20 (11%)	5 (3%)	4 3
All	All	6441/7429 (87%)	5903 (92%)	497 (8%)	41 (1%)	23 30

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	87	ILE
15	O	153	PRO
15	O	155	ILE
15	Q	153	PRO
17	S	103	ALA
32	U	66	PRO
33	V	14	TYR
33	V	70	ARG
3	C	42	PHE
10	J	110	ALA
14	N	186	PHE
17	S	167	PHE
19	X	130	GLU
32	U	7	THR
33	V	82	SER
33	V	112	HIS
7	G	233	THR
13	M	234	THR
15	O	106	MET
17	S	60	LYS
1	A	198	THR
4	D	55	ALA
10	J	152	PHE
15	Q	155	ILE
21	b	557	PRO
32	U	117	PRO
33	V	83	PRO
1	A	48	ASN
14	N	227	PRO
16	R	65	ILE
17	S	55	LEU
32	U	113	MET
32	U	155	PRO
15	P	153	PRO
15	P	154	PRO
17	S	101	PRO
27	j	40	PRO
20	a	158	ILE
3	C	161	PRO
14	N	183	PRO
16	R	67	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	137/137 (100%)	128 (93%)	9 (7%)	15 24
2	B	105/180 (58%)	98 (93%)	7 (7%)	15 23
3	C	131/153 (86%)	122 (93%)	9 (7%)	14 22
4	D	140/163 (86%)	125 (89%)	15 (11%)	6 8
5	E	142/164 (87%)	136 (96%)	6 (4%)	26 42
6	F	142/169 (84%)	135 (95%)	7 (5%)	22 36
7	G	172/193 (89%)	146 (85%)	26 (15%)	3 3
8	H	131/154 (85%)	129 (98%)	2 (2%)	57 75
9	I	124/152 (82%)	101 (82%)	23 (18%)	1 2
10	J	130/154 (84%)	122 (94%)	8 (6%)	16 26
11	K	133/160 (83%)	130 (98%)	3 (2%)	44 64
12	L	159/180 (88%)	159 (100%)	0	100 100
13	M	142/247 (58%)	135 (95%)	7 (5%)	22 36
14	N	176/176 (100%)	170 (97%)	6 (3%)	32 51
15	O	138/159 (87%)	134 (97%)	4 (3%)	37 57
15	P	137/159 (86%)	120 (88%)	17 (12%)	4 6
15	Q	138/159 (87%)	133 (96%)	5 (4%)	31 49
16	R	167/193 (86%)	160 (96%)	7 (4%)	26 42
17	S	177/204 (87%)	169 (96%)	8 (4%)	24 39
18	T	136/163 (83%)	135 (99%)	1 (1%)	76 87
19	W	125/151 (83%)	125 (100%)	0	100 100
19	X	127/151 (84%)	125 (98%)	2 (2%)	55 74
20	a	606/606 (100%)	543 (90%)	63 (10%)	7 9
21	b	593/593 (100%)	517 (87%)	76 (13%)	4 5
22	c	67/69 (97%)	59 (88%)	8 (12%)	5 6
23	d	111/111 (100%)	88 (79%)	23 (21%)	1 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	e	55/55 (100%)	51 (93%)	4 (7%)	13 20
25	f	119/125 (95%)	105 (88%)	14 (12%)	5 6
26	i	29/36 (81%)	20 (69%)	9 (31%)	0 0
27	j	34/35 (97%)	29 (85%)	5 (15%)	3 3
28	l	114/143 (80%)	98 (86%)	16 (14%)	3 4
29	m	20/23 (87%)	17 (85%)	3 (15%)	3 3
31	h	70/109 (64%)	54 (77%)	16 (23%)	1 1
32	U	119/121 (98%)	82 (69%)	37 (31%)	0 0
33	V	137/137 (100%)	83 (61%)	54 (39%)	0 0
All	All	5183/5884 (88%)	4683 (90%)	500 (10%)	10 11

All (500) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	105	ASP
1	A	109	LEU
1	A	119	MET
1	A	126	MET
1	A	163	VAL
1	A	169	GLU
1	A	172	GLU
1	A	196	TRP
2	B	93	LEU
2	B	96	ASP
2	B	105	GLU
2	B	131	HIS
2	B	191	LEU
2	B	194	LEU
2	B	207	GLN
3	C	35	GLU
3	C	36	MET
3	C	40	LEU
3	C	45	ARG
3	C	64	LEU
3	C	114	ILE
3	C	139	LYS
3	C	168	LYS
3	C	172	ILE

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Mol	Chain	Res	Type
4	D	35	LYS
4	D	61	ARG
4	D	97	ARG
4	D	117	LEU
4	D	125	GLN
4	D	145	LEU
4	D	151	ARG
4	D	152	GLU
4	D	155	ASN
4	D	165	LYS
4	D	177	LEU
4	D	180	ILE
4	D	184	ARG
4	D	204	PHE
4	D	206	TYR
5	E	45	ARG
5	E	113	LYS
5	E	152	ARG
5	E	157	ARG
5	E	181	GLN
5	E	189	ARG
6	F	161	LEU
6	F	163	PHE
6	F	166	MET
6	F	171	LYS
6	F	176	GLN
6	F	185	LEU
6	F	214	PHE
7	G	37	LEU
7	G	46	GLN
7	G	47	ARG
7	G	49	LYS
7	G	75	LEU
7	G	93	GLU
7	G	94	LYS
7	G	99	LEU
7	G	103	ARG
7	G	111	ARG
7	G	137	ILE
7	G	148	GLU
7	G	155	SER
7	G	159	MET

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Mol	Chain	Res	Type
7	G	163	LEU
7	G	176	VAL
7	G	180	VAL
7	G	182	LYS
7	G	187	ARG
7	G	193	LYS
7	G	201	LYS
7	G	209	LYS
7	G	210	ARG
7	G	211	MET
7	G	216	ILE
7	G	233	THR
8	H	119	PHE
8	H	121	SER
9	I	35	LYS
9	I	36	ASP
9	I	39	ILE
9	I	40	ILE
9	I	42	ILE
9	I	43	THR
9	I	46	MET
9	I	58	LYS
9	I	72	LYS
9	I	86	ILE
9	I	87	THR
9	I	92	HIS
9	I	95	PHE
9	I	120	LEU
9	I	133	LYS
9	I	143	ILE
9	I	144	LEU
9	I	150	VAL
9	I	169	ARG
9	I	170	LEU
9	I	176	MET
9	I	185	PHE
9	I	194	ARG
10	J	38	ASN
10	J	51	LYS
10	J	87	ILE
10	J	93	ARG
10	J	129	LEU

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Mol	Chain	Res	Type
10	J	132	LEU
10	J	133	VAL
10	J	155	LYS
11	K	53	ARG
11	K	151	ARG
11	K	166	THR
13	M	74	GLU
13	M	75	ILE
13	M	77	ARG
13	M	78	VAL
13	M	172	ARG
13	M	173	ARG
13	M	181	ARG
14	N	63	TRP
14	N	86	MET
14	N	169	LEU
14	N	171	ARG
14	N	178	LEU
14	N	241	MET
15	O	54	LEU
15	O	121	ASN
15	O	152	PHE
15	O	153	PRO
15	P	35	GLU
15	P	54	LEU
15	P	64	ARG
15	P	83	VAL
15	P	84	GLN
15	P	106	MET
15	P	120	LYS
15	P	129	LEU
15	P	137	LYS
15	P	147	LEU
15	P	149	THR
15	P	155	ILE
15	P	156	ASP
15	P	158	SER
15	P	160	VAL
15	P	168	ARG
15	P	192	ILE
15	Q	54	LEU
15	Q	104	SER

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Mol	Chain	Res	Type
15	Q	106	MET
15	Q	121	ASN
15	Q	155	ILE
16	R	49	ASN
16	R	63	THR
16	R	64	THR
16	R	65	ILE
16	R	69	THR
16	R	92	PHE
16	R	215	MET
17	S	55	LEU
17	S	57	LEU
17	S	60	LYS
17	S	86	MET
17	S	136	VAL
17	S	175	HIS
17	S	177	VAL
17	S	178	LEU
18	T	31	ARG
19	X	127	THR
19	X	129	ASP
20	a	17	ASN
20	a	29	THR
20	a	32	GLU
20	a	33	LYS
20	a	49	LYS
20	a	85	GLN
20	a	110	LEU
20	a	115	LYS
20	a	123	VAL
20	a	139	ASN
20	a	147	SER
20	a	154	ARG
20	a	179	LEU
20	a	188	LYS
20	a	192	LYS
20	a	193	LEU
20	a	216	LEU
20	a	217	SER
20	a	250	ILE
20	a	252	ARG
20	a	254	LEU

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Mol	Chain	Res	Type
20	a	280	PHE
20	a	284	LYS
20	a	288	ASN
20	a	304	LEU
20	a	309	LEU
20	a	323	ILE
20	a	326	SER
20	a	327	MET
20	a	335	LYS
20	a	344	LYS
20	a	348	GLU
20	a	353	SER
20	a	358	LEU
20	a	364	MET
20	a	365	ILE
20	a	392	GLN
20	a	393	LEU
20	a	407	VAL
20	a	430	ASN
20	a	432	LEU
20	a	453	LEU
20	a	466	THR
20	a	480	LYS
20	a	503	THR
20	a	518	ASP
20	a	529	MET
20	a	532	LYS
20	a	553	LEU
20	a	556	LEU
20	a	567	LEU
20	a	585	ARG
20	a	588	THR
20	a	626	THR
20	a	652	LEU
20	a	663	VAL
20	a	684	ILE
20	a	696	ARG
20	a	702	LEU
20	a	728	GLN
20	a	739	LEU
20	a	755	SER
20	a	757	THR

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Mol	Chain	Res	Type
21	b	4	LYS
21	b	5	PHE
21	b	10	GLN
21	b	42	LEU
21	b	54	LEU
21	b	78	VAL
21	b	84	THR
21	b	106	LYS
21	b	112	VAL
21	b	114	ILE
21	b	117	SER
21	b	125	THR
21	b	154	LEU
21	b	157	GLN
21	b	159	LYS
21	b	187	LEU
21	b	222	LYS
21	b	228	ASN
21	b	230	THR
21	b	238	SER
21	b	263[A]	GLN
21	b	263[B]	GLN
21	b	291	ARG
21	b	293	ASN
21	b	319	VAL
21	b	324	THR
21	b	333	LEU
21	b	346	LEU
21	b	347	THR
21	b	349	GLN
21	b	354	LEU
21	b	355	THR
21	b	360	LEU
21	b	362	LYS
21	b	375	GLN
21	b	377	ILE
21	b	383	VAL
21	b	395	ARG
21	b	401	LEU
21	b	402	ASN
21	b	404	ASN
21	b	406	VAL

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Mol	Chain	Res	Type
21	b	407	LEU
21	b	414	LYS
21	b	421	LEU
21	b	433	LEU
21	b	440	ASP
21	b	442	VAL
21	b	466	SER
21	b	472	GLU
21	b	490	GLN
21	b	491	VAL
21	b	493	LEU
21	b	500	ILE
21	b	504	LYS
21	b	505	ASN
21	b	507	LEU
21	b	518	VAL
21	b	531	LEU
21	b	545	LEU
21	b	569	ILE
21	b	607	GLN
21	b	615	ILE
21	b	619	LEU
21	b	625	LEU
21	b	628	SER
21	b	643	SER
21	b	673	LEU
21	b	684	THR
21	b	686	LEU
21	b	689	LEU
21	b	709	LEU
21	b	713	SER
21	b	717	ILE
21	b	724	LEU
21	b	725	ILE
22	c	26	LEU
22	c	35	LYS
22	c	37	LYS
22	c	63	LEU
22	c	66	ARG
22	c	69	LEU
22	c	72	GLU
22	c	77	MET

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Mol	Chain	Res	Type
23	d	92	ARG
23	d	98	GLU
23	d	99	LYS
23	d	108	LYS
23	d	123	ARG
23	d	129	LEU
23	d	130	LYS
23	d	138	LEU
23	d	143	ARG
23	d	147	LYS
23	d	150	ILE
23	d	151[A]	LYS
23	d	151[B]	LYS
23	d	160	ASN
23	d	162	GLU
23	d	169	LYS
23	d	175	GLU
23	d	177	VAL
23	d	193	LYS
23	d	195	VAL
23	d	201	LYS
23	d	205	LYS
23	d	206	GLN
24	e	10	LYS
24	e	57	LEU
24	e	60	ILE
24	e	61	GLN
25	f	78	ILE
25	f	99	LYS
25	f	134	LYS
25	f	154	ARG
25	f	164	ILE
25	f	176	VAL
25	f	178	ARG
25	f	179	SER
25	f	201	LEU
25	f	203	SER
25	f	204	ARG
25	f	207	PHE
25	f	218	ARG
25	f	226	VAL
26	i	2	MET

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Mol	Chain	Res	Type
26	i	4	ASN
26	i	12	LEU
26	i	16	LEU
26	i	24	SER
26	i	29	VAL
26	i	31	LYS
26	i	32	ARG
26	i	33	LEU
27	j	1	MET
27	j	37	LEU
27	j	38	THR
27	j	39	PHE
27	j	41	PHE
28	l	32	ILE
28	l	33	LYS
28	l	59	LYS
28	l	72	LEU
28	l	91	LYS
28	l	102	LEU
28	l	129	LYS
28	l	130	GLU
28	l	132	LYS
28	l	134	MET
28	l	136	SER
28	l	138	ASN
28	l	140	ASN
28	l	146	LYS
28	l	149	ASP
28	l	152	LYS
29	m	2	ILE
29	m	24	LEU
29	m	27	GLN
31	h	51	ASP
31	h	52	MET
31	h	61	SER
31	h	67	ILE
31	h	68	MET
31	h	73	SER
31	h	75	LEU
31	h	81	ILE
31	h	94	SER
31	h	99	GLN

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Mol	Chain	Res	Type
31	h	105	GLU
31	h	113	TYR
31	h	127	THR
31	h	128	HIS
31	h	131	SER
31	h	136	LYS
32	U	1	LEU
32	U	2	ASP
32	U	4	MET
32	U	5	VAL
32	U	10	GLU
32	U	14	LYS
32	U	19	LEU
32	U	21	LEU
32	U	23	ASP
32	U	24	TYR
32	U	25	ILE
32	U	29	ARG
32	U	49	VAL
32	U	52	LYS
32	U	56	HIS
32	U	70	ILE
32	U	72	GLN
32	U	74	ASP
32	U	76	GLN
32	U	80	GLN
32	U	82	ILE
32	U	83	ILE
32	U	87	THR
32	U	88	ILE
32	U	92	LYS
32	U	95	MET
32	U	97	LEU
32	U	100	LYS
32	U	110	ILE
32	U	114	LYS
32	U	115	MET
32	U	123	ARG
32	U	125	ASP
32	U	126	MET
32	U	127	GLU
32	U	135	ARG

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Mol	Chain	Res	Type
32	U	150	ILE
33	V	1	THR
33	V	3	LEU
33	V	6	GLU
33	V	8	VAL
33	V	10	ILE
33	V	12	GLU
33	V	18	LEU
33	V	19	THR
33	V	20	LEU
33	V	25	GLU
33	V	27	THR
33	V	29	THR
33	V	37	LYS
33	V	41	SER
33	V	53	LYS
33	V	54	LEU
33	V	56	LEU
33	V	57	THR
33	V	58	LEU
33	V	59	ASN
33	V	61	ILE
33	V	64	HIS
33	V	66	TYR
33	V	69	ILE
33	V	70	ARG
33	V	72	ASN
33	V	73	ILE
33	V	74	LYS
33	V	77	ASP
33	V	84	ILE
33	V	85	GLU
33	V	87	VAL
33	V	88	LYS
33	V	111	THR
33	V	113	ARG
33	V	114	ASN
33	V	116	LYS
33	V	121	GLU
33	V	122	SER
33	V	123	VAL
33	V	132	LEU

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Mol	Chain	Res	Type
33	V	133	THR
33	V	135	ASP
33	V	136	LEU
33	V	141	LEU
33	V	142	ASN
33	V	143	ILE
33	V	144	LYS
33	V	147	ASP
33	V	149	ARG
33	V	151	LEU
33	V	158	ARG
33	V	164	ILE
33	V	173	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	94	GLN
1	A	134	ASN
1	A	137	ASN
1	A	193	HIS
1	A	195	ASN
3	C	68	GLN
3	C	95	GLN
3	C	99	HIS
3	C	107	ASN
3	C	158	ASN
3	C	174	HIS
3	C	193	HIS
4	D	78	HIS
4	D	155	ASN
5	E	66	ASN
5	E	126	HIS
5	E	187	ASN
6	F	94	HIS
6	F	103	HIS
6	F	124	GLN
7	G	46	GLN
7	G	87	GLN
7	G	109	HIS
7	G	156	GLN

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Mol	Chain	Res	Type
7	G	232	GLN
7	G	240	HIS
8	H	46	ASN
8	H	113	HIS
8	H	145	GLN
9	I	64	ASN
9	I	92	HIS
9	I	181	GLN
9	I	191	GLN
10	J	38	ASN
11	K	81	HIS
12	L	36	ASN
12	L	75	HIS
12	L	94	HIS
12	L	163	GLN
13	M	129	HIS
13	M	170	HIS
14	N	104	GLN
14	N	111	HIS
14	N	121	GLN
14	N	187	ASN
14	N	204	ASN
15	O	70	HIS
15	O	84	GLN
15	O	121	ASN
15	O	191	ASN
15	P	121	ASN
15	P	140	HIS
15	P	164	GLN
15	P	174	ASN
15	P	191	ASN
15	Q	70	HIS
15	Q	140	HIS
15	Q	191	ASN
16	R	49	ASN
16	R	100	ASN
16	R	154	HIS
16	R	175	HIS
16	R	205	ASN
16	R	221	GLN
17	S	104	GLN
17	S	154	HIS

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Mol	Chain	Res	Type
17	S	173	ASN
17	S	175	HIS
17	S	204	ASN
17	S	239	GLN
18	T	9	GLN
18	T	23	ASN
18	T	39	HIS
19	W	26	GLN
19	X	157	HIS
20	a	17	ASN
20	a	62	HIS
20	a	99	HIS
20	a	121	GLN
20	a	129	GLN
20	a	141	GLN
20	a	187	HIS
20	a	273	GLN
20	a	288	ASN
20	a	325	HIS
20	a	343	HIS
20	a	392	GLN
20	a	426	ASN
20	a	427	ASN
20	a	429	ASN
20	a	430	ASN
20	a	447	ASN
20	a	456	HIS
20	a	485	GLN
20	a	541	HIS
20	a	596	HIS
20	a	649	ASN
20	a	662	GLN
20	a	700	GLN
20	a	720	GLN
20	a	728	GLN
21	b	14	GLN
21	b	53	HIS
21	b	71	GLN
21	b	89	HIS
21	b	132	GLN
21	b	195	HIS
21	b	276	GLN

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Mol	Chain	Res	Type
21	b	288	HIS
21	b	298	HIS
21	b	350	HIS
21	b	373	HIS
21	b	375	GLN
21	b	388	HIS
21	b	404	ASN
21	b	405	ASN
21	b	490	GLN
21	b	505	ASN
21	b	520	HIS
21	b	527	HIS
21	b	607	GLN
21	b	641	ASN
21	b	671	GLN
21	b	681	HIS
22	c	38	GLN
23	d	136	GLN
23	d	206	GLN
25	f	89	GLN
25	f	146	HIS
25	f	155	HIS
26	i	4	ASN
28	l	43	HIS
28	l	141	ASN
28	l	143	GLN
29	m	5	ASN
31	h	93	GLN
32	U	20	ASN
32	U	56	HIS
32	U	72	GLN
32	U	80	GLN
32	U	148	HIS
33	V	64	HIS
33	V	89	HIS
33	V	112	HIS
33	V	114	ASN
33	V	128	GLN
33	V	142	ASN
33	V	155	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

589 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	CLA	b	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.58	14 (17%)
36	CLA	a	812	-	69,73,73	1.14	9 (13%)	82,113,113	1.38	7 (8%)
36	CLA	a	823	-	59,63,73	1.62	11 (18%)	70,101,113	2.24	21 (30%)
36	CLA	A	314	-	69,73,73	1.27	8 (11%)	82,113,113	1.79	9 (10%)
36	CLA	R	312	-	69,73,73	1.16	9 (13%)	82,113,113	1.50	12 (14%)
36	CLA	b	813	-	58,62,73	1.33	11 (18%)	71,100,113	1.35	9 (12%)
36	CLA	O	306	-	65,69,73	1.19	8 (12%)	77,108,113	1.36	4 (5%)
36	CLA	C	211	-	69,73,73	1.13	10 (14%)	82,113,113	1.34	6 (7%)
36	CLA	W	215	-	52,56,73	1.52	10 (19%)	61,92,113	1.40	6 (9%)
36	CLA	L	313	-	69,73,73	1.11	8 (11%)	82,113,113	1.42	7 (8%)
36	CLA	A	305	1	53,57,73	1.31	8 (15%)	61,93,113	1.40	4 (6%)
37	KC1	E	309	-	49,53,53	2.66	19 (38%)	61,89,89	4.48	38 (62%)
39	LMT	L	303	-	36,36,36	1.31	6 (16%)	47,47,47	0.97	1 (2%)
36	CLA	N	311	-	50,54,73	1.35	6 (12%)	59,90,113	1.71	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	KC1	L	317	-	49,53,53	2.70	19 (38%)	61,89,89	4.44	36 (59%)
44	BCR	a	847	-	41,41,41	1.24	4 (9%)	56,56,56	1.28	5 (8%)
36	CLA	W	216	35	49,53,73	1.82	9 (18%)	58,89,113	2.80	15 (25%)
41	LHG	D	319	42	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
36	CLA	D	307	41	65,69,73	1.16	7 (10%)	77,108,113	1.59	13 (16%)
36	CLA	b	827	-	69,73,73	1.22	9 (13%)	82,113,113	1.38	9 (10%)
41	LHG	I	316	-	48,48,48	0.95	2 (4%)	51,54,54	1.01	2 (3%)
35	A86	P	306	-	47,50,50	1.44	5 (10%)	51,76,76	2.25	16 (31%)
41	LHG	a	842	-	47,47,48	0.78	1 (2%)	50,53,54	1.29	4 (8%)
36	CLA	M	309	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
35	A86	F	306	-	47,50,50	1.51	6 (12%)	51,76,76	2.43	14 (27%)
36	CLA	a	838	-	69,73,73	1.12	9 (13%)	82,113,113	1.35	7 (8%)
36	CLA	P	314	-	64,68,73	1.33	10 (15%)	76,107,113	1.66	15 (19%)
35	A86	X	302	35	47,50,50	1.39	6 (12%)	51,76,76	3.01	17 (33%)
36	CLA	b	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.42	14 (17%)
36	CLA	a	839	46	69,73,73	1.11	8 (11%)	82,113,113	1.36	7 (8%)
37	KC1	J	314	-	49,53,53	2.66	19 (38%)	61,89,89	5.09	36 (59%)
41	LHG	Q	315	36	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
35	A86	R	305	-	47,50,50	1.43	6 (12%)	51,76,76	2.18	14 (27%)
44	BCR	l	207	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	12 (21%)
36	CLA	L	308	-	65,69,73	1.89	13 (20%)	77,108,113	2.70	22 (28%)
39	LMT	h	205	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
35	A86	C	202	36	47,50,50	1.56	7 (14%)	51,76,76	2.89	17 (33%)
35	A86	T	305	-	47,50,50	1.69	6 (12%)	51,76,76	3.74	22 (43%)
44	BCR	j	107	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	8 (14%)
37	KC1	P	317	15	49,53,53	2.56	19 (38%)	61,89,89	4.63	37 (60%)
37	KC1	M	317	-	49,53,53	2.70	20 (40%)	61,89,89	4.30	37 (60%)
36	CLA	E	310	-	69,73,73	1.15	7 (10%)	82,113,113	1.42	9 (10%)
36	CLA	N	316	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	5 (6%)
35	A86	Q	316	36	47,50,50	1.77	10 (21%)	51,76,76	2.18	15 (29%)
36	CLA	b	818	-	59,63,73	1.21	8 (13%)	70,101,113	1.62	12 (17%)
35	A86	M	301	-	47,50,50	1.57	5 (10%)	51,76,76	3.27	22 (43%)
36	CLA	a	813	-	49,53,73	1.38	8 (16%)	58,89,113	1.72	10 (17%)
36	CLA	a	820	-	69,73,73	1.13	9 (13%)	82,113,113	1.37	8 (9%)
35	A86	V	302	-	47,50,50	1.52	6 (12%)	51,76,76	2.64	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	U	307	-	54,58,73	1.30	9 (16%)	64,95,113	1.37	4 (6%)
35	A86	A	302	-	47,50,50	1.76	6 (12%)	51,76,76	4.57	24 (47%)
36	CLA	M	310	35,13	50,54,73	1.99	7 (14%)	59,90,113	1.89	13 (22%)
35	A86	C	204	-	47,50,50	1.90	14 (29%)	51,76,76	2.83	16 (31%)
35	A86	L	301	-	47,50,50	1.50	6 (12%)	51,76,76	2.37	16 (31%)
36	CLA	a	841	41	56,60,73	1.28	9 (16%)	65,97,113	1.55	8 (12%)
36	CLA	B	305	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
36	CLA	E	313	-	69,73,73	1.75	15 (21%)	82,113,113	2.25	23 (28%)
36	CLA	a	801	-	69,73,73	1.20	7 (10%)	82,113,113	1.51	11 (13%)
37	KC1	W	213	-	49,53,53	2.81	20 (40%)	61,89,89	4.57	34 (55%)
34	DD6	A	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.90	11 (21%)
36	CLA	M	316	36	46,50,73	1.36	8 (17%)	53,85,113	1.45	4 (7%)
36	CLA	X	313	-	46,50,73	2.06	11 (23%)	53,85,113	4.30	21 (39%)
44	BCR	b	843	-	41,41,41	1.20	4 (9%)	56,56,56	1.20	6 (10%)
36	CLA	M	311	35,13	69,73,73	1.16	8 (11%)	82,113,113	1.25	4 (4%)
35	A86	F	305	-	47,50,50	1.57	9 (19%)	51,76,76	2.48	21 (41%)
34	DD6	R	308	-	40,45,45	1.56	2 (5%)	51,67,67	2.10	12 (23%)
36	CLA	H	308	-	67,72,73	1.17	11 (16%)	79,112,113	1.32	10 (12%)
35	A86	I	301	-	47,50,50	1.47	5 (10%)	51,76,76	2.58	17 (33%)
36	CLA	b	841	41	69,73,73	1.19	11 (15%)	82,113,113	1.81	16 (19%)
36	CLA	Q	305	-	65,69,73	1.19	8 (12%)	77,108,113	1.36	4 (5%)
44	BCR	h	201	-	41,41,41	1.27	5 (12%)	56,56,56	1.46	11 (19%)
36	CLA	I	307	-	58,62,73	1.23	10 (17%)	68,99,113	1.48	9 (13%)
36	CLA	G	316	-	53,57,73	1.30	9 (16%)	61,93,113	1.48	5 (8%)
35	A86	H	304	-	47,50,50	1.48	6 (12%)	51,76,76	2.51	16 (31%)
36	CLA	J	310	-	69,73,73	1.12	9 (13%)	82,113,113	1.35	7 (8%)
36	CLA	H	316	-	69,73,73	1.13	9 (13%)	82,113,113	1.36	6 (7%)
36	CLA	D	308	-	69,73,73	1.14	10 (14%)	82,113,113	1.54	13 (15%)
36	CLA	V	314	-	69,73,73	1.94	16 (23%)	82,113,113	2.81	26 (31%)
36	CLA	L	312	12	50,54,73	1.37	8 (16%)	59,90,113	1.77	8 (13%)
36	CLA	K	313	-	69,73,73	1.18	11 (15%)	82,113,113	1.47	10 (12%)
36	CLA	a	806	-	69,73,73	1.37	8 (11%)	82,113,113	1.95	19 (23%)
36	CLA	L	314	-	69,73,73	1.14	8 (11%)	82,113,113	1.45	10 (12%)
36	CLA	I	311	9	69,73,73	1.10	9 (13%)	82,113,113	1.48	9 (10%)
41	LHG	F	319	-	40,40,48	1.03	2 (5%)	43,46,54	1.11	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	M	307	-	69,73,73	1.15	10 (14%)	82,113,113	1.45	10 (12%)
36	CLA	N	312	-	51,55,73	1.29	8 (15%)	60,91,113	1.48	5 (8%)
34	DD6	a	849	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	15 (29%)
36	CLA	J	313	-	69,73,73	1.13	9 (13%)	82,113,113	1.35	5 (6%)
41	LHG	F	318	-	32,32,48	0.90	2 (6%)	35,37,54	1.75	6 (17%)
36	CLA	Q	306	-	69,73,73	1.13	10 (14%)	82,113,113	1.35	6 (7%)
35	A86	C	203	-	47,50,50	1.47	6 (12%)	51,76,76	2.42	17 (33%)
43	PQN	a	840	-	34,34,34	1.61	2 (5%)	43,45,45	1.19	4 (9%)
36	CLA	P	312	15	50,54,73	1.35	8 (16%)	59,90,113	1.57	7 (11%)
37	KC1	F	308	6	49,53,53	2.68	21 (42%)	61,89,89	4.86	34 (55%)
36	CLA	a	808	20	69,73,73	1.13	9 (13%)	82,113,113	1.40	9 (10%)
36	CLA	K	307	-	65,69,73	1.89	15 (23%)	77,108,113	2.85	24 (31%)
37	KC1	Q	311	15	49,53,53	2.84	22 (44%)	61,89,89	5.74	38 (62%)
36	CLA	R	311	-	69,73,73	1.14	8 (11%)	82,113,113	1.35	8 (9%)
36	CLA	S	320	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
41	LHG	G	320	-	39,39,48	1.04	2 (5%)	42,45,54	1.13	3 (7%)
34	DD6	R	307	-	40,45,45	1.54	2 (5%)	51,67,67	2.08	15 (29%)
35	A86	W	203	36	47,50,50	1.62	6 (12%)	51,76,76	2.49	18 (35%)
35	A86	h	204	-	47,50,50	1.47	6 (12%)	51,76,76	2.44	14 (27%)
44	BCR	m	101	-	41,41,41	1.17	5 (12%)	56,56,56	1.36	7 (12%)
41	LHG	j	104	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	3 (5%)
36	CLA	M	312	36	51,55,73	1.35	8 (15%)	60,91,113	1.57	6 (10%)
36	CLA	b	832	-	53,57,73	1.21	8 (15%)	61,93,113	1.55	8 (13%)
36	CLA	a	833	-	54,58,73	1.27	8 (14%)	64,95,113	1.61	5 (7%)
35	A86	S	302	-	47,50,50	1.39	5 (10%)	51,76,76	2.46	15 (29%)
41	LHG	G	301	-	48,48,48	0.79	2 (4%)	51,54,54	1.30	6 (11%)
36	CLA	O	314	-	45,49,73	1.40	7 (15%)	54,84,113	1.70	9 (16%)
37	KC1	F	315	-	49,53,53	2.64	18 (36%)	61,89,89	5.50	35 (57%)
34	DD6	W	204	36	40,45,45	1.58	2 (5%)	51,67,67	1.95	11 (21%)
36	CLA	W	218	-	47,51,73	1.40	9 (19%)	55,86,113	1.63	7 (12%)
39	LMT	a	851	-	36,36,36	0.43	0	47,47,47	0.75	1 (2%)
36	CLA	a	814	-	54,58,73	1.29	9 (16%)	64,95,113	1.71	7 (10%)
44	BCR	a	845	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	4 (7%)
36	CLA	H	315	-	69,73,73	1.17	9 (13%)	82,113,113	1.53	12 (14%)
35	A86	N	320	-	47,50,50	1.61	7 (14%)	51,76,76	3.06	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	a	821	-	53,57,73	1.28	9 (16%)	61,93,113	1.52	6 (9%)
44	BCR	f	801	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	5 (8%)
36	CLA	P	301	-	69,73,73	1.13	9 (13%)	82,113,113	1.44	9 (10%)
37	KC1	U	312	35	49,53,53	2.90	22 (44%)	61,89,89	4.00	31 (50%)
36	CLA	W	209	-	61,65,73	1.26	9 (14%)	72,103,113	1.40	10 (13%)
35	A86	N	304	-	47,50,50	2.97	10 (21%)	51,76,76	7.92	20 (39%)
41	LHG	E	322	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	2 (3%)
36	CLA	Q	314	-	69,73,73	1.16	8 (11%)	82,113,113	3.84	13 (15%)
35	A86	Q	304	-	47,50,50	1.62	7 (14%)	51,76,76	3.06	23 (45%)
35	A86	K	306	-	47,50,50	1.32	4 (8%)	51,76,76	3.11	20 (39%)
36	CLA	D	306	4	49,53,73	1.43	10 (20%)	58,89,113	1.65	9 (15%)
35	A86	R	303	-	47,50,50	1.50	6 (12%)	51,76,76	3.36	21 (41%)
36	CLA	O	309	-	69,73,73	1.15	10 (14%)	82,113,113	1.41	10 (12%)
36	CLA	H	309	-	69,73,73	1.15	7 (10%)	82,113,113	1.34	5 (6%)
35	A86	M	304	-	47,50,50	1.48	5 (10%)	51,76,76	2.46	16 (31%)
36	CLA	b	826	46	68,72,73	1.27	10 (14%)	80,111,113	2.00	16 (20%)
36	CLA	a	816	-	69,73,73	1.53	8 (11%)	82,113,113	2.05	18 (21%)
39	LMT	a	853	-	33,33,36	0.42	0	44,44,47	0.75	1 (2%)
36	CLA	I	305	-	65,69,73	1.84	13 (20%)	77,108,113	1.63	13 (16%)
36	CLA	B	307	-	50,54,73	1.36	8 (16%)	59,90,113	1.52	7 (11%)
36	CLA	i	102	-	69,73,73	1.15	9 (13%)	82,113,113	1.43	8 (9%)
36	CLA	J	307	10	65,69,73	1.18	10 (15%)	77,108,113	1.43	11 (14%)
42	LMG	E	319	-	40,40,55	1.04	2 (5%)	48,48,63	1.12	4 (8%)
36	CLA	W	206	-	65,69,73	1.17	6 (9%)	77,108,113	1.45	5 (6%)
36	CLA	O	311	-	62,66,73	1.20	8 (12%)	73,104,113	1.35	6 (8%)
39	LMT	P	321	-	23,23,36	0.44	0	28,28,47	0.61	0
36	CLA	A	313	-	45,49,73	1.39	9 (20%)	54,84,113	1.69	7 (12%)
36	CLA	H	314	-	45,49,73	1.38	10 (22%)	54,84,113	1.72	9 (16%)
36	CLA	b	821	46	69,73,73	1.12	10 (14%)	82,113,113	1.40	6 (7%)
36	CLA	a	819	-	49,53,73	1.39	10 (20%)	58,89,113	2.14	9 (15%)
36	CLA	R	310	-	65,69,73	1.20	9 (13%)	77,108,113	1.38	7 (9%)
36	CLA	N	318	-	51,55,73	1.35	8 (15%)	60,91,113	1.68	9 (15%)
36	CLA	f	804	46	69,73,73	1.98	18 (26%)	82,113,113	2.88	31 (37%)
36	CLA	U	308	35	60,64,73	1.28	8 (13%)	71,102,113	1.62	7 (9%)
36	CLA	b	822	-	50,54,73	1.32	9 (18%)	59,90,113	1.49	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DD6	B	302	-	40,45,45	1.56	2 (5%)	51,67,67	2.05	15 (29%)
37	KC1	K	314	-	49,53,53	2.60	18 (36%)	61,89,89	4.66	36 (59%)
42	LMG	V	315	-	46,46,55	0.99	2 (4%)	54,54,63	4.33	4 (7%)
36	CLA	Q	307	-	54,58,73	1.30	9 (16%)	63,94,113	1.44	5 (7%)
35	A86	R	309	-	47,50,50	1.45	6 (12%)	51,76,76	2.57	15 (29%)
35	A86	G	304	-	47,50,50	1.86	8 (17%)	51,76,76	4.31	25 (49%)
36	CLA	J	311	-	50,54,73	1.37	9 (18%)	59,90,113	1.47	7 (11%)
36	CLA	C	210	3	50,54,73	1.39	8 (16%)	59,90,113	1.54	7 (11%)
36	CLA	I	306	9	69,73,73	1.65	15 (21%)	82,113,113	2.48	26 (31%)
36	CLA	E	314	-	69,73,73	1.11	9 (13%)	82,113,113	1.49	9 (10%)
35	A86	P	303	-	47,50,50	1.61	7 (14%)	51,76,76	3.36	23 (45%)
36	CLA	b	819	-	63,67,73	1.26	8 (12%)	74,105,113	1.85	18 (24%)
36	CLA	a	836	-	69,73,73	1.08	7 (10%)	82,113,113	1.56	9 (10%)
34	DD6	E	306	-	40,45,45	1.57	2 (5%)	51,67,67	2.01	10 (19%)
35	A86	S	301	-	47,50,50	1.84	6 (12%)	51,76,76	4.27	25 (49%)
34	DD6	K	305	-	40,45,45	1.55	2 (5%)	51,67,67	2.00	14 (27%)
36	CLA	S	317	-	45,49,73	1.42	8 (17%)	54,84,113	1.53	6 (11%)
36	CLA	A	310	-	69,73,73	1.14	11 (15%)	82,113,113	1.35	8 (9%)
36	CLA	N	319	-	46,50,73	3.23	12 (26%)	53,85,113	5.26	30 (56%)
36	CLA	a	835	-	55,59,73	1.31	10 (18%)	64,96,113	1.43	6 (9%)
36	CLA	V	308	-	69,73,73	1.14	9 (13%)	82,113,113	1.36	8 (9%)
36	CLA	L	310	-	58,62,73	1.28	8 (13%)	68,99,113	1.30	5 (7%)
36	CLA	N	309	-	55,59,73	1.33	7 (12%)	64,96,113	1.73	7 (10%)
36	CLA	F	313	-	56,60,73	1.24	8 (14%)	65,97,113	1.43	5 (7%)
37	KC1	Q	313	-	49,53,53	2.85	21 (42%)	61,89,89	5.74	38 (62%)
34	DD6	j	103	-	40,45,45	1.54	2 (5%)	51,67,67	1.81	14 (27%)
42	LMG	J	319	-	44,44,55	1.00	2 (4%)	52,52,63	1.12	4 (7%)
35	A86	I	302	-	47,50,50	1.46	6 (12%)	51,76,76	2.33	17 (33%)
36	CLA	J	309	-	69,73,73	1.16	10 (14%)	82,113,113	1.25	6 (7%)
36	CLA	B	311	-	59,63,73	1.29	7 (11%)	70,101,113	1.67	11 (15%)
36	CLA	a	832	-	69,73,73	1.13	7 (10%)	82,113,113	1.49	10 (12%)
36	CLA	I	308	-	69,73,73	1.85	16 (23%)	82,113,113	2.50	22 (26%)
41	LHG	D	318	36	45,45,48	0.30	0	48,51,54	0.40	0
36	CLA	D	317	-	62,66,73	1.20	9 (14%)	73,104,113	1.39	6 (8%)
39	LMT	G	322	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DD6	D	303	-	40,45,45	2.19	7 (17%)	51,67,67	2.63	18 (35%)
37	KC1	M	313	13,36	49,53,53	2.67	20 (40%)	61,89,89	4.95	38 (62%)
36	CLA	I	309	9	50,54,73	1.35	9 (18%)	59,90,113	1.92	8 (13%)
35	A86	S	304	-	47,50,50	1.48	6 (12%)	51,76,76	2.61	18 (35%)
36	CLA	L	320	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	6 (7%)
45	SF4	b	803	20,21	0,12,12	-	-	-		
36	CLA	H	318	-	54,58,73	1.32	11 (20%)	64,95,113	1.52	8 (12%)
36	CLA	G	315	-	60,64,73	1.91	15 (25%)	71,102,113	2.65	21 (29%)
41	LHG	f	809	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	3 (6%)
34	DD6	O	304	-	40,45,45	1.48	2 (5%)	51,67,67	1.95	13 (25%)
36	CLA	a	803	36	59,63,73	1.21	11 (18%)	70,101,113	1.54	11 (15%)
35	A86	U	304	37	47,50,50	1.44	5 (10%)	51,76,76	2.59	23 (45%)
36	CLA	C	208	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
36	CLA	D	312	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
36	CLA	T	313	18	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
34	DD6	A	303	-	40,45,45	1.55	2 (5%)	51,67,67	1.84	10 (19%)
36	CLA	C	214	-	45,49,73	1.37	9 (20%)	54,84,113	1.58	6 (11%)
35	A86	F	304	36	47,50,50	1.49	6 (12%)	51,76,76	2.38	16 (31%)
39	LMT	U	315	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
36	CLA	D	315	-	45,49,73	1.35	9 (20%)	54,84,113	1.79	9 (16%)
36	CLA	U	311	32	69,73,73	1.18	10 (14%)	82,113,113	1.54	12 (14%)
34	DD6	L	305	-	40,45,45	1.57	2 (5%)	51,67,67	1.98	16 (31%)
36	CLA	R	315	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	5 (6%)
35	A86	M	305	-	47,50,50	1.62	6 (12%)	51,76,76	2.59	15 (29%)
36	CLA	a	817	-	69,73,73	1.15	8 (11%)	82,113,113	1.60	14 (17%)
36	CLA	N	308	-	69,73,73	1.30	7 (10%)	82,113,113	1.78	19 (23%)
42	LMG	a	852	-	54,54,55	0.91	2 (3%)	62,62,63	1.04	3 (4%)
35	A86	V	301	35	47,50,50	1.47	6 (12%)	51,76,76	2.51	18 (35%)
36	CLA	W	214	-	45,49,73	1.55	7 (15%)	54,84,113	1.77	11 (20%)
36	CLA	F	314	35,6	69,73,73	1.14	11 (15%)	82,113,113	1.45	8 (9%)
36	CLA	H	312	-	69,73,73	1.13	9 (13%)	82,113,113	1.47	10 (12%)
35	A86	X	314	-	47,50,50	1.50	6 (12%)	51,76,76	2.46	15 (29%)
34	DD6	D	304	-	40,45,45	1.53	2 (5%)	51,67,67	1.90	12 (23%)
34	DD6	W	205	-	40,45,45	1.54	2 (5%)	51,67,67	2.01	14 (27%)
44	BCR	i	103	-	41,41,41	1.19	4 (9%)	56,56,56	1.34	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	W	210	-	50,54,73	1.37	8 (16%)	59,90,113	1.84	15 (25%)
36	CLA	a	811	-	58,62,73	1.23	8 (13%)	68,99,113	1.41	5 (7%)
36	CLA	Q	309	15	50,54,73	1.36	8 (16%)	59,90,113	1.59	7 (11%)
34	DD6	D	301	-	40,45,45	1.54	2 (5%)	51,67,67	2.00	15 (29%)
41	LHG	a	850	-	46,46,48	0.96	2 (4%)	49,52,54	1.05	3 (6%)
42	LMG	h	206	-	45,45,55	0.99	2 (4%)	53,53,63	1.04	4 (7%)
36	CLA	f	802	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	8 (9%)
35	A86	L	307	-	47,50,50	1.47	6 (12%)	51,76,76	2.33	13 (25%)
36	CLA	D	311	-	50,54,73	1.33	8 (16%)	59,90,113	1.46	6 (10%)
36	CLA	N	313	-	45,49,73	1.46	7 (15%)	54,84,113	1.72	13 (24%)
36	CLA	b	808	-	69,73,73	1.11	7 (10%)	82,113,113	1.37	6 (7%)
36	CLA	V	307	-	55,59,73	1.32	8 (14%)	64,96,113	1.37	5 (7%)
34	DD6	M	303	-	40,45,45	1.56	2 (5%)	51,67,67	1.95	12 (23%)
44	BCR	b	844	-	41,41,41	1.13	4 (9%)	56,56,56	1.33	5 (8%)
36	CLA	C	205	-	47,51,73	1.33	8 (17%)	55,86,113	1.53	7 (12%)
36	CLA	a	829	-	69,73,73	1.18	7 (10%)	82,113,113	1.60	12 (14%)
36	CLA	G	312	7	62,66,73	1.19	9 (14%)	73,104,113	1.45	5 (6%)
36	CLA	U	309	-	50,54,73	1.41	7 (14%)	59,90,113	1.69	9 (15%)
44	BCR	b	846	-	41,41,41	1.18	4 (9%)	56,56,56	1.46	11 (19%)
35	A86	K	302	-	47,50,50	1.58	5 (10%)	51,76,76	2.88	20 (39%)
36	CLA	F	309	-	69,73,73	1.14	9 (13%)	82,113,113	1.41	10 (12%)
39	LMT	U	314	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
39	LMT	E	323	-	36,36,36	0.35	0	47,47,47	0.83	1 (2%)
39	LMT	G	323	-	36,36,36	0.39	0	47,47,47	0.83	0
36	CLA	b	817	-	63,67,73	1.66	13 (20%)	74,105,113	2.19	19 (25%)
34	DD6	S	306	-	40,45,45	1.51	2 (5%)	51,67,67	1.95	12 (23%)
34	DD6	K	304	-	40,45,45	1.57	2 (5%)	51,67,67	1.85	11 (21%)
36	CLA	O	308	-	69,73,73	1.16	8 (11%)	82,113,113	1.42	9 (10%)
37	KC1	T	315	-	49,53,53	2.69	19 (38%)	61,89,89	4.53	35 (57%)
39	LMT	F	320	-	36,36,36	0.39	0	47,47,47	0.68	1 (2%)
35	A86	L	306	37	47,50,50	1.34	4 (8%)	51,76,76	2.81	18 (35%)
42	LMG	L	321	40	33,33,55	1.14	2 (6%)	41,41,63	1.16	3 (7%)
36	CLA	B	306	-	50,54,73	1.31	8 (16%)	59,90,113	1.59	5 (8%)
35	A86	V	304	-	47,50,50	2.01	8 (17%)	51,76,76	3.65	18 (35%)
36	CLA	K	309	-	63,67,73	1.22	9 (14%)	74,105,113	1.33	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	V	306	33	69,73,73	1.18	7 (10%)	82,113,113	1.49	10 (12%)
38	SQD	A	315	-	26,28,54	1.40	3 (11%)	36,39,65	1.25	2 (5%)
35	A86	J	302	-	47,50,50	1.50	7 (14%)	51,76,76	2.43	14 (27%)
38	SQD	b	804	-	44,46,54	1.20	3 (6%)	54,57,65	1.18	3 (5%)
35	A86	E	302	-	47,50,50	1.47	6 (12%)	51,76,76	2.49	13 (25%)
35	A86	T	301	36	47,50,50	1.49	6 (12%)	51,76,76	2.47	16 (31%)
36	CLA	S	321	-	56,60,73	1.29	9 (16%)	65,97,113	1.64	8 (12%)
36	CLA	b	811	-	69,73,73	1.15	9 (13%)	82,113,113	1.52	8 (9%)
35	A86	W	202	36	47,50,50	1.70	8 (17%)	51,76,76	3.40	27 (52%)
41	LHG	b	850	36	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
36	CLA	J	308	-	65,69,73	1.19	8 (12%)	77,108,113	1.61	9 (11%)
36	CLA	h	203	-	69,73,73	1.11	8 (11%)	82,113,113	1.45	8 (9%)
35	A86	T	306	-	47,50,50	1.40	6 (12%)	51,76,76	2.85	19 (37%)
35	A86	K	301	-	47,50,50	1.49	6 (12%)	51,76,76	2.55	14 (27%)
36	CLA	G	309	-	69,73,73	1.14	12 (17%)	82,113,113	1.79	13 (15%)
36	CLA	l	204	28	53,57,73	1.97	14 (26%)	61,93,113	2.33	19 (31%)
37	KC1	A	312	-	49,53,53	2.71	19 (38%)	61,89,89	5.93	40 (65%)
36	CLA	G	311	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	8 (9%)
36	CLA	H	306	-	65,69,73	1.17	9 (13%)	77,108,113	1.31	4 (5%)
35	A86	A	316	-	47,50,50	1.48	6 (12%)	51,76,76	2.45	17 (33%)
37	KC1	X	311	-	49,53,53	2.81	18 (36%)	61,89,89	4.08	35 (57%)
36	CLA	a	810	36	66,70,73	1.10	8 (12%)	78,109,113	1.41	6 (7%)
37	KC1	G	318	-	49,53,53	2.69	20 (40%)	61,89,89	4.16	40 (65%)
36	CLA	b	815	-	69,73,73	1.18	10 (14%)	82,113,113	1.36	8 (9%)
36	CLA	E	315	-	69,73,73	1.90	18 (26%)	82,113,113	2.63	29 (35%)
36	CLA	T	311	18	69,73,73	1.17	9 (13%)	82,113,113	1.89	14 (17%)
36	CLA	I	314	-	45,49,73	1.40	6 (13%)	54,84,113	1.60	6 (11%)
41	LHG	O	318	-	48,48,48	0.93	3 (6%)	51,54,54	1.24	5 (9%)
37	KC1	G	317	-	49,53,53	2.67	21 (42%)	61,89,89	4.15	35 (57%)
36	CLA	a	827	-	66,70,73	1.16	8 (12%)	78,109,113	1.50	10 (12%)
35	A86	O	303	-	47,50,50	1.51	7 (14%)	51,76,76	2.22	17 (33%)
36	CLA	I	312	9	56,60,73	1.29	8 (14%)	65,97,113	1.42	5 (7%)
42	LMG	D	320	41	46,46,55	0.98	2 (4%)	54,54,63	1.04	4 (7%)
36	CLA	R	313	-	69,73,73	1.14	10 (14%)	82,113,113	1.23	6 (7%)
42	LMG	G	325	-	55,55,55	0.89	2 (3%)	63,63,63	1.02	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	LMG	V	316	-	46,46,55	0.99	2 (4%)	54,54,63	1.05	3 (5%)
36	CLA	B	308	-	69,73,73	1.21	7 (10%)	82,113,113	1.42	12 (14%)
36	CLA	U	306	32	69,73,73	1.83	16 (23%)	82,113,113	2.48	26 (31%)
36	CLA	a	828	-	69,73,73	1.12	8 (11%)	82,113,113	1.42	9 (10%)
42	LMG	D	321	-	37,37,55	1.09	2 (5%)	45,45,63	1.04	2 (4%)
35	A86	V	303	35	47,50,50	1.38	5 (10%)	51,76,76	3.56	21 (41%)
35	A86	O	301	-	47,50,50	1.51	6 (12%)	51,76,76	2.45	16 (31%)
37	KC1	R	317	-	49,53,53	2.66	20 (40%)	61,89,89	4.92	36 (59%)
35	A86	O	305	-	47,50,50	1.68	6 (12%)	51,76,76	2.54	19 (37%)
36	CLA	a	826	-	69,73,73	1.13	10 (14%)	82,113,113	1.50	10 (12%)
36	CLA	W	201	-	52,56,73	1.33	8 (15%)	61,92,113	1.43	5 (8%)
35	A86	M	302	-	47,50,50	1.45	6 (12%)	51,76,76	2.62	16 (31%)
35	A86	X	305	-	47,50,50	1.55	6 (12%)	51,76,76	2.82	16 (31%)
36	CLA	C	209	-	69,73,73	1.19	9 (13%)	82,113,113	1.37	7 (8%)
36	CLA	O	312	-	44,48,73	1.69	11 (25%)	51,82,113	1.94	8 (15%)
41	LHG	R	323	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
36	CLA	T	309	18	69,73,73	1.13	9 (13%)	82,113,113	1.39	7 (8%)
36	CLA	J	316	-	50,54,73	1.35	7 (14%)	59,90,113	1.70	8 (13%)
36	CLA	b	816	-	64,68,73	1.91	16 (25%)	76,107,113	1.95	18 (23%)
36	CLA	E	316	-	69,73,73	1.15	7 (10%)	82,113,113	1.52	9 (10%)
39	LMT	I	317	-	36,36,36	0.41	0	47,47,47	0.77	1 (2%)
35	A86	G	305	-	47,50,50	1.45	6 (12%)	51,76,76	2.51	17 (33%)
36	CLA	D	310	-	69,73,73	1.09	7 (10%)	82,113,113	1.43	9 (10%)
36	CLA	S	315	17	47,51,73	1.41	7 (14%)	55,86,113	1.97	10 (18%)
34	DD6	P	305	-	40,45,45	1.57	2 (5%)	51,67,67	2.03	13 (25%)
36	CLA	f	805	25	56,60,73	1.24	8 (14%)	65,97,113	1.49	6 (9%)
37	KC1	H	313	-	49,53,53	2.60	20 (40%)	61,89,89	4.19	35 (57%)
36	CLA	V	305	35	65,69,73	1.28	6 (9%)	77,108,113	1.41	8 (10%)
34	DD6	E	301	-	40,45,45	1.53	2 (5%)	51,67,67	1.92	10 (19%)
36	CLA	R	318	35	45,49,73	1.42	8 (17%)	54,84,113	1.55	7 (12%)
37	KC1	S	316	-	49,53,53	2.77	21 (42%)	61,89,89	4.94	38 (62%)
36	CLA	H	310	8	50,54,73	1.73	12 (24%)	59,90,113	2.66	18 (30%)
36	CLA	J	315	-	45,49,73	1.40	8 (17%)	54,84,113	1.62	6 (11%)
36	CLA	D	313	-	69,73,73	1.10	9 (13%)	82,113,113	1.50	10 (12%)
36	CLA	W	212	19	69,73,73	1.17	8 (11%)	82,113,113	1.54	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	LHG	i	104	-	45,45,48	0.98	2 (4%)	48,51,54	1.04	2 (4%)
36	CLA	a	834	20	49,53,73	1.36	10 (20%)	58,89,113	1.54	6 (10%)
36	CLA	b	814	-	59,63,73	1.22	9 (15%)	70,101,113	1.37	4 (5%)
36	CLA	A	309	1	50,54,73	1.35	8 (16%)	59,90,113	1.46	4 (6%)
36	CLA	b	837	-	69,73,73	1.12	8 (11%)	82,113,113	1.43	9 (10%)
36	CLA	C	212	35	69,73,73	1.12	10 (14%)	82,113,113	1.53	12 (14%)
37	KC1	D	314	4	49,53,53	2.61	20 (40%)	61,89,89	4.40	36 (59%)
36	CLA	P	313	-	69,73,73	1.14	8 (11%)	82,113,113	1.30	6 (7%)
45	SF4	c	102	-	0,12,12	-	-	-		
35	A86	P	307	-	47,50,50	1.48	5 (10%)	51,76,76	2.43	15 (29%)
35	A86	X	304	-	47,50,50	1.58	6 (12%)	51,76,76	3.35	19 (37%)
36	CLA	F	312	-	69,73,73	1.14	9 (13%)	82,113,113	1.32	6 (7%)
35	A86	B	303	-	47,50,50	1.55	5 (10%)	51,76,76	3.71	23 (45%)
42	LMG	J	318	-	55,55,55	0.89	2 (3%)	63,63,63	1.03	3 (4%)
36	CLA	E	311	-	69,73,73	1.13	8 (11%)	82,113,113	1.31	7 (8%)
35	A86	R	301	-	47,50,50	1.70	6 (12%)	51,76,76	3.18	22 (43%)
36	CLA	G	307	-	45,50,73	2.18	14 (31%)	52,85,113	3.05	18 (34%)
36	CLA	b	809	-	69,73,73	1.13	9 (13%)	82,113,113	1.29	6 (7%)
44	BCR	f	806	-	41,41,41	1.19	3 (7%)	56,56,56	1.24	8 (14%)
36	CLA	H	317	8	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
36	CLA	b	824	-	57,61,73	1.94	15 (26%)	67,98,113	2.44	24 (35%)
37	KC1	B	310	-	49,53,53	2.83	18 (36%)	61,89,89	4.20	32 (52%)
40	DGD	L	302	42	48,48,67	0.99	2 (4%)	62,62,81	1.07	4 (6%)
35	A86	T	302	-	47,50,50	1.42	5 (10%)	51,76,76	2.56	21 (41%)
44	BCR	l	203	-	41,41,41	1.25	4 (9%)	56,56,56	1.23	6 (10%)
36	CLA	I	310	35	69,73,73	1.13	11 (15%)	82,113,113	1.36	6 (7%)
35	A86	B	301	-	47,50,50	1.48	6 (12%)	51,76,76	2.35	15 (29%)
36	CLA	I	313	-	45,49,73	1.38	9 (20%)	54,84,113	1.56	6 (11%)
36	CLA	W	207	34	69,73,73	1.16	7 (10%)	82,113,113	1.41	7 (8%)
35	A86	R	306	-	47,50,50	1.54	6 (12%)	51,76,76	2.81	15 (29%)
36	CLA	a	831	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
35	A86	J	301	-	47,50,50	1.53	6 (12%)	51,76,76	2.58	19 (37%)
36	CLA	Q	308	-	69,73,73	1.15	10 (14%)	82,113,113	1.41	10 (12%)
39	LMT	K	318	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
35	A86	Q	303	-	47,50,50	1.55	7 (14%)	51,76,76	2.55	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	V	310	33	69,73,73	1.14	7 (10%)	82,113,113	1.31	6 (7%)
36	CLA	b	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.31	5 (6%)
36	CLA	a	805	20	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
36	CLA	S	314	-	69,73,73	1.21	11 (15%)	82,113,113	1.44	9 (10%)
36	CLA	a	815	46	49,53,73	1.34	10 (20%)	58,89,113	1.52	4 (6%)
36	CLA	l	205	-	69,73,73	1.48	13 (18%)	82,113,113	2.18	18 (21%)
43	PQN	b	842	-	34,34,34	1.59	2 (5%)	43,45,45	1.22	4 (9%)
34	DD6	H	303	-	40,45,45	1.54	2 (5%)	51,67,67	1.96	11 (21%)
36	CLA	G	314	7	45,49,73	1.38	8 (17%)	54,84,113	1.68	7 (12%)
36	CLA	J	312	10	69,73,73	1.11	9 (13%)	82,113,113	1.40	8 (9%)
36	CLA	N	315	-	45,49,73	1.43	7 (15%)	54,84,113	1.71	11 (20%)
36	CLA	E	312	-	69,73,73	1.14	9 (13%)	82,113,113	1.42	8 (9%)
36	CLA	a	825	-	69,73,73	1.29	10 (14%)	82,113,113	1.73	10 (12%)
36	CLA	M	308	-	56,60,73	1.29	10 (17%)	65,97,113	1.60	7 (10%)
34	DD6	S	307	-	40,45,45	1.57	2 (5%)	51,67,67	2.07	15 (29%)
36	CLA	B	309	2	56,60,73	1.70	10 (17%)	65,97,113	2.13	20 (30%)
36	CLA	j	106	27	46,50,73	1.33	8 (17%)	53,85,113	1.55	4 (7%)
35	A86	Q	301	-	47,50,50	1.51	7 (14%)	51,76,76	2.22	17 (33%)
36	CLA	L	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.56	6 (11%)
36	CLA	V	309	33	47,51,73	1.37	8 (17%)	55,86,113	1.89	10 (18%)
36	CLA	K	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.50	9 (15%)
42	LMG	m	102	-	37,37,55	1.09	2 (5%)	45,45,63	1.09	3 (6%)
35	A86	S	308	37	47,50,50	1.47	6 (12%)	51,76,76	2.43	17 (33%)
36	CLA	V	311	33	69,73,73	1.14	9 (13%)	82,113,113	1.62	13 (15%)
36	CLA	b	805	36	69,73,73	1.21	8 (11%)	82,113,113	1.31	13 (15%)
36	CLA	b	823	-	59,63,73	1.20	10 (16%)	70,101,113	1.43	7 (10%)
35	A86	N	302	-	47,50,50	1.39	6 (12%)	51,76,76	2.46	15 (29%)
36	CLA	S	319	-	69,73,73	1.19	9 (13%)	82,113,113	1.46	9 (10%)
35	A86	F	302	-	47,50,50	1.48	6 (12%)	51,76,76	2.34	14 (27%)
36	CLA	a	822	-	55,59,73	1.50	9 (16%)	64,96,113	2.15	16 (25%)
36	CLA	M	315	-	51,55,73	1.34	8 (15%)	60,91,113	1.53	5 (8%)
35	A86	U	303	36	47,50,50	1.44	6 (12%)	51,76,76	2.35	14 (27%)
36	CLA	L	311	-	69,73,73	1.14	10 (14%)	82,113,113	1.33	10 (12%)
36	CLA	a	837	-	69,73,73	1.11	7 (10%)	82,113,113	1.39	9 (10%)
36	CLA	S	309	-	65,69,73	1.22	10 (15%)	77,108,113	1.27	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LMT	E	320	-	36,36,36	0.37	0	47,47,47	0.67	0
36	CLA	S	311	35	50,54,73	1.40	9 (18%)	59,90,113	1.52	8 (13%)
35	A86	O	319	35,36	47,50,50	1.44	7 (14%)	51,76,76	2.61	16 (31%)
39	LMT	b	848	-	36,36,36	0.38	0	47,47,47	0.68	1 (2%)
40	DGD	C	215	-	58,58,67	0.90	2 (3%)	72,72,81	0.96	3 (4%)
36	CLA	W	211	-	69,73,73	1.17	7 (10%)	82,113,113	1.47	7 (8%)
36	CLA	D	309	-	59,63,73	2.05	17 (28%)	70,101,113	2.98	29 (41%)
35	A86	O	302	-	47,50,50	1.62	6 (12%)	51,76,76	3.36	23 (45%)
36	CLA	F	310	-	60,64,73	1.20	9 (15%)	71,102,113	1.49	11 (15%)
36	CLA	T	308	-	65,69,73	1.19	7 (10%)	77,108,113	1.40	6 (7%)
35	A86	F	307	-	47,50,50	1.42	5 (10%)	51,76,76	3.67	21 (41%)
41	LHG	f	808	-	48,48,48	0.95	2 (4%)	51,54,54	1.03	3 (5%)
36	CLA	N	317	14	58,62,73	1.29	9 (15%)	68,99,113	1.48	11 (16%)
36	CLA	X	312	-	45,49,73	1.41	8 (17%)	54,84,113	1.71	8 (14%)
36	CLA	P	316	-	45,49,73	1.41	7 (15%)	54,84,113	1.71	9 (16%)
36	CLA	a	830	-	54,58,73	1.67	12 (22%)	64,95,113	3.27	18 (28%)
36	CLA	a	848	36	69,73,73	1.45	13 (18%)	82,113,113	1.90	18 (21%)
37	KC1	V	312	33	49,53,53	2.80	19 (38%)	61,89,89	4.34	33 (54%)
36	CLA	A	307	-	64,68,73	1.16	9 (14%)	76,107,113	1.37	9 (11%)
36	CLA	H	307	-	64,68,73	1.27	9 (14%)	76,107,113	1.81	20 (26%)
36	CLA	T	316	-	45,49,73	1.41	9 (20%)	54,84,113	1.53	6 (11%)
36	CLA	P	311	-	69,73,73	1.15	10 (14%)	82,113,113	1.41	10 (12%)
37	KC1	T	310	-	49,53,53	4.43	27 (55%)	61,89,89	6.41	40 (65%)
36	CLA	b	833	-	62,66,73	1.22	8 (12%)	73,104,113	1.56	11 (15%)
36	CLA	R	322	-	56,60,73	1.30	10 (17%)	65,97,113	1.67	8 (12%)
36	CLA	Q	312	-	45,49,73	1.42	7 (15%)	54,84,113	1.71	9 (16%)
45	SF4	c	101	22	0,12,12	-	-	-		
36	CLA	b	838	-	51,55,73	1.25	6 (11%)	60,91,113	1.43	6 (10%)
36	CLA	l	202	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
44	BCR	i	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
36	CLA	G	319	7	54,58,73	1.99	16 (29%)	64,95,113	3.78	30 (46%)
35	A86	K	303	-	47,50,50	1.48	6 (12%)	51,76,76	2.38	21 (41%)
35	A86	F	301	-	47,50,50	1.50	6 (12%)	51,76,76	2.55	15 (29%)
37	KC1	P	315	35	49,53,53	2.84	20 (40%)	61,89,89	5.74	38 (62%)
35	A86	N	303	-	47,50,50	1.39	6 (12%)	51,76,76	3.18	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	A86	U	301	-	47,50,50	1.59	5 (10%)	51,76,76	3.91	26 (50%)
34	DD6	Q	302	-	40,45,45	1.57	2 (5%)	51,67,67	2.03	14 (27%)
39	LMT	F	321	-	34,34,36	0.64	0	45,45,47	1.62	6 (13%)
39	LMT	B	312	-	36,36,36	0.42	0	47,47,47	0.68	1 (2%)
36	CLA	N	310	-	45,49,73	1.62	10 (22%)	54,84,113	2.22	20 (37%)
34	DD6	J	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.83	13 (25%)
36	CLA	a	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.39	10 (12%)
39	LMT	f	807	-	24,24,36	0.43	0	29,29,47	0.57	0
36	CLA	D	316	-	56,60,73	1.28	8 (14%)	65,97,113	1.66	10 (15%)
36	CLA	b	831	-	54,58,73	1.31	9 (16%)	64,95,113	1.51	9 (14%)
36	CLA	X	307	35	54,58,73	1.38	8 (14%)	64,95,113	1.75	10 (15%)
36	CLA	P	318	-	55,59,73	1.28	9 (16%)	64,96,113	1.45	5 (7%)
35	A86	J	303	-	47,50,50	1.59	6 (12%)	51,76,76	2.63	20 (39%)
37	KC1	O	313	-	49,53,53	2.84	21 (42%)	61,89,89	5.74	38 (62%)
36	CLA	X	306	-	65,69,73	1.21	6 (9%)	77,108,113	1.37	7 (9%)
44	BCR	a	846	-	41,41,41	1.16	3 (7%)	56,56,56	1.21	3 (5%)
36	CLA	F	316	6	45,49,73	1.37	9 (20%)	54,84,113	1.48	6 (11%)
36	CLA	b	830	-	69,73,73	1.20	8 (11%)	82,113,113	1.63	16 (19%)
36	CLA	R	319	-	49,53,73	1.38	7 (14%)	58,89,113	1.82	12 (20%)
36	CLA	P	309	41	69,73,73	1.14	10 (14%)	82,113,113	1.35	6 (7%)
36	CLA	P	310	41	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
39	LMT	E	321	-	23,23,36	0.45	0	28,28,47	0.60	0
36	CLA	E	317	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
44	BCR	a	844	-	41,41,41	1.07	3 (7%)	56,56,56	1.31	6 (10%)
36	CLA	O	310	15	50,54,73	1.35	8 (16%)	59,90,113	1.58	7 (11%)
36	CLA	a	809	-	60,64,73	1.19	9 (15%)	71,102,113	1.39	6 (8%)
42	LMG	I	315	-	55,55,55	0.89	2 (3%)	63,63,63	1.01	3 (4%)
35	A86	S	303	-	47,50,50	1.40	6 (12%)	51,76,76	3.19	22 (43%)
35	A86	T	304	-	47,50,50	1.29	5 (10%)	51,76,76	1.99	10 (19%)
36	CLA	A	311	-	69,73,73	1.14	8 (11%)	82,113,113	1.35	6 (7%)
36	CLA	O	316	-	69,73,73	1.82	15 (21%)	82,113,113	2.66	28 (34%)
36	CLA	K	310	-	66,70,73	1.90	18 (27%)	78,109,113	2.57	28 (35%)
35	A86	T	303	-	47,50,50	1.37	6 (12%)	51,76,76	2.82	23 (45%)
36	CLA	W	208	-	49,53,73	1.38	9 (18%)	58,89,113	1.46	5 (8%)
36	CLA	b	801	46	69,73,73	1.17	10 (14%)	82,113,113	1.39	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LMT	K	317	-	32,32,36	0.44	0	43,43,47	0.70	0
35	A86	G	302	-	47,50,50	1.33	5 (10%)	51,76,76	2.26	14 (27%)
39	LMT	I	318	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
36	CLA	K	316	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	4 (4%)
36	CLA	T	314	-	69,73,73	1.13	8 (11%)	82,113,113	1.52	10 (12%)
36	CLA	b	840	-	69,73,73	1.13	10 (14%)	82,113,113	1.48	12 (14%)
36	CLA	E	308	5	53,57,73	1.29	10 (18%)	61,93,113	1.51	7 (11%)
36	CLA	P	319	-	64,68,73	1.90	12 (18%)	76,107,113	2.06	15 (19%)
36	CLA	U	305	-	65,69,73	1.20	8 (12%)	77,108,113	1.32	5 (6%)
35	A86	L	304	-	47,50,50	1.61	6 (12%)	51,76,76	2.49	15 (29%)
36	CLA	G	310	-	69,73,73	1.14	10 (14%)	82,113,113	1.24	7 (8%)
37	KC1	G	308	-	49,53,53	2.66	20 (40%)	61,89,89	4.49	36 (59%)
36	CLA	N	307	-	65,69,73	1.21	7 (10%)	77,108,113	1.33	4 (5%)
35	A86	D	302	-	47,50,50	1.46	6 (12%)	51,76,76	2.32	13 (25%)
35	A86	R	302	-	47,50,50	1.60	7 (14%)	51,76,76	2.64	16 (31%)
36	CLA	a	818	-	69,73,73	1.16	6 (8%)	82,113,113	1.53	9 (10%)
36	CLA	V	313	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
36	CLA	X	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.57	8 (14%)
35	A86	E	305	-	47,50,50	1.47	6 (12%)	51,76,76	2.36	16 (31%)
35	A86	X	303	36	47,50,50	1.74	6 (12%)	51,76,76	3.74	23 (45%)
36	CLA	b	836	-	62,66,73	1.99	15 (24%)	73,104,113	2.94	25 (34%)
37	KC1	W	217	-	49,53,53	2.81	19 (38%)	61,89,89	4.08	34 (55%)
35	A86	N	301	-	47,50,50	1.84	6 (12%)	51,76,76	4.28	25 (49%)
36	CLA	H	305	-	52,56,73	1.33	7 (13%)	61,92,113	1.47	6 (9%)
35	A86	N	305	-	47,50,50	1.77	9 (19%)	51,76,76	2.18	15 (29%)
34	DD6	F	303	-	40,45,45	1.55	2 (5%)	51,67,67	1.88	13 (25%)
36	CLA	S	313	-	50,54,73	1.34	7 (14%)	59,90,113	1.79	11 (18%)
36	CLA	A	308	-	69,73,73	1.12	9 (13%)	82,113,113	1.43	10 (12%)
36	CLA	P	302	-	46,50,73	1.36	7 (15%)	53,85,113	1.63	7 (13%)
36	CLA	K	308	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
36	CLA	a	807	20	69,73,73	1.11	10 (14%)	82,113,113	1.47	10 (12%)
36	CLA	M	306	37,13	59,63,73	1.25	8 (13%)	70,101,113	1.53	9 (12%)
36	CLA	O	307	-	69,73,73	1.14	10 (14%)	82,113,113	1.34	6 (7%)
36	CLA	R	316	-	50,54,73	1.39	11 (22%)	59,90,113	1.94	13 (22%)
44	BCR	b	847	-	41,41,41	1.19	4 (9%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	T	312	18	50,54,73	1.37	8 (16%)	59,90,113	1.64	10 (16%)
39	LMT	a	854	-	36,36,36	0.40	0	47,47,47	0.76	0
36	CLA	F	317	6	60,64,73	1.89	14 (23%)	71,102,113	2.64	24 (33%)
36	CLA	L	309	-	69,73,73	1.13	9 (13%)	82,113,113	1.32	9 (10%)
36	CLA	K	315	-	45,49,73	1.39	9 (20%)	54,84,113	1.61	7 (12%)
41	LHG	O	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.10	4 (9%)
36	CLA	b	810	-	69,73,73	1.09	6 (8%)	82,113,113	1.30	5 (6%)
35	A86	J	306	-	47,50,50	1.50	5 (10%)	51,76,76	2.35	14 (27%)
36	CLA	X	308	19	51,55,73	2.43	10 (19%)	60,91,113	2.47	20 (33%)
40	DGD	b	849	-	61,61,67	1.04	4 (6%)	75,75,81	1.46	11 (14%)
36	CLA	j	101	-	69,73,73	1.14	9 (13%)	82,113,113	1.26	7 (8%)
41	LHG	a	843	36	26,26,48	1.25	2 (7%)	29,32,54	1.29	3 (10%)
35	A86	T	307	-	47,50,50	1.48	6 (12%)	51,76,76	2.92	19 (37%)
36	CLA	R	320	16	49,53,73	1.42	9 (18%)	58,89,113	1.68	11 (18%)
35	A86	N	306	-	47,50,50	1.47	5 (10%)	51,76,76	2.42	17 (33%)
35	A86	U	302	-	47,50,50	1.47	6 (12%)	51,76,76	2.59	20 (39%)
36	CLA	C	206	-	65,69,73	1.17	7 (10%)	77,108,113	1.36	4 (5%)
36	CLA	f	803	-	69,73,73	1.78	15 (21%)	82,113,113	2.43	28 (34%)
34	DD6	E	303	-	40,45,45	1.54	2 (5%)	51,67,67	1.96	11 (21%)
34	DD6	G	303	-	40,45,45	1.54	2 (5%)	51,67,67	1.86	12 (23%)
36	CLA	S	310	-	69,73,73	1.15	9 (13%)	82,113,113	1.58	12 (14%)
39	LMT	B	313	-	36,36,36	0.43	0	47,47,47	0.74	1 (2%)
34	DD6	H	302	-	40,45,45	1.53	2 (5%)	51,67,67	1.85	13 (25%)
44	BCR	b	845	-	41,41,41	1.19	3 (7%)	56,56,56	1.40	9 (16%)
36	CLA	C	207	-	69,73,73	1.96	17 (24%)	82,113,113	2.78	27 (32%)
36	CLA	R	321	-	69,73,73	1.19	10 (14%)	82,113,113	1.42	11 (13%)
35	A86	L	319	-	47,50,50	1.61	6 (12%)	51,76,76	3.35	23 (45%)
35	A86	X	301	-	47,50,50	1.75	7 (14%)	51,76,76	3.44	28 (54%)
39	LMT	P	320	-	23,23,36	0.43	0	28,28,47	0.61	0
36	CLA	a	824	-	69,73,73	1.19	11 (15%)	82,113,113	1.80	19 (23%)
35	A86	S	305	-	47,50,50	1.65	5 (10%)	51,76,76	3.08	20 (39%)
36	CLA	P	308	-	65,69,73	1.19	8 (12%)	77,108,113	1.36	4 (5%)
36	CLA	U	310	-	69,73,73	1.17	8 (11%)	82,113,113	1.51	12 (14%)
36	CLA	b	807	-	49,53,73	1.30	10 (20%)	58,89,113	1.56	8 (13%)
36	CLA	Q	310	-	69,73,73	2.72	16 (23%)	82,113,113	2.80	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	KC1	M	318	-	49,53,53	4.79	25 (51%)	61,89,89	6.66	36 (59%)
36	CLA	l	201	-	69,73,73	1.12	9 (13%)	82,113,113	1.42	10 (12%)
36	CLA	l	206	46	54,58,73	1.26	8 (14%)	64,95,113	1.47	7 (10%)
36	CLA	b	835	-	49,53,73	1.34	9 (18%)	58,89,113	1.63	8 (13%)
36	CLA	a	802	-	69,73,73	1.24	7 (10%)	82,113,113	1.80	15 (18%)
35	A86	J	305	-	47,50,50	1.49	5 (10%)	51,76,76	2.43	17 (33%)
35	A86	P	304	-	47,50,50	1.50	7 (14%)	51,76,76	2.22	17 (33%)
42	LMG	G	324	-	55,55,55	0.91	2 (3%)	63,63,63	1.01	3 (4%)
34	DD6	A	301	-	40,45,45	1.56	2 (5%)	51,67,67	2.07	14 (27%)
36	CLA	b	820	21	64,68,73	1.20	10 (15%)	76,107,113	1.32	5 (6%)
36	CLA	X	310	-	45,49,73	1.47	8 (17%)	54,84,113	2.04	9 (16%)
36	CLA	M	314	-	45,49,73	1.40	9 (20%)	54,84,113	1.55	5 (9%)
37	KC1	N	314	-	49,53,53	2.81	21 (42%)	61,89,89	3.98	35 (57%)
36	CLA	F	311	-	56,60,73	1.25	8 (14%)	65,97,113	1.52	6 (9%)
34	DD6	C	201	-	40,45,45	1.57	2 (5%)	51,67,67	1.90	12 (23%)
36	CLA	R	314	16	50,54,73	1.38	8 (16%)	59,90,113	1.75	9 (15%)
34	DD6	E	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.77	10 (19%)
35	A86	h	202	-	47,50,50	1.45	6 (12%)	51,76,76	2.14	14 (27%)
34	DD6	I	303	-	40,45,45	1.58	3 (7%)	51,67,67	1.91	12 (23%)
36	CLA	H	311	-	69,73,73	1.10	9 (13%)	82,113,113	1.42	7 (8%)
36	CLA	K	312	-	69,73,73	1.13	9 (13%)	82,113,113	1.32	6 (7%)
36	CLA	S	318	-	46,50,73	1.38	6 (13%)	53,85,113	1.55	5 (9%)
37	KC1	O	315	15	49,53,53	2.84	22 (44%)	61,89,89	5.74	38 (62%)
41	LHG	G	321	36	46,46,48	0.96	2 (4%)	49,52,54	1.07	2 (4%)
36	CLA	b	802	-	69,73,73	1.11	8 (11%)	82,113,113	1.36	7 (8%)
35	A86	G	306	-	47,50,50	1.46	6 (12%)	51,76,76	2.65	20 (39%)
36	CLA	X	309	-	48,53,73	1.40	8 (16%)	56,89,113	1.65	9 (16%)
36	CLA	A	306	-	65,69,73	1.92	17 (26%)	77,108,113	2.56	29 (37%)
36	CLA	b	834	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	5 (6%)
35	A86	I	304	-	47,50,50	1.66	6 (12%)	51,76,76	3.12	21 (41%)
42	LMG	j	105	-	52,52,55	0.91	2 (3%)	60,60,63	1.01	3 (5%)
34	DD6	D	305	-	40,45,45	1.54	2 (5%)	51,67,67	1.63	11 (21%)
42	LMG	E	318	-	46,46,55	0.98	2 (4%)	54,54,63	1.07	3 (5%)
36	CLA	U	313	-	45,49,73	1.41	8 (17%)	54,84,113	1.69	9 (16%)
36	CLA	J	317	-	51,55,73	1.32	9 (17%)	60,91,113	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	LHG	l	208	-	47,47,48	0.95	2 (4%)	50,53,54	1.03	4 (8%)
36	CLA	b	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	8 (9%)
36	CLA	b	839	-	69,73,73	1.11	9 (13%)	82,113,113	1.41	6 (7%)
36	CLA	G	313	7	69,73,73	1.20	7 (10%)	82,113,113	1.82	14 (17%)
35	A86	H	301	-	47,50,50	1.40	5 (10%)	51,76,76	5.19	20 (39%)
37	KC1	L	315	35	49,53,53	2.75	18 (36%)	61,89,89	4.93	36 (59%)
35	A86	R	304	36	47,50,50	1.39	5 (10%)	51,76,76	3.29	18 (35%)
39	LMT	L	318	-	32,32,36	0.46	0	43,43,47	0.80	1 (2%)
37	KC1	C	213	-	49,53,53	2.69	19 (38%)	61,89,89	3.92	33 (54%)
36	CLA	S	312	-	69,73,73	1.17	10 (14%)	82,113,113	1.36	11 (13%)
36	CLA	b	812	21	69,73,73	1.16	8 (11%)	82,113,113	1.46	11 (13%)
35	A86	E	307	36	47,50,50	1.49	6 (12%)	51,76,76	2.39	14 (27%)
39	LMT	b	851	-	24,24,36	0.43	0	29,29,47	0.81	0
34	DD6	B	304	-	40,45,45	1.56	2 (5%)	51,67,67	2.08	14 (27%)
36	CLA	j	102	-	69,73,73	1.59	12 (17%)	82,113,113	2.16	18 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	b	806	-	1/1/15/20	14/39/115/115	-
36	CLA	a	812	-	1/1/15/20	13/39/115/115	-
36	CLA	a	823	-	2/2/13/20	12/27/103/115	-
36	CLA	A	314	-	1/1/15/20	21/39/115/115	-
36	CLA	R	312	-	1/1/15/20	13/39/115/115	-
36	CLA	b	813	-	1/1/13/20	3/25/101/115	-
36	CLA	O	306	-	1/1/14/20	7/35/111/115	-
36	CLA	C	211	-	1/1/15/20	13/39/115/115	-
36	CLA	W	215	-	1/1/11/20	4/19/95/115	-
36	CLA	L	313	-	1/1/15/20	8/39/115/115	-
36	CLA	A	305	1	1/1/11/20	5/20/96/115	-
37	KC1	E	309	-	-	5/15/71/71	-
39	LMT	L	303	-	-	10/21/61/61	0/2/2/2
36	CLA	N	311	-	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC1	L	317	-	-	3/15/71/71	-
44	BCR	a	847	-	-	6/29/63/63	0/2/2/2
36	CLA	W	216	35	1/1/11/20	4/15/91/115	-
41	LHG	D	319	42	-	30/53/53/53	-
36	CLA	D	307	41	1/1/14/20	19/35/111/115	-
36	CLA	b	827	-	1/1/15/20	8/39/115/115	-
41	LHG	I	316	-	-	29/53/53/53	-
35	A86	P	306	-	-	3/34/90/90	0/3/3/3
41	LHG	a	842	-	-	23/52/52/53	-
36	CLA	M	309	-	1/1/15/20	15/39/115/115	-
35	A86	F	306	-	-	0/34/90/90	1/3/3/3
36	CLA	a	838	-	1/1/15/20	8/39/115/115	-
36	CLA	P	314	-	-	20/33/109/115	-
36	CLA	b	828	-	1/1/15/20	14/39/115/115	-
35	A86	X	302	35	-	7/34/90/90	0/3/3/3
36	CLA	a	839	46	1/1/15/20	15/39/115/115	-
37	KC1	J	314	-	-	5/15/71/71	-
41	LHG	Q	315	36	-	31/53/53/53	-
35	A86	R	305	-	-	5/34/90/90	0/3/3/3
44	BCR	l	207	-	-	6/29/63/63	0/2/2/2
36	CLA	L	308	-	2/2/14/20	21/35/111/115	-
39	LMT	h	205	-	-	10/21/61/61	0/2/2/2
35	A86	C	202	36	-	8/34/90/90	0/3/3/3
35	A86	T	305	-	-	7/34/90/90	0/3/3/3
44	BCR	j	107	-	-	3/29/63/63	0/2/2/2
37	KC1	P	317	15	-	4/15/71/71	-
37	KC1	M	317	-	-	4/15/71/71	-
36	CLA	E	310	-	-	5/39/115/115	-
36	CLA	N	316	-	1/1/15/20	13/39/115/115	-
35	A86	Q	316	36	-	2/34/90/90	0/3/3/3
36	CLA	b	818	-	-	4/27/103/115	-
35	A86	M	301	-	-	8/34/90/90	0/3/3/3
36	CLA	a	813	-	1/1/11/20	0/15/91/115	-
36	CLA	a	820	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	U	307	-	1/1/12/20	2/21/97/115	-
35	A86	V	302	-	-	5/34/90/90	0/3/3/3
35	A86	A	302	-	-	9/34/90/90	0/3/3/3
36	CLA	M	310	35,13	1/1/11/20	6/17/93/115	-
35	A86	C	204	-	-	11/34/90/90	0/3/3/3
35	A86	L	301	-	-	5/34/90/90	1/3/3/3
36	CLA	a	841	41	1/1/12/20	6/24/100/115	-
36	CLA	B	305	-	1/1/15/20	21/39/115/115	-
36	CLA	E	313	-	2/2/15/20	10/39/115/115	-
36	CLA	a	801	-	1/1/15/20	10/39/115/115	-
37	KC1	W	213	-	-	5/15/71/71	-
34	DD6	A	304	-	-	4/26/80/80	0/3/3/3
36	CLA	M	316	36	1/1/10/20	6/12/88/115	-
36	CLA	X	313	-	-	6/12/88/115	-
44	BCR	b	843	-	-	9/29/63/63	0/2/2/2
36	CLA	M	311	35,13	1/1/15/20	9/39/115/115	-
35	A86	F	305	-	-	8/34/90/90	0/3/3/3
34	DD6	R	308	-	-	11/26/80/80	0/3/3/3
36	CLA	H	308	-	1/1/15/20	14/37/113/115	-
35	A86	I	301	-	-	11/34/90/90	0/3/3/3
36	CLA	b	841	41	1/1/15/20	7/39/115/115	-
36	CLA	Q	305	-	1/1/14/20	7/35/111/115	-
44	BCR	h	201	-	-	9/29/63/63	0/2/2/2
36	CLA	I	307	-	1/1/12/20	4/26/102/115	-
36	CLA	G	316	-	1/1/11/20	10/20/96/115	-
35	A86	H	304	-	-	8/34/90/90	0/3/3/3
36	CLA	J	310	-	1/1/15/20	10/39/115/115	-
36	CLA	H	316	-	1/1/15/20	18/39/115/115	-
36	CLA	V	314	-	1/1/15/20	18/39/115/115	-
36	CLA	D	308	-	1/1/15/20	14/39/115/115	-
36	CLA	L	312	12	-	7/17/93/115	-
36	CLA	K	313	-	1/1/15/20	11/39/115/115	-
36	CLA	a	806	-	2/2/15/20	11/39/115/115	-
36	CLA	L	314	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	I	311	9	1/1/15/20	14/39/115/115	-
41	LHG	F	319	-	-	32/45/45/53	-
36	CLA	M	307	-	1/1/15/20	12/39/115/115	-
36	CLA	N	312	-	1/1/11/20	9/18/94/115	-
34	DD6	a	849	-	-	6/26/80/80	0/3/3/3
36	CLA	J	313	-	1/1/15/20	14/39/115/115	-
41	LHG	F	318	-	-	15/34/34/53	-
36	CLA	Q	306	-	1/1/15/20	14/39/115/115	-
35	A86	C	203	-	-	7/34/90/90	1/3/3/3
43	PQN	a	840	-	-	7/23/43/43	0/2/2/2
36	CLA	P	312	15	1/1/11/20	9/17/93/115	-
37	KC1	F	308	6	-	7/15/71/71	-
36	CLA	a	808	20	1/1/15/20	11/39/115/115	-
36	CLA	K	307	-	2/2/14/20	21/35/111/115	-
37	KC1	Q	311	15	-	1/15/71/71	-
36	CLA	R	311	-	1/1/15/20	12/39/115/115	-
36	CLA	S	320	-	-	12/39/115/115	-
41	LHG	G	320	-	-	16/44/44/53	-
34	DD6	R	307	-	-	11/26/80/80	0/3/3/3
35	A86	W	203	36	-	6/34/90/90	0/3/3/3
35	A86	h	204	-	-	1/34/90/90	0/3/3/3
44	BCR	m	101	-	-	9/29/63/63	0/2/2/2
41	LHG	j	104	-	-	31/53/53/53	-
36	CLA	M	312	36	1/1/11/20	12/18/94/115	-
36	CLA	b	832	-	1/1/11/20	4/20/96/115	-
36	CLA	a	833	-	1/1/12/20	3/21/97/115	-
35	A86	S	302	-	-	6/34/90/90	0/3/3/3
41	LHG	G	301	-	-	24/53/53/53	-
36	CLA	O	314	-	1/1/10/20	4/10/86/115	-
37	KC1	F	315	-	-	3/15/71/71	-
34	DD6	W	204	36	-	7/26/80/80	0/3/3/3
36	CLA	W	218	-	1/1/10/20	6/13/89/115	-
39	LMT	a	851	-	-	15/21/61/61	0/2/2/2
36	CLA	a	814	-	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	BCR	a	845	-	-	7/29/63/63	0/2/2/2
36	CLA	H	315	-	1/1/15/20	15/39/115/115	-
36	CLA	a	821	-	1/1/11/20	4/20/96/115	-
35	A86	N	320	-	-	10/34/90/90	0/3/3/3
44	BCR	f	801	-	-	5/29/63/63	0/2/2/2
36	CLA	P	301	-	1/1/15/20	18/39/115/115	-
37	KC1	U	312	35	-	4/15/71/71	-
36	CLA	W	209	-	1/1/13/20	15/30/106/115	-
35	A86	N	304	-	-	8/34/90/90	0/3/3/3
41	LHG	E	322	-	-	28/53/53/53	-
36	CLA	Q	314	-	1/1/15/20	22/39/115/115	-
35	A86	Q	304	-	-	10/34/90/90	0/3/3/3
36	CLA	D	306	4	1/1/11/20	5/15/91/115	-
35	A86	K	306	-	-	9/34/90/90	0/3/3/3
35	A86	R	303	-	-	7/34/90/90	0/3/3/3
36	CLA	O	309	-	1/1/15/20	17/39/115/115	-
36	CLA	H	309	-	1/1/15/20	17/39/115/115	-
35	A86	M	304	-	-	14/34/90/90	0/3/3/3
36	CLA	b	826	46	1/1/14/20	11/38/114/115	-
36	CLA	a	816	-	1/1/15/20	20/39/115/115	-
39	LMT	a	853	-	-	10/18/58/61	0/2/2/2
36	CLA	I	305	-	2/2/14/20	11/35/111/115	-
36	CLA	B	307	-	1/1/11/20	7/17/93/115	-
36	CLA	i	102	-	1/1/15/20	17/39/115/115	-
36	CLA	J	307	10	1/1/14/20	11/35/111/115	-
42	LMG	E	319	-	-	22/35/55/70	0/1/1/1
36	CLA	W	206	-	1/1/14/20	8/35/111/115	-
36	CLA	O	311	-	1/1/13/20	9/31/107/115	-
39	LMT	P	321	-	-	10/14/34/61	0/1/1/2
36	CLA	A	313	-	1/1/10/20	4/10/86/115	-
36	CLA	H	314	-	1/1/10/20	2/10/86/115	-
36	CLA	b	821	46	1/1/15/20	11/39/115/115	-
36	CLA	a	819	-	1/1/11/20	5/15/91/115	-
36	CLA	R	310	-	1/1/14/20	15/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	N	318	-	1/1/11/20	7/18/94/115	-
36	CLA	f	804	46	2/2/15/20	10/39/115/115	-
36	CLA	U	308	35	1/1/13/20	11/29/105/115	-
36	CLA	b	822	-	1/1/11/20	4/17/93/115	-
34	DD6	B	302	-	-	4/26/80/80	0/3/3/3
37	KC1	K	314	-	-	5/15/71/71	-
42	LMG	V	315	-	-	24/41/61/70	0/1/1/1
36	CLA	Q	307	-	1/1/11/20	5/21/97/115	-
35	A86	R	309	-	-	8/34/90/90	0/3/3/3
35	A86	G	304	-	-	8/34/90/90	0/3/3/3
36	CLA	J	311	-	1/1/11/20	5/17/93/115	-
36	CLA	C	210	3	1/1/11/20	6/17/93/115	-
36	CLA	I	306	9	2/2/15/20	15/39/115/115	-
36	CLA	E	314	-	1/1/15/20	8/39/115/115	-
35	A86	P	303	-	-	9/34/90/90	0/3/3/3
36	CLA	b	819	-	1/1/13/20	7/32/108/115	-
36	CLA	a	836	-	1/1/15/20	11/39/115/115	-
34	DD6	E	306	-	-	4/26/80/80	0/3/3/3
35	A86	S	301	-	-	9/34/90/90	0/3/3/3
34	DD6	K	305	-	-	0/26/80/80	0/3/3/3
36	CLA	S	317	-	1/1/10/20	4/10/86/115	-
36	CLA	A	310	-	1/1/15/20	11/39/115/115	-
36	CLA	N	319	-	1/1/10/20	6/12/88/115	-
36	CLA	a	835	-	1/1/12/20	3/23/99/115	-
36	CLA	V	308	-	1/1/15/20	16/39/115/115	-
36	CLA	L	310	-	1/1/12/20	4/26/102/115	-
36	CLA	N	309	-	1/1/12/20	8/23/99/115	-
36	CLA	F	313	-	1/1/12/20	8/24/100/115	-
37	KC1	Q	313	-	-	1/15/71/71	-
34	DD6	j	103	-	-	8/26/80/80	0/3/3/3
42	LMG	J	319	-	-	22/39/59/70	0/1/1/1
35	A86	I	302	-	-	7/34/90/90	0/3/3/3
36	CLA	J	309	-	1/1/15/20	8/39/115/115	-
36	CLA	B	311	-	1/1/13/20	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	a	832	-	1/1/15/20	15/39/115/115	-
36	CLA	I	308	-	1/1/15/20	17/39/115/115	-
41	LHG	D	318	36	-	29/50/50/53	-
36	CLA	D	317	-	1/1/13/20	11/31/107/115	-
39	LMT	G	322	-	-	17/21/61/61	0/2/2/2
34	DD6	D	303	-	-	9/26/80/80	0/3/3/3
37	KC1	M	313	13,36	-	5/15/71/71	-
36	CLA	I	309	9	1/1/11/20	8/17/93/115	-
35	A86	S	304	-	-	8/34/90/90	0/3/3/3
36	CLA	L	320	-	1/1/15/20	10/39/115/115	-
45	SF4	b	803	20,21	-	-	0/6/5/5
36	CLA	H	318	-	1/1/12/20	7/21/97/115	-
36	CLA	G	315	-	2/2/13/20	12/29/105/115	-
41	LHG	f	809	-	-	28/46/46/53	-
34	DD6	O	304	-	-	5/26/80/80	0/3/3/3
36	CLA	a	803	36	1/1/13/20	5/27/103/115	-
35	A86	U	304	37	-	10/34/90/90	0/3/3/3
36	CLA	C	208	-	1/1/15/20	19/39/115/115	-
36	CLA	D	312	-	1/1/15/20	13/39/115/115	-
36	CLA	T	313	18	1/1/15/20	8/39/115/115	-
34	DD6	A	303	-	-	5/26/80/80	0/3/3/3
36	CLA	C	214	-	1/1/10/20	4/10/86/115	-
35	A86	F	304	36	-	4/34/90/90	0/3/3/3
39	LMT	U	315	-	-	17/21/61/61	0/2/2/2
36	CLA	D	315	-	1/1/10/20	2/10/86/115	-
36	CLA	U	311	32	1/1/15/20	20/39/115/115	-
34	DD6	L	305	-	-	6/26/80/80	0/3/3/3
36	CLA	R	315	-	1/1/15/20	14/39/115/115	-
36	CLA	a	817	-	1/1/15/20	16/39/115/115	-
35	A86	M	305	-	-	8/34/90/90	0/3/3/3
36	CLA	N	308	-	1/1/15/20	15/39/115/115	-
42	LMG	a	852	-	-	26/49/69/70	0/1/1/1
35	A86	V	301	35	-	10/34/90/90	1/3/3/3
36	CLA	W	214	-	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	F	314	35,6	1/1/15/20	16/39/115/115	-
36	CLA	H	312	-	1/1/15/20	17/39/115/115	-
35	A86	X	314	-	-	3/34/90/90	1/3/3/3
34	DD6	D	304	-	-	8/26/80/80	0/3/3/3
34	DD6	W	205	-	-	8/26/80/80	0/3/3/3
44	BCR	i	103	-	-	11/29/63/63	0/2/2/2
36	CLA	W	210	-	1/1/11/20	8/17/93/115	-
36	CLA	a	811	-	1/1/12/20	5/26/102/115	-
36	CLA	Q	309	15	1/1/11/20	9/17/93/115	-
34	DD6	D	301	-	-	11/26/80/80	0/3/3/3
41	LHG	a	850	-	-	36/51/51/53	-
42	LMG	h	206	-	-	24/40/60/70	0/1/1/1
36	CLA	f	802	-	1/1/15/20	12/39/115/115	-
35	A86	L	307	-	-	8/34/90/90	1/3/3/3
36	CLA	D	311	-	-	7/17/93/115	-
36	CLA	N	313	-	1/1/10/20	0/10/86/115	-
36	CLA	b	808	-	1/1/15/20	13/39/115/115	-
36	CLA	V	307	-	1/1/12/20	6/23/99/115	-
34	DD6	M	303	-	-	3/26/80/80	0/3/3/3
44	BCR	b	844	-	-	6/29/63/63	0/2/2/2
36	CLA	C	205	-	1/1/10/20	4/13/89/115	-
36	CLA	a	829	-	1/1/15/20	12/39/115/115	-
36	CLA	G	312	7	1/1/13/20	6/31/107/115	-
36	CLA	U	309	-	-	6/17/93/115	-
44	BCR	b	846	-	-	8/29/63/63	0/2/2/2
35	A86	K	302	-	-	8/34/90/90	0/3/3/3
36	CLA	F	309	-	1/1/15/20	13/39/115/115	-
39	LMT	U	314	-	-	14/21/61/61	0/2/2/2
39	LMT	E	323	-	-	11/21/61/61	0/2/2/2
39	LMT	G	323	-	-	17/21/61/61	0/2/2/2
36	CLA	b	817	-	2/2/13/20	9/32/108/115	-
34	DD6	S	306	-	-	5/26/80/80	0/3/3/3
34	DD6	K	304	-	-	2/26/80/80	0/3/3/3
36	CLA	O	308	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC1	T	315	-	-	7/15/71/71	-
39	LMT	F	320	-	-	12/21/61/61	0/2/2/2
35	A86	L	306	37	-	10/34/90/90	0/3/3/3
42	LMG	L	321	40	-	15/28/48/70	0/1/1/1
36	CLA	B	306	-	1/1/11/20	6/17/93/115	-
35	A86	V	304	-	-	8/34/90/90	0/3/3/3
36	CLA	K	309	-	1/1/13/20	13/32/108/115	-
36	CLA	V	306	33	1/1/15/20	17/39/115/115	-
38	SQD	A	315	-	-	13/22/42/69	0/1/1/1
35	A86	J	302	-	-	5/34/90/90	1/3/3/3
38	SQD	b	804	-	-	23/41/61/69	0/1/1/1
35	A86	E	302	-	-	4/34/90/90	0/3/3/3
35	A86	T	301	36	-	4/34/90/90	1/3/3/3
36	CLA	S	321	-	-	10/24/100/115	-
36	CLA	b	811	-	1/1/15/20	12/39/115/115	-
35	A86	W	202	36	-	9/34/90/90	0/3/3/3
41	LHG	b	850	36	-	26/53/53/53	-
36	CLA	h	203	-	1/1/15/20	17/39/115/115	-
36	CLA	J	308	-	-	12/35/111/115	-
35	A86	K	301	-	-	6/34/90/90	1/3/3/3
35	A86	T	306	-	-	7/34/90/90	0/3/3/3
36	CLA	G	309	-	1/1/15/20	13/39/115/115	-
36	CLA	l	204	28	-	10/20/96/115	-
37	KC1	A	312	-	-	2/15/71/71	-
36	CLA	G	311	-	1/1/15/20	16/39/115/115	-
36	CLA	H	306	-	1/1/14/20	6/35/111/115	-
35	A86	A	316	-	-	9/34/90/90	0/3/3/3
37	KC1	X	311	-	-	2/15/71/71	-
36	CLA	a	810	36	1/1/14/20	16/36/112/115	-
37	KC1	G	318	-	-	7/15/71/71	-
36	CLA	b	815	-	1/1/15/20	15/39/115/115	-
36	CLA	E	315	-	2/2/15/20	16/39/115/115	-
36	CLA	T	311	18	1/1/15/20	13/39/115/115	-
36	CLA	I	314	-	1/1/10/20	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	O	318	-	-	30/53/53/53	-
37	KC1	G	317	-	-	6/15/71/71	-
36	CLA	a	827	-	1/1/14/20	13/36/112/115	-
35	A86	O	303	-	-	6/34/90/90	0/3/3/3
36	CLA	I	312	9	1/1/12/20	4/24/100/115	-
42	LMG	D	320	41	-	24/41/61/70	0/1/1/1
36	CLA	R	313	-	1/1/15/20	14/39/115/115	-
42	LMG	G	325	-	-	27/50/70/70	0/1/1/1
42	LMG	V	316	-	-	25/41/61/70	0/1/1/1
36	CLA	B	308	-	1/1/15/20	14/39/115/115	-
36	CLA	U	306	32	1/1/15/20	19/39/115/115	-
36	CLA	a	828	-	1/1/15/20	14/39/115/115	-
42	LMG	D	321	-	-	21/32/52/70	0/1/1/1
35	A86	V	303	35	-	8/34/90/90	0/3/3/3
35	A86	O	301	-	-	4/34/90/90	0/3/3/3
37	KC1	R	317	-	-	3/15/71/71	-
35	A86	O	305	-	-	13/34/90/90	0/3/3/3
36	CLA	a	826	-	1/1/15/20	10/39/115/115	-
36	CLA	W	201	-	1/1/11/20	4/19/95/115	-
36	CLA	C	209	-	1/1/15/20	11/39/115/115	-
35	A86	M	302	-	-	7/34/90/90	0/3/3/3
35	A86	X	305	-	-	8/34/90/90	0/3/3/3
36	CLA	O	312	-	-	4/10/82/115	-
41	LHG	R	323	-	-	27/53/53/53	-
36	CLA	T	309	18	1/1/15/20	19/39/115/115	-
36	CLA	J	316	-	1/1/11/20	8/17/93/115	-
36	CLA	b	816	-	2/2/14/20	15/33/109/115	-
36	CLA	E	316	-	1/1/15/20	15/39/115/115	-
39	LMT	I	317	-	-	13/21/61/61	0/2/2/2
36	CLA	D	310	-	1/1/15/20	7/39/115/115	-
36	CLA	S	315	17	1/1/10/20	5/13/89/115	-
35	A86	G	305	-	-	4/34/90/90	0/3/3/3
34	DD6	P	305	-	-	3/26/80/80	0/3/3/3
36	CLA	f	805	25	1/1/12/20	9/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC1	H	313	-	-	6/15/71/71	-
36	CLA	V	305	35	1/1/14/20	11/35/111/115	-
34	DD6	E	301	-	-	3/26/80/80	0/3/3/3
36	CLA	R	318	35	1/1/10/20	4/10/86/115	-
37	KC1	S	316	-	-	6/15/71/71	-
36	CLA	H	310	8	1/1/11/20	7/17/93/115	-
36	CLA	J	315	-	1/1/10/20	2/10/86/115	-
36	CLA	D	313	-	1/1/15/20	8/39/115/115	-
36	CLA	W	212	19	-	12/39/115/115	-
41	LHG	i	104	-	-	29/50/50/53	-
36	CLA	a	834	20	1/1/11/20	5/15/91/115	-
36	CLA	b	814	-	1/1/13/20	5/27/103/115	-
36	CLA	A	309	1	1/1/11/20	7/17/93/115	-
36	CLA	b	837	-	1/1/15/20	7/39/115/115	-
36	CLA	C	212	35	1/1/15/20	22/39/115/115	-
37	KC1	D	314	4	-	4/15/71/71	-
36	CLA	P	313	-	1/1/15/20	10/39/115/115	-
45	SF4	c	102	-	-	-	0/6/5/5
35	A86	P	307	-	-	2/34/90/90	0/3/3/3
35	A86	X	304	-	-	7/34/90/90	0/3/3/3
36	CLA	F	312	-	1/1/15/20	21/39/115/115	-
35	A86	B	303	-	-	13/34/90/90	0/3/3/3
42	LMG	J	318	-	-	28/50/70/70	0/1/1/1
36	CLA	E	311	-	1/1/15/20	16/39/115/115	-
36	CLA	b	809	-	1/1/15/20	16/39/115/115	-
35	A86	R	301	-	-	9/34/90/90	0/3/3/3
36	CLA	G	307	-	-	4/11/87/115	-
44	BCR	f	806	-	-	9/29/63/63	0/2/2/2
36	CLA	H	317	8	1/1/15/20	10/39/115/115	-
36	CLA	b	824	-	1/1/12/20	12/25/101/115	-
37	KC1	B	310	-	-	3/15/71/71	-
40	DGD	L	302	42	-	21/36/76/95	0/2/2/2
35	A86	T	302	-	-	7/34/90/90	0/3/3/3
44	BCR	l	203	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	I	310	35	1/1/15/20	11/39/115/115	-
36	CLA	I	313	-	1/1/10/20	4/10/86/115	-
35	A86	B	301	-	-	10/34/90/90	0/3/3/3
36	CLA	W	207	34	1/1/15/20	15/39/115/115	-
36	CLA	a	831	-	1/1/15/20	16/39/115/115	-
35	A86	R	306	-	-	8/34/90/90	0/3/3/3
35	A86	J	301	-	-	10/34/90/90	0/3/3/3
36	CLA	Q	308	-	1/1/15/20	17/39/115/115	-
39	LMT	K	318	-	-	12/21/61/61	0/2/2/2
35	A86	Q	303	-	-	8/34/90/90	0/3/3/3
36	CLA	V	310	33	1/1/15/20	6/39/115/115	-
36	CLA	b	829	-	1/1/15/20	11/39/115/115	-
36	CLA	a	805	20	1/1/15/20	17/39/115/115	-
36	CLA	a	815	46	1/1/11/20	2/15/91/115	-
36	CLA	l	205	-	2/2/15/20	12/39/115/115	-
36	CLA	S	314	-	-	11/39/115/115	-
43	PQN	b	842	-	-	11/23/43/43	0/2/2/2
34	DD6	H	303	-	-	6/26/80/80	0/3/3/3
36	CLA	G	314	7	1/1/10/20	4/10/86/115	-
36	CLA	J	312	10	1/1/15/20	9/39/115/115	-
36	CLA	N	315	-	-	0/10/86/115	-
36	CLA	E	312	-	1/1/15/20	14/39/115/115	-
36	CLA	a	825	-	2/2/15/20	15/39/115/115	-
36	CLA	M	308	-	1/1/12/20	6/24/100/115	-
36	CLA	B	309	2	1/1/12/20	7/24/100/115	-
34	DD6	S	307	-	-	6/26/80/80	0/3/3/3
36	CLA	j	106	27	1/1/10/20	6/12/88/115	-
36	CLA	V	309	33	1/1/10/20	4/13/89/115	-
36	CLA	L	316	-	1/1/10/20	3/10/86/115	-
35	A86	Q	301	-	-	6/34/90/90	0/3/3/3
36	CLA	K	311	-	1/1/11/20	8/17/93/115	-
42	LMG	m	102	-	-	14/32/52/70	0/1/1/1
35	A86	S	308	37	-	12/34/90/90	0/3/3/3
36	CLA	V	311	33	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	b	805	36	1/1/15/20	15/39/115/115	-
36	CLA	b	823	-	1/1/13/20	5/27/103/115	-
36	CLA	a	822	-	1/1/12/20	4/23/99/115	-
36	CLA	S	319	-	1/1/15/20	7/39/115/115	-
35	A86	F	302	-	-	8/34/90/90	0/3/3/3
35	A86	N	302	-	-	6/34/90/90	0/3/3/3
36	CLA	M	315	-	-	6/18/94/115	-
35	A86	U	303	36	-	16/34/90/90	0/3/3/3
36	CLA	L	311	-	1/1/15/20	13/39/115/115	-
36	CLA	a	837	-	1/1/15/20	8/39/115/115	-
36	CLA	S	309	-	1/1/14/20	8/35/111/115	-
39	LMT	E	320	-	-	13/21/61/61	0/2/2/2
36	CLA	S	311	35	1/1/11/20	4/17/93/115	-
35	A86	O	319	35,36	-	8/34/90/90	0/3/3/3
39	LMT	b	848	-	-	12/21/61/61	0/2/2/2
40	DGD	C	215	-	-	31/46/86/95	0/2/2/2
36	CLA	W	211	-	1/1/15/20	10/39/115/115	-
36	CLA	D	309	-	2/2/13/20	7/27/103/115	-
35	A86	O	302	-	-	9/34/90/90	0/3/3/3
36	CLA	F	310	-	1/1/13/20	9/29/105/115	-
36	CLA	T	308	-	1/1/14/20	8/35/111/115	-
35	A86	F	307	-	-	7/34/90/90	0/3/3/3
41	LHG	f	808	-	-	28/53/53/53	-
36	CLA	N	317	14	1/1/12/20	10/26/102/115	-
36	CLA	X	312	-	1/1/10/20	2/10/86/115	-
36	CLA	P	316	-	1/1/10/20	4/10/86/115	-
36	CLA	a	830	-	-	11/21/97/115	-
36	CLA	a	848	36	2/2/15/20	12/39/115/115	-
37	KC1	V	312	33	-	6/15/71/71	-
36	CLA	A	307	-	1/1/14/20	8/33/109/115	-
36	CLA	H	307	-	1/1/14/20	5/33/109/115	-
36	CLA	T	316	-	1/1/10/20	2/10/86/115	-
36	CLA	P	311	-	1/1/15/20	17/39/115/115	-
37	KC1	T	310	-	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	b	833	-	1/1/13/20	11/31/107/115	-
36	CLA	R	322	-	1/1/12/20	9/24/100/115	-
36	CLA	Q	312	-	1/1/10/20	4/10/86/115	-
45	SF4	c	101	22	-	-	0/6/5/5
36	CLA	b	838	-	1/1/11/20	2/18/94/115	-
36	CLA	l	202	-	1/1/15/20	13/39/115/115	-
44	BCR	i	101	-	-	1/29/63/63	0/2/2/2
36	CLA	G	319	7	1/1/12/20	8/21/97/115	-
35	A86	K	303	-	-	5/34/90/90	0/3/3/3
35	A86	F	301	-	-	5/34/90/90	0/3/3/3
37	KC1	P	315	35	-	1/15/71/71	-
35	A86	N	303	-	-	5/34/90/90	0/3/3/3
35	A86	U	301	-	-	8/34/90/90	0/3/3/3
34	DD6	Q	302	-	-	8/26/80/80	0/3/3/3
39	LMT	F	321	-	-	10/19/59/61	0/2/2/2
39	LMT	B	312	-	-	14/21/61/61	0/2/2/2
36	CLA	N	310	-	1/1/10/20	1/10/86/115	-
34	DD6	J	304	-	-	4/26/80/80	0/3/3/3
36	CLA	a	804	-	1/1/15/20	16/39/115/115	-
39	LMT	f	807	-	-	6/15/35/61	0/1/1/2
36	CLA	D	316	-	1/1/12/20	10/24/100/115	-
36	CLA	b	831	-	1/1/12/20	7/21/97/115	-
36	CLA	X	307	35	-	5/21/97/115	-
36	CLA	P	318	-	1/1/12/20	8/23/99/115	-
35	A86	J	303	-	-	7/34/90/90	0/3/3/3
37	KC1	O	313	-	-	1/15/71/71	-
36	CLA	X	306	-	1/1/14/20	9/35/111/115	-
44	BCR	a	846	-	-	7/29/63/63	0/2/2/2
36	CLA	F	316	6	1/1/10/20	2/10/86/115	-
36	CLA	b	830	-	1/1/15/20	7/39/115/115	-
36	CLA	R	319	-	1/1/11/20	6/15/91/115	-
36	CLA	P	309	41	1/1/15/20	14/39/115/115	-
36	CLA	P	310	41	1/1/15/20	11/39/115/115	-
39	LMT	E	321	-	-	9/15/35/61	0/1/1/2
36	CLA	E	317	-	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	BCR	a	844	-	-	6/29/63/63	0/2/2/2
36	CLA	O	310	15	1/1/11/20	9/17/93/115	-
36	CLA	a	809	-	1/1/13/20	8/29/105/115	-
42	LMG	I	315	-	-	32/50/70/70	0/1/1/1
35	A86	S	303	-	-	5/34/90/90	0/3/3/3
35	A86	T	304	-	-	0/34/90/90	0/3/3/3
36	CLA	A	311	-	1/1/15/20	20/39/115/115	-
36	CLA	O	316	-	1/1/15/20	29/39/115/115	-
36	CLA	K	310	-	2/2/14/20	15/36/112/115	-
35	A86	T	303	-	-	6/34/90/90	0/3/3/3
36	CLA	W	208	-	1/1/11/20	6/15/91/115	-
36	CLA	b	801	46	1/1/15/20	8/39/115/115	-
39	LMT	K	317	-	-	14/17/57/61	0/2/2/2
35	A86	G	302	-	-	7/34/90/90	0/3/3/3
39	LMT	I	318	-	-	17/21/61/61	0/2/2/2
36	CLA	K	316	-	1/1/15/20	11/39/115/115	-
36	CLA	T	314	-	1/1/15/20	13/39/115/115	-
36	CLA	b	840	-	1/1/15/20	12/39/115/115	-
36	CLA	E	308	5	1/1/11/20	8/20/96/115	-
36	CLA	P	319	-	1/1/14/20	15/33/109/115	-
36	CLA	U	305	-	1/1/14/20	11/35/111/115	-
35	A86	L	304	-	-	7/34/90/90	0/3/3/3
36	CLA	G	310	-	1/1/15/20	5/39/115/115	-
37	KC1	G	308	-	-	6/15/71/71	-
36	CLA	N	307	-	1/1/14/20	9/35/111/115	-
35	A86	D	302	-	-	7/34/90/90	0/3/3/3
35	A86	R	302	-	-	6/34/90/90	0/3/3/3
36	CLA	a	818	-	1/1/15/20	11/39/115/115	-
36	CLA	V	313	-	1/1/15/20	14/39/115/115	-
36	CLA	b	836	-	1/1/13/20	8/31/107/115	-
35	A86	E	305	-	-	5/34/90/90	0/3/3/3
35	A86	X	303	36	-	9/34/90/90	0/3/3/3
36	CLA	X	315	-	-	2/10/86/115	-
37	KC1	W	217	-	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	N	301	-	-	9/34/90/90	0/3/3/3
36	CLA	H	305	-	1/1/11/20	5/19/95/115	-
35	A86	N	305	-	-	2/34/90/90	0/3/3/3
34	DD6	F	303	-	-	8/26/80/80	0/3/3/3
36	CLA	S	313	-	1/1/11/20	8/17/93/115	-
36	CLA	A	308	-	1/1/15/20	12/39/115/115	-
36	CLA	P	302	-	-	4/12/88/115	-
36	CLA	K	308	-	1/1/15/20	9/39/115/115	-
36	CLA	a	807	20	1/1/15/20	14/39/115/115	-
36	CLA	M	306	37,13	1/1/13/20	8/27/103/115	-
36	CLA	O	307	-	1/1/15/20	14/39/115/115	-
36	CLA	R	316	-	1/1/11/20	8/17/93/115	-
44	BCR	b	847	-	-	8/29/63/63	0/2/2/2
36	CLA	T	312	18	1/1/11/20	6/17/93/115	-
39	LMT	a	854	-	-	16/21/61/61	0/2/2/2
36	CLA	F	317	6	2/2/13/20	10/29/105/115	-
36	CLA	L	309	-	1/1/15/20	11/39/115/115	-
36	CLA	K	315	-	1/1/10/20	2/10/86/115	-
41	LHG	O	317	-	-	32/46/46/53	-
36	CLA	b	810	-	1/1/15/20	9/39/115/115	-
36	CLA	X	308	19	1/1/11/20	11/18/94/115	-
35	A86	J	306	-	-	7/34/90/90	0/3/3/3
40	DGD	b	849	-	-	21/49/89/95	0/2/2/2
36	CLA	j	101	-	1/1/15/20	17/39/115/115	-
41	LHG	a	843	36	-	9/31/31/53	-
35	A86	T	307	-	-	9/34/90/90	0/3/3/3
36	CLA	R	320	16	1/1/11/20	4/15/91/115	-
36	CLA	C	206	-	1/1/14/20	17/35/111/115	-
36	CLA	f	803	-	2/2/15/20	11/39/115/115	-
35	A86	N	306	-	-	8/34/90/90	0/3/3/3
35	A86	U	302	-	-	9/34/90/90	0/3/3/3
36	CLA	S	310	-	1/1/15/20	17/39/115/115	-
34	DD6	E	303	-	-	7/26/80/80	0/3/3/3
34	DD6	G	303	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMT	B	313	-	-	16/21/61/61	0/2/2/2
34	DD6	H	302	-	-	1/26/80/80	0/3/3/3
44	BCR	b	845	-	-	6/29/63/63	0/2/2/2
36	CLA	C	207	-	1/1/15/20	16/39/115/115	-
36	CLA	R	321	-	-	10/39/115/115	-
35	A86	L	319	-	-	9/34/90/90	0/3/3/3
35	A86	X	301	-	-	9/34/90/90	0/3/3/3
39	LMT	P	320	-	-	8/14/34/61	0/1/1/2
36	CLA	a	824	-	1/1/15/20	11/39/115/115	-
35	A86	S	305	-	-	9/34/90/90	0/3/3/3
36	CLA	P	308	-	1/1/14/20	7/35/111/115	-
36	CLA	U	310	-	1/1/15/20	19/39/115/115	-
36	CLA	b	807	-	1/1/11/20	3/15/91/115	-
36	CLA	Q	310	-	-	20/39/115/115	-
37	KC1	M	318	-	-	9/15/71/71	-
36	CLA	l	201	-	1/1/15/20	14/39/115/115	-
36	CLA	l	206	46	1/1/12/20	6/21/97/115	-
36	CLA	b	835	-	1/1/11/20	5/15/91/115	-
36	CLA	a	802	-	2/2/15/20	11/39/115/115	-
35	A86	J	305	-	-	6/34/90/90	0/3/3/3
35	A86	P	304	-	-	6/34/90/90	0/3/3/3
42	LMG	G	324	-	-	31/50/70/70	0/1/1/1
34	DD6	A	301	-	-	6/26/80/80	0/3/3/3
36	CLA	b	820	21	1/1/14/20	17/33/109/115	-
36	CLA	X	310	-	1/1/10/20	4/10/86/115	-
36	CLA	M	314	-	1/1/10/20	4/10/86/115	-
37	KC1	N	314	-	-	7/15/71/71	-
36	CLA	F	311	-	1/1/12/20	9/24/100/115	-
34	DD6	C	201	-	-	7/26/80/80	0/3/3/3
36	CLA	H	311	-	1/1/15/20	9/39/115/115	-
36	CLA	R	314	16	1/1/11/20	9/17/93/115	-
36	CLA	K	312	-	1/1/15/20	6/39/115/115	-
34	DD6	E	304	-	-	4/26/80/80	0/3/3/3
34	DD6	I	303	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	h	202	-	-	3/34/90/90	1/3/3/3
36	CLA	S	318	-	1/1/10/20	7/12/88/115	-
37	KC1	O	315	15	-	1/15/71/71	-
41	LHG	G	321	36	-	28/51/51/53	-
36	CLA	b	802	-	1/1/15/20	9/39/115/115	-
35	A86	G	306	-	-	6/34/90/90	1/3/3/3
36	CLA	X	309	-	-	7/15/91/115	-
36	CLA	A	306	-	2/2/14/20	17/35/111/115	-
36	CLA	b	834	-	1/1/15/20	8/39/115/115	-
35	A86	I	304	-	-	9/34/90/90	0/3/3/3
42	LMG	j	105	-	-	31/47/67/70	0/1/1/1
34	DD6	D	305	-	-	2/26/80/80	0/3/3/3
42	LMG	E	318	-	-	25/41/61/70	0/1/1/1
36	CLA	U	313	-	1/1/10/20	4/10/86/115	-
36	CLA	J	317	-	1/1/11/20	5/18/94/115	-
41	LHG	l	208	-	-	34/52/52/53	-
36	CLA	b	825	-	1/1/15/20	12/39/115/115	-
36	CLA	b	839	-	1/1/15/20	4/39/115/115	-
36	CLA	G	313	7	1/1/15/20	14/39/115/115	-
35	A86	H	301	-	-	5/34/90/90	0/3/3/3
37	KC1	L	315	35	-	6/15/71/71	-
35	A86	R	304	36	-	8/34/90/90	0/3/3/3
39	LMT	L	318	-	-	12/17/57/61	0/2/2/2
37	KC1	C	213	-	-	5/15/71/71	-
36	CLA	S	312	-	-	15/39/115/115	-
36	CLA	b	812	21	1/1/15/20	6/39/115/115	-
35	A86	E	307	36	-	3/34/90/90	0/3/3/3
39	LMT	b	851	-	-	7/15/35/61	0/1/1/2
34	DD6	B	304	-	-	3/26/80/80	0/3/3/3
36	CLA	j	102	-	1/1/15/20	14/39/115/115	-

All (4548) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Q	310	CLA	CAA-C2A	16.11	1.83	1.54
37	M	318	KC1	C4C-NC	15.94	1.63	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	318	KC1	C1A-NA	14.76	1.68	1.38
37	T	310	KC1	C1A-NA	13.47	1.66	1.38
35	N	304	A86	C19-C18	-13.40	1.33	1.52
37	T	310	KC1	C4C-NC	12.52	1.57	1.37
36	N	319	CLA	C1D-C2D	12.28	1.69	1.45
36	N	319	CLA	C1D-ND	10.97	1.52	1.37
36	X	308	CLA	C1B-NB	-10.33	1.24	1.37
35	N	304	A86	C19-C20	9.85	1.66	1.52
37	M	318	KC1	C3C-C2C	9.57	1.57	1.36
37	M	318	KC1	C2A-C3A	9.38	1.56	1.37
37	T	310	KC1	C2A-C3A	9.24	1.55	1.37
37	M	318	KC1	C4C-C3C	9.00	1.60	1.45
35	V	304	A86	C20-C15	8.69	1.59	1.48
34	L	305	DD6	C30-C31	-8.63	1.25	1.42
34	S	307	DD6	C30-C31	-8.59	1.25	1.42
34	A	301	DD6	C30-C31	-8.59	1.25	1.42
34	Q	302	DD6	C30-C31	-8.58	1.25	1.42
34	W	204	DD6	C30-C31	-8.58	1.25	1.42
34	M	303	DD6	C30-C31	-8.55	1.25	1.42
34	C	201	DD6	C30-C31	-8.53	1.25	1.42
34	R	308	DD6	C30-C31	-8.52	1.25	1.42
34	E	306	DD6	C30-C31	-8.50	1.26	1.42
34	J	304	DD6	C30-C31	-8.49	1.26	1.42
34	K	304	DD6	C30-C31	-8.49	1.26	1.42
34	P	305	DD6	C30-C31	-8.47	1.26	1.42
34	E	303	DD6	C30-C31	-8.46	1.26	1.42
34	D	301	DD6	C30-C31	-8.46	1.26	1.42
34	R	307	DD6	C30-C31	-8.45	1.26	1.42
34	K	305	DD6	C30-C31	-8.44	1.26	1.42
34	I	303	DD6	C30-C31	-8.44	1.26	1.42
34	B	302	DD6	C30-C31	-8.43	1.26	1.42
34	A	304	DD6	C30-C31	-8.43	1.26	1.42
34	a	849	DD6	C30-C31	-8.42	1.26	1.42
34	H	302	DD6	C30-C31	-8.40	1.26	1.42
34	B	304	DD6	C30-C31	-8.39	1.26	1.42
34	W	205	DD6	C30-C31	-8.38	1.26	1.42
34	A	303	DD6	C30-C31	-8.37	1.26	1.42
34	j	103	DD6	C30-C31	-8.37	1.26	1.42
34	G	303	DD6	C30-C31	-8.35	1.26	1.42
34	E	304	DD6	C30-C31	-8.34	1.26	1.42
34	D	304	DD6	C30-C31	-8.32	1.26	1.42
34	S	306	DD6	C30-C31	-8.30	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	301	DD6	C30-C31	-8.30	1.26	1.42
34	H	303	DD6	C30-C31	-8.30	1.26	1.42
34	F	303	DD6	C30-C31	-8.30	1.26	1.42
34	D	303	DD6	C30-C31	-8.29	1.26	1.42
34	D	305	DD6	C30-C31	-8.17	1.26	1.42
37	T	310	KC1	C3C-C2C	8.16	1.54	1.36
35	G	304	A86	C20-C15	7.92	1.58	1.48
36	Q	310	CLA	O1A-CGA	7.91	1.46	1.22
34	O	304	DD6	C30-C31	-7.80	1.27	1.42
43	a	840	PQN	C3-C2	7.75	1.49	1.35
43	b	842	PQN	C3-C2	7.67	1.48	1.35
36	P	319	CLA	C1B-NB	-7.50	1.28	1.37
37	M	318	KC1	C3B-C2B	7.48	1.52	1.37
37	T	310	KC1	C4C-C3C	7.44	1.57	1.45
36	X	308	CLA	C4B-NB	7.42	1.47	1.37
36	I	305	CLA	C11-C12	-7.35	1.21	1.52
37	T	310	KC1	C3B-C2B	7.35	1.52	1.37
37	V	312	KC1	C4C-NC	7.30	1.49	1.37
35	N	301	A86	C20-C15	7.30	1.57	1.48
35	S	301	A86	C20-C15	7.26	1.57	1.48
36	X	308	CLA	MG-NB	-7.23	1.91	2.05
37	Q	313	KC1	C4C-NC	7.22	1.49	1.37
37	B	310	KC1	C4C-NC	7.21	1.49	1.37
37	U	312	KC1	C4C-NC	7.19	1.49	1.37
37	Q	311	KC1	C4C-NC	7.17	1.49	1.37
37	O	315	KC1	C4C-NC	7.17	1.49	1.37
36	M	310	CLA	C1D-ND	7.14	1.47	1.37
37	P	315	KC1	C4C-NC	7.10	1.49	1.37
37	M	318	KC1	C1D-C2D	7.09	1.59	1.43
37	O	313	KC1	C4C-NC	7.07	1.49	1.37
36	X	313	CLA	C4B-NB	6.99	1.47	1.37
36	b	816	CLA	C1D-ND	6.94	1.47	1.37
37	X	311	KC1	C4C-NC	6.91	1.49	1.37
37	W	217	KC1	C4C-NC	6.91	1.49	1.37
37	N	314	KC1	C4C-NC	6.90	1.48	1.37
35	S	305	A86	C20-C15	6.86	1.57	1.48
37	M	317	KC1	C4C-NC	6.86	1.48	1.37
37	S	316	KC1	C4C-NC	6.84	1.48	1.37
37	L	317	KC1	C4C-NC	6.83	1.48	1.37
37	R	317	KC1	C4C-NC	6.81	1.48	1.37
37	J	314	KC1	C4C-NC	6.81	1.48	1.37
34	D	303	DD6	C2-C1	6.80	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	313	KC1	C4C-NC	6.77	1.48	1.37
36	I	305	CLA	C15-C13	-6.77	1.06	1.51
37	W	213	KC1	C4C-NC	6.72	1.48	1.37
37	T	315	KC1	C4C-NC	6.70	1.48	1.37
37	F	308	KC1	C4C-NC	6.69	1.48	1.37
37	L	315	KC1	C4C-NC	6.68	1.48	1.37
37	K	314	KC1	C4C-NC	6.67	1.48	1.37
36	M	310	CLA	MG-ND	-6.65	1.92	2.05
37	D	314	KC1	C4C-NC	6.63	1.48	1.37
37	A	312	KC1	C4C-NC	6.63	1.48	1.37
35	U	301	A86	O4-C38	6.62	1.49	1.35
37	G	308	KC1	C4C-NC	6.61	1.48	1.37
37	C	213	KC1	C4C-NC	6.59	1.48	1.37
37	T	310	KC1	CHB-C4A	-6.59	1.24	1.39
37	H	313	KC1	C4C-NC	6.59	1.48	1.37
37	G	317	KC1	C4C-NC	6.54	1.48	1.37
37	F	315	KC1	C4C-NC	6.53	1.48	1.37
37	G	318	KC1	C4C-NC	6.53	1.48	1.37
36	N	319	CLA	CHD-C4C	6.49	1.54	1.39
36	C	207	CLA	C1D-ND	6.49	1.46	1.37
37	E	309	KC1	C4C-NC	6.46	1.48	1.37
37	P	317	KC1	C4C-NC	6.44	1.48	1.37
36	V	314	CLA	MG-NA	6.28	2.21	2.06
37	T	310	KC1	C1D-C2D	6.19	1.57	1.43
36	U	306	CLA	C1D-ND	6.19	1.46	1.37
36	P	319	CLA	C4B-NB	6.14	1.45	1.37
36	L	308	CLA	CHC-C1C	6.01	1.50	1.38
37	L	315	KC1	C2A-C3A	5.96	1.49	1.37
36	H	310	CLA	O2D-CGD	5.95	1.47	1.33
37	U	312	KC1	C2A-C3A	5.95	1.49	1.37
36	Q	310	CLA	CBA-CGA	5.94	1.67	1.50
37	N	314	KC1	C3C-C2C	5.94	1.49	1.36
37	W	217	KC1	C2A-C3A	5.94	1.49	1.37
37	W	217	KC1	CHD-C4C	5.93	1.50	1.38
36	V	314	CLA	C1D-ND	5.92	1.45	1.37
37	B	310	KC1	CHD-C4C	5.91	1.50	1.38
37	X	311	KC1	C2A-C3A	5.91	1.49	1.37
37	X	311	KC1	CHD-C4C	5.90	1.50	1.38
37	O	315	KC1	C2A-C3A	5.88	1.49	1.37
37	P	315	KC1	C2A-C3A	5.87	1.49	1.37
37	O	313	KC1	C2A-C3A	5.87	1.49	1.37
36	I	308	CLA	C1D-ND	5.86	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Q	311	KC1	C2A-C3A	5.86	1.49	1.37
37	Q	313	KC1	C2A-C3A	5.86	1.49	1.37
37	P	315	KC1	C1A-NA	5.85	1.50	1.38
37	S	316	KC1	C2A-C3A	5.85	1.49	1.37
37	V	312	KC1	CHD-C4C	5.85	1.50	1.38
37	O	315	KC1	C1A-NA	5.82	1.50	1.38
35	X	303	A86	O4-C38	5.81	1.48	1.35
37	W	213	KC1	C2A-C3A	5.81	1.49	1.37
37	Q	311	KC1	C1A-NA	5.81	1.50	1.38
37	A	312	KC1	C1A-NA	5.81	1.50	1.38
37	Q	313	KC1	C1A-NA	5.80	1.50	1.38
37	O	313	KC1	C1A-NA	5.80	1.50	1.38
36	G	307	CLA	C1D-ND	5.76	1.45	1.37
36	N	319	CLA	CHD-C1D	5.76	1.49	1.38
35	T	305	A86	O4-C38	5.74	1.47	1.35
37	F	308	KC1	C3C-C2C	5.73	1.49	1.36
37	E	309	KC1	C3C-C2C	5.73	1.49	1.36
37	S	316	KC1	CHD-C4C	5.72	1.49	1.38
35	X	301	A86	O4-C38	5.72	1.47	1.35
36	L	308	CLA	CHC-C4B	5.71	1.52	1.39
36	K	307	CLA	C1D-ND	5.71	1.45	1.37
35	A	302	A86	O4-C38	5.70	1.47	1.35
37	A	312	KC1	C2A-C3A	5.69	1.48	1.37
37	U	312	KC1	C3B-C2B	5.69	1.48	1.37
37	V	312	KC1	C2A-C3A	5.69	1.48	1.37
37	S	316	KC1	C3C-C2C	5.68	1.49	1.36
36	a	816	CLA	C1D-ND	5.68	1.45	1.37
37	G	318	KC1	C3C-C2C	5.68	1.49	1.36
37	N	314	KC1	CHD-C4C	5.67	1.49	1.38
37	B	310	KC1	C2A-C3A	5.66	1.48	1.37
37	U	312	KC1	CHD-C4C	5.66	1.49	1.38
37	G	318	KC1	CHD-C4C	5.66	1.49	1.38
37	G	308	KC1	CHD-C4C	5.65	1.49	1.38
35	N	301	A86	O4-C38	5.65	1.47	1.35
37	F	315	KC1	C2A-C3A	5.65	1.48	1.37
35	R	304	A86	O4-C38	5.64	1.47	1.35
35	S	301	A86	O4-C38	5.64	1.47	1.35
37	F	308	KC1	CHD-C4C	5.63	1.49	1.38
36	b	836	CLA	C1D-ND	5.63	1.45	1.37
37	V	312	KC1	C3C-C2C	5.60	1.48	1.36
35	M	301	A86	O4-C38	5.60	1.47	1.35
37	W	213	KC1	CHD-C4C	5.60	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	217	KC1	C1A-NA	5.60	1.49	1.38
35	S	303	A86	O4-C38	5.59	1.47	1.35
37	G	318	KC1	C2A-C3A	5.59	1.48	1.37
35	X	304	A86	O4-C38	5.59	1.47	1.35
35	R	301	A86	O4-C38	5.59	1.47	1.35
35	K	302	A86	O4-C38	5.58	1.47	1.35
35	N	303	A86	O4-C38	5.58	1.47	1.35
35	N	304	A86	O1-C15	-5.57	1.36	1.45
37	L	317	KC1	CHD-C4C	5.57	1.49	1.38
37	C	213	KC1	CHD-C4C	5.57	1.49	1.38
35	W	202	A86	O4-C38	5.56	1.47	1.35
37	U	312	KC1	C1A-NA	5.56	1.49	1.38
37	X	311	KC1	C1A-NA	5.56	1.49	1.38
37	N	314	KC1	C2A-C3A	5.55	1.48	1.37
36	W	216	CLA	C1B-C2B	5.55	1.56	1.43
37	M	317	KC1	CHD-C4C	5.54	1.49	1.38
37	G	308	KC1	C3C-C2C	5.53	1.48	1.36
37	M	318	KC1	C1A-CHA	5.53	1.54	1.40
37	W	217	KC1	C3C-C2C	5.52	1.48	1.36
37	X	311	KC1	C3C-C2C	5.51	1.48	1.36
37	U	312	KC1	CHB-C1B	5.50	1.49	1.38
35	X	303	A86	C20-C15	5.50	1.55	1.48
37	T	315	KC1	C2A-C3A	5.50	1.48	1.37
37	E	309	KC1	CHD-C4C	5.49	1.49	1.38
35	R	302	A86	C30-C31	-5.49	1.24	1.30
37	B	310	KC1	C3C-C2C	5.49	1.48	1.36
37	A	312	KC1	CHD-C4C	5.49	1.49	1.38
35	I	302	A86	O4-C38	5.48	1.47	1.35
37	M	317	KC1	C2A-C3A	5.47	1.48	1.37
37	T	315	KC1	CHD-C4C	5.47	1.49	1.38
36	D	309	CLA	C1D-ND	5.47	1.45	1.37
37	M	317	KC1	C3C-C2C	5.45	1.48	1.36
37	J	314	KC1	CHD-C4C	5.45	1.49	1.38
37	H	313	KC1	CHD-C4C	5.44	1.49	1.38
37	R	317	KC1	C3C-C2C	5.44	1.48	1.36
35	R	303	A86	O4-C38	5.43	1.47	1.35
37	B	310	KC1	C1A-NA	5.42	1.49	1.38
37	W	213	KC1	C3C-C2C	5.42	1.48	1.36
37	L	317	KC1	C1A-NA	5.42	1.49	1.38
37	C	213	KC1	C2A-C3A	5.42	1.48	1.37
37	D	314	KC1	CHD-C4C	5.41	1.49	1.38
37	D	314	KC1	C3C-C2C	5.39	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	314	KC1	C3B-C2B	5.39	1.48	1.37
37	O	315	KC1	CHD-C4C	5.39	1.49	1.38
34	D	303	DD6	C-C1	5.38	1.61	1.50
37	Q	311	KC1	CHD-C4C	5.38	1.49	1.38
37	J	314	KC1	C1A-NA	5.38	1.49	1.38
35	I	304	A86	O4-C38	5.38	1.47	1.35
37	G	317	KC1	CHD-C4C	5.38	1.49	1.38
37	T	310	KC1	CHD-C4C	-5.37	1.27	1.38
37	P	317	KC1	C2A-C3A	5.37	1.48	1.37
36	j	102	CLA	C1D-ND	5.37	1.44	1.37
37	F	315	KC1	C1A-NA	5.36	1.49	1.38
37	R	317	KC1	CHD-C4C	5.36	1.49	1.38
37	P	315	KC1	CHD-C4C	5.36	1.49	1.38
37	L	315	KC1	C1A-NA	5.36	1.49	1.38
37	Q	313	KC1	CHD-C4C	5.35	1.49	1.38
35	T	305	A86	C20-C15	5.35	1.55	1.48
35	O	305	A86	C30-C31	-5.34	1.24	1.30
37	O	313	KC1	CHD-C4C	5.32	1.49	1.38
37	R	317	KC1	C1A-NA	5.31	1.49	1.38
36	P	319	CLA	MG-NB	-5.31	1.95	2.05
37	S	316	KC1	C1A-NA	5.31	1.49	1.38
37	K	314	KC1	CHD-C4C	5.30	1.49	1.38
37	P	317	KC1	CHD-C4C	5.30	1.49	1.38
37	M	313	KC1	C3C-C2C	5.30	1.48	1.36
37	C	213	KC1	C3C-C2C	5.30	1.48	1.36
37	J	314	KC1	C2A-C3A	5.30	1.47	1.37
36	P	319	CLA	MG-ND	-5.29	1.95	2.05
37	H	313	KC1	C3C-C2C	5.29	1.48	1.36
37	W	213	KC1	C3B-C2B	5.29	1.47	1.37
37	J	314	KC1	C3C-C2C	5.29	1.48	1.36
37	G	318	KC1	O2D-CGD	5.29	1.46	1.33
35	C	202	A86	O4-C38	5.29	1.46	1.35
37	B	310	KC1	O2D-CGD	5.28	1.46	1.33
37	F	308	KC1	C1A-NA	5.28	1.49	1.38
37	G	317	KC1	O2D-CGD	5.26	1.46	1.33
37	M	313	KC1	CHD-C4C	5.26	1.49	1.38
37	L	317	KC1	C2A-C3A	5.26	1.47	1.37
37	M	313	KC1	C2A-C3A	5.25	1.47	1.37
35	J	303	A86	O4-C38	5.25	1.46	1.35
36	W	214	CLA	C1D-ND	5.24	1.44	1.37
37	T	315	KC1	C3C-C2C	5.24	1.48	1.36
37	C	213	KC1	C3B-C2B	5.24	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Q	313	KC1	C3B-C2B	5.24	1.47	1.37
37	Q	311	KC1	C3B-C2B	5.24	1.47	1.37
36	O	316	CLA	C1D-ND	5.24	1.44	1.37
37	O	313	KC1	C3B-C2B	5.23	1.47	1.37
36	W	215	CLA	OBD-CAD	5.23	1.31	1.22
37	S	316	KC1	C3B-C2B	5.22	1.47	1.37
35	R	306	A86	O4-C38	5.22	1.46	1.35
35	F	307	A86	O4-C38	5.22	1.46	1.35
35	K	303	A86	O4-C38	5.22	1.46	1.35
35	V	303	A86	O4-C38	5.22	1.46	1.35
37	P	315	KC1	C3B-C2B	5.22	1.47	1.37
35	T	303	A86	O4-C38	5.21	1.46	1.35
37	B	310	KC1	C3B-C2B	5.21	1.47	1.37
37	W	213	KC1	C1A-NA	5.20	1.48	1.38
37	L	317	KC1	C3C-C2C	5.20	1.48	1.36
37	O	315	KC1	C3B-C2B	5.20	1.47	1.37
37	G	317	KC1	C2A-C3A	5.19	1.47	1.37
37	L	315	KC1	C3B-C2B	5.18	1.47	1.37
35	X	304	A86	C20-C15	5.18	1.54	1.48
35	P	303	A86	O4-C38	5.18	1.46	1.35
37	G	317	KC1	C3C-C2C	5.17	1.47	1.36
36	U	306	CLA	C3C-C2C	5.16	1.47	1.36
35	L	319	A86	O4-C38	5.16	1.46	1.35
37	N	314	KC1	O2D-CGD	5.16	1.45	1.33
35	O	302	A86	O4-C38	5.16	1.46	1.35
37	G	308	KC1	C2A-C3A	5.16	1.47	1.37
37	G	317	KC1	C1A-NA	5.16	1.48	1.38
37	O	313	KC1	C3C-C2C	5.16	1.47	1.36
37	M	313	KC1	C3B-C2B	5.16	1.47	1.37
37	F	315	KC1	CHD-C4C	5.15	1.48	1.38
37	P	315	KC1	C3C-C2C	5.15	1.47	1.36
35	W	203	A86	O4-C38	5.14	1.46	1.35
35	X	305	A86	O4-C38	5.14	1.46	1.35
37	T	315	KC1	C3B-C2B	5.14	1.47	1.37
37	T	315	KC1	O2D-CGD	5.13	1.45	1.33
37	T	310	KC1	OBD-CAD	5.13	1.31	1.22
37	W	217	KC1	O2D-CGD	5.13	1.45	1.33
37	Q	311	KC1	C3C-C2C	5.12	1.47	1.36
37	S	316	KC1	O2D-CGD	5.12	1.45	1.33
36	B	309	CLA	O2D-CGD	5.12	1.45	1.33
37	Q	313	KC1	C3C-C2C	5.12	1.47	1.36
37	D	314	KC1	C2A-C3A	5.12	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	O	315	KC1	C3C-C2C	5.12	1.47	1.36
37	F	308	KC1	C2A-C3A	5.11	1.47	1.37
35	M	302	A86	O4-C38	5.11	1.46	1.35
37	X	311	KC1	O2D-CGD	5.11	1.45	1.33
37	W	217	KC1	C3B-C2B	5.11	1.47	1.37
37	X	311	KC1	C3B-C2B	5.11	1.47	1.37
37	E	309	KC1	C1A-NA	5.11	1.48	1.38
36	K	310	CLA	O2D-CGD	5.10	1.45	1.33
37	M	317	KC1	C3B-C2B	5.10	1.47	1.37
37	L	317	KC1	C3B-C2B	5.09	1.47	1.37
37	M	318	KC1	O2D-CGD	5.08	1.45	1.33
37	U	312	KC1	O2D-CGD	5.08	1.45	1.33
37	L	317	KC1	O2D-CGD	5.08	1.45	1.33
37	E	309	KC1	C2A-C3A	5.08	1.47	1.37
37	R	317	KC1	C2A-C3A	5.08	1.47	1.37
37	L	315	KC1	CHD-C4C	5.08	1.48	1.38
37	V	312	KC1	C3B-C2B	5.08	1.47	1.37
36	M	310	CLA	C1B-NB	-5.07	1.31	1.37
36	a	802	CLA	O2D-CGD	5.07	1.45	1.33
36	O	316	CLA	O2D-CGD	5.07	1.45	1.33
36	V	314	CLA	O2D-CGD	5.06	1.45	1.33
36	I	308	CLA	O2D-CGD	5.06	1.45	1.33
37	M	318	KC1	OBD-CAD	5.06	1.31	1.22
36	L	308	CLA	O2D-CGD	5.06	1.45	1.33
35	T	302	A86	O4-C38	5.05	1.46	1.35
37	K	314	KC1	O2D-CGD	5.05	1.45	1.33
37	V	312	KC1	O2D-CGD	5.05	1.45	1.33
36	U	306	CLA	O2D-CGD	5.05	1.45	1.33
36	K	310	CLA	C1D-ND	5.05	1.44	1.37
36	D	309	CLA	O2D-CGD	5.05	1.45	1.33
35	M	305	A86	O4-C38	5.04	1.46	1.35
37	W	213	KC1	O2D-CGD	5.04	1.45	1.33
37	L	315	KC1	O2D-CGD	5.04	1.45	1.33
36	G	319	CLA	O2D-CGD	5.03	1.45	1.33
36	F	317	CLA	O2D-CGD	5.03	1.45	1.33
35	V	302	A86	O4-C38	5.03	1.46	1.35
35	Q	303	A86	O4-C38	5.03	1.46	1.35
36	G	315	CLA	C3D-C4D	-5.03	1.32	1.44
36	E	313	CLA	C3D-C4D	-5.03	1.32	1.44
36	K	307	CLA	O2D-CGD	5.03	1.45	1.33
37	K	314	KC1	C2A-C3A	5.03	1.47	1.37
36	a	823	CLA	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	315	CLA	O2D-CGD	5.02	1.45	1.33
37	T	310	KC1	O2D-CGD	5.02	1.45	1.33
37	U	312	KC1	C3C-C2C	5.01	1.47	1.36
37	M	313	KC1	O2D-CGD	5.01	1.45	1.33
36	a	830	CLA	O2D-CGD	5.01	1.45	1.33
37	L	315	KC1	C3C-C2C	5.01	1.47	1.36
36	A	306	CLA	O2D-CGD	5.01	1.45	1.33
36	b	836	CLA	O2D-CGD	5.00	1.45	1.33
36	I	306	CLA	O2D-CGD	5.00	1.45	1.33
37	Q	313	KC1	O2D-CGD	5.00	1.45	1.33
36	K	310	CLA	C3C-C2C	5.00	1.47	1.36
36	f	803	CLA	O2D-CGD	5.00	1.45	1.33
35	X	305	A86	C20-C15	4.99	1.54	1.48
36	b	824	CLA	O2D-CGD	4.99	1.45	1.33
35	K	306	A86	O4-C38	4.99	1.46	1.35
37	R	317	KC1	O2D-CGD	4.99	1.45	1.33
35	D	302	A86	O4-C38	4.98	1.46	1.35
36	E	313	CLA	O2D-CGD	4.98	1.45	1.33
37	Q	311	KC1	O2D-CGD	4.98	1.45	1.33
36	a	825	CLA	O2D-CGD	4.97	1.45	1.33
37	K	314	KC1	C3C-C2C	4.97	1.47	1.36
37	O	315	KC1	O2D-CGD	4.97	1.45	1.33
35	O	305	A86	C32-C31	-4.96	1.46	1.54
36	N	319	CLA	C4C-C3C	4.96	1.53	1.45
35	F	306	A86	O4-C38	4.96	1.46	1.35
36	j	102	CLA	O2D-CGD	4.96	1.45	1.33
37	H	313	KC1	C3B-C2B	4.96	1.47	1.37
37	G	308	KC1	C3B-C2B	4.96	1.47	1.37
36	a	816	CLA	O2D-CGD	4.95	1.45	1.33
37	J	314	KC1	C3B-C2B	4.95	1.47	1.37
37	P	315	KC1	O2D-CGD	4.95	1.45	1.33
37	N	314	KC1	C1A-NA	4.95	1.48	1.38
36	a	848	CLA	O2D-CGD	4.94	1.45	1.33
36	C	207	CLA	O2D-CGD	4.94	1.45	1.33
37	O	313	KC1	O2D-CGD	4.94	1.45	1.33
35	G	304	A86	O4-C38	4.94	1.46	1.35
35	R	302	A86	O4-C38	4.93	1.46	1.35
37	K	314	KC1	C3B-C2B	4.93	1.47	1.37
36	E	315	CLA	O2D-CGD	4.93	1.45	1.33
35	H	301	A86	O4-C38	4.93	1.46	1.35
37	J	314	KC1	O2D-CGD	4.93	1.45	1.33
35	V	304	A86	O4-C38	4.93	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	P	317	KC1	C3C-C2C	4.93	1.47	1.36
36	f	804	CLA	O2D-CGD	4.93	1.45	1.33
37	H	313	KC1	C1A-NA	4.92	1.48	1.38
37	D	314	KC1	O2D-CGD	4.92	1.45	1.33
35	J	306	A86	O4-C38	4.92	1.46	1.35
36	l	204	CLA	O2D-CGD	4.92	1.45	1.33
37	F	315	KC1	C3B-C2B	4.92	1.47	1.37
37	W	213	KC1	CHB-C1B	4.92	1.48	1.38
35	O	303	A86	O4-C38	4.91	1.46	1.35
35	X	302	A86	O4-C38	4.91	1.46	1.35
35	G	304	A86	O1-C20	-4.91	1.39	1.46
36	E	315	CLA	C3C-C2C	4.91	1.47	1.36
36	a	806	CLA	O2D-CGD	4.91	1.45	1.33
37	G	308	KC1	C1A-NA	4.91	1.48	1.38
35	Q	301	A86	O4-C38	4.90	1.46	1.35
36	a	822	CLA	O2D-CGD	4.90	1.45	1.33
35	U	304	A86	O4-C38	4.90	1.46	1.35
35	N	304	A86	O4-C38	4.90	1.46	1.35
37	A	312	KC1	C3B-C2B	4.89	1.47	1.37
36	F	317	CLA	C1D-ND	4.89	1.44	1.37
36	D	309	CLA	C3C-C2C	4.89	1.47	1.36
37	H	313	KC1	O2D-CGD	4.89	1.45	1.33
37	G	317	KC1	C3B-C2B	4.88	1.47	1.37
35	S	308	A86	O4-C38	4.88	1.46	1.35
36	l	205	CLA	O2D-CGD	4.88	1.45	1.33
35	F	301	A86	O4-C38	4.88	1.46	1.35
36	b	817	CLA	O2D-CGD	4.87	1.45	1.33
37	G	318	KC1	C1A-NA	4.87	1.48	1.38
35	O	305	A86	O4-C38	4.87	1.46	1.35
35	I	301	A86	O4-C38	4.87	1.46	1.35
43	a	840	PQN	C10-C5	4.87	1.48	1.40
35	P	304	A86	O4-C38	4.87	1.46	1.35
35	G	302	A86	O4-C38	4.87	1.46	1.35
36	X	313	CLA	C1B-C2B	4.86	1.54	1.43
35	J	302	A86	O4-C38	4.86	1.46	1.35
37	L	315	KC1	CHB-C1B	4.86	1.47	1.38
35	C	203	A86	O4-C38	4.86	1.45	1.35
35	T	301	A86	O4-C38	4.86	1.45	1.35
35	F	302	A86	O4-C38	4.85	1.45	1.35
43	b	842	PQN	C10-C5	4.85	1.48	1.40
37	M	317	KC1	O2D-CGD	4.85	1.45	1.33
35	G	306	A86	O4-C38	4.85	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	204	A86	O4-C38	4.84	1.45	1.35
35	T	306	A86	O4-C38	4.84	1.45	1.35
37	O	315	KC1	CHB-C1B	4.84	1.47	1.38
35	H	304	A86	O4-C38	4.84	1.45	1.35
36	b	824	CLA	C3C-C2C	4.84	1.47	1.36
37	H	313	KC1	C2A-C3A	4.84	1.47	1.37
37	Q	311	KC1	CHB-C1B	4.84	1.47	1.38
37	R	317	KC1	C3B-C2B	4.84	1.47	1.37
36	j	102	CLA	C3C-C2C	4.84	1.47	1.36
35	M	304	A86	O4-C38	4.83	1.45	1.35
35	S	302	A86	O4-C38	4.83	1.45	1.35
37	E	309	KC1	C3B-C2B	4.83	1.47	1.37
35	L	304	A86	O4-C38	4.83	1.45	1.35
37	Q	313	KC1	CHB-C1B	4.83	1.47	1.38
35	N	305	A86	O1-C20	-4.82	1.40	1.46
35	P	306	A86	O4-C38	4.82	1.45	1.35
36	b	836	CLA	C3C-C2C	4.82	1.47	1.36
35	N	306	A86	O4-C38	4.82	1.45	1.35
35	N	302	A86	O4-C38	4.82	1.45	1.35
37	O	313	KC1	CHB-C1B	4.82	1.47	1.38
35	X	314	A86	O4-C38	4.82	1.45	1.35
35	J	305	A86	O4-C38	4.81	1.45	1.35
37	M	313	KC1	C1A-NA	4.81	1.48	1.38
37	C	213	KC1	O2D-CGD	4.81	1.45	1.33
36	B	309	CLA	C3C-C2C	4.81	1.47	1.36
35	S	304	A86	O4-C38	4.81	1.45	1.35
35	L	304	A86	C30-C31	-4.80	1.25	1.30
37	P	315	KC1	CHB-C1B	4.80	1.47	1.38
35	R	305	A86	O4-C38	4.80	1.45	1.35
35	E	307	A86	O4-C38	4.80	1.45	1.35
36	a	816	CLA	C3D-C4D	-4.80	1.33	1.44
36	f	804	CLA	C1D-ND	4.80	1.44	1.37
36	C	207	CLA	C3C-C2C	4.80	1.47	1.36
35	Q	316	A86	O1-C20	-4.79	1.40	1.46
36	f	804	CLA	C3C-C2C	4.79	1.47	1.36
35	A	316	A86	O4-C38	4.79	1.45	1.35
35	G	305	A86	O4-C38	4.78	1.45	1.35
37	V	312	KC1	C1A-NA	4.78	1.48	1.38
35	B	303	A86	O4-C38	4.78	1.45	1.35
35	M	305	A86	C20-C15	4.78	1.54	1.48
35	L	301	A86	O4-C38	4.78	1.45	1.35
35	h	202	A86	O4-C38	4.77	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	O	301	A86	O4-C38	4.77	1.45	1.35
37	M	317	KC1	C1A-NA	4.77	1.47	1.38
35	K	301	A86	O4-C38	4.77	1.45	1.35
36	I	306	CLA	C3C-C2C	4.77	1.47	1.36
35	P	307	A86	O4-C38	4.77	1.45	1.35
37	N	314	KC1	CHC-C4B	4.77	1.47	1.38
35	L	307	A86	O4-C38	4.77	1.45	1.35
37	P	317	KC1	O2D-CGD	4.76	1.44	1.33
37	L	315	KC1	CHC-C4B	4.76	1.47	1.38
35	V	301	A86	O4-C38	4.76	1.45	1.35
36	A	306	CLA	C3C-C2C	4.76	1.47	1.36
37	D	314	KC1	C3B-C2B	4.76	1.46	1.37
36	D	309	CLA	CHC-C1C	4.76	1.48	1.38
35	U	303	A86	O4-C38	4.76	1.45	1.35
37	T	315	KC1	C1A-NA	4.75	1.47	1.38
37	G	308	KC1	O2D-CGD	4.75	1.44	1.33
36	b	824	CLA	CHC-C1C	4.74	1.48	1.38
35	W	202	A86	C20-C15	4.74	1.54	1.48
35	E	305	A86	O4-C38	4.74	1.45	1.35
35	U	302	A86	O4-C38	4.74	1.45	1.35
35	W	203	A86	C30-C31	-4.74	1.25	1.30
35	J	301	A86	O4-C38	4.74	1.45	1.35
36	b	816	CLA	O2D-CGD	4.74	1.44	1.33
35	F	304	A86	O4-C38	4.74	1.45	1.35
36	O	316	CLA	C3C-C2C	4.73	1.47	1.36
37	S	316	KC1	CHC-C4B	4.72	1.47	1.38
35	B	303	A86	C20-C15	4.72	1.54	1.48
35	O	319	A86	O4-C38	4.71	1.45	1.35
35	B	301	A86	O4-C38	4.71	1.45	1.35
37	M	313	KC1	CHC-C4B	4.70	1.47	1.38
37	C	213	KC1	C1A-NA	4.69	1.47	1.38
37	G	318	KC1	C3B-C2B	4.69	1.46	1.37
36	G	319	CLA	C3C-C2C	4.67	1.46	1.36
37	A	312	KC1	C3C-C2C	4.67	1.46	1.36
36	f	804	CLA	CHC-C1C	4.67	1.47	1.38
36	f	803	CLA	C3C-C2C	4.67	1.46	1.36
35	N	305	A86	O4-C38	4.67	1.45	1.35
36	A	306	CLA	C3D-C4D	-4.67	1.33	1.44
37	M	318	KC1	CHC-C4B	4.67	1.47	1.38
36	a	823	CLA	C3C-C2C	4.67	1.46	1.36
35	Q	316	A86	O4-C38	4.67	1.45	1.35
37	E	309	KC1	O2D-CGD	4.66	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	305	CLA	C14-C13	4.66	1.67	1.52
37	A	312	KC1	O2D-CGD	4.65	1.44	1.33
35	E	302	A86	O4-C38	4.65	1.45	1.35
37	W	213	KC1	CHC-C4B	4.65	1.47	1.38
37	B	310	KC1	CHB-C1B	4.65	1.47	1.38
37	M	318	KC1	CHB-C1B	4.64	1.47	1.38
37	F	315	KC1	C3C-C2C	4.64	1.46	1.36
36	G	319	CLA	C1D-ND	4.64	1.44	1.37
35	h	204	A86	O4-C38	4.64	1.45	1.35
37	V	312	KC1	CHC-C4B	4.64	1.47	1.38
36	b	817	CLA	C3C-C2C	4.64	1.46	1.36
37	N	314	KC1	CHB-C1B	4.63	1.47	1.38
37	F	308	KC1	C3B-C2B	4.63	1.46	1.37
35	S	305	A86	O4-C38	4.62	1.45	1.35
36	G	307	CLA	O2D-CGD	4.62	1.45	1.30
37	P	317	KC1	C1A-NA	4.62	1.47	1.38
37	C	213	KC1	CHC-C4B	4.61	1.47	1.38
36	b	836	CLA	CHC-C1C	4.61	1.47	1.38
37	F	315	KC1	O2D-CGD	4.61	1.44	1.33
37	O	313	KC1	CHC-C4B	4.60	1.47	1.38
37	R	317	KC1	CHC-C4B	4.60	1.47	1.38
35	J	303	A86	C30-C31	-4.60	1.25	1.30
35	L	306	A86	O4-C38	4.60	1.45	1.35
37	V	312	KC1	CHB-C1B	4.60	1.47	1.38
36	O	316	CLA	CHC-C1C	4.60	1.47	1.38
35	N	320	A86	C20-C15	4.59	1.54	1.48
37	C	213	KC1	CHB-C1B	4.59	1.47	1.38
37	Q	313	KC1	CHC-C4B	4.59	1.47	1.38
35	Q	304	A86	C20-C15	4.59	1.54	1.48
37	Q	311	KC1	CHC-C4B	4.58	1.47	1.38
35	S	301	A86	O1-C20	-4.58	1.40	1.46
35	N	301	A86	O1-C20	-4.58	1.40	1.46
37	F	308	KC1	O2D-CGD	4.57	1.44	1.33
37	K	314	KC1	C1A-NA	4.57	1.47	1.38
35	R	309	A86	O4-C38	4.57	1.45	1.35
37	M	318	KC1	C3B-C4B	4.56	1.54	1.46
36	C	207	CLA	CHC-C1C	4.56	1.47	1.38
35	P	303	A86	C20-C15	4.55	1.54	1.48
37	O	315	KC1	CHC-C4B	4.54	1.47	1.38
37	M	317	KC1	CHC-C4B	4.54	1.47	1.38
37	T	310	KC1	C4B-NB	-4.54	1.31	1.37
37	P	315	KC1	CHC-C4B	4.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	307	CLA	C3D-C4D	-4.53	1.34	1.44
36	F	317	CLA	C1B-NB	-4.53	1.31	1.37
36	a	848	CLA	C3D-C4D	-4.53	1.34	1.44
37	T	315	KC1	CHC-C4B	4.53	1.47	1.38
36	B	308	CLA	C1D-ND	4.52	1.43	1.37
37	U	312	KC1	CHC-C4B	4.52	1.47	1.38
36	I	306	CLA	C1B-NB	-4.52	1.31	1.37
37	D	314	KC1	C1A-NA	4.52	1.47	1.38
35	L	319	A86	C20-C15	4.52	1.54	1.48
37	K	314	KC1	CHB-C1B	4.51	1.47	1.38
35	O	302	A86	C20-C15	4.51	1.54	1.48
36	I	308	CLA	C3D-C4D	-4.51	1.34	1.44
35	R	301	A86	C20-C15	4.50	1.54	1.48
37	P	317	KC1	C3B-C2B	4.50	1.46	1.37
36	W	216	CLA	C1D-ND	4.49	1.43	1.37
36	A	306	CLA	CHC-C1C	4.48	1.47	1.38
36	G	319	CLA	CHC-C1C	4.48	1.47	1.38
37	X	311	KC1	CHB-C1B	4.48	1.47	1.38
37	H	313	KC1	CHC-C4B	4.48	1.47	1.38
37	M	317	KC1	CHB-C1B	4.47	1.47	1.38
36	E	315	CLA	C1D-ND	4.47	1.43	1.37
36	E	315	CLA	CHC-C1C	4.46	1.47	1.38
38	b	804	SQD	O8-S	4.46	1.64	1.47
35	Q	304	A86	O4-C38	4.45	1.45	1.35
35	A	302	A86	O1-C20	-4.45	1.40	1.46
37	W	217	KC1	CHB-C1B	4.44	1.47	1.38
36	b	836	CLA	C1B-NB	-4.44	1.32	1.37
37	U	312	KC1	CHB-C4A	4.43	1.49	1.39
38	A	315	SQD	O8-S	4.43	1.63	1.47
35	U	302	A86	O1-C20	-4.43	1.40	1.46
35	T	307	A86	C20-C15	4.43	1.53	1.48
35	M	301	A86	O1-C20	-4.42	1.40	1.46
35	A	302	A86	C30-C31	-4.41	1.25	1.30
37	E	309	KC1	CHC-C4B	4.41	1.47	1.38
35	Q	303	A86	C30-C31	-4.40	1.25	1.30
35	N	320	A86	O4-C38	4.40	1.44	1.35
37	B	310	KC1	CHC-C4B	4.40	1.47	1.38
35	A	302	A86	C30-C29	-4.40	1.24	1.31
37	L	317	KC1	CHC-C4B	4.39	1.47	1.38
35	R	301	A86	C30-C29	-4.39	1.24	1.31
36	b	817	CLA	C3D-C4D	-4.38	1.34	1.44
36	l	204	CLA	C3D-C4D	-4.38	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	L	304	A86	O1-C20	-4.38	1.40	1.46
36	N	310	CLA	C1B-NB	-4.38	1.32	1.37
35	X	301	A86	C20-C15	4.37	1.53	1.48
37	D	314	KC1	CHB-C1B	4.36	1.46	1.38
36	f	803	CLA	CHC-C1C	4.36	1.47	1.38
35	S	304	A86	C30-C31	-4.36	1.25	1.30
36	G	319	CLA	O2A-CGA	4.36	1.46	1.33
37	T	310	KC1	CHD-C1D	4.36	1.49	1.39
35	N	306	A86	C20-C15	4.35	1.53	1.48
35	I	304	A86	O1-C20	-4.35	1.40	1.46
37	X	311	KC1	CHC-C4B	4.35	1.46	1.38
37	M	318	KC1	C2A-C1A	4.35	1.58	1.44
35	F	305	A86	O4-C38	4.35	1.44	1.35
42	V	316	LMG	O8-C28	4.35	1.46	1.33
36	N	319	CLA	C4B-NB	4.35	1.43	1.37
35	J	301	A86	C20-C15	4.34	1.53	1.48
37	W	217	KC1	CHC-C4B	4.34	1.46	1.38
37	G	308	KC1	CHB-C1B	4.34	1.46	1.38
41	I	316	LHG	O8-C23	4.34	1.46	1.33
35	T	304	A86	O4-C38	4.33	1.44	1.35
36	I	308	CLA	O2A-CGA	4.33	1.46	1.33
36	V	305	CLA	C1D-ND	4.33	1.43	1.37
42	G	324	LMG	O8-C28	4.33	1.46	1.33
35	O	302	A86	O1-C20	-4.32	1.40	1.46
35	C	202	A86	O1-C20	-4.32	1.40	1.46
35	U	301	A86	C20-C15	4.32	1.53	1.48
37	F	315	KC1	CHC-C4B	4.32	1.46	1.38
35	X	304	A86	O1-C20	-4.31	1.40	1.46
42	V	315	LMG	O8-C28	4.31	1.45	1.33
36	E	315	CLA	C3D-C4D	-4.31	1.34	1.44
40	L	302	DGD	O1G-C1A	4.31	1.45	1.33
42	h	206	LMG	O8-C28	4.31	1.45	1.33
36	W	216	CLA	CHB-C1B	4.31	1.49	1.39
36	K	307	CLA	O2A-CGA	4.31	1.45	1.33
37	G	308	KC1	CHC-C4B	4.31	1.46	1.38
41	F	319	LHG	O8-C23	4.30	1.45	1.33
37	T	310	KC1	C2A-C1A	4.30	1.58	1.44
41	G	320	LHG	O8-C23	4.30	1.45	1.33
41	f	808	LHG	O8-C23	4.30	1.45	1.33
36	U	306	CLA	O2A-CGA	4.29	1.45	1.33
41	f	809	LHG	O8-C23	4.29	1.45	1.33
37	D	314	KC1	CHC-C4B	4.29	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	308	CLA	O2A-CGA	4.29	1.45	1.33
41	i	104	LHG	O8-C23	4.29	1.45	1.33
42	E	318	LMG	O8-C28	4.29	1.45	1.33
36	G	315	CLA	O2A-CGA	4.28	1.45	1.33
36	b	816	CLA	C3D-C4D	-4.28	1.34	1.44
37	T	310	KC1	CAB-C3B	4.28	1.58	1.47
35	R	301	A86	O1-C20	-4.28	1.40	1.46
42	m	102	LMG	O8-C28	4.28	1.45	1.33
36	A	306	CLA	O2A-CGA	4.27	1.45	1.33
41	l	208	LHG	O8-C23	4.27	1.45	1.33
41	G	321	LHG	O8-C23	4.27	1.45	1.33
41	a	850	LHG	O8-C23	4.27	1.45	1.33
36	K	307	CLA	CHC-C1C	4.27	1.47	1.38
35	X	301	A86	C30-C31	-4.27	1.25	1.30
42	G	325	LMG	O8-C28	4.26	1.45	1.33
36	a	822	CLA	O2A-CGA	4.26	1.45	1.33
36	b	817	CLA	O2A-CGA	4.26	1.45	1.33
35	R	304	A86	O1-C20	-4.26	1.40	1.46
36	l	205	CLA	O2A-CGA	4.26	1.45	1.33
37	E	309	KC1	CHB-C1B	4.26	1.46	1.38
36	A	306	CLA	C1D-ND	4.26	1.43	1.37
36	b	816	CLA	O2A-CGA	4.26	1.45	1.33
36	f	803	CLA	O2A-CGA	4.26	1.45	1.33
36	F	317	CLA	O2A-CGA	4.26	1.45	1.33
37	K	314	KC1	CHC-C4B	4.26	1.46	1.38
36	V	314	CLA	C3C-C2C	4.25	1.45	1.36
41	Q	315	LHG	O8-C23	4.25	1.45	1.33
42	D	321	LMG	O8-C28	4.25	1.45	1.33
37	F	315	KC1	CHB-C1B	4.25	1.46	1.38
37	L	317	KC1	CHB-C1B	4.25	1.46	1.38
35	L	319	A86	O1-C20	-4.25	1.40	1.46
35	R	301	A86	C30-C31	-4.25	1.25	1.30
41	R	323	LHG	O8-C23	4.25	1.45	1.33
36	V	314	CLA	O2A-CGA	4.25	1.45	1.33
36	E	313	CLA	C3C-C2C	4.25	1.45	1.36
35	O	303	A86	C30-C31	-4.25	1.25	1.30
36	a	802	CLA	O2A-CGA	4.24	1.45	1.33
36	f	804	CLA	O2A-CGA	4.24	1.45	1.33
35	J	301	A86	C30-C31	-4.24	1.25	1.30
37	G	317	KC1	CHC-C4B	4.24	1.46	1.38
36	a	823	CLA	O2A-CGA	4.24	1.45	1.33
36	j	102	CLA	O2A-CGA	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	H	301	A86	O1-C20	-4.24	1.40	1.46
35	X	303	A86	C30-C31	-4.24	1.25	1.30
42	D	320	LMG	O8-C28	4.24	1.45	1.33
41	E	322	LHG	O8-C23	4.24	1.45	1.33
37	G	317	KC1	CHB-C1B	4.24	1.46	1.38
36	l	204	CLA	O2A-CGA	4.24	1.45	1.33
38	b	804	SQD	O48-C23	4.24	1.45	1.33
35	J	306	A86	C30-C31	-4.23	1.25	1.30
40	C	215	DGD	O1G-C1A	4.23	1.45	1.33
35	P	304	A86	C30-C31	-4.23	1.25	1.30
42	a	852	LMG	O8-C28	4.23	1.45	1.33
42	J	319	LMG	O8-C28	4.23	1.45	1.33
37	P	317	KC1	CHB-C1B	4.23	1.46	1.38
37	M	313	KC1	CHB-C1B	4.23	1.46	1.38
36	b	836	CLA	O2A-CGA	4.23	1.45	1.33
42	E	319	LMG	O8-C28	4.23	1.45	1.33
36	E	313	CLA	O2A-CGA	4.23	1.45	1.33
37	T	310	KC1	CHB-C1B	4.22	1.46	1.38
36	O	312	CLA	C2A-C1A	4.22	1.56	1.51
41	j	104	LHG	O8-C23	4.22	1.45	1.33
35	B	303	A86	O1-C20	-4.22	1.40	1.46
35	Q	301	A86	C30-C31	-4.22	1.25	1.30
36	B	309	CLA	O2A-CGA	4.22	1.45	1.33
36	D	309	CLA	O2A-CGA	4.22	1.45	1.33
35	K	302	A86	O1-C20	-4.22	1.40	1.46
42	L	321	LMG	O8-C28	4.21	1.45	1.33
35	F	301	A86	C20-C15	4.21	1.53	1.48
41	i	104	LHG	O7-C7	4.21	1.46	1.34
35	P	303	A86	O1-C20	-4.21	1.40	1.46
36	a	806	CLA	O2A-CGA	4.21	1.45	1.33
36	K	307	CLA	C3C-C2C	4.21	1.45	1.36
35	T	307	A86	O1-C20	-4.21	1.40	1.46
36	O	316	CLA	O2A-CGA	4.20	1.45	1.33
41	D	319	LHG	O8-C23	4.20	1.45	1.33
37	P	317	KC1	CHC-C4B	4.20	1.46	1.38
35	R	309	A86	O1-C20	-4.20	1.40	1.46
41	b	850	LHG	O8-C23	4.20	1.45	1.33
35	X	303	A86	O1-C20	-4.20	1.40	1.46
37	G	318	KC1	CHB-C1B	4.20	1.46	1.38
36	b	824	CLA	C3D-C4D	-4.20	1.34	1.44
36	E	315	CLA	O2A-CGA	4.20	1.45	1.33
41	a	843	LHG	O8-C23	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	816	CLA	O2A-CGA	4.19	1.45	1.33
36	a	825	CLA	O2A-CGA	4.19	1.45	1.33
35	C	204	A86	C30-C31	-4.19	1.25	1.30
36	K	310	CLA	C3D-C4D	-4.19	1.34	1.44
35	X	305	A86	O1-C20	-4.18	1.40	1.46
41	O	317	LHG	O8-C23	4.18	1.45	1.33
37	T	315	KC1	CHB-C1B	4.18	1.46	1.38
36	X	313	CLA	C1D-ND	4.18	1.43	1.37
36	a	848	CLA	O2A-CGA	4.18	1.45	1.33
42	j	105	LMG	O8-C28	4.18	1.45	1.33
36	I	306	CLA	O2A-CGA	4.18	1.45	1.33
36	b	824	CLA	O2A-CGA	4.17	1.45	1.33
36	a	830	CLA	O2A-CGA	4.17	1.45	1.33
35	K	303	A86	O1-C20	-4.17	1.40	1.46
37	A	312	KC1	CHC-C4B	4.17	1.46	1.38
36	G	307	CLA	C1B-NB	-4.17	1.32	1.37
36	C	207	CLA	O2A-CGA	4.16	1.45	1.33
42	I	315	LMG	O8-C28	4.16	1.45	1.33
36	I	308	CLA	C3C-C2C	4.16	1.45	1.36
37	J	314	KC1	CHC-C4B	4.16	1.46	1.38
41	f	808	LHG	O7-C7	4.16	1.46	1.34
35	G	306	A86	C20-C15	4.15	1.53	1.48
36	l	205	CLA	CHC-C1C	4.15	1.46	1.38
41	G	321	LHG	O7-C7	4.15	1.46	1.34
35	R	306	A86	C20-C15	4.15	1.53	1.48
42	G	324	LMG	O7-C10	4.15	1.46	1.34
35	I	304	A86	C30-C31	-4.14	1.25	1.30
35	R	309	A86	C20-C15	4.14	1.53	1.48
41	G	320	LHG	O7-C7	4.14	1.46	1.34
35	V	302	A86	C30-C31	-4.14	1.25	1.30
35	F	305	A86	C30-C31	-4.14	1.25	1.30
36	F	317	CLA	C3C-C2C	4.14	1.45	1.36
35	Q	304	A86	O1-C20	-4.14	1.40	1.46
35	L	301	A86	C30-C31	-4.14	1.25	1.30
37	G	318	KC1	CHC-C4B	4.13	1.46	1.38
35	M	305	A86	O1-C20	-4.13	1.40	1.46
35	N	320	A86	O1-C20	-4.13	1.40	1.46
35	B	301	A86	C30-C31	-4.13	1.25	1.30
42	J	318	LMG	O8-C28	4.13	1.45	1.33
35	O	301	A86	C30-C31	-4.13	1.25	1.30
41	I	316	LHG	O7-C7	4.12	1.45	1.34
36	K	310	CLA	O2A-CGA	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	J	314	KC1	CHB-C1B	4.12	1.46	1.38
35	M	305	A86	C30-C31	-4.12	1.25	1.30
37	F	308	KC1	CHB-C1B	4.12	1.46	1.38
42	a	852	LMG	O7-C10	4.12	1.45	1.34
35	X	302	A86	O1-C20	-4.11	1.40	1.46
35	W	203	A86	C20-C15	4.11	1.53	1.48
36	H	307	CLA	C1D-ND	4.11	1.43	1.37
42	D	321	LMG	O7-C10	4.11	1.45	1.34
41	F	319	LHG	O7-C7	4.10	1.45	1.34
42	D	320	LMG	O7-C10	4.10	1.45	1.34
42	V	315	LMG	O7-C10	4.10	1.45	1.34
40	C	215	DGD	O2G-C1B	4.10	1.45	1.34
36	f	804	CLA	MG-NA	4.10	2.16	2.06
42	V	316	LMG	O7-C10	4.10	1.45	1.34
41	a	850	LHG	O7-C7	4.09	1.45	1.34
35	J	305	A86	C30-C31	-4.09	1.25	1.30
42	J	318	LMG	O7-C10	4.09	1.45	1.34
38	b	804	SQD	O47-C7	4.08	1.45	1.34
35	F	306	A86	C20-C15	4.08	1.53	1.48
42	E	319	LMG	O7-C10	4.08	1.45	1.34
35	T	307	A86	O4-C38	4.08	1.44	1.35
42	I	315	LMG	O7-C10	4.08	1.45	1.34
35	X	314	A86	C30-C31	-4.08	1.25	1.30
35	K	301	A86	C30-C31	-4.08	1.25	1.30
36	f	804	CLA	C3D-C4D	-4.08	1.35	1.44
42	m	102	LMG	O7-C10	4.08	1.45	1.34
41	f	809	LHG	O7-C7	4.07	1.45	1.34
35	E	307	A86	C30-C31	-4.07	1.25	1.30
41	j	104	LHG	O7-C7	4.07	1.45	1.34
41	E	322	LHG	O7-C7	4.07	1.45	1.34
35	M	301	A86	C20-C15	4.07	1.53	1.48
41	Q	315	LHG	O7-C7	4.07	1.45	1.34
38	A	315	SQD	O47-C7	4.07	1.45	1.34
41	R	323	LHG	O7-C7	4.07	1.45	1.34
35	H	304	A86	C30-C31	-4.06	1.25	1.30
42	J	319	LMG	O7-C10	4.06	1.45	1.34
42	G	325	LMG	O7-C10	4.06	1.45	1.34
41	l	208	LHG	O7-C7	4.05	1.45	1.34
36	C	207	CLA	C3D-C2D	4.05	1.50	1.39
42	L	321	LMG	O7-C10	4.04	1.45	1.34
35	F	306	A86	C30-C31	-4.04	1.25	1.30
41	O	317	LHG	O7-C7	4.04	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	P	307	A86	C20-C15	4.04	1.53	1.48
42	E	318	LMG	O7-C10	4.04	1.45	1.34
35	K	302	A86	C20-C15	4.04	1.53	1.48
35	W	202	A86	C30-C31	-4.03	1.25	1.30
41	D	319	LHG	O7-C7	4.02	1.45	1.34
35	N	302	A86	C20-C15	4.01	1.53	1.48
35	Q	303	A86	C30-C29	-4.01	1.25	1.31
35	E	302	A86	C30-C31	-4.01	1.25	1.30
35	O	301	A86	C20-C15	4.01	1.53	1.48
35	E	305	A86	C30-C31	-4.01	1.25	1.30
37	F	308	KC1	CHC-C4B	4.01	1.46	1.38
35	O	305	A86	C30-C29	-4.01	1.25	1.31
36	X	313	CLA	C1B-NB	-4.00	1.32	1.37
42	h	206	LMG	O7-C10	4.00	1.45	1.34
35	C	202	A86	C20-C15	4.00	1.53	1.48
35	S	305	A86	O1-C20	-4.00	1.41	1.46
41	a	843	LHG	O7-C7	4.00	1.45	1.34
35	P	306	A86	C30-C31	-4.00	1.25	1.30
35	C	203	A86	C20-C15	4.00	1.53	1.48
35	A	316	A86	C30-C31	-3.99	1.25	1.30
35	I	301	A86	C20-C15	3.99	1.53	1.48
35	P	307	A86	C30-C31	-3.98	1.25	1.30
35	A	316	A86	C20-C15	3.98	1.53	1.48
36	A	314	CLA	OBD-CAD	3.98	1.29	1.22
35	R	306	A86	O1-C20	-3.98	1.41	1.46
35	S	302	A86	C20-C15	3.98	1.53	1.48
40	L	302	DGD	O2G-C1B	3.97	1.45	1.34
35	T	301	A86	C30-C31	-3.97	1.26	1.30
35	R	305	A86	C30-C31	-3.97	1.26	1.30
35	T	301	A86	C20-C15	3.97	1.53	1.48
35	W	202	A86	O1-C20	-3.97	1.41	1.46
35	F	302	A86	C30-C31	-3.96	1.26	1.30
35	h	204	A86	C30-C31	-3.96	1.26	1.30
35	V	301	A86	C30-C31	-3.96	1.26	1.30
35	E	305	A86	C20-C15	3.96	1.53	1.48
36	W	216	CLA	CHB-C4A	3.96	1.47	1.37
35	L	307	A86	C30-C31	-3.95	1.26	1.30
35	J	305	A86	C20-C15	3.95	1.53	1.48
35	A	302	A86	C20-C15	3.95	1.53	1.48
35	F	304	A86	C20-C15	3.95	1.53	1.48
35	J	302	A86	C30-C31	-3.95	1.26	1.30
36	G	307	CLA	C3C-C2C	3.95	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	304	A86	C30-C31	-3.95	1.26	1.30
35	X	301	A86	C30-C29	-3.95	1.25	1.31
35	S	308	A86	C30-C31	-3.95	1.26	1.30
35	M	304	A86	C30-C31	-3.94	1.26	1.30
36	Q	310	CLA	C2-C3	3.94	1.42	1.33
37	O	313	KC1	CHB-C4A	3.94	1.48	1.39
35	M	304	A86	C20-C15	3.94	1.53	1.48
42	j	105	LMG	O7-C10	3.94	1.45	1.34
35	T	305	A86	O1-C20	-3.93	1.41	1.46
36	N	308	CLA	C4B-NB	3.93	1.43	1.37
35	T	306	A86	C20-C15	3.93	1.53	1.48
35	U	304	A86	C20-C15	3.93	1.53	1.48
37	P	315	KC1	CHB-C4A	3.93	1.48	1.39
36	B	309	CLA	C1B-NB	-3.93	1.32	1.37
35	T	302	A86	C20-C15	3.92	1.53	1.48
37	Q	313	KC1	CHB-C4A	3.92	1.48	1.39
35	I	301	A86	C30-C31	-3.92	1.26	1.30
35	h	202	A86	C30-C31	-3.91	1.26	1.30
37	O	315	KC1	CHB-C4A	3.91	1.48	1.39
37	L	315	KC1	CHB-C4A	3.91	1.48	1.39
37	Q	311	KC1	CHB-C4A	3.91	1.48	1.39
36	f	803	CLA	C3D-C4D	-3.91	1.35	1.44
35	T	304	A86	C20-C15	3.91	1.53	1.48
35	X	314	A86	C20-C15	3.91	1.53	1.48
35	W	203	A86	C30-C29	-3.90	1.25	1.31
35	B	301	A86	C20-C15	3.90	1.53	1.48
35	S	304	A86	C30-C29	-3.90	1.25	1.31
35	V	301	A86	C20-C15	3.89	1.53	1.48
35	D	302	A86	C30-C31	-3.89	1.26	1.30
41	b	850	LHG	O7-C7	3.89	1.45	1.34
35	X	302	A86	C20-C15	3.89	1.53	1.48
35	L	304	A86	C30-C29	-3.89	1.25	1.31
35	F	305	A86	O1-C20	-3.88	1.41	1.46
35	J	306	A86	C20-C15	3.88	1.53	1.48
35	J	303	A86	O1-C20	-3.88	1.41	1.46
36	E	313	CLA	CHC-C1C	3.88	1.46	1.38
35	U	303	A86	C30-C31	-3.87	1.26	1.30
35	E	307	A86	C20-C15	3.87	1.53	1.48
37	F	308	KC1	CHD-C1D	3.87	1.48	1.39
36	Q	310	CLA	CAA-CBA	3.87	1.64	1.52
35	F	302	A86	C20-C15	3.87	1.53	1.48
37	W	213	KC1	CHD-C1D	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	203	A86	C30-C31	-3.86	1.26	1.30
35	S	308	A86	C20-C15	3.85	1.53	1.48
35	H	304	A86	C20-C15	3.85	1.53	1.48
35	F	301	A86	C30-C31	-3.85	1.26	1.30
37	M	318	KC1	CHB-C4A	-3.85	1.30	1.39
35	D	302	A86	C20-C15	3.85	1.53	1.48
36	F	317	CLA	CHC-C1C	3.84	1.46	1.38
37	A	312	KC1	CHB-C1B	3.84	1.45	1.38
36	U	309	CLA	C1D-ND	3.83	1.42	1.37
35	J	306	A86	C30-C29	-3.83	1.25	1.31
37	G	318	KC1	CHD-C1D	3.83	1.48	1.39
36	S	314	CLA	C1D-ND	3.83	1.42	1.37
35	O	301	A86	C30-C29	-3.83	1.25	1.31
36	V	314	CLA	CHC-C1C	3.82	1.46	1.38
35	G	305	A86	C30-C31	-3.82	1.26	1.30
35	M	301	A86	C30-C31	-3.82	1.26	1.30
35	L	301	A86	C20-C15	3.82	1.53	1.48
35	K	302	A86	C30-C31	-3.82	1.26	1.30
37	B	310	KC1	CHD-C1D	3.82	1.48	1.39
36	X	307	CLA	C1D-ND	3.81	1.42	1.37
35	F	304	A86	C30-C29	-3.81	1.25	1.31
36	b	826	CLA	O2D-CGD	3.80	1.42	1.33
37	B	310	KC1	OBD-CAD	3.80	1.29	1.22
34	D	303	DD6	C24-C1	3.80	1.54	1.46
35	C	204	A86	C30-C29	-3.80	1.25	1.31
36	K	307	CLA	C1B-NB	-3.80	1.32	1.37
35	X	301	A86	O1-C20	-3.79	1.41	1.46
36	X	310	CLA	C1D-ND	3.79	1.42	1.37
36	C	210	CLA	C1D-ND	3.79	1.42	1.37
35	J	301	A86	C30-C29	-3.79	1.25	1.31
36	G	315	CLA	C3C-C2C	3.79	1.44	1.36
36	N	315	CLA	C1D-ND	3.79	1.42	1.37
35	V	304	A86	C17-C18	-3.78	1.47	1.52
35	L	306	A86	O1-C20	-3.78	1.41	1.46
37	R	317	KC1	CHB-C1B	3.78	1.45	1.38
37	W	213	KC1	CHB-C4A	3.78	1.47	1.39
36	V	314	CLA	C1B-NB	-3.77	1.32	1.37
36	G	315	CLA	CHC-C1C	3.77	1.46	1.38
35	V	304	A86	C30-C31	-3.77	1.26	1.30
35	W	203	A86	O1-C20	-3.77	1.41	1.46
35	H	304	A86	C30-C29	-3.77	1.25	1.31
35	J	302	A86	C20-C15	3.77	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	311	KC1	CHD-C1D	3.77	1.47	1.39
37	W	213	KC1	OBD-CAD	3.76	1.29	1.22
35	V	304	A86	C19-C20	3.76	1.57	1.52
35	B	301	A86	C30-C29	-3.76	1.25	1.31
35	T	307	A86	C30-C31	-3.75	1.26	1.30
36	K	310	CLA	CHD-C4C	3.75	1.47	1.39
35	K	306	A86	O1-C20	-3.75	1.41	1.46
36	G	315	CLA	CHD-C4C	3.75	1.47	1.39
35	I	304	A86	C20-C15	3.74	1.53	1.48
36	E	315	CLA	CHD-C4C	3.74	1.47	1.39
44	a	847	BCR	C30-C25	-3.74	1.49	1.53
35	J	305	A86	C30-C29	-3.74	1.25	1.31
37	W	217	KC1	CHD-C1D	3.73	1.47	1.39
35	L	301	A86	C30-C29	-3.73	1.25	1.31
36	U	306	CLA	OBD-CAD	3.73	1.28	1.22
36	l	204	CLA	CHB-C1B	3.73	1.47	1.39
36	E	317	CLA	C1D-ND	3.72	1.42	1.37
35	C	204	A86	C20-C15	3.71	1.52	1.48
35	A	316	A86	C30-C29	-3.71	1.25	1.31
35	Q	301	A86	C30-C29	-3.71	1.25	1.31
37	T	310	KC1	CHC-C4B	3.71	1.45	1.38
36	U	306	CLA	C1B-NB	-3.71	1.33	1.37
35	I	302	A86	O1-C20	-3.71	1.41	1.46
35	J	302	A86	C30-C29	-3.70	1.25	1.31
35	N	304	A86	C30-C31	-3.70	1.26	1.30
36	f	804	CLA	CHD-C4C	3.70	1.47	1.39
35	P	307	A86	C30-C29	-3.70	1.25	1.31
35	V	301	A86	C30-C29	-3.70	1.25	1.31
36	S	315	CLA	C1D-ND	3.70	1.42	1.37
35	K	303	A86	C30-C31	-3.70	1.26	1.30
37	N	314	KC1	CHD-C1D	3.70	1.47	1.39
35	F	305	A86	C20-C15	3.70	1.52	1.48
35	E	305	A86	C30-C29	-3.69	1.25	1.31
35	Q	316	A86	C30-C29	-3.69	1.25	1.31
35	K	301	A86	C30-C29	-3.69	1.25	1.31
35	X	314	A86	C30-C29	-3.69	1.25	1.31
35	T	302	A86	O1-C20	-3.68	1.41	1.46
36	I	308	CLA	OBD-CAD	3.68	1.28	1.22
35	R	303	A86	C20-C15	3.68	1.52	1.48
35	N	305	A86	C30-C29	-3.68	1.25	1.31
37	B	310	KC1	CHB-C4A	3.68	1.47	1.39
35	E	307	A86	C30-C29	-3.68	1.25	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	R	302	A86	O1-C20	-3.68	1.41	1.46
35	I	302	A86	C30-C31	-3.68	1.26	1.30
35	L	307	A86	C20-C15	3.67	1.52	1.48
37	S	316	KC1	CHD-C1D	3.67	1.47	1.39
37	L	315	KC1	OBD-CAD	3.67	1.28	1.22
35	R	303	A86	O1-C20	-3.67	1.41	1.46
37	D	314	KC1	CHD-C1D	3.67	1.47	1.39
35	R	303	A86	C30-C31	-3.67	1.26	1.30
35	U	304	A86	C30-C31	-3.67	1.26	1.30
35	F	302	A86	C30-C29	-3.67	1.25	1.31
35	L	307	A86	C30-C29	-3.66	1.25	1.31
35	O	303	A86	C30-C29	-3.66	1.25	1.31
36	b	824	CLA	CHB-C1B	3.66	1.47	1.39
36	B	309	CLA	OBD-CAD	3.66	1.28	1.22
36	L	308	CLA	OBD-CAD	3.66	1.28	1.22
36	b	816	CLA	CHD-C1D	3.66	1.45	1.38
35	W	202	A86	C30-C29	-3.66	1.25	1.31
36	a	801	CLA	CMD-C2D	-3.66	1.43	1.50
37	V	312	KC1	CHB-C4A	3.66	1.47	1.39
35	P	304	A86	C30-C29	-3.66	1.26	1.31
36	N	308	CLA	MG-NB	-3.66	1.98	2.05
35	P	306	A86	C30-C29	-3.66	1.26	1.31
36	f	804	CLA	CHB-C1B	3.66	1.47	1.39
36	W	209	CLA	C1D-ND	3.65	1.42	1.37
35	U	303	A86	C30-C29	-3.65	1.26	1.31
35	V	302	A86	O1-C20	-3.65	1.41	1.46
35	h	204	A86	C30-C29	-3.65	1.26	1.31
37	S	316	KC1	CHB-C1B	3.65	1.45	1.38
35	N	320	A86	C30-C31	-3.65	1.26	1.30
35	U	301	A86	C30-C31	-3.65	1.26	1.30
35	E	302	A86	C30-C29	-3.64	1.26	1.31
35	S	308	A86	C30-C29	-3.64	1.26	1.31
36	N	309	CLA	C1D-ND	3.64	1.42	1.37
35	F	306	A86	C30-C29	-3.64	1.26	1.31
35	M	302	A86	O1-C20	-3.64	1.41	1.46
35	X	301	A86	C32-C31	3.64	1.60	1.54
36	l	204	CLA	CHC-C1C	3.64	1.45	1.38
44	b	843	BCR	C1-C6	-3.64	1.49	1.53
36	U	305	CLA	C1D-ND	3.63	1.42	1.37
44	l	203	BCR	C30-C25	-3.63	1.49	1.53
37	P	315	KC1	OBD-CAD	3.63	1.28	1.22
35	V	303	A86	O1-C20	-3.63	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	307	CLA	OBD-CAD	3.62	1.28	1.22
36	O	316	CLA	OBD-CAD	3.62	1.28	1.22
37	N	314	KC1	OBD-CAD	3.62	1.28	1.22
36	G	315	CLA	C1D-ND	3.62	1.42	1.37
36	X	306	CLA	C1D-ND	3.62	1.42	1.37
37	O	313	KC1	OBD-CAD	3.62	1.28	1.22
35	C	204	A86	C24-C1	3.62	1.53	1.46
37	V	312	KC1	CHD-C1D	3.62	1.47	1.39
37	G	308	KC1	CHD-C1D	3.62	1.47	1.39
35	V	303	A86	C20-C15	3.62	1.52	1.48
35	M	302	A86	C30-C31	-3.62	1.26	1.30
37	H	313	KC1	CHB-C1B	3.62	1.45	1.38
37	Q	313	KC1	OBD-CAD	3.61	1.28	1.22
35	K	301	A86	C20-C15	3.61	1.52	1.48
35	N	306	A86	O1-C20	-3.61	1.41	1.46
36	S	311	CLA	C1D-ND	3.61	1.42	1.37
44	i	103	BCR	C1-C6	-3.61	1.49	1.53
37	W	217	KC1	CHB-C4A	3.61	1.47	1.39
37	X	311	KC1	CHB-C4A	3.61	1.47	1.39
36	L	316	CLA	C1D-ND	3.61	1.42	1.37
36	G	315	CLA	OBD-CAD	3.61	1.28	1.22
37	A	312	KC1	CHD-C1D	3.61	1.47	1.39
37	N	314	KC1	CHB-C4A	3.61	1.47	1.39
37	C	213	KC1	CHD-C1D	3.61	1.47	1.39
36	D	309	CLA	CHD-C4C	3.60	1.47	1.39
36	I	306	CLA	OBD-CAD	3.60	1.28	1.22
36	L	308	CLA	C3D-C4D	-3.60	1.36	1.44
35	M	304	A86	C30-C29	-3.60	1.26	1.31
36	G	307	CLA	CHC-C1C	3.60	1.45	1.38
35	h	202	A86	C30-C29	-3.60	1.26	1.31
35	I	301	A86	C30-C29	-3.60	1.26	1.31
36	K	307	CLA	OBD-CAD	3.60	1.28	1.22
35	Q	304	A86	C30-C31	-3.60	1.26	1.30
36	b	817	CLA	OBD-CAD	3.60	1.28	1.22
35	X	303	A86	C30-C29	-3.60	1.26	1.31
37	S	316	KC1	CHC-C1C	3.59	1.47	1.39
37	U	312	KC1	CHD-C1D	3.59	1.47	1.39
37	Q	311	KC1	OBD-CAD	3.59	1.28	1.22
37	O	315	KC1	OBD-CAD	3.59	1.28	1.22
36	F	317	CLA	OBD-CAD	3.59	1.28	1.22
36	a	822	CLA	OBD-CAD	3.59	1.28	1.22
37	M	318	KC1	CAB-C3B	3.59	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	D	302	A86	C30-C29	-3.59	1.26	1.31
36	f	803	CLA	C1D-ND	3.59	1.42	1.37
37	R	317	KC1	OBD-CAD	3.59	1.28	1.22
36	V	314	CLA	OBD-CAD	3.59	1.28	1.22
35	T	301	A86	C30-C29	-3.59	1.26	1.31
37	T	315	KC1	CHD-C1D	3.59	1.47	1.39
36	a	829	CLA	CMB-C2B	-3.58	1.43	1.50
35	O	319	A86	C20-C15	3.58	1.52	1.48
35	G	306	A86	C30-C31	-3.58	1.26	1.30
35	R	305	A86	C30-C29	-3.58	1.26	1.31
35	G	305	A86	C30-C29	-3.58	1.26	1.31
37	T	310	KC1	C4A-C3A	3.58	1.51	1.44
36	E	315	CLA	OBD-CAD	3.58	1.28	1.22
37	X	311	KC1	OBD-CAD	3.58	1.28	1.22
36	K	310	CLA	OBD-CAD	3.57	1.28	1.22
37	C	213	KC1	CHB-C4A	3.57	1.47	1.39
36	A	306	CLA	CHD-C4C	3.56	1.47	1.39
36	a	825	CLA	OBD-CAD	3.56	1.28	1.22
37	W	217	KC1	OBD-CAD	3.56	1.28	1.22
36	l	205	CLA	OBD-CAD	3.56	1.28	1.22
37	T	315	KC1	OBD-CAD	3.56	1.28	1.22
36	L	308	CLA	MG-NB	-3.56	1.98	2.05
35	N	306	A86	C30-C31	-3.56	1.26	1.30
36	b	816	CLA	OBD-CAD	3.56	1.28	1.22
36	S	320	CLA	C1D-ND	3.56	1.42	1.37
37	S	316	KC1	OBD-CAD	3.56	1.28	1.22
37	G	317	KC1	CHD-C1D	3.55	1.47	1.39
36	b	824	CLA	CHD-C4C	3.55	1.47	1.39
35	F	301	A86	C30-C29	-3.55	1.26	1.31
36	C	207	CLA	C3D-C4D	-3.55	1.36	1.44
35	C	203	A86	C30-C29	-3.55	1.26	1.31
36	A	306	CLA	OBD-CAD	3.55	1.28	1.22
36	a	823	CLA	OBD-CAD	3.54	1.28	1.22
36	L	312	CLA	C1D-ND	3.53	1.42	1.37
36	X	313	CLA	CHC-C4B	-3.53	1.31	1.39
36	f	804	CLA	OBD-CAD	3.53	1.28	1.22
35	R	306	A86	C30-C31	-3.53	1.26	1.30
36	a	806	CLA	OBD-CAD	3.53	1.28	1.22
35	L	319	A86	C30-C31	-3.53	1.26	1.30
37	A	312	KC1	CHB-C4A	3.53	1.47	1.39
36	D	309	CLA	OBD-CAD	3.53	1.28	1.22
36	W	214	CLA	C4B-NB	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	O	303	A86	O1-C20	-3.52	1.41	1.46
36	E	313	CLA	OBD-CAD	3.52	1.28	1.22
44	h	201	BCR	C1-C6	-3.52	1.49	1.53
36	b	836	CLA	OBD-CAD	3.52	1.28	1.22
37	D	314	KC1	CHB-C4A	3.52	1.47	1.39
36	C	207	CLA	CHD-C4C	3.52	1.47	1.39
35	O	319	A86	O1-C20	-3.52	1.41	1.46
37	J	314	KC1	CHD-C1D	3.51	1.47	1.39
36	l	204	CLA	C1C-NC	-3.51	1.32	1.37
36	C	207	CLA	OBD-CAD	3.51	1.28	1.22
35	P	304	A86	O1-C20	-3.51	1.41	1.46
36	W	210	CLA	C1D-ND	3.51	1.42	1.37
35	O	302	A86	C30-C31	-3.51	1.26	1.30
36	f	803	CLA	OBD-CAD	3.51	1.28	1.22
37	E	309	KC1	CHD-C1D	3.51	1.47	1.39
36	Q	310	CLA	C4B-NB	3.51	1.42	1.37
37	M	318	KC1	CHD-C1D	3.51	1.47	1.39
35	K	302	A86	C30-C29	-3.51	1.26	1.31
37	N	314	KC1	CHC-C1C	3.51	1.47	1.39
37	R	317	KC1	CHD-C1D	3.51	1.47	1.39
36	a	816	CLA	OBD-CAD	3.50	1.28	1.22
35	V	302	A86	C20-C15	3.50	1.52	1.48
35	E	302	A86	C20-C15	3.50	1.52	1.48
35	h	204	A86	C20-C15	3.50	1.52	1.48
36	A	314	CLA	C1D-ND	3.50	1.42	1.37
35	N	302	A86	O1-C20	-3.50	1.41	1.46
37	M	313	KC1	CHD-C1D	3.50	1.47	1.39
35	P	303	A86	C30-C31	-3.50	1.26	1.30
36	B	307	CLA	C1D-ND	3.50	1.42	1.37
36	V	305	CLA	C1B-C2B	3.50	1.51	1.43
36	G	319	CLA	OBD-CAD	3.50	1.28	1.22
37	H	313	KC1	CHD-C1D	3.50	1.47	1.39
36	a	830	CLA	OBD-CAD	3.50	1.28	1.22
37	V	312	KC1	CHC-C1C	3.50	1.47	1.39
36	l	204	CLA	OBD-CAD	3.49	1.28	1.22
36	S	317	CLA	C1D-ND	3.49	1.42	1.37
37	K	314	KC1	CHB-C4A	3.49	1.47	1.39
36	R	319	CLA	C1D-ND	3.48	1.42	1.37
35	R	302	A86	C30-C29	-3.48	1.26	1.31
35	S	302	A86	O1-C20	-3.48	1.41	1.46
36	L	308	CLA	C1D-ND	3.48	1.42	1.37
37	G	317	KC1	OBD-CAD	3.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	816	CLA	CHB-C1B	3.47	1.47	1.39
36	f	804	CLA	MG-ND	-3.47	1.98	2.05
36	U	313	CLA	C1D-ND	3.47	1.42	1.37
36	R	314	CLA	C1D-ND	3.47	1.42	1.37
37	F	315	KC1	OBD-CAD	3.47	1.28	1.22
35	M	305	A86	C30-C29	-3.46	1.26	1.31
36	K	311	CLA	C1D-ND	3.46	1.42	1.37
35	Q	301	A86	O1-C20	-3.46	1.41	1.46
37	P	315	KC1	CHD-C1D	3.45	1.47	1.39
37	F	308	KC1	C1B-NB	-3.45	1.33	1.37
36	D	309	CLA	C3D-C4D	-3.45	1.36	1.44
37	O	315	KC1	CHD-C1D	3.45	1.47	1.39
36	N	313	CLA	C1D-ND	3.45	1.42	1.37
35	N	304	A86	C30-C29	-3.45	1.26	1.31
37	O	313	KC1	CHD-C1D	3.45	1.47	1.39
35	G	305	A86	C20-C15	3.45	1.52	1.48
37	L	317	KC1	CHD-C1D	3.45	1.47	1.39
35	F	307	A86	C20-C15	3.45	1.52	1.48
36	b	836	CLA	C3D-C4D	-3.44	1.36	1.44
37	Q	313	KC1	CHD-C1D	3.44	1.47	1.39
35	U	302	A86	C30-C31	-3.44	1.26	1.30
36	E	313	CLA	CHB-C1B	3.44	1.47	1.39
36	J	308	CLA	C1D-ND	3.44	1.42	1.37
35	F	307	A86	C30-C29	-3.44	1.26	1.31
35	X	305	A86	C30-C31	-3.44	1.26	1.30
36	J	311	CLA	C1D-ND	3.44	1.42	1.37
36	b	824	CLA	OBD-CAD	3.44	1.28	1.22
35	T	303	A86	O1-C20	-3.44	1.41	1.46
37	Q	311	KC1	CHD-C1D	3.43	1.47	1.39
37	L	317	KC1	CHB-C4A	3.43	1.47	1.39
35	H	301	A86	C20-C15	3.43	1.52	1.48
36	I	308	CLA	CHB-C1B	3.43	1.47	1.39
36	N	318	CLA	C1D-ND	3.43	1.42	1.37
37	G	308	KC1	CHB-C4A	3.43	1.47	1.39
36	S	313	CLA	C1D-ND	3.43	1.42	1.37
36	N	307	CLA	C1D-ND	3.43	1.42	1.37
36	O	312	CLA	C4B-NB	3.43	1.42	1.37
36	W	216	CLA	C4B-NB	3.43	1.42	1.37
37	M	317	KC1	CHC-C1C	3.43	1.47	1.39
36	R	320	CLA	C1D-ND	3.43	1.42	1.37
36	N	308	CLA	MG-ND	-3.42	1.99	2.05
36	V	307	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	j	102	CLA	OBD-CAD	3.42	1.28	1.22
36	U	306	CLA	CHD-C4C	3.41	1.47	1.39
36	T	316	CLA	C1D-ND	3.41	1.42	1.37
36	N	311	CLA	C1D-ND	3.41	1.42	1.37
35	C	204	A86	C28-C27	-3.41	1.44	1.50
36	A	306	CLA	C3D-C2D	3.40	1.48	1.39
36	G	319	CLA	CHD-C4C	3.40	1.46	1.39
36	N	317	CLA	C1D-ND	3.40	1.42	1.37
36	P	314	CLA	C4B-NB	3.40	1.42	1.37
36	J	315	CLA	C1D-ND	3.40	1.42	1.37
36	S	321	CLA	C1D-ND	3.40	1.42	1.37
36	T	313	CLA	C1D-ND	3.40	1.42	1.37
36	P	312	CLA	C1D-ND	3.39	1.42	1.37
36	Q	309	CLA	C1D-ND	3.39	1.42	1.37
36	E	313	CLA	C3D-C2D	3.39	1.48	1.39
36	a	802	CLA	OBD-CAD	3.38	1.28	1.22
36	X	312	CLA	C1D-ND	3.38	1.42	1.37
37	M	313	KC1	CHC-C1C	3.38	1.46	1.39
36	G	315	CLA	C4B-NB	-3.38	1.33	1.37
36	M	314	CLA	C1D-ND	3.38	1.42	1.37
35	L	304	A86	C20-C15	3.38	1.52	1.48
36	N	316	CLA	C1D-ND	3.38	1.42	1.37
36	B	311	CLA	C4B-NB	3.37	1.42	1.37
36	W	206	CLA	C1D-ND	3.37	1.42	1.37
36	X	315	CLA	C1D-ND	3.37	1.42	1.37
36	V	308	CLA	C1D-ND	3.37	1.42	1.37
35	K	306	A86	C20-C15	3.37	1.52	1.48
35	F	307	A86	O1-C20	-3.37	1.41	1.46
36	G	307	CLA	CHD-C4C	3.36	1.46	1.39
36	C	207	CLA	CHB-C1B	3.36	1.47	1.39
37	T	315	KC1	CHC-C1C	3.36	1.46	1.39
35	G	306	A86	C30-C29	-3.36	1.26	1.31
37	L	317	KC1	OBD-CAD	3.35	1.28	1.22
36	S	318	CLA	C1D-ND	3.35	1.42	1.37
36	C	206	CLA	C1D-ND	3.35	1.42	1.37
36	T	308	CLA	C1D-ND	3.35	1.42	1.37
36	F	317	CLA	C3D-C4D	-3.35	1.36	1.44
36	B	311	CLA	C1D-ND	3.35	1.42	1.37
35	V	302	A86	C30-C29	-3.35	1.26	1.31
36	f	803	CLA	CHD-C4C	3.35	1.46	1.39
37	M	317	KC1	CHB-C4A	3.35	1.46	1.39
36	G	315	CLA	C3D-C2D	3.35	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	317	KC1	CHD-C1D	3.35	1.46	1.39
37	H	313	KC1	CHC-C1C	3.35	1.46	1.39
36	R	318	CLA	C1D-ND	3.34	1.42	1.37
44	h	201	BCR	C30-C25	-3.34	1.49	1.53
36	K	315	CLA	C1D-ND	3.34	1.42	1.37
35	U	304	A86	C30-C29	-3.34	1.26	1.31
36	b	805	CLA	CMD-C2D	-3.34	1.43	1.50
37	G	318	KC1	CHB-C4A	3.34	1.46	1.39
36	a	830	CLA	C3D-C4D	-3.33	1.36	1.44
36	F	309	CLA	C1D-ND	3.33	1.42	1.37
36	S	319	CLA	C1D-ND	3.33	1.42	1.37
35	T	306	A86	O1-C20	-3.33	1.41	1.46
35	I	302	A86	C20-C15	3.33	1.52	1.48
36	Q	312	CLA	C1D-ND	3.33	1.42	1.37
36	W	207	CLA	C1D-ND	3.33	1.42	1.37
36	V	314	CLA	CHD-C4C	3.33	1.46	1.39
35	Q	316	A86	C30-C31	-3.33	1.26	1.30
36	O	310	CLA	C1D-ND	3.33	1.42	1.37
37	J	314	KC1	CHB-C4A	3.33	1.46	1.39
44	f	806	BCR	C1-C6	-3.33	1.49	1.53
36	F	312	CLA	C1D-ND	3.33	1.42	1.37
35	M	302	A86	C30-C29	-3.32	1.26	1.31
37	A	312	KC1	OBD-CAD	3.32	1.28	1.22
37	L	315	KC1	CHD-C1D	3.32	1.46	1.39
35	S	303	A86	O1-C20	-3.32	1.41	1.46
36	A	305	CLA	C1D-ND	3.31	1.42	1.37
37	X	311	KC1	CHC-C1C	3.31	1.46	1.39
35	R	309	A86	C30-C31	-3.31	1.26	1.30
36	l	205	CLA	C1C-NC	-3.31	1.32	1.37
36	b	811	CLA	CMC-C2C	-3.30	1.44	1.50
37	A	312	KC1	C1B-NB	-3.30	1.33	1.37
37	F	315	KC1	CHB-C4A	3.30	1.46	1.39
36	X	307	CLA	C4B-NB	3.30	1.42	1.37
36	b	816	CLA	CHD-C4C	3.30	1.46	1.39
35	O	302	A86	C30-C29	-3.30	1.26	1.31
36	P	316	CLA	C1D-ND	3.30	1.42	1.37
36	V	313	CLA	C1D-ND	3.30	1.42	1.37
35	N	305	A86	C30-C31	-3.29	1.26	1.30
36	W	201	CLA	C1D-ND	3.29	1.42	1.37
36	b	836	CLA	CHD-C4C	3.29	1.46	1.39
36	W	211	CLA	C1D-ND	3.29	1.42	1.37
36	G	307	CLA	C3D-C2D	3.29	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	208	CLA	C1D-ND	3.29	1.42	1.37
35	G	302	A86	C20-C15	3.28	1.52	1.48
36	M	315	CLA	C4B-NB	3.28	1.42	1.37
36	O	314	CLA	C1D-ND	3.28	1.42	1.37
37	W	217	KC1	CHC-C1C	3.28	1.46	1.39
36	G	313	CLA	C1D-ND	3.28	1.42	1.37
37	C	213	KC1	CHC-C1C	3.28	1.46	1.39
36	K	310	CLA	C4B-NB	-3.28	1.33	1.37
37	E	309	KC1	CHB-C4A	3.28	1.46	1.39
37	K	314	KC1	CHD-C1D	3.28	1.46	1.39
37	P	317	KC1	CHD-C1D	3.27	1.46	1.39
37	R	317	KC1	CHC-C1C	3.27	1.46	1.39
37	M	313	KC1	OBD-CAD	3.27	1.28	1.22
36	b	817	CLA	C3D-C2D	3.27	1.47	1.39
37	U	312	KC1	OBD-CAD	3.27	1.28	1.22
37	P	317	KC1	CHB-C4A	3.27	1.46	1.39
36	b	806	CLA	C1D-ND	3.27	1.42	1.37
35	N	304	A86	C15-C16	-3.27	1.50	1.55
36	P	310	CLA	C1D-ND	3.27	1.42	1.37
35	P	303	A86	C30-C29	-3.26	1.26	1.31
37	Q	313	KC1	CHC-C1C	3.26	1.46	1.39
37	O	315	KC1	CHC-C1C	3.26	1.46	1.39
35	L	319	A86	C30-C29	-3.26	1.26	1.31
35	N	303	A86	O1-C20	-3.26	1.42	1.46
35	N	306	A86	C30-C29	-3.26	1.26	1.31
37	F	308	KC1	OBD-CAD	3.26	1.28	1.22
36	I	308	CLA	C3D-C2D	3.25	1.47	1.39
36	O	308	CLA	C1D-ND	3.25	1.42	1.37
35	U	303	A86	C20-C15	3.25	1.52	1.48
37	Q	311	KC1	CHC-C1C	3.25	1.46	1.39
36	W	215	CLA	C1D-ND	3.25	1.42	1.37
36	f	803	CLA	CHC-C4B	3.25	1.46	1.39
36	T	312	CLA	C1D-ND	3.25	1.42	1.37
37	E	309	KC1	OBD-CAD	3.25	1.28	1.22
37	P	315	KC1	CHC-C1C	3.25	1.46	1.39
36	M	306	CLA	MG-NB	-3.25	1.99	2.05
36	Q	308	CLA	C1D-ND	3.24	1.42	1.37
36	L	308	CLA	C1B-NB	-3.24	1.33	1.37
36	l	204	CLA	C3D-C2D	3.24	1.47	1.39
35	K	303	A86	C20-C15	3.24	1.52	1.48
36	Q	305	CLA	C1D-ND	3.24	1.42	1.37
36	Q	307	CLA	C1D-ND	3.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	S	316	KC1	CHB-C4A	3.24	1.46	1.39
36	R	312	CLA	C1D-ND	3.24	1.42	1.37
36	b	816	CLA	C4B-NB	-3.23	1.33	1.37
35	I	304	A86	C30-C29	-3.23	1.26	1.31
36	S	318	CLA	C4B-NB	3.23	1.42	1.37
36	V	309	CLA	C1D-ND	3.23	1.42	1.37
37	G	308	KC1	OBD-CAD	3.23	1.28	1.22
35	B	303	A86	C30-C31	-3.23	1.26	1.30
36	P	308	CLA	C1D-ND	3.23	1.42	1.37
35	M	302	A86	C20-C15	3.23	1.52	1.48
36	U	307	CLA	C1D-ND	3.22	1.42	1.37
37	M	318	KC1	C4A-C3A	3.22	1.51	1.44
35	N	304	A86	C13-C11	-3.22	1.43	1.49
36	U	309	CLA	C4B-NB	3.22	1.42	1.37
37	O	313	KC1	CHC-C1C	3.22	1.46	1.39
36	R	315	CLA	C1D-ND	3.22	1.42	1.37
36	O	309	CLA	C1D-ND	3.22	1.42	1.37
35	V	304	A86	C30-C29	-3.21	1.26	1.31
36	a	817	CLA	C1B-NB	-3.21	1.33	1.37
37	T	310	KC1	CMD-C2D	3.21	1.57	1.50
37	T	315	KC1	CHB-C4A	3.21	1.46	1.39
37	V	312	KC1	OBD-CAD	3.21	1.28	1.22
35	T	303	A86	C20-C15	3.21	1.52	1.48
37	F	315	KC1	CHD-C1D	3.21	1.46	1.39
37	F	308	KC1	CHB-C4A	3.20	1.46	1.39
35	L	306	A86	C13-C11	-3.20	1.43	1.49
36	L	310	CLA	C1D-ND	3.20	1.42	1.37
37	G	317	KC1	CHB-C4A	3.20	1.46	1.39
36	b	819	CLA	C4B-NB	3.20	1.42	1.37
36	f	804	CLA	C3D-C2D	3.20	1.47	1.39
36	A	309	CLA	C1D-ND	3.20	1.42	1.37
37	M	313	KC1	CHB-C4A	3.20	1.46	1.39
36	b	830	CLA	CMB-C2B	-3.20	1.44	1.50
44	a	846	BCR	C1-C6	-3.20	1.49	1.53
44	a	845	BCR	C30-C25	-3.20	1.49	1.53
35	P	306	A86	C20-C15	3.19	1.52	1.48
37	J	314	KC1	CHC-C1C	3.19	1.46	1.39
36	P	311	CLA	C1D-ND	3.19	1.42	1.37
36	T	309	CLA	C1D-ND	3.19	1.42	1.37
35	B	303	A86	C30-C29	-3.19	1.26	1.31
36	L	313	CLA	C1D-ND	3.18	1.42	1.37
36	M	309	CLA	C1D-ND	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	O	306	CLA	C1D-ND	3.18	1.42	1.37
36	N	319	CLA	MG-ND	3.18	2.12	2.05
36	Q	312	CLA	C1B-C2B	3.18	1.50	1.43
36	O	316	CLA	CHC-C4B	3.17	1.46	1.39
36	C	205	CLA	C1D-ND	3.17	1.42	1.37
36	O	314	CLA	C1B-C2B	3.17	1.50	1.43
35	T	303	A86	C30-C31	-3.17	1.26	1.30
36	F	316	CLA	C1D-ND	3.17	1.42	1.37
36	a	823	CLA	C1D-ND	3.17	1.42	1.37
36	D	309	CLA	CHB-C1B	3.17	1.46	1.39
37	C	213	KC1	OBD-CAD	3.17	1.27	1.22
36	T	311	CLA	C4B-NB	3.17	1.42	1.37
36	b	813	CLA	CAB-C3B	-3.17	1.44	1.50
36	S	310	CLA	C1D-ND	3.17	1.42	1.37
35	S	302	A86	C30-C31	-3.17	1.26	1.30
35	Q	316	A86	O1-C15	-3.16	1.40	1.45
36	b	827	CLA	C1D-ND	3.16	1.42	1.37
36	a	848	CLA	OBD-CAD	3.16	1.27	1.22
35	h	202	A86	C20-C15	3.16	1.52	1.48
36	N	318	CLA	C4B-NB	3.16	1.42	1.37
35	Q	303	A86	C20-C15	3.16	1.52	1.48
36	b	827	CLA	C4B-NB	3.16	1.42	1.37
36	i	102	CLA	C1D-ND	3.16	1.42	1.37
37	M	318	KC1	CMD-C2D	3.16	1.57	1.50
37	M	317	KC1	OBD-CAD	3.16	1.27	1.22
36	K	309	CLA	C1D-ND	3.16	1.42	1.37
36	P	316	CLA	C1B-C2B	3.16	1.50	1.43
35	N	301	A86	C30-C31	-3.15	1.26	1.30
36	P	302	CLA	C1D-ND	3.15	1.42	1.37
35	N	305	A86	O1-C15	-3.15	1.40	1.45
36	b	830	CLA	CMD-C2D	-3.15	1.44	1.50
36	V	310	CLA	C1D-ND	3.15	1.42	1.37
36	a	834	CLA	C1D-ND	3.15	1.42	1.37
37	X	311	KC1	C1A-CHA	3.15	1.48	1.40
36	R	321	CLA	C1D-ND	3.15	1.42	1.37
44	l	203	BCR	C1-C6	-3.15	1.49	1.53
44	b	846	BCR	C30-C25	-3.15	1.49	1.53
37	W	217	KC1	C1A-CHA	3.14	1.48	1.40
36	D	307	CLA	C1D-ND	3.14	1.42	1.37
36	R	316	CLA	C1D-ND	3.14	1.42	1.37
36	O	316	CLA	CHD-C4C	3.14	1.46	1.39
35	F	305	A86	C30-C29	-3.14	1.26	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	310	CLA	C3B-C4B	3.14	1.51	1.42
37	W	213	KC1	CHC-C1C	3.14	1.46	1.39
36	U	308	CLA	C1D-ND	3.14	1.42	1.37
36	l	204	CLA	CHD-C4C	3.14	1.46	1.39
37	L	317	KC1	CHC-C1C	3.14	1.46	1.39
35	O	303	A86	C20-C15	3.14	1.52	1.48
36	a	816	CLA	C3D-C2D	3.13	1.47	1.39
36	D	312	CLA	C1D-ND	3.13	1.42	1.37
36	G	316	CLA	C1D-ND	3.13	1.42	1.37
36	L	311	CLA	C1D-ND	3.13	1.42	1.37
37	H	313	KC1	C1B-NB	-3.13	1.33	1.37
35	S	301	A86	C30-C31	-3.12	1.26	1.30
36	H	317	CLA	C1D-ND	3.12	1.42	1.37
36	W	218	CLA	C1D-ND	3.12	1.42	1.37
36	K	310	CLA	C3D-C2D	3.12	1.47	1.39
36	L	314	CLA	C1D-ND	3.12	1.42	1.37
36	M	315	CLA	C1D-ND	3.12	1.42	1.37
35	S	304	A86	C20-C15	3.12	1.52	1.48
35	O	305	A86	C20-C15	3.12	1.52	1.48
36	A	308	CLA	C1D-ND	3.12	1.42	1.37
35	T	306	A86	C30-C31	-3.12	1.27	1.30
36	f	804	CLA	CHC-C4B	3.11	1.46	1.39
36	S	315	CLA	C4B-NB	3.11	1.42	1.37
36	l	204	CLA	C1D-ND	3.11	1.42	1.37
35	Q	301	A86	C20-C15	3.11	1.52	1.48
35	R	305	A86	C20-C15	3.11	1.52	1.48
36	N	319	CLA	C4D-CHA	3.11	1.49	1.38
37	T	310	KC1	C3B-C4B	3.11	1.51	1.46
35	N	302	A86	C30-C31	-3.11	1.27	1.30
36	U	307	CLA	C4B-NB	3.11	1.41	1.37
36	N	319	CLA	C3C-C2C	3.11	1.43	1.36
36	V	306	CLA	C1D-ND	3.11	1.41	1.37
37	E	309	KC1	CHC-C1C	3.10	1.46	1.39
37	H	313	KC1	OBD-CAD	3.10	1.27	1.22
36	b	816	CLA	C3D-C2D	3.10	1.47	1.39
36	L	320	CLA	C1D-ND	3.10	1.41	1.37
36	X	315	CLA	C4B-NB	3.10	1.41	1.37
36	U	313	CLA	C4B-NB	3.10	1.41	1.37
36	a	814	CLA	C1D-ND	3.10	1.41	1.37
37	B	310	KC1	CHC-C1C	3.10	1.46	1.39
36	E	315	CLA	C3D-C2D	3.09	1.47	1.39
36	J	316	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	X	308	CLA	C1D-ND	3.09	1.41	1.37
36	a	813	CLA	MG-NB	-3.09	1.99	2.05
36	N	308	CLA	C1C-C2C	3.09	1.50	1.44
36	K	307	CLA	C1C-NC	-3.09	1.33	1.37
36	S	309	CLA	C1D-ND	3.09	1.41	1.37
36	N	310	CLA	C1D-C2D	3.09	1.51	1.45
35	N	303	A86	C20-C15	3.09	1.52	1.48
36	W	201	CLA	C4B-NB	3.08	1.41	1.37
36	V	314	CLA	CHB-C1B	3.08	1.46	1.39
36	W	206	CLA	C4B-NB	3.08	1.41	1.37
36	X	310	CLA	C4B-NB	3.08	1.41	1.37
36	a	830	CLA	C4B-NB	3.08	1.41	1.37
36	F	311	CLA	C1D-ND	3.08	1.41	1.37
36	O	311	CLA	C1D-ND	3.08	1.41	1.37
36	I	309	CLA	C4B-NB	3.07	1.41	1.37
36	I	309	CLA	C1D-ND	3.07	1.41	1.37
35	S	303	A86	C20-C15	3.07	1.52	1.48
36	R	318	CLA	C4B-NB	3.07	1.41	1.37
44	a	847	BCR	C1-C6	-3.07	1.49	1.53
36	b	806	CLA	CMC-C2C	-3.07	1.44	1.50
36	J	317	CLA	C1D-ND	3.07	1.41	1.37
36	A	314	CLA	C4B-NB	3.07	1.41	1.37
35	T	302	A86	C30-C29	-3.07	1.26	1.31
36	A	313	CLA	C4B-NB	3.07	1.41	1.37
36	a	835	CLA	CMD-C2D	-3.07	1.44	1.50
36	G	311	CLA	CMD-C2D	-3.07	1.44	1.50
35	P	304	A86	C20-C15	3.06	1.52	1.48
35	U	302	A86	C30-C29	-3.06	1.26	1.31
36	S	314	CLA	C4B-NB	3.06	1.41	1.37
36	C	209	CLA	CMD-C2D	-3.06	1.44	1.50
36	M	311	CLA	C1D-ND	3.06	1.41	1.37
36	b	822	CLA	C1D-ND	3.06	1.41	1.37
36	P	313	CLA	C1D-ND	3.06	1.41	1.37
36	I	306	CLA	CHD-C4C	3.06	1.46	1.39
35	S	301	A86	C32-C31	-3.05	1.49	1.54
36	H	306	CLA	C1D-ND	3.05	1.41	1.37
37	L	315	KC1	CHC-C1C	3.05	1.46	1.39
36	l	202	CLA	C1D-ND	3.05	1.41	1.37
36	S	317	CLA	C4B-NB	3.05	1.41	1.37
36	B	306	CLA	C1D-ND	3.05	1.41	1.37
37	G	317	KC1	CHC-C1C	3.05	1.46	1.39
36	L	309	CLA	C1D-ND	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	316	CLA	C1D-ND	3.05	1.41	1.37
35	U	301	A86	C30-C29	-3.04	1.26	1.31
36	H	314	CLA	C1D-ND	3.04	1.41	1.37
35	M	301	A86	C30-C29	-3.04	1.26	1.31
36	E	310	CLA	C1D-ND	3.04	1.41	1.37
36	L	312	CLA	C4B-NB	3.04	1.41	1.37
35	R	303	A86	C30-C29	-3.04	1.26	1.31
36	S	311	CLA	C4B-NB	3.04	1.41	1.37
36	H	305	CLA	C1D-ND	3.04	1.41	1.37
36	J	310	CLA	C1D-ND	3.04	1.41	1.37
37	M	318	KC1	C1B-NB	-3.04	1.33	1.37
36	b	835	CLA	C1D-ND	3.04	1.41	1.37
36	C	210	CLA	C4B-NB	3.03	1.41	1.37
37	G	308	KC1	CHC-C1C	3.03	1.46	1.39
35	N	301	A86	C32-C31	-3.03	1.49	1.54
36	S	315	CLA	CMC-C2C	-3.03	1.44	1.50
35	I	302	A86	C30-C29	-3.03	1.27	1.31
36	F	317	CLA	CHD-C4C	3.03	1.46	1.39
36	X	306	CLA	C4B-NB	3.03	1.41	1.37
36	T	312	CLA	C4B-NB	3.03	1.41	1.37
35	T	307	A86	C30-C29	-3.03	1.27	1.31
36	H	310	CLA	C4B-NB	3.03	1.41	1.37
36	O	316	CLA	C4B-NB	-3.03	1.33	1.37
37	K	314	KC1	OBD-CAD	3.03	1.27	1.22
36	f	802	CLA	C4B-NB	3.02	1.41	1.37
35	L	306	A86	C20-C15	3.02	1.52	1.48
36	I	313	CLA	C1D-ND	3.02	1.41	1.37
35	R	309	A86	C30-C29	-3.02	1.27	1.31
37	K	314	KC1	CHC-C1C	3.02	1.46	1.39
36	H	305	CLA	C4B-NB	3.02	1.41	1.37
36	b	826	CLA	CMD-C2D	-3.02	1.44	1.50
35	N	320	A86	C32-C31	-3.02	1.49	1.54
37	F	315	KC1	C1B-NB	-3.02	1.33	1.37
36	X	309	CLA	C1D-ND	3.02	1.41	1.37
37	P	317	KC1	CHC-C1C	3.02	1.46	1.39
36	a	830	CLA	C3D-C2D	3.01	1.47	1.39
36	K	313	CLA	C1D-ND	3.01	1.41	1.37
36	a	801	CLA	C1D-ND	3.01	1.41	1.37
36	U	310	CLA	C4B-NB	3.01	1.41	1.37
36	a	806	CLA	C4B-NB	-3.01	1.33	1.37
44	b	845	BCR	C30-C25	-3.01	1.49	1.53
36	P	316	CLA	C4B-NB	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	206	CLA	C1D-ND	3.01	1.41	1.37
36	K	307	CLA	CHB-C1B	3.01	1.46	1.39
36	G	313	CLA	CMD-C2D	-3.01	1.44	1.50
35	K	303	A86	C30-C29	-3.01	1.27	1.31
36	b	815	CLA	CMC-C2C	-3.01	1.44	1.50
36	I	312	CLA	C4B-NB	3.01	1.41	1.37
37	D	314	KC1	CHC-C1C	3.01	1.46	1.39
36	b	814	CLA	C1D-ND	3.01	1.41	1.37
37	U	312	KC1	CHC-C1C	3.00	1.46	1.39
36	j	106	CLA	C1D-ND	3.00	1.41	1.37
36	b	818	CLA	C1D-ND	3.00	1.41	1.37
37	R	317	KC1	CHB-C4A	3.00	1.46	1.39
36	Q	312	CLA	C4B-NB	3.00	1.41	1.37
35	Q	304	A86	C32-C31	-2.99	1.49	1.54
36	S	321	CLA	C4B-NB	2.99	1.41	1.37
36	K	316	CLA	C1D-ND	2.99	1.41	1.37
36	N	313	CLA	C4B-NB	2.99	1.41	1.37
36	a	833	CLA	CMB-C2B	-2.99	1.44	1.50
36	b	831	CLA	CMD-C2D	-2.99	1.44	1.50
36	a	829	CLA	C1B-NB	-2.98	1.33	1.37
36	X	312	CLA	C4B-NB	2.98	1.41	1.37
36	b	813	CLA	CMD-C2D	-2.98	1.44	1.50
36	E	313	CLA	CHD-C4C	2.98	1.46	1.39
44	b	847	BCR	C30-C25	-2.98	1.50	1.53
36	X	313	CLA	O2D-CGD	2.98	1.40	1.33
37	V	312	KC1	C4C-C3C	2.98	1.50	1.45
36	M	312	CLA	C1D-ND	2.97	1.41	1.37
36	C	208	CLA	C1D-ND	2.97	1.41	1.37
36	l	204	CLA	C4B-NB	2.97	1.41	1.37
36	X	309	CLA	C4B-NB	2.97	1.41	1.37
36	H	308	CLA	C1D-ND	2.97	1.41	1.37
36	V	305	CLA	C4B-NB	2.97	1.41	1.37
36	a	826	CLA	C1D-ND	2.97	1.41	1.37
44	m	101	BCR	C30-C25	-2.97	1.50	1.53
36	j	101	CLA	C1D-ND	2.97	1.41	1.37
36	N	307	CLA	C4B-NB	2.97	1.41	1.37
36	P	319	CLA	C3D-C4D	2.96	1.50	1.44
36	X	308	CLA	CMD-C2D	-2.96	1.44	1.50
36	O	314	CLA	C4B-NB	2.96	1.41	1.37
36	P	318	CLA	C4B-NB	2.96	1.41	1.37
36	K	307	CLA	C3D-C4D	-2.96	1.37	1.44
36	A	306	CLA	CHB-C1B	2.96	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	310	CLA	CMD-C2D	-2.96	1.44	1.50
36	K	311	CLA	C4B-NB	2.96	1.41	1.37
37	E	309	KC1	C1B-NB	-2.96	1.34	1.37
44	b	847	BCR	C1-C6	-2.96	1.50	1.53
36	a	832	CLA	C1D-ND	2.96	1.41	1.37
36	b	828	CLA	C1D-ND	2.95	1.41	1.37
36	N	310	CLA	C4B-NB	2.95	1.41	1.37
36	P	318	CLA	C1D-ND	2.95	1.41	1.37
37	J	314	KC1	OBD-CAD	2.95	1.27	1.22
36	R	313	CLA	C1D-ND	2.95	1.41	1.37
36	S	309	CLA	C4B-NB	2.95	1.41	1.37
36	W	216	CLA	C1B-NB	2.95	1.41	1.37
36	E	313	CLA	C1D-ND	2.95	1.41	1.37
36	I	305	CLA	C16-C15	2.95	1.68	1.51
36	Q	314	CLA	C3B-C4B	2.95	1.51	1.42
36	S	320	CLA	C4B-NB	2.94	1.41	1.37
36	V	307	CLA	C4B-NB	2.94	1.41	1.37
36	N	313	CLA	CHC-C1C	2.94	1.44	1.38
36	E	312	CLA	C1D-ND	2.94	1.41	1.37
36	R	321	CLA	CMB-C2B	-2.94	1.44	1.50
36	b	809	CLA	C1D-ND	2.94	1.41	1.37
36	a	830	CLA	C1B-NB	-2.94	1.34	1.37
35	V	304	A86	O1-C20	-2.94	1.42	1.46
36	a	827	CLA	CMC-C2C	-2.94	1.44	1.50
36	a	830	CLA	C1D-ND	2.94	1.41	1.37
44	m	101	BCR	C1-C6	-2.94	1.50	1.53
37	P	317	KC1	OBD-CAD	2.94	1.27	1.22
37	T	310	KC1	CHC-C1C	-2.94	1.32	1.39
36	K	307	CLA	CHD-C4C	2.94	1.45	1.39
36	A	310	CLA	CMD-C2D	-2.93	1.44	1.50
36	W	209	CLA	C4B-NB	2.93	1.41	1.37
36	T	314	CLA	C1D-ND	2.93	1.41	1.37
36	Q	314	CLA	C1D-ND	2.93	1.41	1.37
36	D	316	CLA	C1D-ND	2.93	1.41	1.37
36	Q	314	CLA	CHC-C1C	2.93	1.44	1.38
36	X	313	CLA	CHB-C1B	2.93	1.46	1.39
35	O	319	A86	C30-C31	-2.93	1.27	1.30
36	C	211	CLA	C1D-ND	2.93	1.41	1.37
36	D	311	CLA	C1D-ND	2.93	1.41	1.37
36	D	315	CLA	C1D-ND	2.93	1.41	1.37
36	G	314	CLA	C1D-ND	2.93	1.41	1.37
35	J	303	A86	C20-C15	2.93	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	O	313	KC1	C1B-NB	-2.93	1.34	1.37
36	A	313	CLA	C1D-ND	2.93	1.41	1.37
37	F	315	KC1	CHC-C1C	2.92	1.45	1.39
37	O	315	KC1	C1B-NB	-2.92	1.34	1.37
36	b	801	CLA	CMC-C2C	-2.92	1.44	1.50
36	M	306	CLA	MG-ND	-2.92	2.00	2.05
36	I	308	CLA	CHD-C1D	2.92	1.44	1.38
35	G	302	A86	C30-C31	-2.92	1.27	1.30
36	f	805	CLA	C1D-ND	2.92	1.41	1.37
36	N	315	CLA	C4B-NB	2.92	1.41	1.37
36	K	308	CLA	C4B-NB	2.91	1.41	1.37
36	G	307	CLA	CHB-C1B	2.91	1.45	1.39
36	H	318	CLA	CMD-C2D	-2.91	1.44	1.50
36	I	308	CLA	CHD-C4C	2.91	1.45	1.39
35	G	302	A86	C30-C29	-2.91	1.27	1.31
36	O	316	CLA	CHB-C1B	2.91	1.45	1.39
37	G	318	KC1	CHC-C1C	2.91	1.45	1.39
36	I	312	CLA	C1D-ND	2.91	1.41	1.37
36	b	825	CLA	C1D-ND	2.91	1.41	1.37
36	a	817	CLA	MG-NB	-2.91	2.00	2.05
36	N	317	CLA	C4B-NB	2.91	1.41	1.37
36	I	314	CLA	C1D-ND	2.91	1.41	1.37
36	D	306	CLA	C1D-ND	2.91	1.41	1.37
36	S	313	CLA	C4B-NB	2.91	1.41	1.37
36	F	314	CLA	C1D-ND	2.90	1.41	1.37
37	Q	311	KC1	C1B-NB	-2.90	1.34	1.37
41	O	318	LHG	C13-C12	2.90	1.66	1.51
37	Q	313	KC1	C1B-NB	-2.90	1.34	1.37
36	P	314	CLA	C1B-C2B	2.90	1.49	1.43
36	H	316	CLA	C1D-ND	2.90	1.41	1.37
36	T	314	CLA	C4B-NB	2.90	1.41	1.37
36	U	311	CLA	CMD-C2D	-2.90	1.44	1.50
36	R	322	CLA	C1D-ND	2.90	1.41	1.37
36	I	306	CLA	C1D-ND	2.90	1.41	1.37
36	b	841	CLA	C1D-ND	2.90	1.41	1.37
36	U	306	CLA	CHB-C1B	2.90	1.45	1.39
36	a	837	CLA	C1D-ND	2.89	1.41	1.37
36	V	306	CLA	C4B-NB	2.89	1.41	1.37
35	C	204	A86	C25-C26	2.89	1.52	1.43
35	U	301	A86	O1-C20	-2.89	1.42	1.46
37	P	315	KC1	C1B-NB	-2.89	1.34	1.37
35	J	303	A86	C30-C29	-2.89	1.27	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	828	CLA	CMC-C2C	-2.89	1.44	1.50
35	S	302	A86	C30-C29	-2.89	1.27	1.31
36	a	831	CLA	C1D-ND	2.89	1.41	1.37
36	M	309	CLA	C4B-NB	2.89	1.41	1.37
36	Q	310	CLA	C1D-ND	2.89	1.41	1.37
36	E	315	CLA	CHB-C1B	2.88	1.45	1.39
36	J	313	CLA	C1D-ND	2.88	1.41	1.37
36	P	314	CLA	C1D-ND	2.88	1.41	1.37
36	N	313	CLA	C3B-C4B	2.88	1.51	1.42
35	N	302	A86	C30-C29	-2.88	1.27	1.31
36	I	312	CLA	C3B-C4B	2.88	1.51	1.42
37	F	308	KC1	CHC-C1C	2.88	1.45	1.39
36	b	812	CLA	CMB-C2B	-2.88	1.44	1.50
36	a	812	CLA	CMC-C2C	-2.88	1.44	1.50
36	R	311	CLA	C1D-ND	2.88	1.41	1.37
36	N	309	CLA	C1B-C2B	2.88	1.49	1.43
36	b	834	CLA	C4B-NB	2.88	1.41	1.37
37	M	317	KC1	C1B-NB	-2.88	1.34	1.37
36	U	306	CLA	C4B-NB	2.88	1.41	1.37
36	F	317	CLA	CHB-C1B	2.88	1.45	1.39
36	M	308	CLA	C1D-ND	2.87	1.41	1.37
36	W	212	CLA	MG-NB	-2.87	2.00	2.05
36	b	815	CLA	C1D-ND	2.87	1.41	1.37
37	A	312	KC1	CHC-C1C	2.87	1.45	1.39
36	D	313	CLA	C1D-ND	2.87	1.41	1.37
36	M	314	CLA	C4B-NB	2.87	1.41	1.37
36	I	310	CLA	C1D-ND	2.87	1.41	1.37
36	T	311	CLA	C3C-C2C	2.87	1.43	1.36
36	Q	310	CLA	C1B-C2B	2.87	1.49	1.43
36	M	307	CLA	C1D-ND	2.87	1.41	1.37
35	S	305	A86	C30-C29	-2.87	1.27	1.31
36	l	201	CLA	C1D-ND	2.87	1.41	1.37
44	b	846	BCR	C1-C6	-2.87	1.50	1.53
37	G	318	KC1	C1D-ND	-2.86	1.34	1.37
37	S	316	KC1	C1B-NB	-2.86	1.34	1.37
36	b	833	CLA	MG-NB	-2.86	2.00	2.05
36	L	310	CLA	C4B-NB	2.86	1.41	1.37
35	X	305	A86	C30-C29	-2.86	1.27	1.31
36	H	309	CLA	C1D-ND	2.86	1.41	1.37
37	G	317	KC1	C1B-NB	-2.86	1.34	1.37
36	X	313	CLA	CHB-C4A	2.86	1.44	1.37
36	b	831	CLA	CMB-C2B	-2.86	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	303	A86	C30-C29	-2.86	1.27	1.31
35	T	302	A86	C30-C31	-2.86	1.27	1.30
37	T	315	KC1	C1A-CHA	2.86	1.47	1.40
36	V	310	CLA	C1B-C2B	2.86	1.49	1.43
36	a	815	CLA	C1D-ND	2.86	1.41	1.37
36	R	310	CLA	C4B-NB	2.86	1.41	1.37
36	K	308	CLA	C1D-ND	2.85	1.41	1.37
36	G	313	CLA	MG-NB	-2.85	2.00	2.05
36	O	312	CLA	C1B-C2B	2.85	1.49	1.43
36	b	812	CLA	CMD-C2D	-2.85	1.44	1.50
36	G	311	CLA	C1B-C2B	2.85	1.49	1.43
36	M	316	CLA	C4B-NB	2.85	1.41	1.37
36	O	312	CLA	C1D-ND	2.85	1.41	1.37
36	S	319	CLA	C4B-NB	2.85	1.41	1.37
36	I	309	CLA	C1B-C2B	2.85	1.49	1.43
36	X	306	CLA	C1B-C2B	2.84	1.49	1.43
36	l	205	CLA	C1D-C2D	2.84	1.51	1.45
36	B	311	CLA	C3B-C4B	2.84	1.51	1.42
36	a	828	CLA	C1D-ND	2.84	1.41	1.37
36	W	212	CLA	C4B-NB	2.84	1.41	1.37
36	b	841	CLA	CHC-C4B	-2.84	1.33	1.39
36	T	313	CLA	C4B-NB	2.84	1.41	1.37
36	W	218	CLA	CMD-C2D	-2.84	1.44	1.50
36	Q	310	CLA	O2A-CGA	2.84	1.41	1.33
36	E	311	CLA	C1D-ND	2.84	1.41	1.37
36	T	316	CLA	C4B-NB	2.84	1.41	1.37
36	X	307	CLA	C1B-C2B	2.83	1.49	1.43
36	B	309	CLA	C4B-NB	2.83	1.41	1.37
37	G	317	KC1	C1A-CHA	2.83	1.47	1.40
36	R	320	CLA	C4B-NB	2.83	1.41	1.37
36	U	305	CLA	C4B-NB	2.83	1.41	1.37
35	J	303	A86	C13-C11	-2.83	1.44	1.49
37	H	313	KC1	CHB-C4A	2.83	1.45	1.39
36	O	312	CLA	CMD-C2D	-2.83	1.45	1.50
36	B	305	CLA	C1D-ND	2.83	1.41	1.37
35	C	204	A86	C3-C2	2.83	1.51	1.43
36	Q	309	CLA	C4B-NB	2.83	1.41	1.37
36	b	823	CLA	C1D-ND	2.83	1.41	1.37
37	G	318	KC1	C1B-NB	-2.83	1.34	1.37
37	G	318	KC1	OBD-CAD	2.83	1.27	1.22
37	D	314	KC1	OBD-CAD	2.82	1.27	1.22
36	H	315	CLA	C4B-NB	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	820	CLA	C1D-ND	2.82	1.41	1.37
36	Q	310	CLA	CMD-C2D	-2.82	1.45	1.50
36	F	313	CLA	C1D-ND	2.82	1.41	1.37
36	H	317	CLA	C4B-NB	2.82	1.41	1.37
36	a	807	CLA	C1D-ND	2.82	1.41	1.37
37	O	315	KC1	C1A-CHA	2.82	1.47	1.40
36	a	813	CLA	C1B-NB	-2.82	1.34	1.37
36	H	312	CLA	C1B-C2B	2.82	1.49	1.43
36	J	312	CLA	C1D-ND	2.82	1.41	1.37
36	a	815	CLA	C4B-NB	2.82	1.41	1.37
37	Q	313	KC1	C1A-CHA	2.81	1.47	1.40
36	K	310	CLA	CHB-C1B	2.81	1.45	1.39
36	T	311	CLA	C1B-C2B	2.81	1.49	1.43
36	a	811	CLA	C4B-NB	2.81	1.41	1.37
36	E	314	CLA	C1D-ND	2.81	1.41	1.37
36	I	314	CLA	C4B-NB	2.81	1.41	1.37
36	N	309	CLA	CMB-C2B	-2.81	1.45	1.50
36	N	312	CLA	C1D-ND	2.81	1.41	1.37
36	b	807	CLA	C1D-ND	2.81	1.41	1.37
36	H	310	CLA	C1D-ND	2.81	1.41	1.37
36	a	829	CLA	CMD-C2D	-2.81	1.45	1.50
36	a	818	CLA	C1B-NB	-2.81	1.34	1.37
36	a	821	CLA	CMD-C2D	-2.81	1.45	1.50
35	T	305	A86	C17-C18	-2.81	1.48	1.52
36	C	209	CLA	C4B-NB	2.81	1.41	1.37
36	I	305	CLA	C1D-ND	2.81	1.41	1.37
36	P	312	CLA	C4B-NB	2.81	1.41	1.37
36	S	312	CLA	C1D-ND	2.81	1.41	1.37
36	N	310	CLA	C1D-ND	2.80	1.41	1.37
36	K	316	CLA	C1B-C2B	2.80	1.49	1.43
36	E	316	CLA	C1D-ND	2.80	1.41	1.37
36	B	309	CLA	CHB-C1B	2.80	1.45	1.39
35	C	202	A86	C30-C31	-2.80	1.27	1.30
36	B	309	CLA	C1D-ND	2.80	1.41	1.37
36	a	806	CLA	CHD-C4C	2.80	1.45	1.39
36	a	824	CLA	CMD-C2D	-2.80	1.45	1.50
37	Q	311	KC1	C1A-CHA	2.80	1.47	1.40
36	E	316	CLA	C4B-NB	2.80	1.41	1.37
36	T	309	CLA	C4B-NB	2.80	1.41	1.37
36	a	829	CLA	MG-NB	-2.80	2.00	2.05
36	J	307	CLA	C1D-ND	2.80	1.41	1.37
36	G	310	CLA	C1D-ND	2.80	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	310	CLA	C1B-C2B	2.79	1.49	1.43
36	C	207	CLA	C4B-NB	-2.79	1.34	1.37
36	D	309	CLA	CHC-C4B	2.79	1.45	1.39
36	N	316	CLA	C4B-NB	2.79	1.41	1.37
37	G	308	KC1	C1B-NB	-2.79	1.34	1.37
36	W	211	CLA	C4B-NB	2.79	1.41	1.37
36	S	318	CLA	C1B-C2B	2.79	1.49	1.43
36	I	306	CLA	C1D-C2D	2.79	1.50	1.45
37	P	315	KC1	C1A-CHA	2.79	1.47	1.40
36	V	309	CLA	C4B-NB	2.79	1.41	1.37
36	b	817	CLA	C1D-ND	2.78	1.41	1.37
36	W	207	CLA	C4B-NB	2.78	1.41	1.37
35	R	306	A86	C30-C29	-2.78	1.27	1.31
35	N	304	A86	C21-C20	2.78	1.56	1.51
36	f	802	CLA	C3B-C4B	2.78	1.50	1.42
36	K	313	CLA	MG-NB	-2.78	2.00	2.05
36	I	308	CLA	C1D-C2D	2.78	1.50	1.45
36	P	314	CLA	CMD-C2D	-2.78	1.45	1.50
36	a	808	CLA	C1D-ND	2.78	1.41	1.37
36	b	808	CLA	C1D-ND	2.78	1.41	1.37
36	j	102	CLA	C1D-C2D	2.78	1.50	1.45
35	Q	316	A86	C15-C16	-2.78	1.51	1.55
36	b	810	CLA	C1D-ND	2.78	1.41	1.37
37	M	318	KC1	CHC-C1C	-2.78	1.32	1.39
36	J	309	CLA	C4B-NB	2.78	1.41	1.37
36	a	811	CLA	C1D-ND	2.78	1.41	1.37
35	N	305	A86	C15-C16	-2.78	1.51	1.55
36	M	311	CLA	C4B-NB	2.78	1.41	1.37
36	U	308	CLA	OBD-CAD	2.78	1.27	1.22
36	D	308	CLA	C1D-ND	2.78	1.41	1.37
36	N	312	CLA	C1B-C2B	2.78	1.49	1.43
36	I	311	CLA	C1D-ND	2.77	1.41	1.37
36	B	307	CLA	C4B-NB	2.77	1.41	1.37
35	N	320	A86	C37-C36	-2.77	1.48	1.52
35	V	303	A86	C13-C11	-2.77	1.44	1.49
36	E	317	CLA	C4B-NB	2.77	1.41	1.37
37	L	317	KC1	C1A-CHA	2.77	1.47	1.40
36	R	312	CLA	C4B-NB	2.77	1.41	1.37
37	A	312	KC1	C1D-ND	-2.77	1.34	1.37
36	W	218	CLA	C1B-C2B	2.77	1.49	1.43
35	H	301	A86	C13-C11	-2.77	1.44	1.49
36	N	319	CLA	C3B-C4B	2.77	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	313	CLA	C1B-C2B	2.77	1.49	1.43
36	b	805	CLA	MG-ND	-2.77	2.00	2.05
36	G	307	CLA	C1D-C2D	2.77	1.50	1.45
37	O	313	KC1	C1A-CHA	2.77	1.47	1.40
37	W	213	KC1	C1A-CHA	2.77	1.47	1.40
36	V	311	CLA	CMD-C2D	-2.77	1.45	1.50
44	a	846	BCR	C30-C25	-2.77	1.50	1.53
36	O	310	CLA	C4B-NB	2.77	1.41	1.37
36	S	317	CLA	C1B-C2B	2.77	1.49	1.43
36	b	801	CLA	C1D-ND	2.77	1.41	1.37
36	Q	314	CLA	C4B-NB	2.77	1.41	1.37
36	V	306	CLA	C3B-C4B	2.76	1.50	1.42
36	M	306	CLA	CMD-C2D	-2.76	1.45	1.50
36	a	805	CLA	C1D-ND	2.76	1.41	1.37
36	h	203	CLA	C1D-ND	2.76	1.41	1.37
37	U	312	KC1	C4A-C3A	2.76	1.50	1.44
34	G	303	DD6	O1-C20	-2.76	1.42	1.46
36	V	306	CLA	CHC-C1C	2.76	1.44	1.38
36	b	827	CLA	C3B-C4B	2.76	1.50	1.42
36	L	316	CLA	C1B-C2B	2.76	1.49	1.43
36	S	309	CLA	CMD-C2D	-2.76	1.45	1.50
36	R	314	CLA	C4B-NB	2.76	1.41	1.37
36	R	321	CLA	C4B-NB	2.76	1.41	1.37
44	b	844	BCR	C1-C6	-2.76	1.50	1.53
36	J	312	CLA	C4B-NB	2.76	1.41	1.37
36	V	310	CLA	C4B-NB	2.76	1.41	1.37
36	b	805	CLA	C1B-NB	-2.76	1.34	1.37
36	l	204	CLA	C1B-C2B	2.75	1.49	1.43
35	Q	304	A86	C37-C36	-2.75	1.48	1.52
36	E	310	CLA	CMD-C2D	-2.75	1.45	1.50
36	b	811	CLA	C1D-ND	2.75	1.41	1.37
36	A	306	CLA	CHC-C4B	2.75	1.45	1.39
36	b	827	CLA	CMC-C2C	-2.75	1.45	1.50
37	F	315	KC1	C1D-ND	-2.75	1.34	1.37
37	J	314	KC1	C1B-NB	-2.75	1.34	1.37
36	b	836	CLA	C4B-NB	-2.75	1.34	1.37
36	J	315	CLA	C1B-C2B	2.75	1.49	1.43
36	b	829	CLA	CMD-C2D	-2.75	1.45	1.50
36	I	313	CLA	C4B-NB	2.75	1.41	1.37
36	a	809	CLA	C1D-ND	2.75	1.41	1.37
37	M	317	KC1	C1D-ND	-2.75	1.34	1.37
36	G	313	CLA	CMB-C2B	-2.74	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Q	306	CLA	C1D-ND	2.74	1.41	1.37
36	U	311	CLA	C4B-NB	2.74	1.41	1.37
36	R	311	CLA	C4B-NB	2.74	1.41	1.37
36	b	820	CLA	C1D-ND	2.74	1.41	1.37
36	a	836	CLA	C1D-ND	2.74	1.41	1.37
36	l	205	CLA	C1D-ND	2.74	1.41	1.37
36	b	819	CLA	CMB-C2B	-2.74	1.45	1.50
36	a	819	CLA	CMD-C2D	-2.74	1.45	1.50
36	I	314	CLA	C1B-C2B	2.74	1.49	1.43
44	b	844	BCR	C30-C25	-2.74	1.50	1.53
36	D	317	CLA	C1D-ND	2.74	1.41	1.37
36	a	822	CLA	C1D-ND	2.74	1.41	1.37
37	L	315	KC1	C1A-CHA	2.74	1.47	1.40
36	G	309	CLA	C1D-ND	2.74	1.41	1.37
36	D	310	CLA	C1D-ND	2.74	1.41	1.37
35	R	302	A86	C13-C11	-2.73	1.44	1.49
36	R	310	CLA	C1D-ND	2.73	1.41	1.37
36	V	306	CLA	CMC-C2C	-2.73	1.45	1.50
37	F	308	KC1	C1D-ND	-2.73	1.34	1.37
36	b	833	CLA	CMB-C2B	-2.73	1.45	1.50
36	P	309	CLA	C1D-ND	2.73	1.41	1.37
36	M	308	CLA	C4B-NB	2.73	1.41	1.37
36	b	839	CLA	C1D-ND	2.73	1.41	1.37
37	V	312	KC1	C1A-CHA	2.73	1.47	1.40
36	G	312	CLA	C1D-ND	2.73	1.41	1.37
36	j	102	CLA	C3D-C2D	2.73	1.46	1.39
36	G	307	CLA	CHD-C1D	2.72	1.43	1.38
36	R	319	CLA	C4B-NB	2.72	1.41	1.37
36	M	315	CLA	C1B-C2B	2.72	1.49	1.43
36	B	305	CLA	C4B-NB	2.72	1.41	1.37
36	S	310	CLA	C4B-NB	2.72	1.41	1.37
36	G	314	CLA	C4B-NB	2.72	1.41	1.37
36	a	811	CLA	C3B-C4B	2.72	1.50	1.42
36	a	818	CLA	C1D-ND	2.72	1.41	1.37
36	b	830	CLA	C1B-NB	-2.72	1.34	1.37
36	X	312	CLA	C1B-C2B	2.72	1.49	1.43
36	H	315	CLA	C1D-ND	2.72	1.41	1.37
36	a	819	CLA	C1B-NB	-2.72	1.34	1.37
44	f	801	BCR	C30-C25	-2.72	1.50	1.53
36	O	307	CLA	C1D-ND	2.72	1.41	1.37
36	b	831	CLA	C1B-NB	-2.72	1.34	1.37
36	a	804	CLA	MG-NB	-2.72	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	309	CLA	C1D-ND	2.72	1.41	1.37
36	V	305	CLA	C1D-C2D	2.72	1.50	1.45
36	b	821	CLA	C1D-ND	2.72	1.41	1.37
36	L	316	CLA	C4B-NB	2.72	1.41	1.37
36	P	311	CLA	C4B-NB	2.72	1.41	1.37
36	a	815	CLA	C3B-C4B	2.72	1.50	1.42
36	U	307	CLA	C1B-C2B	2.72	1.49	1.43
36	G	312	CLA	CMD-C2D	-2.71	1.45	1.50
44	b	843	BCR	C30-C25	-2.71	1.50	1.53
36	P	301	CLA	C1D-ND	2.71	1.41	1.37
36	b	825	CLA	CMD-C2D	-2.71	1.45	1.50
36	H	309	CLA	CMD-C2D	-2.71	1.45	1.50
36	a	841	CLA	C1D-ND	2.71	1.41	1.37
36	E	308	CLA	C1D-ND	2.71	1.41	1.37
36	b	824	CLA	C1D-ND	2.71	1.41	1.37
36	E	315	CLA	CHC-C4B	2.71	1.45	1.39
36	a	818	CLA	CMB-C2B	-2.71	1.45	1.50
36	l	205	CLA	C3D-C2D	2.71	1.46	1.39
35	J	301	A86	O1-C20	-2.71	1.42	1.46
36	I	307	CLA	C1D-ND	2.71	1.41	1.37
36	b	838	CLA	C1D-ND	2.71	1.41	1.37
36	C	214	CLA	C1D-ND	2.71	1.41	1.37
36	G	319	CLA	C4B-NB	-2.71	1.34	1.37
36	H	310	CLA	CBD-CGD	2.71	1.60	1.52
36	A	309	CLA	C4B-NB	2.70	1.41	1.37
36	a	848	CLA	C4B-NB	2.70	1.41	1.37
36	G	315	CLA	CHB-C1B	2.70	1.45	1.39
35	U	302	A86	C20-C15	2.70	1.51	1.48
36	a	812	CLA	C1D-ND	2.70	1.41	1.37
36	T	311	CLA	C1D-ND	2.70	1.41	1.37
36	U	308	CLA	C4B-NB	2.70	1.41	1.37
36	A	313	CLA	C1B-C2B	2.70	1.49	1.43
36	W	211	CLA	C1B-C2B	2.70	1.49	1.43
36	D	311	CLA	C4B-NB	2.70	1.41	1.37
36	a	803	CLA	C1D-ND	2.70	1.41	1.37
35	R	302	A86	C20-C15	2.70	1.51	1.48
36	K	310	CLA	CHD-C1D	2.70	1.43	1.38
39	L	303	LMT	O3'-C3'	-2.70	1.36	1.43
36	D	306	CLA	C4B-NB	2.70	1.41	1.37
39	L	303	LMT	O2'-C2'	-2.70	1.36	1.43
36	a	802	CLA	C1D-ND	2.70	1.41	1.37
36	W	218	CLA	C4B-NB	2.70	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	308	CLA	C4B-NB	2.69	1.41	1.37
36	S	312	CLA	C4B-NB	2.69	1.41	1.37
37	B	310	KC1	C4C-C3C	2.69	1.49	1.45
36	F	310	CLA	C1D-ND	2.69	1.41	1.37
36	I	306	CLA	C3D-C2D	2.69	1.46	1.39
36	W	215	CLA	C4B-NB	2.69	1.41	1.37
36	a	841	CLA	CMC-C2C	-2.69	1.45	1.50
36	O	309	CLA	C4B-NB	2.69	1.41	1.37
36	a	826	CLA	CMC-C2C	-2.69	1.45	1.50
36	U	308	CLA	C1B-C2B	2.69	1.49	1.43
36	M	310	CLA	C1B-C2B	2.69	1.49	1.43
36	S	321	CLA	C1B-C2B	2.69	1.49	1.43
36	T	312	CLA	C1B-C2B	2.69	1.49	1.43
36	b	830	CLA	C1D-ND	2.69	1.41	1.37
36	W	208	CLA	C4B-NB	2.69	1.41	1.37
37	L	317	KC1	C1B-NB	-2.69	1.34	1.37
36	J	316	CLA	C1B-C2B	2.69	1.49	1.43
35	Q	316	A86	C13-C11	-2.69	1.44	1.49
36	b	841	CLA	C1B-NB	-2.69	1.34	1.37
36	C	212	CLA	CMD-C2D	-2.68	1.45	1.50
36	l	204	CLA	C1D-C2D	2.68	1.50	1.45
44	j	107	BCR	C1-C6	-2.68	1.50	1.53
36	H	305	CLA	C3B-C4B	2.68	1.50	1.42
41	G	301	LHG	O7-C5	-2.68	1.40	1.46
36	R	322	CLA	C4B-NB	2.68	1.41	1.37
36	M	311	CLA	C1B-C2B	2.68	1.49	1.43
37	E	309	KC1	C1A-CHA	2.68	1.47	1.40
36	H	317	CLA	C1B-C2B	2.68	1.49	1.43
35	N	305	A86	C13-C11	-2.68	1.44	1.49
36	N	315	CLA	C3B-C4B	2.68	1.50	1.42
37	R	317	KC1	C1B-NB	-2.68	1.34	1.37
36	N	310	CLA	CHC-C1C	2.67	1.43	1.38
36	b	826	CLA	C1D-ND	2.67	1.41	1.37
36	B	306	CLA	C4B-NB	2.67	1.41	1.37
36	H	316	CLA	C4B-NB	2.67	1.41	1.37
36	f	805	CLA	C1B-C2B	2.67	1.49	1.43
36	P	309	CLA	C4B-NB	2.66	1.41	1.37
36	Q	305	CLA	C4B-NB	2.66	1.41	1.37
36	K	307	CLA	C1D-C2D	2.66	1.50	1.45
37	F	308	KC1	C4C-C3C	2.66	1.49	1.45
35	F	301	A86	O1-C20	-2.66	1.42	1.46
36	f	803	CLA	C4B-NB	-2.66	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	834	CLA	C3B-C4B	2.66	1.50	1.42
37	G	317	KC1	O1D-CGD	2.66	1.28	1.21
36	O	306	CLA	C4B-NB	2.66	1.41	1.37
36	J	307	CLA	MG-NB	-2.66	2.00	2.05
36	R	318	CLA	C3B-C4B	2.66	1.50	1.42
36	W	214	CLA	C1B-C2B	2.66	1.49	1.43
37	B	310	KC1	C1A-CHA	2.66	1.47	1.40
36	a	804	CLA	CMD-C2D	-2.66	1.45	1.50
36	S	319	CLA	C1B-C2B	2.66	1.49	1.43
35	U	302	A86	C13-C11	-2.66	1.44	1.49
36	b	817	CLA	C1D-C2D	2.65	1.50	1.45
36	K	312	CLA	C1D-ND	2.65	1.41	1.37
37	M	318	KC1	C1C-C2C	2.65	1.49	1.44
36	O	316	CLA	C3D-C2D	2.65	1.46	1.39
36	J	317	CLA	C4B-NB	2.65	1.41	1.37
36	Q	308	CLA	C4B-NB	2.65	1.41	1.37
44	b	845	BCR	C1-C6	-2.65	1.50	1.53
36	b	830	CLA	C4B-NB	2.65	1.41	1.37
36	R	320	CLA	CMD-C2D	-2.65	1.45	1.50
36	a	828	CLA	CMD-C2D	-2.65	1.45	1.50
36	K	309	CLA	C4B-NB	2.65	1.41	1.37
36	F	317	CLA	C3D-C2D	2.65	1.46	1.39
36	W	215	CLA	MG-NB	-2.65	2.00	2.05
36	Q	306	CLA	C4B-NB	2.65	1.41	1.37
35	L	304	A86	C13-C11	-2.65	1.44	1.49
36	b	841	CLA	CMC-C2C	-2.65	1.45	1.50
35	X	304	A86	C30-C29	-2.65	1.27	1.31
36	b	819	CLA	C1B-NB	-2.64	1.34	1.37
36	R	314	CLA	C1B-C2B	2.64	1.49	1.43
34	F	303	DD6	O1-C20	-2.64	1.42	1.46
36	a	834	CLA	C4B-NB	2.64	1.41	1.37
37	U	312	KC1	C1A-CHA	2.64	1.47	1.40
36	X	310	CLA	C1B-C2B	2.64	1.49	1.43
36	T	308	CLA	C1B-C2B	2.64	1.49	1.43
36	U	305	CLA	C1B-C2B	2.64	1.49	1.43
35	F	306	A86	O1-C20	-2.64	1.42	1.46
34	a	849	DD6	O1-C20	-2.64	1.42	1.46
36	C	207	CLA	C1B-C2B	2.64	1.49	1.43
36	S	315	CLA	C1B-C2B	2.64	1.49	1.43
34	B	304	DD6	O1-C20	-2.64	1.42	1.46
37	N	314	KC1	C1A-CHA	2.64	1.47	1.40
36	R	322	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	819	CLA	CMD-C2D	-2.63	1.45	1.50
36	V	314	CLA	C3D-C4D	-2.63	1.38	1.44
36	a	821	CLA	MG-NB	-2.63	2.00	2.05
36	N	309	CLA	C4B-NB	2.63	1.41	1.37
36	T	314	CLA	C1B-C2B	2.63	1.49	1.43
36	f	803	CLA	C1B-C2B	2.63	1.49	1.43
36	R	310	CLA	MG-NB	-2.63	2.00	2.05
36	E	315	CLA	C1D-C2D	2.63	1.50	1.45
36	M	316	CLA	C1B-C2B	2.63	1.49	1.43
37	E	309	KC1	C1D-ND	-2.63	1.34	1.37
37	P	317	KC1	C1D-ND	-2.63	1.34	1.37
36	X	308	CLA	CHC-C1C	2.63	1.43	1.38
36	D	308	CLA	MG-NB	-2.63	2.00	2.05
36	S	309	CLA	C1B-C2B	2.63	1.49	1.43
36	N	311	CLA	C4B-NB	2.62	1.41	1.37
37	A	312	KC1	C1D-C2D	2.62	1.49	1.43
37	G	318	KC1	C1A-CHA	2.62	1.47	1.40
36	G	319	CLA	CHC-C4B	2.62	1.45	1.39
34	D	305	DD6	O1-C20	-2.62	1.42	1.46
36	C	209	CLA	C1D-ND	2.62	1.41	1.37
35	X	302	A86	C30-C31	-2.62	1.27	1.30
41	O	318	LHG	C12-C11	2.62	1.64	1.51
36	M	314	CLA	C1B-C2B	2.62	1.49	1.43
37	S	316	KC1	C1A-CHA	2.62	1.47	1.40
36	N	307	CLA	C1B-C2B	2.62	1.49	1.43
36	b	834	CLA	C1D-ND	2.62	1.41	1.37
34	D	301	DD6	O1-C20	-2.62	1.42	1.46
36	a	829	CLA	MG-ND	-2.62	2.00	2.05
36	R	316	CLA	C4B-NB	2.62	1.41	1.37
37	G	308	KC1	C1D-ND	-2.62	1.34	1.37
36	a	806	CLA	C1B-NB	2.62	1.41	1.37
36	W	201	CLA	C1B-C2B	2.62	1.49	1.43
36	S	320	CLA	C1B-C2B	2.62	1.49	1.43
35	J	305	A86	O1-C20	-2.62	1.42	1.46
36	Q	305	CLA	C1B-C2B	2.61	1.49	1.43
36	a	817	CLA	CMC-C2C	-2.61	1.45	1.50
36	b	826	CLA	C1B-C2B	2.61	1.49	1.43
36	V	314	CLA	C3D-C2D	2.61	1.46	1.39
36	N	317	CLA	CMB-C2B	-2.61	1.45	1.50
35	C	204	A86	C4-C5	2.61	1.51	1.43
36	C	214	CLA	CMD-C2D	-2.61	1.45	1.50
36	J	312	CLA	CMC-C2C	-2.61	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	831	CLA	MG-NB	-2.61	2.00	2.05
35	Q	303	A86	C32-C31	-2.61	1.50	1.54
36	b	829	CLA	C1D-ND	2.61	1.41	1.37
36	S	312	CLA	CMD-C2D	-2.61	1.45	1.50
36	A	314	CLA	C1B-C2B	2.61	1.49	1.43
34	D	303	DD6	C4-C5	2.61	1.51	1.43
35	I	301	A86	O1-C20	-2.61	1.42	1.46
36	C	210	CLA	C1B-C2B	2.61	1.49	1.43
36	P	301	CLA	C4B-NB	2.61	1.41	1.37
34	K	304	DD6	O1-C20	-2.61	1.42	1.46
36	R	310	CLA	CMB-C2B	-2.61	1.45	1.50
36	K	312	CLA	C4B-NB	2.61	1.41	1.37
36	V	314	CLA	CHC-C4B	2.61	1.45	1.39
36	W	206	CLA	C1B-C2B	2.60	1.49	1.43
36	L	310	CLA	C1B-C2B	2.60	1.49	1.43
44	f	801	BCR	C1-C6	-2.60	1.50	1.53
37	R	317	KC1	C1A-CHA	2.60	1.47	1.40
37	F	308	KC1	C1A-CHA	2.60	1.47	1.40
36	O	307	CLA	C4B-NB	2.60	1.41	1.37
36	R	315	CLA	C4B-NB	2.60	1.41	1.37
36	H	315	CLA	CMD-C2D	-2.60	1.45	1.50
36	A	307	CLA	C1D-ND	2.60	1.41	1.37
36	F	312	CLA	C4B-NB	2.60	1.41	1.37
36	i	102	CLA	C4B-NB	2.60	1.41	1.37
36	H	309	CLA	C1B-C2B	2.60	1.49	1.43
35	I	304	A86	C13-C11	-2.60	1.44	1.49
37	C	213	KC1	C1B-NB	-2.59	1.34	1.37
36	F	316	CLA	C4B-NB	2.59	1.41	1.37
36	U	311	CLA	C1D-ND	2.59	1.41	1.37
36	G	309	CLA	O2D-CGD	2.59	1.39	1.33
36	j	106	CLA	C4B-NB	2.59	1.41	1.37
36	a	804	CLA	CMB-C2B	-2.59	1.45	1.50
36	N	311	CLA	C1B-C2B	2.59	1.49	1.43
36	C	212	CLA	C1D-ND	2.59	1.41	1.37
36	a	841	CLA	C4B-NB	2.59	1.41	1.37
36	F	312	CLA	C1B-C2B	2.59	1.49	1.43
36	A	306	CLA	MG-NB	-2.59	2.00	2.05
36	L	320	CLA	C4B-NB	2.59	1.41	1.37
36	b	824	CLA	C1B-C2B	2.59	1.49	1.43
38	A	315	SQD	O48-C23	2.59	1.45	1.33
36	A	311	CLA	MG-NB	-2.59	2.00	2.05
36	N	312	CLA	C4B-NB	2.59	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	316	CLA	C1B-C2B	2.59	1.49	1.43
36	H	310	CLA	O2D-CED	2.59	1.51	1.45
34	D	303	DD6	O1-C20	-2.58	1.42	1.46
35	O	301	A86	O1-C20	-2.58	1.42	1.46
36	l	201	CLA	C1B-NB	-2.58	1.34	1.37
36	O	306	CLA	C1B-C2B	2.58	1.49	1.43
36	M	310	CLA	CMD-C2D	-2.58	1.45	1.50
36	L	309	CLA	MG-NB	-2.58	2.00	2.05
36	b	802	CLA	C4B-NB	2.58	1.41	1.37
37	U	312	KC1	C1B-NB	-2.58	1.34	1.37
35	R	304	A86	C20-C15	2.58	1.51	1.48
36	C	209	CLA	CMB-C2B	-2.58	1.45	1.50
36	I	308	CLA	C1B-C2B	2.58	1.49	1.43
36	R	319	CLA	C1B-C2B	2.58	1.49	1.43
36	a	824	CLA	C4B-NB	2.58	1.41	1.37
36	D	309	CLA	C1B-C2B	2.58	1.49	1.43
36	H	312	CLA	C1D-ND	2.58	1.41	1.37
36	P	308	CLA	C1B-C2B	2.58	1.49	1.43
36	i	102	CLA	CMC-C2C	-2.58	1.45	1.50
36	G	316	CLA	C4B-NB	2.58	1.41	1.37
36	P	310	CLA	C4B-NB	2.58	1.41	1.37
36	I	307	CLA	MG-NB	-2.58	2.00	2.05
36	W	208	CLA	C1B-C2B	2.58	1.49	1.43
36	C	209	CLA	C1B-C2B	2.58	1.49	1.43
36	O	308	CLA	C4B-NB	2.57	1.41	1.37
36	K	315	CLA	C4B-NB	2.57	1.41	1.37
36	J	311	CLA	C4B-NB	2.57	1.41	1.37
35	Q	303	A86	C13-C11	-2.57	1.44	1.49
35	F	307	A86	C30-C31	-2.57	1.27	1.30
36	R	316	CLA	C1B-C2B	2.57	1.49	1.43
36	b	812	CLA	MG-NB	-2.57	2.00	2.05
36	T	309	CLA	C1B-C2B	2.57	1.49	1.43
36	G	319	CLA	C1D-C2D	2.57	1.50	1.45
36	H	307	CLA	C1D-C2D	2.57	1.50	1.45
36	b	830	CLA	MG-NB	-2.57	2.00	2.05
36	H	308	CLA	MG-NB	-2.57	2.00	2.05
37	M	313	KC1	C1B-NB	-2.57	1.34	1.37
35	S	304	A86	C32-C31	-2.57	1.50	1.54
36	K	310	CLA	C1D-C2D	2.57	1.50	1.45
36	T	308	CLA	C4B-NB	2.56	1.41	1.37
36	b	841	CLA	C1B-C2B	2.56	1.49	1.43
36	M	307	CLA	C4B-NB	2.56	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	818	CLA	CMC-C2C	-2.56	1.45	1.50
36	H	314	CLA	C4B-NB	2.56	1.41	1.37
36	Q	307	CLA	C4B-NB	2.56	1.41	1.37
36	A	306	CLA	C1B-C2B	2.56	1.49	1.43
36	b	840	CLA	CMD-C2D	-2.56	1.45	1.50
36	a	827	CLA	C1D-ND	2.56	1.41	1.37
36	I	314	CLA	CMB-C2B	-2.56	1.45	1.50
36	Q	307	CLA	C1B-C2B	2.56	1.49	1.43
36	M	306	CLA	C1D-ND	2.56	1.41	1.37
36	b	812	CLA	C1B-NB	-2.56	1.34	1.37
36	f	804	CLA	C1B-C2B	2.56	1.49	1.43
36	V	311	CLA	C1B-C2B	2.56	1.49	1.43
36	K	307	CLA	C3D-C2D	2.56	1.46	1.39
36	R	315	CLA	C1B-C2B	2.55	1.49	1.43
36	W	207	CLA	C1B-C2B	2.55	1.49	1.43
36	C	214	CLA	C4B-NB	2.55	1.41	1.37
36	a	810	CLA	C1D-ND	2.55	1.41	1.37
36	B	308	CLA	C1B-C2B	2.55	1.49	1.43
36	L	314	CLA	C4B-NB	2.55	1.41	1.37
36	M	312	CLA	C4B-NB	2.55	1.41	1.37
36	a	819	CLA	C1B-C2B	2.55	1.49	1.43
36	J	315	CLA	C4B-NB	2.55	1.41	1.37
36	P	313	CLA	C4B-NB	2.55	1.41	1.37
36	a	818	CLA	MG-NB	-2.55	2.00	2.05
36	U	311	CLA	MG-NB	-2.55	2.00	2.05
36	b	818	CLA	CMC-C2C	-2.55	1.45	1.50
36	D	309	CLA	C4B-NB	-2.55	1.34	1.37
36	R	318	CLA	C1B-C2B	2.55	1.49	1.43
36	C	206	CLA	C1B-C2B	2.55	1.49	1.43
36	O	308	CLA	C1B-C2B	2.55	1.49	1.43
36	J	308	CLA	C1B-C2B	2.55	1.49	1.43
37	G	318	KC1	CBD-CAD	-2.55	1.45	1.56
37	C	213	KC1	C1A-CHA	2.55	1.46	1.40
36	b	836	CLA	CHB-C1B	2.55	1.45	1.39
36	D	316	CLA	CMD-C2D	-2.55	1.45	1.50
36	a	830	CLA	C1B-C2B	2.55	1.49	1.43
36	L	309	CLA	C4B-NB	2.55	1.41	1.37
37	D	314	KC1	C1D-ND	-2.54	1.34	1.37
37	G	317	KC1	C1D-ND	-2.54	1.34	1.37
36	C	209	CLA	MG-NB	-2.54	2.00	2.05
36	V	308	CLA	C4B-NB	2.54	1.41	1.37
36	a	813	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	308	CLA	CMD-C2D	-2.54	1.45	1.50
36	K	313	CLA	OBD-CAD	-2.54	1.18	1.22
36	a	833	CLA	C1D-ND	2.54	1.41	1.37
35	O	303	A86	C32-C31	-2.54	1.50	1.54
35	S	303	A86	C30-C29	-2.54	1.27	1.31
36	H	311	CLA	CMD-C2D	-2.54	1.45	1.50
36	X	312	CLA	CMC-C2C	-2.54	1.45	1.50
36	I	306	CLA	C4D-CHA	2.54	1.47	1.38
36	a	823	CLA	CHD-C1D	2.54	1.43	1.38
36	b	823	CLA	CMD-C2D	-2.54	1.45	1.50
35	E	307	A86	O1-C20	-2.54	1.42	1.46
36	G	310	CLA	MG-NB	-2.54	2.00	2.05
36	U	309	CLA	C1B-C2B	2.54	1.49	1.43
36	E	315	CLA	C1B-C2B	2.54	1.49	1.43
36	b	805	CLA	C1B-C2B	2.54	1.49	1.43
36	F	311	CLA	C4B-NB	2.54	1.41	1.37
34	H	303	DD6	O1-C20	-2.54	1.42	1.46
36	O	311	CLA	C4B-NB	2.54	1.41	1.37
36	b	820	CLA	CMD-C2D	-2.54	1.45	1.50
35	X	302	A86	C30-C29	-2.54	1.27	1.31
36	H	306	CLA	C4B-NB	2.53	1.41	1.37
36	E	311	CLA	MG-NB	-2.53	2.00	2.05
36	a	822	CLA	C4B-NB	2.53	1.41	1.37
37	M	318	KC1	C1D-ND	2.53	1.41	1.37
35	F	304	A86	O1-C20	-2.53	1.42	1.46
36	H	310	CLA	C4D-CHA	2.53	1.47	1.38
36	a	806	CLA	C1D-ND	2.53	1.41	1.37
37	K	314	KC1	C1B-NB	-2.53	1.34	1.37
36	J	309	CLA	MG-NB	-2.53	2.00	2.05
36	a	823	CLA	MG-NB	-2.53	2.00	2.05
36	A	311	CLA	CMB-C2B	-2.53	1.45	1.50
36	L	312	CLA	C1B-C2B	2.53	1.49	1.43
36	M	312	CLA	C1B-C2B	2.53	1.49	1.43
36	L	320	CLA	C1B-C2B	2.53	1.49	1.43
36	R	313	CLA	MG-NB	-2.53	2.00	2.05
36	G	319	CLA	C1B-C2B	2.53	1.49	1.43
36	K	315	CLA	C1B-C2B	2.53	1.49	1.43
36	M	310	CLA	MG-NB	-2.53	2.00	2.05
36	f	802	CLA	C1D-ND	2.53	1.41	1.37
36	a	814	CLA	CMC-C2C	-2.53	1.45	1.50
36	b	808	CLA	CMC-C2C	-2.53	1.45	1.50
36	F	311	CLA	CMC-C2C	-2.53	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	K	311	CLA	C1B-C2B	2.53	1.49	1.43
34	A	303	DD6	O1-C20	-2.53	1.43	1.46
36	a	813	CLA	CMC-C2C	-2.53	1.45	1.50
36	N	318	CLA	C1B-C2B	2.53	1.49	1.43
36	P	319	CLA	C3B-C4B	2.53	1.50	1.42
36	b	818	CLA	MG-NB	-2.53	2.00	2.05
36	a	809	CLA	MG-NB	-2.53	2.00	2.05
36	O	310	CLA	C1B-C2B	2.53	1.49	1.43
34	S	307	DD6	O1-C20	-2.53	1.43	1.46
36	a	805	CLA	MG-NB	-2.52	2.00	2.05
36	H	314	CLA	C1B-C2B	2.52	1.49	1.43
35	X	303	A86	C13-C11	-2.52	1.45	1.49
35	S	305	A86	C30-C31	-2.52	1.27	1.30
36	P	314	CLA	MG-NB	-2.52	2.00	2.05
36	V	311	CLA	MG-NB	-2.52	2.00	2.05
44	a	845	BCR	C1-C6	-2.52	1.50	1.53
36	P	310	CLA	C1B-C2B	2.52	1.49	1.43
36	X	308	CLA	C1B-C2B	2.52	1.49	1.43
44	l	207	BCR	C1-C6	-2.52	1.50	1.53
36	C	209	CLA	CMC-C2C	-2.52	1.45	1.50
36	R	311	CLA	C1B-C2B	2.52	1.49	1.43
35	N	303	A86	C30-C29	-2.52	1.27	1.31
36	Q	310	CLA	MG-NB	-2.52	2.00	2.05
36	J	308	CLA	CMC-C2C	-2.52	1.45	1.50
36	M	309	CLA	C1B-C2B	2.52	1.49	1.43
36	K	316	CLA	MG-NB	-2.52	2.00	2.05
36	O	312	CLA	MG-NB	-2.52	2.00	2.05
36	a	801	CLA	C1B-NB	-2.52	1.34	1.37
35	E	302	A86	O1-C20	-2.52	1.43	1.46
36	E	308	CLA	CMB-C2B	-2.52	1.45	1.50
36	I	306	CLA	C4B-NB	-2.52	1.34	1.37
37	W	217	KC1	C1B-NB	-2.52	1.34	1.37
37	X	311	KC1	C1B-NB	-2.52	1.34	1.37
35	T	305	A86	C13-C11	-2.52	1.45	1.49
36	E	313	CLA	C1B-C2B	2.51	1.49	1.43
36	a	835	CLA	C1D-ND	2.51	1.41	1.37
36	F	313	CLA	CMB-C2B	-2.51	1.45	1.50
35	W	203	A86	C13-C11	-2.51	1.45	1.49
36	A	308	CLA	CMC-C2C	-2.51	1.45	1.50
36	Q	309	CLA	C1B-C2B	2.51	1.49	1.43
36	a	803	CLA	CMD-C2D	-2.51	1.45	1.50
35	A	316	A86	O1-C20	-2.51	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	306	CLA	C1D-C2D	2.51	1.50	1.45
36	O	316	CLA	C4D-CHA	2.51	1.47	1.38
36	b	837	CLA	C1D-ND	2.51	1.41	1.37
35	E	305	A86	O1-C20	-2.51	1.43	1.46
39	L	303	LMT	O2B-C2B	-2.51	1.36	1.43
36	L	314	CLA	C1B-C2B	2.51	1.49	1.43
36	W	212	CLA	MG-ND	-2.51	2.00	2.05
36	b	811	CLA	CMD-C2D	-2.51	1.45	1.50
36	P	319	CLA	CMD-C2D	-2.51	1.45	1.50
36	H	307	CLA	C3B-C4B	2.51	1.50	1.42
36	R	310	CLA	CMD-C2D	-2.51	1.45	1.50
36	K	310	CLA	CHC-C4B	2.51	1.45	1.39
36	P	313	CLA	C1B-C2B	2.51	1.49	1.43
36	D	309	CLA	C3D-C2D	2.51	1.45	1.39
36	a	817	CLA	MG-ND	-2.51	2.00	2.05
36	a	824	CLA	MG-NB	-2.51	2.00	2.05
44	j	107	BCR	C30-C25	-2.51	1.50	1.53
36	R	321	CLA	MG-NB	-2.51	2.00	2.05
36	L	308	CLA	CHB-C4A	-2.51	1.31	1.37
36	b	832	CLA	C1D-ND	2.51	1.41	1.37
36	b	837	CLA	CMD-C2D	-2.51	1.45	1.50
35	P	304	A86	C32-C31	-2.50	1.50	1.54
36	C	208	CLA	CMD-C2D	-2.50	1.45	1.50
36	b	841	CLA	CMB-C2B	-2.50	1.45	1.50
35	G	306	A86	O1-C20	-2.50	1.43	1.46
36	b	802	CLA	C3B-C4B	2.50	1.50	1.42
36	b	829	CLA	CHC-C1C	2.50	1.43	1.38
36	a	801	CLA	MG-NB	-2.50	2.00	2.05
36	b	836	CLA	C3D-C2D	2.50	1.45	1.39
36	a	804	CLA	MG-ND	-2.50	2.00	2.05
37	J	314	KC1	C1A-CHA	2.50	1.46	1.40
36	a	801	CLA	C1B-C2B	2.50	1.49	1.43
37	N	314	KC1	C4C-C3C	2.50	1.49	1.45
36	P	312	CLA	C1B-C2B	2.50	1.49	1.43
36	P	301	CLA	CMC-C2C	-2.50	1.45	1.50
36	E	315	CLA	C4B-NB	-2.50	1.34	1.37
34	j	103	DD6	O1-C20	-2.50	1.43	1.46
36	a	813	CLA	CMD-C2D	-2.50	1.45	1.50
35	L	301	A86	O1-C20	-2.50	1.43	1.46
35	U	304	A86	O1-C20	-2.50	1.43	1.46
36	B	308	CLA	MG-NB	-2.49	2.00	2.05
36	R	316	CLA	MG-NB	-2.49	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	213	KC1	C4A-C3A	2.49	1.49	1.44
36	O	311	CLA	C1B-C2B	2.49	1.49	1.43
36	V	311	CLA	C4B-NB	2.49	1.41	1.37
36	H	309	CLA	C4B-NB	2.49	1.41	1.37
36	S	311	CLA	C3B-C4B	2.49	1.50	1.42
36	I	308	CLA	C4B-NB	2.49	1.41	1.37
36	I	305	CLA	C1B-C2B	2.49	1.49	1.43
36	K	312	CLA	CMD-C2D	-2.49	1.45	1.50
36	C	208	CLA	MG-NB	-2.49	2.00	2.05
36	V	313	CLA	MG-NB	-2.49	2.00	2.05
36	D	317	CLA	C4B-NB	2.49	1.41	1.37
36	a	819	CLA	C4B-NB	2.49	1.41	1.37
36	R	322	CLA	O1D-CGD	2.49	1.27	1.21
36	B	306	CLA	C1B-C2B	2.49	1.49	1.43
36	L	313	CLA	C1B-C2B	2.49	1.49	1.43
36	b	815	CLA	C1B-C2B	2.49	1.49	1.43
44	i	101	BCR	C1-C6	-2.49	1.50	1.53
36	b	813	CLA	C1B-C2B	2.49	1.49	1.43
36	N	317	CLA	MG-NB	-2.49	2.00	2.05
36	C	214	CLA	C1B-C2B	2.49	1.49	1.43
36	K	309	CLA	C1B-C2B	2.49	1.49	1.43
36	A	308	CLA	C4B-NB	2.48	1.41	1.37
37	G	308	KC1	C1A-CHA	2.48	1.46	1.40
34	P	305	DD6	O1-C20	-2.48	1.43	1.46
36	S	310	CLA	C1B-C2B	2.48	1.49	1.43
36	l	202	CLA	CMD-C2D	-2.48	1.45	1.50
36	U	310	CLA	C1B-C2B	2.48	1.49	1.43
36	S	313	CLA	C1B-C2B	2.48	1.49	1.43
35	X	304	A86	C30-C31	-2.48	1.27	1.30
36	J	310	CLA	C1B-C2B	2.48	1.49	1.43
36	b	810	CLA	C1B-C2B	2.48	1.49	1.43
36	a	835	CLA	C1B-NB	-2.48	1.34	1.37
36	b	823	CLA	CMB-C2B	-2.48	1.45	1.50
36	b	813	CLA	C4B-C3B	2.48	1.48	1.43
36	K	316	CLA	C4B-NB	2.48	1.41	1.37
36	M	307	CLA	MG-NB	-2.48	2.00	2.05
35	Q	301	A86	C32-C31	-2.48	1.50	1.54
36	V	313	CLA	C1B-C2B	2.48	1.48	1.43
36	A	311	CLA	C1D-ND	2.48	1.41	1.37
36	K	316	CLA	CMB-C2B	-2.48	1.45	1.50
34	E	301	DD6	O1-C20	-2.48	1.43	1.46
36	D	316	CLA	C1B-C2B	2.48	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	G	301	LHG	O8-C6	-2.48	1.39	1.45
35	G	305	A86	O1-C20	-2.48	1.43	1.46
36	N	308	CLA	CMB-C2B	-2.48	1.45	1.50
35	P	307	A86	O1-C20	-2.48	1.43	1.46
36	C	208	CLA	C1B-C2B	2.48	1.48	1.43
36	b	833	CLA	C1B-NB	-2.48	1.34	1.37
34	E	304	DD6	O1-C20	-2.47	1.43	1.46
36	K	309	CLA	MG-NB	-2.47	2.00	2.05
35	T	306	A86	C30-C29	-2.47	1.27	1.31
34	A	301	DD6	O1-C20	-2.47	1.43	1.46
34	I	303	DD6	O1-C20	-2.47	1.43	1.46
36	a	824	CLA	C1B-NB	-2.47	1.34	1.37
44	a	844	BCR	C1-C6	-2.47	1.50	1.53
36	a	824	CLA	MG-ND	-2.47	2.00	2.05
37	H	313	KC1	C1D-ND	-2.47	1.34	1.37
36	f	804	CLA	CHD-C1D	2.47	1.43	1.38
36	l	202	CLA	MG-NB	-2.47	2.00	2.05
36	l	205	CLA	C4B-NB	-2.47	1.34	1.37
36	U	310	CLA	C1D-ND	2.47	1.41	1.37
37	M	317	KC1	C1A-CHA	2.47	1.46	1.40
37	P	317	KC1	C1B-NB	-2.47	1.34	1.37
37	U	312	KC1	C1D-ND	-2.47	1.34	1.37
36	F	311	CLA	C1B-C2B	2.47	1.48	1.43
37	A	312	KC1	C1A-CHA	2.47	1.46	1.40
36	C	207	CLA	C1D-C2D	2.47	1.50	1.45
36	E	308	CLA	MG-NB	-2.47	2.00	2.05
36	L	311	CLA	MG-NB	-2.47	2.00	2.05
36	A	310	CLA	MG-NB	-2.47	2.00	2.05
36	b	809	CLA	MG-NB	-2.47	2.00	2.05
36	G	314	CLA	C1B-C2B	2.47	1.48	1.43
36	l	206	CLA	C1B-C2B	2.47	1.48	1.43
36	I	305	CLA	CMD-C2D	-2.47	1.45	1.50
36	M	307	CLA	CMB-C2B	-2.46	1.45	1.50
36	b	805	CLA	MG-NB	-2.46	2.00	2.05
36	a	833	CLA	C4B-NB	2.46	1.41	1.37
36	b	824	CLA	C1B-NB	-2.46	1.34	1.37
34	H	302	DD6	O1-C20	-2.46	1.43	1.46
36	L	308	CLA	C4B-NB	-2.46	1.34	1.37
36	b	802	CLA	CMB-C2B	-2.46	1.45	1.50
36	C	214	CLA	MG-NB	-2.46	2.00	2.05
36	b	817	CLA	C4B-NB	2.46	1.41	1.37
37	D	314	KC1	C1B-NB	-2.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	816	CLA	CHC-C4B	2.46	1.44	1.39
36	S	312	CLA	MG-NB	-2.46	2.00	2.05
36	E	310	CLA	C4B-NB	2.46	1.41	1.37
36	J	316	CLA	C4B-NB	2.46	1.41	1.37
35	C	202	A86	C32-C31	-2.46	1.50	1.54
36	b	821	CLA	CMB-C2B	-2.46	1.45	1.50
36	J	308	CLA	C4B-NB	2.46	1.41	1.37
36	J	313	CLA	MG-NB	-2.46	2.00	2.05
36	X	309	CLA	C3B-C4B	2.46	1.49	1.42
36	D	309	CLA	C1D-C2D	2.46	1.50	1.45
36	V	314	CLA	C1D-C2D	2.46	1.50	1.45
36	a	834	CLA	CMB-C2B	-2.46	1.45	1.50
36	X	315	CLA	C1B-C2B	2.46	1.48	1.43
37	X	311	KC1	C4C-C3C	2.46	1.49	1.45
36	f	803	CLA	C3D-C2D	2.46	1.45	1.39
36	P	318	CLA	C3B-C4B	2.46	1.49	1.42
36	A	309	CLA	CMB-C2B	-2.46	1.45	1.50
36	R	318	CLA	CMC-C2C	-2.46	1.45	1.50
36	a	808	CLA	MG-NB	-2.46	2.00	2.05
34	R	308	DD6	O1-C20	-2.46	1.43	1.46
36	a	821	CLA	C1D-ND	2.45	1.41	1.37
36	M	308	CLA	C1B-C2B	2.45	1.48	1.43
36	a	841	CLA	CMB-C2B	-2.45	1.45	1.50
36	B	305	CLA	CHC-C1C	2.45	1.43	1.38
36	a	820	CLA	MG-NB	-2.45	2.00	2.05
36	b	801	CLA	CMB-C2B	-2.45	1.45	1.50
36	a	828	CLA	C1B-NB	-2.45	1.34	1.37
41	F	318	LHG	P-O6	2.45	1.68	1.60
36	S	311	CLA	CHC-C1C	2.45	1.43	1.38
36	P	309	CLA	MG-NB	-2.45	2.00	2.05
37	U	312	KC1	C4C-C3C	2.45	1.49	1.45
36	F	314	CLA	C1B-C2B	2.45	1.48	1.43
36	a	848	CLA	MG-NB	-2.45	2.00	2.05
36	a	838	CLA	CMD-C2D	-2.45	1.45	1.50
36	G	319	CLA	C3D-C2D	2.45	1.45	1.39
37	P	317	KC1	CBD-CAD	-2.45	1.45	1.56
35	W	202	A86	C32-C31	2.45	1.58	1.54
36	R	313	CLA	CMD-C2D	-2.45	1.45	1.50
36	a	814	CLA	CMB-C2B	-2.45	1.45	1.50
36	a	839	CLA	CMB-C2B	-2.45	1.45	1.50
36	H	318	CLA	MG-NB	-2.45	2.00	2.05
36	W	212	CLA	C1B-C2B	2.45	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	217	KC1	C4C-C3C	2.45	1.49	1.45
36	C	208	CLA	C4B-NB	2.45	1.41	1.37
36	l	202	CLA	CMB-C2B	-2.45	1.45	1.50
36	A	311	CLA	CMD-C2D	-2.45	1.45	1.50
35	R	304	A86	C30-C31	-2.45	1.27	1.30
36	R	312	CLA	MG-NB	-2.45	2.00	2.05
36	B	307	CLA	C1B-C2B	2.45	1.48	1.43
36	X	309	CLA	C1B-C2B	2.45	1.48	1.43
39	L	303	LMT	O1'-C1'	-2.45	1.36	1.40
35	K	301	A86	O1-C20	-2.44	1.43	1.46
36	a	839	CLA	C1D-ND	2.44	1.41	1.37
37	P	317	KC1	C1A-CHA	2.44	1.46	1.40
36	W	206	CLA	C3B-C4B	2.44	1.49	1.42
36	X	307	CLA	CMB-C2B	-2.44	1.45	1.50
37	T	310	KC1	C1B-NB	-2.44	1.34	1.37
36	b	827	CLA	CHC-C1C	2.44	1.43	1.38
36	b	829	CLA	MG-NB	-2.44	2.00	2.05
36	G	316	CLA	CMD-C2D	-2.44	1.45	1.50
35	X	314	A86	O1-C20	-2.44	1.43	1.46
35	X	301	A86	C13-C11	-2.44	1.45	1.49
36	K	310	CLA	MG-NB	-2.44	2.01	2.05
36	N	312	CLA	CMD-C2D	-2.44	1.45	1.50
36	U	313	CLA	C3B-C4B	2.44	1.49	1.42
36	b	835	CLA	C4B-NB	2.44	1.41	1.37
36	G	311	CLA	C1D-ND	2.44	1.41	1.37
36	J	307	CLA	C4B-NB	2.44	1.41	1.37
36	S	311	CLA	CMD-C2D	-2.44	1.45	1.50
36	D	312	CLA	C4B-NB	2.44	1.41	1.37
36	F	314	CLA	C4B-NB	2.44	1.41	1.37
36	W	201	CLA	C3B-C4B	2.44	1.49	1.42
36	a	838	CLA	CMB-C2B	-2.44	1.45	1.50
36	b	806	CLA	CMD-C2D	-2.44	1.45	1.50
37	L	317	KC1	C1D-ND	-2.44	1.34	1.37
36	b	828	CLA	MG-ND	-2.43	2.01	2.05
35	G	302	A86	O1-C20	-2.43	1.43	1.46
36	C	206	CLA	C4B-NB	2.43	1.41	1.37
36	R	318	CLA	CHC-C1C	2.43	1.43	1.38
34	B	302	DD6	O1-C20	-2.43	1.43	1.46
35	F	302	A86	O1-C20	-2.43	1.43	1.46
36	W	210	CLA	C4B-NB	2.43	1.41	1.37
36	b	821	CLA	C4B-NB	2.43	1.41	1.37
36	b	829	CLA	CMB-C2B	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	306	CLA	C1B-C2B	2.43	1.48	1.43
34	D	304	DD6	O1-C20	-2.43	1.43	1.46
36	J	317	CLA	CMD-C2D	-2.43	1.45	1.50
36	a	819	CLA	C1D-ND	2.43	1.41	1.37
36	j	101	CLA	MG-NB	-2.43	2.01	2.05
36	B	305	CLA	CMC-C2C	-2.43	1.45	1.50
36	D	308	CLA	CMB-C2B	-2.43	1.45	1.50
36	b	805	CLA	CMC-C2C	-2.43	1.45	1.50
36	R	312	CLA	CMD-C2D	-2.43	1.45	1.50
36	A	311	CLA	C1B-C2B	2.43	1.48	1.43
36	b	840	CLA	CMB-C2B	-2.43	1.45	1.50
35	C	203	A86	O1-C20	-2.43	1.43	1.46
36	b	826	CLA	C1B-NB	-2.43	1.34	1.37
36	H	307	CLA	C1B-NB	-2.42	1.34	1.37
36	O	316	CLA	C1D-C2D	2.42	1.50	1.45
36	O	307	CLA	MG-NB	-2.42	2.01	2.05
36	A	307	CLA	CMC-C2C	-2.42	1.45	1.50
36	b	815	CLA	CMD-C2D	-2.42	1.45	1.50
36	V	307	CLA	C1B-C2B	2.42	1.48	1.43
35	h	204	A86	O1-C20	-2.42	1.43	1.46
36	b	834	CLA	CMD-C2D	-2.42	1.45	1.50
35	C	202	A86	C30-C29	-2.42	1.28	1.31
36	J	309	CLA	CMD-C2D	-2.42	1.45	1.50
36	a	848	CLA	C3D-C2D	2.42	1.45	1.39
36	i	102	CLA	C1B-C2B	2.42	1.48	1.43
36	E	317	CLA	C1B-C2B	2.42	1.48	1.43
34	Q	302	DD6	O1-C20	-2.42	1.43	1.46
36	A	310	CLA	C1B-C2B	2.42	1.48	1.43
36	a	824	CLA	C1B-C2B	2.42	1.48	1.43
36	j	101	CLA	C1B-C2B	2.42	1.48	1.43
36	W	212	CLA	CHC-C1C	2.42	1.43	1.38
36	V	309	CLA	C1B-C2B	2.42	1.48	1.43
36	W	207	CLA	CHC-C1C	2.42	1.43	1.38
36	J	309	CLA	C1B-C2B	2.42	1.48	1.43
34	W	204	DD6	O1-C20	-2.42	1.43	1.46
35	B	301	A86	O1-C20	-2.42	1.43	1.46
36	L	311	CLA	C4B-NB	2.42	1.41	1.37
35	Q	304	A86	C30-C29	-2.42	1.28	1.31
36	G	312	CLA	MG-NB	-2.42	2.01	2.05
36	U	311	CLA	CMC-C2C	-2.41	1.45	1.50
36	A	309	CLA	CMC-C2C	-2.41	1.45	1.50
36	L	309	CLA	CMC-C2C	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	316	CLA	C1B-C2B	2.41	1.48	1.43
36	b	808	CLA	C4B-NB	2.41	1.41	1.37
36	Q	306	CLA	MG-NB	-2.41	2.01	2.05
37	J	314	KC1	CBD-CAD	-2.41	1.45	1.56
36	J	307	CLA	CMD-C2D	-2.41	1.45	1.50
36	R	316	CLA	CMD-C2D	-2.41	1.45	1.50
36	J	315	CLA	MG-NB	-2.41	2.01	2.05
36	M	312	CLA	MG-NB	-2.41	2.01	2.05
36	L	311	CLA	C3B-C4B	2.41	1.49	1.42
36	F	317	CLA	MG-NB	-2.41	2.01	2.05
36	H	318	CLA	C1D-ND	2.41	1.41	1.37
36	L	310	CLA	C3B-C4B	2.41	1.49	1.42
36	U	310	CLA	MG-ND	-2.41	2.01	2.05
34	K	305	DD6	O1-C20	-2.41	1.43	1.46
36	b	818	CLA	C3B-C4B	2.41	1.49	1.42
36	J	309	CLA	CMB-C2B	-2.41	1.45	1.50
36	a	831	CLA	MG-NB	-2.41	2.01	2.05
36	a	833	CLA	C1B-C2B	2.41	1.48	1.43
36	b	838	CLA	CMD-C2D	-2.41	1.45	1.50
36	B	305	CLA	C3B-C4B	2.41	1.49	1.42
36	b	833	CLA	C1D-ND	2.41	1.41	1.37
36	G	316	CLA	C1B-C2B	2.41	1.48	1.43
36	U	311	CLA	CHC-C1C	2.41	1.43	1.38
36	D	317	CLA	C1B-C2B	2.41	1.48	1.43
36	M	311	CLA	MG-NB	-2.41	2.01	2.05
36	Q	308	CLA	MG-NB	-2.41	2.01	2.05
36	R	313	CLA	C1B-C2B	2.41	1.48	1.43
36	G	311	CLA	MG-NB	-2.40	2.01	2.05
36	I	308	CLA	MG-NB	-2.40	2.01	2.05
35	F	305	A86	C13-C11	-2.40	1.45	1.49
36	A	310	CLA	C1D-ND	2.40	1.41	1.37
36	V	313	CLA	C4B-NB	2.40	1.41	1.37
37	K	314	KC1	C1D-ND	-2.40	1.34	1.37
35	P	306	A86	O1-C20	-2.40	1.43	1.46
36	I	306	CLA	CHB-C1B	2.40	1.44	1.39
36	H	312	CLA	CMC-C2C	-2.40	1.45	1.50
36	H	306	CLA	MG-NB	-2.40	2.01	2.05
36	b	826	CLA	MG-NB	-2.40	2.01	2.05
37	G	318	KC1	O2A-CGA	-2.40	1.24	1.30
36	a	841	CLA	C3B-C4B	2.40	1.49	1.42
36	a	810	CLA	C1B-C2B	2.40	1.48	1.43
36	K	308	CLA	C1B-C2B	2.40	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	312	CLA	C1B-C2B	2.40	1.48	1.43
36	D	308	CLA	CMD-C2D	-2.40	1.45	1.50
34	C	201	DD6	O1-C20	-2.40	1.43	1.46
36	L	313	CLA	C4B-NB	2.40	1.41	1.37
36	b	825	CLA	C1B-NB	-2.40	1.34	1.37
36	a	848	CLA	C1D-ND	2.40	1.41	1.37
36	B	309	CLA	CHC-C1C	2.40	1.43	1.38
36	a	839	CLA	MG-NB	-2.40	2.01	2.05
36	A	305	CLA	C4B-NB	2.40	1.41	1.37
36	R	313	CLA	C4B-NB	2.40	1.41	1.37
36	W	215	CLA	C1B-C2B	2.40	1.48	1.43
36	V	311	CLA	CMC-C2C	-2.40	1.45	1.50
36	U	313	CLA	CHC-C1C	2.40	1.43	1.38
36	H	307	CLA	C1B-C2B	2.40	1.48	1.43
36	b	840	CLA	C1D-ND	2.40	1.41	1.37
36	l	206	CLA	C4B-NB	2.40	1.41	1.37
36	E	314	CLA	CMC-C2C	-2.40	1.45	1.50
36	b	822	CLA	MG-NB	-2.40	2.01	2.05
36	D	315	CLA	C1B-C2B	2.40	1.48	1.43
36	R	320	CLA	C1B-C2B	2.40	1.48	1.43
36	C	211	CLA	C4B-NB	2.40	1.41	1.37
36	K	308	CLA	MG-NB	-2.39	2.01	2.05
36	R	322	CLA	MG-NB	-2.39	2.01	2.05
36	G	314	CLA	CMB-C2B	-2.39	1.45	1.50
36	a	804	CLA	CMC-C2C	-2.39	1.45	1.50
36	a	808	CLA	CMD-C2D	-2.39	1.45	1.50
36	V	308	CLA	C1B-C2B	2.39	1.48	1.43
34	M	303	DD6	O1-C20	-2.39	1.43	1.46
36	b	820	CLA	CMB-C2B	-2.39	1.45	1.50
36	I	310	CLA	C4B-NB	2.39	1.41	1.37
36	f	804	CLA	C1D-C2D	2.39	1.50	1.45
34	E	306	DD6	O1-C20	-2.39	1.43	1.46
36	a	841	CLA	CMD-C2D	-2.39	1.45	1.50
36	I	305	CLA	C4B-NB	2.39	1.41	1.37
36	b	827	CLA	CMD-C2D	-2.39	1.45	1.50
36	b	833	CLA	CMC-C2C	-2.39	1.45	1.50
40	b	849	DGD	C3G-C2G	2.39	1.58	1.50
36	L	314	CLA	CMD-C2D	-2.39	1.45	1.50
36	H	307	CLA	CHC-C1C	2.39	1.43	1.38
36	a	828	CLA	C1B-C2B	2.39	1.48	1.43
34	O	304	DD6	O1-C20	-2.39	1.43	1.46
35	S	308	A86	O1-C20	-2.39	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	314	CLA	CMD-C2D	-2.39	1.45	1.50
36	b	836	CLA	MG-NB	-2.39	2.01	2.05
36	C	205	CLA	C1B-C2B	2.39	1.48	1.43
36	B	308	CLA	CMD-C2D	-2.39	1.45	1.50
35	U	303	A86	O1-C20	-2.39	1.43	1.46
36	V	306	CLA	C1B-C2B	2.39	1.48	1.43
36	E	310	CLA	C3B-C4B	2.39	1.49	1.42
36	W	218	CLA	CMC-C2C	-2.38	1.45	1.50
36	b	816	CLA	C1D-C2D	2.38	1.50	1.45
36	a	832	CLA	MG-NB	-2.38	2.01	2.05
35	J	306	A86	O1-C20	-2.38	1.43	1.46
36	P	313	CLA	MG-NB	-2.38	2.01	2.05
36	G	315	CLA	CHC-C4B	2.38	1.44	1.39
36	D	316	CLA	C4B-NB	2.38	1.41	1.37
37	P	317	KC1	C4B-NB	-2.38	1.34	1.37
36	C	207	CLA	MG-NB	-2.38	2.01	2.05
35	C	204	A86	C8-C6	2.38	1.51	1.46
36	L	314	CLA	MG-NB	-2.38	2.01	2.05
36	b	801	CLA	MG-NB	-2.38	2.01	2.05
36	M	306	CLA	CMB-C2B	-2.38	1.45	1.50
36	b	807	CLA	C4B-NB	2.38	1.41	1.37
37	V	312	KC1	C1D-ND	-2.38	1.34	1.37
36	O	309	CLA	MG-NB	-2.38	2.01	2.05
36	a	835	CLA	CMB-C2B	-2.38	1.45	1.50
36	T	312	CLA	C3B-C4B	2.38	1.49	1.42
35	N	320	A86	C30-C29	-2.38	1.28	1.31
37	T	315	KC1	C1B-NB	-2.38	1.34	1.37
36	D	307	CLA	CMB-C2B	-2.38	1.45	1.50
36	b	818	CLA	CMD-C2D	-2.38	1.45	1.50
39	L	303	LMT	O4'-C4B	-2.38	1.37	1.43
36	U	306	CLA	C3D-C2D	2.38	1.45	1.39
36	a	801	CLA	CMB-C2B	-2.38	1.45	1.50
36	M	311	CLA	CMD-C2D	-2.38	1.45	1.50
36	H	316	CLA	C1B-C2B	2.38	1.48	1.43
36	J	307	CLA	CMB-C2B	-2.38	1.45	1.50
36	h	203	CLA	C1B-C2B	2.38	1.48	1.43
35	V	303	A86	C30-C29	-2.38	1.28	1.31
36	K	312	CLA	MG-NB	-2.38	2.01	2.05
36	a	813	CLA	MG-ND	-2.38	2.01	2.05
36	b	835	CLA	CMD-C2D	-2.37	1.45	1.50
36	F	317	CLA	MG-ND	-2.37	2.01	2.05
36	S	312	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	311	CLA	CMB-C2B	-2.37	1.45	1.50
36	a	818	CLA	CMD-C2D	-2.37	1.45	1.50
36	a	807	CLA	CMD-C2D	-2.37	1.45	1.50
36	f	802	CLA	CHC-C1C	2.37	1.43	1.38
36	H	318	CLA	C4B-NB	2.37	1.41	1.37
36	H	309	CLA	MG-NB	-2.37	2.01	2.05
36	l	201	CLA	C3B-C4B	2.37	1.49	1.42
36	E	315	CLA	CHD-C1D	2.37	1.43	1.38
36	L	309	CLA	C1B-C2B	2.37	1.48	1.43
36	L	320	CLA	MG-NB	-2.37	2.01	2.05
36	W	208	CLA	C3B-C4B	2.37	1.49	1.42
36	S	315	CLA	CHC-C1C	2.37	1.43	1.38
36	E	314	CLA	CAC-C3C	-2.37	1.45	1.51
36	b	807	CLA	C1B-C2B	2.37	1.48	1.43
44	l	207	BCR	C30-C25	-2.37	1.50	1.53
36	T	316	CLA	C1B-C2B	2.37	1.48	1.43
36	X	315	CLA	C3B-C4B	2.37	1.49	1.42
36	D	311	CLA	C1B-C2B	2.37	1.48	1.43
36	D	312	CLA	CMD-C2D	-2.37	1.45	1.50
36	P	318	CLA	C1B-C2B	2.37	1.48	1.43
36	K	315	CLA	MG-NB	-2.37	2.01	2.05
41	O	318	LHG	P-O6	2.37	1.68	1.59
36	W	209	CLA	C3B-C4B	2.37	1.49	1.42
36	P	318	CLA	MG-NB	-2.37	2.01	2.05
36	S	310	CLA	MG-NB	-2.37	2.01	2.05
36	S	315	CLA	C3B-C4B	2.37	1.49	1.42
36	J	311	CLA	C1B-C2B	2.37	1.48	1.43
36	b	823	CLA	MG-NB	-2.37	2.01	2.05
36	P	311	CLA	MG-NB	-2.37	2.01	2.05
36	H	311	CLA	C1B-C2B	2.37	1.48	1.43
36	K	308	CLA	CMC-C2C	-2.37	1.45	1.50
35	G	304	A86	C13-C11	-2.37	1.45	1.49
35	C	203	A86	C32-C31	-2.37	1.50	1.54
36	a	812	CLA	CMD-C2D	-2.37	1.45	1.50
36	a	814	CLA	C1B-C2B	2.37	1.48	1.43
36	S	314	CLA	C1B-C2B	2.37	1.48	1.43
37	C	213	KC1	C1D-ND	-2.37	1.34	1.37
36	G	315	CLA	MG-NB	-2.36	2.01	2.05
36	b	806	CLA	MG-NB	-2.36	2.01	2.05
36	B	305	CLA	C1B-C2B	2.36	1.48	1.43
35	V	301	A86	O1-C20	-2.36	1.43	1.46
36	b	839	CLA	CMB-C2B	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	a	842	LHG	O8-C6	-2.36	1.39	1.45
36	a	802	CLA	CHC-C1C	2.36	1.43	1.38
37	X	311	KC1	C1D-C2D	2.36	1.48	1.43
36	A	305	CLA	CMD-C2D	-2.36	1.45	1.50
36	b	827	CLA	CMB-C2B	-2.36	1.45	1.50
34	L	305	DD6	O1-C20	-2.36	1.43	1.46
36	D	306	CLA	CMB-C2B	-2.36	1.45	1.50
37	W	217	KC1	C1D-C2D	2.36	1.48	1.43
36	G	312	CLA	CMB-C2B	-2.36	1.45	1.50
36	P	301	CLA	C1B-C2B	2.36	1.48	1.43
36	a	821	CLA	C1B-C2B	2.36	1.48	1.43
36	E	308	CLA	C4B-NB	2.36	1.41	1.37
36	b	820	CLA	C4B-NB	2.36	1.41	1.37
36	K	307	CLA	MG-NB	-2.36	2.01	2.05
36	A	314	CLA	C3D-C4D	2.36	1.49	1.44
35	h	202	A86	O1-C20	-2.36	1.43	1.46
36	a	839	CLA	C1B-NB	-2.36	1.34	1.37
36	G	316	CLA	CMC-C2C	-2.36	1.45	1.50
36	D	310	CLA	MG-NB	-2.36	2.01	2.05
36	a	817	CLA	C1D-ND	2.36	1.41	1.37
36	B	311	CLA	CMD-C2D	-2.36	1.45	1.50
36	U	306	CLA	CHC-C1C	2.36	1.43	1.38
35	R	302	A86	C32-C31	-2.36	1.50	1.54
36	M	311	CLA	CMB-C2B	-2.36	1.45	1.50
36	R	311	CLA	MG-NB	-2.36	2.01	2.05
36	J	310	CLA	C4B-NB	2.36	1.41	1.37
36	E	313	CLA	C1B-NB	-2.36	1.34	1.37
36	D	311	CLA	CMB-C2B	-2.36	1.45	1.50
36	a	808	CLA	CMB-C2B	-2.36	1.45	1.50
36	b	841	CLA	MG-NB	-2.36	2.01	2.05
35	T	301	A86	O1-C20	-2.36	1.43	1.46
36	a	814	CLA	CMD-C2D	-2.36	1.45	1.50
44	f	806	BCR	C30-C25	-2.36	1.50	1.53
34	A	304	DD6	O1-C20	-2.35	1.43	1.46
36	A	307	CLA	MG-NB	-2.35	2.01	2.05
36	Q	314	CLA	MG-NB	-2.35	2.01	2.05
36	O	312	CLA	CMB-C2B	-2.35	1.45	1.50
36	W	210	CLA	MG-NB	-2.35	2.01	2.05
36	H	306	CLA	C1B-C2B	2.35	1.48	1.43
36	E	314	CLA	CMD-C2D	-2.35	1.45	1.50
37	W	213	KC1	C4C-C3C	2.35	1.49	1.45
36	l	206	CLA	CMD-C2D	-2.35	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	314	CLA	MG-NB	-2.35	2.01	2.05
35	Q	303	A86	O1-C20	-2.35	1.43	1.46
36	C	212	CLA	CHC-C1C	2.35	1.43	1.38
36	K	313	CLA	MG-ND	-2.35	2.01	2.05
36	J	317	CLA	C1B-C2B	2.35	1.48	1.43
37	T	310	KC1	C1A-CHA	2.35	1.46	1.40
35	D	302	A86	O1-C20	-2.35	1.43	1.46
36	T	314	CLA	C3B-C4B	2.35	1.49	1.42
36	A	305	CLA	C1B-C2B	2.35	1.48	1.43
36	D	315	CLA	C1B-NB	-2.35	1.34	1.37
36	P	314	CLA	MG-ND	-2.35	2.01	2.05
36	W	218	CLA	C3B-C4B	2.35	1.49	1.42
36	P	302	CLA	CMC-C2C	-2.35	1.46	1.50
36	b	813	CLA	MG-NB	-2.35	2.01	2.05
36	A	311	CLA	C4B-NB	2.35	1.40	1.37
36	a	839	CLA	CMD-C2D	-2.35	1.46	1.50
36	H	315	CLA	C3B-C4B	2.35	1.49	1.42
36	H	307	CLA	MG-NB	-2.35	2.01	2.05
36	b	824	CLA	MG-NB	-2.35	2.01	2.05
36	E	310	CLA	CHC-C1C	2.35	1.43	1.38
36	H	312	CLA	C4B-NB	2.35	1.40	1.37
36	A	310	CLA	C4B-NB	2.35	1.40	1.37
36	F	310	CLA	C4B-NB	2.35	1.40	1.37
36	C	211	CLA	CMD-C2D	-2.35	1.46	1.50
36	a	820	CLA	C1B-NB	-2.35	1.34	1.37
36	b	806	CLA	C1B-NB	-2.35	1.34	1.37
36	a	820	CLA	CMB-C2B	-2.35	1.46	1.50
37	K	314	KC1	C1A-CHA	2.35	1.46	1.40
36	G	307	CLA	C4B-NB	-2.34	1.34	1.37
36	b	820	CLA	C1B-NB	-2.34	1.34	1.37
36	J	311	CLA	MG-NB	-2.34	2.01	2.05
36	Q	310	CLA	MG-ND	-2.34	2.01	2.05
36	a	828	CLA	MG-NB	-2.34	2.01	2.05
36	H	311	CLA	C1D-ND	2.34	1.40	1.37
36	b	802	CLA	C1D-ND	2.34	1.40	1.37
36	K	309	CLA	CMB-C2B	-2.34	1.46	1.50
36	a	823	CLA	C1B-C2B	2.34	1.48	1.43
36	M	308	CLA	CMB-C2B	-2.34	1.46	1.50
36	P	302	CLA	C1B-C2B	2.34	1.48	1.43
36	a	825	CLA	C1D-ND	2.34	1.40	1.37
36	P	314	CLA	CMB-C2B	-2.34	1.46	1.50
36	W	209	CLA	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	802	CLA	CMD-C2D	-2.34	1.46	1.50
36	E	314	CLA	C1B-C2B	2.34	1.48	1.43
36	O	312	CLA	MG-ND	-2.34	2.01	2.05
35	O	319	A86	C30-C29	-2.34	1.28	1.31
36	b	825	CLA	C1B-C2B	2.34	1.48	1.43
36	H	308	CLA	C4B-NB	2.34	1.40	1.37
36	a	839	CLA	CMC-C2C	-2.34	1.46	1.50
35	F	305	A86	O3-C36	-2.34	1.39	1.43
36	E	308	CLA	C1B-C2B	2.34	1.48	1.43
36	a	811	CLA	CMB-C2B	-2.34	1.46	1.50
36	f	802	CLA	CMD-C2D	-2.34	1.46	1.50
36	C	212	CLA	MG-NB	-2.34	2.01	2.05
36	U	311	CLA	C1B-C2B	2.34	1.48	1.43
35	S	303	A86	C30-C31	-2.34	1.27	1.30
36	J	308	CLA	CHC-C1C	2.34	1.43	1.38
36	N	307	CLA	C3B-C4B	2.34	1.49	1.42
36	b	840	CLA	C3B-C4B	2.34	1.49	1.42
37	G	318	KC1	C4B-NB	-2.34	1.34	1.37
36	b	821	CLA	CMD-C2D	-2.34	1.46	1.50
36	l	201	CLA	CMB-C2B	-2.34	1.46	1.50
36	S	312	CLA	C3B-C4B	2.34	1.49	1.42
36	T	316	CLA	CMB-C2B	-2.34	1.46	1.50
37	S	316	KC1	C3B-C4B	2.34	1.50	1.46
36	O	306	CLA	MG-NB	-2.34	2.01	2.05
44	b	845	BCR	C38-C26	-2.34	1.47	1.50
36	b	815	CLA	MG-NB	-2.34	2.01	2.05
36	C	211	CLA	MG-NB	-2.34	2.01	2.05
36	A	305	CLA	MG-NB	-2.34	2.01	2.05
36	a	835	CLA	C4B-NB	2.33	1.40	1.37
36	M	316	CLA	CMD-C2D	-2.33	1.46	1.50
36	P	302	CLA	CMD-C2D	-2.33	1.46	1.50
35	L	307	A86	O1-C20	-2.33	1.43	1.46
36	D	312	CLA	MG-NB	-2.33	2.01	2.05
36	S	314	CLA	O2D-CGD	2.33	1.39	1.33
37	B	310	KC1	C1D-ND	-2.33	1.34	1.37
36	I	312	CLA	CMC-C2C	-2.33	1.46	1.50
36	a	832	CLA	CMD-C2D	-2.33	1.46	1.50
35	H	304	A86	O1-C20	-2.33	1.43	1.46
36	l	202	CLA	C3B-C4B	2.33	1.49	1.42
36	a	824	CLA	CHC-C1C	2.33	1.43	1.38
36	Q	305	CLA	MG-NB	-2.33	2.01	2.05
36	b	841	CLA	C3C-C2C	2.33	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	316	CLA	CMD-C2D	-2.33	1.46	1.50
36	I	312	CLA	CMB-C2B	-2.33	1.46	1.50
44	a	844	BCR	C30-C25	-2.33	1.50	1.53
36	Q	310	CLA	CMB-C2B	-2.33	1.46	1.50
36	b	815	CLA	CMB-C2B	-2.33	1.46	1.50
36	M	316	CLA	C3B-C4B	2.33	1.49	1.42
36	I	305	CLA	MG-NB	-2.33	2.01	2.05
36	j	102	CLA	MG-NB	-2.33	2.01	2.05
35	N	304	A86	C20-C15	2.33	1.51	1.48
36	M	309	CLA	C3B-C4B	2.33	1.49	1.42
36	X	309	CLA	CHC-C1C	2.33	1.43	1.38
36	a	809	CLA	CMB-C2B	-2.33	1.46	1.50
36	O	316	CLA	MG-NB	-2.33	2.01	2.05
35	T	301	A86	C32-C31	-2.33	1.50	1.54
36	C	208	CLA	CMB-C2B	-2.33	1.46	1.50
36	a	820	CLA	CMD-C2D	-2.33	1.46	1.50
36	a	819	CLA	MG-NB	-2.33	2.01	2.05
36	E	312	CLA	MG-NB	-2.33	2.01	2.05
36	L	311	CLA	CHC-C1C	2.33	1.43	1.38
36	K	309	CLA	CMD-C2D	-2.33	1.46	1.50
36	U	313	CLA	C1B-C2B	2.33	1.48	1.43
35	X	302	A86	C13-C11	-2.33	1.45	1.49
36	b	819	CLA	C1D-ND	2.33	1.40	1.37
36	H	318	CLA	CMB-C2B	-2.33	1.46	1.50
36	b	826	CLA	CMB-C2B	-2.33	1.46	1.50
36	H	314	CLA	MG-NB	-2.33	2.01	2.05
36	F	309	CLA	CHC-C1C	2.33	1.43	1.38
36	b	831	CLA	C4B-NB	2.32	1.40	1.37
37	A	312	KC1	CBD-CAD	-2.32	1.46	1.56
36	b	806	CLA	CHC-C1C	2.32	1.43	1.38
36	A	311	CLA	CMC-C2C	-2.32	1.46	1.50
37	E	309	KC1	C4B-NB	-2.32	1.34	1.37
36	E	312	CLA	C4B-NB	2.32	1.40	1.37
35	O	319	A86	C3-C2	2.32	1.50	1.43
36	S	312	CLA	CHC-C1C	2.32	1.43	1.38
36	W	207	CLA	C3B-C4B	2.32	1.49	1.42
36	f	805	CLA	CMD-C2D	-2.32	1.46	1.50
36	O	311	CLA	MG-NB	-2.32	2.01	2.05
36	K	312	CLA	C1B-C2B	2.32	1.48	1.43
36	b	822	CLA	CMD-C2D	-2.32	1.46	1.50
36	a	803	CLA	CHC-C1C	2.32	1.43	1.38
36	P	309	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	311	CLA	C1B-NB	-2.32	1.34	1.37
36	a	811	CLA	CMD-C2D	-2.32	1.46	1.50
36	b	818	CLA	CHC-C1C	2.32	1.43	1.38
36	X	312	CLA	C3B-C4B	2.32	1.49	1.42
37	M	313	KC1	C1D-ND	-2.32	1.34	1.37
37	M	313	KC1	C1A-CHA	2.32	1.46	1.40
36	A	305	CLA	CMB-C2B	-2.32	1.46	1.50
36	b	839	CLA	C4B-NB	2.32	1.40	1.37
36	G	310	CLA	CMD-C2D	-2.32	1.46	1.50
36	a	837	CLA	CMD-C2D	-2.32	1.46	1.50
36	K	312	CLA	CMB-C2B	-2.32	1.46	1.50
36	U	306	CLA	C4C-C3C	2.32	1.49	1.45
35	R	305	A86	O1-C20	-2.32	1.43	1.46
36	H	310	CLA	CMD-C2D	-2.32	1.46	1.50
36	S	311	CLA	MG-NB	-2.32	2.01	2.05
36	S	321	CLA	C3B-C4B	2.32	1.49	1.42
35	G	304	A86	C30-C29	-2.32	1.28	1.31
36	T	316	CLA	C3B-C4B	2.32	1.49	1.42
36	G	313	CLA	CHC-C1C	2.32	1.43	1.38
36	C	205	CLA	CMD-C2D	-2.32	1.46	1.50
36	b	829	CLA	C3B-C4B	2.32	1.49	1.42
36	a	809	CLA	CMD-C2D	-2.32	1.46	1.50
36	H	317	CLA	MG-NB	-2.32	2.01	2.05
36	N	319	CLA	C1B-C2B	2.32	1.48	1.43
36	a	837	CLA	MG-NB	-2.32	2.01	2.05
37	B	310	KC1	C1D-C2D	2.32	1.48	1.43
36	j	102	CLA	C4B-NB	2.32	1.40	1.37
36	b	802	CLA	CMC-C2C	-2.31	1.46	1.50
36	a	835	CLA	MG-NB	-2.31	2.01	2.05
36	W	209	CLA	CHC-C1C	2.31	1.43	1.38
36	R	316	CLA	CMC-C2C	-2.31	1.46	1.50
36	C	212	CLA	C1B-C2B	2.31	1.48	1.43
36	F	309	CLA	C4B-NB	2.31	1.40	1.37
36	h	203	CLA	C4B-NB	2.31	1.40	1.37
36	b	801	CLA	MG-ND	-2.31	2.01	2.05
36	M	312	CLA	CMD-C2D	-2.31	1.46	1.50
35	T	306	A86	C13-C11	-2.31	1.45	1.49
36	S	320	CLA	C3B-C4B	2.31	1.49	1.42
36	M	308	CLA	MG-NB	-2.31	2.01	2.05
36	P	308	CLA	MG-NB	-2.31	2.01	2.05
37	H	313	KC1	CBD-CAD	-2.31	1.46	1.56
36	H	316	CLA	CMB-C2B	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	819	CLA	CMC-C2C	-2.31	1.46	1.50
36	E	316	CLA	MG-NB	-2.31	2.01	2.05
35	J	302	A86	O1-C20	-2.31	1.43	1.46
36	K	308	CLA	C3B-C4B	2.31	1.49	1.42
34	J	304	DD6	O1-C20	-2.31	1.43	1.46
36	I	313	CLA	C1B-C2B	2.31	1.48	1.43
36	Q	306	CLA	C1B-C2B	2.31	1.48	1.43
36	D	311	CLA	CMD-C2D	-2.31	1.46	1.50
36	E	311	CLA	CMD-C2D	-2.31	1.46	1.50
36	U	307	CLA	CMD-C2D	-2.31	1.46	1.50
36	b	807	CLA	CMD-C2D	-2.31	1.46	1.50
36	a	822	CLA	C1B-C2B	2.31	1.48	1.43
36	B	306	CLA	CMD-C2D	-2.31	1.46	1.50
36	I	310	CLA	C1B-NB	-2.31	1.34	1.37
36	W	211	CLA	O2D-CGD	2.31	1.38	1.33
36	P	310	CLA	MG-NB	-2.31	2.01	2.05
36	a	838	CLA	MG-ND	-2.31	2.01	2.05
36	I	307	CLA	CMD-C2D	-2.31	1.46	1.50
36	R	322	CLA	CMD-C2D	-2.31	1.46	1.50
36	a	827	CLA	CMD-C2D	-2.31	1.46	1.50
36	a	832	CLA	CMB-C2B	-2.31	1.46	1.50
36	H	315	CLA	MG-NB	-2.31	2.01	2.05
36	Q	306	CLA	CHC-C1C	2.31	1.43	1.38
36	i	102	CLA	CMD-C2D	-2.31	1.46	1.50
36	A	309	CLA	C1B-C2B	2.31	1.48	1.43
35	F	301	A86	C32-C31	-2.31	1.50	1.54
36	C	212	CLA	C3B-C4B	2.31	1.49	1.42
36	b	833	CLA	C1B-C2B	2.31	1.48	1.43
36	N	318	CLA	C3B-C4B	2.31	1.49	1.42
36	A	307	CLA	C4B-NB	2.31	1.40	1.37
36	b	808	CLA	CMB-C2B	-2.31	1.46	1.50
36	V	307	CLA	C3B-C4B	2.31	1.49	1.42
36	O	309	CLA	CMB-C2B	-2.31	1.46	1.50
36	A	307	CLA	C1B-C2B	2.31	1.48	1.43
36	V	307	CLA	MG-NB	-2.31	2.01	2.05
36	B	309	CLA	MG-NB	-2.31	2.01	2.05
35	N	303	A86	C30-C31	-2.30	1.27	1.30
36	j	106	CLA	CMB-C2B	-2.30	1.46	1.50
36	R	314	CLA	CMC-C2C	-2.30	1.46	1.50
35	L	301	A86	C32-C31	-2.30	1.50	1.54
36	A	306	CLA	C4C-C3C	2.30	1.48	1.45
36	S	309	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	305	CLA	CMD-C2D	-2.30	1.46	1.50
36	I	310	CLA	CMD-C2D	-2.30	1.46	1.50
37	M	317	KC1	CBD-CAD	-2.30	1.46	1.56
36	S	317	CLA	C3B-C4B	2.30	1.49	1.42
36	a	832	CLA	CMC-C2C	-2.30	1.46	1.50
36	b	811	CLA	CMB-C2B	-2.30	1.46	1.50
36	b	835	CLA	CMB-C2B	-2.30	1.46	1.50
36	b	825	CLA	MG-NB	-2.30	2.01	2.05
36	U	307	CLA	C3B-C4B	2.30	1.49	1.42
37	G	318	KC1	C4C-C3C	2.30	1.48	1.45
36	l	202	CLA	C4B-NB	2.30	1.40	1.37
36	h	203	CLA	CMD-C2D	-2.30	1.46	1.50
36	J	316	CLA	CMB-C2B	-2.30	1.46	1.50
36	A	308	CLA	MG-NB	-2.30	2.01	2.05
36	B	311	CLA	C1B-C2B	2.30	1.48	1.43
36	E	316	CLA	CMB-C2B	-2.30	1.46	1.50
36	P	309	CLA	CHC-C1C	2.30	1.43	1.38
36	F	316	CLA	MG-NB	-2.30	2.01	2.05
36	F	309	CLA	MG-NB	-2.30	2.01	2.05
36	b	832	CLA	CMD-C2D	-2.30	1.46	1.50
34	E	303	DD6	O1-C20	-2.30	1.43	1.46
34	W	205	DD6	O1-C20	-2.30	1.43	1.46
36	F	310	CLA	MG-NB	-2.30	2.01	2.05
36	C	208	CLA	CMC-C2C	-2.30	1.46	1.50
36	a	835	CLA	C3B-C4B	2.30	1.49	1.42
36	U	311	CLA	C3B-C4B	2.30	1.49	1.42
36	D	315	CLA	MG-NB	-2.30	2.01	2.05
36	R	311	CLA	CMD-C2D	-2.30	1.46	1.50
36	V	309	CLA	CMD-C2D	-2.30	1.46	1.50
36	O	307	CLA	CHC-C1C	2.30	1.43	1.38
36	C	211	CLA	CMB-C2B	-2.30	1.46	1.50
36	H	315	CLA	CMB-C2B	-2.30	1.46	1.50
36	a	810	CLA	CMB-C2B	-2.30	1.46	1.50
36	X	315	CLA	CHC-C1C	2.30	1.43	1.38
36	b	826	CLA	MG-ND	-2.30	2.01	2.05
36	K	316	CLA	CMD-C2D	-2.29	1.46	1.50
36	b	828	CLA	CMD-C2D	-2.29	1.46	1.50
35	R	301	A86	C13-C11	-2.29	1.45	1.49
36	b	841	CLA	CMD-C2D	-2.29	1.46	1.50
36	b	809	CLA	C1B-C2B	2.29	1.48	1.43
37	D	314	KC1	CBD-CAD	-2.29	1.46	1.56
36	R	320	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	V	311	CLA	MG-ND	-2.29	2.01	2.05
36	b	814	CLA	C3B-C4B	2.29	1.49	1.42
36	Q	307	CLA	CMB-C2B	-2.29	1.46	1.50
36	a	819	CLA	CMB-C2B	-2.29	1.46	1.50
36	l	206	CLA	CMB-C2B	-2.29	1.46	1.50
36	J	313	CLA	C4B-NB	2.29	1.40	1.37
36	a	808	CLA	C4B-NB	2.29	1.40	1.37
37	W	213	KC1	C1D-C2D	2.29	1.48	1.43
36	J	310	CLA	CMD-C2D	-2.29	1.46	1.50
36	O	307	CLA	C1B-C2B	2.29	1.48	1.43
36	X	306	CLA	C3B-C4B	2.29	1.49	1.42
36	J	307	CLA	MG-ND	-2.29	2.01	2.05
37	O	315	KC1	CAA-C2A	2.29	1.53	1.46
36	L	313	CLA	CMD-C2D	-2.29	1.46	1.50
36	b	813	CLA	C1D-ND	2.29	1.40	1.37
36	b	833	CLA	C4B-NB	2.29	1.40	1.37
36	I	305	CLA	CMB-C2B	-2.29	1.46	1.50
36	Q	308	CLA	CMB-C2B	-2.29	1.46	1.50
36	a	833	CLA	CMC-C2C	-2.29	1.46	1.50
36	S	319	CLA	C3B-C4B	2.29	1.49	1.42
35	C	204	A86	O1-C20	-2.29	1.43	1.46
36	F	313	CLA	CMD-C2D	-2.29	1.46	1.50
36	I	311	CLA	CMC-C2C	-2.29	1.46	1.50
36	b	815	CLA	C1B-NB	-2.29	1.34	1.37
36	a	805	CLA	C1B-C2B	2.29	1.48	1.43
37	G	317	KC1	C4B-NB	-2.29	1.34	1.37
36	F	314	CLA	CMD-C2D	-2.29	1.46	1.50
36	K	313	CLA	CMD-C2D	-2.29	1.46	1.50
36	a	834	CLA	CMD-C2D	-2.29	1.46	1.50
36	A	309	CLA	MG-NB	-2.29	2.01	2.05
36	D	307	CLA	MG-NB	-2.29	2.01	2.05
36	f	803	CLA	C4C-C3C	2.29	1.48	1.45
36	a	803	CLA	C4B-NB	2.29	1.40	1.37
36	a	810	CLA	C4B-NB	2.29	1.40	1.37
36	a	826	CLA	C1B-NB	-2.29	1.34	1.37
36	F	311	CLA	CMB-C2B	-2.29	1.46	1.50
36	P	318	CLA	CMD-C2D	-2.29	1.46	1.50
36	a	808	CLA	CMC-C2C	-2.29	1.46	1.50
36	I	307	CLA	C1B-C2B	2.29	1.48	1.43
36	a	841	CLA	C1B-C2B	2.29	1.48	1.43
36	R	314	CLA	C3B-C4B	2.29	1.49	1.42
36	P	301	CLA	CMD-C2D	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	815	CLA	CMC-C2C	-2.29	1.46	1.50
36	H	308	CLA	C1B-NB	-2.29	1.34	1.37
36	I	313	CLA	CHC-C1C	2.29	1.43	1.38
36	T	313	CLA	C3B-C4B	2.29	1.49	1.42
36	b	828	CLA	CMB-C2B	-2.29	1.46	1.50
36	P	319	CLA	CMB-C2B	-2.29	1.46	1.50
36	a	831	CLA	CMC-C2C	-2.29	1.46	1.50
36	I	311	CLA	CMD-C2D	-2.28	1.46	1.50
39	L	303	LMT	O3B-C3B	-2.28	1.37	1.43
36	Q	307	CLA	MG-NB	-2.28	2.01	2.05
36	b	828	CLA	MG-NB	-2.28	2.01	2.05
36	F	309	CLA	C1B-NB	-2.28	1.34	1.37
36	H	311	CLA	C4B-NB	2.28	1.40	1.37
36	H	317	CLA	CHC-C1C	2.28	1.43	1.38
36	W	215	CLA	CHC-C1C	2.28	1.43	1.38
36	H	305	CLA	CMB-C2B	-2.28	1.46	1.50
36	F	313	CLA	C4B-NB	2.28	1.40	1.37
36	A	313	CLA	MG-NB	-2.28	2.01	2.05
36	b	814	CLA	C1B-C2B	2.28	1.48	1.43
37	M	313	KC1	C4C-C3C	2.28	1.48	1.45
36	a	838	CLA	C4B-NB	2.28	1.40	1.37
36	Q	308	CLA	CMD-C2D	-2.28	1.46	1.50
36	G	311	CLA	MG-ND	-2.28	2.01	2.05
36	a	825	CLA	MG-NB	-2.28	2.01	2.05
36	a	810	CLA	CMD-C2D	-2.28	1.46	1.50
36	E	313	CLA	MG-NB	-2.28	2.01	2.05
36	U	311	CLA	MG-ND	-2.28	2.01	2.05
37	C	213	KC1	CBD-CAD	-2.28	1.46	1.56
37	M	318	KC1	C3D-CAD	2.28	1.53	1.45
36	Q	308	CLA	C1B-C2B	2.28	1.48	1.43
36	a	807	CLA	CMC-C2C	-2.28	1.46	1.50
36	H	314	CLA	CMC-C2C	-2.28	1.46	1.50
36	b	814	CLA	CMC-C2C	-2.28	1.46	1.50
36	I	313	CLA	C3B-C4B	2.28	1.49	1.42
36	b	839	CLA	C3B-C4B	2.28	1.49	1.42
34	D	303	DD6	C3-C2	2.28	1.50	1.43
36	J	311	CLA	CMB-C2B	-2.28	1.46	1.50
36	D	315	CLA	C4B-NB	2.28	1.40	1.37
36	T	316	CLA	MG-NB	-2.28	2.01	2.05
35	V	301	A86	C32-C31	-2.28	1.50	1.54
35	S	301	A86	C13-C11	-2.28	1.45	1.49
36	b	814	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	310	CLA	MG-NB	-2.28	2.01	2.05
36	a	829	CLA	C4B-NB	2.28	1.40	1.37
37	E	309	KC1	CBD-CAD	-2.28	1.46	1.56
36	D	316	CLA	CMB-C2B	-2.28	1.46	1.50
36	L	316	CLA	MG-NB	-2.28	2.01	2.05
36	D	307	CLA	C1B-C2B	2.28	1.48	1.43
36	O	309	CLA	C1B-C2B	2.28	1.48	1.43
36	b	838	CLA	CMB-C2B	-2.28	1.46	1.50
36	H	308	CLA	CMD-C2D	-2.28	1.46	1.50
36	R	321	CLA	C1B-NB	-2.28	1.34	1.37
36	D	317	CLA	CMB-C2B	-2.28	1.46	1.50
36	H	312	CLA	CMB-C2B	-2.28	1.46	1.50
36	b	837	CLA	CHC-C1C	2.28	1.43	1.38
36	E	312	CLA	CMB-C2B	-2.27	1.46	1.50
37	Q	311	KC1	CAA-C2A	2.27	1.53	1.46
37	Q	313	KC1	CAA-C2A	2.27	1.53	1.46
36	a	822	CLA	C3B-C4B	2.27	1.49	1.42
36	G	310	CLA	C4B-NB	2.27	1.40	1.37
35	X	314	A86	C32-C31	-2.27	1.50	1.54
36	F	310	CLA	CMD-C2D	-2.27	1.46	1.50
36	H	316	CLA	CMD-C2D	-2.27	1.46	1.50
36	l	201	CLA	CMD-C2D	-2.27	1.46	1.50
36	C	212	CLA	CMC-C2C	-2.27	1.46	1.50
36	M	308	CLA	CMD-C2D	-2.27	1.46	1.50
36	P	301	CLA	CMB-C2B	-2.27	1.46	1.50
36	a	817	CLA	CMD-C2D	-2.27	1.46	1.50
36	b	810	CLA	CMD-C2D	-2.27	1.46	1.50
36	a	814	CLA	C1B-NB	-2.27	1.34	1.37
36	b	838	CLA	C1B-C2B	2.27	1.48	1.43
37	F	315	KC1	C1A-CHA	2.27	1.46	1.40
36	a	831	CLA	CMD-C2D	-2.27	1.46	1.50
36	b	814	CLA	CMB-C2B	-2.27	1.46	1.50
36	J	316	CLA	MG-NB	-2.27	2.01	2.05
36	b	827	CLA	C1B-NB	-2.27	1.34	1.37
36	l	201	CLA	C4B-NB	2.27	1.40	1.37
36	V	314	CLA	C4B-NB	-2.27	1.34	1.37
36	K	311	CLA	C3B-C4B	2.27	1.49	1.42
36	O	306	CLA	CMD-C2D	-2.27	1.46	1.50
35	M	302	A86	C13-C11	-2.27	1.45	1.49
36	a	821	CLA	MG-ND	-2.27	2.01	2.05
36	a	808	CLA	C1B-C2B	2.27	1.48	1.43
37	R	317	KC1	C4B-NB	-2.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	214	CLA	CMB-C2B	-2.27	1.46	1.50
36	b	833	CLA	CMD-C2D	-2.27	1.46	1.50
36	a	803	CLA	C3B-C4B	2.27	1.49	1.42
36	K	315	CLA	CMD-C2D	-2.27	1.46	1.50
36	O	308	CLA	CMB-C2B	-2.27	1.46	1.50
36	G	307	CLA	MG-NB	-2.27	2.01	2.05
36	N	308	CLA	C3B-C4B	2.27	1.49	1.42
37	B	310	KC1	C1B-NB	-2.27	1.34	1.37
36	G	319	CLA	C4C-C3C	2.27	1.48	1.45
36	H	318	CLA	C1B-C2B	2.27	1.48	1.43
36	J	313	CLA	C1B-C2B	2.27	1.48	1.43
36	b	839	CLA	CMD-C2D	-2.27	1.46	1.50
36	U	309	CLA	C3B-C4B	2.27	1.49	1.42
36	J	317	CLA	MG-NB	-2.27	2.01	2.05
36	P	310	CLA	CMB-C2B	-2.27	1.46	1.50
36	D	317	CLA	C3B-C4B	2.27	1.49	1.42
36	F	311	CLA	CMD-C2D	-2.27	1.46	1.50
36	F	310	CLA	C1B-C2B	2.27	1.48	1.43
36	b	838	CLA	MG-NB	-2.27	2.01	2.05
36	A	307	CLA	CMD-C2D	-2.27	1.46	1.50
36	P	314	CLA	CMC-C2C	-2.27	1.46	1.50
36	J	312	CLA	C1B-C2B	2.27	1.48	1.43
36	R	316	CLA	C1D-C2D	2.27	1.49	1.45
36	b	812	CLA	CMC-C2C	-2.27	1.46	1.50
36	b	834	CLA	CMB-C2B	-2.27	1.46	1.50
36	a	837	CLA	C1B-C2B	2.27	1.48	1.43
36	Q	310	CLA	CMC-C2C	-2.27	1.46	1.50
36	i	102	CLA	CMB-C2B	-2.27	1.46	1.50
37	E	309	KC1	O2A-CGA	-2.27	1.24	1.30
44	i	103	BCR	C38-C26	-2.27	1.47	1.50
36	f	802	CLA	C1B-NB	-2.26	1.34	1.37
36	H	310	CLA	CMB-C2B	-2.26	1.46	1.50
36	b	809	CLA	CMD-C2D	-2.26	1.46	1.50
36	D	313	CLA	CMD-C2D	-2.26	1.46	1.50
36	J	311	CLA	CMD-C2D	-2.26	1.46	1.50
36	K	313	CLA	CMC-C2C	-2.26	1.46	1.50
36	K	310	CLA	C1C-C2C	2.26	1.49	1.44
36	P	311	CLA	C1B-C2B	2.26	1.48	1.43
36	M	314	CLA	MG-NB	-2.26	2.01	2.05
36	H	317	CLA	C3B-C4B	2.26	1.49	1.42
36	a	812	CLA	C4B-NB	2.26	1.40	1.37
36	b	801	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	303	A86	C13-C11	-2.26	1.45	1.49
36	S	313	CLA	C3B-C4B	2.26	1.49	1.42
36	a	823	CLA	CHD-C4C	2.26	1.44	1.39
36	X	315	CLA	MG-NB	-2.26	2.01	2.05
36	b	820	CLA	MG-NB	-2.26	2.01	2.05
36	L	311	CLA	CMC-C2C	-2.26	1.46	1.50
36	J	313	CLA	C3B-C4B	2.26	1.49	1.42
36	X	312	CLA	CHC-C1C	2.26	1.43	1.38
35	N	301	A86	C13-C11	-2.26	1.45	1.49
37	P	315	KC1	CAA-C2A	2.26	1.53	1.46
36	C	205	CLA	MG-NB	-2.26	2.01	2.05
36	A	314	CLA	CMD-C2D	-2.26	1.46	1.50
35	T	305	A86	C30-C29	-2.26	1.28	1.31
37	L	315	KC1	C1D-ND	-2.26	1.34	1.37
36	O	312	CLA	CMC-C2C	-2.26	1.46	1.50
36	G	311	CLA	C1B-NB	-2.26	1.34	1.37
36	E	311	CLA	C1B-C2B	2.26	1.48	1.43
37	F	308	KC1	O2A-CGA	-2.26	1.24	1.30
36	C	210	CLA	C3B-C4B	2.26	1.49	1.42
36	b	840	CLA	MG-NB	-2.26	2.01	2.05
37	R	317	KC1	C1D-ND	-2.26	1.34	1.37
44	f	806	BCR	C33-C5	-2.26	1.47	1.50
36	E	310	CLA	C1B-C2B	2.26	1.48	1.43
36	E	312	CLA	CMC-C2C	-2.26	1.46	1.50
36	I	312	CLA	CMD-C2D	-2.26	1.46	1.50
36	l	202	CLA	CHC-C1C	2.26	1.43	1.38
36	j	101	CLA	C4B-NB	2.26	1.40	1.37
36	R	311	CLA	CMB-C2B	-2.26	1.46	1.50
36	b	816	CLA	C1B-C2B	2.26	1.48	1.43
37	V	312	KC1	C1B-NB	-2.26	1.34	1.37
36	O	309	CLA	CMD-C2D	-2.26	1.46	1.50
35	M	304	A86	O1-C20	-2.26	1.43	1.46
35	h	202	A86	C32-C31	-2.26	1.50	1.54
36	U	309	CLA	CMD-C2D	-2.26	1.46	1.50
36	O	308	CLA	MG-NB	-2.26	2.01	2.05
36	I	310	CLA	C3B-C4B	2.26	1.49	1.42
36	N	310	CLA	CMD-C2D	-2.26	1.46	1.50
36	a	815	CLA	CMB-C2B	-2.26	1.46	1.50
36	b	810	CLA	CMB-C2B	-2.26	1.46	1.50
36	S	314	CLA	C3B-C4B	2.26	1.49	1.42
36	F	313	CLA	MG-NB	-2.26	2.01	2.05
36	L	312	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	314	CLA	CMD-C2D	-2.26	1.46	1.50
36	T	309	CLA	CMC-C2C	-2.26	1.46	1.50
36	P	312	CLA	C3B-C4B	2.26	1.49	1.42
36	A	313	CLA	CMD-C2D	-2.26	1.46	1.50
36	b	821	CLA	MG-NB	-2.26	2.01	2.05
36	D	312	CLA	C1B-C2B	2.26	1.48	1.43
36	M	310	CLA	CMB-C2B	-2.26	1.46	1.50
37	M	317	KC1	O2A-CGA	-2.26	1.24	1.30
36	f	803	CLA	MG-NB	-2.25	2.01	2.05
36	H	318	CLA	C3B-C4B	2.25	1.49	1.42
36	D	306	CLA	O2A-CGA	2.25	1.38	1.30
36	a	816	CLA	C1B-C2B	2.25	1.48	1.43
36	B	311	CLA	CMB-C2B	-2.25	1.46	1.50
36	F	310	CLA	CMC-C2C	-2.25	1.46	1.50
36	P	311	CLA	CMB-C2B	-2.25	1.46	1.50
36	V	307	CLA	CMB-C2B	-2.25	1.46	1.50
36	D	310	CLA	C1B-C2B	2.25	1.48	1.43
36	f	805	CLA	MG-NB	-2.25	2.01	2.05
36	F	309	CLA	C3B-C4B	2.25	1.49	1.42
35	R	306	A86	O3-C36	-2.25	1.39	1.43
36	l	205	CLA	C1B-C2B	2.25	1.48	1.43
36	j	101	CLA	C1B-NB	-2.25	1.34	1.37
36	b	832	CLA	CMC-C2C	-2.25	1.46	1.50
35	S	303	A86	C13-C11	-2.25	1.45	1.49
36	N	307	CLA	CMD-C2D	-2.25	1.46	1.50
36	Q	305	CLA	CMD-C2D	-2.25	1.46	1.50
36	D	309	CLA	MG-NB	-2.25	2.01	2.05
36	a	826	CLA	C1B-C2B	2.25	1.48	1.43
35	K	303	A86	C13-C11	-2.25	1.45	1.49
36	S	311	CLA	CMB-C2B	-2.25	1.46	1.50
36	W	207	CLA	CMC-C2C	-2.25	1.46	1.50
36	F	316	CLA	CHC-C1C	2.25	1.43	1.38
36	j	106	CLA	MG-NB	-2.25	2.01	2.05
36	a	826	CLA	CMD-C2D	-2.25	1.46	1.50
37	D	314	KC1	C1A-CHA	2.25	1.46	1.40
37	O	313	KC1	CAA-C2A	2.25	1.53	1.46
36	a	833	CLA	CMD-C2D	-2.25	1.46	1.50
36	a	806	CLA	C1B-C2B	2.25	1.48	1.43
35	C	204	A86	C32-C31	-2.25	1.50	1.54
36	b	805	CLA	CMB-C2B	-2.25	1.46	1.50
36	f	802	CLA	CMB-C2B	-2.25	1.46	1.50
36	S	320	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	218	CLA	CHC-C1C	2.25	1.43	1.38
36	A	314	CLA	C3B-C4B	2.25	1.49	1.42
36	b	835	CLA	C3B-C4B	2.25	1.49	1.42
36	K	315	CLA	C3B-C4B	2.25	1.49	1.42
36	Q	314	CLA	C1B-C2B	2.25	1.48	1.43
36	M	315	CLA	CMC-C2C	-2.25	1.46	1.50
35	O	305	A86	O1-C20	-2.25	1.43	1.46
36	N	313	CLA	CMC-C2C	-2.25	1.46	1.50
36	P	311	CLA	CMD-C2D	-2.25	1.46	1.50
36	a	805	CLA	CMB-C2B	-2.25	1.46	1.50
36	b	834	CLA	CMC-C2C	-2.25	1.46	1.50
35	N	305	A86	C17-C16	-2.25	1.51	1.54
36	G	313	CLA	C3B-C4B	2.25	1.49	1.42
36	N	315	CLA	C1B-C2B	2.25	1.48	1.43
36	K	308	CLA	CHC-C1C	2.25	1.43	1.38
36	P	312	CLA	MG-NB	-2.25	2.01	2.05
36	D	310	CLA	CMD-C2D	-2.25	1.46	1.50
36	V	307	CLA	CMD-C2D	-2.25	1.46	1.50
37	N	314	KC1	C1D-C2D	2.25	1.48	1.43
36	E	314	CLA	MG-NB	-2.25	2.01	2.05
36	A	308	CLA	CHC-C1C	2.25	1.43	1.38
36	I	310	CLA	MG-NB	-2.25	2.01	2.05
36	P	308	CLA	CMD-C2D	-2.25	1.46	1.50
36	b	822	CLA	C1B-NB	-2.25	1.34	1.37
35	V	302	A86	C17-C18	-2.24	1.49	1.52
36	O	307	CLA	C3B-C4B	2.24	1.49	1.42
36	C	206	CLA	CMB-C2B	-2.24	1.46	1.50
36	C	211	CLA	C1B-C2B	2.24	1.48	1.43
34	S	306	DD6	O1-C20	-2.24	1.43	1.46
36	D	307	CLA	C4B-NB	2.24	1.40	1.37
36	J	313	CLA	CMB-C2B	-2.24	1.46	1.50
36	F	316	CLA	C1B-C2B	2.24	1.48	1.43
36	I	307	CLA	C4B-NB	2.24	1.40	1.37
36	b	813	CLA	C4B-NB	2.24	1.40	1.37
36	b	824	CLA	C4B-NB	2.24	1.40	1.37
36	W	212	CLA	C1A-CHA	-2.24	1.33	1.43
36	F	310	CLA	CMB-C2B	-2.24	1.46	1.50
36	P	319	CLA	CMC-C2C	-2.24	1.46	1.50
36	a	817	CLA	CMB-C2B	-2.24	1.46	1.50
35	W	202	A86	C13-C11	-2.24	1.45	1.49
36	I	313	CLA	MG-NB	-2.24	2.01	2.05
36	a	821	CLA	C1B-NB	-2.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	824	CLA	C1C-C2C	2.24	1.49	1.44
36	J	312	CLA	CMB-C2B	-2.24	1.46	1.50
36	K	315	CLA	CMC-C2C	-2.24	1.46	1.50
36	W	211	CLA	CMD-C2D	-2.24	1.46	1.50
36	I	314	CLA	MG-NB	-2.24	2.01	2.05
36	B	306	CLA	CMB-C2B	-2.24	1.46	1.50
36	T	309	CLA	CMD-C2D	-2.24	1.46	1.50
36	R	311	CLA	CHC-C1C	2.24	1.43	1.38
36	A	310	CLA	CMC-C2C	-2.24	1.46	1.50
36	b	807	CLA	CMC-C2C	-2.24	1.46	1.50
36	G	319	CLA	C3D-C4D	-2.24	1.39	1.44
36	G	316	CLA	CMB-C2B	-2.24	1.46	1.50
36	G	312	CLA	CMC-C2C	-2.24	1.46	1.50
36	a	803	CLA	CMC-C2C	-2.24	1.46	1.50
36	A	308	CLA	C3B-C4B	2.24	1.49	1.42
36	O	310	CLA	C3B-C4B	2.24	1.49	1.42
35	G	304	A86	C17-C18	-2.24	1.49	1.52
36	j	106	CLA	CMD-C2D	-2.24	1.46	1.50
36	R	322	CLA	CHC-C1C	2.24	1.43	1.38
36	M	309	CLA	MG-NB	-2.24	2.01	2.05
36	N	313	CLA	MG-NB	-2.24	2.01	2.05
36	W	214	CLA	C3B-C4B	2.24	1.49	1.42
36	a	825	CLA	CHC-C1C	2.24	1.43	1.38
36	L	311	CLA	CMD-C2D	-2.24	1.46	1.50
36	R	314	CLA	CMD-C2D	-2.24	1.46	1.50
36	b	829	CLA	C4B-NB	2.24	1.40	1.37
36	H	309	CLA	CMB-C2B	-2.24	1.46	1.50
36	R	314	CLA	CMB-C2B	-2.24	1.46	1.50
36	R	319	CLA	C3B-C4B	2.24	1.49	1.42
36	P	302	CLA	MG-NB	-2.24	2.01	2.05
36	O	307	CLA	CMC-C2C	-2.24	1.46	1.50
36	b	832	CLA	C1B-C2B	2.24	1.48	1.43
36	U	306	CLA	C1C-NC	2.24	1.41	1.37
36	H	306	CLA	CMB-C2B	-2.23	1.46	1.50
36	R	312	CLA	CHC-C1C	2.23	1.43	1.38
36	B	307	CLA	C3B-C4B	2.23	1.49	1.42
36	a	834	CLA	C3B-C4B	2.23	1.49	1.42
36	H	311	CLA	MG-NB	-2.23	2.01	2.05
36	a	848	CLA	MG-ND	-2.23	2.01	2.05
36	V	308	CLA	MG-NB	-2.23	2.01	2.05
36	A	307	CLA	CMB-C2B	-2.23	1.46	1.50
36	D	313	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	O	307	CLA	CMD-C2D	-2.23	1.46	1.50
36	a	805	CLA	CMD-C2D	-2.23	1.46	1.50
36	P	313	CLA	CMD-C2D	-2.23	1.46	1.50
36	b	801	CLA	CMD-C2D	-2.23	1.46	1.50
36	b	825	CLA	CMC-C2C	-2.23	1.46	1.50
36	P	309	CLA	CMD-C2D	-2.23	1.46	1.50
44	h	201	BCR	C39-C30	-2.23	1.49	1.53
36	Q	309	CLA	MG-NB	-2.23	2.01	2.05
36	C	211	CLA	CMC-C2C	-2.23	1.46	1.50
37	L	315	KC1	C1B-NB	-2.23	1.34	1.37
36	J	317	CLA	CHC-C1C	2.23	1.43	1.38
36	D	307	CLA	CMD-C2D	-2.23	1.46	1.50
36	b	837	CLA	CMC-C2C	-2.23	1.46	1.50
36	G	309	CLA	C1B-C2B	2.23	1.48	1.43
35	S	304	A86	O1-C20	-2.23	1.43	1.46
36	b	822	CLA	CMB-C2B	-2.23	1.46	1.50
37	S	316	KC1	C4C-C3C	2.23	1.48	1.45
36	T	309	CLA	C3B-C4B	2.23	1.49	1.42
35	Q	316	A86	C17-C16	-2.23	1.51	1.54
36	a	836	CLA	C1B-C2B	2.23	1.48	1.43
35	D	302	A86	C32-C31	-2.23	1.50	1.54
36	b	811	CLA	C4B-NB	2.23	1.40	1.37
37	D	314	KC1	C4B-NB	-2.23	1.34	1.37
36	H	315	CLA	MG-ND	-2.23	2.01	2.05
36	T	311	CLA	C3B-C4B	2.23	1.49	1.42
36	J	312	CLA	CHC-C1C	2.23	1.43	1.38
36	a	835	CLA	CMC-C2C	-2.23	1.46	1.50
36	O	310	CLA	MG-NB	-2.23	2.01	2.05
36	f	805	CLA	C4B-NB	2.23	1.40	1.37
35	C	202	A86	C13-C11	-2.23	1.45	1.49
36	M	315	CLA	CMD-C2D	-2.23	1.46	1.50
35	L	307	A86	C32-C31	-2.23	1.50	1.54
36	K	311	CLA	CMB-C2B	-2.23	1.46	1.50
36	X	308	CLA	C3B-C4B	2.23	1.49	1.42
36	a	838	CLA	MG-NB	-2.23	2.01	2.05
36	b	808	CLA	C1B-C2B	2.23	1.48	1.43
36	H	316	CLA	CMC-C2C	-2.23	1.46	1.50
36	N	319	CLA	CHC-C1C	2.23	1.42	1.38
36	N	317	CLA	C1B-NB	-2.23	1.34	1.37
36	B	307	CLA	CMD-C2D	-2.23	1.46	1.50
36	L	310	CLA	CMB-C2B	-2.23	1.46	1.50
36	L	314	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	313	CLA	CMB-C2B	-2.23	1.46	1.50
36	R	315	CLA	CMD-C2D	-2.23	1.46	1.50
36	V	313	CLA	CMB-C2B	-2.23	1.46	1.50
36	K	312	CLA	CMC-C2C	-2.23	1.46	1.50
36	S	319	CLA	MG-NB	-2.23	2.01	2.05
35	O	303	A86	C13-C11	-2.23	1.45	1.49
36	P	309	CLA	C3B-C4B	2.23	1.49	1.42
36	I	312	CLA	CHC-C1C	2.23	1.42	1.38
36	P	309	CLA	CMC-C2C	-2.23	1.46	1.50
36	a	812	CLA	CMB-C2B	-2.23	1.46	1.50
35	Q	316	A86	C17-C18	-2.23	1.49	1.52
36	b	836	CLA	C1D-C2D	2.23	1.49	1.45
36	D	317	CLA	CMD-C2D	-2.23	1.46	1.50
35	R	303	A86	C13-C11	-2.22	1.45	1.49
36	D	313	CLA	C3B-C4B	2.22	1.49	1.42
36	T	309	CLA	CHC-C1C	2.22	1.42	1.38
36	a	807	CLA	C1B-C2B	2.22	1.48	1.43
36	M	307	CLA	CHC-C1C	2.22	1.42	1.38
36	S	321	CLA	CHC-C1C	2.22	1.42	1.38
36	b	825	CLA	MG-ND	-2.22	2.01	2.05
36	W	208	CLA	MG-NB	-2.22	2.01	2.05
44	h	201	BCR	C33-C5	-2.22	1.47	1.50
36	C	206	CLA	CMD-C2D	-2.22	1.46	1.50
36	b	806	CLA	C3B-C4B	2.22	1.49	1.42
36	N	309	CLA	CMD-C2D	-2.22	1.46	1.50
36	H	318	CLA	C1B-NB	-2.22	1.34	1.37
36	H	308	CLA	C1B-C2B	2.22	1.48	1.43
36	E	317	CLA	C3B-C4B	2.22	1.49	1.42
36	R	321	CLA	CMD-C2D	-2.22	1.46	1.50
37	L	317	KC1	C4C-C3C	2.22	1.48	1.45
36	E	315	CLA	MG-NB	-2.22	2.01	2.05
36	G	316	CLA	MG-NB	-2.22	2.01	2.05
37	K	314	KC1	CBD-CAD	-2.22	1.46	1.56
36	B	308	CLA	CAC-C3C	-2.22	1.45	1.51
35	P	304	A86	C13-C11	-2.22	1.45	1.49
36	Q	309	CLA	C3B-C4B	2.22	1.49	1.42
36	F	314	CLA	MG-NB	-2.22	2.01	2.05
36	b	837	CLA	C4B-NB	2.22	1.40	1.37
36	W	210	CLA	C1B-NB	-2.22	1.34	1.37
36	N	312	CLA	C3B-C4B	2.22	1.49	1.42
36	N	312	CLA	MG-NB	-2.22	2.01	2.05
36	a	804	CLA	C1D-ND	2.22	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	316	CLA	MG-NB	-2.22	2.01	2.05
36	W	207	CLA	MG-NB	-2.22	2.01	2.05
36	M	315	CLA	CMB-C2B	-2.22	1.46	1.50
36	Q	306	CLA	CMC-C2C	-2.22	1.46	1.50
36	C	207	CLA	C4C-C3C	2.22	1.48	1.45
36	H	316	CLA	C3B-C4B	2.22	1.49	1.42
35	Q	301	A86	C13-C11	-2.22	1.45	1.49
36	a	821	CLA	CMC-C2C	-2.22	1.46	1.50
36	b	825	CLA	CMB-C2B	-2.22	1.46	1.50
36	H	312	CLA	C1B-NB	-2.22	1.34	1.37
36	E	310	CLA	MG-NB	-2.22	2.01	2.05
37	S	316	KC1	C1D-ND	-2.22	1.34	1.37
36	Q	306	CLA	CMD-C2D	-2.22	1.46	1.50
36	I	309	CLA	C3B-C4B	2.22	1.49	1.42
36	D	312	CLA	CMB-C2B	-2.21	1.46	1.50
36	E	317	CLA	CHC-C1C	2.21	1.42	1.38
36	K	310	CLA	C1B-C2B	2.21	1.48	1.43
36	W	201	CLA	CMB-C2B	-2.21	1.46	1.50
36	a	807	CLA	MG-NB	-2.21	2.01	2.05
36	Q	306	CLA	C3B-C4B	2.21	1.49	1.42
37	T	315	KC1	C4C-C3C	2.21	1.48	1.45
36	H	311	CLA	CMC-C2C	-2.21	1.46	1.50
36	P	312	CLA	CMD-C2D	-2.21	1.46	1.50
36	j	102	CLA	C1B-C2B	2.21	1.48	1.43
36	b	812	CLA	MG-ND	-2.21	2.01	2.05
36	O	310	CLA	CMC-C2C	-2.21	1.46	1.50
36	a	821	CLA	CMB-C2B	-2.21	1.46	1.50
36	b	809	CLA	CMB-C2B	-2.21	1.46	1.50
36	b	836	CLA	C1C-C2C	2.21	1.49	1.44
36	E	312	CLA	C3B-C4B	2.21	1.49	1.42
36	a	829	CLA	CMC-C2C	-2.21	1.46	1.50
36	S	309	CLA	C3B-C4B	2.21	1.49	1.42
36	a	848	CLA	CHC-C1C	2.21	1.42	1.38
36	H	318	CLA	MG-ND	-2.21	2.01	2.05
36	a	808	CLA	MG-ND	-2.21	2.01	2.05
36	b	830	CLA	MG-ND	-2.21	2.01	2.05
37	V	312	KC1	CBD-CAD	-2.21	1.46	1.56
36	D	313	CLA	CHC-C1C	2.21	1.42	1.38
36	a	826	CLA	C3B-C4B	2.21	1.49	1.42
36	G	310	CLA	CMC-C2C	-2.21	1.46	1.50
36	J	313	CLA	CMC-C2C	-2.21	1.46	1.50
36	j	101	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	305	CLA	CMD-C2D	-2.21	1.46	1.50
37	U	312	KC1	C1D-C2D	2.21	1.48	1.43
36	C	206	CLA	MG-NB	-2.21	2.01	2.05
36	K	311	CLA	MG-NB	-2.21	2.01	2.05
36	J	312	CLA	CMD-C2D	-2.21	1.46	1.50
36	I	312	CLA	C1B-C2B	2.21	1.48	1.43
36	C	209	CLA	MG-ND	-2.21	2.01	2.05
36	R	320	CLA	CMB-C2B	-2.21	1.46	1.50
36	V	311	CLA	C3B-C4B	2.21	1.49	1.42
36	R	313	CLA	MG-ND	-2.21	2.01	2.05
36	J	315	CLA	CMB-C2B	-2.21	1.46	1.50
36	I	306	CLA	C3D-C4D	-2.21	1.39	1.44
36	b	834	CLA	CHC-C1C	2.21	1.42	1.38
36	H	312	CLA	CMD-C2D	-2.21	1.46	1.50
36	K	312	CLA	CHC-C1C	2.21	1.42	1.38
36	A	313	CLA	CMB-C2B	-2.21	1.46	1.50
36	b	839	CLA	CMC-C2C	-2.21	1.46	1.50
36	F	310	CLA	C1B-NB	-2.21	1.35	1.37
36	W	208	CLA	CHC-C1C	2.21	1.42	1.38
36	J	316	CLA	CMC-C2C	-2.21	1.46	1.50
35	J	301	A86	C32-C31	-2.21	1.50	1.54
36	V	311	CLA	C1D-ND	2.21	1.40	1.37
36	l	201	CLA	MG-NB	-2.21	2.01	2.05
37	U	312	KC1	C1B-C2B	2.21	1.49	1.45
36	D	313	CLA	MG-NB	-2.20	2.01	2.05
36	J	310	CLA	MG-NB	-2.20	2.01	2.05
36	J	311	CLA	C3B-C4B	2.20	1.49	1.42
36	O	311	CLA	CMD-C2D	-2.20	1.46	1.50
36	W	216	CLA	C3D-C4D	2.20	1.49	1.44
36	b	817	CLA	CHC-C1C	2.20	1.42	1.38
36	a	805	CLA	CMC-C2C	-2.20	1.46	1.50
36	b	821	CLA	C1B-NB	-2.20	1.35	1.37
36	N	316	CLA	CHC-C1C	2.20	1.42	1.38
36	G	309	CLA	C1B-NB	-2.20	1.35	1.37
36	J	316	CLA	CMD-C2D	-2.20	1.46	1.50
36	L	320	CLA	CMB-C2B	-2.20	1.46	1.50
36	N	316	CLA	MG-NB	-2.20	2.01	2.05
36	b	813	CLA	MG-ND	-2.20	2.01	2.05
36	H	315	CLA	C1B-C2B	2.20	1.48	1.43
35	F	306	A86	C32-C31	-2.20	1.50	1.54
36	W	201	CLA	CMD-C2D	-2.20	1.46	1.50
36	a	826	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	312	CLA	CMC-C2C	-2.20	1.46	1.50
35	U	303	A86	C32-C31	-2.20	1.50	1.54
44	b	846	BCR	C33-C5	-2.20	1.47	1.50
36	L	308	CLA	MG-ND	2.20	2.10	2.05
36	E	311	CLA	CMC-C2C	-2.20	1.46	1.50
36	b	811	CLA	C1B-C2B	2.20	1.48	1.43
36	R	313	CLA	C3B-C4B	2.20	1.49	1.42
44	i	101	BCR	C30-C25	-2.20	1.51	1.53
36	H	308	CLA	CMB-C2B	-2.20	1.46	1.50
36	R	316	CLA	CMB-C2B	-2.20	1.46	1.50
36	b	813	CLA	CMC-C2C	-2.20	1.46	1.50
36	E	317	CLA	MG-NB	-2.20	2.01	2.05
36	P	314	CLA	C3B-C4B	2.20	1.49	1.42
36	a	812	CLA	C1B-C2B	2.20	1.48	1.43
36	a	836	CLA	CMC-C2C	-2.20	1.46	1.50
36	b	832	CLA	CMB-C2B	-2.20	1.46	1.50
36	E	313	CLA	C4B-NB	2.20	1.40	1.37
36	E	312	CLA	C1B-C2B	2.20	1.48	1.43
36	I	305	CLA	CMC-C2C	-2.20	1.46	1.50
36	U	310	CLA	MG-NB	-2.20	2.01	2.05
36	V	308	CLA	C3B-C4B	2.20	1.49	1.42
36	b	817	CLA	C1B-C2B	2.20	1.48	1.43
36	I	313	CLA	CMD-C2D	-2.20	1.46	1.50
36	L	310	CLA	CMD-C2D	-2.20	1.46	1.50
36	N	311	CLA	CMD-C2D	-2.20	1.46	1.50
36	b	837	CLA	CMB-C2B	-2.20	1.46	1.50
36	G	309	CLA	C3B-C4B	2.20	1.49	1.42
36	S	312	CLA	MG-ND	-2.20	2.01	2.05
36	X	312	CLA	CMD-C2D	-2.20	1.46	1.50
36	a	836	CLA	MG-NB	-2.20	2.01	2.05
36	a	839	CLA	C4B-NB	2.20	1.40	1.37
36	T	313	CLA	CHC-C1C	2.20	1.42	1.38
36	Q	305	CLA	C3B-C4B	2.20	1.49	1.42
36	a	834	CLA	MG-NB	-2.20	2.01	2.05
36	K	311	CLA	CMD-C2D	-2.20	1.46	1.50
36	K	309	CLA	CHC-C1C	2.20	1.42	1.38
35	F	305	A86	C32-C31	-2.20	1.50	1.54
37	H	313	KC1	C3B-C4B	2.20	1.49	1.46
36	J	310	CLA	CMC-C2C	-2.19	1.46	1.50
36	D	308	CLA	CHC-C1C	2.19	1.42	1.38
37	L	317	KC1	CBD-CAD	-2.19	1.46	1.56
36	b	828	CLA	C1B-C2B	2.19	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	O	312	CLA	C3B-C4B	2.19	1.49	1.42
36	M	306	CLA	CAB-C3B	-2.19	1.41	1.47
37	P	317	KC1	O2A-CGA	-2.19	1.24	1.30
36	V	310	CLA	CMB-C2B	-2.19	1.46	1.50
36	H	307	CLA	CAC-C3C	-2.19	1.45	1.51
36	h	203	CLA	CMB-C2B	-2.19	1.46	1.50
35	N	305	A86	C17-C18	-2.19	1.49	1.52
36	I	311	CLA	MG-NB	-2.19	2.01	2.05
36	N	317	CLA	CMC-C2C	-2.19	1.46	1.50
36	b	808	CLA	CMD-C2D	-2.19	1.46	1.50
36	J	317	CLA	C3B-C4B	2.19	1.49	1.42
36	L	320	CLA	CMD-C2D	-2.19	1.46	1.50
36	K	313	CLA	C1B-NB	-2.19	1.35	1.37
34	R	307	DD6	O1-C20	-2.19	1.43	1.46
36	X	310	CLA	C3B-C4B	2.19	1.49	1.42
36	X	308	CLA	MG-ND	-2.19	2.01	2.05
36	a	833	CLA	MG-NB	-2.19	2.01	2.05
36	K	309	CLA	C3B-C4B	2.19	1.49	1.42
36	H	309	CLA	CMC-C2C	-2.19	1.46	1.50
36	Q	309	CLA	CMD-C2D	-2.19	1.46	1.50
36	b	832	CLA	MG-NB	-2.19	2.01	2.05
36	I	309	CLA	CMD-C2D	-2.19	1.46	1.50
36	E	315	CLA	C4C-C3C	2.19	1.48	1.45
37	C	213	KC1	C4C-C3C	2.19	1.48	1.45
36	b	839	CLA	MG-NB	-2.19	2.01	2.05
36	D	308	CLA	CMC-C2C	-2.19	1.46	1.50
36	Q	312	CLA	CMD-C2D	-2.19	1.46	1.50
36	G	310	CLA	C1B-C2B	2.19	1.48	1.43
36	R	319	CLA	CMC-C2C	-2.19	1.46	1.50
36	a	836	CLA	CMD-C2D	-2.19	1.46	1.50
36	D	317	CLA	CMC-C2C	-2.19	1.46	1.50
36	M	309	CLA	CMC-C2C	-2.19	1.46	1.50
36	N	316	CLA	C3B-C4B	2.19	1.49	1.42
37	G	317	KC1	O2A-CGA	-2.19	1.24	1.30
36	D	316	CLA	CMC-C2C	-2.19	1.46	1.50
36	P	301	CLA	C3B-C4B	2.19	1.49	1.42
36	R	310	CLA	C3B-C4B	2.19	1.49	1.42
36	M	308	CLA	C3B-C4B	2.19	1.49	1.42
36	Q	310	CLA	C3B-C4B	2.19	1.49	1.42
36	a	832	CLA	C1B-C2B	2.19	1.48	1.43
44	i	103	BCR	C30-C25	-2.19	1.51	1.53
36	U	310	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	302	CLA	CMB-C2B	-2.19	1.46	1.50
36	E	308	CLA	C1B-NB	-2.19	1.35	1.37
37	F	308	KC1	C4B-NB	-2.19	1.35	1.37
35	O	301	A86	C32-C31	-2.19	1.50	1.54
36	W	215	CLA	C3B-C4B	2.19	1.49	1.42
36	Q	309	CLA	CMC-C2C	-2.19	1.46	1.50
36	a	838	CLA	C3B-C4B	2.19	1.49	1.42
36	a	807	CLA	C1B-NB	-2.18	1.35	1.37
36	b	809	CLA	C4B-NB	2.18	1.40	1.37
36	D	317	CLA	MG-NB	-2.18	2.01	2.05
35	G	306	A86	C32-C31	-2.18	1.50	1.54
36	M	309	CLA	CHC-C1C	2.18	1.42	1.38
36	b	817	CLA	MG-NB	-2.18	2.01	2.05
36	b	825	CLA	C4B-NB	2.18	1.40	1.37
36	I	311	CLA	C1B-NB	-2.18	1.35	1.37
36	T	316	CLA	CMD-C2D	-2.18	1.46	1.50
36	U	308	CLA	CMD-C2D	-2.18	1.46	1.50
36	I	307	CLA	CMC-C2C	-2.18	1.46	1.50
36	b	810	CLA	MG-NB	-2.18	2.01	2.05
36	a	820	CLA	C4B-NB	2.18	1.40	1.37
37	H	313	KC1	C1A-CHA	2.18	1.45	1.40
36	I	307	CLA	CMB-C2B	-2.18	1.46	1.50
36	j	101	CLA	CMB-C2B	-2.18	1.46	1.50
36	V	310	CLA	CMD-C2D	-2.18	1.46	1.50
36	M	316	CLA	MG-NB	-2.18	2.01	2.05
36	O	311	CLA	CMB-C2B	-2.18	1.46	1.50
36	L	316	CLA	C3B-C4B	2.18	1.49	1.42
36	b	811	CLA	C3B-C4B	2.18	1.49	1.42
36	E	317	CLA	CMB-C2B	-2.18	1.46	1.50
36	N	318	CLA	CMD-C2D	-2.18	1.46	1.50
36	P	312	CLA	CMB-C2B	-2.18	1.46	1.50
36	G	312	CLA	C4B-NB	2.18	1.40	1.37
36	a	823	CLA	C4B-NB	2.18	1.40	1.37
36	b	815	CLA	C4B-NB	2.18	1.40	1.37
36	S	321	CLA	CMD-C2D	-2.18	1.46	1.50
36	b	830	CLA	CMC-C2C	-2.18	1.46	1.50
36	M	307	CLA	C1B-C2B	2.18	1.48	1.43
36	a	813	CLA	CMA-C3A	-2.18	1.48	1.53
36	F	309	CLA	CMC-C2C	-2.18	1.46	1.50
36	M	312	CLA	CMB-C2B	-2.18	1.46	1.50
36	W	210	CLA	CMB-C2B	-2.18	1.46	1.50
36	L	310	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	309	CLA	CMB-C2B	-2.18	1.46	1.50
36	H	306	CLA	C3B-C4B	2.18	1.49	1.42
36	h	203	CLA	MG-NB	-2.18	2.01	2.05
36	b	820	CLA	C1B-C2B	2.18	1.48	1.43
36	a	809	CLA	CMC-C2C	-2.18	1.46	1.50
44	b	847	BCR	C38-C26	-2.18	1.47	1.50
36	b	837	CLA	C3B-C4B	2.18	1.49	1.42
36	R	321	CLA	C3B-C4B	2.18	1.49	1.42
36	C	205	CLA	C4B-NB	2.18	1.40	1.37
37	L	317	KC1	O2A-CGA	-2.18	1.24	1.30
36	D	312	CLA	CMC-C2C	-2.18	1.46	1.50
36	a	801	CLA	CMC-C2C	-2.18	1.46	1.50
36	K	316	CLA	CMC-C2C	-2.18	1.46	1.50
36	T	314	CLA	CMC-C2C	-2.18	1.46	1.50
36	D	310	CLA	CMC-C2C	-2.18	1.46	1.50
36	D	313	CLA	C1B-C2B	2.18	1.48	1.43
36	a	839	CLA	C1B-C2B	2.18	1.48	1.43
36	E	312	CLA	CMD-C2D	-2.17	1.46	1.50
36	J	315	CLA	CMC-C2C	-2.17	1.46	1.50
36	b	820	CLA	CMC-C2C	-2.17	1.46	1.50
36	b	801	CLA	C4B-NB	2.17	1.40	1.37
36	b	818	CLA	C4B-NB	2.17	1.40	1.37
36	a	823	CLA	C1B-NB	-2.17	1.35	1.37
36	K	307	CLA	CHC-C4B	2.17	1.44	1.39
36	i	102	CLA	MG-NB	-2.17	2.01	2.05
36	b	841	CLA	C1C-NC	-2.17	1.34	1.37
36	A	307	CLA	CHC-C1C	2.17	1.42	1.38
36	S	310	CLA	CHC-C1C	2.17	1.42	1.38
36	a	812	CLA	CHC-C1C	2.17	1.42	1.38
36	b	802	CLA	CHC-C1C	2.17	1.42	1.38
36	a	848	CLA	CHD-C1D	2.17	1.42	1.38
36	W	215	CLA	CMB-C2B	-2.17	1.46	1.50
36	b	829	CLA	CMC-C2C	-2.17	1.46	1.50
36	b	831	CLA	C1D-ND	2.17	1.40	1.37
36	a	824	CLA	C3C-C2C	2.17	1.41	1.36
36	G	309	CLA	MG-NB	-2.17	2.01	2.05
35	I	302	A86	C13-C11	-2.17	1.45	1.49
37	G	308	KC1	O2A-CGA	-2.17	1.24	1.30
36	N	311	CLA	C3B-C4B	2.17	1.49	1.42
36	A	306	CLA	C4B-NB	-2.17	1.35	1.37
36	M	315	CLA	CAC-C3C	-2.17	1.45	1.51
36	C	205	CLA	CMB-C2B	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	831	CLA	CMB-C2B	-2.17	1.46	1.50
36	V	309	CLA	CMB-C2B	-2.17	1.46	1.50
36	X	307	CLA	MG-NB	-2.17	2.01	2.05
36	b	812	CLA	C4B-NB	2.17	1.40	1.37
36	G	309	CLA	CMD-C2D	-2.17	1.46	1.50
36	A	309	CLA	C3B-C4B	2.17	1.49	1.42
36	a	811	CLA	CHC-C1C	2.17	1.42	1.38
36	b	835	CLA	CHC-C1C	2.17	1.42	1.38
36	V	308	CLA	CMD-C2D	-2.17	1.46	1.50
37	T	310	KC1	C1C-C2C	2.17	1.48	1.44
36	b	829	CLA	C1B-NB	-2.17	1.35	1.37
35	T	304	A86	C30-C29	-2.17	1.28	1.31
36	A	305	CLA	CMC-C2C	-2.17	1.46	1.50
36	b	814	CLA	C4B-NB	2.17	1.40	1.37
36	Q	309	CLA	CMB-C2B	-2.17	1.46	1.50
36	b	812	CLA	C1D-ND	2.17	1.40	1.37
37	R	317	KC1	C1D-C2D	2.17	1.48	1.43
36	H	314	CLA	CMB-C2B	-2.17	1.46	1.50
36	M	307	CLA	CMC-C2C	-2.17	1.46	1.50
36	U	307	CLA	CMB-C2B	-2.17	1.46	1.50
36	O	306	CLA	CMC-C2C	-2.17	1.46	1.50
36	L	313	CLA	MG-NB	-2.17	2.01	2.05
36	O	316	CLA	C1B-C2B	2.17	1.48	1.43
36	I	311	CLA	C3B-C4B	2.17	1.49	1.42
36	S	319	CLA	CMD-C2D	-2.17	1.46	1.50
37	F	315	KC1	CBD-CAD	-2.17	1.46	1.56
36	I	311	CLA	C1B-C2B	2.17	1.48	1.43
44	a	847	BCR	C33-C5	-2.17	1.47	1.50
36	I	314	CLA	CMD-C2D	-2.17	1.46	1.50
36	Q	308	CLA	MG-ND	-2.17	2.01	2.05
36	S	309	CLA	CHC-C1C	2.17	1.42	1.38
36	H	317	CLA	CMB-C2B	-2.17	1.46	1.50
36	P	311	CLA	MG-ND	-2.17	2.01	2.05
36	P	316	CLA	CMD-C2D	-2.16	1.46	1.50
36	Q	306	CLA	CMB-C2B	-2.16	1.46	1.50
36	a	815	CLA	CMD-C2D	-2.16	1.46	1.50
36	a	825	CLA	C3B-C4B	2.16	1.49	1.42
36	M	315	CLA	MG-NB	-2.16	2.01	2.05
36	b	822	CLA	CHC-C1C	2.16	1.42	1.38
36	D	311	CLA	CMC-C2C	-2.16	1.46	1.50
36	P	319	CLA	C1B-C2B	2.16	1.48	1.43
36	R	313	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	210	CLA	C3B-C4B	2.16	1.49	1.42
36	H	317	CLA	CMD-C2D	-2.16	1.46	1.50
36	K	313	CLA	CMB-C2B	-2.16	1.46	1.50
36	j	102	CLA	C1B-NB	-2.16	1.35	1.37
35	E	307	A86	C32-C31	-2.16	1.50	1.54
36	M	307	CLA	CMD-C2D	-2.16	1.46	1.50
36	I	310	CLA	C1B-C2B	2.16	1.48	1.43
36	M	312	CLA	MG-ND	-2.16	2.01	2.05
36	A	313	CLA	CMC-C2C	-2.16	1.46	1.50
36	b	813	CLA	CMB-C2B	-2.16	1.46	1.50
36	b	823	CLA	CMC-C2C	-2.16	1.46	1.50
37	Q	313	KC1	C1D-C2D	2.16	1.48	1.43
36	V	310	CLA	MG-NB	-2.16	2.01	2.05
36	b	826	CLA	CMC-C2C	-2.16	1.46	1.50
36	X	313	CLA	C3D-C4D	2.16	1.49	1.44
37	G	308	KC1	C4C-C3C	2.16	1.48	1.45
36	a	809	CLA	C1B-C2B	2.16	1.48	1.43
37	M	313	KC1	CBD-CAD	-2.16	1.46	1.56
36	R	315	CLA	C3B-C4B	2.16	1.49	1.42
36	Q	305	CLA	CMC-C2C	-2.16	1.46	1.50
36	a	837	CLA	CMB-C2B	-2.16	1.46	1.50
37	U	312	KC1	CBD-CAD	-2.16	1.46	1.56
36	O	308	CLA	CMD-C2D	-2.16	1.46	1.50
36	O	310	CLA	CMD-C2D	-2.16	1.46	1.50
36	S	317	CLA	MG-NB	-2.16	2.01	2.05
35	F	302	A86	C32-C31	-2.16	1.50	1.54
36	H	316	CLA	CHC-C1C	2.16	1.42	1.38
36	a	824	CLA	C3B-C4B	2.16	1.49	1.42
36	D	317	CLA	CHC-C1C	2.16	1.42	1.38
36	K	313	CLA	CHC-C1C	2.16	1.42	1.38
36	N	311	CLA	MG-NB	-2.16	2.01	2.05
36	Q	308	CLA	C3B-C4B	2.16	1.49	1.42
36	a	809	CLA	C1B-NB	-2.16	1.35	1.37
37	Q	313	KC1	C1D-ND	-2.16	1.35	1.37
36	A	309	CLA	CMD-C2D	-2.16	1.46	1.50
36	F	314	CLA	CMB-C2B	-2.16	1.46	1.50
36	I	313	CLA	CMC-C2C	-2.16	1.46	1.50
37	F	315	KC1	O2A-CGA	-2.16	1.24	1.30
36	H	305	CLA	C1B-C2B	2.16	1.48	1.43
36	O	306	CLA	C3B-C4B	2.16	1.49	1.42
36	a	825	CLA	C4B-NB	2.16	1.40	1.37
36	H	305	CLA	MG-NB	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	206	CLA	MG-NB	-2.16	2.01	2.05
36	D	306	CLA	CMD-C2D	-2.16	1.46	1.50
36	a	811	CLA	CMC-C2C	-2.16	1.46	1.50
36	X	306	CLA	CHC-C1C	2.16	1.42	1.38
36	i	102	CLA	CHC-C1C	2.16	1.42	1.38
36	D	309	CLA	C1C-C2C	2.16	1.48	1.44
37	L	315	KC1	C4A-C3A	2.16	1.48	1.44
36	M	314	CLA	C3B-C4B	2.16	1.49	1.42
36	D	306	CLA	MG-NB	-2.16	2.01	2.05
36	R	310	CLA	MG-ND	-2.16	2.01	2.05
36	P	308	CLA	C3B-C4B	2.16	1.49	1.42
36	a	848	CLA	C1B-C2B	2.16	1.48	1.43
36	b	816	CLA	MG-NB	-2.15	2.01	2.05
36	F	316	CLA	CMD-C2D	-2.15	1.46	1.50
36	R	319	CLA	CMD-C2D	-2.15	1.46	1.50
36	f	802	CLA	MG-NB	-2.15	2.01	2.05
36	b	810	CLA	CMC-C2C	-2.15	1.46	1.50
36	O	310	CLA	CMB-C2B	-2.15	1.46	1.50
36	F	316	CLA	C3B-C4B	2.15	1.49	1.42
36	A	310	CLA	MG-ND	-2.15	2.01	2.05
36	D	308	CLA	MG-ND	-2.15	2.01	2.05
36	E	311	CLA	C4B-NB	2.15	1.40	1.37
36	C	211	CLA	CHC-C1C	2.15	1.42	1.38
36	X	313	CLA	CMB-C2B	2.15	1.55	1.50
36	j	106	CLA	C1B-C2B	2.15	1.48	1.43
36	K	312	CLA	C3B-C4B	2.15	1.49	1.42
36	P	310	CLA	CMD-C2D	-2.15	1.46	1.50
36	B	311	CLA	C1B-NB	-2.15	1.35	1.37
36	a	827	CLA	C1B-NB	-2.15	1.35	1.37
36	F	312	CLA	C3B-C4B	2.15	1.49	1.42
36	O	309	CLA	C3B-C4B	2.15	1.49	1.42
36	a	834	CLA	C1B-C2B	2.15	1.48	1.43
35	T	303	A86	C13-C11	-2.15	1.45	1.49
36	Q	307	CLA	CMD-C2D	-2.15	1.46	1.50
36	f	805	CLA	CMB-C2B	-2.15	1.46	1.50
36	N	318	CLA	MG-NB	-2.15	2.01	2.05
36	M	308	CLA	CHC-C1C	2.15	1.42	1.38
36	f	805	CLA	CHC-C1C	2.15	1.42	1.38
36	S	318	CLA	C3B-C4B	2.15	1.49	1.42
36	O	311	CLA	CMC-C2C	-2.15	1.46	1.50
36	L	314	CLA	MG-ND	-2.15	2.01	2.05
36	D	315	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	836	CLA	CMB-C2B	-2.15	1.46	1.50
36	X	307	CLA	CAC-C3C	-2.15	1.45	1.51
37	W	213	KC1	C1B-NB	-2.15	1.35	1.37
36	T	313	CLA	CMD-C2D	-2.15	1.46	1.50
36	T	314	CLA	CMD-C2D	-2.15	1.46	1.50
37	Q	311	KC1	C1D-C2D	2.15	1.48	1.43
36	R	314	CLA	MG-NB	-2.15	2.01	2.05
36	X	310	CLA	MG-NB	-2.15	2.01	2.05
35	V	304	A86	C17-C16	-2.15	1.51	1.54
36	N	318	CLA	CMB-C2B	-2.15	1.46	1.50
35	J	302	A86	C32-C31	-2.15	1.50	1.54
36	a	807	CLA	CMB-C2B	-2.15	1.46	1.50
37	G	317	KC1	C4C-C3C	2.15	1.48	1.45
36	b	837	CLA	MG-NB	-2.15	2.01	2.05
36	W	212	CLA	C3B-C4B	2.15	1.49	1.42
36	M	306	CLA	C1B-C2B	2.15	1.48	1.43
36	F	313	CLA	CHC-C1C	2.15	1.42	1.38
36	R	316	CLA	MG-ND	-2.15	2.01	2.05
36	a	831	CLA	MG-ND	-2.15	2.01	2.05
36	D	313	CLA	CMB-C2B	-2.15	1.46	1.50
36	N	316	CLA	CMD-C2D	-2.15	1.46	1.50
36	b	809	CLA	CMC-C2C	-2.15	1.46	1.50
36	j	106	CLA	CMC-C2C	-2.15	1.46	1.50
36	P	313	CLA	CMC-C2C	-2.15	1.46	1.50
36	Q	312	CLA	CMB-C2B	-2.15	1.46	1.50
36	T	316	CLA	CMC-C2C	-2.15	1.46	1.50
35	X	304	A86	C13-C11	-2.15	1.45	1.49
36	F	312	CLA	CMD-C2D	-2.15	1.46	1.50
36	J	317	CLA	CMC-C2C	-2.15	1.46	1.50
36	M	314	CLA	CMC-C2C	-2.15	1.46	1.50
36	b	834	CLA	C1B-C2B	2.14	1.48	1.43
36	j	101	CLA	CMC-C2C	-2.14	1.46	1.50
37	T	315	KC1	CBD-CAD	-2.14	1.46	1.56
36	b	840	CLA	C4B-NB	2.14	1.40	1.37
36	I	309	CLA	CAC-C3C	-2.14	1.45	1.51
36	A	307	CLA	C3B-C4B	2.14	1.49	1.42
36	U	307	CLA	CHC-C1C	2.14	1.42	1.38
36	U	306	CLA	C1C-C2C	2.14	1.48	1.44
36	T	308	CLA	CMB-C2B	-2.14	1.46	1.50
36	D	315	CLA	C3B-C4B	2.14	1.49	1.42
36	P	302	CLA	C4B-NB	2.14	1.40	1.37
36	M	314	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	311	CLA	C3B-C4B	2.14	1.49	1.42
36	i	102	CLA	C3B-C4B	2.14	1.49	1.42
36	B	305	CLA	CMD-C2D	-2.14	1.46	1.50
36	E	314	CLA	CMB-C2B	-2.14	1.46	1.50
36	L	312	CLA	CMD-C2D	-2.14	1.46	1.50
36	R	313	CLA	CMB-C2B	-2.14	1.46	1.50
36	a	812	CLA	C3B-C4B	2.14	1.49	1.42
36	H	318	CLA	CMC-C2C	-2.14	1.46	1.50
36	U	308	CLA	CMB-C2B	-2.14	1.46	1.50
36	X	309	CLA	C3D-C4D	2.14	1.49	1.44
36	M	309	CLA	CMB-C2B	-2.14	1.46	1.50
36	V	308	CLA	CMB-C2B	-2.14	1.46	1.50
36	b	823	CLA	C1B-C2B	2.14	1.48	1.43
37	T	310	KC1	C3D-CAD	2.14	1.52	1.45
36	G	309	CLA	CHC-C1C	2.14	1.42	1.38
35	S	308	A86	C32-C31	-2.14	1.51	1.54
36	D	311	CLA	C3B-C4B	2.14	1.49	1.42
36	j	106	CLA	C3B-C4B	2.14	1.49	1.42
36	l	201	CLA	CHC-C1C	2.14	1.42	1.38
36	J	315	CLA	CMD-C2D	-2.14	1.46	1.50
36	W	214	CLA	MG-NB	-2.14	2.01	2.05
36	O	314	CLA	CMB-C2B	-2.14	1.46	1.50
36	U	305	CLA	C3B-C4B	2.14	1.49	1.42
36	b	835	CLA	C1B-C2B	2.14	1.48	1.43
35	K	301	A86	C32-C31	-2.14	1.51	1.54
36	A	306	CLA	C1C-C2C	2.14	1.48	1.44
36	S	310	CLA	CMD-C2D	-2.14	1.46	1.50
36	E	314	CLA	C1B-NB	-2.14	1.35	1.37
35	F	304	A86	C32-C31	-2.14	1.51	1.54
36	I	311	CLA	CHC-C1C	2.14	1.42	1.38
36	J	317	CLA	CMB-C2B	-2.14	1.46	1.50
36	W	208	CLA	CMD-C2D	-2.14	1.46	1.50
37	W	213	KC1	C1D-ND	-2.14	1.35	1.37
36	M	314	CLA	CHC-C1C	2.14	1.42	1.38
36	b	801	CLA	C1B-C2B	2.14	1.48	1.43
36	O	309	CLA	CHC-C1C	2.14	1.42	1.38
36	J	310	CLA	CMB-C2B	-2.14	1.46	1.50
36	W	216	CLA	CMD-C2D	-2.14	1.46	1.50
36	b	807	CLA	MG-NB	-2.14	2.01	2.05
36	a	812	CLA	C1B-NB	-2.14	1.35	1.37
36	I	306	CLA	MG-NB	-2.14	2.01	2.05
36	a	822	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	319	CLA	CMB-C2B	-2.14	1.46	1.50
36	S	314	CLA	MG-NB	-2.14	2.01	2.05
36	a	827	CLA	CMB-C2B	-2.14	1.46	1.50
36	O	309	CLA	MG-ND	-2.14	2.01	2.05
36	V	313	CLA	MG-ND	-2.14	2.01	2.05
36	a	803	CLA	C1B-NB	-2.14	1.35	1.37
36	b	809	CLA	C1B-NB	-2.14	1.35	1.37
35	H	304	A86	C32-C31	-2.14	1.51	1.54
36	D	315	CLA	CMD-C2D	-2.14	1.46	1.50
36	D	308	CLA	C1B-C2B	2.14	1.48	1.43
36	J	312	CLA	C3B-C4B	2.14	1.49	1.42
36	T	314	CLA	CHC-C1C	2.14	1.42	1.38
37	O	313	KC1	C1D-C2D	2.14	1.48	1.43
36	b	807	CLA	C3B-C4B	2.14	1.49	1.42
37	F	308	KC1	CBD-CAD	-2.14	1.46	1.56
37	G	308	KC1	CBD-CAD	-2.14	1.46	1.56
36	L	312	CLA	CMC-C2C	-2.13	1.46	1.50
36	F	309	CLA	C1B-C2B	2.13	1.48	1.43
37	O	315	KC1	C1D-C2D	2.13	1.48	1.43
36	F	309	CLA	CMB-C2B	-2.13	1.46	1.50
36	L	309	CLA	CMD-C2D	-2.13	1.46	1.50
36	S	315	CLA	CMB-C2B	-2.13	1.46	1.50
36	R	315	CLA	MG-NB	-2.13	2.01	2.05
36	C	214	CLA	CMC-C2C	-2.13	1.46	1.50
36	f	805	CLA	CMC-C2C	-2.13	1.46	1.50
36	b	823	CLA	C1B-NB	-2.13	1.35	1.37
44	b	843	BCR	C33-C5	-2.13	1.47	1.50
36	b	822	CLA	C1B-C2B	2.13	1.48	1.43
36	a	824	CLA	CMB-C2B	-2.13	1.46	1.50
36	W	211	CLA	C3B-C4B	2.13	1.49	1.42
37	N	314	KC1	C3B-C4B	2.13	1.49	1.46
37	J	314	KC1	C1D-ND	-2.13	1.35	1.37
36	S	314	CLA	CMB-C2B	-2.13	1.46	1.50
36	X	313	CLA	CMD-C2D	-2.13	1.46	1.50
36	b	835	CLA	MG-NB	-2.13	2.01	2.05
36	S	314	CLA	CMD-C2D	-2.13	1.46	1.50
37	H	313	KC1	O2A-CGA	-2.13	1.25	1.30
36	G	315	CLA	C1B-C2B	2.13	1.48	1.43
37	S	316	KC1	C1D-C2D	2.13	1.48	1.43
36	P	308	CLA	CMC-C2C	-2.13	1.46	1.50
36	W	212	CLA	CMB-C2B	-2.13	1.46	1.50
36	S	311	CLA	C1B-C2B	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	X	305	A86	C13-C11	-2.13	1.45	1.49
36	S	319	CLA	CMB-C2B	-2.13	1.46	1.50
36	K	313	CLA	C3B-C4B	2.13	1.48	1.42
36	F	312	CLA	MG-NB	-2.13	2.01	2.05
36	b	831	CLA	CMC-C2C	-2.13	1.46	1.50
36	R	322	CLA	C3B-C4B	2.13	1.48	1.42
36	a	802	CLA	MG-NB	-2.13	2.01	2.05
44	m	101	BCR	C38-C26	-2.13	1.47	1.50
44	h	201	BCR	C38-C26	-2.13	1.47	1.50
36	a	830	CLA	C1D-C2D	2.13	1.49	1.45
36	a	837	CLA	C4B-NB	2.13	1.40	1.37
36	b	823	CLA	C3B-C4B	2.13	1.48	1.42
36	a	819	CLA	C3C-C2C	2.13	1.41	1.36
36	b	838	CLA	CMC-C2C	-2.13	1.46	1.50
36	L	309	CLA	C3B-C4B	2.13	1.48	1.42
35	C	204	A86	C9-C10	2.13	1.49	1.43
36	H	317	CLA	CMC-C2C	-2.13	1.46	1.50
36	f	802	CLA	CMC-C2C	-2.13	1.46	1.50
36	J	307	CLA	C1B-C2B	2.13	1.48	1.43
36	P	312	CLA	CMC-C2C	-2.13	1.46	1.50
36	B	305	CLA	MG-NB	-2.13	2.01	2.05
36	a	810	CLA	MG-NB	-2.13	2.01	2.05
36	H	312	CLA	MG-NB	-2.13	2.01	2.05
36	W	218	CLA	MG-NB	-2.13	2.01	2.05
36	G	309	CLA	CMB-C2B	-2.12	1.46	1.50
36	S	310	CLA	CMB-C2B	-2.12	1.46	1.50
36	J	312	CLA	MG-NB	-2.12	2.01	2.05
36	A	308	CLA	CMD-C2D	-2.12	1.46	1.50
36	W	216	CLA	CMC-C2C	-2.12	1.46	1.50
36	a	803	CLA	MG-ND	-2.12	2.01	2.05
36	H	308	CLA	CMC-C2C	-2.12	1.46	1.50
36	M	311	CLA	MG-ND	-2.12	2.01	2.05
36	U	305	CLA	CHC-C1C	2.12	1.42	1.38
36	E	315	CLA	C1C-C2C	2.12	1.48	1.44
36	H	310	CLA	C3B-C4B	2.12	1.48	1.42
36	L	312	CLA	CMB-C2B	-2.12	1.46	1.50
36	l	202	CLA	CMC-C2C	-2.12	1.46	1.50
36	L	309	CLA	CHC-C1C	2.12	1.42	1.38
36	a	835	CLA	CHC-C1C	2.12	1.42	1.38
36	P	316	CLA	CMB-C2B	-2.12	1.46	1.50
36	C	210	CLA	CMB-C2B	-2.12	1.46	1.50
36	L	313	CLA	CMC-C2C	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	320	CLA	MG-NB	-2.12	2.01	2.05
37	J	314	KC1	O2A-CGA	-2.12	1.25	1.30
36	O	307	CLA	CMB-C2B	-2.12	1.46	1.50
36	H	306	CLA	CMD-C2D	-2.12	1.46	1.50
36	L	320	CLA	CMC-C2C	-2.12	1.46	1.50
36	M	306	CLA	CMC-C2C	-2.12	1.46	1.50
36	a	836	CLA	O2D-CED	-2.12	1.40	1.45
36	W	209	CLA	CMD-C2D	-2.12	1.46	1.50
36	O	314	CLA	CMD-C2D	-2.12	1.46	1.50
36	N	317	CLA	C3B-C4B	2.12	1.48	1.42
36	N	307	CLA	MG-NB	-2.12	2.01	2.05
37	G	308	KC1	C4B-NB	-2.12	1.35	1.37
36	D	312	CLA	CHC-C1C	2.12	1.42	1.38
36	S	317	CLA	CHC-C1C	2.12	1.42	1.38
36	J	308	CLA	MG-NB	-2.12	2.01	2.05
36	V	314	CLA	C4D-CHA	2.12	1.45	1.38
36	U	308	CLA	C3B-C4B	2.12	1.48	1.42
36	a	811	CLA	C1B-NB	-2.12	1.35	1.37
36	W	209	CLA	MG-NB	-2.12	2.01	2.05
36	U	306	CLA	MG-NB	-2.12	2.01	2.05
36	G	310	CLA	CHC-C1C	2.12	1.42	1.38
36	H	308	CLA	CHC-C1C	2.12	1.42	1.38
36	N	307	CLA	CHC-C1C	2.12	1.42	1.38
37	M	317	KC1	C4B-NB	-2.12	1.35	1.37
37	N	314	KC1	C1D-ND	-2.12	1.35	1.37
36	b	813	CLA	CHC-C1C	2.12	1.42	1.38
36	a	802	CLA	C3B-C4B	2.12	1.48	1.42
36	L	312	CLA	MG-NB	-2.12	2.01	2.05
36	A	306	CLA	MG-ND	-2.12	2.01	2.05
36	S	311	CLA	MG-ND	-2.12	2.01	2.05
36	G	311	CLA	C4B-NB	2.12	1.40	1.37
36	D	315	CLA	CMB-C2B	-2.12	1.46	1.50
36	l	206	CLA	CMC-C2C	-2.12	1.46	1.50
37	Q	313	KC1	C4A-C3A	2.12	1.48	1.44
36	b	828	CLA	C1B-NB	-2.12	1.35	1.37
36	H	314	CLA	C1B-NB	-2.11	1.35	1.37
36	G	310	CLA	MG-ND	-2.11	2.01	2.05
36	A	305	CLA	C3B-C4B	2.11	1.48	1.42
36	N	308	CLA	C1B-C2B	2.11	1.48	1.43
36	I	313	CLA	CMB-C2B	-2.11	1.46	1.50
44	m	101	BCR	C33-C5	-2.11	1.47	1.50
36	b	817	CLA	C3B-C4B	2.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	313	CLA	MG-ND	-2.11	2.01	2.05
36	G	310	CLA	CMB-C2B	-2.11	1.46	1.50
36	h	203	CLA	CMC-C2C	-2.11	1.46	1.50
36	W	210	CLA	MG-ND	-2.11	2.01	2.05
36	B	306	CLA	MG-NB	-2.11	2.01	2.05
36	b	831	CLA	CHC-C1C	2.11	1.42	1.38
36	Q	305	CLA	CMB-C2B	-2.11	1.46	1.50
36	R	315	CLA	CHC-C1C	2.11	1.42	1.38
36	b	821	CLA	C3B-C4B	2.11	1.48	1.42
36	P	319	CLA	CHC-C1C	2.11	1.42	1.38
44	b	844	BCR	C27-C26	-2.11	1.47	1.51
36	S	313	CLA	CMD-C2D	-2.11	1.46	1.50
44	l	203	BCR	C38-C26	-2.11	1.47	1.50
36	J	308	CLA	C3B-C4B	2.11	1.48	1.42
36	a	805	CLA	C4B-NB	2.11	1.40	1.37
36	a	828	CLA	C4B-NB	2.11	1.40	1.37
36	a	803	CLA	MG-NB	-2.11	2.01	2.05
36	V	309	CLA	C3B-C4B	2.11	1.48	1.42
36	C	212	CLA	C4B-NB	2.11	1.40	1.37
36	a	824	CLA	C1D-ND	2.11	1.40	1.37
36	a	826	CLA	C4B-NB	2.11	1.40	1.37
36	S	319	CLA	CMC-C2C	-2.11	1.46	1.50
36	S	321	CLA	CMC-C2C	-2.11	1.46	1.50
36	H	316	CLA	MG-NB	-2.11	2.01	2.05
36	b	823	CLA	C4B-NB	2.11	1.40	1.37
36	M	316	CLA	CMB-C2B	-2.11	1.46	1.50
36	G	313	CLA	C1B-C2B	2.11	1.48	1.43
36	T	308	CLA	MG-NB	-2.11	2.01	2.05
36	P	301	CLA	CHC-C1C	2.11	1.42	1.38
36	a	822	CLA	CHC-C1C	2.11	1.42	1.38
36	G	314	CLA	CMC-C2C	-2.11	1.46	1.50
37	O	313	KC1	C4A-C3A	2.11	1.48	1.44
36	W	206	CLA	CHC-C1C	2.11	1.42	1.38
36	a	827	CLA	CHC-C1C	2.11	1.42	1.38
36	S	309	CLA	CMC-C2C	-2.11	1.46	1.50
36	a	835	CLA	MG-ND	-2.11	2.01	2.05
36	b	820	CLA	MG-ND	-2.11	2.01	2.05
36	L	308	CLA	MG-NA	2.11	2.11	2.06
36	X	309	CLA	CMB-C2B	-2.11	1.46	1.50
36	X	306	CLA	MG-NB	-2.11	2.01	2.05
36	J	309	CLA	CHC-C1C	2.11	1.42	1.38
36	J	308	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	312	CLA	C1B-C2B	2.11	1.48	1.43
37	R	317	KC1	C4C-C3C	2.11	1.48	1.45
36	H	311	CLA	CHC-C1C	2.10	1.42	1.38
36	a	803	CLA	CMB-C2B	-2.10	1.46	1.50
36	T	312	CLA	CHC-C1C	2.10	1.42	1.38
36	P	319	CLA	MG-NA	2.10	2.11	2.06
36	b	822	CLA	C4B-NB	2.10	1.40	1.37
36	C	207	CLA	CHC-C4B	2.10	1.44	1.39
36	D	306	CLA	MG-ND	-2.10	2.01	2.05
36	b	806	CLA	MG-ND	-2.10	2.01	2.05
36	P	311	CLA	CHC-C1C	2.10	1.42	1.38
37	P	315	KC1	C4C-C3C	2.10	1.48	1.45
36	K	311	CLA	CMC-C2C	-2.10	1.46	1.50
36	b	807	CLA	CMB-C2B	-2.10	1.46	1.50
36	P	310	CLA	C3B-C4B	2.10	1.48	1.42
36	j	101	CLA	C3B-C4B	2.10	1.48	1.42
36	a	807	CLA	C4B-NB	2.10	1.40	1.37
36	S	314	CLA	CHC-C1C	2.10	1.42	1.38
36	O	308	CLA	C3B-C4B	2.10	1.48	1.42
36	F	316	CLA	CMB-C2B	-2.10	1.46	1.50
36	a	815	CLA	C1B-NB	-2.10	1.35	1.37
36	P	318	CLA	CMC-C2C	-2.10	1.46	1.50
36	a	838	CLA	CMC-C2C	-2.10	1.46	1.50
37	M	313	KC1	O2A-CGA	-2.10	1.25	1.30
36	N	309	CLA	CMC-C2C	-2.10	1.46	1.50
36	b	835	CLA	CMC-C2C	-2.10	1.46	1.50
36	a	848	CLA	C3B-C4B	2.10	1.48	1.42
36	Q	306	CLA	MG-ND	-2.10	2.01	2.05
36	U	309	CLA	MG-NB	-2.10	2.01	2.05
36	H	312	CLA	MG-ND	-2.10	2.01	2.05
36	Q	312	CLA	CMC-C2C	-2.10	1.46	1.50
35	O	319	A86	C13-C11	-2.10	1.45	1.49
36	f	804	CLA	C1C-C2C	2.10	1.48	1.44
44	b	846	BCR	C38-C26	-2.10	1.47	1.50
36	S	309	CLA	CMB-C2B	-2.10	1.46	1.50
36	b	824	CLA	C4C-C3C	2.10	1.48	1.45
44	b	844	BCR	C38-C26	-2.10	1.47	1.50
36	a	804	CLA	C1B-NB	-2.10	1.35	1.37
36	H	311	CLA	C3B-C4B	2.10	1.48	1.42
36	J	313	CLA	CHC-C1C	2.10	1.42	1.38
36	b	831	CLA	MG-ND	-2.10	2.01	2.05
36	a	816	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	204	CLA	MG-NB	-2.10	2.01	2.05
36	H	311	CLA	CMB-C2B	-2.10	1.46	1.50
36	M	308	CLA	CMC-C2C	-2.10	1.46	1.50
36	L	313	CLA	C3B-C4B	2.10	1.48	1.42
36	V	311	CLA	CMB-C2B	-2.10	1.46	1.50
36	l	206	CLA	CHC-C1C	2.10	1.42	1.38
36	A	310	CLA	CMB-C2B	-2.10	1.46	1.50
36	J	311	CLA	CMC-C2C	-2.10	1.46	1.50
36	N	317	CLA	CHC-C1C	2.10	1.42	1.38
44	a	847	BCR	C38-C26	-2.09	1.47	1.50
36	W	208	CLA	CMB-C2B	-2.09	1.46	1.50
36	a	828	CLA	CMC-C2C	-2.09	1.46	1.50
36	b	821	CLA	CMC-C2C	-2.09	1.46	1.50
36	H	310	CLA	MG-NB	-2.09	2.01	2.05
36	b	814	CLA	MG-NB	-2.09	2.01	2.05
36	a	804	CLA	C1B-C2B	2.09	1.48	1.43
36	b	839	CLA	C1B-C2B	2.09	1.48	1.43
36	L	311	CLA	MG-ND	-2.09	2.01	2.05
44	l	203	BCR	C33-C5	-2.09	1.47	1.50
36	b	840	CLA	CMC-C2C	-2.09	1.46	1.50
37	P	315	KC1	C1D-C2D	2.09	1.48	1.43
36	W	209	CLA	CMB-C2B	-2.09	1.46	1.50
36	T	311	CLA	CMD-C2D	-2.09	1.46	1.50
36	G	312	CLA	C1B-NB	-2.09	1.35	1.37
36	L	309	CLA	CMB-C2B	-2.09	1.46	1.50
36	X	310	CLA	CHC-C1C	2.09	1.42	1.38
36	A	308	CLA	C1B-C2B	2.09	1.48	1.43
36	R	310	CLA	C1B-C2B	2.09	1.48	1.43
36	X	308	CLA	CMC-C2C	-2.09	1.46	1.50
35	A	316	A86	C32-C31	-2.09	1.51	1.54
37	O	313	KC1	C4C-C3C	2.09	1.48	1.45
36	a	807	CLA	CHC-C1C	2.09	1.42	1.38
36	f	804	CLA	C4C-C3C	2.09	1.48	1.45
36	P	310	CLA	CMC-C2C	-2.09	1.46	1.50
36	S	310	CLA	CMC-C2C	-2.09	1.46	1.50
36	I	307	CLA	C3B-C4B	2.09	1.48	1.42
36	V	310	CLA	CMC-C2C	-2.09	1.46	1.50
36	G	312	CLA	MG-ND	-2.09	2.01	2.05
36	D	306	CLA	C3B-C4B	2.09	1.48	1.42
36	V	313	CLA	C3B-C4B	2.09	1.48	1.42
36	E	312	CLA	CHC-C1C	2.09	1.42	1.38
35	T	304	A86	C13-C11	-2.09	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	314	KC1	C1B-NB	-2.09	1.35	1.37
36	S	320	CLA	CMB-C2B	-2.09	1.46	1.50
36	V	305	CLA	C3B-C4B	2.09	1.48	1.42
36	T	309	CLA	MG-NB	-2.09	2.01	2.05
35	O	302	A86	C13-C11	-2.09	1.45	1.49
36	N	313	CLA	CMD-C2D	-2.09	1.46	1.50
36	Q	307	CLA	CMC-C2C	-2.09	1.46	1.50
37	G	317	KC1	CBD-CAD	-2.09	1.47	1.56
36	Q	307	CLA	C3B-C4B	2.09	1.48	1.42
36	G	316	CLA	CHC-C1C	2.09	1.42	1.38
36	K	310	CLA	MG-ND	-2.09	2.01	2.05
36	F	314	CLA	C3B-C4B	2.09	1.48	1.42
36	M	307	CLA	C3B-C4B	2.09	1.48	1.42
36	P	318	CLA	CMB-C2B	-2.09	1.46	1.50
36	A	311	CLA	CHC-C1C	2.09	1.42	1.38
36	W	214	CLA	CMB-C2B	-2.09	1.46	1.50
36	X	310	CLA	CMB-C2B	-2.09	1.46	1.50
36	F	313	CLA	CMC-C2C	-2.09	1.46	1.50
36	O	308	CLA	CMC-C2C	-2.09	1.46	1.50
36	P	308	CLA	CMB-C2B	-2.09	1.46	1.50
36	h	203	CLA	C3B-C4B	2.09	1.48	1.42
36	F	314	CLA	CHC-C1C	2.08	1.42	1.38
36	B	307	CLA	MG-NB	-2.08	2.01	2.05
35	K	306	A86	C13-C11	-2.08	1.45	1.49
36	S	320	CLA	MG-NB	-2.08	2.01	2.05
36	C	211	CLA	C3B-C4B	2.08	1.48	1.42
36	H	314	CLA	C3B-C4B	2.08	1.48	1.42
36	V	305	CLA	CHC-C1C	2.08	1.42	1.38
36	V	307	CLA	CHC-C1C	2.08	1.42	1.38
36	B	306	CLA	C3B-C4B	2.08	1.48	1.42
36	b	816	CLA	CHC-C1C	2.08	1.42	1.38
36	C	214	CLA	C3B-C4B	2.08	1.48	1.42
36	R	311	CLA	C3B-C4B	2.08	1.48	1.42
36	K	315	CLA	CMB-C2B	-2.08	1.46	1.50
36	l	202	CLA	C1B-C2B	2.08	1.48	1.43
36	I	311	CLA	C4B-NB	2.08	1.40	1.37
36	b	815	CLA	MG-ND	-2.08	2.01	2.05
36	X	307	CLA	CMD-C2D	-2.08	1.46	1.50
36	G	319	CLA	C1B-NB	-2.08	1.35	1.37
36	a	821	CLA	C4B-NB	2.08	1.40	1.37
36	b	814	CLA	C1B-NB	-2.08	1.35	1.37
37	M	318	KC1	C4B-NB	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	313	CLA	C3B-C4B	2.08	1.48	1.42
36	M	309	CLA	CMD-C2D	-2.08	1.46	1.50
44	m	101	BCR	C4-C5	-2.08	1.47	1.51
36	N	316	CLA	CMC-C2C	-2.08	1.46	1.50
36	O	314	CLA	CMC-C2C	-2.08	1.46	1.50
36	V	313	CLA	CMD-C2D	-2.08	1.46	1.50
36	b	815	CLA	C3B-C4B	2.08	1.48	1.42
36	C	210	CLA	CMD-C2D	-2.08	1.46	1.50
36	W	214	CLA	CMD-C2D	-2.08	1.46	1.50
36	b	808	CLA	MG-NB	-2.08	2.01	2.05
36	a	837	CLA	CMC-C2C	-2.08	1.46	1.50
36	E	308	CLA	MG-ND	-2.08	2.01	2.05
36	H	308	CLA	MG-ND	-2.08	2.01	2.05
36	F	316	CLA	CMC-C2C	-2.08	1.46	1.50
36	S	320	CLA	CMC-C2C	-2.08	1.46	1.50
36	W	209	CLA	CMC-C2C	-2.08	1.46	1.50
36	I	308	CLA	C1B-NB	-2.08	1.35	1.37
36	a	817	CLA	C3B-C4B	2.08	1.48	1.42
36	a	830	CLA	C4D-CHA	2.08	1.45	1.38
36	E	314	CLA	C3B-C4B	2.08	1.48	1.42
35	T	307	A86	O4-C34	-2.08	1.41	1.46
36	E	313	CLA	MG-ND	-2.08	2.01	2.05
37	A	312	KC1	C4B-NB	-2.08	1.35	1.37
37	O	315	KC1	C4A-C3A	2.08	1.48	1.44
36	V	308	CLA	CMC-C2C	-2.08	1.46	1.50
36	a	838	CLA	C1B-C2B	2.08	1.48	1.43
36	a	820	CLA	CMC-C2C	-2.08	1.46	1.50
36	L	311	CLA	C1B-C2B	2.08	1.48	1.43
35	R	304	A86	C30-C29	-2.08	1.28	1.31
36	I	310	CLA	CMB-C2B	-2.08	1.46	1.50
36	X	307	CLA	C3B-C4B	2.08	1.48	1.42
36	E	308	CLA	CMC-C2C	-2.08	1.46	1.50
36	R	310	CLA	C1B-NB	-2.08	1.35	1.37
36	P	316	CLA	MG-NB	-2.08	2.01	2.05
37	P	315	KC1	CBD-CAD	-2.08	1.47	1.56
36	S	318	CLA	CMD-C2D	-2.08	1.46	1.50
36	G	316	CLA	C3B-C4B	2.08	1.48	1.42
36	J	307	CLA	C3B-C4B	2.08	1.48	1.42
36	J	311	CLA	MG-ND	-2.08	2.01	2.05
36	U	305	CLA	MG-NB	-2.08	2.01	2.05
37	Q	311	KC1	C4A-C3A	2.08	1.48	1.44
36	K	313	CLA	C1B-C2B	2.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	313	CLA	C4B-NB	2.07	1.40	1.37
36	G	309	CLA	C4B-NB	2.07	1.40	1.37
36	B	307	CLA	CMB-C2B	-2.07	1.46	1.50
36	V	308	CLA	CHC-C1C	2.07	1.42	1.38
36	R	315	CLA	CMB-C2B	-2.07	1.46	1.50
44	a	846	BCR	C38-C26	-2.07	1.47	1.50
36	b	829	CLA	C1B-C2B	2.07	1.48	1.43
36	J	310	CLA	C3B-C4B	2.07	1.48	1.42
36	P	301	CLA	MG-NB	-2.07	2.01	2.05
36	a	810	CLA	CHC-C1C	2.07	1.42	1.38
36	P	309	CLA	MG-ND	-2.07	2.01	2.05
36	S	317	CLA	CMD-C2D	-2.07	1.46	1.50
36	b	840	CLA	C1B-C2B	2.07	1.48	1.43
36	E	316	CLA	C3B-C4B	2.07	1.48	1.42
36	R	320	CLA	CHC-C1C	2.07	1.42	1.38
36	G	309	CLA	O2A-CGA	2.07	1.39	1.33
36	a	814	CLA	C4B-NB	2.07	1.40	1.37
36	H	315	CLA	CMC-C2C	-2.07	1.46	1.50
36	a	813	CLA	CMB-C2B	-2.07	1.46	1.50
36	a	820	CLA	C1B-C2B	2.07	1.48	1.43
36	R	316	CLA	C3B-C4B	2.07	1.48	1.42
36	L	316	CLA	CMD-C2D	-2.07	1.46	1.50
36	B	308	CLA	CMB-C2B	-2.07	1.46	1.50
36	l	201	CLA	CMC-C2C	-2.07	1.46	1.50
36	V	313	CLA	CHC-C1C	2.07	1.42	1.38
37	T	315	KC1	O2A-CGA	-2.07	1.25	1.30
36	b	807	CLA	CHC-C1C	2.07	1.42	1.38
35	P	303	A86	C37-C36	-2.07	1.49	1.52
36	D	308	CLA	C4B-NB	2.07	1.40	1.37
36	b	832	CLA	C1B-NB	-2.07	1.35	1.37
36	C	212	CLA	MG-ND	-2.07	2.01	2.05
37	W	217	KC1	CBD-CAD	-2.07	1.47	1.56
36	O	309	CLA	CMC-C2C	-2.07	1.46	1.50
35	R	309	A86	C13-C11	-2.07	1.45	1.49
36	X	312	CLA	MG-NB	-2.07	2.01	2.05
36	P	316	CLA	CMC-C2C	-2.07	1.46	1.50
36	U	313	CLA	CMC-C2C	-2.07	1.46	1.50
36	I	306	CLA	CHC-C1C	2.07	1.42	1.38
37	H	313	KC1	C1D-C2D	2.07	1.48	1.43
36	T	312	CLA	MG-NB	-2.07	2.01	2.05
37	Q	311	KC1	C1D-ND	-2.07	1.35	1.37
37	P	315	KC1	C4A-C3A	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L	315	KC1	CBD-CAD	-2.07	1.47	1.56
36	N	318	CLA	CHC-C1C	2.07	1.42	1.38
36	M	316	CLA	CMC-C2C	-2.07	1.46	1.50
36	b	840	CLA	MG-ND	-2.07	2.01	2.05
36	S	313	CLA	CHC-C1C	2.07	1.42	1.38
36	R	322	CLA	CMB-C2B	-2.07	1.46	1.50
36	l	205	CLA	MG-NB	-2.07	2.01	2.05
36	b	811	CLA	MG-NB	-2.06	2.01	2.05
36	K	309	CLA	CMC-C2C	-2.06	1.46	1.50
36	N	315	CLA	CMD-C2D	-2.06	1.46	1.50
36	H	308	CLA	C3B-C4B	2.06	1.48	1.42
36	K	315	CLA	CHC-C1C	2.06	1.42	1.38
36	O	311	CLA	C3B-C4B	2.06	1.48	1.42
36	a	825	CLA	C1B-C2B	2.06	1.48	1.43
35	h	204	A86	C32-C31	-2.06	1.51	1.54
36	Q	314	CLA	CMD-C2D	-2.06	1.46	1.50
36	W	211	CLA	CMB-C2B	-2.06	1.46	1.50
36	D	312	CLA	C3B-C4B	2.06	1.48	1.42
36	C	208	CLA	C1B-NB	-2.06	1.35	1.37
36	U	311	CLA	C1B-NB	-2.06	1.35	1.37
36	F	312	CLA	CMB-C2B	-2.06	1.46	1.50
36	O	306	CLA	CMB-C2B	-2.06	1.46	1.50
36	T	311	CLA	CMB-C2B	-2.06	1.46	1.50
35	L	319	A86	C13-C11	-2.06	1.45	1.49
36	J	310	CLA	CHC-C1C	2.06	1.42	1.38
44	i	103	BCR	C33-C5	-2.06	1.47	1.50
36	U	307	CLA	CMC-C2C	-2.06	1.46	1.50
36	G	319	CLA	C1A-CHA	2.06	1.51	1.43
36	a	814	CLA	MG-NB	-2.06	2.01	2.05
36	N	312	CLA	CHC-C1C	2.06	1.42	1.38
36	R	318	CLA	CMD-C2D	-2.06	1.46	1.50
37	M	317	KC1	C4C-C3C	2.06	1.48	1.45
37	N	314	KC1	C4A-C3A	2.06	1.48	1.44
37	O	313	KC1	CBD-CAD	-2.06	1.47	1.56
37	O	315	KC1	C1D-ND	-2.06	1.35	1.37
37	O	315	KC1	CBD-CAD	-2.06	1.47	1.56
36	a	815	CLA	C1B-C2B	2.06	1.48	1.43
37	S	316	KC1	CBD-CAD	-2.06	1.47	1.56
36	R	320	CLA	CMC-C2C	-2.06	1.46	1.50
36	C	205	CLA	C3B-C4B	2.06	1.48	1.42
36	H	314	CLA	MG-ND	-2.06	2.01	2.05
36	Q	312	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	311	KC1	CBD-CAD	-2.06	1.47	1.56
36	R	312	CLA	CMC-C2C	-2.06	1.46	1.50
35	P	303	A86	C13-C11	-2.06	1.45	1.49
36	F	317	CLA	C4B-NB	-2.06	1.35	1.37
36	T	311	CLA	CHC-C4B	-2.06	1.34	1.39
36	F	311	CLA	C3B-C4B	2.06	1.48	1.42
36	S	310	CLA	C3B-C4B	2.06	1.48	1.42
35	R	305	A86	C32-C31	-2.06	1.51	1.54
36	H	306	CLA	CMC-C2C	-2.06	1.46	1.50
36	R	313	CLA	CMC-C2C	-2.06	1.46	1.50
35	F	305	A86	C37-C36	-2.06	1.49	1.52
37	T	315	KC1	C1D-ND	-2.06	1.35	1.37
36	C	207	CLA	C1C-C2C	2.06	1.48	1.44
36	F	310	CLA	C3B-C4B	2.06	1.48	1.42
36	T	312	CLA	CMD-C2D	-2.05	1.46	1.50
36	T	313	CLA	MG-NB	-2.05	2.01	2.05
37	N	314	KC1	CBD-CAD	-2.05	1.47	1.56
36	K	310	CLA	C4C-C3C	2.05	1.48	1.45
36	S	309	CLA	MG-ND	-2.05	2.01	2.05
36	A	308	CLA	CMB-C2B	-2.05	1.46	1.50
36	I	310	CLA	CMC-C2C	-2.05	1.46	1.50
36	a	815	CLA	MG-NB	-2.05	2.01	2.05
36	K	308	CLA	CMD-C2D	-2.05	1.46	1.50
36	Q	308	CLA	CHC-C1C	2.05	1.42	1.38
40	b	849	DGD	C1E-C2E	2.05	1.58	1.52
36	W	210	CLA	CMD-C2D	-2.05	1.46	1.50
36	b	819	CLA	C3B-C4B	2.05	1.48	1.42
36	W	215	CLA	MG-ND	-2.05	2.01	2.05
37	K	314	KC1	C4A-C3A	2.05	1.48	1.44
36	H	318	CLA	CAA-C2A	-2.05	1.50	1.54
35	M	305	A86	C13-C11	-2.05	1.45	1.49
36	M	314	CLA	CMB-C2B	-2.05	1.46	1.50
37	W	213	KC1	O2A-CGA	-2.05	1.25	1.30
36	H	306	CLA	CHC-C1C	2.05	1.42	1.38
36	b	806	CLA	CMB-C2B	-2.05	1.46	1.50
37	Q	313	KC1	CBD-CAD	-2.05	1.47	1.56
36	D	311	CLA	MG-NB	-2.05	2.01	2.05
36	F	311	CLA	MG-NB	-2.05	2.01	2.05
40	b	849	DGD	C2A-C1A	-2.05	1.44	1.50
36	L	316	CLA	CMB-C2B	-2.05	1.46	1.50
36	a	810	CLA	CMC-C2C	-2.05	1.46	1.50
36	b	821	CLA	MG-ND	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	212	CLA	CMB-C2B	-2.05	1.46	1.50
36	C	210	CLA	CHC-C1C	2.05	1.42	1.38
36	L	320	CLA	C3B-C4B	2.05	1.48	1.42
36	b	822	CLA	C3B-C4B	2.05	1.48	1.42
36	G	309	CLA	CMC-C2C	-2.05	1.46	1.50
36	N	312	CLA	CMB-C2B	-2.05	1.46	1.50
36	a	831	CLA	C1B-NB	-2.05	1.35	1.37
36	A	313	CLA	C3B-C4B	2.05	1.48	1.42
36	I	309	CLA	CMB-C2B	-2.05	1.46	1.50
36	N	315	CLA	CMB-C2B	-2.05	1.46	1.50
37	Q	311	KC1	CBD-CAD	-2.05	1.47	1.56
36	R	312	CLA	C3B-C4B	2.05	1.48	1.42
36	C	214	CLA	CHC-C1C	2.05	1.42	1.38
36	J	309	CLA	C3B-C4B	2.05	1.48	1.42
36	P	311	CLA	CMC-C2C	-2.05	1.46	1.50
36	T	311	CLA	C4C-C3C	-2.05	1.41	1.45
36	b	809	CLA	CHC-C1C	2.05	1.42	1.38
36	b	807	CLA	C1B-NB	-2.05	1.35	1.37
36	O	307	CLA	MG-ND	-2.05	2.01	2.05
36	a	827	CLA	MG-NB	-2.05	2.01	2.05
36	a	834	CLA	C1B-NB	-2.05	1.35	1.37
36	L	313	CLA	CMB-C2B	-2.05	1.46	1.50
36	T	308	CLA	CMC-C2C	-2.05	1.46	1.50
36	a	809	CLA	C4B-NB	2.04	1.40	1.37
34	I	303	DD6	C36-C31	-2.04	1.32	1.35
35	T	304	A86	C15-C16	-2.04	1.52	1.55
36	R	316	CLA	CHC-C1C	2.04	1.42	1.38
36	O	314	CLA	MG-NB	-2.04	2.01	2.05
37	M	313	KC1	C1D-C2D	2.04	1.47	1.43
36	S	317	CLA	CMB-C2B	-2.04	1.46	1.50
36	T	308	CLA	CMD-C2D	-2.04	1.46	1.50
36	M	312	CLA	C3B-C4B	2.04	1.48	1.42
36	D	310	CLA	CMB-C2B	-2.04	1.46	1.50
36	J	307	CLA	CMC-C2C	-2.04	1.46	1.50
36	a	803	CLA	C1B-C2B	2.04	1.47	1.43
35	B	301	A86	C32-C31	-2.04	1.51	1.54
36	W	206	CLA	CMD-C2D	-2.04	1.46	1.50
36	a	834	CLA	CMC-C2C	-2.04	1.46	1.50
36	W	208	CLA	O2A-CGA	2.04	1.37	1.30
36	N	317	CLA	CMD-C2D	-2.04	1.46	1.50
36	L	314	CLA	C3B-C4B	2.04	1.48	1.42
36	D	306	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	831	CLA	C1B-C2B	2.04	1.47	1.43
36	C	206	CLA	C3B-C4B	2.04	1.48	1.42
36	F	314	CLA	C1B-NB	-2.04	1.35	1.37
36	a	808	CLA	C1B-NB	-2.04	1.35	1.37
36	a	841	CLA	MG-NB	-2.04	2.01	2.05
36	b	819	CLA	CHC-C1C	2.04	1.42	1.38
36	a	820	CLA	MG-ND	-2.04	2.01	2.05
36	D	309	CLA	C4C-C3C	2.04	1.48	1.45
37	R	317	KC1	CBD-CAD	-2.04	1.47	1.56
36	a	825	CLA	C1B-NB	-2.04	1.35	1.37
36	l	205	CLA	CHC-C4B	2.04	1.44	1.39
36	S	312	CLA	CMB-C2B	-2.03	1.46	1.50
36	b	811	CLA	C1B-NB	-2.03	1.35	1.37
36	I	308	CLA	MG-ND	-2.03	2.01	2.05
36	B	307	CLA	CMC-C2C	-2.03	1.46	1.50
36	F	314	CLA	CMC-C2C	-2.03	1.46	1.50
36	J	309	CLA	CMC-C2C	-2.03	1.46	1.50
36	a	814	CLA	CHC-C4B	-2.03	1.34	1.39
36	H	310	CLA	C1B-NB	-2.03	1.35	1.37
36	b	840	CLA	C1B-NB	-2.03	1.35	1.37
36	I	305	CLA	CHC-C1C	2.03	1.42	1.38
36	R	312	CLA	CMB-C2B	-2.03	1.46	1.50
36	S	314	CLA	O1D-CGD	2.03	1.26	1.21
36	C	210	CLA	MG-NB	-2.03	2.01	2.05
35	G	304	A86	O4-C34	-2.03	1.41	1.46
36	Q	314	CLA	CMC-C2C	-2.03	1.46	1.50
35	H	301	A86	C30-C31	-2.03	1.28	1.30
36	I	310	CLA	MG-ND	-2.03	2.01	2.05
44	b	847	BCR	C33-C5	-2.03	1.47	1.50
36	R	321	CLA	CMC-C2C	-2.03	1.46	1.50
36	a	805	CLA	MG-ND	-2.03	2.01	2.05
36	M	311	CLA	CMC-C2C	-2.03	1.46	1.50
36	R	318	CLA	MG-NB	-2.03	2.01	2.05
40	b	849	DGD	O3D-C3D	-2.03	1.37	1.43
35	A	302	A86	C13-C11	-2.03	1.45	1.49
36	U	313	CLA	CMB-C2B	-2.03	1.46	1.50
44	b	843	BCR	C38-C26	-2.03	1.47	1.50
36	I	307	CLA	C1B-NB	-2.03	1.35	1.37
36	F	312	CLA	CHC-C1C	2.03	1.42	1.38
36	b	802	CLA	MG-NB	-2.03	2.01	2.05
35	Q	316	A86	C20-C15	2.03	1.50	1.48
36	G	311	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	309	CLA	CMB-C2B	-2.03	1.46	1.50
36	O	312	CLA	C2A-C3A	2.03	1.58	1.53
36	a	805	CLA	C1B-NB	-2.03	1.35	1.37
36	a	807	CLA	C3B-C4B	2.03	1.48	1.42
37	O	313	KC1	O2A-CGA	-2.03	1.25	1.30
36	b	839	CLA	CHC-C1C	2.03	1.42	1.38
37	Q	313	KC1	C4C-C3C	2.03	1.48	1.45
37	D	314	KC1	O2A-CGA	-2.03	1.25	1.30
36	a	832	CLA	C1B-NB	-2.03	1.35	1.37
36	b	805	CLA	C4B-NB	2.03	1.40	1.37
35	G	304	A86	C30-C31	-2.03	1.28	1.30
36	R	321	CLA	MG-ND	-2.03	2.01	2.05
37	C	213	KC1	O2A-CGA	-2.03	1.25	1.30
36	J	307	CLA	C1B-NB	-2.03	1.35	1.37
36	S	312	CLA	CMC-C2C	-2.03	1.46	1.50
37	O	315	KC1	O2A-CGA	-2.03	1.25	1.30
36	I	310	CLA	CHC-C1C	2.03	1.42	1.38
36	T	316	CLA	CHC-C1C	2.03	1.42	1.38
36	N	310	CLA	C1B-C2B	2.03	1.47	1.43
35	E	302	A86	C32-C31	-2.03	1.51	1.54
36	M	308	CLA	MG-ND	-2.03	2.01	2.05
36	A	314	CLA	CMB-C2B	-2.03	1.46	1.50
36	S	318	CLA	CMB-C2B	-2.03	1.46	1.50
37	U	312	KC1	O2A-CGA	-2.03	1.25	1.30
36	N	315	CLA	MG-NB	-2.03	2.01	2.05
36	X	315	CLA	CMD-C2D	-2.03	1.46	1.50
36	U	308	CLA	CMC-C2C	-2.03	1.46	1.50
36	a	834	CLA	CHC-C1C	2.03	1.42	1.38
36	F	314	CLA	MG-ND	-2.02	2.01	2.05
36	b	816	CLA	C1B-NB	-2.02	1.35	1.37
36	G	315	CLA	MG-ND	-2.02	2.01	2.05
36	I	309	CLA	MG-NB	-2.02	2.01	2.05
36	S	319	CLA	MG-ND	-2.02	2.01	2.05
36	b	832	CLA	MG-ND	-2.02	2.01	2.05
36	P	318	CLA	CHC-C1C	2.02	1.42	1.38
36	a	838	CLA	C1D-ND	2.02	1.40	1.37
36	Q	310	CLA	MG-NA	2.02	2.11	2.06
36	W	218	CLA	MG-ND	-2.02	2.01	2.05
36	b	827	CLA	MG-NB	-2.02	2.01	2.05
36	V	306	CLA	MG-NB	-2.02	2.01	2.05
36	B	308	CLA	CMC-C2C	-2.02	1.46	1.50
36	S	321	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	310	CLA	C1B-NB	-2.02	1.35	1.37
44	a	844	BCR	C33-C5	-2.02	1.47	1.50
37	Q	311	KC1	C4C-C3C	2.02	1.48	1.45
36	S	321	CLA	MG-NB	-2.02	2.01	2.05
36	D	310	CLA	CHC-C1C	2.02	1.42	1.38
36	V	309	CLA	CHC-C1C	2.02	1.42	1.38
36	j	102	CLA	MG-ND	-2.02	2.01	2.05
37	V	312	KC1	C4B-NB	-2.02	1.35	1.37
37	S	316	KC1	O2A-CGA	-2.02	1.25	1.30
36	J	309	CLA	C1B-NB	-2.02	1.35	1.37
36	R	322	CLA	CMC-C2C	-2.02	1.46	1.50
36	T	309	CLA	CMB-C2B	-2.02	1.46	1.50
36	b	826	CLA	C4B-NB	2.02	1.40	1.37
36	G	310	CLA	C1B-NB	-2.02	1.35	1.37
36	X	309	CLA	CMD-C2D	-2.02	1.46	1.50
36	b	818	CLA	CMB-C2B	-2.02	1.46	1.50
36	F	313	CLA	C1B-C2B	2.02	1.47	1.43
37	O	315	KC1	C4C-C3C	2.02	1.48	1.45
36	L	316	CLA	CMC-C2C	-2.02	1.46	1.50
36	f	803	CLA	C1C-C2C	2.02	1.48	1.44
36	a	826	CLA	MG-NB	-2.02	2.01	2.05
35	W	202	A86	C33-C34	2.02	1.56	1.51
36	a	815	CLA	CHC-C1C	2.02	1.42	1.38
36	U	305	CLA	CMB-C2B	-2.02	1.46	1.50
36	W	201	CLA	MG-NB	-2.02	2.01	2.05
36	I	305	CLA	C3B-C4B	2.02	1.48	1.42
36	J	315	CLA	C3B-C4B	2.02	1.48	1.42
36	E	308	CLA	C3B-C4B	2.02	1.48	1.42
36	D	316	CLA	C3B-C4B	2.02	1.48	1.42
36	T	312	CLA	CMC-C2C	-2.02	1.46	1.50
36	N	310	CLA	C3C-C2C	2.02	1.41	1.36
35	C	204	A86	C26-C27	2.01	1.40	1.35
36	B	306	CLA	CHC-C1C	2.01	1.42	1.38
36	B	305	CLA	CMB-C2B	-2.01	1.46	1.50
36	H	307	CLA	CMC-C2C	-2.01	1.46	1.50
36	Q	308	CLA	CMC-C2C	-2.01	1.46	1.50
36	N	310	CLA	MG-ND	-2.01	2.01	2.05
36	Q	307	CLA	MG-ND	-2.01	2.01	2.05
37	T	310	KC1	C1D-ND	2.01	1.40	1.37
36	S	314	CLA	CMC-C2C	-2.01	1.46	1.50
36	a	828	CLA	CMB-C2B	-2.01	1.46	1.50
35	J	302	A86	C15-C16	-2.01	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	309	CLA	CMC-C2C	-2.01	1.46	1.50
36	D	307	CLA	C3B-C4B	2.01	1.48	1.42
36	K	308	CLA	C1B-NB	-2.01	1.35	1.37
36	T	314	CLA	CMB-C2B	-2.01	1.46	1.50
36	b	841	CLA	MG-ND	-2.01	2.01	2.05
36	V	309	CLA	MG-NB	-2.01	2.01	2.05
36	b	820	CLA	C3B-C4B	2.01	1.48	1.42
37	F	308	KC1	C1D-C2D	2.01	1.47	1.43
36	a	819	CLA	CHC-C4B	-2.01	1.34	1.39
36	A	310	CLA	C3B-C4B	2.01	1.48	1.42
36	C	205	CLA	MG-ND	-2.01	2.01	2.05
36	C	209	CLA	C3B-C4B	2.01	1.48	1.42
36	a	827	CLA	C4B-NB	2.01	1.40	1.37
37	T	310	KC1	O2A-CGA	-2.01	1.25	1.30
36	a	833	CLA	MG-ND	-2.01	2.01	2.05
36	U	307	CLA	MG-NB	-2.01	2.01	2.05
36	l	205	CLA	C1B-NB	-2.01	1.35	1.37
36	X	310	CLA	CMD-C2D	-2.01	1.46	1.50
36	b	834	CLA	C1B-NB	-2.01	1.35	1.37
36	S	320	CLA	CMD-C2D	-2.01	1.46	1.50
36	a	809	CLA	CHC-C1C	2.01	1.42	1.38
36	D	308	CLA	C3B-C4B	2.01	1.48	1.42
36	U	310	CLA	CMC-C2C	-2.01	1.46	1.50
36	R	321	CLA	C1B-C2B	2.01	1.47	1.43
37	D	314	KC1	C1D-C2D	2.01	1.47	1.43
37	W	217	KC1	O2A-CGA	-2.01	1.25	1.30
36	P	314	CLA	MG-NA	2.01	2.11	2.06
35	N	302	A86	C13-C11	-2.01	1.45	1.49
36	A	313	CLA	CHC-C1C	2.01	1.42	1.38
36	b	821	CLA	CHC-C1C	2.01	1.42	1.38
36	I	307	CLA	MG-ND	-2.01	2.01	2.05
41	F	318	LHG	P-O3	2.01	1.62	1.54
36	a	826	CLA	CHC-C1C	2.01	1.42	1.38
36	a	819	CLA	CAC-C3C	-2.01	1.46	1.51
37	Q	311	KC1	O2A-CGA	-2.01	1.25	1.30
36	S	313	CLA	CMB-C2B	-2.00	1.46	1.50
36	L	311	CLA	C1B-NB	-2.00	1.35	1.37
36	N	309	CLA	CHC-C4B	-2.00	1.34	1.39
36	a	841	CLA	C1B-NB	-2.00	1.35	1.37
36	C	211	CLA	MG-ND	-2.00	2.01	2.05
36	W	201	CLA	CHC-C1C	2.00	1.42	1.38
35	E	305	A86	C32-C31	-2.00	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	823	CLA	CHC-C1C	2.00	1.42	1.38
35	G	305	A86	C15-C16	-2.00	1.52	1.55
36	G	314	CLA	C3B-C4B	2.00	1.48	1.42
36	b	801	CLA	C3B-C4B	2.00	1.48	1.42
37	J	314	KC1	C4C-C3C	2.00	1.48	1.45
36	A	310	CLA	CHC-C1C	2.00	1.42	1.38
36	W	215	CLA	CMD-C2D	-2.00	1.46	1.50
36	U	313	CLA	CMD-C2D	-2.00	1.46	1.50
36	M	307	CLA	MG-ND	-2.00	2.01	2.05
36	a	830	CLA	MG-NB	-2.00	2.01	2.05

All (7109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	304	A86	O1-C20-C21	-50.47	58.64	115.05
36	Q	314	CLA	C4-C3-C5	-23.62	74.22	115.23
37	M	318	KC1	C1D-ND-C4D	-23.03	90.15	106.31
42	V	315	LMG	O7-C10-C11	22.21	159.53	111.48
35	A	302	A86	C33-C32-C31	-21.39	88.43	109.21
37	T	310	KC1	CHD-C4C-NC	20.49	155.17	124.31
35	H	301	A86	O4-C38-O5	20.38	162.35	122.99
42	V	315	LMG	O7-C10-O9	-19.08	79.09	123.70
37	P	315	KC1	C1A-NA-C4A	-18.84	98.08	106.68
37	O	315	KC1	C1A-NA-C4A	-18.84	98.09	106.68
37	Q	313	KC1	C1A-NA-C4A	-18.81	98.10	106.68
37	Q	311	KC1	C1A-NA-C4A	-18.81	98.10	106.68
37	O	313	KC1	C1A-NA-C4A	-18.79	98.11	106.68
37	A	312	KC1	C1A-NA-C4A	-18.39	98.29	106.68
37	A	312	KC1	CMD-C2D-C1D	-18.30	97.55	125.42
36	N	319	CLA	CMD-C2D-C1D	18.11	156.62	124.73
36	X	313	CLA	C4A-NA-C1A	17.80	114.80	106.68
36	N	319	CLA	C1D-ND-C4D	-17.61	93.96	106.31
35	H	301	A86	O4-C38-C39	-17.12	80.54	111.09
37	W	213	KC1	CMD-C2D-C1D	-17.12	99.35	125.42
36	Q	314	CLA	C4-C3-C2	-16.72	80.68	123.63
37	M	318	KC1	C3C-C4C-NC	-16.51	92.23	109.90
37	F	315	KC1	CMD-C2D-C1D	-16.46	100.35	125.42
35	R	304	A86	C29-C30-C31	-15.94	158.86	177.66
37	P	317	KC1	CMD-C2D-C1D	-15.92	101.17	125.42
35	G	304	A86	C20-O1-C15	15.70	67.78	61.03
37	L	315	KC1	CMD-C2D-C1D	-15.61	101.64	125.42
36	G	319	CLA	C4A-NA-C1A	15.57	113.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	M	313	KC1	CMD-C2D-C1D	-15.56	101.72	125.42
36	a	830	CLA	C4A-NA-C1A	15.56	113.78	106.68
35	V	303	A86	C29-C30-C31	-15.55	159.31	177.66
37	S	316	KC1	CMD-C2D-C1D	-15.54	101.76	125.42
37	J	314	KC1	CMD-C2D-C1D	-15.48	101.85	125.42
37	O	313	KC1	CMD-C2D-C1D	-15.48	101.85	125.42
37	P	315	KC1	CMD-C2D-C1D	-15.47	101.86	125.42
37	O	315	KC1	CMD-C2D-C1D	-15.46	101.88	125.42
37	Q	311	KC1	CMD-C2D-C1D	-15.45	101.89	125.42
37	Q	313	KC1	CMD-C2D-C1D	-15.42	101.94	125.42
37	O	313	KC1	C1A-C2A-C3A	-15.33	93.18	107.28
37	O	315	KC1	C1A-C2A-C3A	-15.32	93.20	107.28
37	Q	311	KC1	C1A-C2A-C3A	-15.30	93.21	107.28
37	P	315	KC1	C1A-C2A-C3A	-15.28	93.23	107.28
37	Q	313	KC1	C1A-C2A-C3A	-15.28	93.23	107.28
36	Q	314	CLA	C5-C3-C2	15.01	154.87	121.17
37	F	315	KC1	C1A-NA-C4A	-14.90	99.88	106.68
36	W	216	CLA	C4A-NA-C1A	14.86	113.46	106.68
37	M	318	KC1	C1A-C2A-C3A	14.83	120.91	107.28
35	V	304	A86	C20-O1-C15	14.81	67.40	61.03
35	H	301	A86	C29-C30-C31	-14.68	160.34	177.66
37	T	310	KC1	C3C-C4C-NC	-14.54	94.34	109.90
37	F	308	KC1	CMD-C2D-C1D	-14.32	103.61	125.42
35	N	301	A86	C20-O1-C15	14.29	67.17	61.03
35	S	301	A86	C20-O1-C15	14.24	67.15	61.03
37	K	314	KC1	CMD-C2D-C1D	-14.21	103.78	125.42
36	N	319	CLA	CHD-C1D-ND	-14.17	104.86	124.80
35	F	307	A86	C41-C32-C31	14.01	123.01	110.47
35	A	302	A86	C40-C32-C31	13.98	122.98	110.47
37	T	310	KC1	C1A-C2A-C3A	13.81	119.97	107.28
37	A	312	KC1	C1A-C2A-C3A	-13.79	94.61	107.28
35	F	307	A86	C33-C32-C31	-13.37	96.21	109.21
37	T	310	KC1	CHD-C4C-C3C	-13.29	100.73	125.23
35	T	305	A86	C29-C30-C31	-13.21	162.07	177.66
36	f	804	CLA	C4A-NA-C1A	13.05	112.63	106.68
37	T	310	KC1	CHB-C4A-C3A	-13.04	104.43	125.03
37	F	315	KC1	C1A-C2A-C3A	-13.01	95.32	107.28
37	R	317	KC1	CMD-C2D-C1D	-12.85	105.85	125.42
37	T	315	KC1	CMD-C2D-C1D	-12.76	105.98	125.42
35	S	305	A86	C20-O1-C15	12.70	66.49	61.03
35	X	303	A86	O1-C20-C21	-12.58	100.98	115.05
35	N	301	A86	C29-C30-C31	-12.58	162.82	177.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	S	301	A86	C29-C30-C31	-12.57	162.83	177.66
35	B	303	A86	C40-C32-C31	-12.44	99.34	110.47
37	S	316	KC1	CAB-C3B-C4B	12.34	154.28	124.82
37	D	314	KC1	CMD-C2D-C1D	-12.25	106.77	125.42
36	X	313	CLA	CMB-C2B-C1B	-12.09	107.01	125.42
37	M	318	KC1	C1A-NA-C4A	12.06	112.18	106.68
35	G	304	A86	C29-C30-C31	-11.96	163.55	177.66
36	Q	310	CLA	CAA-CBA-CGA	11.92	147.04	113.21
37	F	308	KC1	C1A-NA-C4A	-11.85	101.27	106.68
37	M	313	KC1	CAB-C3B-C4B	11.83	153.06	124.82
35	N	304	A86	C21-C20-C19	11.76	127.45	114.24
35	H	301	A86	O5-C38-C39	-11.65	83.52	124.77
37	H	313	KC1	C1A-NA-C4A	-11.65	101.37	106.68
37	R	317	KC1	CAB-C3B-C4B	11.54	152.38	124.82
36	X	313	CLA	C4B-C3B-C2B	-11.53	92.96	107.30
34	D	303	DD6	C-C1-C24	-11.43	100.62	118.09
35	G	304	A86	O1-C20-C21	-11.39	102.32	115.05
37	N	314	KC1	CAB-C3B-C4B	11.29	151.77	124.82
37	T	310	KC1	C2A-C3A-C4A	-11.23	97.98	106.41
37	M	318	KC1	C2D-C1D-ND	11.22	121.96	110.33
42	V	315	LMG	O9-C10-C11	-11.08	80.44	123.78
36	a	830	CLA	C4D-CHA-C1A	-11.07	108.04	121.24
36	V	314	CLA	C4A-NA-C1A	11.00	111.70	106.68
37	A	312	KC1	CHD-C4C-C3C	-10.98	104.98	125.23
37	V	312	KC1	CMD-C2D-C1D	-10.94	108.76	125.42
36	A	314	CLA	C4A-NA-C1A	10.90	111.65	106.68
37	V	312	KC1	CAC-C3C-C4C	10.88	138.95	124.79
37	K	314	KC1	CHD-C4C-C3C	-10.88	105.16	125.23
35	B	303	A86	C35-C34-C33	-10.86	90.37	109.89
37	A	312	KC1	CAB-C3B-C4B	10.83	150.68	124.82
37	L	315	KC1	CHD-C4C-C3C	-10.83	105.26	125.23
37	C	213	KC1	CAB-C3B-C4B	10.80	150.60	124.82
37	M	318	KC1	OBD-CAD-C3D	-10.78	103.21	128.42
35	V	304	A86	O1-C20-C19	10.78	123.59	113.49
36	N	319	CLA	C3D-C2D-C1D	-10.77	91.14	105.83
37	G	308	KC1	CAB-C3B-C4B	10.75	150.49	124.82
35	X	304	A86	C29-C30-C31	-10.75	164.98	177.66
37	U	312	KC1	C1A-C2A-C3A	-10.68	97.46	107.28
36	G	319	CLA	C1D-ND-C4D	-10.68	98.82	106.31
37	J	314	KC1	CAB-C3B-C4B	10.67	150.29	124.82
35	X	303	A86	C20-O1-C15	10.64	65.60	61.03
37	T	310	KC1	OBD-CAD-C3D	-10.63	103.56	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	304	A86	O1-C20-C15	-10.63	54.96	59.23
37	V	312	KC1	CAB-C3B-C4B	10.60	150.12	124.82
37	M	318	KC1	C2A-C1A-NA	-10.58	92.40	109.34
37	Q	313	KC1	CAB-C3B-C4B	10.55	150.00	124.82
37	Q	311	KC1	CAB-C3B-C4B	10.54	150.00	124.82
37	O	313	KC1	CAB-C3B-C4B	10.54	149.98	124.82
37	M	317	KC1	CAB-C3B-C4B	10.52	149.95	124.82
37	O	315	KC1	CAB-C3B-C4B	10.52	149.95	124.82
37	T	315	KC1	CAB-C3B-C4B	10.52	149.93	124.82
37	F	315	KC1	CAB-C3B-C4B	10.51	149.91	124.82
37	P	315	KC1	CAB-C3B-C4B	10.51	149.91	124.82
37	G	318	KC1	CAB-C3B-C4B	10.51	149.91	124.82
37	L	317	KC1	CAB-C3B-C4B	10.48	149.84	124.82
35	X	302	A86	C29-C30-C31	-10.42	165.37	177.66
37	P	315	KC1	CHD-C4C-C3C	-10.40	106.05	125.23
37	O	313	KC1	CHD-C4C-C3C	-10.40	106.05	125.23
35	N	304	A86	O1-C20-C19	-10.40	103.74	113.49
36	b	836	CLA	C1D-ND-C4D	-10.39	99.03	106.31
37	Q	311	KC1	CHD-C4C-C3C	-10.37	106.10	125.23
37	E	309	KC1	CAB-C3B-C4B	10.37	149.59	124.82
37	O	315	KC1	CHD-C4C-C3C	-10.37	106.11	125.23
37	Q	313	KC1	CHD-C4C-C3C	-10.36	106.12	125.23
37	L	315	KC1	C1A-C2A-C3A	-10.35	97.76	107.28
37	J	314	KC1	C1A-NA-C4A	-10.33	101.97	106.68
35	J	303	A86	C29-C30-C31	-10.28	165.53	177.66
37	J	314	KC1	CHD-C4C-C3C	-10.28	106.28	125.23
35	T	305	A86	C20-O1-C15	10.27	65.44	61.03
37	K	314	KC1	CAB-C3B-C4B	10.26	149.31	124.82
35	X	304	A86	C20-O1-C15	10.25	65.44	61.03
37	F	315	KC1	CHD-C4C-C3C	-10.18	106.45	125.23
35	S	303	A86	C29-C30-C31	-10.16	165.67	177.66
37	F	308	KC1	C1A-C2A-C3A	-10.16	97.94	107.28
37	P	317	KC1	CHD-C4C-C3C	-10.14	106.53	125.23
37	R	317	KC1	C1A-NA-C4A	-10.14	102.05	106.68
35	R	303	A86	C33-C32-C31	-10.13	99.36	109.21
35	N	303	A86	C29-C30-C31	-10.13	165.71	177.66
35	L	306	A86	C29-C30-C31	-10.11	165.73	177.66
35	T	306	A86	C29-C30-C31	-10.10	165.75	177.66
37	U	312	KC1	CHD-C4C-C3C	-10.08	106.64	125.23
37	E	309	KC1	CMD-C2D-C1D	-10.07	110.08	125.42
35	M	301	A86	C29-C30-C31	-10.00	165.87	177.66
37	L	315	KC1	CHD-C4C-NC	9.98	139.34	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L	317	KC1	CHD-C4C-C3C	-9.97	106.84	125.23
37	W	217	KC1	CAB-C3B-C4B	9.97	148.62	124.82
37	B	310	KC1	CAB-C3B-C4B	9.97	148.62	124.82
37	X	311	KC1	CAB-C3B-C4B	9.96	148.61	124.82
37	J	314	KC1	C1A-C2A-C3A	-9.96	98.12	107.28
35	R	306	A86	C29-C30-C31	-9.96	165.91	177.66
37	A	312	KC1	CMD-C2D-C3D	9.96	157.08	125.67
37	G	308	KC1	CMD-C2D-C1D	-9.96	110.26	125.42
37	R	317	KC1	CHD-C4C-C3C	-9.87	107.03	125.23
37	W	213	KC1	CMD-C2D-C3D	9.81	156.59	125.67
37	L	317	KC1	C1A-C2A-C3A	-9.80	98.27	107.28
37	J	314	KC1	CHD-C4C-NC	9.75	139.00	124.31
35	X	305	A86	C20-O1-C15	9.75	65.22	61.03
37	M	318	KC1	C2A-C3A-C4A	-9.74	99.09	106.41
35	R	302	A86	C29-C30-C31	-9.74	166.17	177.66
37	M	313	KC1	CHD-C4C-C3C	-9.74	107.28	125.23
37	W	213	KC1	CHD-C4C-C3C	-9.73	107.29	125.23
37	F	315	KC1	CHD-C4C-NC	9.70	138.92	124.31
37	W	213	KC1	CAB-C3B-C4B	9.69	147.96	124.82
36	b	826	CLA	C4A-NA-C1A	9.68	111.09	106.68
37	G	317	KC1	CHD-C4C-C3C	-9.66	107.42	125.23
36	K	307	CLA	C4A-NA-C1A	9.66	111.08	106.68
37	T	315	KC1	CHD-C4C-C3C	-9.65	107.43	125.23
37	G	317	KC1	CHD-C4C-NC	9.60	138.77	124.31
37	C	213	KC1	CHD-C4C-C3C	-9.59	107.54	125.23
37	B	310	KC1	C1A-C2A-C3A	-9.58	98.48	107.28
37	M	318	KC1	C3D-C4D-ND	9.57	123.55	110.20
35	J	301	A86	C20-O1-C15	9.57	65.14	61.03
36	Q	310	CLA	C1-O2A-CGA	9.57	139.81	116.65
37	M	318	KC1	CHD-C1D-ND	-9.56	109.70	124.05
35	B	303	A86	C20-O1-C15	9.54	65.13	61.03
37	L	315	KC1	CMD-C2D-C3D	9.53	155.73	125.67
35	M	305	A86	C20-O1-C15	9.52	65.12	61.03
37	P	317	KC1	CMD-C2D-C3D	9.47	155.54	125.67
37	T	315	KC1	CHD-C4C-NC	9.46	138.56	124.31
37	F	315	KC1	CMD-C2D-C3D	9.45	155.47	125.67
35	C	204	A86	C-C1-C2	-9.44	107.53	122.82
37	M	318	KC1	C4C-C3C-C2C	9.43	120.62	106.89
36	I	309	CLA	C4A-NA-C1A	9.41	110.97	106.68
36	N	309	CLA	C4A-NA-C1A	9.41	110.97	106.68
35	U	301	A86	C20-O1-C15	9.38	65.06	61.03
37	T	310	KC1	CHB-C4A-NA	9.37	138.76	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	G	317	KC1	CAB-C3B-C4B	9.36	147.17	124.82
35	O	302	A86	C20-O1-C15	9.34	65.04	61.03
35	K	306	A86	C33-C32-C31	-9.34	100.13	109.21
37	H	313	KC1	CHD-C4C-C3C	-9.34	108.01	125.23
35	U	301	A86	C3-C2-C1	-9.33	114.19	127.28
37	Q	311	KC1	CMD-C2D-C3D	9.33	155.11	125.67
36	T	311	CLA	C4A-NA-C1A	9.33	110.94	106.68
37	O	315	KC1	CMD-C2D-C3D	9.33	155.10	125.67
37	O	313	KC1	CMD-C2D-C3D	9.33	155.10	125.67
37	Q	313	KC1	CMD-C2D-C3D	9.33	155.08	125.67
35	R	301	A86	C20-O1-C15	9.32	65.04	61.03
37	P	315	KC1	CMD-C2D-C3D	9.32	155.08	125.67
37	M	318	KC1	C4B-C3B-C2B	-9.32	98.73	106.81
35	L	319	A86	C20-O1-C15	9.31	65.03	61.03
35	P	303	A86	C20-O1-C15	9.30	65.02	61.03
36	a	833	CLA	C4A-NA-C1A	9.29	110.92	106.68
35	Q	316	A86	C20-O1-C15	9.28	65.02	61.03
35	T	307	A86	O1-C20-C21	-9.28	104.68	115.05
35	T	305	A86	O1-C20-C19	9.28	122.18	113.49
37	G	308	KC1	CHD-C4C-C3C	-9.27	108.13	125.23
37	D	314	KC1	CAB-C3B-C4B	9.27	146.95	124.82
35	F	301	A86	C20-O1-C15	9.26	65.01	61.03
37	V	312	KC1	CHD-C4C-C3C	-9.25	108.17	125.23
35	T	307	A86	C20-O1-C15	9.25	65.00	61.03
35	M	302	A86	C29-C30-C31	-9.25	166.75	177.66
35	W	202	A86	C20-O1-C15	9.23	65.00	61.03
37	M	313	KC1	CMD-C2D-C3D	9.23	154.77	125.67
35	N	305	A86	C20-O1-C15	9.22	64.99	61.03
37	S	316	KC1	CHD-C4C-C3C	-9.22	108.24	125.23
37	M	317	KC1	CMD-C2D-C1D	-9.21	111.39	125.42
37	P	317	KC1	CHD-C4C-NC	9.21	138.18	124.31
36	C	207	CLA	CMD-C2D-C1D	9.21	140.95	124.73
35	N	320	A86	C20-O1-C15	9.19	64.98	61.03
35	F	306	A86	C20-O1-C15	9.18	64.97	61.03
35	Q	304	A86	C20-O1-C15	9.17	64.97	61.03
37	J	314	KC1	CMD-C2D-C3D	9.16	154.57	125.67
36	b	841	CLA	C4A-NA-C1A	9.11	110.83	106.68
35	G	306	A86	C20-O1-C15	9.09	64.94	61.03
36	O	312	CLA	C3A-C2A-C1A	-9.09	97.00	106.30
35	U	301	A86	C3-C4-C5	-9.07	104.95	123.52
37	L	315	KC1	OBD-CAD-C3D	-9.06	107.23	128.42
37	D	314	KC1	OBD-CAD-C3D	-9.05	107.25	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	G	308	KC1	OBD-CAD-C3D	-9.05	107.25	128.42
36	U	308	CLA	C4A-NA-C1A	9.02	110.80	106.68
36	L	308	CLA	C3B-C2B-C1B	-9.01	96.55	107.17
35	I	304	A86	O4-C38-C39	9.01	127.15	111.09
36	H	310	CLA	O2D-CGD-CBD	8.99	126.95	111.23
37	B	310	KC1	CHD-C4C-C3C	-8.99	108.65	125.23
36	I	306	CLA	C4A-NA-C1A	8.99	110.78	106.68
35	O	301	A86	C20-O1-C15	8.98	64.89	61.03
35	J	305	A86	C20-O1-C15	8.98	64.89	61.03
35	O	302	A86	O4-C38-C39	8.97	127.09	111.09
37	T	310	KC1	CHC-C4B-NB	8.97	137.43	124.80
36	S	321	CLA	C4A-NA-C1A	8.97	110.77	106.68
35	L	319	A86	O4-C38-C39	8.97	127.09	111.09
35	P	303	A86	O4-C38-C39	8.97	127.09	111.09
35	I	301	A86	C20-O1-C15	8.97	64.88	61.03
37	S	316	KC1	CMD-C2D-C3D	8.96	153.93	125.67
37	K	314	KC1	OBD-CAD-C3D	-8.96	107.47	128.42
37	M	318	KC1	CHB-C4A-C3A	-8.96	110.89	125.03
37	F	308	KC1	OBD-CAD-C3D	-8.95	107.50	128.42
35	W	202	A86	O4-C38-C39	8.94	127.04	111.09
35	X	303	A86	O4-C38-C39	8.94	127.04	111.09
35	N	304	A86	C20-O1-C15	8.94	64.87	61.03
35	F	304	A86	C20-O1-C15	8.93	64.87	61.03
37	M	317	KC1	OBD-CAD-C3D	-8.93	107.54	128.42
37	F	308	KC1	CHD-C4C-C3C	-8.92	108.77	125.23
37	E	309	KC1	OBD-CAD-C3D	-8.92	107.57	128.42
35	M	301	A86	C20-O1-C15	8.91	64.86	61.03
35	A	316	A86	C20-O1-C15	8.89	64.85	61.03
36	G	313	CLA	C4A-NA-C1A	8.88	110.73	106.68
35	A	302	A86	C20-O1-C15	8.87	64.84	61.03
35	S	301	A86	O4-C38-C39	8.87	126.90	111.09
35	P	307	A86	C20-O1-C15	8.84	64.83	61.03
35	E	305	A86	C20-O1-C15	8.84	64.83	61.03
35	N	301	A86	O4-C38-C39	8.83	126.84	111.09
35	X	301	A86	O4-C38-C39	8.83	126.84	111.09
35	C	203	A86	C20-O1-C15	8.83	64.82	61.03
36	K	307	CLA	C1D-ND-C4D	-8.82	100.12	106.31
36	U	306	CLA	CMD-C2D-C1D	8.81	140.25	124.73
36	a	819	CLA	C4A-NA-C1A	8.81	110.70	106.68
37	X	311	KC1	CHD-C4C-C3C	-8.81	108.98	125.23
37	W	217	KC1	CHD-C4C-C3C	-8.80	108.99	125.23
36	P	319	CLA	C4A-NA-C1A	8.79	110.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	T	315	KC1	OBD-CAD-C3D	-8.79	107.88	128.42
35	R	301	A86	O4-C38-C39	8.78	126.75	111.09
37	R	317	KC1	OBD-CAD-C3D	-8.78	107.89	128.42
37	G	308	KC1	C1A-C2A-C3A	-8.78	99.21	107.28
37	K	314	KC1	CMD-C2D-C3D	8.77	153.34	125.67
35	E	307	A86	C20-O1-C15	8.77	64.80	61.03
35	R	303	A86	O4-C38-C39	8.76	126.72	111.09
37	S	316	KC1	C1A-C2A-C3A	-8.76	99.23	107.28
35	U	304	A86	C20-O1-C15	8.76	64.79	61.03
36	S	315	CLA	C4A-NA-C1A	8.75	110.67	106.68
35	T	301	A86	C20-O1-C15	8.74	64.78	61.03
35	R	309	A86	C20-O1-C15	8.73	64.78	61.03
36	D	309	CLA	C1D-ND-C4D	-8.72	100.19	106.31
35	L	301	A86	C20-O1-C15	8.71	64.77	61.03
35	X	314	A86	C20-O1-C15	8.71	64.77	61.03
37	M	313	KC1	OBD-CAD-C3D	-8.68	108.13	128.42
35	F	302	A86	C20-O1-C15	8.66	64.75	61.03
35	S	308	A86	C20-O1-C15	8.66	64.75	61.03
37	T	310	KC1	CHC-C4B-C3B	-8.65	110.62	125.21
35	H	301	A86	O1-C20-C21	-8.65	105.39	115.05
37	A	312	KC1	CHD-C4C-NC	8.64	137.33	124.31
35	H	304	A86	C20-O1-C15	8.64	64.74	61.03
35	B	301	A86	C20-O1-C15	8.64	64.74	61.03
35	J	306	A86	C20-O1-C15	8.63	64.74	61.03
37	F	315	KC1	OBD-CAD-C3D	-8.62	108.28	128.42
35	V	301	A86	C20-O1-C15	8.61	64.73	61.03
35	C	202	A86	C20-O1-C15	8.60	64.73	61.03
37	P	315	KC1	OBD-CAD-C3D	-8.60	108.32	128.42
36	D	309	CLA	CMD-C2D-C1D	8.60	139.87	124.73
37	L	317	KC1	OBD-CAD-C3D	-8.59	108.33	128.42
36	G	319	CLA	CMD-C2D-C1D	8.59	139.85	124.73
37	Q	311	KC1	OBD-CAD-C3D	-8.59	108.35	128.42
37	Q	313	KC1	OBD-CAD-C3D	-8.58	108.35	128.42
37	O	315	KC1	OBD-CAD-C3D	-8.58	108.36	128.42
37	O	313	KC1	OBD-CAD-C3D	-8.58	108.37	128.42
36	K	307	CLA	CMD-C2D-C1D	8.57	139.82	124.73
35	M	304	A86	C20-O1-C15	8.56	64.71	61.03
35	K	302	A86	C20-O1-C15	8.56	64.71	61.03
36	H	310	CLA	CED-O2D-CGD	8.56	135.33	115.92
36	R	316	CLA	C4A-NA-C1A	8.55	110.58	106.68
37	H	313	KC1	C1A-C2A-C3A	-8.55	99.42	107.28
36	T	314	CLA	C4A-NA-C1A	8.54	110.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	E	309	KC1	CHD-C4C-C3C	-8.54	109.49	125.23
37	G	317	KC1	OBD-CAD-C3D	-8.51	108.53	128.42
35	K	301	A86	C20-O1-C15	8.49	64.68	61.03
36	b	836	CLA	CMD-C2D-C1D	8.49	139.68	124.73
37	S	316	KC1	OBD-CAD-C3D	-8.49	108.58	128.42
35	R	306	A86	C20-O1-C15	8.48	64.67	61.03
37	C	213	KC1	OBD-CAD-C3D	-8.48	108.60	128.42
36	V	314	CLA	CMD-C2D-C1D	8.48	139.65	124.73
37	M	317	KC1	CHD-C4C-C3C	-8.47	109.61	125.23
35	J	302	A86	C20-O1-C15	8.47	64.67	61.03
35	T	303	A86	O4-C38-C39	8.46	126.18	111.09
35	D	302	A86	C20-O1-C15	8.45	64.66	61.03
36	S	313	CLA	C4A-NA-C1A	8.45	110.53	106.68
36	X	307	CLA	C4A-NA-C1A	8.45	110.53	106.68
37	N	314	KC1	CHD-C4C-C3C	-8.45	109.65	125.23
37	R	317	KC1	C1A-C2A-C3A	-8.44	99.52	107.28
36	X	313	CLA	C3B-C4B-NB	8.43	118.06	110.53
36	N	319	CLA	CHD-C1D-C2D	8.43	143.01	125.49
35	N	306	A86	C20-O1-C15	8.42	64.65	61.03
37	V	312	KC1	OBD-CAD-C3D	-8.42	108.75	128.42
35	E	302	A86	C20-O1-C15	8.41	64.64	61.03
37	B	310	KC1	OBD-CAD-C3D	-8.41	108.76	128.42
36	O	316	CLA	C1D-ND-C4D	-8.40	100.42	106.31
37	U	312	KC1	OBD-CAD-C3D	-8.40	108.78	128.42
36	a	813	CLA	C4A-NA-C1A	8.40	110.51	106.68
35	X	301	A86	C20-O1-C15	8.40	64.64	61.03
35	h	204	A86	C20-O1-C15	8.39	64.64	61.03
36	V	309	CLA	C4A-NA-C1A	8.39	110.51	106.68
35	I	304	A86	C20-O1-C15	8.36	64.62	61.03
36	f	803	CLA	CMD-C2D-C1D	8.35	139.43	124.73
37	F	308	KC1	CMD-C2D-C3D	8.35	151.99	125.67
36	O	316	CLA	CMD-C2D-C1D	8.34	139.41	124.73
36	F	317	CLA	CMD-C2D-C1D	8.32	139.39	124.73
36	b	811	CLA	C4A-NA-C1A	8.31	110.47	106.68
36	N	319	CLA	C3C-C4C-NC	-8.30	99.79	110.43
35	G	305	A86	C20-O1-C15	8.30	64.60	61.03
35	L	307	A86	C20-O1-C15	8.30	64.60	61.03
37	N	314	KC1	OBD-CAD-C3D	-8.28	109.07	128.42
36	F	311	CLA	C4A-NA-C1A	8.28	110.45	106.68
35	P	303	A86	C29-C30-C31	-8.27	167.90	177.66
36	E	315	CLA	CMD-C2D-C1D	8.27	139.30	124.73
35	O	302	A86	C29-C30-C31	-8.27	167.90	177.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L	317	KC1	CHD-C4C-NC	8.27	136.76	124.31
35	L	319	A86	C29-C30-C31	-8.27	167.91	177.66
35	C	202	A86	O4-C38-C39	8.26	125.82	111.09
35	W	203	A86	C20-O1-C15	8.24	64.57	61.03
36	K	310	CLA	CMD-C2D-C1D	8.24	139.24	124.73
37	T	310	KC1	C2A-C1A-NA	-8.24	96.15	109.34
36	a	814	CLA	C4A-NA-C1A	8.24	110.44	106.68
36	b	817	CLA	C4A-NA-C1A	8.23	110.43	106.68
36	a	836	CLA	C4A-NA-C1A	8.22	110.43	106.68
36	G	309	CLA	C4A-NA-C1A	8.22	110.43	106.68
37	H	313	KC1	OBD-CAD-C3D	-8.21	109.22	128.42
37	W	213	KC1	OBD-CAD-C3D	-8.21	109.23	128.42
35	C	204	A86	C20-O1-C15	8.20	64.55	61.03
35	T	305	A86	O4-C38-C39	8.20	125.71	111.09
36	a	826	CLA	C4A-NA-C1A	8.19	110.42	106.68
37	J	314	KC1	OBD-CAD-C3D	-8.18	109.29	128.42
36	l	205	CLA	C4A-NA-C1A	8.18	110.41	106.68
37	G	318	KC1	CHD-C4C-C3C	-8.18	110.15	125.23
35	N	303	A86	O4-C38-C39	8.17	125.66	111.09
35	V	303	A86	O4-C38-C39	8.17	125.65	111.09
36	W	206	CLA	C4A-NA-C1A	8.16	110.40	106.68
35	X	305	A86	O1-C20-C21	-8.16	105.92	115.05
35	S	303	A86	O4-C38-C39	8.16	125.64	111.09
36	I	306	CLA	CMD-C2D-C1D	8.15	139.08	124.73
37	S	316	KC1	CAB-C3B-C2B	-8.14	101.97	128.43
37	D	314	KC1	CHD-C4C-C3C	-8.13	110.24	125.23
36	N	318	CLA	C4A-NA-C1A	8.13	110.39	106.68
36	H	312	CLA	C4A-NA-C1A	8.10	110.38	106.68
36	X	313	CLA	C3B-C2B-C1B	8.10	116.72	107.17
35	T	304	A86	C20-O1-C15	8.10	64.51	61.03
37	W	217	KC1	OBD-CAD-C3D	-8.10	109.49	128.42
37	X	311	KC1	OBD-CAD-C3D	-8.10	109.49	128.42
36	B	306	CLA	C4A-NA-C1A	8.08	110.37	106.68
36	B	311	CLA	C4A-NA-C1A	8.08	110.37	106.68
37	P	317	KC1	OBD-CAD-C3D	-8.08	109.53	128.42
36	l	205	CLA	CMD-C2D-C1D	8.07	138.94	124.73
36	b	826	CLA	CED-O2D-CGD	8.07	134.22	115.92
36	b	835	CLA	C4A-NA-C1A	8.04	110.35	106.68
37	T	315	KC1	CMD-C2D-C3D	8.03	150.99	125.67
36	L	312	CLA	C4A-NA-C1A	8.03	110.34	106.68
36	j	102	CLA	CMD-C2D-C1D	8.03	138.86	124.73
37	M	318	KC1	C1C-C2C-C3C	-8.02	98.54	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	V	311	CLA	C4A-NA-C1A	8.02	110.34	106.68
35	S	302	A86	C29-C30-C31	-8.02	168.20	177.66
36	N	311	CLA	C4A-NA-C1A	8.00	110.33	106.68
36	N	319	CLA	C4D-C3D-CAD	-8.00	99.42	108.11
36	H	309	CLA	C4A-NA-C1A	7.99	110.33	106.68
36	G	307	CLA	CMD-C2D-C1D	7.99	138.80	124.73
35	N	302	A86	C29-C30-C31	-7.98	168.24	177.66
37	R	317	KC1	CAB-C3B-C2B	-7.97	102.52	128.43
36	D	315	CLA	C4A-NA-C1A	7.96	110.31	106.68
36	R	314	CLA	C4A-NA-C1A	7.96	110.31	106.68
35	O	305	A86	C29-C30-C31	-7.96	168.27	177.66
36	Q	312	CLA	C4A-NA-C1A	7.95	110.31	106.68
37	L	317	KC1	C1A-NA-C4A	-7.95	103.05	106.68
36	P	316	CLA	C4A-NA-C1A	7.94	110.30	106.68
35	N	302	A86	C20-O1-C15	7.94	64.44	61.03
37	M	318	KC1	CAC-C3C-C2C	-7.94	112.97	127.56
36	J	312	CLA	C4A-NA-C1A	7.93	110.30	106.68
37	P	317	KC1	CHC-C4B-NB	7.93	135.96	124.80
36	A	313	CLA	C4A-NA-C1A	7.92	110.29	106.68
35	X	304	A86	O1-C20-C21	-7.92	106.20	115.05
36	I	308	CLA	CMD-C2D-C1D	7.91	138.65	124.73
36	L	313	CLA	C4A-NA-C1A	7.91	110.29	106.68
37	Q	311	KC1	C2A-C3A-C4A	7.90	112.34	106.41
37	O	315	KC1	C2A-C3A-C4A	7.89	112.34	106.41
35	K	302	A86	O4-C38-C39	7.89	125.16	111.09
37	M	318	KC1	CHD-C4C-C3C	-7.88	110.70	125.23
36	O	314	CLA	C4A-NA-C1A	7.87	110.27	106.68
36	J	308	CLA	C4A-NA-C1A	7.87	110.27	106.68
36	b	816	CLA	CMD-C2D-C1D	7.87	138.58	124.73
37	O	313	KC1	C2A-C3A-C4A	7.86	112.31	106.41
37	P	315	KC1	C2A-C3A-C4A	7.86	112.31	106.41
37	M	313	KC1	C1A-C2A-C3A	-7.86	100.06	107.28
35	G	302	A86	C20-O1-C15	7.85	64.40	61.03
37	K	314	KC1	C1A-C2A-C3A	-7.85	100.07	107.28
36	G	307	CLA	C1C-C2C-C3C	-7.85	98.73	106.98
35	S	302	A86	C20-O1-C15	7.84	64.40	61.03
36	T	312	CLA	C4A-NA-C1A	7.84	110.26	106.68
35	X	302	A86	C20-O1-C15	7.84	64.40	61.03
37	R	317	KC1	CMD-C2D-C3D	7.83	150.37	125.67
37	Q	313	KC1	C2A-C3A-C4A	7.82	112.29	106.41
35	L	304	A86	C20-O1-C15	7.82	64.39	61.03
36	U	306	CLA	C4A-NA-C1A	7.81	110.24	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	I	311	CLA	C4A-NA-C1A	7.81	110.24	106.68
36	R	319	CLA	C4A-NA-C1A	7.81	110.24	106.68
37	X	311	KC1	C1A-C2A-C3A	-7.80	100.11	107.28
37	W	217	KC1	C1A-C2A-C3A	-7.80	100.11	107.28
36	f	804	CLA	CMD-C2D-C1D	7.80	138.47	124.73
36	b	807	CLA	C4A-NA-C1A	7.80	110.24	106.68
35	F	305	A86	C20-O1-C15	7.79	64.38	61.03
36	X	312	CLA	C4A-NA-C1A	7.79	110.23	106.68
37	E	309	KC1	C1A-C2A-C3A	-7.78	100.13	107.28
35	T	302	A86	C20-O1-C15	7.77	64.37	61.03
37	A	312	KC1	CHB-C4A-C3A	-7.77	112.76	125.03
36	b	806	CLA	C4A-NA-C1A	7.76	110.22	106.68
35	M	301	A86	O4-C38-C39	7.74	124.89	111.09
36	b	817	CLA	CMD-C2D-C1D	7.73	138.35	124.73
36	a	828	CLA	C4A-NA-C1A	7.72	110.20	106.68
36	l	204	CLA	CMD-C2D-C1D	7.72	138.32	124.73
37	U	312	KC1	C1A-NA-C4A	-7.71	103.16	106.68
37	S	316	KC1	CHB-C4A-C3A	-7.71	112.86	125.03
37	M	313	KC1	CAB-C3B-C2B	-7.70	103.41	128.43
35	U	303	A86	C20-O1-C15	7.70	64.34	61.03
36	i	102	CLA	C4A-NA-C1A	7.69	110.19	106.68
36	D	313	CLA	C4A-NA-C1A	7.69	110.19	106.68
36	b	819	CLA	C4A-NA-C1A	7.69	110.19	106.68
37	G	308	KC1	CHD-C4C-NC	7.69	135.89	124.31
36	b	839	CLA	C4A-NA-C1A	7.68	110.18	106.68
37	P	317	KC1	CAB-C3B-C4B	7.68	143.16	124.82
35	K	306	A86	C40-C32-C31	7.68	117.34	110.47
36	A	306	CLA	CMD-C2D-C1D	7.68	138.25	124.73
36	S	318	CLA	C4A-NA-C1A	7.68	110.18	106.68
35	N	301	A86	O1-C20-C21	-7.67	106.48	115.05
35	S	301	A86	O1-C20-C21	-7.66	106.49	115.05
35	h	202	A86	C20-O1-C15	7.65	64.32	61.03
35	H	301	A86	C20-O1-C15	7.65	64.31	61.03
36	f	805	CLA	C4A-NA-C1A	7.65	110.17	106.68
35	P	306	A86	C20-O1-C15	7.64	64.31	61.03
37	B	310	KC1	C1A-NA-C4A	-7.63	103.20	106.68
36	a	824	CLA	C4A-NA-C1A	7.63	110.16	106.68
37	R	317	KC1	CHB-C4A-C3A	-7.62	112.99	125.03
37	O	315	KC1	C2A-C1A-NA	7.62	121.56	109.34
37	M	318	KC1	CHC-C4B-C3B	-7.62	112.36	125.21
37	O	313	KC1	C2A-C1A-NA	7.62	121.54	109.34
37	Q	313	KC1	C2A-C1A-NA	7.61	121.54	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	830	CLA	CMD-C2D-C1D	7.61	138.13	124.73
36	K	312	CLA	C4A-NA-C1A	7.61	110.15	106.68
37	Q	311	KC1	C2A-C1A-NA	7.61	121.53	109.34
37	M	317	KC1	C1D-ND-C4D	7.60	111.65	106.31
35	R	301	A86	O1-C20-C21	-7.60	106.55	115.05
37	P	315	KC1	C2A-C1A-NA	7.60	121.51	109.34
36	T	309	CLA	C4A-NA-C1A	7.59	110.14	106.68
36	E	314	CLA	C4A-NA-C1A	7.59	110.14	106.68
35	R	303	A86	C20-O1-C15	7.58	64.29	61.03
36	a	802	CLA	C4A-NA-C1A	7.57	110.13	106.68
36	b	832	CLA	C4A-NA-C1A	7.57	110.13	106.68
36	h	203	CLA	C4A-NA-C1A	7.56	110.13	106.68
35	Q	303	A86	C20-O1-C15	7.56	64.28	61.03
36	a	818	CLA	C4A-NA-C1A	7.56	110.13	106.68
37	K	314	KC1	CHD-C4C-NC	7.56	135.69	124.31
36	L	308	CLA	CHB-C4A-NA	7.55	135.29	124.40
36	a	808	CLA	C4A-NA-C1A	7.54	110.12	106.68
36	C	209	CLA	C4A-NA-C1A	7.54	110.12	106.68
36	X	310	CLA	O1D-CGD-CBD	7.53	139.36	124.52
36	Q	309	CLA	C4A-NA-C1A	7.52	110.11	106.68
37	D	314	KC1	CMD-C2D-C3D	7.52	149.38	125.67
36	b	824	CLA	CMD-C2D-C1D	7.52	137.96	124.73
35	R	305	A86	C20-O1-C15	7.51	64.25	61.03
35	X	304	A86	O4-C38-C39	7.50	124.47	111.09
37	O	313	KC1	CHD-C4C-NC	7.50	135.60	124.31
36	H	310	CLA	C4D-CHA-C1A	-7.49	112.31	121.24
37	T	310	KC1	C1D-ND-C4D	-7.49	101.06	106.31
36	a	823	CLA	C4A-NA-C1A	7.49	110.09	106.68
36	H	316	CLA	C4A-NA-C1A	7.48	110.09	106.68
37	F	308	KC1	C2C-C1C-NC	7.48	119.71	110.45
37	P	315	KC1	CHD-C4C-NC	7.47	135.57	124.31
36	b	825	CLA	C4A-NA-C1A	7.47	110.09	106.68
35	S	304	A86	C20-O1-C15	7.47	64.24	61.03
35	G	304	A86	C21-C20-C19	-7.47	105.85	114.24
37	G	318	KC1	OBD-CAD-C3D	-7.47	110.96	128.42
35	S	301	A86	C21-C20-C19	-7.47	105.85	114.24
35	N	301	A86	C21-C20-C19	-7.46	105.86	114.24
36	D	310	CLA	C4A-NA-C1A	7.46	110.08	106.68
36	a	807	CLA	C4A-NA-C1A	7.46	110.08	106.68
37	Q	311	KC1	CHD-C4C-NC	7.45	135.54	124.31
36	O	310	CLA	C4A-NA-C1A	7.45	110.08	106.68
37	O	315	KC1	CHD-C4C-NC	7.45	135.53	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Q	313	KC1	CHD-C4C-NC	7.45	135.53	124.31
36	S	310	CLA	C4A-NA-C1A	7.45	110.08	106.68
35	T	306	A86	C20-O1-C15	7.45	64.23	61.03
37	L	315	KC1	CAB-C3B-C4B	7.44	142.59	124.82
36	V	314	CLA	C1D-ND-C4D	-7.42	101.10	106.31
35	G	304	A86	O4-C38-C39	7.42	124.32	111.09
35	O	305	A86	C20-O1-C15	7.42	64.22	61.03
35	K	302	A86	C35-C34-C33	-7.41	96.57	109.89
36	A	308	CLA	C4A-NA-C1A	7.41	110.06	106.68
36	E	316	CLA	C4A-NA-C1A	7.41	110.06	106.68
36	a	816	CLA	CMD-C2D-C1D	7.41	137.78	124.73
36	V	314	CLA	C1C-C2C-C3C	-7.41	99.19	106.98
36	a	841	CLA	C4A-NA-C1A	7.41	110.06	106.68
37	H	313	KC1	CHB-C4A-C3A	-7.40	113.34	125.03
36	G	315	CLA	C1C-C2C-C3C	-7.40	99.19	106.98
37	F	308	KC1	CHD-C4C-NC	7.40	135.46	124.31
35	V	303	A86	C20-O1-C15	7.40	64.21	61.03
36	C	206	CLA	C4A-NA-C1A	7.39	110.05	106.68
36	H	307	CLA	C4A-NA-C1A	7.38	110.05	106.68
35	V	304	A86	O1-C20-C21	7.38	123.30	115.05
36	G	312	CLA	C4A-NA-C1A	7.38	110.05	106.68
37	D	314	KC1	CHD-C1D-ND	-7.38	112.98	124.05
36	V	306	CLA	C4A-NA-C1A	7.36	110.04	106.68
36	B	305	CLA	C4A-NA-C1A	7.36	110.04	106.68
36	C	207	CLA	C1D-ND-C4D	-7.36	101.15	106.31
36	J	315	CLA	C4A-NA-C1A	7.36	110.04	106.68
36	a	815	CLA	C4A-NA-C1A	7.36	110.04	106.68
37	T	310	KC1	CHD-C1D-ND	-7.35	113.02	124.05
36	A	306	CLA	C2B-C1B-NB	7.35	117.95	110.33
36	P	301	CLA	C4A-NA-C1A	7.35	110.03	106.68
36	L	314	CLA	C4A-NA-C1A	7.34	110.03	106.68
35	L	304	A86	O1-C20-C21	-7.33	106.85	115.05
36	C	207	CLA	C3D-C2D-C1D	-7.33	95.83	105.83
36	N	312	CLA	C4A-NA-C1A	7.33	110.02	106.68
37	M	313	KC1	CHD-C4C-NC	7.32	135.34	124.31
36	P	312	CLA	C4A-NA-C1A	7.32	110.02	106.68
36	W	218	CLA	C4A-NA-C1A	7.32	110.02	106.68
36	a	827	CLA	C4A-NA-C1A	7.32	110.02	106.68
36	R	315	CLA	C4A-NA-C1A	7.31	110.02	106.68
36	G	316	CLA	C4A-NA-C1A	7.31	110.01	106.68
36	L	320	CLA	C4A-NA-C1A	7.31	110.01	106.68
37	G	318	KC1	C2C-C1C-NC	7.30	119.49	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Q	304	A86	C33-C32-C31	-7.30	102.12	109.21
36	C	212	CLA	C4A-NA-C1A	7.29	110.01	106.68
37	D	314	KC1	CHC-C4B-NB	7.29	135.06	124.80
36	Q	308	CLA	C4A-NA-C1A	7.29	110.00	106.68
36	C	210	CLA	C4A-NA-C1A	7.28	110.00	106.68
36	U	310	CLA	C4A-NA-C1A	7.28	110.00	106.68
36	L	308	CLA	CMD-C2D-C1D	7.27	137.54	124.73
36	a	834	CLA	C4A-NA-C1A	7.27	110.00	106.68
35	N	320	A86	C33-C32-C31	-7.27	102.15	109.21
37	F	308	KC1	C1D-ND-C4D	7.27	111.41	106.31
36	a	821	CLA	C4A-NA-C1A	7.27	109.99	106.68
36	G	314	CLA	C4A-NA-C1A	7.26	109.99	106.68
35	K	303	A86	C20-O1-C15	7.26	64.15	61.03
36	T	311	CLA	CAC-C3C-C4C	-7.25	115.35	124.79
36	P	311	CLA	C4A-NA-C1A	7.25	109.99	106.68
35	K	306	A86	C20-O1-C15	7.25	64.14	61.03
36	O	311	CLA	C4A-NA-C1A	7.24	109.98	106.68
36	G	315	CLA	CMD-C2D-C1D	7.24	137.48	124.73
36	E	315	CLA	C2B-C1B-NB	7.23	117.83	110.33
37	Q	313	KC1	C1D-ND-C4D	7.23	111.38	106.31
35	O	319	A86	C20-O1-C15	7.21	64.13	61.03
36	J	310	CLA	C4A-NA-C1A	7.21	109.97	106.68
36	O	309	CLA	C4A-NA-C1A	7.21	109.97	106.68
36	X	308	CLA	C4A-NA-C1A	7.21	109.97	106.68
36	a	817	CLA	CMB-C2B-C1B	-7.20	114.46	125.42
37	N	314	KC1	CAB-C3B-C2B	-7.19	105.04	128.43
36	a	848	CLA	CMD-C2D-C1D	7.18	137.38	124.73
36	b	808	CLA	C4A-NA-C1A	7.18	109.96	106.68
36	a	812	CLA	C4A-NA-C1A	7.18	109.95	106.68
36	a	810	CLA	C4A-NA-C1A	7.17	109.95	106.68
37	Q	311	KC1	C1D-ND-C4D	7.17	111.34	106.31
35	R	304	A86	O4-C38-C39	7.17	123.87	111.09
35	S	301	A86	C25-C26-C27	-7.16	117.23	127.28
37	D	314	KC1	C1A-C2A-C3A	-7.16	100.69	107.28
36	J	313	CLA	C4A-NA-C1A	7.16	109.95	106.68
35	I	302	A86	C20-O1-C15	7.16	64.11	61.03
35	N	301	A86	C25-C26-C27	-7.16	117.24	127.28
37	A	312	KC1	CHD-C1D-ND	-7.15	113.33	124.05
36	P	313	CLA	C4A-NA-C1A	7.15	109.94	106.68
36	F	314	CLA	C4A-NA-C1A	7.14	109.94	106.68
37	S	316	KC1	CHD-C4C-NC	7.14	135.07	124.31
36	Q	306	CLA	C4A-NA-C1A	7.14	109.94	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	F	315	KC1	CAC-C3C-C4C	7.14	134.08	124.79
37	T	310	KC1	CAC-C3C-C2C	-7.13	114.46	127.56
37	N	314	KC1	CHD-C1D-ND	-7.13	113.35	124.05
36	M	307	CLA	C4A-NA-C1A	7.13	109.93	106.68
37	O	315	KC1	C1D-ND-C4D	7.13	111.31	106.31
36	X	306	CLA	C4A-NA-C1A	7.12	109.93	106.68
37	W	217	KC1	CHB-C4A-C3A	-7.12	113.78	125.03
36	U	309	CLA	C4A-NA-C1A	7.12	109.93	106.68
37	X	311	KC1	CHB-C4A-C3A	-7.12	113.79	125.03
36	H	314	CLA	C4A-NA-C1A	7.12	109.93	106.68
36	a	837	CLA	C4A-NA-C1A	7.11	109.92	106.68
36	P	308	CLA	C4A-NA-C1A	7.11	109.92	106.68
36	b	815	CLA	C4A-NA-C1A	7.10	109.92	106.68
37	D	314	KC1	CHC-C4B-C3B	-7.10	113.23	125.21
35	M	301	A86	C35-C34-C33	-7.10	97.13	109.89
36	a	832	CLA	C4A-NA-C1A	7.10	109.92	106.68
36	V	310	CLA	C4A-NA-C1A	7.10	109.92	106.68
35	F	301	A86	O1-C20-C19	-7.09	106.84	113.49
36	a	819	CLA	CAC-C3C-C4C	-7.09	115.56	124.79
36	P	309	CLA	C4A-NA-C1A	7.09	109.91	106.68
36	O	306	CLA	C4A-NA-C1A	7.09	109.91	106.68
37	E	309	KC1	C1D-ND-C4D	7.08	111.28	106.31
37	E	309	KC1	C2C-C1C-NC	7.08	119.22	110.45
36	I	308	CLA	C1D-ND-C4D	-7.08	101.34	106.31
36	T	308	CLA	C4A-NA-C1A	7.08	109.91	106.68
36	V	308	CLA	C4A-NA-C1A	7.08	109.91	106.68
37	M	318	KC1	CHB-C4A-NA	7.07	135.20	124.23
36	U	311	CLA	C4A-NA-C1A	7.07	109.91	106.68
37	G	318	KC1	C1A-C2A-C3A	-7.07	100.78	107.28
36	G	315	CLA	C3B-C2B-C1B	-7.07	98.84	107.17
36	M	315	CLA	C4A-NA-C1A	7.06	109.90	106.68
37	T	310	KC1	CHB-C1B-NB	7.06	134.74	124.80
36	O	307	CLA	C4A-NA-C1A	7.06	109.90	106.68
36	b	820	CLA	C4A-NA-C1A	7.05	109.90	106.68
35	F	307	A86	C20-O1-C15	7.05	64.06	61.03
36	C	211	CLA	C4A-NA-C1A	7.04	109.89	106.68
36	a	829	CLA	C4A-NA-C1A	7.04	109.89	106.68
36	O	316	CLA	C3B-C2B-C1B	-7.04	98.88	107.17
36	a	816	CLA	C4A-NA-C1A	7.04	109.89	106.68
36	I	307	CLA	C4A-NA-C1A	7.03	109.89	106.68
36	b	810	CLA	C4A-NA-C1A	7.03	109.89	106.68
35	C	202	A86	C29-C30-C31	-7.03	169.36	177.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	V	312	KC1	CMD-C2D-C3D	7.03	147.84	125.67
36	W	207	CLA	C4A-NA-C1A	7.03	109.89	106.68
35	U	301	A86	C4-C3-C2	7.03	137.90	123.52
37	P	315	KC1	C1D-ND-C4D	7.02	111.24	106.31
36	Q	305	CLA	C4A-NA-C1A	7.02	109.88	106.68
37	A	312	KC1	CHC-C4B-NB	7.02	134.69	124.80
37	P	317	KC1	CHC-C4B-C3B	-7.02	113.37	125.21
36	E	313	CLA	CMD-C2D-C1D	7.02	137.09	124.73
36	W	201	CLA	C4A-NA-C1A	7.02	109.88	106.68
36	V	305	CLA	C4A-NA-C1A	7.01	109.88	106.68
36	I	308	CLA	C4A-NA-C1A	7.01	109.88	106.68
37	A	312	KC1	CHC-C4B-C3B	-7.01	113.39	125.21
36	O	316	CLA	C2B-C1B-NB	7.01	117.59	110.33
35	R	309	A86	C29-C30-C31	-7.01	169.39	177.66
36	l	206	CLA	C4A-NA-C1A	7.01	109.88	106.68
37	O	313	KC1	C1D-ND-C4D	7.01	111.23	106.31
35	V	302	A86	C20-O1-C15	7.00	64.04	61.03
36	H	315	CLA	C4A-NA-C1A	6.98	109.86	106.68
36	F	317	CLA	C1C-C2C-C3C	-6.98	99.64	106.98
36	A	311	CLA	C4A-NA-C1A	6.98	109.86	106.68
36	a	839	CLA	C4A-NA-C1A	6.98	109.86	106.68
36	E	310	CLA	C4A-NA-C1A	6.98	109.86	106.68
36	X	309	CLA	C4A-NA-C1A	6.97	109.86	106.68
35	X	301	A86	C29-C30-C31	-6.97	169.44	177.66
35	V	304	A86	C29-C30-C31	-6.96	169.44	177.66
35	U	302	A86	C20-O1-C15	6.96	64.02	61.03
36	U	305	CLA	C4A-NA-C1A	6.95	109.85	106.68
37	G	318	KC1	C1D-ND-C4D	6.95	111.19	106.31
36	M	311	CLA	C4A-NA-C1A	6.95	109.85	106.68
37	F	315	KC1	CHB-C4A-C3A	-6.95	114.06	125.03
37	X	311	KC1	CHC-C4B-C3B	-6.95	113.50	125.21
37	W	217	KC1	CHC-C4B-C3B	-6.94	113.51	125.21
36	N	307	CLA	C4A-NA-C1A	6.94	109.84	106.68
35	M	302	A86	C20-O1-C15	6.93	64.01	61.03
36	R	320	CLA	C4A-NA-C1A	6.93	109.84	106.68
37	A	312	KC1	CAB-C3B-C2B	-6.92	105.93	128.43
37	K	314	KC1	CHC-C4B-C3B	-6.92	113.54	125.21
36	K	310	CLA	C3B-C2B-C1B	-6.92	99.01	107.17
36	b	823	CLA	C4A-NA-C1A	6.91	109.83	106.68
37	F	308	KC1	CHB-C1B-NB	6.91	134.53	124.80
37	A	312	KC1	C2A-C1A-NA	6.91	120.41	109.34
37	C	213	KC1	CAB-C3B-C2B	-6.91	105.97	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	S	316	KC1	C1A-NA-C4A	-6.91	103.53	106.68
36	I	305	CLA	C4A-NA-C1A	6.90	109.83	106.68
35	S	304	A86	C33-C32-C31	6.90	115.92	109.21
36	F	310	CLA	C4A-NA-C1A	6.90	109.83	106.68
35	U	301	A86	C29-C30-C31	-6.89	169.53	177.66
36	b	836	CLA	C4A-NA-C1A	6.89	109.82	106.68
37	T	310	KC1	C4C-C3C-C2C	6.89	116.92	106.89
36	j	106	CLA	C4A-NA-C1A	6.89	109.82	106.68
37	D	314	KC1	C1D-ND-C4D	6.89	111.14	106.31
36	L	308	CLA	C4D-C3D-CAD	6.89	115.58	108.11
37	L	315	KC1	CHC-C4B-NB	6.88	134.49	124.80
35	P	303	A86	O1-C20-C21	-6.88	107.36	115.05
37	G	308	KC1	CAB-C3B-C2B	-6.88	106.07	128.43
37	V	312	KC1	CAB-C3B-C2B	-6.86	106.12	128.43
37	M	317	KC1	CAB-C3B-C2B	-6.86	106.12	128.43
35	L	319	A86	O1-C20-C21	-6.86	107.38	115.05
35	O	303	A86	C20-O1-C15	6.85	63.97	61.03
37	L	317	KC1	CHB-C4A-C3A	-6.85	114.21	125.03
36	N	315	CLA	C4A-NA-C1A	6.85	109.81	106.68
36	G	315	CLA	C2B-C1B-NB	6.85	117.43	110.33
37	G	317	KC1	CHB-C4A-C3A	-6.85	114.22	125.03
37	B	310	KC1	CHC-C4B-NB	6.85	134.44	124.80
35	O	302	A86	O1-C20-C21	-6.84	107.40	115.05
36	F	312	CLA	C4A-NA-C1A	6.84	109.80	106.68
37	J	314	KC1	CHC-C4B-C3B	-6.84	113.67	125.21
36	N	319	CLA	CMD-C2D-C3D	-6.84	112.01	127.69
37	G	317	KC1	CHC-C4B-NB	6.83	134.42	124.80
36	f	802	CLA	C4A-NA-C1A	6.83	109.80	106.68
37	O	315	KC1	C2C-C1C-NC	6.83	118.91	110.45
36	E	313	CLA	C1C-C2C-C3C	-6.83	99.80	106.98
35	R	303	A86	C40-C32-C31	6.83	116.58	110.47
37	Q	313	KC1	C2C-C1C-NC	6.83	118.90	110.45
37	H	313	KC1	CHD-C4C-NC	6.82	134.59	124.31
36	a	816	CLA	C1D-ND-C4D	-6.82	101.53	106.31
35	R	306	A86	C25-C26-C27	-6.82	117.72	127.28
37	Q	311	KC1	C2C-C1C-NC	6.82	118.89	110.45
37	H	313	KC1	CHB-C1B-NB	6.82	134.40	124.80
36	P	318	CLA	C4A-NA-C1A	6.82	109.79	106.68
35	B	303	A86	C25-C26-C27	-6.81	117.72	127.28
37	X	311	KC1	CHC-C4B-NB	6.81	134.39	124.80
37	P	315	KC1	C2C-C1C-NC	6.81	118.88	110.45
37	K	314	KC1	CHC-C4B-NB	6.81	134.39	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L	317	KC1	CHC-C4B-NB	6.81	134.39	124.80
37	W	217	KC1	CHC-C4B-NB	6.80	134.38	124.80
36	A	310	CLA	C4A-NA-C1A	6.80	109.78	106.68
36	K	316	CLA	C4A-NA-C1A	6.80	109.78	106.68
36	M	308	CLA	C4A-NA-C1A	6.79	109.78	106.68
36	a	806	CLA	C4A-NA-C1A	6.79	109.78	106.68
36	M	309	CLA	C4A-NA-C1A	6.78	109.77	106.68
36	b	830	CLA	C4A-NA-C1A	6.78	109.77	106.68
36	b	814	CLA	C4A-NA-C1A	6.78	109.77	106.68
37	G	318	KC1	CAB-C3B-C2B	-6.78	106.38	128.43
35	P	304	A86	C20-O1-C15	6.78	63.94	61.03
37	T	315	KC1	CAB-C3B-C2B	-6.78	106.40	128.43
36	K	308	CLA	C4A-NA-C1A	6.78	109.77	106.68
36	E	308	CLA	C4A-NA-C1A	6.77	109.77	106.68
37	T	310	KC1	CHC-C1C-C2C	6.77	135.72	125.03
35	Q	301	A86	C20-O1-C15	6.77	63.94	61.03
35	K	301	A86	O1-C20-C19	-6.77	107.15	113.49
36	Q	310	CLA	O2A-CGA-CBA	-6.76	91.22	111.83
36	U	307	CLA	C4A-NA-C1A	6.76	109.76	106.68
36	H	317	CLA	C4A-NA-C1A	6.75	109.76	106.68
36	l	204	CLA	C4A-NA-C1A	6.75	109.76	106.68
36	M	316	CLA	C4A-NA-C1A	6.75	109.76	106.68
37	O	313	KC1	C2C-C1C-NC	6.75	118.80	110.45
35	L	306	A86	C20-O1-C15	6.74	63.92	61.03
36	D	307	CLA	C4A-NA-C1A	6.73	109.75	106.68
37	G	318	KC1	C1A-NA-C4A	-6.73	103.61	106.68
37	J	314	KC1	CAB-C3B-C2B	-6.72	106.57	128.43
35	O	319	A86	C29-C30-C31	-6.72	169.73	177.66
36	M	314	CLA	C4A-NA-C1A	6.72	109.75	106.68
35	I	304	A86	C29-C30-C31	-6.72	169.73	177.66
37	L	317	KC1	CAB-C3B-C2B	-6.72	106.59	128.43
37	G	308	KC1	CHC-C4B-NB	6.72	134.26	124.80
37	G	318	KC1	CHD-C4C-NC	6.72	134.43	124.31
36	a	809	CLA	C4A-NA-C1A	6.72	109.74	106.68
37	H	313	KC1	CHD-C1D-ND	-6.71	113.98	124.05
36	W	208	CLA	C4A-NA-C1A	6.71	109.74	106.68
37	G	308	KC1	CHC-C4B-C3B	-6.71	113.89	125.21
37	E	309	KC1	CAB-C3B-C2B	-6.71	106.62	128.43
35	T	303	A86	C20-O1-C15	6.71	63.91	61.03
36	C	208	CLA	C4A-NA-C1A	6.70	109.74	106.68
36	b	821	CLA	C4A-NA-C1A	6.70	109.74	106.68
37	F	315	KC1	CAB-C3B-C2B	-6.70	106.66	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	317	CLA	C4A-NA-C1A	6.70	109.73	106.68
36	I	314	CLA	C4A-NA-C1A	6.70	109.73	106.68
37	Q	313	KC1	CAB-C3B-C2B	-6.70	106.66	128.43
37	L	315	KC1	CHC-C1C-NC	-6.69	113.85	124.23
37	M	313	KC1	C1A-NA-C4A	-6.69	103.62	106.68
37	O	313	KC1	CHC-C4B-NB	6.69	134.22	124.80
37	Q	311	KC1	CAB-C3B-C2B	-6.69	106.67	128.43
37	O	313	KC1	CAB-C3B-C2B	-6.69	106.67	128.43
35	U	302	A86	O1-C20-C21	-6.69	107.58	115.05
37	L	315	KC1	CHC-C4B-C3B	-6.69	113.94	125.21
37	M	317	KC1	CHD-C1D-ND	-6.68	114.02	124.05
36	K	310	CLA	C2B-C1B-NB	6.68	117.26	110.33
37	O	315	KC1	CHC-C4B-NB	6.68	134.21	124.80
36	W	214	CLA	C4A-NA-C1A	6.68	109.73	106.68
37	P	315	KC1	CAB-C3B-C2B	-6.68	106.72	128.43
37	P	315	KC1	CHC-C4B-NB	6.68	134.20	124.80
37	O	315	KC1	CAB-C3B-C2B	-6.68	106.72	128.43
36	P	302	CLA	C4A-NA-C1A	6.68	109.72	106.68
36	j	102	CLA	C4A-NA-C1A	6.67	109.72	106.68
37	J	314	KC1	CHB-C4A-C3A	-6.67	114.50	125.03
35	N	301	A86	C35-C34-C33	-6.66	97.92	109.89
37	Q	313	KC1	CHC-C4B-NB	6.66	134.18	124.80
37	R	317	KC1	CHD-C4C-NC	6.66	134.34	124.31
36	D	312	CLA	C4A-NA-C1A	6.66	109.72	106.68
37	W	217	KC1	C1D-ND-C4D	6.66	110.98	106.31
36	B	307	CLA	C4A-NA-C1A	6.66	109.72	106.68
37	Q	311	KC1	CHC-C4B-NB	6.66	134.17	124.80
35	S	301	A86	C35-C34-C33	-6.66	97.93	109.89
36	C	214	CLA	C4A-NA-C1A	6.65	109.72	106.68
37	B	310	KC1	C1D-ND-C4D	6.65	110.98	106.31
37	M	313	KC1	CAC-C3C-C4C	6.65	133.45	124.79
37	L	315	KC1	C1A-NA-C4A	-6.65	103.64	106.68
36	U	313	CLA	C4A-NA-C1A	6.65	109.71	106.68
37	G	318	KC1	CHC-C4B-NB	6.65	134.16	124.80
37	U	312	KC1	CAC-C3C-C4C	6.64	133.43	124.79
36	N	316	CLA	C4A-NA-C1A	6.64	109.71	106.68
37	G	318	KC1	CHC-C4B-C3B	-6.64	114.02	125.21
36	D	308	CLA	C4A-NA-C1A	6.64	109.71	106.68
34	S	307	DD6	C21-C20-C19	6.64	121.70	114.24
35	E	302	A86	O1-C20-C19	-6.63	107.27	113.49
37	F	308	KC1	CHC-C4B-C3B	-6.63	114.03	125.21
37	M	317	KC1	C1A-C2A-C3A	-6.63	101.19	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	E	309	KC1	CHC-C4B-NB	6.63	134.13	124.80
36	a	811	CLA	C4A-NA-C1A	6.63	109.70	106.68
37	L	317	KC1	CHC-C4B-C3B	-6.62	114.04	125.21
37	M	317	KC1	CHC-C4B-NB	6.62	134.12	124.80
37	R	317	KC1	CHC-C4B-NB	6.62	134.12	124.80
37	G	317	KC1	C1D-ND-C4D	6.62	110.95	106.31
37	F	315	KC1	CHC-C4B-C3B	-6.61	114.06	125.21
37	F	315	KC1	CHC-C4B-NB	6.60	134.10	124.80
37	B	310	KC1	CHC-C4B-C3B	-6.60	114.08	125.21
37	X	311	KC1	C1D-ND-C4D	6.60	110.94	106.31
36	b	829	CLA	C4A-NA-C1A	6.60	109.69	106.68
35	J	303	A86	C20-O1-C15	6.60	63.86	61.03
36	F	309	CLA	C4A-NA-C1A	6.60	109.69	106.68
36	P	310	CLA	C4A-NA-C1A	6.60	109.69	106.68
37	X	311	KC1	CHD-C1D-ND	-6.60	114.16	124.05
37	W	217	KC1	CHD-C1D-ND	-6.59	114.16	124.05
35	W	202	A86	C35-C34-C33	-6.59	98.05	109.89
37	G	317	KC1	CHC-C4B-C3B	-6.59	114.10	125.21
37	T	310	KC1	C1B-CHB-C4A	-6.58	112.03	126.02
37	O	313	KC1	CHB-C4A-C3A	-6.58	114.64	125.03
37	Q	313	KC1	CHB-C4A-C3A	-6.58	114.64	125.03
36	Q	307	CLA	C4A-NA-C1A	6.58	109.68	106.68
36	K	315	CLA	C4A-NA-C1A	6.58	109.68	106.68
37	T	315	KC1	CHC-C4B-NB	6.58	134.06	124.80
35	X	303	A86	C3-C2-C1	-6.58	118.06	127.28
37	O	315	KC1	CHB-C4A-C3A	-6.57	114.65	125.03
37	F	308	KC1	CHB-C4A-C3A	-6.57	114.65	125.03
36	R	312	CLA	C4A-NA-C1A	6.57	109.68	106.68
37	Q	311	KC1	CHB-C4A-C3A	-6.57	114.66	125.03
36	W	211	CLA	C4A-NA-C1A	6.56	109.67	106.68
37	J	314	KC1	CHC-C4B-NB	6.56	134.04	124.80
36	E	311	CLA	C4A-NA-C1A	6.56	109.67	106.68
35	h	204	A86	O1-C20-C19	-6.56	107.34	113.49
35	V	302	A86	C29-C30-C31	-6.56	169.92	177.66
36	O	308	CLA	C4A-NA-C1A	6.56	109.67	106.68
37	P	315	KC1	CHB-C4A-C3A	-6.56	114.68	125.03
36	H	306	CLA	C4A-NA-C1A	6.55	109.67	106.68
35	L	319	A86	C35-C34-C33	-6.55	98.12	109.89
35	I	302	A86	C29-C30-C31	-6.55	169.93	177.66
35	X	302	A86	O1-C20-C21	-6.55	107.73	115.05
35	O	302	A86	C35-C34-C33	-6.54	98.13	109.89
36	a	805	CLA	C4A-NA-C1A	6.54	109.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	R	310	CLA	C4A-NA-C1A	6.54	109.66	106.68
34	S	307	DD6	C3-C2-C1	-6.54	118.11	127.28
36	R	318	CLA	C4A-NA-C1A	6.53	109.66	106.68
34	D	303	DD6	C21-C20-C19	6.53	121.58	114.24
35	G	305	A86	O1-C20-C19	-6.53	107.37	113.49
36	D	316	CLA	C4A-NA-C1A	6.53	109.66	106.68
36	K	311	CLA	C4A-NA-C1A	6.52	109.66	106.68
37	A	312	KC1	C2A-C3A-C4A	6.52	111.31	106.41
35	P	303	A86	C35-C34-C33	-6.52	98.18	109.89
36	G	307	CLA	C4A-NA-C1A	6.52	109.65	106.68
37	U	312	KC1	CHD-C1D-ND	-6.52	114.28	124.05
35	N	303	A86	C35-C34-C33	-6.51	98.18	109.89
35	A	302	A86	O1-C20-C21	-6.51	107.77	115.05
36	D	309	CLA	C4A-NA-C1A	6.51	109.65	106.68
36	H	311	CLA	C4A-NA-C1A	6.51	109.65	106.68
35	S	303	A86	C35-C34-C33	-6.51	98.19	109.89
37	F	308	KC1	CHC-C4B-NB	6.51	133.97	124.80
36	a	848	CLA	C4A-NA-C1A	6.51	109.65	106.68
36	D	309	CLA	C2B-C1B-NB	6.50	117.07	110.33
36	L	308	CLA	CHC-C1C-NC	-6.50	114.52	124.31
35	R	302	A86	C25-C26-C27	-6.50	118.16	127.28
37	O	313	KC1	CHC-C4B-C3B	-6.50	114.25	125.21
37	T	310	KC1	C4B-C3B-C2B	-6.49	101.18	106.81
36	J	309	CLA	C4A-NA-C1A	6.49	109.64	106.68
36	G	315	CLA	C2C-C1C-NC	6.49	116.79	109.98
37	Q	313	KC1	CHC-C4B-C3B	-6.48	114.28	125.21
37	K	314	KC1	CAB-C3B-C2B	-6.48	107.36	128.43
36	S	317	CLA	C4A-NA-C1A	6.47	109.63	106.68
37	T	315	KC1	CHC-C4B-C3B	-6.47	114.29	125.21
37	A	312	KC1	C2C-C1C-NC	6.47	118.46	110.45
35	N	320	A86	C25-C26-C27	-6.47	118.20	127.28
37	Q	311	KC1	CHC-C4B-C3B	-6.47	114.30	125.21
37	L	315	KC1	C2C-C1C-NC	6.47	118.45	110.45
37	P	315	KC1	CHC-C4B-C3B	-6.46	114.32	125.21
37	F	315	KC1	CHD-C1D-ND	-6.46	114.36	124.05
37	B	310	KC1	CAB-C3B-C2B	-6.46	107.44	128.43
37	O	315	KC1	CHC-C4B-C3B	-6.45	114.33	125.21
35	Q	303	A86	C29-C30-C31	-6.45	170.05	177.66
35	Q	304	A86	C25-C26-C27	-6.44	118.24	127.28
37	M	318	KC1	CHC-C4B-NB	6.44	133.87	124.80
37	M	318	KC1	CHC-C1C-NC	-6.44	114.25	124.23
37	E	309	KC1	CMD-C2D-C3D	6.43	145.95	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	J	314	KC1	C2C-C1C-NC	6.43	118.41	110.45
35	I	301	A86	O1-C20-C19	-6.43	107.47	113.49
36	a	803	CLA	C4A-NA-C1A	6.42	109.61	106.68
34	E	301	DD6	C21-C20-C19	6.42	121.46	114.24
35	M	304	A86	C4-C5-C6	-6.42	118.27	127.28
37	S	316	KC1	C1D-ND-C4D	6.42	110.82	106.31
36	b	809	CLA	C4A-NA-C1A	6.41	109.61	106.68
36	S	320	CLA	C4A-NA-C1A	6.41	109.60	106.68
34	K	305	DD6	C21-C20-C19	6.41	121.44	114.24
37	H	313	KC1	CHB-C1B-C2B	-6.41	112.16	125.49
36	G	319	CLA	CHD-C1D-ND	-6.41	115.79	124.80
37	G	308	KC1	CMD-C2D-C3D	6.40	145.86	125.67
36	A	307	CLA	C4A-NA-C1A	6.40	109.60	106.68
37	U	312	KC1	CHC-C4B-C3B	-6.40	114.42	125.21
36	J	317	CLA	C4A-NA-C1A	6.40	109.60	106.68
37	E	309	KC1	CHD-C1D-ND	-6.40	114.45	124.05
37	S	316	KC1	CHD-C1D-ND	-6.39	114.46	124.05
34	E	306	DD6	C21-C20-C19	6.39	121.42	114.24
36	j	102	CLA	C1D-ND-C4D	-6.39	101.83	106.31
36	I	312	CLA	C4A-NA-C1A	6.39	109.59	106.68
34	O	304	DD6	C21-C20-C19	6.39	121.42	114.24
37	E	309	KC1	CHC-C4B-C3B	-6.39	114.44	125.21
36	a	820	CLA	C4A-NA-C1A	6.38	109.59	106.68
37	G	308	KC1	C2C-C1C-NC	6.38	118.34	110.45
35	S	304	A86	C29-C30-C31	-6.38	170.14	177.66
36	b	833	CLA	C4A-NA-C1A	6.37	109.59	106.68
34	R	308	DD6	C9-C10-C11	-6.37	118.34	127.28
36	W	216	CLA	C2B-C1B-NB	-6.37	103.72	110.33
35	S	303	A86	C20-O1-C15	6.37	63.77	61.03
36	A	309	CLA	C4A-NA-C1A	6.36	109.58	106.68
34	H	303	DD6	C21-C20-C19	6.36	121.39	114.24
37	R	317	KC1	CHC-C1C-NC	-6.36	114.37	124.23
36	G	307	CLA	CHD-C1D-ND	-6.36	115.85	124.80
35	R	304	A86	C20-O1-C15	6.36	63.76	61.03
35	U	304	A86	C4-C5-C6	-6.35	118.37	127.28
37	T	310	KC1	C1D-CHD-C4C	-6.35	111.31	126.25
34	A	301	DD6	C3-C2-C1	-6.35	118.37	127.28
35	C	202	A86	O1-C20-C21	-6.35	107.95	115.05
36	N	317	CLA	C4A-NA-C1A	6.35	109.58	106.68
35	T	306	A86	C23-C16-C22	-6.35	98.15	107.37
36	b	837	CLA	C4A-NA-C1A	6.34	109.57	106.68
37	F	315	KC1	C2A-C3A-C4A	6.34	111.17	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	213	KC1	C2C-C1C-NC	6.33	118.29	110.45
37	W	213	KC1	C1A-C2A-C3A	-6.33	101.46	107.28
36	a	825	CLA	C4A-NA-C1A	6.33	109.57	106.68
36	b	822	CLA	C4A-NA-C1A	6.33	109.57	106.68
35	N	303	A86	C20-O1-C15	6.33	63.75	61.03
37	C	213	KC1	CHC-C4B-NB	6.33	133.71	124.80
37	U	312	KC1	C2C-C1C-NC	6.33	118.28	110.45
34	S	306	DD6	C21-C20-C19	6.33	121.35	114.24
36	B	309	CLA	CMD-C2D-C1D	6.32	135.86	124.73
36	R	322	CLA	C4A-NA-C1A	6.32	109.56	106.68
36	b	840	CLA	C4A-NA-C1A	6.31	109.56	106.68
36	I	313	CLA	C4A-NA-C1A	6.31	109.56	106.68
37	W	217	KC1	CAB-C3B-C2B	-6.31	107.92	128.43
36	l	201	CLA	C4A-NA-C1A	6.31	109.56	106.68
37	M	317	KC1	CAC-C3C-C4C	6.30	132.99	124.79
37	G	308	KC1	C1D-ND-C4D	6.30	110.73	106.31
37	W	213	KC1	CHC-C4B-C3B	-6.30	114.59	125.21
36	j	101	CLA	C4A-NA-C1A	6.30	109.55	106.68
37	X	311	KC1	CAB-C3B-C2B	-6.29	107.97	128.43
34	D	304	DD6	C21-C20-C19	6.29	121.31	114.24
36	S	319	CLA	C4A-NA-C1A	6.29	109.55	106.68
37	W	213	KC1	CHC-C4B-NB	6.29	133.66	124.80
35	R	301	A86	C35-C34-C33	-6.29	98.59	109.89
37	G	318	KC1	O2D-CGD-CBD	6.29	122.22	111.23
37	R	317	KC1	CHB-C1B-NB	6.29	133.65	124.80
36	a	822	CLA	CMD-C2D-C1D	6.28	135.79	124.73
34	L	305	DD6	C3-C2-C1	-6.28	118.47	127.28
37	X	311	KC1	C2C-C1C-NC	6.28	118.22	110.45
37	B	310	KC1	C2C-C1C-NC	6.27	118.22	110.45
36	b	834	CLA	C4A-NA-C1A	6.27	109.54	106.68
37	W	217	KC1	C2C-C1C-NC	6.27	118.21	110.45
36	S	314	CLA	C4A-NA-C1A	6.27	109.54	106.68
37	M	313	KC1	CHB-C1B-NB	6.26	133.62	124.80
35	X	304	A86	C35-C34-C33	-6.26	98.64	109.89
34	B	302	DD6	C3-C2-C1	-6.26	118.50	127.28
36	L	309	CLA	C4A-NA-C1A	6.26	109.53	106.68
37	R	317	KC1	CHD-C1D-ND	-6.26	114.66	124.05
36	I	310	CLA	C4A-NA-C1A	6.25	109.53	106.68
35	S	305	A86	C29-C30-C31	-6.25	170.29	177.66
36	N	308	CLA	CMC-C2C-C1C	6.24	134.79	125.03
35	T	307	A86	C29-C30-C31	-6.24	170.30	177.66
34	C	201	DD6	C21-C20-C19	6.24	121.25	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	209	CLA	C4A-NA-C1A	6.24	109.52	106.68
34	G	303	DD6	C21-C20-C19	6.23	121.24	114.24
35	O	305	A86	C3-C2-C1	-6.23	118.54	127.28
36	L	316	CLA	C4A-NA-C1A	6.23	109.52	106.68
36	R	311	CLA	C4A-NA-C1A	6.23	109.52	106.68
36	J	316	CLA	C4A-NA-C1A	6.22	109.52	106.68
35	R	302	A86	C20-O1-C15	6.22	63.70	61.03
37	G	317	KC1	C2C-C1C-NC	6.22	118.15	110.45
36	b	838	CLA	C4A-NA-C1A	6.22	109.52	106.68
36	X	310	CLA	C4A-NA-C1A	6.21	109.51	106.68
36	W	210	CLA	C4A-NA-C1A	6.21	109.51	106.68
36	b	841	CLA	CMC-C2C-C1C	-6.21	115.33	125.03
36	b	836	CLA	C3B-C4B-NB	6.21	116.07	110.53
35	N	320	A86	C29-C30-C31	-6.20	170.34	177.66
37	R	317	KC1	C2C-C1C-NC	6.20	118.13	110.45
36	J	307	CLA	C4A-NA-C1A	6.20	109.51	106.68
36	X	308	CLA	CHC-C4B-NB	6.20	133.34	124.05
36	H	310	CLA	C4A-NA-C1A	6.19	109.50	106.68
36	T	316	CLA	C4A-NA-C1A	6.19	109.50	106.68
37	F	315	KC1	C2A-C1A-NA	6.19	119.26	109.34
37	G	308	KC1	C1A-NA-C4A	-6.19	103.86	106.68
36	a	825	CLA	CMD-C2D-C1D	6.18	135.62	124.73
34	E	303	DD6	C21-C20-C19	6.18	121.19	114.24
37	B	310	KC1	CHB-C4A-C3A	-6.18	115.27	125.03
36	b	802	CLA	C4A-NA-C1A	6.18	109.50	106.68
37	M	313	KC1	CHC-C4B-NB	6.18	133.50	124.80
35	T	305	A86	O2-C18-C17	-6.17	97.12	109.75
37	D	314	KC1	C2C-C1C-NC	6.17	118.09	110.45
34	M	303	DD6	C21-C20-C19	6.16	121.16	114.24
36	P	319	CLA	C1D-ND-C4D	-6.16	101.99	106.31
36	I	308	CLA	CHD-C1D-ND	-6.15	116.14	124.80
37	L	317	KC1	C2C-C1C-NC	6.15	118.07	110.45
36	E	312	CLA	C4A-NA-C1A	6.15	109.49	106.68
36	S	309	CLA	C4A-NA-C1A	6.15	109.49	106.68
35	R	303	A86	C34-O4-C38	6.15	128.70	117.85
35	S	305	A86	C21-C20-C19	-6.14	107.34	114.24
36	X	315	CLA	C4A-NA-C1A	6.14	109.48	106.68
37	F	308	KC1	CAA-C2A-C1A	6.14	151.53	124.64
36	M	310	CLA	C4A-NA-C1A	6.13	109.48	106.68
37	W	213	KC1	C1D-ND-C4D	6.13	110.61	106.31
36	H	305	CLA	C4A-NA-C1A	6.13	109.48	106.68
37	U	312	KC1	C1D-ND-C4D	6.13	110.61	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	P	317	KC1	CHC-C1C-NC	-6.13	114.73	124.23
37	B	310	KC1	CHD-C1D-ND	-6.12	114.86	124.05
34	I	303	DD6	C21-C20-C19	6.12	121.12	114.24
34	E	304	DD6	C21-C20-C19	6.12	121.11	114.24
34	J	304	DD6	C21-C20-C19	6.12	121.11	114.24
35	Q	304	A86	C29-C30-C31	-6.11	170.45	177.66
36	U	306	CLA	C3D-C2D-C1D	-6.11	97.49	105.83
36	K	313	CLA	C4A-NA-C1A	6.11	109.47	106.68
37	W	213	KC1	CAB-C3B-C2B	-6.11	108.56	128.43
37	S	316	KC1	CHB-C4A-NA	6.11	133.70	124.23
37	T	310	KC1	C2D-C1D-ND	6.10	116.66	110.33
35	X	303	A86	C29-C30-C31	-6.10	170.46	177.66
37	N	314	KC1	CHC-C1C-NC	-6.10	114.78	124.23
36	C	205	CLA	C4A-NA-C1A	6.10	109.46	106.68
37	M	313	KC1	CHC-C4B-C3B	-6.09	114.94	125.21
36	L	308	CLA	C2B-C1B-NB	6.09	116.64	110.33
36	a	806	CLA	CMD-C2D-C1D	6.09	135.45	124.73
36	M	306	CLA	C4A-NA-C1A	6.09	109.46	106.68
37	U	312	KC1	C2A-C3A-C4A	6.08	110.98	106.41
37	A	312	KC1	C4B-CHC-C1C	-6.08	113.09	126.02
35	R	301	A86	C25-C26-C27	-6.08	118.75	127.28
37	C	213	KC1	CHC-C4B-C3B	-6.08	114.96	125.21
37	N	314	KC1	C1D-ND-C4D	6.08	110.58	106.31
36	D	311	CLA	C4A-NA-C1A	6.07	109.45	106.68
34	R	307	DD6	C21-C20-C19	6.06	121.05	114.24
37	R	317	KC1	C1D-ND-C4D	6.06	110.57	106.31
36	f	804	CLA	C2B-C1B-NB	6.06	116.61	110.33
36	a	823	CLA	CMD-C2D-C1D	6.06	135.40	124.73
37	L	317	KC1	C1D-ND-C4D	6.06	110.56	106.31
37	M	317	KC1	CHC-C4B-C3B	-6.06	114.99	125.21
35	W	202	A86	C23-C16-C17	-6.06	98.32	108.97
37	E	309	KC1	CHB-C4A-C3A	-6.06	115.47	125.03
37	O	315	KC1	CHC-C1C-NC	-6.05	114.85	124.23
36	V	307	CLA	C4A-NA-C1A	6.05	109.44	106.68
36	G	307	CLA	C2C-C1C-NC	6.05	116.34	109.98
37	P	315	KC1	CHC-C1C-NC	-6.05	114.85	124.23
37	M	317	KC1	CHC-C1C-NC	-6.04	114.86	124.23
37	Q	311	KC1	CHC-C1C-NC	-6.03	114.88	124.23
37	Q	313	KC1	CHC-C1C-NC	-6.03	114.88	124.23
35	X	301	A86	C35-C34-C33	-6.03	99.06	109.89
34	W	204	DD6	C21-C20-C19	6.02	121.00	114.24
35	F	307	A86	O4-C38-C39	6.02	121.82	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	307	CLA	C1D-ND-C4D	-6.02	102.09	106.31
37	E	309	KC1	CHC-C1C-NC	-6.01	114.91	124.23
36	b	801	CLA	C4A-NA-C1A	6.01	109.42	106.68
36	C	207	CLA	C3B-C4B-NB	6.01	115.89	110.53
36	G	319	CLA	C2B-C1B-NB	6.01	116.56	110.33
37	K	314	KC1	C2C-C1C-NC	6.01	117.89	110.45
36	A	306	CLA	C3B-C2B-C1B	-6.00	100.09	107.17
35	T	303	A86	C29-C30-C31	-6.00	170.58	177.66
37	O	313	KC1	CHC-C1C-NC	-6.00	114.93	124.23
36	E	315	CLA	C3B-C2B-C1B	-6.00	100.10	107.17
37	V	312	KC1	CHC-C4B-NB	5.99	133.24	124.80
36	a	822	CLA	C4A-NA-C1A	5.99	109.41	106.68
36	f	803	CLA	C2C-C1C-NC	5.99	116.27	109.98
36	b	828	CLA	C4A-NA-C1A	5.99	109.41	106.68
36	L	310	CLA	C4A-NA-C1A	5.99	109.41	106.68
36	K	309	CLA	C4A-NA-C1A	5.98	109.41	106.68
37	G	317	KC1	CAB-C3B-C2B	-5.98	108.98	128.43
35	I	304	A86	O1-C20-C21	-5.98	108.36	115.05
34	A	304	DD6	C21-C20-C19	5.98	120.96	114.24
37	T	315	KC1	CHB-C4A-C3A	-5.98	115.59	125.03
37	V	312	KC1	CHC-C4B-C3B	-5.97	115.14	125.21
36	l	205	CLA	O2D-CGD-CBD	5.97	121.67	111.23
36	f	804	CLA	CHD-C1D-ND	-5.97	116.40	124.80
37	M	313	KC1	CHC-C1C-NC	-5.97	114.98	124.23
36	Q	310	CLA	C1-C2-C3	5.96	135.97	126.20
36	G	307	CLA	C3B-C4B-NB	5.96	115.85	110.53
36	l	204	CLA	O2D-CGD-CBD	5.96	121.65	111.23
36	M	312	CLA	C4A-NA-C1A	5.96	109.40	106.68
37	T	310	KC1	CHC-C1C-NC	-5.95	115.01	124.23
36	N	319	CLA	CHD-C4C-C3C	5.94	133.44	124.77
36	V	314	CLA	CHD-C1D-ND	-5.94	116.44	124.80
37	P	315	KC1	CHD-C1D-ND	-5.94	115.14	124.05
37	O	313	KC1	CHD-C1D-ND	-5.94	115.14	124.05
36	D	306	CLA	C4A-NA-C1A	5.94	109.39	106.68
36	X	308	CLA	CAA-C2A-C1A	-5.94	92.53	111.97
37	P	317	KC1	C2C-C1C-NC	5.93	117.79	110.45
37	W	213	KC1	CHC-C1C-NC	-5.93	115.04	124.23
37	D	314	KC1	CAB-C3B-C2B	-5.93	109.15	128.43
35	U	301	A86	C8-C6-C5	5.93	128.33	119.01
35	X	301	A86	C40-C32-C31	-5.92	105.17	110.47
36	T	313	CLA	C4A-NA-C1A	5.92	109.38	106.68
36	a	835	CLA	C4A-NA-C1A	5.92	109.38	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	305	A86	C35-C34-C33	-5.92	99.26	109.89
36	H	318	CLA	C4A-NA-C1A	5.91	109.38	106.68
35	V	301	A86	C4-C5-C6	-5.91	118.99	127.28
34	R	307	DD6	C3-C2-C1	-5.91	118.99	127.28
37	F	315	KC1	C2C-C1C-NC	5.90	117.76	110.45
34	A	303	DD6	C21-C20-C19	5.90	120.87	114.24
35	M	305	A86	O1-C20-C21	-5.90	108.45	115.05
34	W	205	DD6	C21-C20-C19	5.90	120.87	114.24
36	E	313	CLA	C4A-NA-C1A	5.90	109.37	106.68
36	S	311	CLA	C4A-NA-C1A	5.90	109.37	106.68
35	U	301	A86	C25-C24-C1	-5.89	110.20	126.36
36	Q	310	CLA	CAA-C2A-C3A	5.89	128.92	113.00
37	T	315	KC1	C4D-CHA-C1A	-5.89	104.50	122.45
37	L	317	KC1	CAA-C2A-C1A	5.89	150.45	124.64
37	C	213	KC1	C1D-ND-C4D	5.89	110.44	106.31
35	T	302	A86	C29-C30-C31	-5.88	170.72	177.66
37	O	315	KC1	CHD-C1D-ND	-5.88	115.22	124.05
36	l	205	CLA	C3B-C4B-NB	5.88	115.78	110.53
36	a	801	CLA	C4A-NA-C1A	5.88	109.36	106.68
35	K	301	A86	C4-C5-C6	-5.88	119.03	127.28
36	J	311	CLA	C4A-NA-C1A	5.88	109.36	106.68
36	A	305	CLA	C4A-NA-C1A	5.88	109.36	106.68
37	D	314	KC1	C4B-CHC-C1C	-5.88	113.53	126.02
37	V	312	KC1	C1D-ND-C4D	5.87	110.43	106.31
36	R	321	CLA	C4A-NA-C1A	5.87	109.36	106.68
37	P	317	KC1	C1A-C2A-C3A	-5.87	101.88	107.28
37	Q	311	KC1	CHD-C1D-ND	-5.87	115.25	124.05
36	I	306	CLA	C3B-C4B-NB	5.87	115.77	110.53
36	A	306	CLA	C2C-C1C-NC	5.87	116.15	109.98
35	X	302	A86	C4-C5-C6	-5.87	119.05	127.28
36	a	802	CLA	CMD-C2D-C1D	5.86	135.05	124.73
36	b	817	CLA	O2D-CGD-CBD	5.86	121.47	111.23
37	Q	313	KC1	CHD-C1D-ND	-5.85	115.27	124.05
35	J	301	A86	O1-C20-C21	-5.85	108.51	115.05
36	b	812	CLA	C4A-NA-C1A	5.85	109.35	106.68
34	D	303	DD6	C24-C1-C2	-5.84	109.82	119.01
37	H	313	KC1	C4B-CHC-C1C	-5.84	113.60	126.02
37	S	316	KC1	CHC-C4B-C3B	-5.84	115.36	125.21
37	N	314	KC1	C2C-C1C-NC	5.84	117.68	110.45
37	G	318	KC1	CHB-C4A-C3A	-5.84	115.81	125.03
37	M	313	KC1	CHB-C4A-C3A	-5.84	115.81	125.03
37	J	314	KC1	CAA-C2A-C1A	5.84	150.22	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	F	313	CLA	C4A-NA-C1A	5.84	109.34	106.68
35	O	319	A86	C25-C26-C27	-5.84	119.09	127.28
37	U	312	KC1	C4B-C3B-C2B	-5.83	101.76	106.81
36	F	317	CLA	C3D-C2D-C1D	-5.83	97.87	105.83
36	F	317	CLA	C2C-C1C-NC	5.83	116.11	109.98
36	b	818	CLA	C4A-NA-C1A	5.83	109.34	106.68
35	U	301	A86	O1-C20-C19	-5.83	108.03	113.49
37	C	213	KC1	CHC-C1C-NC	-5.82	115.21	124.23
34	H	302	DD6	C21-C20-C19	5.82	120.78	114.24
35	T	303	A86	C25-C26-C27	-5.80	119.14	127.28
37	N	314	KC1	C4B-CHC-C1C	-5.80	113.68	126.02
37	L	315	KC1	C2A-C3A-C4A	5.80	110.77	106.41
35	J	301	A86	O1-C20-C19	-5.80	108.06	113.49
37	L	315	KC1	CAC-C3C-C4C	5.79	132.33	124.79
37	G	317	KC1	CHC-C1C-NC	-5.79	115.26	124.23
34	D	301	DD6	C3-C2-C1	-5.79	119.16	127.28
36	G	319	CLA	C2C-C1C-NC	5.79	116.06	109.98
36	X	313	CLA	C2B-C1B-NB	-5.78	104.33	110.33
37	G	308	KC1	CHC-C1C-NC	-5.78	115.27	124.23
36	E	315	CLA	C3B-C4B-NB	5.78	115.69	110.53
36	K	310	CLA	CHD-C1D-ND	-5.78	116.67	124.80
36	a	822	CLA	O2D-CGD-CBD	5.77	121.32	111.23
36	O	316	CLA	C1C-C2C-C3C	-5.77	100.91	106.98
37	M	313	KC1	CHD-C1D-ND	-5.77	115.40	124.05
37	T	310	KC1	C2A-C1A-CHA	5.77	152.64	128.96
35	V	302	A86	C35-C34-C33	-5.76	99.54	109.89
36	E	313	CLA	C2C-C1C-NC	5.76	116.03	109.98
35	J	302	A86	C4-C5-C6	-5.76	119.20	127.28
36	b	831	CLA	C4A-NA-C1A	5.76	109.31	106.68
35	G	306	A86	C25-C26-C27	-5.75	119.21	127.28
37	N	314	KC1	CMD-C2D-C1D	-5.75	116.66	125.42
36	E	315	CLA	CHD-C1D-ND	-5.75	116.71	124.80
35	I	304	A86	C34-O4-C38	5.75	128.00	117.85
37	W	217	KC1	CHB-C4A-NA	5.75	133.14	124.23
37	X	311	KC1	CHB-C4A-NA	5.75	133.14	124.23
35	K	306	A86	O4-C38-C39	5.75	121.34	111.09
36	D	309	CLA	C3B-C2B-C1B	-5.74	100.40	107.17
37	R	317	KC1	CHC-C4B-C3B	-5.74	115.53	125.21
37	S	316	KC1	CHC-C4B-NB	5.74	132.88	124.80
37	J	314	KC1	CHC-C1C-NC	-5.74	115.33	124.23
37	M	317	KC1	CMD-C2D-C3D	5.73	143.75	125.67
36	f	803	CLA	C3D-C2D-C1D	-5.73	98.01	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	T	315	KC1	CHC-C1C-NC	-5.73	115.35	124.23
36	C	207	CLA	C4A-NA-C1A	5.73	109.29	106.68
36	a	801	CLA	O2D-CGD-CBD	5.73	121.24	111.23
37	L	317	KC1	CHB-C4A-NA	5.72	133.10	124.23
36	J	316	CLA	CAC-C3C-C4C	5.71	132.22	124.79
37	R	317	KC1	CHB-C1B-C2B	-5.71	113.61	125.49
36	a	816	CLA	O2D-CGD-CBD	5.71	121.21	111.23
34	R	308	DD6	C4-C5-C6	-5.71	119.27	127.28
35	X	301	A86	O1-C20-C21	-5.71	108.67	115.05
35	U	301	A86	C4-C5-C6	5.71	135.28	127.28
36	G	319	CLA	C3D-C2D-C1D	-5.70	98.05	105.83
34	D	303	DD6	C-C1-C2	-5.70	113.58	122.82
35	h	204	A86	C3-C2-C1	-5.70	119.28	127.28
34	E	306	DD6	C14-C13-C11	-5.70	116.69	125.53
36	N	319	CLA	CHA-C4D-ND	5.70	144.31	132.55
36	C	207	CLA	C2C-C1C-NC	5.70	115.97	109.98
37	T	315	KC1	CAC-C3C-C4C	5.69	132.20	124.79
37	M	318	KC1	C1D-CHD-C4C	-5.69	112.86	126.25
36	V	314	CLA	C3D-C2D-C1D	-5.69	98.07	105.83
36	K	307	CLA	C3B-C4B-NB	5.69	115.61	110.53
36	I	308	CLA	C2B-C1B-NB	5.68	116.22	110.33
37	L	317	KC1	C2A-C3A-C4A	5.68	110.68	106.41
37	T	315	KC1	C2C-C1C-NC	5.67	117.47	110.45
37	H	313	KC1	CHC-C1C-NC	-5.67	115.44	124.23
37	C	213	KC1	C2C-C1C-NC	5.67	117.47	110.45
37	Q	313	KC1	C4B-CHC-C1C	-5.67	113.97	126.02
41	F	318	LHG	O4-P-O5	5.67	132.92	110.83
35	A	302	A86	C36-C31-C32	5.67	125.32	119.70
37	U	312	KC1	CHC-C4B-NB	5.67	132.78	124.80
37	G	317	KC1	C1A-C2A-C3A	-5.67	102.07	107.28
35	T	303	A86	C34-O4-C38	5.66	127.85	117.85
37	G	317	KC1	CAC-C3C-C4C	5.66	132.16	124.79
37	F	308	KC1	C4B-CHC-C1C	-5.66	113.99	126.02
37	O	313	KC1	C4B-CHC-C1C	-5.66	113.99	126.02
36	b	836	CLA	C3D-C2D-C1D	-5.66	98.11	105.83
36	N	310	CLA	C2B-C1B-NB	5.66	116.19	110.33
37	F	315	KC1	C4B-CHC-C1C	-5.65	114.00	126.02
37	L	317	KC1	CHC-C1C-NC	-5.65	115.47	124.23
37	Q	311	KC1	C4B-CHC-C1C	-5.65	114.01	126.02
37	N	314	KC1	C4D-CHA-C1A	-5.65	105.24	122.45
37	P	315	KC1	C4B-CHC-C1C	-5.64	114.03	126.02
37	O	315	KC1	C4B-CHC-C1C	-5.64	114.03	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	K	306	A86	O3-C36-C37	-5.64	98.50	109.22
37	G	318	KC1	CHC-C1C-NC	-5.64	115.49	124.23
37	C	213	KC1	CHD-C4C-NC	5.63	132.80	124.31
36	A	306	CLA	C3B-C4B-NB	5.63	115.55	110.53
36	S	319	CLA	CBA-CAA-C2A	-5.63	97.06	113.79
37	T	315	KC1	CHB-C1B-NB	5.62	132.71	124.80
35	N	304	A86	C21-C20-C15	-5.62	105.21	123.35
36	j	102	CLA	O2D-CGD-CBD	5.62	121.05	111.23
37	C	213	KC1	CHD-C1D-ND	-5.61	115.63	124.05
37	S	316	KC1	C2C-C1C-NC	5.61	117.40	110.45
35	V	302	A86	O1-C20-C19	5.61	118.75	113.49
37	F	308	KC1	O2D-CGD-CBD	5.61	121.03	111.23
36	X	308	CLA	C3B-C4B-NB	-5.61	105.53	110.53
34	L	305	DD6	C21-C20-C19	5.60	120.54	114.24
37	P	317	KC1	CHD-C1D-ND	-5.60	115.64	124.05
34	E	303	DD6	C14-C13-C11	-5.60	116.83	125.53
37	G	308	KC1	CHB-C4A-C3A	-5.60	116.18	125.03
35	Q	304	A86	O1-C20-C21	-5.60	108.79	115.05
36	C	207	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
36	C	207	CLA	C2B-C1B-NB	5.59	116.13	110.33
36	b	827	CLA	C4A-NA-C1A	5.59	109.23	106.68
37	P	317	KC1	CHB-C1B-NB	5.59	132.67	124.80
36	F	317	CLA	C3B-C4B-NB	5.59	115.52	110.53
37	M	313	KC1	C1D-ND-C4D	5.59	110.23	106.31
36	W	215	CLA	C4A-NA-C1A	5.59	109.23	106.68
37	G	318	KC1	CHD-C1D-ND	-5.59	115.67	124.05
35	N	320	A86	O1-C20-C21	-5.59	108.81	115.05
37	W	213	KC1	CHD-C1D-ND	-5.58	115.67	124.05
37	C	213	KC1	CHB-C1B-NB	5.58	132.66	124.80
37	B	310	KC1	CAA-C2A-C1A	5.58	149.10	124.64
35	N	305	A86	O4-C38-C39	5.58	121.04	111.09
36	a	824	CLA	CAC-C3C-C4C	-5.58	117.53	124.79
37	B	310	KC1	CHC-C1C-NC	-5.58	115.58	124.23
37	G	308	KC1	CAA-C2A-C1A	5.57	149.07	124.64
36	G	307	CLA	C4B-C3B-C2B	-5.57	100.37	107.30
36	G	319	CLA	C2D-C1D-ND	5.57	115.64	110.13
36	B	309	CLA	C4A-NA-C1A	5.57	109.22	106.68
35	C	202	A86	C34-O4-C38	5.57	127.68	117.85
36	G	310	CLA	C4A-NA-C1A	5.57	109.22	106.68
36	E	315	CLA	C2C-C1C-NC	5.56	115.83	109.98
36	C	207	CLA	O2D-CGD-CBD	5.56	120.96	111.23
35	X	303	A86	C4-C5-C6	-5.56	119.47	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Q	316	A86	O4-C38-C39	5.56	121.01	111.09
36	F	316	CLA	C4A-NA-C1A	5.56	109.22	106.68
36	Q	310	CLA	CAA-C2A-C1A	5.56	130.18	111.97
36	b	813	CLA	C4A-NA-C1A	5.55	109.21	106.68
37	H	313	KC1	CHC-C4B-C3B	-5.55	115.85	125.21
36	E	317	CLA	C4A-NA-C1A	5.55	109.21	106.68
35	X	305	A86	C29-C30-C31	-5.55	171.11	177.66
37	A	312	KC1	OBD-CAD-C3D	-5.55	115.44	128.42
36	a	830	CLA	CHB-C4A-NA	5.55	132.41	124.40
36	G	311	CLA	C4A-NA-C1A	5.55	109.21	106.68
35	A	316	A86	C4-C5-C6	-5.54	119.50	127.28
37	A	312	KC1	O2D-CGD-CBD	5.54	120.92	111.23
34	K	305	DD6	C3-C2-C1	-5.54	119.51	127.28
35	G	305	A86	O1-C20-C21	-5.54	108.86	115.05
37	N	314	KC1	CHB-C1B-NB	5.53	132.59	124.80
37	G	308	KC1	CHD-C1D-ND	-5.53	115.75	124.05
37	N	314	KC1	CHC-C4B-C3B	-5.53	115.89	125.21
37	J	314	KC1	C1D-ND-C4D	5.52	110.19	106.31
36	Q	310	CLA	O2A-C1-C2	5.52	129.35	108.11
37	X	311	KC1	C4B-CHC-C1C	-5.52	114.30	126.02
35	V	303	A86	C34-O4-C38	5.51	127.58	117.85
37	W	217	KC1	C4B-CHC-C1C	-5.51	114.31	126.02
37	T	315	KC1	C1D-ND-C4D	5.51	110.18	106.31
37	J	314	KC1	CHB-C1B-NB	5.51	132.55	124.80
35	X	304	A86	C25-C26-C27	-5.51	119.56	127.28
37	W	213	KC1	C4B-CHC-C1C	-5.50	114.34	126.02
36	V	314	CLA	C2C-C1C-NC	5.49	115.75	109.98
36	U	306	CLA	O2D-CGD-CBD	5.49	120.83	111.23
37	R	317	KC1	CHB-C4A-NA	5.48	132.74	124.23
36	l	202	CLA	C4A-NA-C1A	5.48	109.18	106.68
35	G	304	A86	O1-C15-C20	-5.48	54.80	59.45
37	M	313	KC1	C2C-C1C-NC	5.48	117.23	110.45
37	J	314	KC1	C4B-CHC-C1C	-5.48	114.37	126.02
37	B	310	KC1	CAC-C3C-C4C	5.48	131.92	124.79
37	H	313	KC1	C2C-C1C-NC	5.48	117.23	110.45
35	S	308	A86	C4-C5-C6	-5.47	119.61	127.28
36	a	804	CLA	C4A-NA-C1A	5.47	109.17	106.68
36	E	313	CLA	C2B-C1B-NB	5.47	116.00	110.33
37	M	317	KC1	C2C-C1C-NC	5.47	117.22	110.45
35	H	304	A86	C25-C26-C27	-5.46	119.62	127.28
37	K	314	KC1	CHC-C1C-NC	-5.46	115.77	124.23
36	N	310	CLA	C4A-NA-C1A	5.46	109.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	304	A86	O1-C20-C15	-5.46	57.04	59.23
35	V	302	A86	C23-C16-C22	-5.46	99.44	107.37
36	U	306	CLA	CHD-C1D-ND	-5.45	117.13	124.80
36	a	806	CLA	O2D-CGD-CBD	5.45	120.77	111.23
34	S	306	DD6	C3-C2-C1	-5.45	119.63	127.28
36	b	836	CLA	C2C-C1C-NC	5.45	115.71	109.98
36	a	824	CLA	CAC-C3C-C2C	5.45	137.57	127.56
37	B	310	KC1	C4B-CHC-C1C	-5.45	114.44	126.02
37	G	317	KC1	C4B-CHC-C1C	-5.45	114.44	126.02
35	U	301	A86	C9-C8-C6	-5.45	111.43	126.36
35	V	303	A86	C4-C5-C6	-5.44	119.65	127.28
35	G	306	A86	O1-C20-C19	-5.44	108.39	113.49
37	M	313	KC1	C4B-CHC-C1C	-5.44	114.46	126.02
34	F	303	DD6	C9-C10-C11	-5.44	119.65	127.28
35	G	304	A86	C21-C20-C15	5.44	140.90	123.35
37	M	313	KC1	O2D-CGD-CBD	5.43	120.72	111.23
37	D	314	KC1	CHC-C1C-NC	-5.43	115.82	124.23
36	X	313	CLA	C4D-CHA-C1A	-5.43	114.77	121.24
37	M	317	KC1	C1A-NA-C4A	-5.42	104.20	106.68
35	A	316	A86	O1-C20-C19	-5.42	108.41	113.49
36	G	319	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
35	C	204	A86	C8-C6-C5	5.41	127.53	119.01
37	P	317	KC1	C4B-CHC-C1C	-5.41	114.52	126.02
37	K	314	KC1	CHB-C1B-NB	5.41	132.41	124.80
36	I	306	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
35	X	301	A86	C4-C5-C6	-5.41	119.70	127.28
37	E	309	KC1	CAA-C2A-C1A	5.40	148.32	124.64
36	L	308	CLA	O2D-CGD-CBD	5.40	120.68	111.23
36	O	316	CLA	O2D-CGD-CBD	5.40	120.67	111.23
35	R	303	A86	O3-C36-C37	-5.40	98.96	109.22
36	U	306	CLA	C2D-C1D-ND	5.40	115.47	110.13
36	E	315	CLA	O2D-CGD-CBD	5.40	120.66	111.23
37	H	313	KC1	C1B-CHB-C4A	-5.39	114.56	126.02
37	T	310	KC1	O2D-CGD-CBD	5.39	120.65	111.23
36	F	317	CLA	C4B-C3B-C2B	-5.38	100.61	107.30
35	M	302	A86	C3-C2-C1	-5.38	119.73	127.28
36	f	804	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
37	C	213	KC1	C1A-C2A-C3A	-5.38	102.33	107.28
36	f	804	CLA	C2C-C1C-NC	5.38	115.63	109.98
35	U	304	A86	C3-C2-C1	-5.38	119.74	127.28
36	I	306	CLA	O2D-CGD-CBD	5.38	120.63	111.23
36	W	216	CLA	CMB-C2B-C1B	5.37	133.60	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	309	CLA	C2C-C1C-NC	5.37	115.62	109.98
36	C	207	CLA	CHD-C1D-ND	-5.37	117.25	124.80
37	V	312	KC1	CHB-C4A-C3A	-5.37	116.56	125.03
37	F	308	KC1	CHC-C1C-NC	-5.36	115.92	124.23
37	F	315	KC1	CHC-C1C-NC	-5.36	115.92	124.23
37	T	310	KC1	CHB-C1B-C2B	-5.36	114.33	125.49
36	a	830	CLA	O2D-CGD-CBD	5.36	120.61	111.23
37	M	313	KC1	CHB-C1B-C2B	-5.36	114.33	125.49
36	a	838	CLA	C4A-NA-C1A	5.36	109.12	106.68
36	D	316	CLA	CAC-C3C-C4C	5.36	131.76	124.79
37	W	213	KC1	CHD-C4C-NC	5.36	132.38	124.31
35	N	306	A86	C25-C26-C27	-5.36	119.77	127.28
36	F	317	CLA	C4A-NA-C1A	5.36	109.12	106.68
35	U	302	A86	C4-C5-C6	-5.36	119.77	127.28
35	T	306	A86	O4-C38-C39	5.35	120.64	111.09
36	b	836	CLA	O2D-CGD-CBD	5.35	120.58	111.23
36	X	313	CLA	CED-O2D-CGD	5.35	128.05	115.92
36	K	310	CLA	C4A-NA-C1A	5.35	109.12	106.68
37	F	308	KC1	CHB-C1B-C2B	-5.35	114.36	125.49
36	R	313	CLA	C4A-NA-C1A	5.35	109.12	106.68
37	X	311	KC1	CAA-C2A-C1A	5.34	148.06	124.64
36	K	310	CLA	O2D-CGD-CBD	5.34	120.57	111.23
37	W	217	KC1	CAA-C2A-C1A	5.34	148.05	124.64
37	A	312	KC1	CHC-C1C-NC	-5.34	115.95	124.23
37	F	308	KC1	C4B-C3B-C2B	-5.34	102.18	106.81
37	F	315	KC1	O2D-CGD-CBD	5.34	120.57	111.23
37	G	317	KC1	CHB-C4A-NA	5.34	132.51	124.23
36	L	311	CLA	C4A-NA-C1A	5.34	109.11	106.68
35	W	203	A86	C4-C5-C6	-5.34	119.79	127.28
37	P	317	KC1	C1D-ND-C4D	5.34	110.06	106.31
35	N	320	A86	C3-C2-C1	-5.33	119.80	127.28
34	B	304	DD6	C4-C5-C6	-5.33	119.80	127.28
36	P	319	CLA	C3B-C4B-NB	-5.33	105.77	110.53
37	S	316	KC1	C4B-CHC-C1C	-5.33	114.69	126.02
37	L	315	KC1	O2D-CGD-CBD	5.33	120.55	111.23
37	X	311	KC1	C1A-NA-C4A	-5.33	104.25	106.68
35	L	306	A86	C4-C5-C6	-5.32	119.81	127.28
37	U	312	KC1	CHC-C1C-NC	-5.32	115.98	124.23
37	S	316	KC1	CHC-C1C-NC	-5.32	115.98	124.23
35	C	204	A86	C-C1-C24	5.32	126.22	118.09
36	b	824	CLA	C2C-C1C-NC	5.32	115.57	109.98
37	X	311	KC1	CHC-C1C-NC	-5.32	115.99	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	825	CLA	O2D-CGD-CBD	5.32	120.52	111.23
36	a	823	CLA	O2D-CGD-CBD	5.31	120.52	111.23
37	N	314	KC1	CHC-C4B-NB	5.31	132.28	124.80
35	F	304	A86	O1-C20-C19	-5.31	108.51	113.49
34	B	304	DD6	C9-C10-C11	-5.31	119.83	127.28
37	S	316	KC1	CHB-C1B-C2B	-5.31	114.44	125.49
36	D	309	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
35	R	309	A86	C4-C5-C6	-5.30	119.84	127.28
37	W	217	KC1	CHC-C1C-NC	-5.30	116.01	124.23
37	K	314	KC1	C4B-CHC-C1C	-5.30	114.75	126.02
35	W	202	A86	C25-C26-C27	-5.30	119.84	127.28
35	U	303	A86	C3-C2-C1	-5.30	119.84	127.28
36	S	310	CLA	C1-C2-C3	5.30	134.87	126.20
37	L	315	KC1	C1D-ND-C4D	5.29	110.02	106.31
36	b	816	CLA	O2D-CGD-CBD	5.29	120.48	111.23
37	P	317	KC1	CHB-C4A-C3A	-5.29	116.68	125.03
35	K	303	A86	O1-C20-C21	-5.29	109.14	115.05
35	B	303	A86	O4-C38-C39	5.28	120.51	111.09
35	V	304	A86	C21-C20-C15	-5.28	106.29	123.35
37	C	213	KC1	C4B-CHC-C1C	-5.28	114.79	126.02
37	K	314	KC1	C4D-CHA-C1A	-5.28	106.35	122.45
37	W	217	KC1	C1A-NA-C4A	-5.28	104.27	106.68
35	N	303	A86	C3-C4-C5	-5.28	112.71	123.52
35	S	303	A86	C3-C4-C5	-5.28	112.72	123.52
36	R	312	CLA	O2D-CGD-CBD	5.28	120.46	111.23
35	V	304	A86	C35-C34-C33	-5.28	100.41	109.89
37	A	312	KC1	C4D-CHA-C1A	5.28	138.54	122.45
35	Q	304	A86	C3-C2-C1	-5.28	119.88	127.28
37	R	317	KC1	C1B-CHB-C4A	-5.27	114.81	126.02
35	E	307	A86	O1-C20-C19	-5.27	108.55	113.49
35	P	307	A86	C3-C2-C1	-5.27	119.88	127.28
37	T	315	KC1	C1B-CHB-C4A	-5.27	114.81	126.02
37	U	312	KC1	CAB-C3B-C4B	5.27	137.41	124.82
37	E	309	KC1	C1A-NA-C4A	-5.27	104.27	106.68
37	A	312	KC1	CAC-C3C-C4C	5.26	131.64	124.79
36	M	310	CLA	C3B-C4B-NB	-5.26	105.83	110.53
37	H	313	KC1	CHC-C4B-NB	5.26	132.20	124.80
37	V	312	KC1	C4D-CHA-C1A	-5.26	106.43	122.45
36	D	309	CLA	C3B-C4B-NB	5.25	115.22	110.53
35	W	203	A86	C25-C26-C27	-5.25	119.91	127.28
35	S	305	A86	C25-C26-C27	-5.25	119.91	127.28
35	G	304	A86	C35-C34-C33	-5.24	100.47	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	K	307	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
37	V	312	KC1	CHC-C1C-NC	-5.24	116.11	124.23
35	U	301	A86	O1-C20-C21	-5.24	109.19	115.05
37	M	317	KC1	CHB-C1B-NB	5.24	132.17	124.80
35	C	203	A86	C3-C2-C1	-5.23	119.94	127.28
37	L	317	KC1	C4B-CHC-C1C	-5.23	114.90	126.02
36	X	310	CLA	O2D-CGD-O1D	-5.23	113.67	123.85
37	R	317	KC1	CAA-C2A-C1A	5.23	147.55	124.64
36	O	316	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
36	K	307	CLA	O2D-CGD-CBD	5.22	120.36	111.23
35	S	301	A86	C21-C20-C15	5.22	140.21	123.35
35	U	302	A86	C25-C26-C27	-5.22	119.96	127.28
37	F	308	KC1	CHD-C1D-ND	-5.22	116.22	124.05
35	N	301	A86	C21-C20-C15	5.22	140.19	123.35
34	Q	302	DD6	C3-C2-C1	-5.21	119.97	127.28
35	X	303	A86	C34-O4-C38	5.21	127.05	117.85
35	W	203	A86	C35-C34-C33	-5.21	100.53	109.89
37	V	312	KC1	C2C-C1C-NC	5.20	116.89	110.45
36	X	310	CLA	CAA-C2A-C3A	-5.19	104.32	116.23
36	b	836	CLA	C4B-C3B-C2B	-5.19	100.84	107.30
35	T	302	A86	C35-C34-C33	-5.18	100.58	109.89
36	a	817	CLA	CMB-C2B-C3B	5.18	138.73	126.55
36	a	829	CLA	CMB-C2B-C1B	-5.18	117.54	125.42
34	D	301	DD6	C21-C20-C19	5.18	120.05	114.24
34	B	302	DD6	C9-C10-C11	-5.17	120.02	127.28
35	L	301	A86	C4-C5-C6	-5.17	120.02	127.28
35	Q	303	A86	C3-C2-C1	-5.17	120.02	127.28
35	F	305	A86	C29-C30-C31	-5.17	171.56	177.66
36	S	312	CLA	C4A-NA-C1A	5.17	109.04	106.68
35	X	302	A86	O4-C38-C39	5.17	120.30	111.09
37	M	318	KC1	CHB-C1B-NB	5.17	132.07	124.80
35	D	302	A86	O1-C20-C19	-5.16	108.65	113.49
37	T	310	KC1	C1A-NA-C4A	5.16	109.03	106.68
37	K	314	KC1	C1B-CHB-C4A	-5.16	115.06	126.02
37	R	317	KC1	C4B-CHC-C1C	-5.15	115.07	126.02
34	Q	302	DD6	C9-C10-C11	-5.14	120.06	127.28
35	E	305	A86	O1-C20-C19	-5.14	108.67	113.49
34	W	204	DD6	C3-C2-C1	-5.14	120.07	127.28
37	T	315	KC1	CHB-C4A-NA	5.14	132.20	124.23
35	B	303	A86	C4-C5-C6	-5.14	120.07	127.28
36	I	306	CLA	C4B-C3B-C2B	-5.14	100.91	107.30
37	T	310	KC1	C3A-C4A-NA	5.13	116.81	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L	315	KC1	C3C-C4C-NC	5.13	115.40	109.90
37	B	310	KC1	C2A-C3A-C4A	5.13	110.26	106.41
37	T	315	KC1	C4B-CHC-C1C	-5.13	115.12	126.02
34	P	305	DD6	C9-C10-C11	-5.13	120.09	127.28
35	U	303	A86	C25-C26-C27	-5.12	120.09	127.28
35	J	305	A86	O1-C20-C19	-5.12	108.69	113.49
37	M	318	KC1	O2D-CGD-CBD	5.12	120.18	111.23
37	G	308	KC1	CHB-C1B-NB	5.12	132.01	124.80
35	X	301	A86	C3-C2-C1	-5.12	120.10	127.28
37	L	317	KC1	CHD-C1D-ND	-5.12	116.37	124.05
35	B	303	A86	O1-C20-C21	-5.12	109.33	115.05
37	F	315	KC1	C1D-ND-C4D	5.12	109.90	106.31
35	N	301	A86	O1-C15-C20	-5.11	55.11	59.45
35	I	301	A86	C4-C5-C6	-5.11	120.11	127.28
35	X	314	A86	C4-C5-C6	-5.11	120.11	127.28
36	b	805	CLA	C4A-NA-C1A	5.11	109.01	106.68
35	X	304	A86	C23-C16-C17	-5.10	100.00	108.97
35	S	301	A86	O1-C15-C20	-5.10	55.12	59.45
34	W	205	DD6	C3-C2-C1	-5.10	120.12	127.28
35	R	302	A86	C35-C34-C33	-5.10	100.73	109.89
36	U	306	CLA	C1D-ND-C4D	-5.10	102.74	106.31
36	V	313	CLA	C4A-NA-C1A	5.09	109.00	106.68
35	R	304	A86	C21-C20-C19	5.09	119.96	114.24
37	L	317	KC1	CHB-C1B-NB	5.09	131.97	124.80
37	M	313	KC1	C1B-CHB-C4A	-5.09	115.21	126.02
35	X	301	A86	C23-C16-C17	-5.08	100.03	108.97
35	J	305	A86	O1-C20-C21	-5.08	109.37	115.05
36	Q	310	CLA	C4A-NA-C1A	5.08	109.00	106.68
37	P	317	KC1	CAB-C3B-C2B	-5.08	111.92	128.43
37	D	314	KC1	C4D-CHA-C1A	-5.07	106.98	122.45
36	b	824	CLA	C2B-C1B-NB	5.07	115.59	110.33
35	I	301	A86	C25-C26-C27	-5.07	120.17	127.28
35	X	302	A86	C23-C16-C22	-5.07	100.01	107.37
36	H	310	CLA	O2D-CGD-O1D	-5.06	113.99	123.85
37	U	312	KC1	C4B-CHC-C1C	-5.06	115.26	126.02
36	Q	310	CLA	C5-C3-C2	5.06	132.53	121.17
36	V	314	CLA	O2D-CGD-CBD	5.06	120.08	111.23
36	P	314	CLA	C4A-NA-C1A	5.06	108.99	106.68
35	h	202	A86	C4-C5-C6	-5.05	120.19	127.28
37	R	317	KC1	O2D-CGD-CBD	5.05	120.06	111.23
37	T	315	KC1	CHB-C1B-C2B	-5.05	114.99	125.49
36	G	315	CLA	C4A-NA-C1A	5.05	108.98	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	309	CLA	O2D-CGD-CBD	5.04	120.05	111.23
37	D	314	KC1	C1B-CHB-C4A	-5.04	115.30	126.02
37	J	314	KC1	CHD-C1D-ND	-5.04	116.48	124.05
37	P	315	KC1	O2D-CGD-CBD	5.04	120.04	111.23
36	G	319	CLA	C3B-C4B-NB	5.04	115.03	110.53
37	H	313	KC1	C1D-ND-C4D	5.04	109.85	106.31
35	B	301	A86	C4-C5-C6	-5.04	120.22	127.28
35	M	302	A86	O4-C38-C39	5.04	120.07	111.09
37	E	309	KC1	CHB-C4A-NA	5.03	132.04	124.23
37	E	309	KC1	O2D-CGD-CBD	5.03	120.03	111.23
34	A	301	DD6	C9-C10-C11	-5.03	120.22	127.28
35	H	304	A86	O1-C20-C19	-5.03	108.77	113.49
37	M	317	KC1	CHB-C4A-C3A	-5.03	117.08	125.03
36	b	836	CLA	CHD-C1D-ND	-5.03	117.72	124.80
37	C	213	KC1	C4D-CHA-C1A	-5.03	107.12	122.45
35	M	304	A86	O1-C20-C21	-5.03	109.43	115.05
34	P	305	DD6	C4-C5-C6	-5.03	120.23	127.28
35	W	203	A86	C3-C2-C1	-5.03	120.23	127.28
36	a	848	CLA	O2D-CGD-CBD	5.03	120.02	111.23
35	M	305	A86	O4-C38-C39	5.03	120.05	111.09
37	G	318	KC1	C4B-CHC-C1C	-5.02	115.34	126.02
35	S	308	A86	O1-C20-C21	-5.02	109.44	115.05
36	K	307	CLA	C4B-C3B-C2B	-5.02	101.06	107.30
37	V	312	KC1	CHB-C1B-NB	5.02	131.87	124.80
37	B	310	KC1	CHB-C4A-NA	5.02	132.01	124.23
35	K	301	A86	O1-C20-C21	-5.02	109.44	115.05
35	E	302	A86	O1-C20-C21	-5.01	109.44	115.05
35	H	304	A86	C4-C5-C6	-5.01	120.25	127.28
36	Q	310	CLA	C6-C5-C3	5.01	125.68	113.47
36	f	803	CLA	O2D-CGD-CBD	5.01	119.99	111.23
35	N	303	A86	C-C1-C24	5.01	125.74	118.09
37	O	313	KC1	O2D-CGD-CBD	5.01	119.99	111.23
34	Q	302	DD6	C4-C5-C6	-5.01	120.25	127.28
35	R	305	A86	C3-C2-C1	-5.01	120.26	127.28
35	K	303	A86	C35-C34-C33	-5.01	100.89	109.89
37	G	308	KC1	C4B-CHC-C1C	-5.01	115.38	126.02
37	E	309	KC1	CHB-C1B-NB	5.00	131.84	124.80
34	R	308	DD6	C21-C20-C19	5.00	119.86	114.24
36	P	319	CLA	C2D-C1D-ND	5.00	115.08	110.13
35	F	306	A86	O1-C20-C19	-5.00	108.81	113.49
36	O	312	CLA	C4A-NA-C1A	5.00	108.96	106.68
36	I	308	CLA	O2D-CGD-CBD	5.00	119.96	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	S	303	A86	C-C1-C24	4.99	125.71	118.09
35	L	307	A86	O1-C20-C21	-4.99	109.47	115.05
35	J	303	A86	C25-C26-C27	-4.99	120.28	127.28
37	Q	313	KC1	O2D-CGD-CBD	4.99	119.95	111.23
35	W	202	A86	C34-O4-C38	4.99	126.66	117.85
37	L	315	KC1	C4B-CHC-C1C	-4.99	115.42	126.02
35	O	319	A86	O4-C38-C39	4.99	119.98	111.09
37	P	317	KC1	O2D-CGD-CBD	4.99	119.95	111.23
35	O	301	A86	O1-C20-C21	-4.99	109.47	115.05
37	Q	311	KC1	O2D-CGD-CBD	4.99	119.94	111.23
37	E	309	KC1	CAC-C3C-C2C	4.98	136.71	127.56
35	N	306	A86	O4-C38-C39	4.98	119.97	111.09
35	F	305	A86	C4-C5-C6	-4.98	120.30	127.28
37	M	313	KC1	CAA-C2A-C1A	4.97	146.44	124.64
34	B	304	DD6	C21-C20-C19	4.97	119.82	114.24
35	X	305	A86	C35-C34-C33	-4.97	100.96	109.89
37	G	317	KC1	CHD-C1D-ND	-4.97	116.60	124.05
35	H	304	A86	O4-C38-C39	4.97	119.95	111.09
35	J	302	A86	O1-C20-C21	-4.97	109.50	115.05
37	O	315	KC1	O2D-CGD-CBD	4.97	119.91	111.23
34	I	303	DD6	C3-C2-C1	-4.96	120.32	127.28
36	l	204	CLA	C2B-C1B-NB	4.96	115.47	110.33
37	E	309	KC1	C4B-CHC-C1C	-4.96	115.47	126.02
35	W	202	A86	O1-C20-C21	-4.96	109.50	115.05
36	G	315	CLA	O2D-CGD-CBD	4.96	119.90	111.23
35	R	302	A86	C3-C2-C1	-4.96	120.33	127.28
37	H	313	KC1	CAA-C2A-C1A	4.96	146.35	124.64
37	J	314	KC1	CHB-C4A-NA	4.95	131.91	124.23
36	Q	314	CLA	C4A-NA-C1A	4.95	108.94	106.68
37	S	316	KC1	CHB-C1B-NB	4.95	131.77	124.80
36	f	804	CLA	O2D-CGD-CBD	4.95	119.89	111.23
37	G	318	KC1	CHB-C1B-NB	4.95	131.77	124.80
35	G	306	A86	O4-C38-C39	4.95	119.91	111.09
35	J	306	A86	O1-C20-C21	-4.94	109.53	115.05
37	W	213	KC1	O2D-CGD-CBD	4.94	119.87	111.23
35	G	305	A86	C4-C5-C6	-4.94	120.35	127.28
37	K	314	KC1	C1D-ND-C4D	4.94	109.78	106.31
37	J	314	KC1	O2D-CGD-CBD	4.94	119.86	111.23
35	U	301	A86	C24-C1-C2	4.93	126.77	119.01
37	L	315	KC1	CHD-C1D-ND	-4.93	116.65	124.05
37	A	312	KC1	CHB-C4A-NA	4.93	131.87	124.23
37	J	314	KC1	CHB-C1B-C2B	-4.93	115.24	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	302	A86	C29-C30-C31	-4.93	171.85	177.66
37	P	317	KC1	C1B-CHB-C4A	-4.92	115.55	126.02
35	G	305	A86	O4-C38-C39	4.92	119.87	111.09
35	L	304	A86	C4-C5-C6	-4.92	120.38	127.28
36	b	824	CLA	O2D-CGD-CBD	4.92	119.82	111.23
35	G	304	A86	O1-C20-C19	4.91	118.10	113.49
35	M	301	A86	C3-C2-C1	-4.91	120.39	127.28
37	V	312	KC1	C1B-CHB-C4A	-4.91	115.58	126.02
36	l	205	CLA	C4B-C3B-C2B	-4.91	101.19	107.30
36	Q	310	CLA	O1A-CGA-CBA	4.91	142.99	123.78
37	G	317	KC1	CMD-C2D-C1D	-4.91	117.94	125.42
35	M	301	A86	O1-C20-C21	-4.91	109.56	115.05
37	P	317	KC1	CAC-C3C-C4C	4.91	131.17	124.79
36	B	309	CLA	O2D-CGD-CBD	4.91	119.81	111.23
35	J	302	A86	O1-C20-C19	-4.90	108.90	113.49
37	X	311	KC1	CHD-C4C-NC	4.90	131.69	124.31
37	A	312	KC1	CHB-C1B-NB	4.89	131.69	124.80
37	J	314	KC1	C2A-C3A-C4A	4.89	110.08	106.41
35	F	305	A86	C23-C16-C17	-4.89	100.37	108.97
35	T	301	A86	C4-C5-C6	-4.89	120.42	127.28
36	D	309	CLA	CHD-C1D-ND	-4.89	117.92	124.80
35	N	301	A86	C3-C2-C1	-4.89	120.42	127.28
36	K	307	CLA	C4C-C3C-C2C	-4.89	99.78	106.89
35	E	302	A86	C4-C5-C6	-4.88	120.43	127.28
35	V	301	A86	O1-C20-C19	-4.88	108.91	113.49
35	S	301	A86	C3-C2-C1	-4.88	120.43	127.28
35	D	302	A86	C3-C2-C1	-4.88	120.43	127.28
35	G	304	A86	O-C13-C11	-4.88	110.53	121.04
35	F	306	A86	O1-C20-C21	-4.88	109.60	115.05
37	M	317	KC1	C4B-CHC-C1C	-4.88	115.66	126.02
37	H	313	KC1	CHB-C4A-NA	4.87	131.79	124.23
35	O	301	A86	O1-C20-C19	-4.87	108.92	113.49
37	N	314	KC1	C1B-CHB-C4A	-4.87	115.67	126.02
37	V	312	KC1	C1A-C2A-C3A	-4.87	102.81	107.28
36	b	826	CLA	C4D-CHA-C1A	-4.87	115.44	121.24
35	W	202	A86	C4-C5-C6	-4.87	120.45	127.28
37	H	313	KC1	O2D-CGD-CBD	4.86	119.73	111.23
37	W	217	KC1	CHD-C4C-NC	4.86	131.63	124.31
36	T	311	CLA	CAC-C3C-C2C	4.86	136.49	127.56
35	P	306	A86	C4-C5-C6	-4.86	120.47	127.28
37	K	314	KC1	CAA-C2A-C1A	4.86	145.92	124.64
36	I	308	CLA	C3B-C2B-C1B	-4.85	101.45	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	301	DD6	C21-C20-C19	4.85	119.69	114.24
36	K	310	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
34	M	303	DD6	C3-C2-C1	-4.85	120.48	127.28
34	A	304	DD6	C3-C2-C1	-4.85	120.48	127.28
36	F	317	CLA	O2D-CGD-CBD	4.85	119.70	111.23
37	T	315	KC1	CHD-C1D-ND	-4.84	116.78	124.05
37	F	308	KC1	C2A-C3A-C4A	4.84	110.05	106.41
37	B	310	KC1	O2D-CGD-CBD	4.84	119.70	111.23
34	P	305	DD6	C21-C20-C19	4.84	119.68	114.24
36	N	308	CLA	C4A-NA-C1A	4.84	108.89	106.68
37	L	317	KC1	CAC-C3C-C4C	4.83	131.08	124.79
37	U	312	KC1	O2D-CGD-CBD	4.83	119.68	111.23
35	E	305	A86	O4-C38-C39	4.83	119.70	111.09
36	E	315	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
36	X	313	CLA	O2D-CGD-O1D	-4.83	114.45	123.85
36	G	319	CLA	O2D-CGD-CBD	4.83	119.67	111.23
35	J	301	A86	C4-C5-C6	-4.82	120.51	127.28
37	M	317	KC1	O2D-CGD-CBD	4.82	119.65	111.23
37	D	314	KC1	CHB-C1B-NB	4.81	131.58	124.80
34	R	307	DD6	C9-C10-C11	-4.81	120.53	127.28
35	L	304	A86	O4-C38-C39	4.81	119.67	111.09
36	H	308	CLA	C4A-NA-C1A	4.81	108.87	106.68
36	E	313	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
35	P	304	A86	C3-C2-C1	-4.80	120.54	127.28
37	U	312	KC1	CMD-C2D-C1D	-4.80	118.11	125.42
35	X	303	A86	C25-C26-C27	-4.80	120.55	127.28
35	X	305	A86	O4-C38-C39	4.80	119.64	111.09
37	W	213	KC1	CHB-C1B-NB	4.80	131.55	124.80
35	M	301	A86	O4-C34-C33	4.79	119.91	107.64
36	a	806	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
35	N	306	A86	C4-C5-C6	-4.79	120.56	127.28
35	K	306	A86	C29-C30-C31	-4.79	172.01	177.66
35	U	303	A86	C4-C5-C6	-4.78	120.57	127.28
36	N	308	CLA	C3B-C4B-NB	-4.78	106.26	110.53
36	V	314	CLA	C4B-C3B-C2B	-4.78	101.36	107.30
35	P	307	A86	O1-C20-C21	-4.78	109.71	115.05
39	F	321	LMT	C3B-C4B-C5B	-4.78	101.57	110.23
36	b	830	CLA	CMB-C2B-C1B	-4.77	118.15	125.42
35	C	203	A86	O4-C38-C39	4.77	119.60	111.09
36	A	306	CLA	O2D-CGD-CBD	4.77	119.57	111.23
34	K	304	DD6	C4-C5-C6	-4.77	120.59	127.28
37	K	314	KC1	CHD-C1D-ND	-4.77	116.89	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	f	804	CLA	C3B-C4B-NB	4.77	114.79	110.53
35	F	301	A86	O1-C20-C21	-4.77	109.72	115.05
37	F	308	KC1	C1B-CHB-C4A	-4.77	115.89	126.02
35	Q	301	A86	C3-C2-C1	-4.77	120.59	127.28
35	Q	303	A86	O4-C38-C39	4.77	119.59	111.09
35	O	303	A86	C3-C2-C1	-4.77	120.59	127.28
37	A	312	KC1	CHB-C1B-C2B	-4.76	115.58	125.49
36	I	308	CLA	C4C-C3C-C2C	-4.76	99.96	106.89
36	K	307	CLA	CHD-C1D-ND	-4.76	118.11	124.80
35	X	302	A86	C3-C2-C1	-4.76	120.61	127.28
36	R	322	CLA	O1D-CGD-CBD	4.75	133.90	124.52
35	H	304	A86	C3-C2-C1	-4.75	120.61	127.28
37	L	315	KC1	CHB-C4A-C3A	-4.75	117.52	125.03
35	O	305	A86	O4-C38-C39	4.75	119.56	111.09
37	K	314	KC1	C2A-C3A-C4A	4.75	109.98	106.41
37	E	309	KC1	CHD-C4C-NC	4.75	131.47	124.31
35	K	306	A86	C41-C32-C31	4.75	114.72	110.47
37	N	314	KC1	CHB-C4A-C3A	-4.75	117.53	125.03
35	W	202	A86	C12-C11-C13	4.75	123.70	116.00
35	R	309	A86	O4-C38-C39	4.74	119.55	111.09
37	C	213	KC1	CHB-C4A-C3A	-4.74	117.54	125.03
35	S	305	A86	O1-C15-C20	-4.74	55.43	59.45
35	U	301	A86	O4-C38-C39	4.74	119.54	111.09
36	O	316	CLA	CHD-C1D-ND	-4.74	118.13	124.80
35	F	306	A86	C3-C2-C1	-4.74	120.63	127.28
37	F	315	KC1	CHB-C4A-NA	4.74	131.57	124.23
35	U	301	A86	C7-C6-C5	-4.74	115.14	122.82
35	M	305	A86	C29-C30-C31	-4.73	172.07	177.66
35	P	306	A86	O4-C38-C39	4.73	119.53	111.09
35	H	301	A86	C4-C5-C6	-4.73	120.64	127.28
35	X	302	A86	C25-C26-C27	-4.73	120.64	127.28
35	U	301	A86	C25-C26-C27	4.73	133.91	127.28
35	I	302	A86	C35-C34-C33	-4.73	101.39	109.89
35	J	303	A86	C35-C34-C33	-4.73	101.39	109.89
35	U	304	A86	O1-C20-C21	-4.73	109.76	115.05
37	N	314	KC1	CHB-C1B-C2B	-4.73	115.66	125.49
35	G	302	A86	O1-C20-C21	-4.72	109.77	115.05
35	I	304	A86	C3-C2-C1	-4.72	120.66	127.28
35	L	307	A86	C3-C2-C1	-4.72	120.66	127.28
34	S	307	DD6	C15-C14-C13	-4.72	116.02	125.99
37	M	313	KC1	C3C-C4C-NC	4.72	114.95	109.90
35	W	202	A86	C3-C2-C1	-4.72	120.66	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	L	306	A86	C24-C1-C2	4.72	126.43	119.01
35	J	306	A86	O4-C38-C39	4.72	119.50	111.09
36	a	819	CLA	CAC-C3C-C2C	4.71	136.22	127.56
34	H	303	DD6	C9-C10-C11	-4.71	120.67	127.28
35	U	302	A86	O4-C38-C39	4.71	119.50	111.09
37	G	308	KC1	C2A-C3A-C4A	4.71	109.95	106.41
36	b	824	CLA	C4D-C3D-CAD	4.71	113.22	108.11
35	F	307	A86	C29-C30-C31	-4.71	172.10	177.66
36	N	310	CLA	CMD-C2D-C1D	4.71	133.02	124.73
35	F	302	A86	O4-C38-C39	4.70	119.48	111.09
35	M	304	A86	O4-C38-C39	4.70	119.48	111.09
36	M	310	CLA	C1D-ND-C4D	-4.70	103.01	106.31
35	P	304	A86	O4-C38-C39	4.70	119.47	111.09
37	V	312	KC1	O2D-CGD-CBD	4.70	119.45	111.23
36	a	831	CLA	C4A-NA-C1A	4.70	108.82	106.68
34	j	103	DD6	C14-C13-C11	-4.70	118.24	125.53
37	V	312	KC1	CHB-C4A-NA	4.70	131.51	124.23
35	R	309	A86	O1-C20-C21	-4.70	109.80	115.05
36	S	315	CLA	CBA-CAA-C2A	4.69	123.75	114.05
37	S	316	KC1	O2D-CGD-CBD	4.69	119.43	111.23
37	G	308	KC1	CHB-C4A-NA	4.69	131.50	124.23
36	f	803	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
35	X	314	A86	O1-C20-C21	-4.69	109.81	115.05
37	L	315	KC1	CHB-C1B-NB	4.69	131.40	124.80
35	G	302	A86	C3-C2-C1	-4.69	120.70	127.28
36	E	312	CLA	CAA-C2A-C3A	-4.69	100.33	113.00
35	K	303	A86	C4-C5-C6	-4.69	120.70	127.28
35	K	302	A86	O4-C34-C33	4.68	119.62	107.64
37	N	314	KC1	C1A-C2A-C3A	-4.68	102.98	107.28
35	W	202	A86	O4-C38-O5	-4.68	113.95	122.99
34	P	305	DD6	C3-C2-C1	-4.68	120.72	127.28
35	R	305	A86	O4-C38-C39	4.67	119.42	111.09
34	H	303	DD6	C3-C2-C1	-4.67	120.72	127.28
37	B	310	KC1	CHB-C1B-NB	4.67	131.38	124.80
35	B	301	A86	O4-C38-C39	4.67	119.42	111.09
35	G	302	A86	O4-C38-C39	4.67	119.42	111.09
35	O	303	A86	O4-C38-C39	4.67	119.42	111.09
37	K	314	KC1	CHB-C1B-C2B	-4.67	115.77	125.49
35	R	306	A86	C35-C34-C33	-4.67	101.50	109.89
35	S	305	A86	C4-C5-C6	-4.67	120.73	127.28
35	F	302	A86	C4-C5-C6	-4.67	120.73	127.28
36	X	308	CLA	CAC-C3C-C4C	4.66	130.86	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	I	301	A86	O4-C38-C39	4.66	119.40	111.09
36	W	211	CLA	O2D-CGD-CBD	4.66	119.38	111.23
35	F	301	A86	C4-C5-C6	-4.66	120.74	127.28
35	Q	301	A86	O4-C38-C39	4.66	119.40	111.09
36	F	317	CLA	C4D-CHA-C1A	-4.66	115.69	121.24
35	P	304	A86	C4-C5-C6	-4.66	120.74	127.28
35	T	304	A86	O4-C38-C39	4.66	119.39	111.09
35	h	202	A86	O4-C38-C39	4.66	119.39	111.09
34	H	303	DD6	C4-C5-C6	-4.65	120.75	127.28
35	U	304	A86	O1-C20-C19	-4.65	109.13	113.49
35	J	306	A86	C3-C2-C1	-4.65	120.75	127.28
35	T	303	A86	C35-C34-C33	-4.65	101.53	109.89
35	L	307	A86	O4-C38-C39	4.65	119.38	111.09
35	Q	301	A86	C4-C5-C6	-4.65	120.76	127.28
35	E	307	A86	O1-C20-C21	-4.65	109.85	115.05
36	L	312	CLA	O1D-CGD-CBD	4.65	133.68	124.52
34	A	304	DD6	C9-C10-C11	-4.65	120.76	127.28
35	M	304	A86	C25-C26-C27	-4.65	120.76	127.28
35	T	306	A86	C3-C2-C1	-4.64	120.77	127.28
35	O	303	A86	C4-C5-C6	-4.64	120.77	127.28
35	N	304	A86	C19-C18-C17	-4.64	102.11	110.79
35	U	303	A86	O4-C38-C39	4.64	119.36	111.09
37	T	315	KC1	O2D-CGD-CBD	4.64	119.33	111.23
35	T	301	A86	O4-C38-C39	4.63	119.35	111.09
36	G	309	CLA	O2D-CGD-CBD	4.63	119.33	111.23
35	Q	304	A86	O4-C38-C39	4.63	119.35	111.09
37	S	316	KC1	C1B-CHB-C4A	-4.63	116.17	126.02
35	N	320	A86	O4-C38-C39	4.63	119.35	111.09
35	N	304	A86	C3-C2-C1	-4.63	120.78	127.28
35	L	306	A86	C3-C2-C1	-4.62	120.79	127.28
35	F	304	A86	O4-C38-C39	4.62	119.34	111.09
35	B	303	A86	C3-C2-C1	-4.62	120.80	127.28
35	T	301	A86	C3-C2-C1	-4.62	120.80	127.28
35	T	301	A86	C25-C26-C27	-4.62	120.80	127.28
35	N	301	A86	C4-C5-C6	-4.62	120.80	127.28
37	J	314	KC1	C1B-CHB-C4A	-4.62	116.21	126.02
35	S	305	A86	O4-C38-C39	4.62	119.32	111.09
36	B	309	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
35	G	306	A86	O1-C20-C21	-4.61	109.90	115.05
35	F	301	A86	O4-C38-C39	4.61	119.31	111.09
35	C	203	A86	O1-C20-C21	-4.61	109.90	115.05
37	P	317	KC1	CHB-C1B-C2B	-4.61	115.91	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	V	312	KC1	CHD-C1D-ND	-4.61	117.14	124.05
35	S	304	A86	O4-C38-C39	4.60	119.30	111.09
35	X	314	A86	C25-C26-C27	-4.60	120.82	127.28
35	L	301	A86	O4-C38-C39	4.60	119.29	111.09
37	M	317	KC1	C3C-C4C-NC	4.60	114.83	109.90
35	R	303	A86	C3-C2-C1	-4.60	120.83	127.28
35	J	302	A86	O4-C38-C39	4.60	119.29	111.09
35	S	301	A86	C4-C5-C6	-4.60	120.83	127.28
35	I	304	A86	O4-C38-O5	-4.59	114.12	122.99
35	R	306	A86	O1-C20-C21	-4.59	109.92	115.05
35	B	301	A86	O1-C20-C21	-4.59	109.92	115.05
35	V	301	A86	O4-C38-C39	4.59	119.27	111.09
36	O	316	CLA	C2C-C1C-NC	4.59	114.80	109.98
35	T	301	A86	O1-C20-C21	-4.59	109.92	115.05
37	P	315	KC1	C3C-C4C-NC	4.59	114.81	109.90
37	C	213	KC1	CHB-C1B-C2B	-4.58	115.95	125.49
35	J	305	A86	O4-C38-C39	4.58	119.26	111.09
35	L	319	A86	C3-C2-C1	-4.58	120.85	127.28
34	H	302	DD6	C3-C2-C1	-4.58	120.85	127.28
36	B	308	CLA	C4A-NA-C1A	4.58	108.77	106.68
35	V	304	A86	O1-C15-C20	-4.58	55.57	59.45
35	R	306	A86	C4-C5-C6	-4.58	120.86	127.28
35	O	302	A86	C3-C2-C1	-4.58	120.86	127.28
35	S	304	A86	C3-C2-C1	-4.57	120.86	127.28
35	B	303	A86	C23-C16-C17	-4.57	100.94	108.97
35	D	302	A86	O4-C38-C39	4.57	119.24	111.09
36	a	823	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
35	I	304	A86	C4-C5-C6	-4.57	120.87	127.28
37	M	317	KC1	C1B-CHB-C4A	-4.57	116.31	126.02
34	C	201	DD6	C3-C2-C1	-4.57	120.87	127.28
35	X	305	A86	C25-C26-C27	-4.57	120.87	127.28
35	O	319	A86	C4-C3-C2	-4.57	114.18	123.52
35	X	314	A86	O4-C38-C39	4.57	119.23	111.09
35	P	303	A86	C3-C2-C1	-4.56	120.88	127.28
36	a	822	CLA	C3B-C2B-C1B	-4.56	101.79	107.17
36	b	836	CLA	C3C-C4C-NC	4.56	116.27	110.43
34	K	304	DD6	C21-C20-C19	4.56	119.36	114.24
35	h	204	A86	O1-C20-C21	-4.56	109.95	115.05
37	O	313	KC1	C3C-C4C-NC	4.56	114.78	109.90
35	C	204	A86	C24-C1-C2	4.56	126.17	119.01
37	W	217	KC1	CHB-C1B-NB	4.56	131.22	124.80
37	Q	313	KC1	C3C-C4C-NC	4.55	114.78	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	316	A86	O4-C38-C39	4.55	119.21	111.09
35	R	304	A86	C3-C4-C5	-4.55	114.20	123.52
34	E	306	DD6	C4-C5-C6	-4.55	120.89	127.28
37	G	317	KC1	CHB-C1B-NB	4.55	131.21	124.80
36	l	205	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
36	L	308	CLA	C4A-NA-C1A	4.55	108.76	106.68
35	C	204	A86	O4-C38-C39	4.55	119.21	111.09
36	I	314	CLA	CMA-C3A-C2A	-4.55	105.80	116.23
37	Q	311	KC1	C3C-C4C-NC	4.55	114.78	109.90
37	W	213	KC1	CHB-C4A-C3A	-4.55	117.85	125.03
35	S	304	A86	O1-C20-C21	-4.55	109.97	115.05
36	b	819	CLA	CMB-C2B-C1B	-4.54	118.50	125.42
35	L	319	A86	O4-C34-C35	4.54	119.26	107.64
35	V	303	A86	O1-C20-C19	-4.54	109.23	113.49
35	J	301	A86	O4-C38-C39	4.54	119.18	111.09
35	S	308	A86	O4-C38-C39	4.54	119.18	111.09
37	G	317	KC1	C1B-CHB-C4A	-4.53	116.38	126.02
36	G	315	CLA	C3B-C4B-NB	4.53	114.58	110.53
36	f	803	CLA	C1D-ND-C4D	-4.53	103.13	106.31
35	O	301	A86	O4-C38-C39	4.53	119.16	111.09
37	C	213	KC1	C1B-CHB-C4A	-4.53	116.40	126.02
35	K	301	A86	O4-C38-C39	4.53	119.16	111.09
37	O	315	KC1	C3C-C4C-NC	4.52	114.75	109.90
35	M	302	A86	C4-C5-C6	-4.52	120.93	127.28
35	K	306	A86	C23-C16-C17	-4.52	101.02	108.97
35	O	302	A86	O4-C34-C35	4.52	119.21	107.64
36	a	814	CLA	CMC-C2C-C1C	-4.52	117.97	125.03
37	V	312	KC1	C4B-CHC-C1C	-4.52	116.41	126.02
35	P	303	A86	O4-C34-C35	4.52	119.21	107.64
37	F	308	KC1	C2A-C1A-NA	4.52	116.58	109.34
35	T	306	A86	C4-C5-C6	-4.52	120.94	127.28
35	F	304	A86	O1-C20-C21	-4.52	110.00	115.05
37	L	317	KC1	CHB-C1B-C2B	-4.52	116.09	125.49
35	X	305	A86	C4-C5-C6	-4.51	120.95	127.28
35	L	301	A86	O1-C20-C19	-4.51	109.26	113.49
35	S	302	A86	O4-C38-C39	4.51	119.14	111.09
37	G	318	KC1	CHB-C1B-C2B	-4.51	116.10	125.49
35	T	307	A86	C3-C2-C1	-4.51	120.95	127.28
37	X	311	KC1	CHB-C1B-NB	4.51	131.15	124.80
37	L	317	KC1	O2D-CGD-CBD	4.51	119.11	111.23
36	W	212	CLA	CHD-C1D-ND	-4.51	118.46	124.80
37	L	317	KC1	C1B-CHB-C4A	-4.51	116.44	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	F	303	DD6	C4-C5-C6	-4.50	120.97	127.28
35	P	307	A86	O4-C38-C39	4.50	119.11	111.09
35	W	203	A86	C23-C16-C17	-4.50	101.06	108.97
37	F	308	KC1	CHB-C4A-NA	4.49	131.20	124.23
35	K	306	A86	C36-C31-C32	-4.49	115.24	119.70
35	M	305	A86	C35-C34-C33	-4.49	101.81	109.89
36	U	313	CLA	CAA-C2A-C3A	-4.49	105.93	116.23
35	S	303	A86	C24-C1-C2	-4.49	111.94	119.01
35	E	307	A86	C4-C5-C6	-4.49	120.98	127.28
37	N	314	KC1	CMD-C2D-C3D	4.49	139.83	125.67
35	E	302	A86	C3-C2-C1	-4.49	120.98	127.28
37	E	309	KC1	C1B-CHB-C4A	-4.49	116.48	126.02
34	F	303	DD6	C21-C20-C19	4.49	119.28	114.24
34	W	205	DD6	C4-C5-C6	-4.49	120.98	127.28
35	N	303	A86	C24-C1-C2	-4.49	111.95	119.01
35	G	304	A86	O1-C20-C15	-4.49	57.42	59.23
35	N	302	A86	O4-C38-C39	4.49	119.09	111.09
36	G	319	CLA	C3C-C4C-NC	4.49	116.18	110.43
35	X	303	A86	O1-C15-C20	-4.48	55.65	59.45
35	J	305	A86	C4-C5-C6	-4.48	120.99	127.28
35	A	302	A86	C26-C25-C24	-4.48	110.21	123.20
37	F	315	KC1	CHB-C1B-NB	4.48	131.11	124.80
35	X	303	A86	O4-C38-O5	-4.48	114.34	122.99
35	N	303	A86	C40-C32-C31	4.48	114.48	110.47
35	V	301	A86	C25-C26-C27	-4.48	121.00	127.28
37	N	314	KC1	CHB-C4A-NA	4.47	131.17	124.23
37	E	309	KC1	CHB-C1B-C2B	-4.47	116.19	125.49
36	b	819	CLA	CAA-C2A-C3A	-4.47	100.92	113.00
37	L	315	KC1	CAB-C3B-C2B	-4.47	113.90	128.43
35	T	302	A86	C3-C2-C1	-4.47	121.01	127.28
35	S	303	A86	C40-C32-C31	4.47	114.47	110.47
35	N	304	A86	O4-C38-C39	4.46	119.05	111.09
34	C	201	DD6	C4-C5-C6	-4.46	121.02	127.28
37	D	314	KC1	CHB-C4A-C3A	-4.46	117.98	125.03
37	U	312	KC1	C2A-C1A-NA	4.46	116.49	109.34
37	G	308	KC1	CHB-C1B-C2B	-4.46	116.21	125.49
35	M	301	A86	C23-C16-C17	-4.46	101.13	108.97
37	D	314	KC1	CHB-C4A-NA	4.46	131.14	124.23
37	M	318	KC1	CHC-C1C-C2C	4.46	132.06	125.03
35	F	307	A86	O4-C34-C33	4.46	119.04	107.64
34	Q	302	DD6	C21-C20-C19	4.45	119.25	114.24
35	M	302	A86	C35-C34-C33	-4.45	101.88	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	X	304	A86	O1-C15-C20	-4.45	55.67	59.45
37	K	314	KC1	O2D-CGD-CBD	4.45	119.02	111.23
36	L	312	CLA	O2D-CGD-O1D	-4.45	115.18	123.85
36	b	824	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
36	W	216	CLA	CHC-C4B-NB	4.45	130.72	124.05
35	E	302	A86	O4-C38-C39	4.45	119.02	111.09
36	f	803	CLA	C3C-C4C-NC	4.45	116.13	110.43
36	G	309	CLA	O2D-CGD-O1D	-4.44	115.20	123.85
35	T	302	A86	O1-C20-C21	-4.44	110.08	115.05
36	M	306	CLA	C3B-C4B-NB	-4.44	106.57	110.53
35	B	303	A86	C29-C30-C31	-4.44	172.42	177.66
34	E	306	DD6	C3-C2-C1	-4.44	121.05	127.28
37	M	317	KC1	CHB-C1B-C2B	-4.44	116.26	125.49
35	X	305	A86	C3-C2-C1	-4.43	121.06	127.28
36	W	212	CLA	C4A-NA-C1A	4.43	108.70	106.68
37	V	312	KC1	C4C-C3C-C2C	-4.43	100.44	106.89
35	P	303	A86	O4-C38-O5	-4.43	114.43	122.99
35	L	301	A86	O1-C20-C21	-4.43	110.10	115.05
37	D	314	KC1	CAA-C2A-C1A	4.43	144.04	124.64
36	A	306	CLA	C3C-C4C-NC	4.43	116.10	110.43
36	f	802	CLA	C3B-C4B-NB	-4.43	106.58	110.53
37	P	317	KC1	CHB-C4A-NA	4.42	131.09	124.23
37	M	313	KC1	CHB-C4A-NA	4.42	131.09	124.23
37	G	308	KC1	C1B-CHB-C4A	-4.42	116.63	126.02
36	E	313	CLA	O2D-CGD-CBD	4.42	118.95	111.23
36	l	204	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
37	C	213	KC1	O2D-CGD-CBD	4.41	118.95	111.23
35	X	301	A86	O4-C38-O5	-4.41	114.47	122.99
35	E	307	A86	O4-C38-C39	4.41	118.96	111.09
36	X	308	CLA	CBC-CAC-C3C	4.41	124.38	112.42
34	D	304	DD6	C3-C2-C1	-4.41	121.09	127.28
41	G	301	LHG	O4-P-O5	4.41	132.96	112.44
37	V	312	KC1	CHB-C1B-C2B	-4.41	116.32	125.49
35	X	314	A86	O1-C20-C19	-4.40	109.36	113.49
35	O	302	A86	O4-C38-O5	-4.40	114.49	122.99
35	F	306	A86	O4-C38-C39	4.40	118.94	111.09
35	U	304	A86	O4-C38-C39	4.40	118.93	111.09
36	P	314	CLA	CAA-C2A-C3A	-4.40	101.12	113.00
35	R	303	A86	C25-C26-C27	-4.39	121.12	127.28
35	G	304	A86	O4-C38-O5	-4.39	114.51	122.99
35	L	319	A86	O4-C38-O5	-4.39	114.51	122.99
35	N	301	A86	C34-O4-C38	4.39	125.60	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	302	A86	O4-C34-C33	4.39	118.87	107.64
35	I	301	A86	C3-C2-C1	-4.39	121.12	127.28
35	C	203	A86	O1-C20-C19	-4.39	109.38	113.49
37	D	314	KC1	CAC-C3C-C4C	4.39	130.50	124.79
34	a	849	DD6	C21-C20-C19	4.39	119.17	114.24
36	H	315	CLA	CBC-CAC-C3C	4.39	124.31	112.42
36	W	210	CLA	CMB-C2B-C1B	-4.39	118.74	125.42
35	M	301	A86	C25-C26-C27	-4.38	121.13	127.28
36	a	802	CLA	CMD-C2D-C3D	-4.38	117.64	127.69
35	M	305	A86	C25-C26-C27	-4.38	121.14	127.28
37	A	312	KC1	C1D-ND-C4D	4.38	109.38	106.31
41	O	318	LHG	O4-P-O5	4.38	132.80	112.44
41	F	318	LHG	O3-P-O6	-4.38	95.26	106.67
36	j	102	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
35	O	302	A86	C4-C5-C6	-4.37	121.15	127.28
35	S	301	A86	C34-O4-C38	4.37	125.57	117.85
36	I	306	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
35	V	301	A86	O1-C20-C21	-4.37	110.17	115.05
35	R	303	A86	C4-C5-C6	-4.36	121.16	127.28
37	W	217	KC1	O2D-CGD-CBD	4.36	118.86	111.23
36	N	319	CLA	C2B-C1B-NB	4.36	114.85	110.33
35	T	305	A86	C3-C2-C1	-4.36	121.16	127.28
35	O	301	A86	C3-C2-C1	-4.36	121.16	127.28
35	R	304	A86	O1-C20-C21	-4.36	110.18	115.05
35	T	302	A86	C23-C16-C22	-4.36	101.04	107.37
35	X	305	A86	O1-C15-C20	-4.35	55.76	59.45
36	G	319	CLA	C4D-C3D-CAD	-4.35	103.38	108.11
36	b	836	CLA	C2D-C1D-ND	4.35	114.43	110.13
37	X	311	KC1	O2D-CGD-CBD	4.35	118.83	111.23
35	O	319	A86	C36-C31-C32	-4.35	115.38	119.70
35	K	302	A86	C3-C2-C1	-4.35	121.18	127.28
35	S	308	A86	C3-C2-C1	-4.35	121.18	127.28
35	P	303	A86	C4-C5-C6	-4.35	121.18	127.28
35	P	304	A86	C35-C34-C33	-4.34	102.08	109.89
35	D	302	A86	O1-C20-C21	-4.34	110.19	115.05
35	h	204	A86	C25-C26-C27	-4.34	121.19	127.28
35	O	301	A86	C4-C5-C6	-4.34	121.19	127.28
36	C	207	CLA	C2D-C1D-ND	4.34	114.42	110.13
36	I	309	CLA	CBA-CAA-C2A	-4.34	100.89	113.79
35	M	301	A86	O1-C20-C19	-4.34	109.43	113.49
35	S	301	A86	O4-C38-O5	-4.33	114.62	122.99
36	a	823	CLA	CHD-C4C-C3C	-4.33	118.46	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	305	A86	O1-C20-C21	-4.33	110.21	115.05
36	P	319	CLA	CHD-C1D-ND	-4.33	118.70	124.80
35	L	319	A86	C4-C5-C6	-4.33	121.20	127.28
35	C	204	A86	C3-C2-C1	-4.33	121.20	127.28
35	P	307	A86	C4-C5-C6	-4.33	121.20	127.28
35	M	302	A86	C25-C26-C27	-4.33	121.20	127.28
35	Q	303	A86	O1-C20-C21	-4.33	110.21	115.05
35	T	307	A86	C40-C32-C31	4.33	114.35	110.47
35	L	304	A86	C35-C34-C33	-4.32	102.12	109.89
37	G	308	KC1	O2D-CGD-CBD	4.32	118.79	111.23
35	Q	301	A86	C35-C34-C33	-4.32	102.12	109.89
35	O	303	A86	C35-C34-C33	-4.32	102.12	109.89
35	R	301	A86	O4-C38-O5	-4.32	114.65	122.99
37	M	318	KC1	CHB-C1B-C2B	-4.32	116.51	125.49
35	N	301	A86	O4-C38-O5	-4.32	114.66	122.99
39	F	321	LMT	O5B-C1B-C2B	-4.31	101.50	110.37
37	N	314	KC1	CAA-C2A-C1A	4.31	143.54	124.64
41	a	842	LHG	O4-P-O5	4.31	132.50	112.44
37	G	318	KC1	C1B-CHB-C4A	-4.31	116.86	126.02
37	W	217	KC1	C1B-CHB-C4A	-4.31	116.86	126.02
35	Q	303	A86	C4-C5-C6	-4.31	121.23	127.28
35	F	302	A86	O1-C20-C21	-4.31	110.23	115.05
35	P	306	A86	O1-C20-C21	-4.31	110.23	115.05
35	U	303	A86	O1-C20-C21	-4.31	110.23	115.05
36	A	306	CLA	C4A-NA-C1A	4.31	108.64	106.68
36	U	309	CLA	CBA-CAA-C2A	-4.30	100.98	113.79
34	O	304	DD6	C9-C10-C11	-4.30	121.24	127.28
36	f	803	CLA	C1C-C2C-C3C	-4.30	102.45	106.98
35	L	304	A86	C25-C26-C27	-4.30	121.24	127.28
37	J	314	KC1	C2A-C1A-NA	4.30	116.24	109.34
35	F	304	A86	C4-C5-C6	-4.30	121.25	127.28
35	P	307	A86	O1-C20-C19	-4.30	109.46	113.49
34	B	302	DD6	C21-C20-C19	4.30	119.07	114.24
35	J	301	A86	O1-C20-C15	-4.30	57.50	59.23
37	X	311	KC1	C1B-CHB-C4A	-4.30	116.88	126.02
36	b	816	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
34	A	303	DD6	C3-C2-C1	-4.30	121.25	127.28
35	h	204	A86	O1-C20-C15	-4.30	57.50	59.23
35	T	303	A86	C4-C5-C6	-4.29	121.25	127.28
36	G	307	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
35	F	302	A86	C3-C2-C1	-4.29	121.26	127.28
35	J	306	A86	O1-C20-C19	-4.29	109.47	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	V	309	CLA	CBA-CAA-C2A	-4.29	105.18	114.05
35	K	306	A86	C25-C26-C27	-4.29	121.27	127.28
35	N	305	A86	C34-O4-C38	-4.29	110.27	117.85
35	V	303	A86	O4-C38-O5	-4.29	114.71	122.99
34	E	301	DD6	C9-C10-C11	-4.29	121.27	127.28
35	R	301	A86	C4-C5-C6	-4.29	121.27	127.28
36	J	308	CLA	O2D-CGD-CBD	4.29	118.72	111.23
36	B	309	CLA	CMD-C2D-C3D	-4.28	117.86	127.69
35	O	319	A86	C3-C2-C1	4.28	133.28	127.28
36	D	307	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
41	G	321	LHG	O7-C7-C8	4.28	120.74	111.48
35	X	303	A86	C21-C20-C19	-4.28	109.44	114.24
35	R	301	A86	C3-C2-C1	-4.28	121.28	127.28
34	E	303	DD6	C4-C5-C6	-4.27	121.28	127.28
35	Q	316	A86	C34-O4-C38	-4.27	110.30	117.85
35	Q	301	A86	C25-C26-C27	-4.27	121.28	127.28
35	H	304	A86	O1-C20-C15	-4.27	57.51	59.23
36	f	803	CLA	C2B-C1B-NB	4.27	114.76	110.33
44	f	801	BCR	C2-C1-C6	4.27	116.64	110.44
35	T	306	A86	O1-C20-C21	-4.27	110.28	115.05
36	b	824	CLA	C3C-C4C-NC	4.27	115.90	110.43
35	R	301	A86	C34-O4-C38	4.27	125.38	117.85
36	V	314	CLA	C2D-C1D-ND	4.27	114.35	110.13
36	b	827	CLA	C3B-C4B-NB	-4.27	106.72	110.53
35	F	305	A86	O4-C38-C39	4.27	118.70	111.09
35	h	204	A86	O4-C38-C39	4.26	118.69	111.09
37	R	317	KC1	C3B-C2B-C1B	-4.26	103.01	107.05
34	S	306	DD6	C9-C10-C11	-4.26	121.30	127.28
37	G	317	KC1	CMD-C2D-C3D	4.26	139.11	125.67
37	J	314	KC1	C3C-C4C-NC	4.26	114.47	109.90
35	O	303	A86	C25-C26-C27	-4.26	121.30	127.28
35	F	301	A86	C3-C2-C1	-4.26	121.31	127.28
35	E	307	A86	C3-C2-C1	-4.26	121.31	127.28
36	C	207	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
35	P	304	A86	C25-C26-C27	-4.25	121.31	127.28
34	R	307	DD6	C4-C5-C6	-4.25	121.31	127.28
36	G	319	CLA	CHB-C4A-NA	4.25	130.53	124.40
37	L	315	KC1	CAA-C2A-C1A	4.25	143.26	124.64
37	J	314	KC1	C4B-C3B-C2B	-4.24	103.14	106.81
35	P	303	A86	C34-O4-C38	4.24	125.34	117.85
35	R	303	A86	C29-C30-C31	-4.24	172.66	177.66
36	I	305	CLA	O2D-CGD-O1D	-4.24	115.59	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	217	KC1	CAC-C3C-C4C	4.24	130.31	124.79
37	X	311	KC1	CAC-C3C-C4C	4.24	130.31	124.79
34	M	303	DD6	C4-C5-C6	-4.24	121.33	127.28
35	T	305	A86	O1-C15-C20	-4.24	55.86	59.45
36	f	804	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
34	J	304	DD6	C3-C2-C1	-4.23	121.34	127.28
37	K	314	KC1	CAC-C3C-C4C	4.23	130.30	124.79
35	H	304	A86	O1-C20-C21	-4.23	110.32	115.05
36	I	306	CLA	C2B-C1B-NB	4.23	114.72	110.33
35	K	301	A86	O1-C20-C15	-4.23	57.53	59.23
35	h	202	A86	O1-C20-C21	-4.23	110.32	115.05
35	B	303	A86	O1-C15-C20	-4.23	55.86	59.45
36	Q	314	CLA	C3B-C4B-NB	-4.23	106.75	110.53
35	X	314	A86	C3-C2-C1	-4.23	121.35	127.28
35	L	319	A86	C34-O4-C38	4.23	125.31	117.85
35	O	302	A86	C34-O4-C38	4.23	125.31	117.85
37	W	217	KC1	CHB-C1B-C2B	-4.22	116.70	125.49
35	B	301	A86	O1-C20-C19	-4.22	109.53	113.49
35	R	301	A86	O4-C34-C35	4.22	118.44	107.64
37	H	313	KC1	C4B-C3B-C2B	-4.22	103.16	106.81
35	H	301	A86	C23-C16-C17	-4.22	101.56	108.97
34	E	301	DD6	C3-C2-C1	-4.22	121.36	127.28
36	F	314	CLA	C7-C6-C5	-4.22	102.02	113.26
37	D	314	KC1	CHB-C1B-C2B	-4.22	116.72	125.49
35	F	304	A86	O1-C20-C15	-4.22	57.53	59.23
36	V	309	CLA	C2A-C1A-CHA	4.22	131.18	123.87
37	X	311	KC1	CHB-C1B-C2B	-4.21	116.72	125.49
35	N	301	A86	O4-C34-C33	4.21	118.42	107.64
35	O	302	A86	O1-C15-C20	-4.21	55.88	59.45
37	W	213	KC1	C1B-CHB-C4A	-4.21	117.07	126.02
36	C	212	CLA	CAC-C3C-C4C	4.21	130.27	124.79
35	M	305	A86	O1-C15-C20	-4.21	55.88	59.45
35	F	306	A86	O1-C20-C15	-4.21	57.54	59.23
35	A	316	A86	O1-C20-C21	-4.21	110.35	115.05
36	K	307	CLA	C3C-C4C-NC	4.21	115.82	110.43
35	S	301	A86	O4-C34-C33	4.21	118.40	107.64
37	D	314	KC1	C2A-C3A-C4A	4.20	109.57	106.41
37	O	313	KC1	CHB-C1B-NB	4.20	130.72	124.80
36	b	818	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
36	I	308	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
35	T	306	A86	C25-C26-C27	-4.20	121.39	127.28
36	E	315	CLA	C1C-C2C-C3C	-4.20	102.57	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	A	312	KC1	CAA-C2A-C1A	4.20	143.03	124.64
34	W	205	DD6	C9-C10-C11	-4.20	121.39	127.28
36	C	207	CLA	C3C-C4C-NC	4.19	115.80	110.43
40	L	302	DGD	O2G-C1B-C2B	4.19	120.55	111.48
37	Q	311	KC1	CHB-C1B-NB	4.19	130.71	124.80
35	G	306	A86	O1-C20-C15	-4.19	57.54	59.23
35	O	319	A86	O1-C20-C21	-4.19	110.36	115.05
35	T	301	A86	O1-C20-C15	-4.19	57.54	59.23
36	f	804	CLA	C3C-C4C-NC	4.19	115.80	110.43
37	N	314	KC1	C4B-C3B-C2B	-4.19	103.18	106.81
35	S	308	A86	O1-C20-C15	-4.19	57.54	59.23
36	N	308	CLA	CHC-C1C-NC	-4.19	118.01	124.31
35	O	305	A86	O1-C20-C21	-4.19	110.37	115.05
35	C	202	A86	C33-C32-C31	4.18	113.28	109.21
34	K	304	DD6	C3-C2-C1	-4.18	121.41	127.28
36	b	841	CLA	CMC-C2C-C3C	4.18	137.47	126.15
37	O	315	KC1	CHB-C1B-NB	4.18	130.69	124.80
44	a	844	BCR	C2-C1-C6	4.18	116.52	110.44
35	R	301	A86	O1-C15-C20	-4.18	55.90	59.45
36	I	309	CLA	C2A-C1A-CHA	4.18	131.12	123.87
37	H	313	KC1	CAC-C3C-C4C	4.18	130.23	124.79
36	P	314	CLA	CAA-C2A-C1A	-4.18	98.29	111.97
35	N	303	A86	C25-C26-C27	-4.18	121.42	127.28
37	Q	313	KC1	CHB-C1B-NB	4.17	130.68	124.80
35	Q	304	A86	O1-C15-C20	-4.17	55.91	59.45
35	L	319	A86	O1-C15-C20	-4.17	55.91	59.45
36	D	309	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
36	R	321	CLA	CMB-C2B-C1B	-4.17	119.07	125.42
35	S	303	A86	C25-C26-C27	-4.17	121.43	127.28
37	V	312	KC1	C3C-C4C-NC	4.17	114.37	109.90
36	F	317	CLA	CHD-C1D-ND	-4.17	118.94	124.80
35	P	303	A86	O1-C15-C20	-4.17	55.92	59.45
35	D	302	A86	C4-C5-C6	-4.17	121.44	127.28
35	R	309	A86	C35-C34-C33	-4.16	102.41	109.89
37	B	310	KC1	C1B-CHB-C4A	-4.16	117.17	126.02
35	N	320	A86	O1-C15-C20	-4.16	55.92	59.45
35	I	304	A86	C12-C11-C13	-4.16	109.25	116.00
37	P	315	KC1	CHB-C1B-NB	4.16	130.66	124.80
36	P	302	CLA	O2D-CGD-O1D	-4.16	115.75	123.85
35	T	305	A86	O4-C38-O5	-4.16	114.96	122.99
42	J	318	LMG	O7-C10-C11	4.16	120.47	111.48
36	D	309	CLA	C3C-C4C-NC	4.16	115.75	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	V	316	LMG	O7-C10-C11	4.16	120.47	111.48
37	F	315	KC1	CAA-C2A-C1A	4.16	142.85	124.64
35	K	306	A86	C4-C5-C6	-4.16	121.45	127.28
35	J	302	A86	O1-C20-C15	-4.16	57.56	59.23
36	a	804	CLA	C3B-C4B-NB	-4.15	106.82	110.53
36	L	308	CLA	CMB-C2B-C1B	4.15	131.74	125.42
36	Q	310	CLA	C2A-C3A-C4A	4.15	108.58	101.87
34	B	302	DD6	C4-C5-C6	-4.15	121.45	127.28
35	C	203	A86	O1-C20-C15	-4.15	57.56	59.23
35	R	303	A86	O4-C38-O5	-4.15	114.98	122.99
42	E	319	LMG	O7-C10-C11	4.15	120.46	111.48
35	K	302	A86	C4-C5-C6	-4.15	121.46	127.28
34	A	304	DD6	C4-C5-C6	-4.15	121.46	127.28
37	D	314	KC1	O2D-CGD-CBD	4.15	118.48	111.23
35	J	306	A86	C4-C5-C6	-4.14	121.47	127.28
36	b	816	CLA	C3B-C4B-NB	4.14	114.23	110.53
36	a	806	CLA	CMD-C2D-C3D	-4.14	118.19	127.69
37	N	314	KC1	O2D-CGD-CBD	4.14	118.47	111.23
35	O	302	A86	C23-C16-C17	-4.14	101.69	108.97
36	b	836	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
35	E	302	A86	O1-C20-C15	-4.14	57.56	59.23
36	P	314	CLA	C2A-C3A-C4A	4.14	108.55	101.87
35	S	304	A86	C41-C32-C31	-4.14	106.77	110.47
36	G	309	CLA	C1-C2-C3	4.14	132.97	126.20
36	R	322	CLA	CED-O2D-CGD	4.14	125.30	115.92
35	J	305	A86	O1-C20-C15	-4.14	57.57	59.23
36	a	822	CLA	CMD-C2D-C3D	-4.13	118.21	127.69
35	N	302	A86	C35-C34-C33	-4.13	102.46	109.89
37	B	310	KC1	CHB-C1B-C2B	-4.13	116.89	125.49
36	I	308	CLA	C3C-C4C-NC	4.13	115.72	110.43
34	E	301	DD6	C14-C13-C11	-4.13	119.12	125.53
42	J	319	LMG	O7-C10-C11	4.13	120.41	111.48
35	C	202	A86	O4-C38-O5	-4.13	115.02	122.99
37	F	315	KC1	CHB-C1B-C2B	-4.13	116.90	125.49
35	M	304	A86	O1-C20-C15	-4.12	57.57	59.23
34	j	103	DD6	C9-C10-C11	-4.12	121.50	127.28
35	A	316	A86	O1-C20-C15	-4.12	57.57	59.23
35	L	319	A86	C23-C16-C17	-4.12	101.72	108.97
35	P	303	A86	C23-C16-C17	-4.12	101.72	108.97
35	L	307	A86	C4-C5-C6	-4.12	121.50	127.28
35	L	301	A86	O1-C20-C15	-4.12	57.57	59.23
35	W	202	A86	O1-C15-C20	-4.12	55.95	59.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	G	305	A86	O1-C20-C15	-4.12	57.57	59.23
35	S	302	A86	C35-C34-C33	-4.12	102.48	109.89
36	G	319	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
34	D	304	DD6	C9-C10-C11	-4.12	121.50	127.28
36	D	315	CLA	CAA-C2A-C3A	-4.12	106.78	116.23
37	M	318	KC1	C2A-C1A-CHA	4.12	145.87	128.96
35	L	306	A86	C23-C16-C17	-4.12	101.73	108.97
41	F	319	LHG	O7-C7-C8	4.11	120.38	111.48
36	K	310	CLA	C3B-C4B-NB	4.11	114.20	110.53
34	W	204	DD6	C4-C5-C6	-4.11	121.51	127.28
36	K	307	CLA	CAC-C3C-C4C	4.11	130.14	124.79
41	a	843	LHG	O7-C7-C8	4.11	120.37	111.48
34	A	303	DD6	C9-C10-C11	-4.11	121.51	127.28
42	G	325	LMG	O7-C10-C11	4.11	120.37	111.48
36	f	804	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
37	U	312	KC1	CAA-C2A-C1A	4.11	142.64	124.64
35	F	305	A86	C3-C2-C1	-4.11	121.52	127.28
40	C	215	DGD	O2G-C1B-C2B	4.10	120.36	111.48
41	j	104	LHG	O7-C7-C8	4.10	120.36	111.48
36	A	306	CLA	C1C-C2C-C3C	-4.10	102.66	106.98
36	E	315	CLA	C4A-NA-C1A	4.10	108.55	106.68
42	a	852	LMG	O7-C10-C11	4.10	120.36	111.48
35	S	303	A86	C23-C16-C17	-4.10	101.76	108.97
36	N	313	CLA	C3B-C4B-NB	-4.10	106.87	110.53
35	T	306	A86	C35-C34-C33	-4.10	102.52	109.89
35	V	301	A86	C3-C2-C1	-4.10	121.53	127.28
35	J	305	A86	C3-C2-C1	-4.10	121.53	127.28
37	M	313	KC1	C4C-C3C-C2C	-4.10	100.93	106.89
41	G	320	LHG	O7-C7-C8	4.10	120.35	111.48
35	M	301	A86	O1-C15-C20	-4.10	55.98	59.45
36	A	314	CLA	CHB-C4A-NA	4.10	130.31	124.40
37	E	309	KC1	C2A-C3A-C4A	4.09	109.48	106.41
35	C	204	A86	O1-C20-C21	-4.09	110.48	115.05
35	N	303	A86	C23-C16-C17	-4.09	101.78	108.97
35	O	301	A86	O1-C20-C15	-4.09	57.58	59.23
37	G	317	KC1	CAA-C2A-C1A	4.09	142.56	124.64
35	J	306	A86	O1-C20-C15	-4.09	57.58	59.23
35	Q	304	A86	C36-C31-C32	-4.09	115.64	119.70
35	T	304	A86	O1-C20-C15	-4.09	57.58	59.23
41	f	808	LHG	O7-C7-C8	4.09	120.33	111.48
36	b	817	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
35	N	320	A86	C36-C31-C32	-4.09	115.64	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	303	A86	C23-C16-C17	-4.09	101.79	108.97
37	F	315	KC1	C3C-C4C-NC	4.09	114.28	109.90
35	S	308	A86	O1-C20-C19	-4.08	109.66	113.49
35	T	301	A86	O1-C20-C19	-4.08	109.66	113.49
35	O	319	A86	C35-C34-C33	-4.08	102.55	109.89
35	U	301	A86	C26-C25-C24	4.08	135.03	123.20
37	L	315	KC1	C1B-CHB-C4A	-4.08	117.35	126.02
35	P	307	A86	C25-C26-C27	-4.08	121.56	127.28
35	F	302	A86	O1-C20-C15	-4.08	57.59	59.23
35	X	314	A86	O1-C20-C15	-4.08	57.59	59.23
44	m	101	BCR	C2-C1-C6	4.08	116.36	110.44
35	S	303	A86	O4-C38-O5	-4.08	115.12	122.99
35	V	301	A86	O1-C20-C15	-4.08	57.59	59.23
37	G	317	KC1	C1A-NA-C4A	-4.07	104.82	106.68
37	O	315	KC1	CHB-C4A-NA	4.07	130.55	124.23
35	T	307	A86	O1-C15-C20	-4.07	56.00	59.45
36	X	315	CLA	CAA-C2A-C3A	-4.07	106.89	116.23
35	N	303	A86	O4-C38-O5	-4.07	115.13	122.99
35	F	304	A86	C3-C2-C1	-4.07	121.57	127.28
35	E	305	A86	O1-C20-C15	-4.07	57.59	59.23
36	U	306	CLA	C2B-C1B-NB	4.07	114.55	110.33
36	a	830	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
35	V	303	A86	C9-C10-C11	-4.07	115.14	126.64
42	D	320	LMG	O7-C10-C11	4.07	120.28	111.48
37	Q	311	KC1	CHB-C4A-NA	4.07	130.54	124.23
35	V	302	A86	C3-C2-C1	-4.07	121.58	127.28
37	C	213	KC1	CHB-C4A-NA	4.07	130.53	124.23
37	Q	313	KC1	CHB-C4A-NA	4.07	130.53	124.23
37	O	313	KC1	CHB-C4A-NA	4.06	130.53	124.23
44	b	847	BCR	C2-C1-C6	4.06	116.34	110.44
36	B	311	CLA	O1D-CGD-CBD	4.06	132.53	124.52
35	F	301	A86	O1-C20-C15	-4.06	57.60	59.23
36	V	314	CLA	C3B-C4B-NB	4.06	114.15	110.53
35	I	301	A86	O1-C20-C15	-4.06	57.60	59.23
35	N	306	A86	C29-C30-C31	-4.06	172.88	177.66
36	U	311	CLA	C1-C2-C3	-4.05	119.56	126.20
34	R	308	DD6	C3-C2-C1	-4.05	121.59	127.28
34	E	301	DD6	C4-C5-C6	-4.05	121.59	127.28
35	C	202	A86	O1-C15-C20	-4.05	56.02	59.45
42	h	206	LMG	O7-C10-C11	4.05	120.24	111.48
35	E	307	A86	O1-C20-C15	-4.05	57.60	59.23
41	f	809	LHG	O7-C7-C8	4.05	120.23	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	R	302	A86	C23-C16-C17	-4.04	101.86	108.97
35	I	301	A86	O1-C20-C21	-4.04	110.53	115.05
36	b	829	CLA	C3B-C4B-NB	-4.04	106.92	110.53
35	X	301	A86	C41-C32-C31	4.04	114.09	110.47
36	a	830	CLA	C4D-C3D-CAD	4.04	112.49	108.11
42	I	315	LMG	O7-C10-C11	4.04	120.22	111.48
41	i	104	LHG	O7-C7-C8	4.04	120.22	111.48
35	M	305	A86	C4-C5-C6	-4.04	121.61	127.28
37	M	317	KC1	CHD-C4C-NC	4.04	130.39	124.31
36	E	315	CLA	C3C-C4C-NC	4.04	115.60	110.43
37	H	313	KC1	C2A-C1A-NA	4.04	115.81	109.34
38	A	315	SQD	O47-C7-C8	4.04	120.21	111.48
35	X	302	A86	O1-C15-C20	-4.04	56.03	59.45
35	A	302	A86	O1-C15-C20	-4.03	56.03	59.45
35	U	302	A86	C21-C20-C19	4.03	118.77	114.24
34	P	305	DD6	C14-C13-C11	-4.03	119.27	125.53
36	a	825	CLA	CMD-C2D-C3D	-4.03	118.44	127.69
36	b	824	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
37	P	315	KC1	CHB-C4A-NA	4.03	130.48	124.23
38	b	804	SQD	O47-C7-C8	4.03	120.20	111.48
41	l	208	LHG	O7-C7-C8	4.03	120.20	111.48
37	G	317	KC1	CHB-C1B-C2B	-4.03	117.11	125.49
41	R	323	LHG	O7-C7-C8	4.03	120.19	111.48
35	W	202	A86	O4-C34-C33	4.03	117.94	107.64
37	W	213	KC1	CHB-C1B-C2B	-4.03	117.11	125.49
34	E	304	DD6	C3-C2-C1	-4.02	121.63	127.28
37	F	315	KC1	C1B-CHB-C4A	-4.02	117.47	126.02
35	M	305	A86	C3-C2-C1	-4.02	121.64	127.28
37	M	317	KC1	C4C-C3C-C2C	-4.02	101.04	106.89
36	N	315	CLA	CMB-C2B-C1B	-4.02	119.30	125.42
37	K	314	KC1	C4B-C3B-C2B	-4.02	103.33	106.81
37	O	315	KC1	C4B-C3B-C2B	-4.02	103.33	106.81
37	Q	311	KC1	C4B-C3B-C2B	-4.02	103.33	106.81
35	N	302	A86	C4-C5-C6	-4.02	121.65	127.28
35	U	304	A86	O1-C20-C15	-4.02	57.61	59.23
36	l	204	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
37	Q	313	KC1	C4B-C3B-C2B	-4.01	103.33	106.81
37	S	316	KC1	C2A-C3A-C4A	4.01	109.42	106.41
36	a	848	CLA	CHD-C4C-NC	4.01	130.45	124.23
35	R	309	A86	O1-C15-C20	-4.01	56.05	59.45
34	G	303	DD6	C3-C2-C1	-4.01	121.65	127.28
41	Q	315	LHG	O7-C7-C8	4.01	120.16	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	302	A86	O4-C38-C39	4.01	118.24	111.09
35	B	301	A86	O1-C20-C15	-4.01	57.62	59.23
37	L	315	KC1	C2A-C1A-NA	4.00	115.76	109.34
35	S	302	A86	C4-C5-C6	-4.00	121.67	127.28
37	O	313	KC1	C4B-C3B-C2B	-4.00	103.34	106.81
35	K	302	A86	C23-C16-C17	-4.00	101.94	108.97
35	P	307	A86	O1-C20-C15	-4.00	57.62	59.23
36	a	802	CLA	O2D-CGD-CBD	4.00	118.22	111.23
35	X	301	A86	O4-C34-C35	4.00	117.87	107.64
35	K	302	A86	O1-C15-C20	-4.00	56.06	59.45
35	I	302	A86	C25-C26-C27	-4.00	121.67	127.28
41	O	317	LHG	O7-C7-C8	3.99	120.12	111.48
36	W	216	CLA	CMB-C2B-C3B	-3.99	117.16	126.55
36	a	824	CLA	CBC-CAC-C3C	3.99	123.24	112.42
36	a	801	CLA	C1D-ND-C4D	-3.99	103.51	106.31
41	a	850	LHG	O7-C7-C8	3.99	120.11	111.48
35	T	307	A86	C25-C26-C27	-3.99	121.68	127.28
35	H	301	A86	C35-C34-C33	-3.99	102.72	109.89
37	R	317	KC1	C3C-C4C-NC	3.99	114.17	109.90
36	f	803	CLA	CHD-C1D-ND	-3.99	119.19	124.80
37	L	315	KC1	CHB-C4A-NA	3.99	130.41	124.23
36	a	835	CLA	C3B-C4B-NB	-3.99	106.97	110.53
36	a	823	CLA	CMD-C2D-C3D	-3.98	118.56	127.69
34	D	305	DD6	C21-C20-C19	3.98	118.71	114.24
42	G	324	LMG	O7-C10-C11	3.98	120.09	111.48
35	X	302	A86	C35-C34-C33	-3.98	102.73	109.89
36	a	830	CLA	CHA-C4D-ND	3.98	140.76	132.55
35	T	303	A86	O4-C38-O5	-3.98	115.31	122.99
35	L	307	A86	O1-C20-C15	-3.98	57.63	59.23
36	I	308	CLA	CAC-C3C-C4C	3.98	129.97	124.79
42	m	102	LMG	O7-C10-C11	3.98	120.08	111.48
37	P	315	KC1	C4B-C3B-C2B	-3.98	103.37	106.81
34	D	304	DD6	C14-C13-C11	-3.97	119.36	125.53
36	N	309	CLA	O2A-CGA-O1A	-3.97	113.69	123.63
37	U	312	KC1	CHB-C1B-NB	3.97	130.40	124.80
35	R	309	A86	C3-C2-C1	-3.97	121.71	127.28
34	O	304	DD6	C4-C5-C6	-3.97	121.71	127.28
37	A	312	KC1	C3A-C4A-NA	3.97	115.36	110.45
35	S	305	A86	C3-C2-C1	-3.97	121.72	127.28
36	X	312	CLA	CAA-C2A-C3A	-3.97	107.14	116.23
36	W	210	CLA	C2A-C1A-CHA	3.97	130.75	123.87
35	A	302	A86	C3-C4-C5	-3.97	115.41	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	308	CLA	CAC-C3C-C4C	3.96	129.95	124.79
36	b	840	CLA	CAC-C3C-C4C	3.96	129.95	124.79
36	l	201	CLA	O2D-CGD-O1D	-3.96	116.14	123.85
35	X	301	A86	C12-C11-C13	3.96	122.42	116.00
37	L	315	KC1	CHB-C1B-C2B	-3.96	117.25	125.49
37	W	213	KC1	CAC-C3C-C4C	3.96	129.94	124.79
37	S	316	KC1	C3B-C2B-C1B	-3.96	103.30	107.05
37	M	317	KC1	C4D-CHA-C1A	-3.96	110.39	122.45
36	b	826	CLA	O2D-CGD-O1D	-3.95	116.15	123.85
35	R	303	A86	C23-C16-C17	-3.95	102.02	108.97
37	A	312	KC1	C4B-C3B-C2B	-3.95	103.39	106.81
35	L	306	A86	O4-C38-C39	3.95	118.13	111.09
35	X	303	A86	C35-C34-C33	-3.95	102.79	109.89
42	L	321	LMG	O7-C10-C11	3.95	120.03	111.48
41	I	316	LHG	O7-C7-C8	3.95	120.02	111.48
35	I	304	A86	O1-C15-C20	-3.95	56.10	59.45
34	O	304	DD6	C15-C14-C13	-3.95	117.64	125.99
37	G	318	KC1	CHB-C4A-NA	3.95	130.35	124.23
36	R	319	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
37	T	310	KC1	C1C-C2C-C3C	-3.94	102.83	106.98
34	A	303	DD6	C4-C5-C6	-3.94	121.75	127.28
36	a	817	CLA	C4A-NA-C1A	3.94	108.48	106.68
35	X	303	A86	C21-C20-C15	3.94	136.08	123.35
35	X	301	A86	O1-C15-C20	-3.94	56.11	59.45
36	K	307	CLA	C2D-C1D-ND	3.94	114.03	110.13
36	J	308	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
35	T	307	A86	C4-C5-C6	-3.93	121.76	127.28
35	L	306	A86	C9-C8-C6	-3.93	115.58	126.36
36	b	817	CLA	C4C-C3C-C2C	-3.93	101.17	106.89
35	S	301	A86	O4-C34-C35	3.93	117.70	107.64
35	Q	303	A86	C12-C11-C13	3.93	122.37	116.00
35	U	301	A86	C-C1-C2	-3.93	116.45	122.82
42	E	318	LMG	O7-C10-C11	3.93	119.98	111.48
39	F	321	LMT	O5B-C5B-C4B	3.93	116.78	109.70
36	f	803	CLA	C4A-NA-C1A	3.93	108.47	106.68
41	D	319	LHG	O7-C7-C8	3.92	119.97	111.48
36	A	313	CLA	CAA-C2A-C3A	-3.92	107.23	116.23
35	F	307	A86	C25-C26-C27	-3.92	121.78	127.28
44	h	201	BCR	C40-C30-C25	3.92	116.39	110.24
34	B	304	DD6	C14-C13-C11	-3.92	119.44	125.53
36	a	829	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
35	F	307	A86	C3-C2-C1	-3.92	121.78	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	301	A86	O4-C34-C35	3.92	117.67	107.64
35	S	305	A86	C35-C34-C33	-3.92	102.84	109.89
34	E	303	DD6	C3-C2-C1	-3.92	121.78	127.28
35	I	304	A86	C7-C6-C5	-3.92	116.47	122.82
37	S	316	KC1	CAA-C2A-C1A	3.92	141.81	124.64
36	A	306	CLA	CHD-C1D-ND	-3.92	119.29	124.80
35	I	304	A86	C25-C26-C27	-3.92	121.79	127.28
36	X	308	CLA	O2A-CGA-O1A	-3.92	113.83	123.63
36	a	832	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
35	J	301	A86	C3-C2-C1	-3.91	121.79	127.28
34	B	304	DD6	C3-C2-C1	-3.91	121.79	127.28
35	X	304	A86	C4-C5-C6	-3.91	121.79	127.28
37	X	311	KC1	C4B-C3B-C2B	-3.91	103.42	106.81
41	b	850	LHG	O7-C7-C8	3.91	119.94	111.48
35	G	305	A86	C3-C2-C1	-3.91	121.79	127.28
36	E	316	CLA	CBC-CAC-C3C	3.91	123.02	112.42
36	I	305	CLA	C11-C12-C13	3.91	128.95	115.97
35	N	320	A86	C23-C16-C17	-3.91	102.11	108.97
35	V	303	A86	C40-C32-C31	3.91	113.97	110.47
36	A	314	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
35	S	305	A86	C21-C20-C15	3.90	135.95	123.35
36	B	311	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
37	F	315	KC1	C4B-C3B-C2B	-3.90	103.43	106.81
36	T	316	CLA	CAA-C2A-C3A	-3.90	107.29	116.23
35	D	302	A86	O1-C20-C15	-3.90	57.66	59.23
35	R	306	A86	O1-C15-C20	-3.90	56.14	59.45
35	W	202	A86	O4-C34-C35	3.90	117.61	107.64
36	R	318	CLA	CAA-C2A-C3A	-3.90	107.30	116.23
37	C	213	KC1	C4B-C3B-C2B	-3.90	103.44	106.81
34	K	305	DD6	C4-C5-C6	-3.89	121.82	127.28
36	b	833	CLA	O2D-CGD-O1D	-3.89	116.27	123.85
37	G	308	KC1	C4B-C3B-C2B	-3.89	103.44	106.81
34	j	103	DD6	C4-C5-C6	-3.89	121.82	127.28
36	D	308	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
35	E	307	A86	C25-C26-C27	-3.89	121.82	127.28
36	a	848	CLA	CHD-C4C-C3C	-3.88	119.11	124.77
36	W	216	CLA	CHB-C4A-NA	3.88	130.00	124.40
36	M	308	CLA	CBC-CAC-C3C	3.88	122.94	112.42
37	W	217	KC1	C4B-C3B-C2B	-3.88	103.45	106.81
36	j	102	CLA	C2D-C1D-ND	3.88	113.96	110.13
35	S	308	A86	C25-C26-C27	-3.88	121.84	127.28
35	T	302	A86	O4-C38-C39	3.87	118.00	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	305	A86	C23-C16-C22	-3.87	101.74	107.37
36	E	315	CLA	C1-C2-C3	-3.87	119.86	126.20
35	E	305	A86	C3-C2-C1	-3.87	121.85	127.28
37	P	315	KC1	O2D-CGD-O1D	-3.87	116.32	123.85
35	Q	304	A86	C23-C16-C17	-3.87	102.17	108.97
36	E	315	CLA	CHB-C4A-NA	3.86	129.98	124.40
37	U	312	KC1	CMD-C2D-C3D	3.86	137.85	125.67
35	L	304	A86	O1-C15-C20	-3.86	56.18	59.45
36	K	313	CLA	O2D-CGD-O1D	-3.86	116.34	123.85
36	a	802	CLA	C1-C2-C3	-3.85	119.88	126.20
35	N	302	A86	C25-C26-C27	-3.85	121.87	127.28
35	C	204	A86	C7-C6-C8	-3.85	112.20	118.09
34	a	849	DD6	C4-C5-C6	-3.85	121.88	127.28
35	J	303	A86	C4-C5-C6	-3.85	121.88	127.28
34	A	301	DD6	C14-C13-C11	-3.85	119.56	125.53
37	W	213	KC1	C4B-C3B-C2B	-3.85	103.48	106.81
37	Q	313	KC1	O2D-CGD-O1D	-3.85	116.36	123.85
36	l	202	CLA	O2D-CGD-O1D	-3.84	116.36	123.85
35	R	301	A86	C23-C16-C17	-3.84	102.21	108.97
35	S	302	A86	C25-C26-C27	-3.84	121.89	127.28
36	b	821	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
35	I	302	A86	O4-C38-C39	3.84	117.94	111.09
36	L	316	CLA	CAA-C2A-C3A	-3.84	107.42	116.23
34	a	849	DD6	C3-C2-C1	-3.84	121.89	127.28
35	K	302	A86	O4-C38-O5	-3.84	115.58	122.99
35	H	301	A86	O1-C15-C20	-3.84	56.19	59.45
36	N	319	CLA	C4D-CHA-C1A	3.84	125.82	121.24
36	b	802	CLA	C3B-C4B-NB	-3.84	107.11	110.53
37	H	313	KC1	C3C-C4C-NC	3.84	114.01	109.90
37	K	314	KC1	CHB-C4A-NA	3.84	130.18	124.23
37	M	313	KC1	C4B-C3B-C2B	-3.84	103.49	106.81
37	W	213	KC1	CAA-C2A-C1A	3.83	141.45	124.64
35	Q	316	A86	O1-C20-C15	-3.83	57.69	59.23
35	R	304	A86	C3-C2-C1	-3.83	121.90	127.28
36	G	309	CLA	C1-O2A-CGA	3.83	125.93	116.65
34	I	303	DD6	C4-C5-C6	-3.83	121.90	127.28
35	G	304	A86	C41-C32-C31	3.83	113.90	110.47
36	D	309	CLA	C2D-C1D-ND	3.83	113.92	110.13
36	H	314	CLA	CAA-C2A-C3A	-3.83	107.45	116.23
42	j	105	LMG	O7-C10-C11	3.83	119.76	111.48
37	Q	311	KC1	O2D-CGD-O1D	-3.83	116.40	123.85
37	O	313	KC1	O2D-CGD-O1D	-3.83	116.40	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	N	310	CLA	CAA-C2A-C3A	-3.83	107.46	116.23
36	X	313	CLA	CMB-C2B-C3B	3.82	135.54	126.55
36	b	806	CLA	CMB-C2B-C1B	-3.82	119.60	125.42
35	G	306	A86	C9-C8-C6	-3.82	115.88	126.36
36	O	316	CLA	C2D-C1D-ND	3.82	113.91	110.13
36	G	315	CLA	CMC-C2C-C1C	3.82	131.01	125.03
36	a	830	CLA	C2A-C3A-C4A	3.82	108.04	101.87
37	D	314	KC1	C3C-C4C-NC	3.82	113.99	109.90
36	P	316	CLA	CMA-C3A-C2A	-3.82	107.47	116.23
36	G	309	CLA	CED-O2D-CGD	3.82	124.58	115.92
36	Q	312	CLA	CMA-C3A-C2A	-3.82	107.48	116.23
36	P	319	CLA	C2A-C1A-CHA	3.81	130.49	123.87
37	L	315	KC1	C4B-C3B-C2B	-3.81	103.51	106.81
37	M	318	KC1	CMD-C2D-C3D	3.81	137.70	125.67
36	M	312	CLA	CAA-C2A-C3A	-3.81	102.69	113.00
35	C	204	A86	O1-C20-C15	-3.81	57.70	59.23
36	O	314	CLA	CMA-C3A-C2A	-3.81	107.49	116.23
36	a	848	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
35	X	304	A86	O4-C38-O5	-3.81	115.64	122.99
35	M	304	A86	C3-C2-C1	-3.81	121.94	127.28
35	T	307	A86	C35-C34-C33	-3.81	103.05	109.89
35	X	304	A86	C3-C2-C1	-3.80	121.94	127.28
37	O	315	KC1	O2D-CGD-O1D	-3.80	116.44	123.85
44	b	846	BCR	C2-C1-C6	3.80	115.97	110.44
36	V	309	CLA	CAA-C2A-C1A	3.80	124.44	111.97
42	D	321	LMG	O7-C10-C11	3.80	119.71	111.48
36	O	308	CLA	C4-C3-C5	3.80	121.83	115.23
36	S	313	CLA	C2A-C1A-CHA	3.80	130.46	123.87
36	Q	312	CLA	CAA-C2A-C3A	-3.80	107.52	116.23
37	G	318	KC1	C3C-C4C-NC	3.80	113.97	109.90
37	K	314	KC1	CHB-C4A-C3A	-3.80	119.03	125.03
36	U	306	CLA	C3C-C4C-NC	3.80	115.30	110.43
35	X	301	A86	C34-O4-C38	3.80	124.55	117.85
36	P	316	CLA	CAA-C2A-C3A	-3.79	107.53	116.23
36	G	313	CLA	CAA-C2A-C3A	-3.79	102.75	113.00
37	V	312	KC1	CAC-C3C-C2C	-3.79	120.59	127.56
34	F	303	DD6	C3-C2-C1	-3.79	121.96	127.28
34	E	303	DD6	C9-C10-C11	-3.79	121.96	127.28
36	W	218	CLA	CBC-CAC-C3C	3.79	122.70	112.42
36	a	822	CLA	C1-C2-C3	-3.79	119.99	126.20
36	I	308	CLA	C3D-C4D-ND	3.79	116.15	109.99
37	A	312	KC1	C1B-CHB-C4A	-3.79	117.97	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	O	314	CLA	CAA-C2A-C3A	-3.79	107.55	116.23
36	a	836	CLA	O2D-CGD-O1D	-3.79	116.48	123.85
36	E	313	CLA	CHB-C4A-NA	3.79	129.86	124.40
35	M	301	A86	O4-C38-O5	-3.78	115.68	122.99
36	a	819	CLA	CMC-C2C-C3C	3.78	136.38	126.15
36	G	315	CLA	CMD-C2D-C3D	-3.78	119.02	127.69
36	N	313	CLA	CMB-C2B-C1B	-3.78	119.67	125.42
40	b	849	DGD	O5D-C6D-C5D	-3.78	100.91	109.42
36	K	310	CLA	CHB-C4A-NA	3.78	129.85	124.40
35	S	304	A86	C4-C5-C6	-3.77	121.99	127.28
35	Q	304	A86	C41-C32-C31	3.77	113.85	110.47
36	O	316	CLA	C1-C2-C3	-3.77	120.02	126.20
35	A	302	A86	C8-C6-C5	-3.77	113.08	119.01
35	K	301	A86	C34-O4-C38	-3.77	111.19	117.85
36	B	309	CLA	C2B-C1B-NB	3.77	114.23	110.33
36	P	314	CLA	CBA-CAA-C2A	3.77	125.01	113.79
37	M	318	KC1	CMC-C2C-C1C	3.77	130.92	125.03
35	N	301	A86	O1-C20-C15	-3.76	57.72	59.23
41	E	322	LHG	O7-C7-C8	3.76	119.62	111.48
35	I	304	A86	C23-C16-C17	-3.76	102.36	108.97
36	N	313	CLA	CAA-C2A-C3A	-3.76	107.60	116.23
35	U	302	A86	C35-C34-C33	-3.76	103.14	109.89
35	N	305	A86	O1-C20-C15	-3.76	57.72	59.23
35	W	203	A86	O1-C15-C20	-3.75	56.27	59.45
35	S	303	A86	C3-C2-C1	-3.75	122.02	127.28
36	W	211	CLA	O2D-CGD-O1D	-3.75	116.54	123.85
37	T	315	KC1	C3C-C4C-NC	3.75	113.92	109.90
37	A	312	KC1	CBC-CAC-C3C	-3.75	102.25	112.42
36	f	804	CLA	C4D-CHA-C1A	-3.75	116.77	121.24
36	M	314	CLA	CAA-C2A-C3A	-3.75	107.63	116.23
36	N	310	CLA	CHD-C1D-C2D	3.75	133.29	125.49
34	K	305	DD6	C9-C10-C11	-3.75	122.02	127.28
35	R	305	A86	C4-C5-C6	-3.75	122.02	127.28
36	W	212	CLA	CMA-C3A-C2A	-3.75	99.48	113.98
35	N	306	A86	O1-C15-C20	-3.75	56.27	59.45
37	B	310	KC1	C2A-C1A-NA	3.75	115.35	109.34
36	E	315	CLA	C3D-C4D-ND	3.75	116.08	109.99
34	B	304	DD6	O1-C20-C19	-3.75	109.98	113.49
36	K	310	CLA	C2C-C1C-NC	3.75	113.92	109.98
37	D	314	KC1	CHD-C1D-C2D	3.75	138.30	127.43
36	N	310	CLA	C2D-C1D-ND	-3.75	106.42	110.13
35	K	303	A86	O1-C15-C20	-3.75	56.27	59.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	307	CLA	CMC-C2C-C1C	3.74	130.88	125.03
35	N	303	A86	C3-C2-C1	-3.74	122.03	127.28
37	O	313	KC1	CAC-C3C-C4C	3.74	129.66	124.79
37	M	313	KC1	C4D-CHA-C1A	-3.74	111.05	122.45
37	L	317	KC1	C4B-C3B-C2B	-3.74	103.57	106.81
36	M	307	CLA	C1-C2-C3	3.74	132.32	126.20
34	j	103	DD6	C3-C2-C1	-3.74	122.04	127.28
36	X	309	CLA	C2A-C1A-CHA	3.74	130.35	123.87
36	R	314	CLA	CAC-C3C-C4C	3.74	129.65	124.79
34	G	303	DD6	C4-C5-C6	-3.74	122.04	127.28
36	f	804	CLA	CHB-C4A-NA	3.74	129.79	124.40
35	F	302	A86	O1-C20-C19	-3.73	109.99	113.49
35	V	304	A86	C25-C26-C27	-3.73	122.05	127.28
35	K	302	A86	O1-C20-C21	-3.73	110.88	115.05
36	f	803	CLA	C1-C2-C3	-3.73	120.08	126.20
37	P	315	KC1	CAC-C3C-C4C	3.73	129.64	124.79
36	N	310	CLA	CMB-C2B-C3B	3.73	135.32	126.55
37	L	317	KC1	C2A-C1A-NA	3.73	115.31	109.34
35	S	301	A86	O1-C20-C15	-3.73	57.73	59.23
37	Q	313	KC1	CAC-C3C-C4C	3.73	129.64	124.79
36	D	313	CLA	O2A-CGA-O1A	-3.73	114.31	123.63
37	Q	311	KC1	CAC-C3C-C4C	3.72	129.63	124.79
35	T	303	A86	C3-C2-C1	-3.72	122.06	127.28
34	j	103	DD6	C21-C20-C19	3.72	118.42	114.24
35	F	305	A86	C35-C34-C33	-3.72	103.20	109.89
34	D	303	DD6	C15-C14-C13	-3.72	118.13	125.99
35	R	305	A86	O1-C20-C21	-3.72	110.89	115.05
35	M	305	A86	C23-C16-C17	-3.72	102.43	108.97
36	l	202	CLA	C3B-C4B-NB	-3.72	107.21	110.53
35	N	306	A86	C35-C34-C33	-3.72	103.21	109.89
36	G	315	CLA	C1-C2-C3	-3.72	120.11	126.20
36	f	804	CLA	C1D-ND-C4D	-3.72	103.70	106.31
36	a	802	CLA	C4D-C3D-CAD	-3.71	104.07	108.11
36	I	310	CLA	CMB-C2B-C1B	-3.71	119.76	125.42
37	O	315	KC1	CAC-C3C-C4C	3.71	129.62	124.79
36	a	801	CLA	CGD-CBD-CAD	3.71	122.87	110.85
37	T	315	KC1	CAD-C3D-C2D	-3.71	136.45	144.26
35	X	301	A86	O4-C34-C33	3.71	117.13	107.64
36	b	824	CLA	C1-C2-C3	-3.71	120.12	126.20
34	D	301	DD6	C9-C10-C11	-3.71	122.08	127.28
35	E	302	A86	C25-C26-C27	-3.71	122.08	127.28
35	N	320	A86	C41-C32-C31	3.71	113.79	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	T	310	KC1	CMA-C3A-C4A	3.71	130.82	125.03
35	K	306	A86	C34-O4-C38	-3.71	111.30	117.85
36	L	308	CLA	CHC-C4B-NB	3.70	129.61	124.05
34	Q	302	DD6	C14-C13-C11	-3.70	119.78	125.53
35	N	306	A86	C3-C2-C1	-3.70	122.09	127.28
36	H	311	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
36	K	315	CLA	CAA-C2A-C3A	-3.70	107.75	116.23
37	F	308	KC1	O2D-CGD-O1D	-3.70	116.65	123.85
36	X	308	CLA	CBA-CAA-C2A	3.70	124.79	113.79
35	C	204	A86	C25-C26-C27	3.70	132.46	127.28
35	G	304	A86	C28-C27-C26	-3.70	116.83	122.82
35	S	304	A86	O1-C20-C15	-3.69	57.74	59.23
37	M	317	KC1	CHD-C1D-C2D	3.69	138.15	127.43
35	B	301	A86	C34-O4-C38	-3.69	111.33	117.85
35	T	302	A86	O1-C15-C20	-3.69	56.32	59.45
37	G	318	KC1	CAC-C3C-C2C	3.69	134.34	127.56
36	V	305	CLA	CMD-C2D-C1D	3.69	131.23	124.73
37	L	315	KC1	C4D-CHA-C1A	-3.69	111.21	122.45
37	A	312	KC1	CHD-C1D-C2D	3.69	138.13	127.43
37	S	316	KC1	C2B-C1B-NB	3.69	113.77	110.13
35	X	301	A86	C23-C16-C22	-3.69	102.02	107.37
37	M	318	KC1	C1B-CHB-C4A	-3.69	118.19	126.02
35	X	301	A86	C25-C26-C27	-3.69	122.11	127.28
35	h	202	A86	O1-C20-C15	-3.68	57.75	59.23
36	K	307	CLA	CHD-C4C-C3C	-3.68	119.40	124.77
36	I	308	CLA	CHB-C4A-NA	3.68	129.71	124.40
37	W	213	KC1	CHB-C4A-NA	3.68	129.94	124.23
37	O	313	KC1	CHB-C1B-C2B	-3.68	117.83	125.49
36	A	306	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
35	U	302	A86	C41-C32-C31	3.68	113.76	110.47
37	Q	311	KC1	CHB-C1B-C2B	-3.68	117.84	125.49
35	P	303	A86	O4-C34-C33	3.67	117.04	107.64
35	F	305	A86	O1-C15-C20	-3.67	56.33	59.45
35	F	306	A86	C4-C5-C6	-3.67	122.13	127.28
37	O	315	KC1	CHB-C1B-C2B	-3.67	117.85	125.49
37	Q	313	KC1	CHB-C1B-C2B	-3.67	117.85	125.49
35	Q	303	A86	C33-C32-C31	3.67	112.78	109.21
37	P	315	KC1	CHB-C1B-C2B	-3.67	117.86	125.49
36	G	315	CLA	CHB-C4A-NA	3.67	129.69	124.40
35	L	319	A86	O4-C34-C33	3.67	117.03	107.64
35	G	302	A86	O1-C20-C15	-3.67	57.75	59.23
37	W	217	KC1	C2A-C3A-C4A	3.67	109.16	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	201	DD6	C9-C10-C11	-3.66	122.14	127.28
37	C	213	KC1	CAC-C3C-C4C	3.66	129.55	124.79
36	S	311	CLA	O2D-CGD-O1D	-3.66	116.73	123.85
35	K	303	A86	C23-C16-C17	-3.66	102.54	108.97
37	G	318	KC1	O2D-CGD-O1D	-3.66	116.73	123.85
35	O	302	A86	O4-C34-C33	3.66	116.99	107.64
36	N	319	CLA	O1D-CGD-CBD	3.65	131.72	124.52
37	O	313	KC1	CAA-C2A-C1A	3.65	140.65	124.64
36	G	314	CLA	CAA-C2A-C3A	-3.65	107.86	116.23
37	X	311	KC1	C2A-C3A-C4A	3.65	109.15	106.41
36	J	316	CLA	CAC-C3C-C2C	-3.65	120.85	127.56
34	J	304	DD6	C4-C5-C6	-3.65	122.16	127.28
44	b	846	BCR	C11-C10-C9	-3.65	122.16	127.28
35	C	202	A86	C3-C2-C1	-3.65	122.17	127.28
35	R	304	A86	C25-C26-C27	-3.65	122.17	127.28
35	X	305	A86	C23-C16-C17	-3.64	102.56	108.97
37	R	317	KC1	C2A-C1A-NA	3.64	115.18	109.34
37	P	315	KC1	CAA-C2A-C1A	3.64	140.60	124.64
36	M	310	CLA	CHC-C4B-NB	3.64	129.51	124.05
37	O	315	KC1	CAA-C2A-C1A	3.64	140.59	124.64
36	L	308	CLA	CMD-C2D-C3D	-3.64	119.34	127.69
37	Q	311	KC1	CAA-C2A-C1A	3.64	140.59	124.64
36	b	817	CLA	CAC-C3C-C4C	3.64	129.52	124.79
37	U	312	KC1	CHB-C4A-C3A	-3.64	119.28	125.03
35	L	306	A86	C26-C25-C24	-3.64	112.66	123.20
37	Q	313	KC1	CAA-C2A-C1A	3.64	140.58	124.64
35	U	302	A86	O1-C15-C20	-3.64	56.37	59.45
34	D	303	DD6	C3-C4-C5	3.63	130.95	123.52
37	T	315	KC1	C4B-C3B-C2B	-3.63	103.67	106.81
35	U	301	A86	O1-C20-C15	-3.63	57.77	59.23
35	P	306	A86	C34-O4-C38	-3.62	111.44	117.85
35	F	305	A86	C41-C32-C31	3.62	113.72	110.47
35	C	204	A86	C4-C3-C2	3.62	130.93	123.52
36	X	307	CLA	CBC-CAC-C3C	-3.62	102.61	112.42
35	K	302	A86	C29-C30-C31	-3.62	173.39	177.66
36	a	830	CLA	C1-C2-C3	-3.62	120.91	126.76
43	b	842	PQN	C11-C12-C13	-3.62	120.60	126.83
36	a	823	CLA	C1D-CHD-C4C	-3.62	118.33	126.02
37	F	315	KC1	C4C-C3C-C2C	-3.62	101.63	106.89
35	A	316	A86	C3-C2-C1	-3.61	122.21	127.28
36	I	313	CLA	CAA-C2A-C3A	-3.61	107.95	116.23
35	J	303	A86	O1-C20-C21	-3.61	111.01	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	P	317	KC1	CAA-C2A-C1A	3.61	140.46	124.64
36	a	819	CLA	CMC-C2C-C1C	-3.61	119.39	125.03
36	A	308	CLA	CMB-C2B-C1B	-3.61	119.92	125.42
35	J	301	A86	C34-O4-C38	-3.61	111.48	117.85
36	I	306	CLA	C1D-ND-C4D	-3.61	103.78	106.31
36	a	836	CLA	O1D-CGD-CBD	3.60	131.63	124.52
35	R	304	A86	O1-C15-C20	-3.60	56.40	59.45
36	E	308	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
34	S	306	DD6	C15-C14-C13	-3.60	118.38	125.99
34	D	305	DD6	C3-C2-C1	-3.60	122.23	127.28
36	a	816	CLA	C1-C2-C3	-3.60	120.30	126.20
34	W	204	DD6	C9-C10-C11	-3.60	122.23	127.28
35	F	306	A86	C25-C26-C27	-3.60	122.23	127.28
35	X	302	A86	C9-C8-C6	-3.60	116.50	126.36
37	G	317	KC1	C3C-C4C-NC	3.60	113.75	109.90
36	a	811	CLA	C3B-C4B-NB	-3.60	107.32	110.53
35	T	302	A86	C4-C5-C6	-3.60	122.23	127.28
35	R	305	A86	O1-C20-C15	-3.60	57.78	59.23
35	W	202	A86	C41-C32-C31	-3.59	107.25	110.47
34	H	302	DD6	C4-C5-C6	-3.59	122.24	127.28
37	E	309	KC1	C3C-C4C-NC	3.59	113.75	109.90
34	M	303	DD6	C15-C14-C13	-3.59	118.40	125.99
35	R	301	A86	O4-C34-C33	3.59	116.83	107.64
36	D	316	CLA	CAC-C3C-C2C	-3.59	120.96	127.56
36	T	314	CLA	CHB-C4A-NA	3.59	129.58	124.40
36	f	804	CLA	C1-C2-C3	-3.59	120.32	126.20
36	b	812	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
36	J	313	CLA	C3B-C4B-NB	-3.59	107.33	110.53
36	V	314	CLA	CHB-C4A-NA	3.59	129.57	124.40
36	H	310	CLA	CMD-C2D-C1D	-3.59	118.41	124.73
35	V	302	A86	O1-C15-C20	-3.58	56.41	59.45
36	J	315	CLA	CAA-C2A-C3A	-3.58	108.01	116.23
34	D	304	DD6	C4-C5-C6	-3.58	122.25	127.28
35	T	302	A86	C41-C32-C31	-3.58	107.27	110.47
37	G	318	KC1	C4B-C3B-C2B	-3.58	103.71	106.81
35	E	305	A86	C4-C5-C6	-3.58	122.26	127.28
35	F	302	A86	C25-C26-C27	-3.58	122.26	127.28
36	D	309	CLA	C1-C2-C3	-3.58	120.34	126.20
36	X	313	CLA	O1D-CGD-CBD	3.57	131.57	124.52
35	W	203	A86	C9-C8-C6	-3.57	116.57	126.36
37	H	313	KC1	C3A-C4A-NA	3.57	114.87	110.45
36	H	318	CLA	O2D-CGD-O1D	-3.57	116.90	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	828	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
35	K	303	A86	C4-C3-C2	-3.57	116.21	123.52
37	L	315	KC1	C4C-C3C-C2C	-3.57	101.69	106.89
36	E	313	CLA	C1-C2-C3	-3.57	120.35	126.20
36	a	838	CLA	C3B-C4B-NB	-3.57	107.34	110.53
36	j	102	CLA	C4C-C3C-C2C	-3.57	101.70	106.89
36	I	306	CLA	C1-C2-C3	-3.57	120.36	126.20
36	j	102	CLA	CAC-C3C-C4C	3.57	129.43	124.79
35	C	203	A86	C4-C5-C6	-3.56	122.28	127.28
36	L	308	CLA	C3B-C4B-NB	-3.56	107.35	110.53
35	N	303	A86	C28-C27-C26	-3.56	117.05	122.82
36	Q	312	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
36	N	317	CLA	CMB-C2B-C1B	-3.56	120.00	125.42
35	U	301	A86	C9-C10-C11	-3.56	116.58	126.64
36	a	822	CLA	C4-C3-C5	3.56	120.32	116.13
35	O	305	A86	O1-C20-C15	-3.56	57.80	59.23
36	R	316	CLA	CBC-CAC-C3C	3.56	122.06	112.42
35	I	302	A86	C4-C5-C6	-3.56	122.29	127.28
36	P	316	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
35	R	303	A86	O1-C20-C21	-3.55	111.08	115.05
35	A	302	A86	C3-C2-C1	-3.55	122.30	127.28
36	b	836	CLA	C2B-C1B-NB	3.55	114.01	110.33
36	V	306	CLA	CMC-C2C-C1C	3.55	130.58	125.03
37	P	315	KC1	C3A-C4A-NA	3.55	114.84	110.45
37	A	312	KC1	CAD-C3D-C2D	3.55	151.75	144.26
35	A	316	A86	C25-C26-C27	-3.55	122.30	127.28
36	O	314	CLA	O2D-CGD-O1D	-3.55	116.95	123.85
36	L	311	CLA	CMB-C2B-C1B	-3.54	120.02	125.42
36	N	313	CLA	C4A-NA-C1A	3.54	108.30	106.68
36	H	315	CLA	C3B-C4B-NB	-3.54	107.37	110.53
35	R	303	A86	O1-C15-C20	-3.54	56.45	59.45
36	X	308	CLA	C2B-C1B-NB	3.54	114.00	110.33
36	J	317	CLA	C3B-C4B-NB	-3.54	107.37	110.53
37	O	313	KC1	C3A-C4A-NA	3.54	114.83	110.45
36	C	214	CLA	CAA-C2A-C3A	-3.54	108.12	116.23
36	C	207	CLA	C1-C2-C3	-3.54	120.40	126.20
35	U	303	A86	C34-O4-C38	-3.54	111.60	117.85
35	U	303	A86	O1-C20-C15	-3.54	57.81	59.23
35	T	307	A86	C41-C32-C31	-3.54	107.31	110.47
35	S	303	A86	C28-C27-C26	-3.54	117.09	122.82
36	W	212	CLA	CAA-C2A-C3A	-3.54	103.44	113.00
36	X	313	CLA	C2C-C1C-NC	3.54	113.69	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	b	844	BCR	C28-C27-C26	-3.54	107.75	114.06
35	X	302	A86	C9-C10-C11	-3.53	116.65	126.64
36	R	316	CLA	CAA-C2A-C3A	-3.53	103.45	113.00
37	Q	313	KC1	C3A-C4A-NA	3.53	114.82	110.45
37	S	316	KC1	C4B-C3B-C2B	-3.53	103.75	106.81
35	Q	303	A86	O1-C20-C15	-3.53	57.81	59.23
36	I	305	CLA	C12-C11-C10	3.53	129.11	113.28
35	B	303	A86	O-C13-C14	-3.53	114.52	121.76
36	E	315	CLA	C1D-ND-C4D	-3.53	103.83	106.31
35	N	302	A86	O1-C15-C20	-3.53	56.46	59.45
36	N	312	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
35	X	303	A86	C23-C16-C22	-3.53	102.24	107.37
36	U	311	CLA	C3B-C4B-NB	-3.53	107.38	110.53
35	G	304	A86	C33-C32-C31	-3.53	105.78	109.21
36	K	307	CLA	CHB-C4A-NA	3.53	129.49	124.40
34	D	301	DD6	C14-C13-C11	-3.53	120.06	125.53
36	X	309	CLA	CAA-C2A-C1A	3.53	123.53	111.97
36	R	319	CLA	CMC-C2C-C1C	-3.53	119.53	125.03
36	b	835	CLA	C3B-C4B-NB	-3.53	107.38	110.53
44	h	201	BCR	C39-C30-C25	-3.53	104.72	110.24
36	H	311	CLA	O2D-CGD-CBD	3.52	117.39	111.23
36	G	307	CLA	C3D-C4D-ND	3.52	115.72	109.99
37	C	213	KC1	CAA-C2A-C1A	3.52	140.08	124.64
36	h	203	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
37	A	312	KC1	O2D-CGD-O1D	-3.52	116.99	123.85
36	H	307	CLA	C3C-C4C-NC	-3.52	105.92	110.43
37	T	310	KC1	C3D-C4D-ND	3.52	115.11	110.20
37	V	312	KC1	C4B-C3B-C2B	-3.52	103.76	106.81
35	S	302	A86	O1-C15-C20	-3.52	56.47	59.45
36	L	308	CLA	C1-C2-C3	-3.52	120.44	126.20
36	R	312	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
35	J	302	A86	C3-C2-C1	-3.51	122.35	127.28
35	J	302	A86	C25-C26-C27	-3.51	122.35	127.28
37	O	315	KC1	C3A-C4A-NA	3.51	114.80	110.45
37	Q	311	KC1	C3A-C4A-NA	3.51	114.80	110.45
36	W	210	CLA	CMB-C2B-C3B	3.51	134.81	126.55
35	V	303	A86	O1-C15-C20	-3.51	56.47	59.45
36	G	313	CLA	CBA-CAA-C2A	3.51	124.24	113.79
36	b	819	CLA	CAA-C2A-C1A	-3.51	100.47	111.97
35	R	306	A86	C23-C16-C17	-3.51	102.80	108.97
34	D	305	DD6	O1-C20-C19	-3.51	110.20	113.49
37	G	308	KC1	C3C-C4C-NC	3.51	113.66	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	303	A86	C28-C27-C26	-3.51	117.13	122.82
35	G	306	A86	C8-C6-C5	3.51	124.53	119.01
35	P	306	A86	O1-C20-C15	-3.51	57.82	59.23
35	T	305	A86	O2-C18-C19	-3.51	102.57	109.75
34	K	305	DD6	C15-C14-C13	-3.51	118.58	125.99
34	O	304	DD6	C3-C2-C1	-3.51	122.36	127.28
34	a	849	DD6	C14-C13-C11	-3.50	120.09	125.53
36	N	313	CLA	CMB-C2B-C3B	3.50	134.79	126.55
35	R	302	A86	C4-C5-C6	-3.50	122.37	127.28
37	B	310	KC1	CHD-C4C-NC	3.50	129.59	124.31
35	Q	304	A86	C25-C24-C1	-3.50	116.77	126.36
36	M	310	CLA	C2A-C1A-CHA	3.50	129.94	123.87
35	V	304	A86	C4-C5-C6	-3.50	122.37	127.28
35	N	320	A86	C25-C24-C1	-3.50	116.77	126.36
36	a	818	CLA	CMB-C2B-C1B	-3.50	120.09	125.42
34	L	305	DD6	C4-C5-C6	-3.50	122.37	127.28
36	I	314	CLA	CAA-C2A-C3A	-3.49	108.22	116.23
37	E	309	KC1	C4B-C3B-C2B	-3.49	103.78	106.81
36	f	803	CLA	C3B-C4B-NB	3.49	113.65	110.53
36	R	322	CLA	O2D-CGD-CBD	-3.49	105.12	111.23
36	G	313	CLA	CAA-CBA-CGA	3.49	123.12	113.21
36	L	308	CLA	CHB-C1B-NB	-3.49	118.81	124.05
36	b	830	CLA	O2D-CGD-CBD	3.49	117.32	111.23
37	P	317	KC1	C4D-CHA-C1A	-3.49	111.83	122.45
34	W	204	DD6	C14-C13-C11	-3.48	120.12	125.53
35	T	306	A86	O1-C15-C20	-3.48	56.50	59.45
37	R	317	KC1	CAC-C3C-C4C	3.48	129.32	124.79
35	L	306	A86	C9-C10-C11	-3.48	116.80	126.64
37	V	312	KC1	CHD-C4C-NC	3.48	129.55	124.31
35	M	301	A86	C4-C5-C6	-3.48	122.40	127.28
39	F	321	LMT	C1B-C2B-C3B	3.48	117.33	110.01
35	R	305	A86	C25-C26-C27	-3.48	122.40	127.28
36	H	318	CLA	C3B-C4B-NB	-3.47	107.43	110.53
36	K	310	CLA	C3D-C4D-ND	3.47	115.63	109.99
36	V	314	CLA	C4D-C3D-CAD	-3.47	104.33	108.11
36	b	817	CLA	C1-C2-C3	-3.47	120.51	126.20
37	F	308	KC1	C3C-C4C-NC	3.47	113.62	109.90
35	T	305	A86	C25-C26-C27	-3.47	122.41	127.28
36	b	821	CLA	C3B-C4B-NB	-3.47	107.43	110.53
35	T	305	A86	C10-C9-C8	-3.47	113.15	123.20
34	A	301	DD6	C4-C5-C6	-3.47	122.41	127.28
36	G	309	CLA	CHB-C4A-NA	3.47	129.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	202	A86	C33-C32-C31	-3.47	105.84	109.21
36	O	316	CLA	CMB-C2B-C1B	3.47	130.70	125.42
37	C	213	KC1	CMD-C2D-C1D	-3.47	120.14	125.42
36	a	803	CLA	O2A-CGA-O1A	-3.47	114.96	123.63
35	G	302	A86	C34-O4-C38	-3.47	111.73	117.85
37	D	314	KC1	C4C-C3C-C2C	-3.46	101.85	106.89
35	H	301	A86	C4-C3-C2	-3.46	116.43	123.52
36	K	310	CLA	C3C-C4C-NC	3.46	114.87	110.43
35	K	306	A86	O1-C15-C20	-3.46	56.52	59.45
35	L	306	A86	C36-C31-C32	-3.46	116.26	119.70
36	S	312	CLA	CMA-C3A-C2A	-3.46	100.60	113.98
36	W	215	CLA	C3B-C4B-NB	-3.46	107.44	110.53
36	W	210	CLA	CAA-C2A-C1A	3.45	123.30	111.97
35	B	301	A86	C3-C2-C1	-3.45	122.44	127.28
34	H	302	DD6	C15-C14-C13	-3.45	118.69	125.99
36	K	313	CLA	O2D-CGD-CBD	3.45	117.26	111.23
36	D	312	CLA	C3B-C4B-NB	-3.45	107.45	110.53
35	J	303	A86	O1-C15-C20	-3.45	56.52	59.45
36	I	306	CLA	CHB-C4A-NA	3.45	129.38	124.40
37	P	317	KC1	C3B-C2B-C1B	-3.45	103.78	107.05
36	N	311	CLA	C2A-C1A-CHA	3.45	129.86	123.87
35	A	302	A86	C23-C16-C17	-3.45	102.91	108.97
34	K	304	DD6	C9-C10-C11	-3.45	122.44	127.28
34	R	308	DD6	C14-C13-C11	-3.45	120.18	125.53
36	D	308	CLA	CBC-CAC-C3C	3.45	121.76	112.42
36	b	819	CLA	C3A-C2A-C1A	3.44	106.50	101.34
36	U	306	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
36	U	306	CLA	C1-C2-C3	-3.44	120.56	126.20
36	F	317	CLA	CMC-C2C-C1C	3.44	130.41	125.03
35	K	303	A86	O4-C38-C39	3.44	117.22	111.09
37	C	213	KC1	CMD-C2D-C3D	3.44	136.52	125.67
37	M	317	KC1	CHB-C4A-NA	3.44	129.57	124.23
35	O	319	A86	O1-C15-C20	-3.44	56.53	59.45
35	R	306	A86	O4-C38-C39	3.44	117.22	111.09
36	G	313	CLA	CMB-C2B-C1B	-3.44	120.18	125.42
36	D	306	CLA	CAA-CBA-CGA	3.44	121.66	112.49
36	a	825	CLA	C1-C2-C3	-3.44	120.57	126.20
35	G	306	A86	C25-C24-C1	-3.43	116.94	126.36
34	a	849	DD6	C9-C10-C11	-3.43	122.46	127.28
36	K	310	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
35	K	301	A86	C9-C10-C11	-3.43	116.94	126.64
35	U	302	A86	C4-C3-C2	-3.43	116.50	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	828	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
35	L	304	A86	C3-C2-C1	-3.43	122.47	127.28
35	F	307	A86	C41-C32-C33	3.43	125.30	109.06
37	G	317	KC1	O1D-CGD-CBD	3.43	131.28	124.52
36	F	317	CLA	C4D-C3D-CAD	3.43	111.83	108.11
35	I	302	A86	O1-C15-C20	-3.43	56.55	59.45
35	L	307	A86	C34-O4-C38	-3.42	111.80	117.85
35	I	304	A86	C7-C6-C8	3.42	123.32	118.09
36	R	311	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
36	f	803	CLA	CAC-C3C-C4C	3.42	129.24	124.79
36	G	319	CLA	C1-C2-C3	-3.42	121.22	126.76
35	G	302	A86	C4-C5-C6	-3.42	122.48	127.28
36	b	808	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
35	V	303	A86	O1-C20-C21	-3.42	111.22	115.05
36	R	315	CLA	CHB-C4A-NA	3.42	129.34	124.40
37	G	317	KC1	C4B-C3B-C2B	-3.42	103.85	106.81
36	S	311	CLA	C3B-C4B-NB	-3.42	107.48	110.53
36	H	307	CLA	C4D-CHA-C1A	3.42	125.32	121.24
36	I	308	CLA	CHD-C4C-C3C	-3.42	119.79	124.77
34	D	301	DD6	O1-C15-C14	-3.42	107.09	116.88
36	P	314	CLA	CHA-C1A-NA	-3.42	118.66	126.39
37	K	314	KC1	C2A-C1A-CHA	-3.41	114.94	128.96
36	b	841	CLA	CAC-C3C-C2C	3.41	133.83	127.56
36	V	314	CLA	C1-C2-C3	-3.41	120.60	126.20
34	E	304	DD6	C4-C5-C6	-3.41	122.49	127.28
36	Q	310	CLA	CHA-C1A-NA	-3.41	118.66	126.39
37	R	317	KC1	C2A-C3A-C4A	3.41	108.97	106.41
36	S	321	CLA	CHB-C4A-NA	3.41	129.32	124.40
37	L	317	KC1	C3C-C4C-NC	3.41	113.55	109.90
36	b	816	CLA	C1-C2-C3	-3.41	120.61	126.20
37	M	318	KC1	CMA-C3A-C4A	3.41	130.36	125.03
35	T	307	A86	O4-C34-C35	-3.40	98.92	107.64
36	S	313	CLA	CHB-C4A-NA	3.40	129.31	124.40
35	V	302	A86	C4-C5-C6	-3.40	122.50	127.28
36	a	809	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
36	b	840	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
37	M	318	KC1	C3D-C2D-C1D	-3.40	95.53	106.40
35	N	304	A86	C24-C1-C2	3.40	124.36	119.01
36	a	827	CLA	CMB-C2B-C1B	-3.40	120.24	125.42
35	K	302	A86	O1-C20-C19	-3.40	110.31	113.49
36	b	818	CLA	CMB-C2B-C1B	-3.40	120.25	125.42
36	F	313	CLA	C3B-C4B-NB	-3.40	107.50	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	207	CLA	CHB-C4A-NA	3.39	129.30	124.40
34	R	307	DD6	C21-C20-C15	-3.39	116.72	122.30
35	A	302	A86	C34-O4-C38	3.39	123.84	117.85
35	E	305	A86	C34-O4-C38	-3.39	111.86	117.85
36	H	318	CLA	C1-O2A-CGA	3.39	124.86	116.65
36	C	214	CLA	CMA-C3A-C2A	-3.39	108.46	116.23
36	D	315	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
35	L	306	A86	O1-C15-C20	-3.39	56.58	59.45
36	V	306	CLA	C3B-C4B-NB	-3.39	107.51	110.53
36	G	314	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
36	D	306	CLA	CAC-C3C-C4C	3.38	129.19	124.79
36	b	823	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
37	E	309	KC1	CAC-C3C-C4C	-3.38	120.39	124.79
36	I	312	CLA	C3B-C4B-NB	-3.38	107.51	110.53
36	H	307	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
36	S	317	CLA	CAA-C2A-C3A	-3.38	108.48	116.23
36	j	106	CLA	C3B-C4B-NB	-3.38	107.52	110.53
34	P	305	DD6	C37-C36-C35	3.38	120.63	114.42
35	K	306	A86	C28-C27-C26	-3.37	117.35	122.82
35	G	306	A86	C9-C10-C11	-3.37	117.10	126.64
36	P	319	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
36	a	821	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
36	b	821	CLA	O2D-CGD-CBD	3.37	117.12	111.23
36	L	308	CLA	C4B-C3B-C2B	3.37	111.49	107.30
36	W	212	CLA	C4D-C3D-CAD	-3.37	104.44	108.11
36	a	830	CLA	C2B-C1B-NB	3.37	113.82	110.33
35	B	303	A86	O1-C20-C19	-3.37	110.33	113.49
36	O	312	CLA	CHA-C1A-NA	-3.37	118.66	126.33
36	b	830	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
36	K	307	CLA	C4D-C3D-CAD	-3.37	104.45	108.11
36	a	816	CLA	CMD-C2D-C3D	-3.37	119.97	127.69
35	X	303	A86	C3-C4-C5	-3.37	116.63	123.52
35	R	302	A86	C3-C4-C5	-3.37	116.63	123.52
36	a	837	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
35	J	303	A86	C4-C3-C2	-3.37	116.63	123.52
35	L	304	A86	C23-C16-C17	-3.37	103.05	108.97
35	G	304	A86	C7-C6-C8	3.37	123.23	118.09
39	F	321	LMT	C1B-O5B-C5B	3.37	120.29	113.72
36	K	307	CLA	C3D-C4D-ND	3.37	115.46	109.99
37	D	314	KC1	C4B-C3B-C2B	-3.36	103.90	106.81
36	a	839	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
37	E	309	KC1	C1C-C2C-C3C	-3.36	103.44	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	831	CLA	C3B-C4B-NB	-3.36	107.53	110.53
35	X	303	A86	C25-C24-C1	-3.36	117.16	126.36
35	M	302	A86	O1-C15-C20	-3.36	56.60	59.45
36	X	310	CLA	C3B-C4B-NB	-3.36	107.53	110.53
35	N	306	A86	C23-C16-C17	-3.36	103.07	108.97
37	G	317	KC1	O2D-CGD-O1D	-3.36	117.32	123.85
36	F	313	CLA	O2D-CGD-O1D	-3.36	117.32	123.85
35	I	304	A86	C35-C34-C33	-3.36	103.86	109.89
36	N	310	CLA	CHD-C1D-ND	-3.35	120.08	124.80
35	U	301	A86	C34-O4-C38	3.35	123.76	117.85
37	N	314	KC1	CHD-C1D-C2D	3.35	137.15	127.43
36	A	314	CLA	CGD-CBD-CAD	3.35	121.69	110.85
35	P	303	A86	C41-C32-C31	-3.35	107.47	110.47
36	U	313	CLA	C2A-C1A-CHA	3.35	129.66	123.86
35	B	303	A86	C34-O4-C38	-3.35	111.93	117.85
36	b	834	CLA	C3B-C4B-NB	-3.35	107.54	110.53
36	a	822	CLA	C3B-C4B-NB	-3.35	107.54	110.53
34	E	306	DD6	C37-C36-C35	3.35	120.57	114.42
37	H	313	KC1	C2B-C1B-NB	3.35	113.44	110.13
36	a	817	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
35	R	309	A86	C23-C16-C17	-3.34	103.09	108.97
36	b	805	CLA	C7-C6-C5	-3.34	104.36	113.26
36	U	310	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
35	L	306	A86	C21-C20-C19	3.34	117.99	114.24
36	V	310	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
36	b	831	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
36	a	832	CLA	O2D-CGD-CBD	3.34	117.06	111.23
35	O	302	A86	C41-C32-C31	-3.33	107.49	110.47
36	L	311	CLA	C3B-C4B-NB	-3.33	107.55	110.53
36	b	812	CLA	CMB-C2B-C1B	-3.33	120.34	125.42
36	J	311	CLA	C3B-C4B-NB	-3.33	107.56	110.53
36	N	316	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
36	a	823	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
36	N	310	CLA	CMB-C2B-C1B	-3.33	120.35	125.42
37	G	308	KC1	C2A-C1A-NA	3.33	114.67	109.34
34	B	304	DD6	C37-C36-C35	3.33	120.54	114.42
37	M	317	KC1	C4B-C3B-C2B	-3.33	103.93	106.81
36	G	310	CLA	C3B-C4B-NB	-3.32	107.56	110.53
36	H	307	CLA	C1-O2A-CGA	3.32	124.70	116.65
36	E	310	CLA	CMB-C2B-C1B	-3.32	120.36	125.42
35	X	301	A86	C28-C27-C26	-3.32	117.43	122.82
36	S	315	CLA	CHB-C4A-NA	3.32	129.20	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	834	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
35	G	304	A86	C4-C3-C2	-3.32	116.72	123.52
37	H	313	KC1	C4C-C3C-C2C	-3.32	102.06	106.89
36	b	806	CLA	C3B-C4B-NB	-3.32	107.56	110.53
36	G	315	CLA	CMB-C2B-C1B	3.32	130.48	125.42
35	I	302	A86	C3-C2-C1	-3.32	122.62	127.28
35	L	319	A86	C41-C32-C31	-3.32	107.50	110.47
36	D	309	CLA	C3D-C4D-ND	3.32	115.39	109.99
35	X	314	A86	C34-O4-C38	-3.32	111.98	117.85
36	l	202	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
36	G	319	CLA	C3D-C4D-ND	3.32	115.38	109.99
36	b	819	CLA	CHB-C4A-NA	3.32	129.19	124.40
36	U	308	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
37	B	310	KC1	C4B-C3B-C2B	-3.32	103.94	106.81
44	a	845	BCR	C2-C1-C6	3.32	115.26	110.44
35	O	301	A86	C34-O4-C38	-3.32	111.99	117.85
36	F	312	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
36	B	311	CLA	CHB-C4A-NA	3.31	129.18	124.40
35	A	316	A86	C34-O4-C38	-3.31	111.99	117.85
35	V	302	A86	C12-C11-C13	3.31	121.37	116.00
35	X	303	A86	C7-C6-C8	3.31	123.15	118.09
35	T	301	A86	C34-O4-C38	-3.31	112.00	117.85
35	W	203	A86	C9-C10-C11	-3.31	117.28	126.64
36	H	310	CLA	CHB-C4A-NA	3.31	129.18	124.40
36	G	315	CLA	CHD-C1D-ND	-3.31	120.14	124.80
35	I	301	A86	C34-O4-C38	-3.31	112.00	117.85
36	I	313	CLA	C3B-C4B-NB	-3.31	107.58	110.53
35	S	305	A86	C19-C18-C17	-3.31	104.60	110.79
36	I	311	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
36	U	313	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
36	U	309	CLA	CAA-C2A-C1A	3.31	122.81	111.97
35	O	301	A86	C25-C26-C27	-3.30	122.64	127.28
36	Q	310	CLA	C3B-C4B-NB	-3.30	107.58	110.53
36	a	808	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
35	H	301	A86	C25-C26-C27	-3.30	122.65	127.28
35	L	301	A86	C3-C2-C1	-3.30	122.65	127.28
35	V	301	A86	C34-O4-C38	-3.30	112.02	117.85
36	a	838	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
36	a	822	CLA	C2B-C1B-NB	3.30	113.75	110.33
35	T	305	A86	C23-C16-C17	-3.30	103.17	108.97
35	K	303	A86	C25-C26-C27	-3.30	122.65	127.28
36	a	815	CLA	C3B-C4B-NB	-3.30	107.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	N	319	CLA	CHB-C1B-C2B	-3.30	117.86	127.43
36	N	315	CLA	CAA-C2A-C3A	-3.30	108.67	116.23
36	a	832	CLA	C3B-C4B-NB	-3.30	107.59	110.53
36	G	307	CLA	CHB-C4A-NA	3.29	129.16	124.40
36	I	311	CLA	CMB-C2B-C1B	-3.29	120.40	125.42
36	X	313	CLA	CHC-C1C-C2C	-3.29	117.59	126.95
36	G	319	CLA	CAC-C3C-C4C	3.29	129.07	124.79
36	H	307	CLA	O2D-CGD-CBD	3.29	116.99	111.23
36	b	813	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
36	S	312	CLA	CMB-C2B-C1B	-3.29	120.41	125.42
36	D	306	CLA	C2A-C1A-CHA	3.29	129.58	123.87
36	b	826	CLA	CHB-C4A-NA	3.29	129.15	124.40
37	T	310	KC1	C4B-CHC-C1C	-3.29	119.03	126.02
35	N	301	A86	O-C13-C11	-3.29	113.95	121.04
35	L	307	A86	C25-C26-C27	-3.29	122.66	127.28
35	S	304	A86	C40-C32-C31	-3.29	107.53	110.47
36	K	310	CLA	CMB-C2B-C1B	3.29	130.43	125.42
36	T	308	CLA	CAC-C3C-C4C	3.29	129.07	124.79
36	K	307	CLA	C2B-C1B-NB	3.29	113.73	110.33
35	A	302	A86	C9-C10-C11	-3.29	117.35	126.64
37	W	217	KC1	CHD-C1D-C2D	3.29	136.96	127.43
36	G	307	CLA	C2B-C1B-NB	3.29	113.73	110.33
35	S	301	A86	O-C13-C11	-3.28	113.97	121.04
35	R	305	A86	C34-O4-C38	-3.28	112.05	117.85
34	E	306	DD6	C9-C10-C11	-3.28	122.67	127.28
36	X	313	CLA	C1D-ND-C4D	-3.28	104.01	106.31
35	U	304	A86	C25-C26-C27	-3.28	122.68	127.28
36	a	830	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
36	A	314	CLA	C2A-C1A-CHA	3.28	129.56	123.87
35	C	202	A86	C23-C16-C17	-3.28	103.20	108.97
36	b	836	CLA	C1-C2-C3	-3.28	120.83	126.20
34	I	303	DD6	C37-C36-C35	3.28	120.44	114.42
37	F	308	KC1	C1C-C2C-C3C	-3.28	103.53	106.98
37	E	309	KC1	CHD-C1D-C2D	3.27	136.93	127.43
35	R	304	A86	C35-C34-C33	-3.27	104.00	109.89
35	T	304	A86	O1-C20-C19	-3.27	110.42	113.49
36	S	318	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
36	R	314	CLA	C2A-C1A-CHA	3.27	129.54	123.87
36	a	806	CLA	C1-C2-C3	-3.27	120.84	126.20
34	G	303	DD6	C15-C14-C13	-3.27	119.08	125.99
36	a	824	CLA	CMB-C2B-C1B	-3.27	120.44	125.42
37	J	314	KC1	CAC-C3C-C4C	3.27	129.04	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	311	KC1	CHD-C1D-C2D	3.27	136.91	127.43
36	K	309	CLA	C3B-C4B-NB	-3.27	107.61	110.53
36	F	317	CLA	C1-C2-C3	-3.27	120.85	126.20
36	S	310	CLA	C1-O2A-CGA	3.27	124.56	116.65
37	J	314	KC1	C4C-C3C-C2C	-3.27	102.14	106.89
44	b	845	BCR	C31-C1-C6	3.27	115.36	110.24
36	H	316	CLA	C3B-C4B-NB	-3.27	107.61	110.53
37	B	310	KC1	C3C-C4C-NC	3.26	113.40	109.90
36	L	313	CLA	CMB-C2B-C1B	-3.26	120.45	125.42
36	b	824	CLA	C4A-NA-C1A	3.26	108.17	106.68
36	V	311	CLA	CMB-C2B-C1B	-3.26	120.45	125.42
36	H	311	CLA	CHB-C4A-NA	3.26	129.11	124.40
36	N	308	CLA	CMA-C3A-C4A	3.26	120.54	111.77
36	a	809	CLA	C3B-C4B-NB	-3.26	107.62	110.53
36	l	205	CLA	C2D-C1D-ND	3.26	113.35	110.13
35	A	302	A86	C40-C32-C33	3.26	124.51	109.06
36	O	310	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
36	B	305	CLA	C3B-C4B-NB	-3.26	107.62	110.53
36	E	313	CLA	CMC-C2C-C1C	3.26	130.13	125.03
36	I	306	CLA	C2C-C1C-NC	3.26	113.40	109.98
36	b	805	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
35	X	305	A86	C9-C8-C6	-3.26	117.43	126.36
36	E	313	CLA	CMD-C2D-C3D	-3.26	120.22	127.69
36	F	310	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
37	M	313	KC1	C2A-C3A-C4A	3.26	108.86	106.41
44	j	107	BCR	C2-C1-C6	3.26	115.17	110.44
39	F	321	LMT	C4B-C3B-C2B	3.26	116.55	110.83
36	a	801	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
36	P	312	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
35	V	303	A86	C9-C8-C6	-3.25	117.44	126.36
35	M	302	A86	C23-C16-C17	-3.25	103.26	108.97
36	U	309	CLA	C2A-C1A-CHA	3.25	129.51	123.87
37	P	317	KC1	C3C-C4C-NC	3.25	113.38	109.90
37	G	318	KC1	CMD-C2D-C1D	3.25	130.37	125.42
36	H	305	CLA	C3B-C4B-NB	-3.25	107.63	110.53
36	l	204	CLA	C2C-C1C-NC	3.24	113.39	109.98
34	D	301	DD6	O1-C20-C19	-3.24	110.45	113.49
36	Q	309	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
36	O	312	CLA	C3B-C4B-NB	-3.24	107.63	110.53
36	b	839	CLA	C3B-C4B-NB	-3.24	107.63	110.53
36	I	305	CLA	C14-C13-C12	-3.24	99.71	111.27
36	E	316	CLA	CAC-C3C-C4C	-3.24	120.57	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	F	307	A86	O1-C15-C20	-3.24	56.70	59.45
36	a	803	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
35	V	303	A86	C4-C3-C2	-3.24	116.89	123.52
36	b	822	CLA	C3B-C4B-NB	-3.24	107.64	110.53
36	N	308	CLA	CMC-C2C-C3C	-3.24	117.39	126.15
37	U	312	KC1	CHD-C1D-C2D	3.24	136.82	127.43
36	W	209	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
36	b	809	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
36	b	826	CLA	CHA-C4D-ND	3.23	139.22	132.55
36	H	307	CLA	CHB-C4A-NA	3.23	129.07	124.40
36	N	318	CLA	CHB-C4A-NA	3.23	129.07	124.40
35	M	304	A86	C34-O4-C38	-3.23	112.14	117.85
35	F	307	A86	O4-C34-C35	-3.23	99.37	107.64
34	A	303	DD6	C21-C20-C15	-3.23	116.99	122.30
36	P	314	CLA	C3B-C4B-NB	-3.23	107.65	110.53
35	T	303	A86	O1-C15-C20	-3.23	56.71	59.45
35	V	302	A86	C41-C32-C31	-3.23	107.58	110.47
36	B	309	CLA	CHD-C1D-ND	-3.23	120.26	124.80
37	U	312	KC1	C3C-C4C-NC	3.23	113.36	109.90
36	R	322	CLA	C3B-C4B-NB	-3.23	107.65	110.53
36	D	313	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
36	N	311	CLA	CHB-C4A-NA	3.22	129.05	124.40
37	H	313	KC1	C3B-C2B-C1B	-3.22	104.00	107.05
39	E	323	LMT	C1B-O1B-C4'	-3.22	110.34	117.98
37	S	316	KC1	CHD-C1D-C2D	3.22	136.78	127.43
35	O	319	A86	C23-C16-C17	-3.22	103.31	108.97
36	A	306	CLA	CMD-C2D-C3D	-3.22	120.30	127.69
36	G	319	CLA	CHD-C4C-C3C	-3.22	120.08	124.77
36	b	818	CLA	CAA-CBA-CGA	3.22	122.35	113.21
36	V	309	CLA	CHB-C4A-NA	3.22	129.05	124.40
36	I	309	CLA	CAA-C2A-C1A	3.22	122.52	111.97
37	H	313	KC1	CHD-C1D-C2D	3.22	136.76	127.43
36	X	308	CLA	CAA-C2A-C3A	-3.21	104.31	113.00
34	W	204	DD6	C37-C36-C35	3.21	120.33	114.42
36	U	306	CLA	C4D-C3D-CAD	-3.21	104.62	108.11
37	A	312	KC1	C3B-C2B-C1B	-3.21	104.00	107.05
37	P	315	KC1	CMA-C3A-C4A	-3.21	120.01	125.03
36	U	311	CLA	CHB-C4A-NA	3.21	129.04	124.40
36	B	311	CLA	C4D-CHA-C1A	-3.21	117.41	121.24
36	M	310	CLA	CAA-C2A-C1A	3.21	122.50	111.97
36	D	317	CLA	C3B-C4B-NB	-3.21	107.66	110.53
36	M	306	CLA	O2D-CGD-O1D	-3.21	117.60	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	824	CLA	CMD-C2D-C3D	-3.21	120.33	127.69
37	E	309	KC1	C4D-CHA-C1A	-3.21	112.67	122.45
37	O	313	KC1	CMA-C3A-C4A	-3.21	120.02	125.03
36	a	820	CLA	CMB-C2B-C1B	-3.21	120.54	125.42
36	T	314	CLA	CAA-C2A-C3A	-3.21	104.34	113.00
36	j	106	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
36	b	816	CLA	C3D-C4D-ND	3.20	115.19	109.99
36	b	830	CLA	CAC-C3C-C4C	3.20	128.96	124.79
35	A	302	A86	C4-C3-C2	-3.20	116.97	123.52
36	P	318	CLA	C3B-C4B-NB	-3.20	107.67	110.53
35	R	302	A86	O1-C15-C20	-3.20	56.74	59.45
44	b	843	BCR	C29-C30-C25	3.20	115.09	110.44
36	b	837	CLA	O1D-CGD-CBD	3.20	130.83	124.52
36	D	308	CLA	C3B-C4B-NB	-3.20	107.67	110.53
36	H	308	CLA	O2D-CGD-O1D	-3.20	116.82	124.08
36	R	321	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
36	N	311	CLA	CAA-C2A-C1A	3.20	122.45	111.97
34	R	307	DD6	C14-C13-C11	-3.20	120.57	125.53
36	V	314	CLA	CMC-C2C-C1C	3.20	130.03	125.03
37	Q	311	KC1	CMA-C3A-C4A	-3.20	120.04	125.03
36	T	312	CLA	C2A-C1A-CHA	3.20	129.42	123.87
34	E	304	DD6	C9-C10-C11	-3.20	122.79	127.28
35	W	202	A86	C10-C9-C8	-3.20	113.94	123.20
35	K	303	A86	C29-C30-C31	-3.20	173.89	177.66
36	H	306	CLA	C3B-C4B-NB	-3.19	107.68	110.53
35	O	303	A86	O1-C15-C20	-3.19	56.74	59.45
36	I	307	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
34	I	303	DD6	C14-C13-C11	-3.19	120.58	125.53
37	G	318	KC1	C1C-C2C-C3C	-3.19	103.62	106.98
36	a	823	CLA	C1-C2-C3	-3.19	120.97	126.20
35	P	306	A86	C3-C2-C1	-3.19	122.80	127.28
37	S	316	KC1	CMA-C3A-C4A	-3.19	120.05	125.03
36	H	314	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
36	V	311	CLA	CAA-C2A-C3A	-3.19	104.39	113.00
37	O	315	KC1	CMA-C3A-C4A	-3.19	120.05	125.03
36	G	312	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
36	a	824	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
37	D	314	KC1	C1D-CHD-C4C	-3.18	118.76	126.25
37	Q	313	KC1	CMA-C3A-C4A	-3.18	120.06	125.03
36	K	310	CLA	C1D-ND-C4D	-3.18	104.08	106.31
36	G	313	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
36	a	841	CLA	O2D-CGD-O1D	-3.18	117.65	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	307	CLA	O2D-CGD-CBD	3.18	116.79	111.23
36	b	837	CLA	C3B-C4B-NB	-3.18	107.69	110.53
36	b	813	CLA	CMA-C3A-C2A	-3.18	101.69	113.98
36	D	310	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
36	R	316	CLA	CHB-C4A-NA	3.18	128.99	124.40
36	a	813	CLA	C3B-C4B-NB	-3.18	107.69	110.53
36	E	316	CLA	CAC-C3C-C2C	3.18	133.39	127.56
35	I	304	A86	C36-C31-C32	-3.17	116.55	119.70
36	F	316	CLA	CAA-C2A-C3A	-3.17	108.95	116.23
35	O	301	A86	C9-C8-C6	-3.17	117.66	126.36
37	B	310	KC1	C3B-C2B-C1B	-3.17	104.04	107.05
36	P	319	CLA	CHC-C4B-NB	3.17	128.81	124.05
34	a	849	DD6	O1-C15-C14	-3.17	107.80	116.88
36	W	208	CLA	C3B-C4B-NB	-3.17	107.70	110.53
36	G	313	CLA	C3A-C2A-C1A	3.17	106.09	101.34
35	T	305	A86	C4-C5-C6	-3.17	122.83	127.28
36	M	315	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
36	U	306	CLA	C2C-C1C-NC	3.17	113.31	109.98
36	H	308	CLA	C3B-C4B-NB	-3.17	107.70	110.53
36	A	307	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
36	F	313	CLA	O2D-CGD-CBD	3.16	116.76	111.23
37	N	314	KC1	C2A-C1A-CHA	-3.16	115.97	128.96
36	b	809	CLA	C3B-C4B-NB	-3.16	107.70	110.53
35	J	305	A86	C34-O4-C38	-3.16	112.26	117.85
37	F	315	KC1	C3A-C4A-NA	3.16	114.37	110.45
36	K	313	CLA	CMB-C2B-C1B	-3.16	120.60	125.42
36	b	835	CLA	CHB-C4A-NA	3.16	128.97	124.40
36	b	832	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
37	T	310	KC1	C3D-C2D-C1D	-3.16	96.30	106.40
36	S	314	CLA	CED-O2D-CGD	3.16	123.09	115.92
36	H	310	CLA	C2D-C1D-ND	-3.16	107.00	110.13
36	i	102	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
36	E	316	CLA	C3B-C4B-NB	-3.16	107.71	110.53
35	K	302	A86	C25-C26-C27	-3.16	122.85	127.28
36	M	306	CLA	CHC-C4B-NB	3.16	128.79	124.05
37	G	317	KC1	C4C-C3C-C2C	-3.16	102.30	106.89
37	T	310	KC1	CMD-C2D-C3D	3.16	135.63	125.67
36	R	319	CLA	CHB-C4A-NA	3.16	128.96	124.40
35	L	306	A86	C41-C32-C31	3.16	113.30	110.47
36	V	309	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
34	S	307	DD6	C37-C36-C35	3.16	120.22	114.42
36	b	820	CLA	O2D-CGD-O1D	-3.15	117.71	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	K	301	A86	C25-C26-C27	-3.15	122.86	127.28
36	b	831	CLA	CMB-C2B-C1B	-3.15	120.62	125.42
36	j	102	CLA	C1-C2-C3	-3.15	121.03	126.20
37	T	315	KC1	C4C-C3C-C2C	-3.15	102.30	106.89
36	W	214	CLA	C3C-C4C-NC	-3.15	106.39	110.43
36	W	215	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
34	K	304	DD6	C15-C14-C13	-3.15	119.33	125.99
36	R	312	CLA	C3B-C4B-NB	-3.15	107.72	110.53
37	S	316	KC1	C2A-C1A-NA	3.15	114.39	109.34
35	T	303	A86	C23-C16-C17	-3.15	103.43	108.97
36	f	803	CLA	CHB-C1B-C2B	-3.15	118.28	127.43
36	W	216	CLA	CMA-C3A-C4A	3.15	120.24	111.77
35	P	304	A86	O1-C15-C20	-3.15	56.78	59.45
36	X	308	CLA	C2A-C1A-CHA	3.15	129.33	123.87
35	V	304	A86	O4-C38-C39	3.15	116.70	111.09
36	i	102	CLA	CHB-C4A-NA	3.15	128.94	124.40
36	b	827	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
36	K	309	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
34	J	304	DD6	C15-C14-C13	-3.15	119.34	125.99
36	a	831	CLA	C3B-C4B-NB	-3.14	107.72	110.53
37	S	316	KC1	C3C-C4C-NC	3.14	113.27	109.90
37	F	315	KC1	CHD-C1D-C2D	3.14	136.55	127.43
36	M	308	CLA	C3B-C4B-NB	-3.14	107.72	110.53
36	a	848	CLA	C3D-C2D-C1D	-3.14	101.54	105.83
35	Q	301	A86	O1-C15-C20	-3.14	56.79	59.45
36	R	310	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
36	R	314	CLA	CHB-C4A-NA	3.14	128.93	124.40
36	a	830	CLA	CMD-C2D-C3D	-3.14	120.50	127.69
37	B	310	KC1	CHD-C1D-C2D	3.13	136.53	127.43
36	a	814	CLA	CMC-C2C-C3C	3.13	134.63	126.15
36	b	801	CLA	CMB-C2B-C1B	-3.13	120.65	125.42
36	a	814	CLA	CHB-C4A-NA	3.13	128.92	124.40
36	C	212	CLA	CHB-C4A-NA	3.13	128.92	124.40
37	M	313	KC1	C2A-C1A-NA	3.13	114.36	109.34
36	P	301	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
36	b	836	CLA	CHD-C4C-C3C	-3.13	120.21	124.77
35	S	303	A86	O1-C15-C20	-3.13	56.80	59.45
37	G	318	KC1	C4D-CHA-C1A	-3.12	112.93	122.45
36	I	310	CLA	CMB-C2B-C3B	3.12	133.90	126.55
36	K	315	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
36	E	310	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
35	T	307	A86	C33-C32-C31	-3.12	106.18	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	303	A86	C25-C26-C27	-3.12	122.90	127.28
36	b	839	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
34	M	303	DD6	C9-C10-C11	-3.12	122.90	127.28
36	b	806	CLA	CMB-C2B-C3B	3.12	133.89	126.55
35	F	304	A86	C34-O4-C38	-3.12	112.34	117.85
35	C	204	A86	C34-O4-C38	-3.12	112.34	117.85
36	A	306	CLA	C1-C2-C3	-3.12	121.09	126.20
36	b	816	CLA	C4B-C3B-C2B	-3.12	103.43	107.30
36	W	201	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
35	G	304	A86	C26-C25-C24	-3.12	114.17	123.20
35	F	307	A86	C23-C16-C17	-3.12	103.49	108.97
36	J	307	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
36	h	203	CLA	CBA-CAA-C2A	3.11	123.06	113.79
44	b	845	BCR	C27-C26-C25	3.11	126.91	122.70
36	E	315	CLA	CHD-C4C-C3C	-3.11	120.23	124.77
36	M	308	CLA	CAC-C3C-C2C	3.11	133.28	127.56
34	L	305	DD6	C25-C24-C1	-3.11	117.82	126.36
36	R	319	CLA	CBC-CAC-C3C	3.11	120.86	112.42
36	a	824	CLA	C3B-C4B-NB	-3.11	107.75	110.53
36	X	307	CLA	CMB-C2B-C1B	-3.11	120.68	125.42
36	B	307	CLA	C3B-C4B-NB	-3.11	107.75	110.53
35	E	305	A86	C25-C26-C27	-3.11	122.91	127.28
36	C	205	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
37	G	318	KC1	C3B-C2B-C1B	-3.11	104.10	107.05
36	b	841	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
36	a	816	CLA	C3D-C2D-C1D	-3.11	101.59	105.83
36	b	810	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
34	W	204	DD6	C21-C20-C15	-3.11	117.19	122.30
35	W	203	A86	O4-C38-C39	3.11	116.63	111.09
34	L	305	DD6	C37-C36-C35	3.11	120.14	114.42
36	O	316	CLA	C4D-C3D-CAD	-3.11	104.73	108.11
36	b	825	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
36	b	836	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
36	a	823	CLA	C3B-C4B-NB	-3.10	107.76	110.53
34	B	302	DD6	C14-C13-C11	-3.10	120.72	125.53
35	F	307	A86	O4-C38-O5	-3.10	117.00	122.99
37	N	314	KC1	C3C-C4C-NC	3.10	113.22	109.90
36	U	308	CLA	CHB-C4A-NA	3.10	128.88	124.40
35	N	303	A86	O1-C15-C20	-3.10	56.82	59.45
37	W	213	KC1	C4D-CHA-C1A	-3.10	113.00	122.45
35	R	309	A86	C25-C26-C27	-3.10	122.93	127.28
36	V	311	CLA	CMD-C2D-C1D	-3.10	119.27	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	202	A86	C4-C5-C6	-3.10	122.93	127.28
37	A	312	KC1	C1C-C2C-C3C	-3.10	103.72	106.98
35	V	303	A86	C3-C2-C1	-3.10	122.93	127.28
36	W	216	CLA	CAA-C2A-C1A	-3.10	101.82	111.97
36	W	207	CLA	C1-C2-C3	3.10	131.27	126.20
35	T	305	A86	O1-C20-C21	-3.10	111.59	115.05
35	T	304	A86	C25-C26-C27	-3.10	122.93	127.28
36	S	315	CLA	C3B-C4B-NB	-3.10	107.77	110.53
36	W	214	CLA	CAC-C3C-C2C	-3.10	121.87	127.56
36	S	315	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
36	K	307	CLA	C1-C2-C3	-3.09	121.13	126.20
36	f	804	CLA	O2A-CGA-CBA	3.09	121.27	111.83
37	R	317	KC1	CHD-C1D-C2D	3.09	136.40	127.43
36	f	803	CLA	C2D-C1D-ND	3.09	113.19	110.13
36	T	309	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
35	M	302	A86	C9-C10-C11	-3.09	117.90	126.64
36	H	312	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
35	G	306	A86	C7-C6-C5	-3.09	117.81	122.82
37	R	317	KC1	C3A-C4A-NA	3.09	114.27	110.45
35	L	319	A86	C28-C27-C26	-3.09	117.81	122.82
34	R	307	DD6	C37-C36-C35	3.09	120.10	114.42
36	H	310	CLA	CHA-C4D-ND	3.09	138.92	132.55
35	R	306	A86	C3-C2-C1	-3.09	122.95	127.28
39	I	317	LMT	C1B-O1B-C4'	-3.09	110.66	117.98
36	J	309	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
35	T	305	A86	O-C13-C11	-3.09	114.39	121.04
37	E	309	KC1	C3B-C2B-C1B	-3.09	104.12	107.05
36	H	315	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
35	Q	303	A86	C41-C32-C31	-3.09	107.71	110.47
36	b	829	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
36	B	307	CLA	C2A-C1A-CHA	3.08	129.22	123.87
44	b	845	BCR	C40-C30-C25	3.08	115.08	110.24
36	a	823	CLA	C2B-C1B-NB	3.08	113.52	110.33
35	T	303	A86	C28-C27-C26	-3.08	117.82	122.82
36	U	310	CLA	C3B-C4B-NB	-3.08	107.78	110.53
36	A	306	CLA	CHD-C4C-C3C	-3.08	120.28	124.77
35	L	301	A86	C34-O4-C38	-3.08	112.40	117.85
35	G	306	A86	C24-C1-C2	3.08	123.86	119.01
36	A	311	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
36	H	314	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
35	M	302	A86	C3-C4-C5	-3.08	117.22	123.52
36	b	825	CLA	CHB-C4A-NA	3.08	128.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	802	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
34	M	303	DD6	C21-C20-C15	-3.08	117.23	122.30
35	L	304	A86	C4-C3-C2	-3.08	117.22	123.52
36	O	316	CLA	C3B-C4B-NB	3.08	113.28	110.53
36	f	803	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
37	R	317	KC1	C4C-C3C-C2C	-3.08	102.41	106.89
36	L	309	CLA	C3B-C4B-NB	-3.08	107.78	110.53
44	i	103	BCR	C15-C16-C17	-3.08	117.22	123.52
37	L	315	KC1	CAD-C3D-C2D	-3.08	137.78	144.26
34	O	304	DD6	C21-C20-C15	-3.07	117.24	122.30
36	a	820	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
36	b	833	CLA	O2D-CGD-CBD	3.07	116.61	111.23
35	R	303	A86	C41-C32-C31	3.07	113.22	110.47
35	h	202	A86	C3-C2-C1	-3.07	122.97	127.28
36	a	825	CLA	C3B-C4B-NB	-3.07	107.79	110.53
35	S	304	A86	C34-O4-C38	-3.07	112.42	117.85
36	b	824	CLA	C3D-C2D-C1D	-3.07	101.64	105.83
36	b	826	CLA	OBD-CAD-C3D	-3.07	121.24	128.42
35	V	304	A86	C23-C16-C17	-3.07	103.57	108.97
34	B	302	DD6	C21-C20-C15	-3.07	117.25	122.30
36	C	208	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
36	N	310	CLA	CMD-C2D-C3D	-3.07	120.65	127.69
37	G	317	KC1	C3B-C2B-C1B	-3.07	104.14	107.05
36	D	313	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
36	K	310	CLA	C1-C2-C3	-3.07	121.17	126.20
36	S	319	CLA	CHB-C4A-NA	3.07	128.83	124.40
36	b	811	CLA	CHB-C4A-NA	3.07	128.83	124.40
36	R	320	CLA	CHB-C4A-NA	3.07	128.82	124.40
36	a	805	CLA	C3B-C4B-NB	-3.07	107.79	110.53
36	b	841	CLA	CAC-C3C-C4C	-3.07	120.80	124.79
36	N	313	CLA	CHB-C1B-NB	3.07	128.65	124.05
34	E	303	DD6	C21-C20-C15	-3.06	117.26	122.30
36	H	316	CLA	CED-O2D-CGD	3.06	122.86	115.92
41	a	843	LHG	O8-C23-C24	3.06	120.45	111.15
34	B	302	DD6	C37-C36-C35	3.06	120.05	114.42
35	R	303	A86	O4-C34-C35	3.06	115.47	107.64
36	D	312	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
36	A	311	CLA	C3B-C4B-NB	-3.06	107.80	110.53
36	C	211	CLA	C3B-C4B-NB	-3.06	107.80	110.53
37	T	315	KC1	C3B-C2B-C1B	-3.06	104.15	107.05
36	M	316	CLA	C3B-C4B-NB	-3.06	107.80	110.53
36	L	312	CLA	CHB-C4A-NA	3.06	128.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	O	302	A86	C28-C27-C26	-3.06	117.86	122.82
35	J	303	A86	O4-C38-C39	3.06	116.54	111.09
34	D	305	DD6	C15-C14-C13	-3.06	119.53	125.99
35	N	306	A86	O1-C20-C21	-3.06	111.63	115.05
36	V	305	CLA	CMA-C3A-C2A	-3.06	102.16	113.98
36	V	313	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
36	N	315	CLA	CMB-C2B-C3B	3.06	133.74	126.55
35	K	301	A86	C3-C2-C1	-3.06	122.99	127.28
36	S	315	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
35	P	307	A86	C34-O4-C38	-3.06	112.45	117.85
36	K	311	CLA	CHB-C4A-NA	3.06	128.81	124.40
36	A	313	CLA	C3B-C4B-NB	-3.05	107.80	110.53
36	a	834	CLA	C3B-C4B-NB	-3.05	107.80	110.53
36	a	823	CLA	CAC-C3C-C4C	3.05	128.76	124.79
43	a	840	PQN	C11-C12-C13	-3.05	121.57	126.83
36	a	803	CLA	C3B-C4B-NB	-3.05	107.81	110.53
36	X	309	CLA	CHB-C4A-NA	3.05	128.80	124.40
36	P	301	CLA	CHB-C4A-NA	3.05	128.80	124.40
36	H	311	CLA	C3B-C4B-NB	-3.05	107.81	110.53
35	C	202	A86	C35-C34-C33	-3.05	104.41	109.89
35	P	303	A86	C28-C27-C26	-3.05	117.88	122.82
36	a	811	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
35	T	304	A86	O1-C20-C21	-3.05	111.64	115.05
36	H	307	CLA	CMD-C2D-C1D	3.05	130.09	124.73
36	U	310	CLA	O1D-CGD-CBD	3.04	130.52	124.52
36	T	312	CLA	CHB-C4A-NA	3.04	128.79	124.40
36	L	311	CLA	CMB-C2B-C3B	3.04	133.71	126.55
35	O	319	A86	C25-C24-C1	-3.04	118.02	126.36
44	l	203	BCR	C27-C26-C25	3.04	126.82	122.70
36	E	308	CLA	C3B-C4B-NB	-3.04	107.81	110.53
39	B	312	LMT	C1B-O1B-C4'	-3.04	110.77	117.98
36	J	315	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
37	V	312	KC1	C3B-C2B-C1B	-3.04	104.17	107.05
36	H	305	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
34	G	303	DD6	O1-C15-C14	-3.04	108.17	116.88
35	Q	303	A86	C34-O4-C38	-3.04	112.47	117.85
36	F	316	CLA	C3B-C4B-NB	-3.04	107.82	110.53
36	I	308	CLA	C1-C2-C3	-3.04	121.22	126.20
36	a	812	CLA	CMB-C2B-C1B	-3.04	120.79	125.42
36	J	312	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
37	P	315	KC1	C4C-C3C-C2C	-3.04	102.47	106.89
36	D	306	CLA	CHB-C4A-NA	3.04	128.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	208	CLA	C3B-C4B-NB	-3.04	107.82	110.53
36	C	212	CLA	CBC-CAC-C3C	3.04	120.65	112.42
36	A	305	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
36	L	316	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
36	D	306	CLA	CAA-C2A-C1A	3.04	121.92	111.97
37	U	312	KC1	CHB-C1B-C2B	-3.04	119.17	125.49
36	i	102	CLA	CMB-C2B-C1B	-3.03	120.80	125.42
44	j	107	BCR	C29-C30-C25	3.03	114.84	110.44
37	O	313	KC1	C4C-C3C-C2C	-3.03	102.48	106.89
37	W	213	KC1	C1A-NA-C4A	-3.03	105.30	106.68
37	Q	313	KC1	C4C-C3C-C2C	-3.03	102.48	106.89
36	Q	305	CLA	C3B-C4B-NB	-3.03	107.82	110.53
36	W	212	CLA	C3B-C4B-NB	-3.03	107.82	110.53
36	W	211	CLA	CHB-C4A-NA	3.03	128.77	124.40
36	G	313	CLA	C3B-C4B-NB	-3.03	107.83	110.53
36	E	314	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
36	b	811	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
36	G	314	CLA	C3B-C4B-NB	-3.03	107.83	110.53
36	f	804	CLA	CMB-C2B-C1B	3.03	130.03	125.42
36	W	207	CLA	O2A-CGA-O1A	-3.03	116.05	123.63
37	V	312	KC1	CAD-C3D-C2D	-3.03	137.88	144.26
36	B	309	CLA	C1-C2-C3	-3.03	121.24	126.20
35	B	303	A86	O-C13-C11	-3.03	114.52	121.04
37	G	318	KC1	CHD-C1D-C2D	3.03	136.21	127.43
35	F	307	A86	C3-C4-C5	-3.03	117.33	123.52
36	Q	306	CLA	C3B-C4B-NB	-3.03	107.83	110.53
36	A	306	CLA	CMB-C2B-C1B	3.03	130.03	125.42
35	M	304	A86	O1-C20-C19	-3.02	110.66	113.49
36	a	810	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
44	l	207	BCR	C2-C1-C6	3.02	114.83	110.44
36	A	314	CLA	C3A-C2A-C1A	3.02	105.87	101.34
35	B	303	A86	O4-C38-O5	-3.02	117.16	122.99
35	N	304	A86	C29-C30-C31	-3.02	174.09	177.66
36	b	818	CLA	CMB-C2B-C3B	3.02	133.66	126.55
36	V	311	CLA	C1-C2-C3	-3.02	121.25	126.20
36	a	823	CLA	CHD-C4C-NC	3.02	128.91	124.23
36	H	317	CLA	C3B-C4B-NB	-3.02	107.83	110.53
36	A	306	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
36	O	307	CLA	C3B-C4B-NB	-3.02	107.83	110.53
36	b	840	CLA	C3B-C4B-NB	-3.02	107.83	110.53
34	R	307	DD6	C15-C14-C13	-3.02	119.61	125.99
44	a	847	BCR	C27-C26-C25	3.02	126.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	302	A86	C-C1-C24	3.02	122.70	118.09
36	G	313	CLA	CHB-C1B-NB	3.02	128.57	124.05
36	O	306	CLA	C3B-C4B-NB	-3.02	107.84	110.53
37	D	314	KC1	C3B-C2B-C1B	-3.02	104.19	107.05
34	S	307	DD6	C4-C5-C6	-3.02	123.05	127.28
34	S	307	DD6	C3-C4-C5	-3.01	117.35	123.52
36	C	214	CLA	C3B-C4B-NB	-3.01	107.84	110.53
36	P	308	CLA	C3B-C4B-NB	-3.01	107.84	110.53
36	a	802	CLA	CHB-C1B-NB	3.01	128.57	124.05
37	Q	311	KC1	C4C-C3C-C2C	-3.01	102.51	106.89
36	I	309	CLA	CHB-C4A-NA	3.01	128.75	124.40
35	A	302	A86	C7-C6-C8	3.01	122.69	118.09
36	b	819	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
36	E	317	CLA	C3B-C4B-NB	-3.01	107.84	110.53
36	a	804	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
36	a	806	CLA	CHB-C1B-NB	3.01	128.57	124.05
36	R	319	CLA	O2D-CGD-CBD	3.01	116.49	111.23
36	a	828	CLA	CMB-C2B-C1B	-3.01	120.84	125.42
36	A	306	CLA	CHB-C4A-NA	3.01	128.74	124.40
36	a	835	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
37	L	317	KC1	CMD-C2D-C3D	3.01	135.16	125.67
36	G	313	CLA	CMA-C3A-C4A	3.01	119.86	111.77
35	U	302	A86	C29-C30-C31	-3.01	174.11	177.66
36	R	314	CLA	CBA-CAA-C2A	-3.01	104.85	113.79
44	i	101	BCR	C31-C1-C6	3.00	114.95	110.24
36	M	308	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
35	V	303	A86	C33-C32-C31	3.00	112.13	109.21
36	b	819	CLA	CMB-C2B-C3B	3.00	133.61	126.55
36	E	311	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
36	N	316	CLA	C3B-C4B-NB	-3.00	107.85	110.53
36	M	308	CLA	CAC-C3C-C4C	-3.00	120.88	124.79
36	R	314	CLA	CAA-C2A-C1A	3.00	121.81	111.97
36	l	206	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
35	N	302	A86	O1-C20-C21	-3.00	111.69	115.05
39	K	318	LMT	C1B-O1B-C4'	-3.00	110.87	117.98
36	a	836	CLA	O2A-CGA-O1A	-3.00	116.13	123.63
36	L	310	CLA	C3B-C4B-NB	-3.00	107.85	110.53
36	S	319	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
37	O	315	KC1	C4C-C3C-C2C	-3.00	102.53	106.89
34	R	308	DD6	C15-C14-C13	-3.00	119.65	125.99
35	N	320	A86	C4-C5-C6	-3.00	123.07	127.28
37	F	308	KC1	CAC-C3C-C2C	3.00	133.06	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	V	307	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
36	P	311	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
37	W	213	KC1	C3C-C4C-NC	2.99	113.11	109.90
36	b	838	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
35	O	305	A86	C12-C11-C13	2.99	120.85	116.00
37	M	317	KC1	CAD-C3D-C2D	-2.99	137.96	144.26
36	O	309	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
44	m	101	BCR	C3-C4-C5	-2.99	108.72	114.06
44	b	844	BCR	C29-C30-C25	2.99	114.78	110.44
35	S	303	A86	C4-C5-C6	-2.99	123.08	127.28
34	E	304	DD6	C14-C13-C11	-2.99	120.89	125.53
36	A	306	CLA	CAC-C3C-C4C	2.99	128.68	124.79
36	G	319	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
35	U	302	A86	C9-C8-C6	-2.99	118.17	126.36
36	a	841	CLA	C3B-C4B-NB	-2.99	107.86	110.53
34	W	205	DD6	C14-C13-C11	-2.99	120.89	125.53
36	R	316	CLA	C2A-C1A-CHA	2.99	129.05	123.87
34	W	205	DD6	C15-C14-C13	-2.99	119.68	125.99
35	N	303	A86	C4-C5-C6	-2.99	123.09	127.28
37	F	308	KC1	C3A-C4A-NA	2.99	114.15	110.45
36	C	209	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
36	a	807	CLA	CHB-C4A-NA	2.99	128.71	124.40
34	W	205	DD6	C21-C20-C15	-2.99	117.39	122.30
36	J	309	CLA	C3B-C4B-NB	-2.99	107.86	110.53
36	a	826	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
36	a	818	CLA	CHB-C4A-NA	2.98	128.71	124.40
37	M	317	KC1	C3B-C2B-C1B	-2.98	104.22	107.05
36	a	816	CLA	CHD-C1D-ND	-2.98	120.61	124.80
36	C	212	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
35	L	304	A86	O-C13-C11	-2.98	114.62	121.04
36	S	310	CLA	C3B-C4B-NB	-2.98	107.87	110.53
35	F	301	A86	C34-O4-C38	-2.98	112.58	117.85
36	a	815	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
36	J	312	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
44	i	101	BCR	C29-C30-C25	2.98	114.77	110.44
36	A	307	CLA	C3B-C4B-NB	-2.98	107.87	110.53
36	B	309	CLA	C4-C3-C5	2.98	120.40	115.23
36	a	848	CLA	O2A-CGA-CBA	2.98	120.92	111.83
36	P	309	CLA	C3B-C4B-NB	-2.98	107.87	110.53
36	X	306	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
36	E	315	CLA	CMB-C2B-C1B	2.98	129.96	125.42
35	S	302	A86	O1-C20-C21	-2.98	111.72	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	210	CLA	CHB-C4A-NA	2.98	128.70	124.40
36	a	826	CLA	CHB-C4A-NA	2.98	128.70	124.40
36	b	816	CLA	O2A-CGA-CBA	2.98	120.92	111.83
35	Q	304	A86	C4-C5-C6	-2.98	123.10	127.28
36	l	205	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
36	a	827	CLA	CMB-C2B-C3B	2.98	133.55	126.55
36	a	819	CLA	CHB-C4A-NA	2.98	128.70	124.40
36	l	205	CLA	CHB-C4A-NA	2.98	128.70	124.40
36	J	310	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
36	W	214	CLA	C1D-ND-C4D	-2.98	104.22	106.31
35	G	302	A86	C3-C4-C5	-2.97	117.43	123.52
36	b	808	CLA	C3B-C4B-NB	-2.97	107.88	110.53
36	H	317	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
36	b	837	CLA	CHB-C4A-NA	2.97	128.69	124.40
37	H	313	KC1	C1D-CHD-C4C	-2.97	119.26	126.25
36	a	833	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
36	b	808	CLA	CHB-C4A-NA	2.97	128.69	124.40
37	T	310	KC1	C4D-CHA-C1A	2.97	131.51	122.45
36	b	825	CLA	O2D-CGD-CBD	2.97	116.42	111.23
36	X	312	CLA	CMB-C2B-C1B	-2.97	120.90	125.42
36	E	315	CLA	O2A-CGA-CBA	2.97	120.89	111.83
36	C	210	CLA	CHB-C4A-NA	2.97	128.68	124.40
36	N	319	CLA	CHB-C4A-NA	2.97	128.68	124.40
36	b	824	CLA	C4-C3-C5	2.97	120.38	115.23
36	S	313	CLA	CAA-C2A-C1A	2.97	121.70	111.97
36	I	313	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
36	b	815	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
36	U	305	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
36	Q	309	CLA	CHB-C4A-NA	2.97	128.68	124.40
36	b	833	CLA	C3B-C4B-NB	-2.97	107.88	110.53
36	Q	308	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
36	N	319	CLA	CED-O2D-CGD	2.97	122.65	115.92
35	W	202	A86	C4-C3-C2	-2.97	117.45	123.52
35	G	306	A86	C-C1-C2	-2.96	118.01	122.82
36	O	309	CLA	C3B-C4B-NB	-2.96	107.88	110.53
36	b	830	CLA	CMB-C2B-C3B	2.96	133.52	126.55
36	Q	310	CLA	C4-C3-C2	-2.96	116.02	123.63
37	G	308	KC1	C4C-C3C-C2C	-2.96	102.58	106.89
36	b	811	CLA	O2A-CGA-O1A	-2.96	116.22	123.63
37	G	318	KC1	C4C-C3C-C2C	-2.96	102.58	106.89
35	F	305	A86	O-C13-C11	-2.96	114.66	121.04
36	b	824	CLA	C4C-C3C-C2C	-2.96	102.58	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	824	CLA	O2A-CGA-CBA	2.96	120.86	111.83
35	K	306	A86	O4-C38-O5	-2.96	117.28	122.99
36	A	309	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
36	b	841	CLA	CHC-C1C-NC	2.96	128.77	124.31
35	T	303	A86	C33-C32-C31	-2.96	106.34	109.21
36	f	802	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
35	V	304	A86	C40-C32-C31	2.96	113.12	110.47
37	G	308	KC1	C4D-CHA-C1A	-2.96	113.44	122.45
36	F	316	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
35	M	304	A86	C9-C10-C11	-2.96	118.28	126.64
36	b	814	CLA	CHB-C4A-NA	2.96	128.67	124.40
35	R	304	A86	C21-C20-C15	-2.96	113.81	123.35
35	F	307	A86	C23-C16-C22	-2.96	103.08	107.37
36	a	848	CLA	CMD-C2D-C3D	-2.96	120.91	127.69
36	S	320	CLA	C3B-C4B-NB	-2.96	107.89	110.53
35	N	304	A86	C34-O4-C38	-2.95	112.63	117.85
36	B	308	CLA	CMB-C2B-C1B	-2.95	120.92	125.42
37	K	314	KC1	C3C-C4C-NC	2.95	113.07	109.90
35	T	302	A86	C25-C26-C27	-2.95	123.14	127.28
35	R	302	A86	O4-C38-C39	2.95	116.36	111.09
36	G	316	CLA	CHB-C4A-NA	2.95	128.66	124.40
36	O	316	CLA	CHB-C4A-NA	2.95	128.66	124.40
36	R	316	CLA	CAC-C3C-C2C	2.95	132.98	127.56
36	I	312	CLA	CHB-C4A-NA	2.95	128.66	124.40
36	J	311	CLA	CHB-C4A-NA	2.95	128.66	124.40
36	H	316	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
36	J	316	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
41	D	319	LHG	O8-C23-C24	2.95	120.83	111.83
37	U	312	KC1	CHB-C4A-NA	2.95	128.81	124.23
36	j	102	CLA	C4-C3-C5	2.95	120.35	115.23
34	S	306	DD6	C37-C36-C31	-2.95	118.64	124.16
36	J	308	CLA	CHB-C4A-NA	2.95	128.66	124.40
36	D	309	CLA	CMB-C2B-C1B	2.95	129.91	125.42
36	G	319	CLA	CHB-C1B-C2B	-2.95	118.87	127.43
36	H	318	CLA	O1D-CGD-CBD	2.95	130.33	124.52
34	L	305	DD6	C15-C14-C13	-2.95	119.76	125.99
35	T	304	A86	C3-C4-C5	-2.95	117.49	123.52
36	M	309	CLA	C3B-C4B-NB	-2.95	107.90	110.53
36	W	207	CLA	C3B-C4B-NB	-2.95	107.90	110.53
36	O	312	CLA	C2A-C3A-C4A	2.95	108.57	103.57
36	W	212	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
35	N	304	A86	C-C1-C2	-2.95	118.04	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	816	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
36	f	805	CLA	CHB-C4A-NA	2.94	128.65	124.40
36	B	306	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
36	b	824	CLA	CHB-C4A-NA	2.94	128.65	124.40
36	O	316	CLA	CHD-C4C-C3C	-2.94	120.48	124.77
36	I	306	CLA	O2A-CGA-CBA	2.94	120.81	111.83
37	G	318	KC1	CED-O2D-CGD	2.94	122.59	115.92
35	C	203	A86	C25-C26-C27	-2.94	123.15	127.28
36	b	817	CLA	C3B-C4B-NB	-2.94	107.91	110.53
34	D	303	DD6	C10-C9-C8	-2.94	114.68	123.20
44	i	103	BCR	C29-C30-C25	2.94	114.71	110.44
37	M	318	KC1	C4B-CHC-C1C	-2.94	119.77	126.02
36	W	209	CLA	CHB-C4A-NA	2.94	128.64	124.40
36	P	311	CLA	C3B-C4B-NB	-2.94	107.91	110.53
36	V	313	CLA	C3B-C4B-NB	-2.94	107.91	110.53
36	L	312	CLA	C2A-C1A-CHA	2.94	128.96	123.87
35	E	302	A86	C9-C10-C11	-2.94	118.34	126.64
37	T	310	KC1	CAC-C3C-C4C	2.94	128.61	124.79
36	b	831	CLA	O2D-CGD-CBD	2.94	116.36	111.23
34	O	304	DD6	C28-C27-C26	-2.94	118.48	124.18
36	M	307	CLA	C3B-C4B-NB	-2.94	107.91	110.53
36	a	810	CLA	C3B-C4B-NB	-2.94	107.91	110.53
36	b	811	CLA	C3B-C4B-NB	-2.94	107.91	110.53
36	b	818	CLA	C3B-C4B-NB	-2.94	107.91	110.53
37	W	217	KC1	C3B-C2B-C1B	-2.94	104.27	107.05
36	A	308	CLA	CMB-C2B-C3B	2.93	133.45	126.55
35	J	305	A86	C25-C26-C27	-2.93	123.16	127.28
40	b	849	DGD	O3E-C3E-C2E	-2.93	103.46	110.38
35	L	307	A86	C12-C11-C13	2.93	120.76	116.00
35	F	306	A86	C12-C11-C13	2.93	120.75	116.00
36	N	307	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	Q	314	CLA	O2D-CGD-CBD	2.93	116.36	111.23
34	A	303	DD6	C14-C13-C11	-2.93	120.98	125.53
36	a	807	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	J	313	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	b	835	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	a	803	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
36	D	309	CLA	C4-C3-C5	2.93	120.31	115.23
44	a	847	BCR	C24-C23-C22	-2.93	121.90	126.23
36	b	824	CLA	CHD-C4C-C3C	-2.93	120.50	124.77
36	B	308	CLA	C2D-C1D-ND	-2.93	107.23	110.13
36	B	305	CLA	O2D-CGD-O1D	-2.93	118.15	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	301	A86	C19-C18-C17	-2.93	105.32	110.79
36	a	822	CLA	O2A-CGA-CBA	2.93	120.76	111.83
36	Q	314	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
35	G	302	A86	O1-C20-C19	-2.93	110.75	113.49
44	b	847	BCR	C27-C26-C25	2.93	126.66	122.70
36	S	320	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
36	G	311	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
34	R	308	DD6	C37-C36-C35	2.92	119.80	114.42
36	I	312	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
36	B	307	CLA	CHB-C4A-NA	2.92	128.62	124.40
37	K	314	KC1	CBC-CAC-C3C	-2.92	104.50	112.42
37	B	310	KC1	C4C-C3C-C2C	-2.92	102.64	106.89
36	F	317	CLA	C2B-C1B-NB	2.92	113.35	110.33
35	R	306	A86	C4-C3-C2	-2.92	117.55	123.52
37	M	313	KC1	O2D-CGD-O1D	-2.92	118.17	123.85
34	I	303	DD6	C25-C26-C27	-2.92	118.44	126.61
36	R	313	CLA	C3B-C4B-NB	-2.92	107.92	110.53
34	J	304	DD6	C37-C36-C31	-2.92	118.70	124.16
36	P	302	CLA	O2D-CGD-CBD	2.92	116.33	111.23
36	F	309	CLA	C3B-C4B-NB	-2.92	107.92	110.53
35	W	203	A86	O1-C20-C21	-2.92	111.79	115.05
37	K	314	KC1	CAD-C3D-C2D	-2.92	138.12	144.26
35	M	301	A86	C34-O4-C38	2.92	123.00	117.85
36	O	310	CLA	CHB-C4A-NA	2.92	128.61	124.40
36	a	821	CLA	CMB-C2B-C1B	-2.91	120.98	125.42
36	T	308	CLA	CHB-C4A-NA	2.91	128.61	124.40
35	M	301	A86	C41-C32-C31	-2.91	107.86	110.47
35	R	304	A86	O4-C38-O5	-2.91	117.36	122.99
36	f	804	CLA	C3D-C4D-ND	2.91	114.72	109.99
37	X	311	KC1	C3B-C2B-C1B	-2.91	104.29	107.05
35	S	301	A86	C19-C18-C17	-2.91	105.34	110.79
36	Q	310	CLA	C3A-C2A-C1A	-2.91	96.98	101.34
36	b	826	CLA	O2D-CGD-CBD	2.91	116.32	111.23
36	X	308	CLA	CHC-C4B-C3B	-2.91	114.74	127.37
34	A	304	DD6	C14-C13-C11	-2.91	121.01	125.53
34	I	303	DD6	C9-C10-C11	-2.91	123.20	127.28
36	S	321	CLA	CGD-CBD-CAD	-2.91	101.43	110.85
34	G	303	DD6	C14-C13-C11	-2.91	121.02	125.53
35	B	303	A86	C25-C24-C1	-2.91	118.39	126.36
36	X	306	CLA	C3B-C4B-NB	-2.91	107.94	110.53
36	F	314	CLA	CHB-C4A-NA	2.91	128.59	124.40
37	W	217	KC1	C3C-C4C-NC	2.91	113.02	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	M	314	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
36	X	312	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
37	L	317	KC1	C3B-C2B-C1B	-2.91	104.30	107.05
35	N	301	A86	C33-C32-C31	-2.90	106.39	109.21
35	T	302	A86	C40-C32-C31	2.90	113.07	110.47
37	U	312	KC1	C4C-C3C-C2C	-2.90	102.67	106.89
36	Q	308	CLA	C3B-C4B-NB	-2.90	107.94	110.53
36	j	101	CLA	C3B-C4B-NB	-2.90	107.94	110.53
35	R	301	A86	C25-C24-C1	-2.90	118.40	126.36
36	H	311	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
36	D	309	CLA	CHD-C4C-C3C	-2.90	120.54	124.77
36	b	811	CLA	O2D-CGD-CBD	2.90	116.30	111.23
36	f	802	CLA	C6-C7-C8	-2.90	106.32	115.97
36	P	319	CLA	CHB-C1B-C2B	-2.90	119.00	127.43
36	b	817	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
37	O	313	KC1	CHD-C1D-C2D	2.90	135.85	127.43
34	Q	302	DD6	C37-C36-C35	2.90	119.76	114.42
37	P	315	KC1	CHD-C1D-C2D	2.90	135.85	127.43
35	T	307	A86	C3-C4-C5	-2.90	117.58	123.52
36	l	201	CLA	C3B-C4B-NB	-2.90	107.94	110.53
34	A	301	DD6	C3-C4-C5	-2.90	117.58	123.52
35	N	304	A86	C26-C25-C24	-2.90	114.80	123.20
36	E	316	CLA	CHB-C4A-NA	2.90	128.59	124.40
36	a	803	CLA	CHB-C4A-NA	2.90	128.59	124.40
36	b	821	CLA	CHB-C4A-NA	2.90	128.58	124.40
36	X	309	CLA	C3B-C4B-NB	-2.90	107.94	110.53
36	F	309	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
36	L	314	CLA	O2A-CGA-O1A	-2.90	116.38	123.63
42	E	318	LMG	O8-C28-C29	2.90	120.67	111.83
36	b	819	CLA	CHB-C1B-NB	2.90	128.40	124.05
36	b	807	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
42	D	320	LMG	O8-C28-C29	2.90	120.67	111.83
44	h	201	BCR	C29-C30-C25	2.90	114.65	110.44
36	I	306	CLA	CMD-C2D-C3D	-2.90	121.05	127.69
36	N	308	CLA	CMB-C2B-C1B	-2.90	121.01	125.42
36	I	311	CLA	CMB-C2B-C3B	2.90	133.36	126.55
35	G	305	A86	C9-C10-C11	-2.89	118.46	126.64
35	G	302	A86	C12-C11-C13	2.89	120.69	116.00
35	Q	303	A86	C40-C32-C31	-2.89	107.88	110.47
36	f	804	CLA	CAC-C3C-C4C	2.89	128.55	124.79
36	G	316	CLA	C3B-C4B-NB	-2.89	107.95	110.53
36	T	309	CLA	CHB-C4A-NA	2.89	128.57	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	b	844	BCR	C30-C25-C26	-2.89	118.69	122.64
35	U	302	A86	C23-C16-C17	-2.89	103.89	108.97
41	I	316	LHG	O8-C23-C24	2.89	120.65	111.83
36	D	311	CLA	CHB-C4A-NA	2.89	128.57	124.40
36	a	824	CLA	C2A-C1A-CHA	2.89	128.88	123.87
36	D	309	CLA	O2A-CGA-CBA	2.89	120.64	111.83
36	K	313	CLA	C3B-C4B-NB	-2.89	107.95	110.53
35	L	301	A86	C25-C26-C27	-2.89	123.23	127.28
36	D	317	CLA	CHB-C4A-NA	2.89	128.57	124.40
36	J	308	CLA	C6-C5-C3	2.89	120.50	113.47
36	U	311	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
36	I	310	CLA	CHB-C4A-NA	2.89	128.56	124.40
36	N	319	CLA	C1D-CHD-C4C	2.89	132.15	126.02
36	U	311	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
36	A	305	CLA	C3B-C4B-NB	-2.89	107.95	110.53
37	W	213	KC1	C1C-C2C-C3C	-2.88	103.95	106.98
36	K	311	CLA	C3B-C4B-NB	-2.88	107.95	110.53
36	V	308	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
34	j	103	DD6	C37-C36-C31	-2.88	118.77	124.16
36	C	214	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
37	X	311	KC1	C3C-C4C-NC	2.88	112.99	109.90
35	G	305	A86	C25-C26-C27	-2.88	123.24	127.28
37	V	312	KC1	CAA-C2A-C1A	2.88	137.27	124.64
36	W	214	CLA	CAA-C2A-C3A	-2.88	109.62	116.23
36	B	306	CLA	CHB-C4A-NA	2.88	128.56	124.40
36	a	818	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
36	P	312	CLA	CHB-C4A-NA	2.88	128.56	124.40
37	G	318	KC1	C2A-C1A-NA	2.88	113.96	109.34
36	N	319	CLA	CAA-C2A-C1A	-2.88	105.77	112.14
40	L	302	DGD	C2G-O2G-C1B	-2.88	110.90	117.80
36	a	829	CLA	CMB-C2B-C3B	2.88	133.32	126.55
34	H	303	DD6	C14-C13-C11	-2.88	121.06	125.53
36	N	319	CLA	CHA-C1A-NA	-2.88	119.87	126.39
36	P	314	CLA	C3A-C2A-C1A	-2.88	97.03	101.34
36	U	313	CLA	CHB-C4A-NA	2.88	128.55	124.40
37	O	315	KC1	CHD-C1D-C2D	2.88	135.78	127.43
35	L	306	A86	C-C1-C2	-2.88	118.16	122.82
34	D	305	DD6	O1-C15-C14	-2.88	108.64	116.88
36	H	307	CLA	CHD-C1D-ND	-2.88	120.75	124.80
37	Q	311	KC1	CHD-C1D-C2D	2.88	135.77	127.43
36	G	307	CLA	CMD-C2D-C3D	-2.88	121.09	127.69
36	h	203	CLA	O1D-CGD-CBD	2.88	130.19	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	H	316	CLA	CHB-C4A-NA	2.88	128.55	124.40
37	T	315	KC1	CAA-C2A-C1A	2.87	137.24	124.64
36	l	201	CLA	O2D-CGD-CBD	2.87	116.25	111.23
40	L	302	DGD	O1G-C1A-C2A	2.87	120.60	111.83
35	K	301	A86	C9-C8-C6	-2.87	118.48	126.36
35	I	302	A86	O1-C20-C21	-2.87	111.84	115.05
36	a	816	CLA	C4-C3-C5	2.87	120.22	115.23
36	b	841	CLA	CHB-C4A-NA	2.87	128.55	124.40
36	j	102	CLA	CHD-C1D-ND	-2.87	120.76	124.80
35	R	303	A86	C9-C10-C11	-2.87	118.52	126.64
36	S	314	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
36	D	316	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
36	D	309	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
36	C	207	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
36	b	806	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
36	V	307	CLA	C3B-C4B-NB	-2.87	107.97	110.53
36	E	315	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
36	b	833	CLA	CAA-C2A-C1A	-2.87	102.57	111.97
34	J	304	DD6	C9-C10-C11	-2.87	123.25	127.28
36	K	313	CLA	CMB-C2B-C3B	2.87	133.30	126.55
36	a	810	CLA	CAA-CBA-CGA	2.87	121.35	113.21
36	M	316	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
36	E	315	CLA	C4-C3-C5	2.87	120.21	115.23
36	S	317	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
44	b	845	BCR	C30-C25-C26	-2.87	118.72	122.64
36	L	314	CLA	CHB-C4A-NA	2.87	128.53	124.40
36	A	306	CLA	O2A-CGA-CBA	2.86	120.57	111.83
37	Q	313	KC1	CHD-C1D-C2D	2.86	135.74	127.43
36	N	319	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
41	F	318	LHG	O8-C23-C24	2.86	120.56	111.83
41	b	850	LHG	O8-C23-C24	2.86	120.56	111.83
36	b	833	CLA	CAA-CBA-CGA	-2.86	105.08	113.21
36	R	316	CLA	CAC-C3C-C4C	-2.86	121.07	124.79
42	D	321	LMG	O8-C28-C29	2.86	120.56	111.83
36	b	830	CLA	C2D-C1D-ND	-2.86	107.30	110.13
35	S	301	A86	C33-C32-C31	-2.86	106.43	109.21
36	D	315	CLA	CMB-C2B-C3B	2.86	133.28	126.55
36	b	825	CLA	C2A-C1A-CHA	2.86	128.83	123.87
35	O	319	A86	O4-C38-O5	-2.86	117.47	122.99
36	C	206	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
36	D	310	CLA	CHB-C4A-NA	2.86	128.53	124.40
34	S	306	DD6	C4-C5-C6	-2.86	123.27	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	827	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
36	Q	308	CLA	CHB-C4A-NA	2.86	128.53	124.40
36	E	316	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
35	P	306	A86	O1-C20-C19	-2.86	110.81	113.49
36	X	308	CLA	CHB-C1B-C2B	-2.86	119.13	127.43
36	f	804	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
35	F	307	A86	C41-C32-C40	-2.86	100.46	108.63
36	T	313	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
36	U	306	CLA	O2A-CGA-CBA	2.85	120.54	111.83
35	N	306	A86	C40-C32-C31	2.85	113.03	110.47
37	N	314	KC1	C1D-CHD-C4C	-2.85	119.53	126.25
37	F	315	KC1	C3B-C2B-C1B	-2.85	104.34	107.05
36	T	311	CLA	CHB-C4A-NA	2.85	128.52	124.40
36	E	313	CLA	C4-C3-C5	2.85	120.18	115.23
36	a	823	CLA	O2A-CGA-CBA	2.85	120.53	111.83
35	F	302	A86	C34-O4-C38	-2.85	112.81	117.85
36	C	211	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
36	b	837	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
36	G	315	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
36	b	802	CLA	CHB-C4A-NA	2.85	128.51	124.40
35	T	303	A86	C40-C32-C31	2.85	113.02	110.47
35	G	304	A86	C19-C18-C17	-2.85	105.46	110.79
36	I	308	CLA	CMD-C2D-C3D	-2.85	121.15	127.69
36	B	309	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
36	U	313	CLA	C3B-C4B-NB	-2.85	107.99	110.53
37	F	308	KC1	C4C-C3C-C2C	-2.85	102.74	106.89
36	Q	314	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
36	j	106	CLA	CHB-C4A-NA	2.85	128.51	124.40
44	b	846	BCR	C27-C26-C25	2.85	126.55	122.70
35	S	304	A86	C12-C11-C13	2.85	120.62	116.00
36	b	817	CLA	CHB-C4A-NA	2.85	128.51	124.40
42	I	315	LMG	O8-C28-C29	2.85	120.52	111.83
41	R	323	LHG	O8-C23-C24	2.85	120.51	111.83
36	a	806	CLA	O2A-CGA-CBA	2.85	120.51	111.83
36	N	318	CLA	C2A-C1A-CHA	2.85	128.81	123.87
35	N	320	A86	C40-C32-C31	2.84	113.02	110.47
42	j	105	LMG	O8-C28-C29	2.84	120.51	111.83
36	X	307	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
37	F	308	KC1	CHD-C1D-C2D	2.84	135.68	127.43
36	R	322	CLA	CMA-C3A-C2A	-2.84	102.99	113.98
36	b	833	CLA	CMD-C2D-C1D	-2.84	119.72	124.73
36	L	308	CLA	C4-C3-C5	2.84	120.16	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	833	CLA	CHB-C4A-NA	2.84	128.50	124.40
36	D	315	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
36	C	207	CLA	CAC-C3C-C4C	2.84	128.49	124.79
35	S	305	A86	O1-C20-C15	-2.84	58.09	59.23
36	a	827	CLA	CHB-C4A-NA	2.84	128.50	124.40
34	E	304	DD6	C37-C36-C31	-2.84	118.85	124.16
36	N	315	CLA	C2A-C1A-CHA	2.84	128.78	123.86
42	G	324	LMG	O8-C28-C29	2.84	120.50	111.83
37	M	313	KC1	C3B-C2B-C1B	-2.84	104.36	107.05
36	F	311	CLA	CHB-C4A-NA	2.84	128.50	124.40
36	N	319	CLA	CMC-C2C-C3C	2.84	133.83	126.15
36	M	314	CLA	C3B-C4B-NB	-2.84	108.00	110.53
36	R	316	CLA	C3B-C4B-NB	-2.84	108.00	110.53
34	H	302	DD6	C21-C20-C15	-2.84	117.63	122.30
36	W	212	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
34	E	303	DD6	C37-C36-C31	-2.84	118.86	124.16
36	N	308	CLA	C1-C2-C3	2.84	130.84	126.20
36	S	310	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
35	X	302	A86	C25-C24-C1	-2.84	118.59	126.36
36	a	805	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
36	a	814	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
35	h	204	A86	C3-C4-C5	-2.83	117.72	123.52
36	P	311	CLA	CHB-C4A-NA	2.83	128.49	124.40
36	E	314	CLA	CMB-C2B-C1B	-2.83	121.10	125.42
36	I	309	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
36	b	801	CLA	CAC-C3C-C4C	2.83	128.48	124.79
36	C	210	CLA	C2A-C1A-CHA	2.83	128.78	123.87
36	T	314	CLA	CMA-C3A-C4A	-2.83	104.16	111.77
36	N	319	CLA	CAC-C3C-C2C	-2.83	122.36	127.56
36	D	306	CLA	CHA-C1A-NA	-2.83	119.98	126.39
41	G	320	LHG	O8-C23-C24	2.83	120.47	111.83
36	a	802	CLA	C4-C3-C5	2.83	120.14	115.23
36	E	310	CLA	CMB-C2B-C3B	2.83	133.21	126.55
36	E	315	CLA	CMD-C2D-C3D	-2.83	121.20	127.69
36	I	307	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
36	R	316	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
36	b	801	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
36	U	306	CLA	CHB-C4A-NA	2.83	128.48	124.40
35	S	302	A86	C23-C16-C17	-2.83	104.00	108.97
36	A	308	CLA	CHB-C4A-NA	2.83	128.48	124.40
36	D	311	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
35	J	306	A86	C25-C26-C27	-2.83	123.31	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	Q	315	LHG	O8-C23-C24	2.83	120.45	111.83
36	C	207	CLA	C4-C3-C5	2.83	120.13	115.23
36	X	315	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
37	H	313	KC1	C2A-C3A-C4A	2.83	108.53	106.41
36	f	804	CLA	CMD-C2D-C3D	-2.83	121.21	127.69
36	E	314	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
36	a	833	CLA	C3B-C4B-NB	-2.83	108.01	110.53
42	a	852	LMG	O8-C28-C29	2.83	120.45	111.83
36	a	813	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
36	b	816	CLA	CHD-C4C-NC	2.82	128.61	124.23
34	G	303	DD6	C37-C36-C31	-2.82	118.88	124.16
35	N	302	A86	C23-C16-C17	-2.82	104.00	108.97
36	j	102	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
41	F	319	LHG	O8-C23-C24	2.82	120.44	111.83
36	b	818	CLA	O2D-CGD-CBD	2.82	116.17	111.23
42	L	321	LMG	O8-C28-C29	2.82	120.44	111.83
36	O	309	CLA	CHB-C4A-NA	2.82	128.47	124.40
34	j	103	DD6	C9-C8-C6	-2.82	118.63	126.36
36	N	313	CLA	CHB-C1B-C2B	-2.82	119.24	127.43
36	R	322	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
35	K	301	A86	C4-C3-C2	-2.82	117.75	123.52
35	O	305	A86	C3-C4-C5	-2.82	117.75	123.52
37	G	308	KC1	C3B-C2B-C1B	-2.82	104.38	107.05
35	R	306	A86	C25-C24-C1	-2.82	118.64	126.36
37	L	317	KC1	C4C-C3C-C2C	-2.82	102.79	106.89
34	O	304	DD6	C34-C35-C36	-2.82	105.16	112.18
36	I	306	CLA	C2D-C1D-ND	2.82	112.92	110.13
36	h	203	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
41	a	850	LHG	O8-C23-C24	2.82	120.43	111.83
41	b	850	LHG	C5-O7-C7	-2.82	111.05	117.80
36	D	310	CLA	C3B-C4B-NB	-2.82	108.02	110.53
37	E	309	KC1	CBC-CAC-C3C	2.82	120.06	112.42
36	W	206	CLA	CHB-C4A-NA	2.82	128.47	124.40
36	M	312	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
36	K	310	CLA	CMD-C2D-C3D	-2.82	121.23	127.69
36	P	319	CLA	CHA-C1A-NA	-2.81	120.02	126.39
36	C	211	CLA	CHB-C4A-NA	2.81	128.46	124.40
34	D	304	DD6	C37-C36-C31	-2.81	118.90	124.16
36	a	821	CLA	C3B-C4B-NB	-2.81	108.02	110.53
44	f	801	BCR	C27-C26-C25	2.81	126.51	122.70
36	b	816	CLA	CMD-C2D-C3D	-2.81	121.24	127.69
36	R	310	CLA	O2D-CGD-O1D	-2.81	118.37	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	818	CLA	CHB-C1B-NB	2.81	128.27	124.05
36	S	319	CLA	C3B-C4B-NB	-2.81	108.02	110.53
35	E	307	A86	C34-O4-C38	-2.81	112.88	117.85
35	J	302	A86	C9-C10-C11	-2.81	118.69	126.64
37	E	309	KC1	O2D-CGD-O1D	-2.81	118.38	123.85
35	S	305	A86	C28-C27-C26	-2.81	118.26	122.82
36	G	315	CLA	C4-C3-C5	2.81	120.11	115.23
35	U	302	A86	C9-C10-C11	-2.81	118.69	126.64
36	a	819	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
36	A	308	CLA	C3B-C4B-NB	-2.81	108.02	110.53
36	b	815	CLA	CBC-CAC-C3C	2.81	120.04	112.42
36	a	829	CLA	CMD-C2D-C1D	-2.81	119.78	124.73
42	V	315	LMG	O8-C28-C29	2.81	120.40	111.83
36	T	312	CLA	CBA-CAA-C2A	-2.81	105.43	113.79
34	O	304	DD6	C37-C36-C31	-2.81	118.91	124.16
36	P	302	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
35	J	306	A86	C12-C11-C13	2.81	120.55	116.00
36	N	318	CLA	C3B-C4B-NB	-2.81	108.02	110.53
35	R	303	A86	C3-C4-C5	-2.81	117.77	123.52
36	P	308	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
36	A	310	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
35	S	301	A86	C25-C24-C1	-2.81	118.67	126.36
36	W	216	CLA	C1D-ND-C4D	-2.81	104.34	106.31
35	S	302	A86	C23-C16-C22	-2.81	103.29	107.37
36	C	207	CLA	CMB-C2B-C1B	2.81	129.69	125.42
35	Q	304	A86	C40-C32-C31	2.80	112.98	110.47
36	a	812	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
35	N	320	A86	O4-C34-C33	2.80	114.81	107.64
36	j	102	CLA	CMD-C2D-C3D	-2.80	121.26	127.69
36	b	816	CLA	C4D-CHA-C1A	-2.80	117.90	121.24
34	C	201	DD6	C15-C14-C13	-2.80	120.07	125.99
36	M	310	CLA	CHA-C1A-NA	-2.80	120.05	126.39
36	W	209	CLA	C3B-C4B-NB	-2.80	108.03	110.53
36	b	812	CLA	CAC-C3C-C4C	2.80	128.43	124.79
36	I	305	CLA	O2D-CGD-CBD	2.80	116.12	111.23
36	Q	305	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
36	I	306	CLA	CHD-C4C-C3C	-2.80	120.69	124.77
36	R	319	CLA	CMC-C2C-C3C	2.80	133.72	126.15
44	b	846	BCR	C3-C4-C5	-2.80	109.07	114.06
36	N	307	CLA	CHB-C4A-NA	2.80	128.44	124.40
36	N	309	CLA	CHB-C4A-NA	2.80	128.44	124.40
35	G	304	A86	C9-C8-C6	2.80	134.03	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	O	316	CLA	O2A-CGA-CBA	2.80	120.36	111.83
36	S	321	CLA	O2D-CGD-CBD	2.80	116.12	111.23
36	X	313	CLA	CHC-C1C-NC	2.80	128.52	124.31
36	R	313	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
37	M	318	KC1	C3A-C4A-NA	2.80	113.91	110.45
36	N	309	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
42	G	325	LMG	O8-C28-C29	2.79	120.36	111.83
36	N	307	CLA	C3B-C4B-NB	-2.79	108.03	110.53
35	V	304	A86	C3-C2-C1	-2.79	123.36	127.28
36	J	310	CLA	CHB-C4A-NA	2.79	128.43	124.40
36	N	318	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
36	X	308	CLA	C3A-C2A-C1A	2.79	105.52	101.34
36	h	203	CLA	CHB-C4A-NA	2.79	128.43	124.40
35	N	302	A86	C23-C16-C22	-2.79	103.31	107.37
35	U	304	A86	C9-C8-C6	-2.79	118.71	126.36
36	G	319	CLA	CHA-C4D-ND	-2.79	126.79	132.55
36	S	309	CLA	C3B-C4B-NB	-2.79	108.04	110.53
35	X	304	A86	O-C13-C11	-2.79	115.03	121.04
36	N	308	CLA	C1-O2A-CGA	2.79	123.41	116.65
36	b	801	CLA	C4D-C3D-CAD	-2.79	105.08	108.11
36	T	312	CLA	CAA-C2A-C1A	2.79	121.12	111.97
36	H	310	CLA	O1D-CGD-CBD	-2.79	119.02	124.52
36	C	207	CLA	CHD-C4C-C3C	-2.79	120.71	124.77
36	J	311	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
36	M	307	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
36	b	832	CLA	CHB-C4A-NA	2.79	128.43	124.40
41	G	301	LHG	O8-C23-C24	2.79	120.34	111.83
35	S	305	A86	O-C13-C11	-2.79	115.04	121.04
35	J	303	A86	C26-C25-C24	-2.79	115.12	123.20
36	f	804	CLA	CHD-C4C-C3C	-2.79	120.71	124.77
36	G	314	CLA	CHB-C4A-NA	2.79	128.42	124.40
36	A	309	CLA	C3B-C4B-NB	-2.79	108.04	110.53
36	b	837	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
34	C	201	DD6	C21-C20-C15	-2.79	117.72	122.30
36	A	313	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
36	T	316	CLA	C3B-C4B-NB	-2.79	108.04	110.53
35	E	305	A86	C12-C11-C13	2.79	120.52	116.00
36	a	824	CLA	O2D-CGD-CBD	2.79	116.10	111.23
35	O	301	A86	C3-C4-C5	-2.78	117.82	123.52
37	A	312	KC1	C2A-C1A-CHA	2.78	140.40	128.96
36	W	218	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
36	j	102	CLA	O2A-CGA-CBA	2.78	120.32	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	j	104	LHG	O8-C23-C24	2.78	120.32	111.83
35	N	301	A86	C25-C24-C1	-2.78	118.73	126.36
35	R	303	A86	C9-C8-C6	-2.78	118.73	126.36
34	K	304	DD6	C37-C36-C35	2.78	119.54	114.42
34	a	849	DD6	C25-C26-C27	-2.78	118.83	126.61
36	a	802	CLA	O2A-CGA-CBA	2.78	120.32	111.83
35	X	303	A86	C10-C9-C8	-2.78	115.14	123.20
40	C	215	DGD	O1G-C1A-C2A	2.78	120.32	111.83
35	J	303	A86	C3-C2-C1	-2.78	123.38	127.28
36	l	204	CLA	CMD-C2D-C3D	-2.78	121.31	127.69
36	V	309	CLA	C3B-C4B-NB	-2.78	108.05	110.53
36	a	822	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
36	F	312	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
36	R	320	CLA	CMD-C2D-C1D	2.78	129.62	124.73
36	a	832	CLA	CHB-C4A-NA	2.78	128.41	124.40
36	b	811	CLA	C1-C2-C3	-2.78	121.64	126.20
36	b	826	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
36	L	313	CLA	CMB-C2B-C3B	2.78	133.09	126.55
37	U	312	KC1	C1B-CHB-C4A	-2.78	120.11	126.02
36	f	805	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
36	F	317	CLA	O2A-CGA-CBA	2.78	120.31	111.83
36	E	317	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
36	a	806	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
41	G	321	LHG	O8-C23-C24	2.78	120.30	111.83
35	B	301	A86	C26-C25-C24	-2.78	115.15	123.20
35	O	305	A86	C4-C5-C6	-2.78	123.38	127.28
35	Q	304	A86	O4-C34-C33	2.78	114.75	107.64
41	E	322	LHG	O8-C23-C24	2.78	120.30	111.83
36	a	825	CLA	O2A-CGA-CBA	2.78	120.30	111.83
37	G	318	KC1	CBC-CAC-C3C	2.78	119.94	112.42
36	E	313	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
36	K	308	CLA	C3B-C4B-NB	-2.77	108.05	110.53
36	a	825	CLA	C4-C3-C5	2.77	120.04	115.23
36	b	837	CLA	CMB-C2B-C1B	-2.77	121.19	125.42
35	K	302	A86	C34-O4-C38	2.77	122.75	117.85
36	S	312	CLA	C3B-C4B-NB	-2.77	108.05	110.53
35	N	306	A86	C28-C27-C26	-2.77	118.32	122.82
35	K	302	A86	O4-C34-C35	2.77	114.73	107.64
35	O	303	A86	C25-C24-C1	-2.77	118.76	126.36
36	O	306	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
36	M	309	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
34	M	303	DD6	C37-C36-C31	-2.77	118.98	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	O	316	CLA	CMC-C2C-C1C	2.77	129.36	125.03
36	L	309	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
35	J	301	A86	C26-C25-C24	-2.77	115.17	123.20
34	E	306	DD6	C21-C20-C15	-2.77	117.74	122.30
36	N	315	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
35	L	307	A86	O1-C20-C19	-2.77	110.90	113.49
36	D	307	CLA	CHB-C4A-NA	2.77	128.40	124.40
36	G	312	CLA	CHB-C4A-NA	2.77	128.40	124.40
36	W	207	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
36	G	309	CLA	C6-C5-C3	2.77	120.21	113.47
37	L	317	KC1	CED-O2D-CGD	2.77	122.19	115.92
35	T	305	A86	C3-C4-C5	-2.77	117.86	123.52
37	G	318	KC1	CAA-CBA-CGA	-2.77	112.99	127.05
35	U	302	A86	C23-C16-C22	-2.77	103.35	107.37
36	P	318	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
36	b	816	CLA	C1D-ND-C4D	-2.76	104.37	106.31
36	V	305	CLA	CHD-C1D-ND	-2.76	120.91	124.80
35	P	304	A86	C25-C24-C1	-2.76	118.78	126.36
36	N	311	CLA	C3B-C4B-NB	-2.76	108.06	110.53
36	A	306	CLA	C2A-C1A-CHA	-2.76	119.07	123.87
36	a	825	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
36	P	309	CLA	CHB-C4A-NA	2.76	128.39	124.40
35	J	302	A86	C34-O4-C38	-2.76	112.97	117.85
35	B	301	A86	C4-C3-C2	-2.76	117.87	123.52
37	D	314	KC1	C2A-C1A-CHA	-2.76	117.62	128.96
36	C	206	CLA	CHB-C4A-NA	2.76	128.38	124.40
35	X	302	A86	O4-C38-O5	-2.76	117.66	122.99
37	S	316	KC1	C4C-C3C-C2C	-2.76	102.87	106.89
36	M	307	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
36	K	315	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
36	b	839	CLA	CHB-C4A-NA	2.76	128.38	124.40
36	J	312	CLA	CHB-C4A-NA	2.76	128.38	124.40
36	U	307	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
35	K	306	A86	C3-C2-C1	-2.76	123.41	127.28
35	F	301	A86	C25-C26-C27	-2.76	123.41	127.28
36	B	309	CLA	CHA-C4D-ND	2.76	138.24	132.55
36	a	836	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
36	L	314	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
36	J	316	CLA	CBC-CAC-C3C	2.76	119.89	112.42
34	B	304	DD6	O1-C20-C21	-2.75	111.97	115.05
35	V	304	A86	C19-C18-C17	-2.75	105.64	110.79
44	a	844	BCR	C24-C23-C22	-2.75	122.16	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	V	311	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
36	G	319	CLA	O2A-CGA-CBA	2.75	120.23	111.83
36	a	841	CLA	CAC-C3C-C4C	2.75	128.37	124.79
42	m	102	LMG	O8-C28-C29	2.75	120.23	111.83
36	V	308	CLA	CHB-C4A-NA	2.75	128.37	124.40
35	M	302	A86	C9-C8-C6	-2.75	118.82	126.36
36	D	317	CLA	CMA-C3A-C2A	-2.75	103.34	113.98
36	b	834	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
34	C	201	DD6	C25-C26-C27	-2.75	118.92	126.61
42	h	206	LMG	O8-C28-C29	2.75	120.22	111.83
35	S	308	A86	C34-O4-C38	-2.75	112.99	117.85
35	Q	301	A86	C25-C24-C1	-2.75	118.82	126.36
36	H	309	CLA	C3B-C4B-NB	-2.75	108.08	110.53
36	b	836	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
34	A	301	DD6	C37-C36-C31	-2.75	119.02	124.16
36	G	310	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
36	D	315	CLA	CHB-C4A-NA	2.75	128.37	124.40
35	K	302	A86	C9-C10-C11	-2.75	118.87	126.64
36	G	310	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
36	b	802	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
36	b	814	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
37	C	213	KC1	C3C-C4C-NC	2.75	112.84	109.90
37	F	308	KC1	CMC-C2C-C3C	2.75	133.58	126.15
43	a	840	PQN	C2M-C2-C3	-2.75	119.94	124.45
35	h	204	A86	C4-C5-C6	-2.75	123.43	127.28
37	L	317	KC1	CMD-C2D-C1D	-2.75	121.24	125.42
37	L	315	KC1	CMC-C2C-C1C	2.75	129.32	125.03
36	H	306	CLA	CHB-C4A-NA	2.75	128.36	124.40
36	Q	306	CLA	CHB-C4A-NA	2.75	128.36	124.40
35	B	303	A86	C8-C6-C5	2.75	123.33	119.01
36	b	817	CLA	CMD-C2D-C3D	-2.74	121.39	127.69
36	E	311	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
35	R	304	A86	C9-C10-C11	-2.74	118.88	126.64
36	D	307	CLA	CAA-CBA-CGA	-2.74	105.42	113.21
37	N	314	KC1	C4C-C3C-C2C	-2.74	102.90	106.89
36	O	307	CLA	CHB-C4A-NA	2.74	128.36	124.40
36	I	307	CLA	CHB-C4A-NA	2.74	128.36	124.40
35	R	303	A86	O1-C20-C19	-2.74	110.92	113.49
36	T	309	CLA	CAA-C2A-C3A	-2.74	105.59	113.00
36	b	824	CLA	CAC-C3C-C4C	2.74	128.36	124.79
35	O	305	A86	C41-C32-C31	-2.74	108.02	110.47
44	a	844	BCR	C27-C26-C25	2.74	126.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	E	309	KC1	C4C-C3C-C2C	-2.74	102.90	106.89
34	B	302	DD6	C25-C26-C27	-2.74	118.94	126.61
43	b	842	PQN	C2M-C2-C3	-2.74	119.94	124.45
37	D	314	KC1	CAA-CBA-CGA	-2.74	113.11	127.05
35	Q	303	A86	O1-C20-C19	-2.74	110.92	113.49
36	D	309	CLA	CAC-C3C-C4C	2.74	128.36	124.79
36	M	310	CLA	CAC-C3C-C4C	2.74	128.36	124.79
36	V	314	CLA	O2A-CGA-CBA	2.74	120.19	111.83
36	S	312	CLA	CMB-C2B-C3B	2.74	132.99	126.55
34	I	303	DD6	C21-C20-C15	-2.74	117.79	122.30
36	F	311	CLA	C3B-C4B-NB	-2.74	108.08	110.53
36	G	307	CLA	CHD-C1D-C2D	2.74	131.18	125.49
36	I	307	CLA	CMB-C2B-C3B	2.74	132.99	126.55
37	G	318	KC1	C3A-C4A-NA	2.74	113.84	110.45
36	b	817	CLA	O2A-CGA-CBA	2.74	120.18	111.83
36	a	823	CLA	C4-C3-C5	2.74	119.98	115.23
35	U	304	A86	C41-C32-C31	-2.74	108.02	110.47
36	K	316	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
35	F	304	A86	C12-C11-C13	2.74	120.44	116.00
34	K	305	DD6	C21-C20-C15	-2.74	117.80	122.30
41	a	842	LHG	O8-C23-C24	2.74	120.18	111.83
36	V	314	CLA	C4-C3-C5	2.74	119.98	115.23
42	J	318	LMG	O8-C28-C29	2.74	120.17	111.83
36	N	315	CLA	CHB-C4A-NA	2.73	128.35	124.40
36	B	309	CLA	O2A-CGA-CBA	2.73	120.17	111.83
36	l	204	CLA	O2A-CGA-CBA	2.73	120.17	111.83
36	O	310	CLA	C3B-C4B-NB	-2.73	108.09	110.53
36	l	205	CLA	CMD-C2D-C3D	-2.73	121.42	127.69
36	l	204	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
36	f	803	CLA	C4-C3-C5	2.73	119.97	115.23
36	a	823	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
35	V	303	A86	C35-C34-C33	-2.73	104.98	109.89
34	K	305	DD6	C14-C13-C11	-2.73	121.29	125.53
42	E	319	LMG	O8-C28-C29	2.73	120.17	111.83
34	A	303	DD6	C37-C36-C31	-2.73	119.05	124.16
37	P	317	KC1	C4C-C3C-C2C	-2.73	102.92	106.89
41	f	808	LHG	O8-C23-C24	2.73	120.16	111.83
35	V	301	A86	C9-C10-C11	-2.73	118.92	126.64
36	R	320	CLA	C2A-C1A-CHA	2.73	128.61	123.87
41	f	809	LHG	O8-C23-C24	2.73	120.16	111.83
36	R	312	CLA	C6-C7-C8	-2.73	106.89	115.97
36	B	308	CLA	CMA-C3A-C2A	-2.73	103.42	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	313	CLA	C3B-C4B-NB	-2.73	108.09	110.53
34	B	302	DD6	C15-C14-C13	-2.73	120.22	125.99
36	K	312	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
35	A	316	A86	C4-C3-C2	-2.73	117.94	123.52
36	U	305	CLA	C3B-C4B-NB	-2.73	108.09	110.53
37	G	317	KC1	CED-O2D-CGD	2.73	122.11	115.92
37	W	213	KC1	CHD-C1D-C2D	2.73	135.35	127.43
36	F	310	CLA	C3B-C4B-NB	-2.73	108.09	110.53
36	F	311	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
36	D	313	CLA	CHB-C4A-NA	2.73	128.34	124.40
36	K	307	CLA	O2A-CGA-CBA	2.73	120.15	111.83
41	i	104	LHG	O8-C23-C24	2.73	120.15	111.83
35	T	302	A86	C36-C31-C32	-2.73	116.99	119.70
35	P	306	A86	C25-C26-C27	-2.73	123.45	127.28
36	N	317	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
36	U	306	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
36	b	814	CLA	C3B-C4B-NB	-2.72	108.10	110.53
35	F	302	A86	C12-C11-C13	2.72	120.42	116.00
34	B	304	DD6	O1-C15-C14	-2.72	109.07	116.88
36	L	308	CLA	O2A-CGA-CBA	2.72	120.14	111.83
35	B	301	A86	C12-C11-C13	2.72	120.42	116.00
36	a	822	CLA	CHB-C1B-C2B	-2.72	119.52	127.43
34	C	201	DD6	C37-C36-C35	2.72	119.43	114.42
36	B	308	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
37	J	314	KC1	C3B-C2B-C1B	-2.72	104.47	107.05
43	a	840	PQN	C14-C13-C15	2.72	119.95	115.23
36	F	314	CLA	C3B-C4B-NB	-2.72	108.10	110.53
34	S	306	DD6	C21-C20-C15	-2.72	117.82	122.30
34	F	303	DD6	C21-C20-C15	-2.72	117.82	122.30
35	U	304	A86	C12-C11-C13	2.72	120.41	116.00
36	U	305	CLA	CHB-C4A-NA	2.72	128.33	124.40
36	P	312	CLA	C3B-C4B-NB	-2.72	108.10	110.53
36	b	841	CLA	O2D-CGD-CBD	2.72	115.98	111.23
37	F	315	KC1	O2D-CGD-O1D	-2.72	118.56	123.85
37	Q	311	KC1	C1B-CHB-C4A	-2.72	120.24	126.02
36	D	308	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
36	E	313	CLA	O2A-CGA-CBA	2.72	120.12	111.83
37	O	313	KC1	C1B-CHB-C4A	-2.72	120.24	126.02
36	P	308	CLA	CHB-C4A-NA	2.72	128.32	124.40
37	O	315	KC1	C1B-CHB-C4A	-2.72	120.25	126.02
34	Q	302	DD6	C21-C20-C15	-2.72	117.83	122.30
36	P	313	CLA	O2D-CGD-O1D	-2.72	118.56	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	S	313	CLA	C3A-C2A-C1A	2.72	105.41	101.34
41	O	317	LHG	O8-C23-C24	2.71	120.11	111.83
36	a	816	CLA	CHB-C4A-NA	2.71	128.32	124.40
36	a	831	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
44	m	101	BCR	C27-C26-C25	2.71	126.37	122.70
34	H	303	DD6	C37-C36-C31	-2.71	119.08	124.16
36	b	810	CLA	CHB-C4A-NA	2.71	128.32	124.40
36	J	307	CLA	CAA-C2A-C3A	-2.71	105.67	113.00
36	G	315	CLA	O2A-CGA-CBA	2.71	120.11	111.83
36	K	307	CLA	C2C-C1C-NC	2.71	112.83	109.98
37	Q	313	KC1	C1B-CHB-C4A	-2.71	120.25	126.02
36	W	216	CLA	C2A-C3A-C4A	2.71	106.25	101.87
36	a	816	CLA	O2A-CGA-CBA	2.71	120.10	111.83
34	C	201	DD6	C14-C13-C11	-2.71	121.32	125.53
36	J	308	CLA	CHD-C1D-ND	-2.71	120.99	124.80
34	a	849	DD6	O1-C20-C19	-2.71	110.95	113.49
36	H	314	CLA	CAC-C3C-C4C	2.71	128.32	124.79
36	a	817	CLA	C3B-C4B-NB	-2.71	108.11	110.53
35	G	304	A86	C36-C31-C32	-2.71	117.01	119.70
37	W	217	KC1	C1C-C2C-C3C	-2.71	104.13	106.98
36	b	805	CLA	CMA-C3A-C2A	-2.71	103.51	113.98
36	L	313	CLA	CHB-C4A-NA	2.71	128.31	124.40
36	N	308	CLA	CMA-C3A-C2A	-2.71	103.51	113.98
36	R	316	CLA	CMC-C2C-C1C	-2.71	120.80	125.03
34	L	305	DD6	C3-C4-C5	-2.71	117.98	123.52
36	F	314	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
36	K	310	CLA	C4-C3-C5	2.71	119.93	115.23
35	L	319	A86	C28-C27-C29	2.71	124.95	118.94
36	a	830	CLA	O2A-CGA-CBA	2.71	120.09	111.83
36	j	102	CLA	C3B-C4B-NB	-2.71	108.11	110.53
36	G	316	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
36	P	309	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
36	b	838	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
36	a	829	CLA	CHB-C1B-NB	2.71	128.11	124.05
41	D	319	LHG	C5-O7-C7	-2.71	111.32	117.80
41	l	208	LHG	O8-C23-C24	2.71	120.08	111.83
36	K	307	CLA	CMD-C2D-C3D	-2.71	121.48	127.69
35	C	203	A86	C12-C11-C13	2.71	120.39	116.00
36	O	307	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
36	S	313	CLA	CAC-C3C-C4C	2.70	128.31	124.79
36	b	836	CLA	CHB-C4A-NA	2.70	128.30	124.40
36	D	312	CLA	CHB-C4A-NA	2.70	128.30	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	301	A86	C3-C4-C5	-2.70	117.99	123.52
36	F	317	CLA	C4-C3-C5	2.70	119.92	115.23
37	S	316	KC1	CAC-C3C-C4C	2.70	128.31	124.79
36	Q	305	CLA	CHB-C4A-NA	2.70	128.30	124.40
36	E	312	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
36	O	306	CLA	CHB-C4A-NA	2.70	128.30	124.40
35	W	202	A86	C25-C24-C1	-2.70	118.95	126.36
34	D	301	DD6	C25-C26-C27	-2.70	119.06	126.61
36	O	316	CLA	CHB-C1B-C2B	-2.70	119.59	127.43
36	P	301	CLA	C3B-C4B-NB	-2.70	108.12	110.53
36	R	311	CLA	C3B-C4B-NB	-2.70	108.12	110.53
37	G	308	KC1	CHD-C1D-C2D	2.70	135.26	127.43
37	X	311	KC1	C1C-C2C-C3C	-2.70	104.14	106.98
36	B	307	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
35	R	304	A86	C25-C24-C1	-2.70	118.96	126.36
35	I	302	A86	C23-C16-C22	-2.70	103.45	107.37
36	C	209	CLA	C3B-C4B-NB	-2.70	108.12	110.53
34	W	205	DD6	C28-C27-C26	-2.70	118.94	124.18
35	B	303	A86	C10-C9-C8	-2.70	115.38	123.20
35	N	320	A86	C3-C4-C5	-2.70	118.00	123.52
36	b	834	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
36	B	309	CLA	CMC-C2C-C1C	2.70	129.25	125.03
36	A	306	CLA	C4-C3-C5	2.70	119.91	115.23
36	S	317	CLA	C3B-C4B-NB	-2.70	108.12	110.53
36	M	316	CLA	CHB-C4A-NA	2.70	128.29	124.40
36	O	308	CLA	CHB-C4A-NA	2.70	128.29	124.40
36	a	818	CLA	CMB-C2B-C3B	2.70	132.89	126.55
36	B	305	CLA	CHB-C4A-NA	2.70	128.29	124.40
35	S	301	A86	C3-C4-C5	-2.70	118.00	123.52
35	P	303	A86	C28-C27-C29	2.69	124.92	118.94
36	K	308	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
36	W	216	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
34	j	103	DD6	O1-C20-C21	-2.69	112.04	115.05
36	B	308	CLA	CHB-C4A-NA	2.69	128.29	124.40
36	K	308	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
35	T	306	A86	O4-C38-O5	-2.69	117.79	122.99
36	H	309	CLA	CHB-C4A-NA	2.69	128.29	124.40
35	S	303	A86	C9-C8-C6	-2.69	118.98	126.36
36	a	810	CLA	CHB-C4A-NA	2.69	128.29	124.40
36	O	311	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
36	I	308	CLA	C4-C3-C5	2.69	119.90	115.23
36	Q	309	CLA	C3B-C4B-NB	-2.69	108.13	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	E	315	CLA	CAC-C3C-C4C	2.69	128.29	124.79
37	P	315	KC1	C1B-CHB-C4A	-2.69	120.30	126.02
35	U	301	A86	O1-C15-C20	-2.69	57.17	59.45
36	V	311	CLA	CMD-C2D-C3D	2.69	133.86	127.69
36	F	309	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
35	O	302	A86	C28-C27-C29	2.69	124.91	118.94
36	G	309	CLA	CBA-CAA-C2A	2.69	121.79	113.79
36	f	803	CLA	O2A-CGA-CBA	2.69	120.03	111.83
35	T	307	A86	C23-C16-C17	-2.69	104.24	108.97
36	G	309	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
36	L	314	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
36	E	315	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
37	C	213	KC1	CAD-C3D-C2D	-2.69	138.60	144.26
36	I	314	CLA	C3B-C4B-NB	-2.69	108.13	110.53
36	F	309	CLA	C1-C2-C3	2.69	130.60	126.20
36	b	836	CLA	C3D-C4D-ND	2.69	114.35	109.99
36	S	314	CLA	CHB-C4A-NA	2.69	128.28	124.40
36	I	306	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
35	Q	304	A86	C3-C4-C5	-2.69	118.03	123.52
36	R	315	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
36	H	315	CLA	CAA-C2A-C1A	2.68	120.77	111.97
36	N	308	CLA	CHB-C1B-NB	2.68	128.08	124.05
36	D	309	CLA	CMD-C2D-C3D	-2.68	121.53	127.69
35	Q	304	A86	O3-C36-C37	-2.68	104.12	109.22
36	W	201	CLA	CHB-C4A-NA	2.68	128.27	124.40
36	G	319	CLA	CMB-C2B-C1B	2.68	129.50	125.42
36	V	306	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
36	K	310	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
36	a	816	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
34	R	308	DD6	C21-C20-C15	-2.68	117.89	122.30
35	N	303	A86	C9-C8-C6	-2.68	119.01	126.36
36	W	211	CLA	CED-O2D-CGD	2.68	122.00	115.92
36	a	811	CLA	CHB-C4A-NA	2.68	128.27	124.40
36	P	309	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
35	h	202	A86	C34-O4-C38	-2.68	113.11	117.85
36	W	207	CLA	CHB-C4A-NA	2.68	128.27	124.40
36	a	837	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
36	l	201	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
35	S	303	A86	C9-C10-C11	-2.68	119.07	126.64
36	K	310	CLA	O2A-CGA-CBA	2.68	120.00	111.83
36	L	320	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
36	b	832	CLA	CMB-C2B-C1B	-2.68	121.34	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	208	CLA	CHB-C4A-NA	2.68	128.26	124.40
36	P	310	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
35	H	304	A86	O4-C38-O5	-2.68	117.82	122.99
36	Q	307	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
36	l	205	CLA	C1-C2-C3	-2.68	121.81	126.20
42	J	318	LMG	C8-O7-C10	-2.68	111.39	117.80
37	A	312	KC1	CMA-C3A-C4A	-2.68	120.85	125.03
36	G	307	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
35	J	301	A86	C12-C11-C13	2.68	120.34	116.00
36	S	312	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
36	H	315	CLA	C2A-C1A-CHA	2.68	128.51	123.87
34	W	205	DD6	C37-C36-C31	-2.68	119.16	124.16
36	L	312	CLA	CAA-C2A-C1A	2.68	120.75	111.97
36	F	312	CLA	CHB-C4A-NA	2.68	128.26	124.40
36	A	310	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
36	R	320	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
36	I	306	CLA	CMC-C2C-C1C	2.67	129.21	125.03
34	a	849	DD6	C37-C36-C31	-2.67	119.16	124.16
43	a	840	PQN	C11-C3-C2	-2.67	120.31	124.89
36	J	307	CLA	C3B-C4B-NB	-2.67	108.14	110.53
36	a	807	CLA	C3B-C4B-NB	-2.67	108.14	110.53
35	P	306	A86	C40-C32-C31	-2.67	108.08	110.47
36	X	309	CLA	CHA-C1A-NA	-2.67	120.34	126.39
34	B	302	DD6	C25-C24-C1	-2.67	119.03	126.36
35	N	303	A86	C9-C10-C11	-2.67	119.08	126.64
36	O	308	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
36	N	318	CLA	C3A-C2A-C1A	2.67	105.34	101.34
36	K	307	CLA	C4-C3-C5	2.67	119.86	115.23
36	D	308	CLA	O2D-CGD-CBD	2.67	115.90	111.23
36	C	207	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
35	N	303	A86	C26-C25-C24	-2.67	115.46	123.20
35	N	306	A86	O4-C38-O5	-2.67	117.84	122.99
36	j	101	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
36	U	306	CLA	C4-C3-C5	2.67	119.86	115.23
36	W	210	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
35	X	305	A86	C9-C10-C11	-2.67	119.10	126.64
36	Q	306	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
36	B	305	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
36	N	316	CLA	CHB-C4A-NA	2.67	128.25	124.40
44	a	846	BCR	C27-C26-C25	2.67	126.31	122.70
35	N	320	A86	O3-C36-C37	-2.67	104.15	109.22
36	B	308	CLA	CMB-C2B-C3B	2.67	132.82	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	804	CLA	O2A-CGA-O1A	-2.67	116.96	123.63
36	b	807	CLA	C3B-C4B-NB	-2.67	108.15	110.53
36	b	833	CLA	CMD-C2D-C3D	2.67	133.80	127.69
44	l	203	BCR	C15-C16-C17	-2.67	118.06	123.52
36	a	830	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
36	a	823	CLA	CHB-C4A-NA	2.66	128.25	124.40
37	E	309	KC1	C2A-C1A-NA	2.66	113.61	109.34
36	a	817	CLA	CHB-C1B-NB	2.66	128.04	124.05
36	K	315	CLA	CMB-C2B-C3B	2.66	132.81	126.55
42	E	319	LMG	C8-O7-C10	-2.66	111.42	117.80
34	O	304	DD6	C25-C26-C27	-2.66	119.16	126.61
36	b	805	CLA	C1-C2-C3	-2.66	121.83	126.20
36	Q	306	CLA	CMB-C2B-C1B	-2.66	121.36	125.42
34	J	304	DD6	C21-C20-C15	-2.66	117.92	122.30
36	a	813	CLA	CHB-C4A-NA	2.66	128.24	124.40
44	b	846	BCR	C8-C9-C10	2.66	123.20	119.01
36	D	317	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
42	V	316	LMG	O8-C28-C29	2.66	119.95	111.83
35	F	306	A86	C34-O4-C38	-2.66	113.15	117.85
36	S	310	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
38	A	315	SQD	C45-O47-C7	-2.66	111.43	117.80
36	O	307	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
35	V	302	A86	O1-C20-C21	-2.66	112.08	115.05
35	T	307	A86	C9-C10-C11	-2.66	119.12	126.64
36	N	319	CLA	CMC-C2C-C1C	-2.66	120.88	125.03
35	X	314	A86	C12-C11-C13	2.66	120.31	116.00
42	J	319	LMG	O8-C28-C29	2.66	119.94	111.83
36	B	306	CLA	C3B-C4B-NB	-2.66	108.16	110.53
37	F	315	KC1	CMA-C3A-C4A	-2.66	120.88	125.03
40	b	849	DGD	CDB-CCB-CBB	-2.66	100.93	114.37
36	S	311	CLA	CHB-C4A-NA	2.66	128.24	124.40
36	X	312	CLA	CHB-C4A-NA	2.66	128.24	124.40
35	A	302	A86	O-C13-C11	-2.66	115.31	121.04
39	b	848	LMT	C1B-O1B-C4'	-2.66	111.68	117.98
35	J	305	A86	C12-C11-C13	2.66	120.31	116.00
36	a	812	CLA	C3B-C4B-NB	-2.66	108.16	110.53
36	b	836	CLA	C4-C3-C5	2.66	119.84	115.23
36	a	834	CLA	CHB-C4A-NA	2.66	128.24	124.40
36	M	315	CLA	CBC-CAC-C3C	-2.66	105.22	112.42
36	a	801	CLA	C2A-C1A-CHA	2.66	128.48	123.87
36	A	310	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
36	K	311	CLA	O2D-CGD-O1D	-2.66	118.68	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	206	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
34	E	301	DD6	C37-C36-C31	-2.66	119.19	124.16
35	U	302	A86	O4-C38-O5	-2.66	117.86	122.99
36	P	310	CLA	CHB-C4A-NA	2.66	128.23	124.40
36	f	802	CLA	CHB-C4A-NA	2.66	128.23	124.40
36	R	321	CLA	CMB-C2B-C3B	2.66	132.79	126.55
35	S	303	A86	C26-C25-C24	-2.66	115.51	123.20
36	H	312	CLA	CHB-C4A-NA	2.65	128.23	124.40
36	K	311	CLA	CAA-C2A-C1A	2.65	120.67	111.97
44	b	846	BCR	C15-C14-C13	-2.65	123.56	127.28
36	E	312	CLA	CHB-C4A-NA	2.65	128.23	124.40
36	I	311	CLA	CHB-C4A-NA	2.65	128.23	124.40
36	a	807	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
36	D	316	CLA	CHB-C4A-NA	2.65	128.23	124.40
44	b	843	BCR	C7-C8-C9	-2.65	122.31	126.23
37	G	318	KC1	CMC-C2C-C3C	2.65	133.32	126.15
36	C	210	CLA	C3B-C4B-NB	-2.65	108.16	110.53
36	I	314	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
36	V	311	CLA	CHB-C4A-NA	2.65	128.22	124.40
36	N	313	CLA	C2A-C1A-CHA	2.65	128.45	123.86
35	R	304	A86	C23-C16-C17	-2.65	104.31	108.97
37	W	213	KC1	C3B-C2B-C1B	-2.65	104.54	107.05
36	V	314	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
36	E	317	CLA	CHB-C4A-NA	2.65	128.22	124.40
36	K	310	CLA	CAC-C3C-C4C	2.65	128.24	124.79
36	K	312	CLA	C3B-C4B-NB	-2.65	108.17	110.53
36	a	836	CLA	CHB-C4A-NA	2.65	128.22	124.40
36	N	312	CLA	C3B-C4B-NB	-2.65	108.17	110.53
36	a	801	CLA	CHA-C1A-NA	-2.65	120.40	126.39
36	Q	307	CLA	CHB-C4A-NA	2.64	128.22	124.40
36	J	308	CLA	C3B-C4B-NB	-2.64	108.17	110.53
36	W	206	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
34	L	305	DD6	C10-C9-C8	-2.64	115.54	123.20
37	K	314	KC1	C3B-C2B-C1B	-2.64	104.54	107.05
38	b	804	SQD	O48-C23-C24	2.64	119.89	111.83
35	F	307	A86	C40-C32-C33	-2.64	96.54	109.06
36	U	307	CLA	CHB-C4A-NA	2.64	128.21	124.40
36	V	306	CLA	CHB-C4A-NA	2.64	128.21	124.40
35	J	301	A86	C25-C26-C27	-2.64	123.57	127.28
36	H	310	CLA	CHD-C4C-C3C	2.64	128.63	124.77
36	R	319	CLA	CAC-C3C-C2C	2.64	132.41	127.56
36	X	315	CLA	CMB-C2B-C1B	-2.64	121.40	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	J	313	CLA	CHB-C4A-NA	2.64	128.21	124.40
36	S	313	CLA	CBA-CAA-C2A	-2.64	105.94	113.79
41	F	318	LHG	C11-C10-C9	-2.64	101.02	114.37
34	P	305	DD6	C21-C20-C15	-2.64	117.96	122.30
36	B	309	CLA	C2C-C1C-NC	2.64	112.75	109.98
34	S	307	DD6	C25-C24-C1	-2.64	119.13	126.36
36	a	815	CLA	CHB-C4A-NA	2.64	128.21	124.40
35	X	302	A86	C23-C16-C17	-2.64	104.33	108.97
35	K	306	A86	C4-C3-C2	-2.64	118.12	123.52
36	T	316	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
34	L	305	DD6	C25-C26-C27	-2.64	119.24	126.61
34	K	305	DD6	C37-C36-C31	-2.64	119.23	124.16
36	C	207	CLA	O2A-CGA-CBA	2.64	119.87	111.83
36	L	309	CLA	CMB-C2B-C1B	-2.64	121.41	125.42
35	P	306	A86	C12-C11-C13	2.64	120.27	116.00
37	R	317	KC1	C2B-C1B-NB	2.64	112.73	110.13
36	B	308	CLA	CHD-C1D-C2D	2.63	130.97	125.49
36	N	310	CLA	C3C-C4C-NC	-2.63	107.06	110.43
36	b	834	CLA	CHB-C4A-NA	2.63	128.20	124.40
36	i	102	CLA	CMB-C2B-C3B	2.63	132.75	126.55
35	E	305	A86	O4-C38-O5	-2.63	117.91	122.99
34	W	205	DD6	O1-C20-C19	2.63	115.96	113.49
41	F	318	LHG	C20-C19-C18	-2.63	101.06	114.37
36	l	204	CLA	CAC-C3C-C4C	2.63	128.22	124.79
34	I	303	DD6	C28-C27-C26	-2.63	119.07	124.18
34	S	307	DD6	C21-C20-C15	-2.63	117.97	122.30
35	O	305	A86	C35-C34-C33	-2.63	105.16	109.89
36	M	310	CLA	C3D-C4D-ND	2.63	114.27	109.99
36	A	313	CLA	CHB-C4A-NA	2.63	128.20	124.40
36	l	205	CLA	C4-C3-C5	2.63	119.80	115.23
35	X	304	A86	C40-C32-C31	-2.63	108.12	110.47
36	H	318	CLA	CAA-CBA-CGA	-2.63	105.74	113.21
37	M	313	KC1	CHD-C1D-C2D	2.63	135.06	127.43
36	a	804	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
36	a	814	CLA	CHC-C1C-NC	2.63	128.27	124.31
36	D	313	CLA	CMB-C2B-C3B	2.63	132.74	126.55
35	R	301	A86	O-C13-C11	-2.63	115.38	121.04
36	a	819	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
35	X	302	A86	C4-C3-C2	-2.63	118.14	123.52
35	V	301	A86	C9-C8-C6	-2.63	119.16	126.36
36	F	310	CLA	O2D-CGD-CBD	2.63	115.82	111.23
36	D	310	CLA	CMB-C2B-C1B	-2.63	121.42	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	301	DD6	C37-C36-C35	2.63	119.25	114.42
36	b	802	CLA	C1-C2-C3	-2.63	121.89	126.20
36	T	311	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
36	b	823	CLA	C3B-C4B-NB	-2.63	108.19	110.53
37	L	315	KC1	O2D-CGD-O1D	-2.63	118.74	123.85
36	N	315	CLA	CAA-C2A-C1A	2.63	118.29	111.81
35	P	303	A86	C9-C10-C11	-2.62	119.22	126.64
36	O	316	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
35	O	303	A86	C23-C16-C17	-2.62	104.36	108.97
35	R	302	A86	C9-C10-C11	-2.62	119.22	126.64
36	b	823	CLA	CMB-C2B-C1B	-2.62	121.42	125.42
37	E	309	KC1	CMC-C2C-C3C	2.62	133.25	126.15
36	H	307	CLA	C2A-C1A-CHA	2.62	128.42	123.87
36	b	816	CLA	CHD-C1D-ND	-2.62	121.11	124.80
44	m	101	BCR	C11-C10-C9	-2.62	123.60	127.28
35	P	304	A86	C23-C16-C17	-2.62	104.36	108.97
36	I	310	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
36	V	306	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
36	S	320	CLA	CHB-C4A-NA	2.62	128.18	124.40
36	K	313	CLA	C4D-C3D-CAD	-2.62	105.26	108.11
36	E	312	CLA	C3B-C4B-NB	-2.62	108.19	110.53
36	C	208	CLA	O2D-CGD-CBD	2.62	115.81	111.23
36	b	822	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
35	L	319	A86	C9-C10-C11	-2.62	119.23	126.64
36	l	205	CLA	O2A-CGA-CBA	2.62	119.82	111.83
35	Q	301	A86	C23-C16-C17	-2.62	104.36	108.97
36	a	812	CLA	CHB-C4A-NA	2.62	128.18	124.40
36	W	201	CLA	C3B-C4B-NB	-2.62	108.19	110.53
36	a	808	CLA	C3B-C4B-NB	-2.62	108.19	110.53
34	W	205	DD6	C32-C33-C34	-2.62	107.85	113.59
37	A	312	KC1	C2B-C1B-NB	2.62	112.72	110.13
36	a	806	CLA	CHB-C1B-C2B	-2.62	119.83	127.43
36	H	315	CLA	CHB-C4A-NA	2.62	128.18	124.40
36	P	319	CLA	CHB-C4A-NA	2.62	128.18	124.40
36	I	311	CLA	O2D-CGD-CBD	2.62	115.80	111.23
36	b	807	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
36	b	823	CLA	CHB-C4A-NA	2.62	128.17	124.40
34	L	305	DD6	C14-C13-C11	-2.61	121.47	125.53
37	A	312	KC1	C4D-C3D-C2D	-2.61	103.90	107.42
36	a	835	CLA	CHB-C4A-NA	2.61	128.17	124.40
34	D	303	DD6	C37-C36-C35	2.61	119.23	114.42
34	S	307	DD6	C9-C10-C11	-2.61	123.61	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	202	A86	C3-C4-C5	-2.61	118.17	123.52
36	I	306	CLA	C2A-C3A-C4A	2.61	106.09	101.87
35	O	305	A86	C25-C26-C27	-2.61	123.61	127.28
36	M	312	CLA	C3B-C4B-NB	-2.61	108.20	110.53
36	a	820	CLA	C3B-C4B-NB	-2.61	108.20	110.53
36	a	839	CLA	CHB-C4A-NA	2.61	128.17	124.40
35	G	305	A86	O4-C38-O5	-2.61	117.95	122.99
36	X	306	CLA	CHB-C4A-NA	2.61	128.17	124.40
36	a	808	CLA	CHB-C4A-NA	2.61	128.16	124.40
36	E	313	CLA	CHD-C4C-C3C	-2.61	120.97	124.77
42	a	852	LMG	C8-O7-C10	-2.61	111.55	117.80
35	M	301	A86	O4-C34-C35	2.61	114.31	107.64
35	O	302	A86	C9-C10-C11	-2.61	119.27	126.64
39	L	318	LMT	C1B-O1B-C4'	-2.61	111.80	117.98
36	G	312	CLA	C3B-C4B-NB	-2.61	108.20	110.53
36	a	824	CLA	CMB-C2B-C3B	2.61	132.68	126.55
36	I	308	CLA	C4D-CHA-C1A	-2.61	118.14	121.24
36	C	205	CLA	CHB-C4A-NA	2.61	128.16	124.40
36	L	311	CLA	CHB-C4A-NA	2.61	128.16	124.40
34	D	304	DD6	C21-C20-C15	-2.61	118.01	122.30
35	G	302	A86	C26-C25-C24	-2.61	115.65	123.20
36	P	312	CLA	C2A-C1A-CHA	2.61	128.39	123.87
36	W	208	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
36	b	813	CLA	C3B-C4B-NB	-2.60	107.63	110.33
36	V	314	CLA	CHB-C1B-C2B	-2.60	119.87	127.43
40	b	849	DGD	C1E-O6E-C5E	2.60	118.80	113.72
35	K	302	A86	C9-C8-C6	-2.60	119.23	126.36
35	K	303	A86	C36-C31-C32	-2.60	117.11	119.70
36	f	805	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
36	W	216	CLA	CAA-CBA-CGA	2.60	119.43	112.49
36	J	317	CLA	CHB-C4A-NA	2.60	128.15	124.40
36	R	311	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
36	M	309	CLA	CHB-C4A-NA	2.60	128.15	124.40
36	H	311	CLA	CMB-C2B-C3B	2.60	132.66	126.55
35	B	303	A86	C41-C32-C31	2.60	112.80	110.47
36	a	839	CLA	C3B-C4B-NB	-2.60	108.21	110.53
36	a	806	CLA	C4-C3-C5	2.60	119.73	115.23
36	O	310	CLA	C2A-C1A-CHA	2.60	128.37	123.87
35	H	301	A86	C9-C10-C11	-2.60	119.30	126.64
36	a	828	CLA	CMB-C2B-C3B	2.60	132.66	126.55
36	U	309	CLA	CHB-C4A-NA	2.60	128.15	124.40
36	Q	309	CLA	C2A-C1A-CHA	2.59	128.37	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	I	306	CLA	C4-C3-C5	2.59	119.73	115.23
35	X	305	A86	C25-C24-C1	-2.59	119.25	126.36
36	b	805	CLA	C3B-C4B-NB	-2.59	108.22	110.53
36	T	311	CLA	CHD-C4C-C3C	-2.59	120.99	124.77
36	O	316	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
34	a	849	DD6	C28-C27-C26	-2.59	119.15	124.18
36	L	320	CLA	CHB-C4A-NA	2.59	128.14	124.40
36	M	306	CLA	CHB-C4A-NA	2.59	128.14	124.40
34	A	301	DD6	O1-C20-C21	-2.59	112.15	115.05
36	Q	314	CLA	CMB-C2B-C3B	2.59	132.65	126.55
34	E	306	DD6	O1-C15-C14	-2.59	109.45	116.88
36	P	302	CLA	CMB-C2B-C3B	2.59	132.64	126.55
36	T	314	CLA	CAA-C2A-C1A	-2.59	103.48	111.97
36	a	826	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
36	b	807	CLA	CHB-C4A-NA	2.59	128.14	124.40
35	G	304	A86	C34-O4-C38	2.59	122.42	117.85
44	f	801	BCR	C30-C25-C26	-2.59	119.10	122.64
34	W	205	DD6	C25-C26-C27	-2.59	119.37	126.61
37	M	317	KC1	C2A-C1A-NA	2.59	113.49	109.34
36	N	310	CLA	CHC-C4B-NB	-2.59	120.17	124.05
34	H	302	DD6	C37-C36-C31	-2.59	119.32	124.16
37	K	314	KC1	C4C-C3C-C2C	-2.59	103.13	106.89
36	E	314	CLA	CHB-C4A-NA	2.59	128.13	124.40
35	O	319	A86	C-C1-C24	-2.59	114.14	118.09
36	D	308	CLA	CMB-C2B-C1B	-2.58	121.48	125.42
36	F	310	CLA	CMB-C2B-C1B	-2.58	121.48	125.42
44	f	806	BCR	C27-C26-C25	2.58	126.20	122.70
36	R	311	CLA	O2D-CGD-CBD	2.58	115.75	111.23
36	E	314	CLA	C1-O2A-CGA	2.58	122.91	116.65
36	V	311	CLA	CMB-C2B-C3B	2.58	132.63	126.55
34	D	301	DD6	C21-C20-C15	-2.58	118.05	122.30
36	G	309	CLA	C3B-C4B-NB	-2.58	108.22	110.53
36	O	311	CLA	CHB-C4A-NA	2.58	128.13	124.40
36	I	308	CLA	CHD-C1D-C2D	2.58	130.86	125.49
36	b	823	CLA	O2D-CGD-CBD	2.58	115.74	111.23
36	S	321	CLA	C2A-C1A-CHA	2.58	128.35	123.87
36	b	817	CLA	C4-C3-C5	2.58	119.71	115.23
36	H	312	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
37	C	213	KC1	O2D-CGD-O1D	-2.58	118.82	123.85
44	b	844	BCR	C2-C1-C6	2.58	114.19	110.44
36	D	307	CLA	C2A-C1A-CHA	2.58	128.34	123.87
34	a	849	DD6	C15-C14-C13	-2.58	120.54	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	O	301	A86	C9-C10-C11	-2.58	119.35	126.64
36	D	311	CLA	C3B-C4B-NB	-2.58	108.23	110.53
36	a	803	CLA	CMB-C2B-C3B	2.58	132.62	126.55
37	T	310	KC1	O2D-CGD-O1D	-2.58	118.83	123.85
36	S	315	CLA	C3A-C2A-C1A	2.58	105.20	101.34
35	P	306	A86	C21-C20-C15	2.58	131.67	123.35
35	S	305	A86	O4-C38-O5	-2.58	118.01	122.99
35	C	203	A86	C34-O4-C38	-2.58	113.29	117.85
36	L	316	CLA	CHB-C4A-NA	2.58	128.12	124.40
34	F	303	DD6	C15-C14-C13	-2.58	120.54	125.99
34	W	204	DD6	C15-C14-C13	-2.58	120.54	125.99
35	N	305	A86	O4-C38-O5	-2.58	118.02	122.99
35	W	202	A86	O2-C18-C19	2.58	115.02	109.75
36	K	315	CLA	CHB-C4A-NA	2.58	128.12	124.40
35	J	302	A86	C9-C8-C6	-2.58	119.30	126.36
35	I	302	A86	C23-C16-C17	-2.58	104.44	108.97
35	A	302	A86	C24-C1-C2	-2.58	114.96	119.01
34	D	301	DD6	C37-C36-C31	-2.58	119.34	124.16
44	m	101	BCR	C15-C14-C13	-2.57	123.67	127.28
35	U	301	A86	C36-C31-C32	2.57	122.25	119.70
34	A	304	DD6	C37-C36-C31	-2.57	119.35	124.16
35	N	302	A86	C4-C3-C2	-2.57	118.25	123.52
35	S	302	A86	C4-C3-C2	-2.57	118.25	123.52
36	a	839	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
35	F	301	A86	C19-C18-C17	-2.57	105.98	110.79
35	I	304	A86	C4-C3-C2	-2.57	118.26	123.52
35	V	303	A86	O4-C34-C35	2.57	114.22	107.64
36	U	306	CLA	CAC-C3C-C4C	2.57	128.13	124.79
36	f	803	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
36	b	828	CLA	C1-C2-C3	-2.57	121.99	126.20
36	b	836	CLA	O2A-CGA-CBA	2.57	119.67	111.83
34	Q	302	DD6	C37-C36-C31	-2.57	119.36	124.16
36	L	310	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
36	a	848	CLA	OBD-CAD-C3D	-2.57	122.41	128.42
36	L	308	CLA	CHC-C1C-C2C	2.57	134.25	126.95
36	P	313	CLA	CHB-C4A-NA	2.57	128.11	124.40
36	M	310	CLA	CHB-C4A-NA	2.57	128.10	124.40
36	b	822	CLA	CHB-C4A-NA	2.57	128.10	124.40
36	S	315	CLA	C1D-ND-C4D	-2.57	104.51	106.31
35	C	203	A86	C3-C4-C5	-2.57	118.27	123.52
35	H	301	A86	C21-C20-C19	-2.57	111.36	114.24
36	R	318	CLA	CHB-C4A-NA	2.57	128.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	G	305	A86	C41-C32-C31	-2.57	108.17	110.47
37	O	313	KC1	C3B-C2B-C1B	-2.57	104.62	107.05
36	T	309	CLA	C3B-C4B-NB	-2.57	108.24	110.53
36	a	803	CLA	C1-O2A-CGA	2.57	122.86	116.65
36	l	206	CLA	CHB-C4A-NA	2.56	128.10	124.40
35	P	306	A86	C4-C3-C2	-2.56	118.27	123.52
44	b	846	BCR	C15-C16-C17	-2.56	118.27	123.52
35	N	304	A86	C40-C32-C31	-2.56	108.18	110.47
36	a	801	CLA	OBD-CAD-C3D	2.56	134.41	128.42
36	M	307	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
36	W	214	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
35	H	304	A86	C9-C10-C11	-2.56	119.40	126.64
36	D	310	CLA	CMB-C2B-C3B	2.56	132.58	126.55
36	N	317	CLA	CHB-C1B-NB	2.56	127.89	124.05
36	G	315	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
37	C	213	KC1	C4C-C3C-C2C	-2.56	103.16	106.89
36	F	317	CLA	CHD-C4C-C3C	-2.56	121.04	124.77
35	S	305	A86	C25-C24-C1	-2.56	119.34	126.36
35	T	303	A86	C25-C24-C1	-2.56	119.34	126.36
35	Q	316	A86	O4-C38-O5	-2.56	118.05	122.99
34	D	301	DD6	C37-C36-C35	2.56	119.13	114.42
36	H	307	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
36	b	811	CLA	CBA-CAA-C2A	2.56	121.41	113.79
36	X	310	CLA	O2D-CGD-CBD	-2.56	106.76	111.23
35	J	301	A86	C4-C3-C2	-2.56	118.28	123.52
36	F	309	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
36	T	312	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
36	N	309	CLA	CMC-C2C-C1C	-2.56	121.04	125.03
36	K	312	CLA	CHB-C4A-NA	2.56	128.09	124.40
43	b	842	PQN	C14-C13-C15	2.56	119.67	115.23
36	M	312	CLA	CHB-C4A-NA	2.56	128.09	124.40
35	F	305	A86	C4-C3-C2	-2.56	118.29	123.52
36	a	821	CLA	CHB-C4A-NA	2.56	128.09	124.40
37	B	310	KC1	O2D-CGD-O1D	-2.56	118.87	123.85
35	Q	301	A86	C29-C30-C31	-2.56	174.65	177.66
36	M	314	CLA	CHB-C4A-NA	2.55	128.09	124.40
34	Q	302	DD6	C15-C14-C13	-2.55	120.59	125.99
36	H	307	CLA	CHB-C1B-NB	2.55	127.88	124.05
36	a	841	CLA	CHB-C4A-NA	2.55	128.09	124.40
35	S	308	A86	C12-C11-C13	2.55	120.14	116.00
36	S	314	CLA	C17-C16-C15	-2.55	101.83	113.28
37	H	313	KC1	CMD-C2D-C3D	2.55	133.72	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	b	845	BCR	C38-C26-C27	-2.55	108.15	113.60
35	F	304	A86	C25-C26-C27	-2.55	123.70	127.28
36	S	314	CLA	C2A-C1A-CHA	2.55	128.29	123.87
36	N	318	CLA	CGD-CBD-CAD	-2.55	102.59	110.85
36	b	805	CLA	O2D-CGD-CBD	2.55	115.69	111.23
35	L	301	A86	C4-C3-C2	-2.55	118.30	123.52
35	J	303	A86	C23-C16-C17	-2.55	104.49	108.97
36	a	813	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
34	K	305	DD6	C37-C36-C35	2.55	119.11	114.42
36	A	309	CLA	CHB-C4A-NA	2.55	128.08	124.40
35	V	303	A86	C25-C24-C1	-2.55	119.38	126.36
36	E	308	CLA	O2D-CGD-CBD	2.55	115.68	111.23
36	M	315	CLA	CHC-C4B-NB	2.55	127.87	124.05
37	O	315	KC1	C1D-CHD-C4C	-2.55	120.26	126.25
36	A	311	CLA	C1-C2-C3	-2.55	122.02	126.20
36	l	204	CLA	CMB-C2B-C1B	2.55	129.30	125.42
44	a	845	BCR	C27-C26-C25	2.55	126.15	122.70
34	a	849	DD6	O1-C20-C21	-2.55	112.20	115.05
35	N	303	A86	C7-C6-C8	2.55	121.98	118.09
35	N	305	A86	O1-C15-C20	-2.55	57.29	59.45
36	a	802	CLA	CED-O2D-CGD	2.55	121.69	115.92
36	F	313	CLA	CHB-C4A-NA	2.55	128.07	124.40
35	T	305	A86	C34-O4-C38	2.55	122.34	117.85
36	b	817	CLA	CHD-C4C-C3C	-2.54	121.06	124.77
35	B	301	A86	O4-C38-O5	-2.54	118.08	122.99
37	T	310	KC1	C4D-C3D-C2D	2.54	110.84	107.42
36	j	102	CLA	CHB-C4A-NA	2.54	128.07	124.40
37	N	314	KC1	C1C-C2C-C3C	-2.54	104.30	106.98
35	U	301	A86	C40-C32-C31	-2.54	108.19	110.47
36	X	313	CLA	C2A-C1A-CHA	2.54	128.28	123.87
36	b	817	CLA	C3D-C4D-ND	2.54	114.12	109.99
35	R	302	A86	C9-C8-C6	-2.54	119.39	126.36
43	b	842	PQN	C11-C3-C2	-2.54	120.53	124.89
44	l	207	BCR	C3-C4-C5	-2.54	109.52	114.06
44	b	843	BCR	C27-C26-C25	2.54	126.14	122.70
36	P	301	CLA	C5-C3-C2	-2.54	115.46	121.17
36	G	313	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
36	U	306	CLA	C4B-C3B-C2B	-2.54	104.14	107.30
36	H	318	CLA	CHB-C4A-NA	2.54	128.07	124.40
36	S	313	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
35	V	304	A86	C4-C3-C2	-2.54	118.32	123.52
37	Q	311	KC1	C1D-CHD-C4C	-2.54	120.27	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	S	315	CLA	CBC-CAC-C3C	2.54	119.31	112.42
36	V	310	CLA	CHB-C4A-NA	2.54	128.07	124.40
36	R	318	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
37	X	311	KC1	C2A-C1A-NA	2.54	113.41	109.34
36	I	313	CLA	CHB-C4A-NA	2.54	128.06	124.40
35	Q	316	A86	O1-C15-C20	-2.54	57.30	59.45
36	R	312	CLA	CHB-C4A-NA	2.54	128.06	124.40
35	U	304	A86	C34-O4-C38	-2.54	113.36	117.85
35	C	203	A86	O4-C38-O5	-2.54	118.09	122.99
36	V	311	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
35	D	302	A86	C25-C26-C27	-2.54	123.72	127.28
37	M	317	KC1	C2D-C1D-ND	-2.54	107.69	110.33
37	P	315	KC1	C3B-C2B-C1B	-2.54	104.64	107.05
35	X	301	A86	C25-C24-C1	-2.54	119.41	126.36
35	X	301	A86	C9-C8-C6	-2.54	119.41	126.36
36	S	321	CLA	C3B-C4B-NB	-2.54	108.27	110.53
35	L	304	A86	O4-C38-O5	-2.54	118.09	122.99
34	j	103	DD6	C4-C3-C2	-2.54	118.33	123.52
35	M	301	A86	C3-C4-C5	-2.54	118.33	123.52
36	a	829	CLA	CMD-C2D-C3D	2.54	133.51	127.69
36	K	316	CLA	CHB-C4A-NA	2.54	128.06	124.40
37	M	318	KC1	C2C-C1C-NC	2.54	113.59	110.45
36	N	318	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
35	N	304	A86	C41-C32-C31	-2.54	108.20	110.47
35	U	301	A86	O4-C38-O5	-2.54	118.09	122.99
36	L	311	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
35	R	301	A86	C23-C16-C22	-2.54	103.69	107.37
35	O	303	A86	C29-C30-C31	-2.54	174.67	177.66
36	J	316	CLA	CHB-C4A-NA	2.54	128.06	124.40
36	T	312	CLA	C3B-C4B-NB	-2.54	108.27	110.53
36	a	826	CLA	C3B-C4B-NB	-2.54	108.27	110.53
37	O	315	KC1	C1C-C2C-C3C	-2.53	104.31	106.98
39	U	314	LMT	C1B-O1B-C4'	-2.53	111.97	117.98
37	Q	313	KC1	C1D-CHD-C4C	-2.53	120.29	126.25
35	P	304	A86	C9-C10-C11	-2.53	119.48	126.64
36	G	312	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
37	W	217	KC1	O2D-CGD-O1D	-2.53	118.92	123.85
35	T	307	A86	C9-C8-C6	-2.53	119.42	126.36
36	X	313	CLA	CMC-C2C-C3C	2.53	133.00	126.15
37	C	213	KC1	CHD-C1D-C2D	2.53	134.78	127.43
36	T	311	CLA	CMC-C2C-C3C	2.53	133.00	126.15
35	U	302	A86	C25-C24-C1	-2.53	119.42	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	S	305	A86	C4-C3-C2	-2.53	118.34	123.52
35	Q	303	A86	C10-C9-C8	-2.53	115.86	123.20
36	a	813	CLA	O2D-CGD-CBD	2.53	115.66	111.23
37	Q	313	KC1	C3B-C2B-C1B	-2.53	104.65	107.05
36	F	310	CLA	CHB-C4A-NA	2.53	128.05	124.40
35	O	302	A86	C3-C4-C5	-2.53	118.34	123.52
36	f	803	CLA	CMB-C2B-C1B	2.53	129.27	125.42
35	X	303	A86	O1-C20-C19	2.53	115.86	113.49
35	L	319	A86	C3-C4-C5	-2.53	118.34	123.52
36	O	308	CLA	C3B-C4B-NB	-2.53	108.27	110.53
34	A	301	DD6	C15-C14-C13	-2.53	120.64	125.99
34	I	303	DD6	C15-C14-C13	-2.53	120.64	125.99
37	J	314	KC1	C3A-C4A-NA	2.53	113.58	110.45
35	P	303	A86	C3-C4-C5	-2.53	118.34	123.52
36	C	212	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
37	R	317	KC1	C1D-CHD-C4C	-2.53	120.30	126.25
35	V	302	A86	C22-C16-C17	2.53	113.41	108.97
36	J	307	CLA	CHB-C4A-NA	2.53	128.05	124.40
37	Q	311	KC1	C3B-C2B-C1B	-2.53	104.65	107.05
36	B	311	CLA	C3B-C4B-NB	-2.53	108.27	110.53
36	H	314	CLA	CMB-C2B-C3B	2.53	132.49	126.55
36	b	840	CLA	CHB-C4A-NA	2.53	128.05	124.40
36	P	319	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
35	N	320	A86	C9-C10-C11	-2.53	119.50	126.64
35	F	305	A86	C10-C9-C8	-2.53	115.88	123.20
37	M	317	KC1	CAA-C2A-C1A	2.53	135.72	124.64
35	O	303	A86	C9-C10-C11	-2.53	119.50	126.64
36	G	314	CLA	CAC-C3C-C4C	2.53	128.08	124.79
35	R	309	A86	C9-C8-C6	-2.53	119.44	126.36
37	P	315	KC1	C1D-CHD-C4C	-2.53	120.31	126.25
35	D	302	A86	C12-C11-C13	2.53	120.09	116.00
35	Q	304	A86	C-C1-C2	-2.52	118.73	122.82
35	M	305	A86	O4-C38-O5	-2.52	118.12	122.99
37	X	311	KC1	O2D-CGD-O1D	-2.52	118.94	123.85
34	W	205	DD6	C37-C36-C35	2.52	119.06	114.42
36	b	813	CLA	O2D-CGD-CBD	2.52	115.64	111.23
36	V	305	CLA	CMA-C3A-C4A	2.52	118.55	111.77
34	K	304	DD6	C14-C13-C11	-2.52	121.62	125.53
37	Q	311	KC1	C1C-C2C-C3C	-2.52	104.33	106.98
36	G	315	CLA	C3D-C2D-C1D	-2.52	102.39	105.83
35	G	302	A86	C21-C20-C15	2.52	131.49	123.35
36	f	803	CLA	CHD-C4C-C3C	-2.52	121.10	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	302	A86	C3-C4-C5	-2.52	118.36	123.52
37	O	313	KC1	C1D-CHD-C4C	-2.52	120.32	126.25
35	F	304	A86	O4-C38-O5	-2.52	118.12	122.99
36	B	311	CLA	C3A-C2A-C1A	2.52	105.11	101.34
36	S	314	CLA	C4D-CHA-C1A	2.52	124.25	121.24
44	i	101	BCR	C2-C1-C6	2.52	114.10	110.44
35	P	307	A86	C12-C11-C13	2.52	120.08	116.00
36	b	836	CLA	CAC-C3C-C4C	2.52	128.07	124.79
35	h	202	A86	C4-C3-C2	-2.52	118.36	123.52
36	M	312	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
36	a	822	CLA	CHB-C4A-NA	2.52	128.03	124.40
36	H	315	CLA	O2D-CGD-CBD	2.52	115.63	111.23
35	Q	303	A86	C35-C34-C33	-2.52	105.36	109.89
35	S	303	A86	C7-C6-C8	2.52	121.94	118.09
34	S	306	DD6	C3-C4-C5	-2.52	118.37	123.52
36	S	310	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
37	P	315	KC1	C1C-C2C-C3C	-2.52	104.33	106.98
35	K	303	A86	C9-C8-C6	-2.52	119.46	126.36
36	H	306	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
36	X	315	CLA	C3B-C4B-NB	-2.52	108.28	110.53
34	L	305	DD6	C9-C10-C11	-2.52	123.75	127.28
35	P	304	A86	C29-C30-C31	-2.52	174.69	177.66
37	W	217	KC1	C2A-C1A-NA	2.52	113.38	109.34
35	E	302	A86	C34-O4-C38	-2.52	113.40	117.85
36	X	312	CLA	CMB-C2B-C3B	2.52	132.47	126.55
36	F	317	CLA	CHA-C4D-ND	2.52	137.74	132.55
35	G	306	A86	C34-O4-C38	-2.52	113.40	117.85
34	F	303	DD6	C14-C13-C11	-2.52	121.63	125.53
35	N	305	A86	C23-C16-C17	-2.52	104.55	108.97
36	Q	310	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
36	N	317	CLA	CMB-C2B-C3B	2.52	132.47	126.55
36	f	804	CLA	CHB-C1B-C2B	-2.52	120.12	127.43
36	H	308	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
36	Q	312	CLA	CHB-C4A-NA	2.51	128.03	124.40
36	N	311	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
35	P	306	A86	O4-C38-O5	-2.51	118.14	122.99
36	J	315	CLA	C3B-C4B-NB	-2.51	108.29	110.53
36	a	806	CLA	CHB-C4A-NA	2.51	128.03	124.40
36	O	312	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
36	b	828	CLA	CHB-C4A-NA	2.51	128.03	124.40
36	B	308	CLA	C3C-C4C-NC	-2.51	107.21	110.43
36	P	316	CLA	CHB-C4A-NA	2.51	128.02	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	U	304	A86	C25-C24-C1	-2.51	119.48	126.36
35	R	309	A86	O4-C38-O5	-2.51	118.14	122.99
34	R	307	DD6	C25-C26-C27	-2.51	119.59	126.61
44	a	847	BCR	C11-C10-C9	-2.51	123.76	127.28
35	U	301	A86	C12-C11-C13	2.51	120.07	116.00
36	b	806	CLA	O1D-CGD-CBD	2.51	129.47	124.52
36	H	317	CLA	CHB-C4A-NA	2.51	128.02	124.40
39	L	303	LMT	C3'-C4'-C5'	-2.51	105.37	110.93
36	a	807	CLA	C11-C10-C8	-2.51	107.63	115.97
35	Q	303	A86	C26-C25-C24	-2.51	115.93	123.20
36	P	314	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
35	F	305	A86	C40-C32-C31	2.51	112.72	110.47
36	X	308	CLA	CAA-CBA-CGA	2.51	120.33	113.21
36	W	209	CLA	O2D-CGD-CBD	2.51	115.61	111.23
36	U	311	CLA	CMB-C2B-C3B	2.51	132.45	126.55
36	a	827	CLA	C6-C5-C3	-2.51	107.36	113.47
36	C	210	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
35	J	306	A86	O4-C38-O5	-2.51	118.15	122.99
37	L	315	KC1	C3B-C2B-C1B	-2.51	104.67	107.05
37	G	308	KC1	CED-O2D-CGD	2.51	121.60	115.92
35	h	202	A86	C26-C25-C24	-2.51	115.94	123.20
36	L	312	CLA	C3B-C4B-NB	-2.51	108.29	110.53
36	N	308	CLA	CHD-C4C-C3C	-2.51	121.12	124.77
35	Q	304	A86	C9-C10-C11	-2.51	119.56	126.64
36	b	816	CLA	C1D-CHD-C4C	-2.51	120.69	126.02
36	U	310	CLA	CMC-C2C-C1C	-2.51	121.12	125.03
36	a	827	CLA	O1D-CGD-CBD	2.51	129.46	124.52
36	V	309	CLA	C3A-C2A-C1A	2.50	105.09	101.34
36	H	308	CLA	O1A-CGA-CBA	2.50	133.58	123.78
35	S	301	A86	C9-C10-C11	-2.50	119.56	126.64
35	Q	301	A86	C9-C10-C11	-2.50	119.56	126.64
44	l	207	BCR	C11-C10-C9	-2.50	123.77	127.28
36	a	808	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
36	S	318	CLA	O2D-CGD-CBD	2.50	115.61	111.23
39	I	318	LMT	C1B-O1B-C4'	-2.50	112.04	117.98
41	G	320	LHG	C5-O7-C7	-2.50	111.80	117.80
36	A	308	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
44	b	847	BCR	C30-C25-C26	-2.50	119.22	122.64
35	N	320	A86	C-C1-C2	-2.50	118.76	122.82
37	O	313	KC1	C1C-C2C-C3C	-2.50	104.35	106.98
36	b	840	CLA	CBC-CAC-C3C	2.50	119.20	112.42
36	D	309	CLA	CMC-C2C-C1C	2.50	128.94	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	302	A86	C9-C10-C11	-2.50	119.57	126.64
36	S	317	CLA	CHB-C4A-NA	2.50	128.01	124.40
36	a	809	CLA	CHB-C4A-NA	2.50	128.01	124.40
40	b	849	DGD	C6D-O5D-C1E	2.50	119.16	113.80
35	Q	303	A86	C3-C4-C5	-2.50	118.41	123.52
37	P	317	KC1	CHD-C1D-C2D	2.50	134.68	127.43
36	b	824	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
39	F	320	LMT	C1B-O1B-C4'	-2.50	112.06	117.98
36	S	321	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
35	U	303	A86	O4-C38-O5	-2.50	118.17	122.99
36	U	308	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
36	b	832	CLA	C3B-C4B-NB	-2.50	108.30	110.53
36	a	812	CLA	CMB-C2B-C3B	2.50	132.42	126.55
37	H	313	KC1	C4D-CHA-C1A	-2.50	114.84	122.45
36	b	836	CLA	CMC-C2C-C1C	2.50	128.94	125.03
35	N	301	A86	C9-C10-C11	-2.50	119.58	126.64
35	Q	316	A86	C23-C16-C17	-2.50	104.58	108.97
37	G	318	KC1	CBA-CAA-C2A	2.49	135.47	125.45
35	V	302	A86	C25-C26-C27	-2.49	123.78	127.28
35	G	304	A86	C10-C9-C8	-2.49	115.98	123.20
35	J	302	A86	C4-C3-C2	-2.49	118.42	123.52
36	A	314	CLA	O1D-CGD-CBD	2.49	129.44	124.52
36	C	212	CLA	C3B-C4B-NB	-2.49	108.31	110.53
36	b	828	CLA	C4D-C3D-CAD	-2.49	105.40	108.11
37	G	308	KC1	C1C-C2C-C3C	-2.49	104.36	106.98
36	a	803	CLA	O2A-CGA-CBA	2.49	119.43	111.83
36	a	820	CLA	CMB-C2B-C3B	2.49	132.41	126.55
36	b	837	CLA	CMB-C2B-C3B	2.49	132.41	126.55
36	K	313	CLA	CHB-C4A-NA	2.49	128.00	124.40
35	M	301	A86	C9-C10-C11	-2.49	119.60	126.64
36	J	307	CLA	CMB-C2B-C3B	2.49	132.41	126.55
36	O	314	CLA	CHB-C4A-NA	2.49	128.00	124.40
35	P	303	A86	C9-C8-C6	-2.49	119.53	126.36
35	M	302	A86	O4-C38-O5	-2.49	118.18	122.99
36	W	218	CLA	CMB-C2B-C3B	2.49	132.41	126.55
36	V	314	CLA	C3D-C4D-ND	2.49	114.03	109.99
37	O	315	KC1	C3B-C2B-C1B	-2.49	104.69	107.05
36	N	317	CLA	C3B-C4B-NB	-2.49	108.31	110.53
34	C	201	DD6	C28-C27-C26	-2.49	119.35	124.18
37	C	213	KC1	C2A-C1A-CHA	-2.49	118.74	128.96
36	f	804	CLA	C4-C3-C5	2.49	119.55	115.23
34	F	303	DD6	O1-C15-C14	-2.49	109.75	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	J	301	A86	O4-C38-O5	-2.49	118.19	122.99
35	L	319	A86	C9-C8-C6	-2.49	119.54	126.36
35	A	316	A86	C12-C11-C13	2.49	120.03	116.00
42	G	325	LMG	C8-O7-C10	-2.49	111.84	117.80
37	Q	313	KC1	C1C-C2C-C3C	-2.49	104.36	106.98
37	N	314	KC1	CAD-C3D-C2D	-2.49	139.02	144.26
36	W	210	CLA	CBA-CAA-C2A	-2.49	106.39	113.79
36	R	311	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
36	D	309	CLA	C4D-C3D-CAD	-2.49	105.41	108.11
36	U	310	CLA	C2D-C1D-ND	-2.49	107.67	110.13
35	O	305	A86	O4-C38-O5	-2.49	118.19	122.99
35	R	309	A86	C4-C3-C2	-2.49	118.43	123.52
36	H	309	CLA	C1-C2-C3	-2.49	122.12	126.20
36	I	306	CLA	C4D-CHA-C1A	2.49	124.21	121.24
36	C	205	CLA	C3B-C4B-NB	-2.49	108.31	110.53
34	H	302	DD6	C37-C36-C35	2.49	118.99	114.42
36	b	826	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
37	G	318	KC1	CAA-C2A-C1A	2.48	135.53	124.64
36	H	305	CLA	CHB-C4A-NA	2.48	127.99	124.40
37	X	311	KC1	C4C-C3C-C2C	-2.48	103.28	106.89
36	A	308	CLA	O1D-CGD-CBD	2.48	129.42	124.52
36	J	312	CLA	CMB-C2B-C3B	2.48	132.39	126.55
35	G	305	A86	C9-C8-C6	-2.48	119.55	126.36
37	W	217	KC1	C4C-C3C-C2C	-2.48	103.28	106.89
35	X	304	A86	C25-C24-C1	-2.48	119.55	126.36
36	a	806	CLA	C4D-C3D-CAD	-2.48	105.41	108.11
35	F	307	A86	C40-C32-C31	2.48	112.69	110.47
36	f	803	CLA	CMC-C2C-C1C	2.48	128.91	125.03
36	F	317	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
39	h	205	LMT	C1B-O1B-C4'	-2.48	112.10	117.98
36	F	317	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
36	l	206	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
36	O	308	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
36	f	804	CLA	CHA-C4D-ND	2.48	137.67	132.55
36	Q	307	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
36	G	309	CLA	CMB-C2B-C3B	2.48	132.38	126.55
35	C	203	A86	C28-C27-C26	-2.48	118.80	122.82
36	b	801	CLA	CMB-C2B-C3B	2.48	132.38	126.55
35	G	306	A86	O4-C38-O5	-2.48	118.20	122.99
34	F	303	DD6	C37-C36-C35	2.48	118.98	114.42
35	T	301	A86	C33-C32-C31	-2.48	106.80	109.21
35	N	305	A86	C3-C2-C1	-2.48	123.80	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	214	CLA	CAC-C3C-C4C	2.48	128.01	124.79
35	L	307	A86	O4-C38-O5	-2.48	118.21	122.99
37	C	213	KC1	C3B-C2B-C1B	-2.48	104.70	107.05
41	Q	315	LHG	C5-O7-C7	-2.48	111.87	117.80
44	i	103	BCR	C28-C27-C26	-2.48	109.64	114.06
35	O	301	A86	C12-C11-C13	2.48	120.02	116.00
36	R	318	CLA	C3B-C4B-NB	-2.48	108.32	110.53
36	N	317	CLA	C2A-C1A-CHA	2.48	128.16	123.87
34	A	301	DD6	O1-C15-C14	-2.48	109.79	116.88
35	L	301	A86	C12-C11-C13	2.47	120.01	116.00
34	B	302	DD6	C3-C4-C5	-2.47	118.46	123.52
35	O	302	A86	C9-C8-C6	-2.47	119.58	126.36
39	a	853	LMT	C1B-O1B-C4'	-2.47	112.11	117.98
35	F	305	A86	C36-C31-C32	-2.47	117.24	119.70
35	Q	316	A86	C3-C2-C1	-2.47	123.81	127.28
44	j	107	BCR	C11-C10-C9	-2.47	123.81	127.28
36	b	824	CLA	CMC-C2C-C1C	2.47	128.90	125.03
35	F	302	A86	O4-C38-O5	-2.47	118.22	122.99
36	a	823	CLA	CMB-C2B-C1B	2.47	129.18	125.42
35	R	303	A86	C25-C24-C1	-2.47	119.59	126.36
36	I	305	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
41	O	318	LHG	O8-C23-C24	2.47	119.36	111.83
35	F	307	A86	C9-C10-C11	-2.47	119.66	126.64
36	J	315	CLA	CHB-C4A-NA	2.47	127.96	124.40
35	Q	303	A86	O4-C38-O5	-2.47	118.23	122.99
36	E	308	CLA	CHB-C4A-NA	2.47	127.96	124.40
36	L	308	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
36	N	313	CLA	CMA-C3A-C2A	-2.47	110.57	116.23
44	f	806	BCR	C16-C15-C14	-2.47	118.47	123.52
36	J	310	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
35	J	301	A86	O1-C15-C20	-2.47	57.36	59.45
35	S	302	A86	O4-C38-O5	-2.47	118.23	122.99
35	Q	304	A86	C24-C1-C2	2.47	122.89	119.01
36	P	310	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
34	K	304	DD6	O1-C15-C14	-2.46	109.82	116.88
35	T	306	A86	O1-C20-C19	2.46	115.80	113.49
36	P	301	CLA	O2D-CGD-CBD	2.46	115.54	111.23
35	V	301	A86	O4-C38-O5	-2.46	118.24	122.99
36	I	308	CLA	O2A-CGA-CBA	2.46	119.34	111.83
36	Q	307	CLA	C3B-C4B-NB	-2.46	108.33	110.53
36	M	315	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	S	318	CLA	CHB-C4A-NA	2.46	127.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	X	301	A86	C4-C3-C2	-2.46	118.48	123.52
35	C	202	A86	C36-C31-C32	-2.46	117.25	119.70
36	H	307	CLA	CHB-C1B-C2B	-2.46	120.28	127.43
36	b	838	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
44	b	844	BCR	C24-C23-C22	-2.46	122.60	126.23
35	h	204	A86	C9-C10-C11	-2.46	119.69	126.64
36	Q	314	CLA	CED-O2D-CGD	2.46	121.49	115.92
35	M	301	A86	C9-C8-C6	-2.46	119.62	126.36
36	M	308	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	G	315	CLA	CHB-C1B-C2B	-2.46	120.29	127.43
36	S	310	CLA	O2A-C1-C2	2.46	117.57	108.11
36	A	305	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	a	836	CLA	CMB-C2B-C3B	2.46	132.33	126.55
37	L	317	KC1	CAD-C3D-C2D	-2.46	139.09	144.26
36	a	804	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	U	306	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
36	L	316	CLA	C3B-C4B-NB	-2.46	108.34	110.53
36	b	826	CLA	C3B-C4B-NB	-2.46	108.34	110.53
35	Q	301	A86	C9-C8-C6	-2.46	119.63	126.36
35	R	305	A86	C40-C32-C31	-2.46	108.27	110.47
35	P	304	A86	C9-C8-C6	-2.46	119.63	126.36
36	P	310	CLA	C3B-C4B-NB	-2.46	108.34	110.53
36	a	836	CLA	C3B-C4B-NB	-2.46	108.34	110.53
36	b	820	CLA	C3B-C4B-NB	-2.46	108.34	110.53
35	G	304	A86	C8-C6-C5	-2.45	115.15	119.01
44	i	101	BCR	C30-C25-C26	-2.45	119.28	122.64
36	a	837	CLA	CHB-C4A-NA	2.45	127.94	124.40
36	R	310	CLA	C3B-C4B-NB	-2.45	108.34	110.53
35	N	301	A86	C4-C3-C2	-2.45	118.50	123.52
36	T	311	CLA	CMC-C2C-C1C	-2.45	121.20	125.03
36	b	818	CLA	C4D-CHA-C1A	2.45	124.17	121.24
34	H	302	DD6	C9-C10-C11	-2.45	123.84	127.28
36	D	306	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
36	E	313	CLA	CMB-C2B-C1B	2.45	129.15	125.42
36	b	806	CLA	CHB-C4A-NA	2.45	127.94	124.40
41	f	809	LHG	C5-O7-C7	-2.45	111.93	117.80
34	D	305	DD6	C25-C24-C1	-2.45	119.65	126.36
34	F	303	DD6	O1-C20-C21	-2.45	112.31	115.05
36	F	309	CLA	CMB-C2B-C3B	2.45	132.31	126.55
36	O	316	CLA	C3C-C4C-NC	2.45	113.57	110.43
35	O	303	A86	C9-C8-C6	-2.45	119.65	126.36
36	G	313	CLA	C6-C7-C8	-2.45	107.83	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	840	CLA	CAA-CBA-CGA	-2.45	106.26	113.21
36	G	319	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
36	U	310	CLA	C1D-ND-C4D	2.45	108.03	106.31
36	V	308	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
36	l	201	CLA	CMB-C2B-C3B	2.45	132.31	126.55
36	H	314	CLA	CHB-C4A-NA	2.45	127.93	124.40
36	b	826	CLA	CAA-C2A-C1A	-2.45	103.96	111.97
36	G	316	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
36	a	837	CLA	C3B-C4B-NB	-2.45	108.35	110.53
35	T	307	A86	C21-C20-C19	-2.45	111.49	114.24
35	Q	316	A86	O4-C34-C33	2.45	113.90	107.64
35	K	301	A86	O4-C38-O5	-2.45	118.27	122.99
36	N	316	CLA	CAA-C2A-C3A	-2.45	106.39	113.00
37	T	315	KC1	C1A-C2A-C3A	-2.45	105.03	107.28
36	N	319	CLA	CMB-C2B-C3B	2.45	132.30	126.55
36	E	314	CLA	CMB-C2B-C3B	2.45	132.30	126.55
34	O	304	DD6	C37-C36-C35	2.45	118.92	114.42
36	b	806	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
36	A	306	CLA	CHB-C1B-C2B	-2.44	120.33	127.43
37	W	213	KC1	C4C-C3C-C2C	-2.44	103.33	106.89
36	C	208	CLA	CHB-C4A-NA	2.44	127.93	124.40
35	N	302	A86	O4-C38-O5	-2.44	118.27	122.99
37	N	314	KC1	CAA-CBA-CGA	-2.44	114.62	127.05
35	T	302	A86	C34-O4-C38	2.44	122.16	117.85
36	X	313	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
36	V	308	CLA	C3B-C4B-NB	-2.44	108.35	110.53
35	S	301	A86	C4-C3-C2	-2.44	118.52	123.52
36	X	308	CLA	C1D-ND-C4D	-2.44	104.60	106.31
35	N	305	A86	O4-C34-C33	2.44	113.89	107.64
37	V	312	KC1	C2A-C1A-CHA	-2.44	118.93	128.96
36	N	313	CLA	CHB-C4A-NA	2.44	127.92	124.40
35	U	304	A86	C28-C27-C26	-2.44	118.86	122.82
36	a	805	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
34	A	304	DD6	C25-C26-C27	-2.44	119.78	126.61
37	P	317	KC1	C1A-NA-C4A	-2.44	105.56	106.68
36	b	816	CLA	C4-C3-C5	2.44	119.47	115.23
35	L	301	A86	O4-C38-O5	-2.44	118.28	122.99
36	a	821	CLA	CMB-C2B-C3B	2.44	132.29	126.55
37	N	314	KC1	C3B-C2B-C1B	-2.44	104.74	107.05
37	K	314	KC1	C2A-C1A-NA	2.44	113.25	109.34
34	E	304	DD6	C15-C14-C13	-2.44	120.83	125.99
36	N	313	CLA	CHA-C1A-NA	-2.44	120.87	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	815	CLA	C3B-C4B-NB	-2.44	108.35	110.53
35	U	301	A86	C41-C32-C31	-2.44	108.29	110.47
35	R	305	A86	O4-C38-O5	-2.44	118.28	122.99
36	N	308	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
36	R	321	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
36	b	826	CLA	C3A-C2A-C1A	2.44	104.99	101.34
34	D	303	DD6	C3-C2-C1	-2.44	123.86	127.28
37	P	317	KC1	O2D-CGD-O1D	-2.44	119.11	123.85
35	N	304	A86	C9-C10-C11	-2.44	119.75	126.64
36	O	308	CLA	C4-C3-C2	-2.44	117.37	123.63
37	R	317	KC1	O2D-CGD-O1D	-2.43	119.11	123.85
35	T	306	A86	C9-C10-C11	-2.43	119.76	126.64
35	T	307	A86	O4-C34-C33	2.43	113.87	107.64
35	U	304	A86	C7-C6-C5	-2.43	118.87	122.82
35	A	302	A86	C12-C11-C13	-2.43	112.05	116.00
35	N	320	A86	C24-C1-C2	2.43	122.84	119.01
36	R	315	CLA	C3B-C4B-NB	-2.43	108.36	110.53
36	W	216	CLA	O2A-CGA-O1A	-2.43	117.08	123.33
35	Q	304	A86	O4-C38-O5	-2.43	118.30	122.99
34	A	304	DD6	C28-C27-C26	-2.43	119.46	124.18
36	A	306	CLA	CMC-C2C-C1C	2.43	128.84	125.03
36	b	831	CLA	CHB-C1B-NB	2.43	127.70	124.05
36	R	321	CLA	CHB-C4A-NA	2.43	127.91	124.40
36	M	306	CLA	CMD-C2D-C1D	-2.43	120.45	124.73
35	T	306	A86	C3-C4-C5	-2.43	118.54	123.52
35	Q	303	A86	C21-C20-C15	2.43	131.20	123.35
36	B	308	CLA	C3B-C4B-NB	-2.43	108.36	110.53
35	G	305	A86	C34-O4-C38	-2.43	113.55	117.85
37	A	312	KC1	C3C-C4C-NC	2.43	112.50	109.90
34	K	304	DD6	O1-C20-C21	-2.43	112.33	115.05
36	H	310	CLA	CAC-C3C-C4C	2.43	127.95	124.79
36	E	310	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
36	a	848	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
36	X	310	CLA	CHB-C4A-NA	2.43	127.90	124.40
36	U	310	CLA	CHB-C4A-NA	2.43	127.90	124.40
37	T	315	KC1	C2A-C1A-CHA	-2.43	119.00	128.96
35	I	301	A86	C40-C32-C31	-2.43	108.30	110.47
34	D	303	DD6	C7-C6-C8	2.43	121.80	118.09
36	V	311	CLA	CBA-CAA-C2A	2.43	121.01	113.79
36	a	808	CLA	O1D-CGD-CBD	2.43	129.30	124.52
36	a	806	CLA	CHD-C4C-C3C	-2.43	121.24	124.77
34	K	304	DD6	C21-C20-C15	-2.43	118.31	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	848	CLA	C3B-C4B-NB	-2.43	108.36	110.53
36	f	805	CLA	C3B-C4B-NB	-2.43	108.36	110.53
35	X	314	A86	O4-C38-O5	-2.43	118.31	122.99
36	U	309	CLA	C3A-C2A-C1A	2.42	104.97	101.34
34	D	301	DD6	C28-C27-C26	-2.42	119.47	124.18
36	b	829	CLA	CHB-C4A-NA	2.42	127.90	124.40
35	X	304	A86	C28-C27-C26	-2.42	118.89	122.82
36	M	306	CLA	CMD-C2D-C3D	2.42	133.25	127.69
35	F	301	A86	O1-C15-C20	-2.42	57.40	59.45
36	H	310	CLA	C3B-C4B-NB	-2.42	108.37	110.53
36	M	311	CLA	O1D-CGD-CBD	2.42	129.30	124.52
35	X	305	A86	C12-C11-C13	2.42	119.93	116.00
36	B	308	CLA	CHD-C1D-ND	-2.42	121.39	124.80
34	W	204	DD6	C25-C26-C27	-2.42	119.83	126.61
36	a	823	CLA	CHB-C1B-C2B	-2.42	120.39	127.43
36	b	838	CLA	CMB-C2B-C3B	2.42	132.25	126.55
35	I	302	A86	C9-C8-C6	-2.42	119.72	126.36
36	l	201	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	V	308	CLA	C1-C2-C3	-2.42	122.23	126.20
36	b	830	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	J	308	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
35	T	301	A86	C12-C11-C13	2.42	119.92	116.00
36	a	831	CLA	C4D-C3D-CAD	-2.42	105.48	108.11
36	K	315	CLA	C3B-C4B-NB	-2.42	108.37	110.53
35	O	305	A86	C-C1-C2	-2.42	118.90	122.82
36	a	824	CLA	CHA-C1A-NA	-2.42	120.91	126.39
36	a	807	CLA	CMB-C2B-C3B	2.42	132.24	126.55
36	N	309	CLA	CMC-C2C-C3C	2.42	132.69	126.15
41	G	301	LHG	C11-C10-C9	-2.42	102.15	114.37
36	O	309	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
36	b	818	CLA	CHB-C1B-C2B	-2.42	120.41	127.43
36	K	310	CLA	CHC-C1C-C2C	-2.42	120.08	126.95
35	R	305	A86	C12-C11-C13	2.42	119.92	116.00
36	X	315	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	D	308	CLA	CAA-CBA-CGA	-2.42	106.35	113.21
36	N	319	CLA	C2A-C1A-CHA	2.42	128.06	123.87
35	T	306	A86	C28-C27-C26	-2.42	118.90	122.82
36	a	805	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	a	828	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	E	310	CLA	C3B-C4B-NB	-2.42	108.37	110.53
36	a	839	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
35	T	302	A86	O4-C34-C35	-2.42	101.45	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	307	A86	C12-C11-C13	2.42	119.92	116.00
36	N	317	CLA	CHB-C4A-NA	2.42	127.89	124.40
36	E	312	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
36	T	311	CLA	CHC-C4B-NB	2.42	127.67	124.05
35	V	301	A86	C33-C32-C31	-2.41	106.86	109.21
35	H	304	A86	C34-O4-C38	-2.41	113.58	117.85
35	R	306	A86	C9-C8-C6	-2.41	119.74	126.36
37	W	213	KC1	C2A-C3A-C4A	2.41	108.22	106.41
36	A	307	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
36	H	312	CLA	CBA-CAA-C2A	2.41	120.98	113.79
35	N	320	A86	O4-C38-O5	-2.41	118.33	122.99
36	N	310	CLA	C3B-C2B-C1B	-2.41	104.32	107.17
36	M	310	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
36	P	318	CLA	CHB-C4A-NA	2.41	127.88	124.40
36	W	210	CLA	CHA-C1A-NA	-2.41	120.93	126.39
35	R	302	A86	C25-C24-C1	-2.41	119.75	126.36
37	S	316	KC1	C4D-CHA-C1A	-2.41	115.10	122.45
36	H	310	CLA	C1D-ND-C4D	2.41	108.00	106.31
36	L	313	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
36	F	314	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
44	i	103	BCR	C30-C25-C26	-2.41	119.34	122.64
35	I	301	A86	O4-C38-O5	-2.41	118.33	122.99
37	W	213	KC1	O2D-CGD-O1D	-2.41	119.15	123.85
34	H	303	DD6	C15-C14-C13	-2.41	120.89	125.99
36	N	310	CLA	CHA-C1A-NA	-2.41	120.93	126.39
36	a	816	CLA	C3B-C4B-NB	-2.41	108.38	110.53
36	U	307	CLA	C3B-C4B-NB	-2.41	108.38	110.53
36	D	309	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
36	N	311	CLA	C3A-C2A-C1A	2.41	104.95	101.34
36	M	307	CLA	C1-O2A-CGA	2.41	122.48	116.65
44	b	845	BCR	C24-C23-C22	-2.41	122.67	126.23
34	Q	302	DD6	C25-C24-C1	-2.41	119.76	126.36
36	G	311	CLA	C3B-C4B-NB	-2.41	108.38	110.53
37	M	318	KC1	O2D-CGD-O1D	-2.41	119.16	123.85
36	b	829	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
36	S	311	CLA	O1D-CGD-CBD	2.41	129.27	124.52
34	E	304	DD6	C32-C33-C34	-2.41	108.31	113.59
35	S	305	A86	C9-C10-C11	-2.41	119.83	126.64
37	S	316	KC1	C3A-C4A-NA	2.41	113.43	110.45
44	i	101	BCR	C1-C6-C5	-2.41	119.34	122.64
36	l	206	CLA	C1-C2-C3	-2.41	122.86	126.76
35	T	302	A86	O4-C34-C33	2.41	113.80	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	L	306	A86	C25-C24-C1	2.41	132.97	126.36
36	b	830	CLA	CAC-C3C-C2C	-2.41	123.14	127.56
36	b	816	CLA	C2A-C1A-CHA	-2.41	119.69	123.87
36	a	807	CLA	C1-C2-C3	-2.41	122.25	126.20
41	O	318	LHG	C20-C19-C18	-2.41	102.20	114.37
36	G	319	CLA	CHC-C1C-C2C	-2.41	120.11	126.95
35	M	302	A86	C25-C24-C1	-2.41	119.76	126.36
34	H	303	DD6	C37-C36-C35	2.41	118.85	114.42
35	H	301	A86	C28-C27-C26	-2.41	118.92	122.82
37	H	313	KC1	CAA-CBA-CGA	-2.41	114.81	127.05
44	m	101	BCR	C7-C8-C9	-2.41	122.68	126.23
35	I	304	A86	C40-C32-C31	2.41	112.62	110.47
36	P	311	CLA	CMB-C2B-C1B	-2.41	121.76	125.42
36	V	314	CLA	CMD-C2D-C3D	-2.40	122.17	127.69
36	a	830	CLA	C5-C3-C4	2.40	120.12	114.59
36	a	813	CLA	CMB-C2B-C3B	2.40	132.20	126.55
36	S	311	CLA	CHB-C1B-NB	2.40	127.65	124.05
36	a	808	CLA	C2A-C1A-CHA	2.40	128.04	123.87
36	a	802	CLA	CHB-C4A-NA	2.40	127.87	124.40
34	Q	302	DD6	C25-C26-C27	-2.40	119.89	126.61
36	S	313	CLA	C3B-C4B-NB	-2.40	108.39	110.53
36	V	311	CLA	C3B-C4B-NB	-2.40	108.39	110.53
35	I	301	A86	C41-C32-C31	-2.40	108.32	110.47
36	J	310	CLA	C3B-C4B-NB	-2.40	108.39	110.53
36	U	308	CLA	C3B-C4B-NB	-2.40	108.39	110.53
36	b	812	CLA	CHB-C4A-NA	2.40	127.86	124.40
36	J	307	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
37	L	317	KC1	CHD-C1D-C2D	2.40	134.39	127.43
36	K	310	CLA	CHD-C1D-C2D	2.40	130.48	125.49
36	E	311	CLA	CMB-C2B-C3B	2.40	132.19	126.55
36	b	828	CLA	CGD-CBD-CAD	2.40	118.61	110.85
36	I	309	CLA	C3B-C4B-NB	-2.40	108.39	110.53
35	R	309	A86	C9-C10-C11	-2.40	119.86	126.64
35	R	305	A86	C3-C4-C5	-2.40	118.61	123.52
35	F	305	A86	C26-C25-C24	-2.40	116.25	123.20
35	h	202	A86	C12-C11-C13	2.40	119.89	116.00
36	E	313	CLA	CHC-C1C-C2C	-2.40	120.13	126.95
44	a	844	BCR	C40-C30-C25	2.40	114.00	110.24
36	A	307	CLA	CHB-C4A-NA	2.40	127.86	124.40
36	T	313	CLA	CHB-C4A-NA	2.40	127.86	124.40
36	G	319	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
35	M	304	A86	O4-C38-O5	-2.40	118.36	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	l	206	CLA	C3B-C4B-NB	-2.40	108.39	110.53
44	h	201	BCR	C27-C26-C25	2.40	125.94	122.70
36	S	314	CLA	CHA-C1A-NA	-2.40	120.96	126.39
39	B	313	LMT	C1B-O1B-C4'	-2.40	112.30	117.98
36	a	824	CLA	CHD-C4C-C3C	-2.40	121.28	124.77
36	T	316	CLA	CHB-C4A-NA	2.39	127.86	124.40
36	W	214	CLA	CHB-C4A-NA	2.39	127.86	124.40
37	R	317	KC1	CBB-CAB-C3B	-2.39	115.56	127.53
36	L	314	CLA	CAA-C2A-C3A	-2.39	106.53	113.00
36	X	307	CLA	C1-C2-C3	-2.39	122.89	126.76
36	N	308	CLA	C6-C5-C3	2.39	119.30	113.47
36	B	309	CLA	C3A-C2A-C1A	2.39	104.92	101.34
36	C	212	CLA	C3A-C2A-C1A	2.39	104.92	101.34
44	b	846	BCR	C1-C6-C5	-2.39	119.37	122.64
35	J	305	A86	O4-C38-O5	-2.39	118.37	122.99
37	E	309	KC1	CAD-C3D-C2D	-2.39	139.22	144.26
36	a	832	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
35	A	302	A86	C4-C5-C6	-2.39	123.92	127.28
36	I	305	CLA	C3B-C4B-NB	-2.39	108.40	110.53
36	b	806	CLA	C2A-C1A-CHA	2.39	128.01	123.87
36	a	827	CLA	C3B-C4B-NB	-2.39	108.40	110.53
36	a	820	CLA	CHB-C4A-NA	2.39	127.85	124.40
36	b	836	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
35	J	303	A86	C3-C4-C5	-2.39	118.63	123.52
44	l	203	BCR	C2-C1-C6	2.39	113.91	110.44
35	J	303	A86	C-C1-C24	2.39	121.74	118.09
34	H	303	DD6	C28-C27-C26	-2.39	119.54	124.18
37	S	316	KC1	C1D-CHD-C4C	-2.39	120.63	126.25
36	a	822	CLA	CMB-C2B-C1B	2.39	129.06	125.42
37	M	317	KC1	O2D-CGD-O1D	-2.39	119.20	123.85
34	F	303	DD6	O1-C20-C19	-2.39	111.25	113.49
34	D	305	DD6	C9-C10-C11	-2.39	123.93	127.28
35	O	301	A86	O4-C38-O5	-2.39	118.38	122.99
36	K	316	CLA	C3B-C4B-NB	-2.39	108.40	110.53
35	G	302	A86	O4-C38-O5	-2.39	118.39	122.99
37	C	213	KC1	C1C-C2C-C3C	-2.39	104.47	106.98
36	J	312	CLA	C3B-C4B-NB	-2.38	108.40	110.53
39	U	315	LMT	C1B-O1B-C4'	-2.38	112.33	117.98
34	D	301	DD6	C4-C5-C6	-2.38	123.93	127.28
36	A	314	CLA	C1D-ND-C4D	-2.38	104.64	106.31
34	J	304	DD6	C14-C13-C11	-2.38	121.83	125.53
36	R	313	CLA	CMB-C2B-C1B	-2.38	121.79	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	K	303	A86	C28-C27-C26	-2.38	118.95	122.82
35	H	301	A86	C3-C2-C1	-2.38	123.94	127.28
36	a	806	CLA	CAC-C3C-C4C	2.38	127.89	124.79
35	h	202	A86	C21-C20-C15	2.38	131.04	123.35
35	S	308	A86	C9-C8-C6	-2.38	119.83	126.36
35	U	303	A86	O1-C20-C19	-2.38	111.26	113.49
35	C	202	A86	C28-C27-C26	-2.38	118.96	122.82
36	b	837	CLA	CBA-CAA-C2A	2.38	120.88	113.79
36	l	204	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
36	H	307	CLA	C4D-C3D-CAD	-2.38	105.52	108.11
36	D	313	CLA	C1-C2-C3	-2.38	122.30	126.20
36	b	835	CLA	CGD-CBD-CAD	-2.38	103.14	110.85
36	A	311	CLA	CHB-C4A-NA	2.38	127.83	124.40
36	f	804	CLA	CMC-C2C-C1C	2.38	128.75	125.03
36	C	212	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
35	S	304	A86	O4-C38-O5	-2.38	118.40	122.99
37	R	317	KC1	C1C-C2C-C3C	-2.38	104.48	106.98
36	I	308	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
36	M	307	CLA	CHB-C4A-NA	2.38	127.83	124.40
35	T	305	A86	C12-C11-C13	2.38	119.85	116.00
36	D	307	CLA	C3A-C2A-C1A	2.38	104.90	101.34
36	G	310	CLA	CMB-C2B-C3B	2.38	132.14	126.55
34	R	308	DD6	O1-C15-C14	-2.38	110.07	116.88
36	Q	308	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
36	I	307	CLA	C3B-C4B-NB	-2.37	108.41	110.53
36	R	320	CLA	C3B-C4B-NB	-2.37	108.41	110.53
36	L	310	CLA	CHB-C4A-NA	2.37	127.83	124.40
35	C	204	A86	O4-C38-O5	-2.37	118.41	122.99
36	U	306	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
35	X	301	A86	O3-C36-C37	-2.37	104.71	109.22
36	N	310	CLA	CHB-C1B-C2B	-2.37	120.54	127.43
34	D	304	DD6	C37-C36-C35	2.37	118.78	114.42
36	K	307	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
36	U	309	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
35	G	306	A86	C3-C4-C5	-2.37	118.66	123.52
36	R	320	CLA	C2D-C1D-ND	-2.37	107.78	110.13
36	X	313	CLA	CHA-C4D-ND	2.37	137.44	132.55
36	H	305	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
36	b	832	CLA	CMB-C2B-C3B	2.37	132.13	126.55
35	O	303	A86	O4-C38-O5	-2.37	118.41	122.99
36	a	838	CLA	CHB-C4A-NA	2.37	127.82	124.40
36	W	209	CLA	C2A-C1A-CHA	2.37	127.98	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	H	315	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
36	V	309	CLA	O2D-CGD-CBD	2.37	115.37	111.23
36	O	314	CLA	C2A-C3A-C4A	2.37	104.37	101.59
36	E	313	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
36	L	309	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
36	b	819	CLA	CHB-C1B-C2B	-2.37	120.55	127.43
36	L	314	CLA	CMB-C2B-C3B	2.37	132.12	126.55
36	C	209	CLA	CMD-C2D-C1D	-2.37	120.56	124.73
36	S	309	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
35	C	202	A86	C26-C25-C24	-2.37	116.34	123.20
35	M	304	A86	C25-C24-C1	-2.37	119.88	126.36
37	V	312	KC1	O2D-CGD-O1D	-2.37	119.24	123.85
36	N	312	CLA	CHB-C4A-NA	2.37	127.81	124.40
34	B	302	DD6	C28-C27-C26	-2.37	119.59	124.18
36	a	822	CLA	C4D-C3D-CAD	-2.37	105.54	108.11
36	F	312	CLA	C3B-C4B-NB	-2.36	108.42	110.53
36	R	316	CLA	CHA-C1A-NA	-2.36	121.04	126.39
35	Q	301	A86	O4-C38-O5	-2.36	118.43	122.99
34	M	303	DD6	C37-C36-C35	2.36	118.77	114.42
37	D	314	KC1	CHD-C4C-NC	2.36	127.87	124.31
34	D	304	DD6	C28-C27-C26	-2.36	119.59	124.18
36	a	824	CLA	CMC-C2C-C1C	-2.36	121.34	125.03
41	O	317	LHG	C5-O7-C7	-2.36	112.14	117.80
36	f	804	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
35	X	304	A86	C36-C31-C32	-2.36	117.35	119.70
36	a	803	CLA	CAA-CBA-CGA	-2.36	106.50	113.21
35	F	301	A86	C9-C10-C11	-2.36	119.97	126.64
35	S	305	A86	O1-C20-C21	-2.36	112.41	115.05
36	B	305	CLA	CMB-C2B-C3B	2.36	132.10	126.55
36	a	848	CLA	C4-C3-C5	2.36	119.32	115.23
35	N	302	A86	C28-C27-C26	-2.36	118.99	122.82
36	I	305	CLA	C15-C13-C12	2.36	133.40	113.58
34	R	307	DD6	C25-C24-C1	-2.36	119.89	126.36
34	D	301	DD6	C15-C14-C13	-2.36	121.00	125.99
35	C	202	A86	C9-C10-C11	-2.36	119.97	126.64
36	H	314	CLA	C3B-C4B-NB	-2.36	108.42	110.53
36	a	801	CLA	C3B-C4B-NB	-2.36	108.42	110.53
35	h	202	A86	O1-C20-C19	-2.36	111.28	113.49
36	K	310	CLA	CHB-C1B-C2B	-2.36	120.58	127.43
35	E	305	A86	C41-C32-C31	-2.36	108.36	110.47
36	F	309	CLA	CHD-C1D-ND	-2.36	121.48	124.80
36	E	315	CLA	CMC-C2C-C1C	2.36	128.72	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	841	CLA	C2A-C1A-CHA	2.36	127.96	123.87
36	I	311	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
36	H	318	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
36	I	305	CLA	CHB-C4A-NA	2.36	127.80	124.40
36	b	830	CLA	CHB-C1B-NB	2.36	127.58	124.05
36	R	318	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
36	B	309	CLA	CHB-C1B-C2B	-2.36	120.58	127.43
36	b	827	CLA	CHB-C4A-NA	2.36	127.80	124.40
36	D	312	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
37	D	314	KC1	CAD-C3D-C2D	-2.36	139.30	144.26
41	F	319	LHG	C5-O7-C7	-2.36	112.16	117.80
36	M	310	CLA	CHB-C1B-NB	2.36	127.58	124.05
36	P	316	CLA	C2A-C3A-C4A	2.36	104.35	101.59
35	J	303	A86	C21-C20-C19	2.36	116.89	114.24
36	G	314	CLA	O1D-CGD-CBD	2.36	129.16	124.52
35	L	306	A86	C35-C34-C33	-2.36	105.66	109.89
36	f	802	CLA	CHB-C1B-NB	2.36	127.58	124.05
35	A	316	A86	O4-C38-O5	-2.35	118.44	122.99
36	C	212	CLA	CMB-C2B-C1B	-2.35	121.83	125.42
35	K	303	A86	C-C1-C24	2.35	121.68	118.09
36	Q	310	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
36	A	307	CLA	C1-C2-C3	-2.35	122.34	126.20
36	D	309	CLA	CHB-C4A-NA	2.35	127.79	124.40
35	T	304	A86	C4-C5-C6	-2.35	123.98	127.28
42	I	315	LMG	C8-O7-C10	-2.35	112.17	117.80
34	P	305	DD6	C15-C14-C13	-2.35	121.02	125.99
34	B	302	DD6	O1-C20-C21	-2.35	112.42	115.05
35	N	305	A86	C-C1-C2	-2.35	119.01	122.82
37	K	314	KC1	C1C-C2C-C3C	-2.35	104.51	106.98
35	P	307	A86	C41-C32-C31	-2.35	108.37	110.47
35	H	301	A86	C26-C25-C24	-2.35	116.39	123.20
36	P	319	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
36	a	838	CLA	CMD-C2D-C1D	-2.35	120.59	124.73
36	b	828	CLA	CHA-C4D-ND	2.35	137.40	132.55
36	Q	312	CLA	C2A-C3A-C4A	2.35	104.34	101.59
36	N	319	CLA	CHC-C1C-NC	2.35	127.85	124.31
36	a	837	CLA	CMB-C2B-C3B	2.35	132.07	126.55
35	S	302	A86	C28-C27-C26	-2.35	119.01	122.82
36	a	817	CLA	CHB-C4A-NA	2.35	127.79	124.40
34	A	304	DD6	C37-C36-C35	2.35	118.74	114.42
36	N	313	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
41	O	318	LHG	C13-C12-C11	-2.35	102.51	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	E	313	CLA	C4D-CHA-C1A	-2.35	118.45	121.24
36	G	307	CLA	O2D-CGD-O1D	-2.35	118.76	124.08
36	F	310	CLA	C1-C2-C3	-2.35	122.35	126.20
42	G	324	LMG	C8-O7-C10	-2.35	112.18	117.80
36	a	832	CLA	CBA-CAA-C2A	2.35	120.77	113.79
35	P	304	A86	O4-C38-O5	-2.34	118.46	122.99
36	F	317	CLA	CHB-C4A-NA	2.34	127.78	124.40
36	b	818	CLA	CHB-C4A-NA	2.34	127.78	124.40
37	H	313	KC1	O2D-CGD-O1D	-2.34	119.28	123.85
36	J	307	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
37	M	317	KC1	C3A-C4A-NA	2.34	113.35	110.45
36	U	313	CLA	O1D-CGD-CBD	2.34	129.14	124.52
36	X	315	CLA	CMB-C2B-C3B	2.34	132.06	126.55
36	F	309	CLA	C4-C3-C2	-2.34	117.61	123.63
35	Q	316	A86	C-C1-C2	-2.34	119.02	122.82
36	a	816	CLA	CHB-C1B-NB	2.34	127.56	124.05
36	L	312	CLA	CBA-CAA-C2A	-2.34	106.82	113.79
36	a	805	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
36	f	803	CLA	C3D-C4D-ND	2.34	113.79	109.99
35	N	305	A86	C41-C32-C31	-2.34	108.38	110.47
36	X	312	CLA	C2A-C1A-CHA	2.34	127.92	123.86
36	a	801	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
36	K	308	CLA	C1-C2-C3	-2.34	122.36	126.20
36	a	848	CLA	C4D-C3D-CAD	2.34	110.65	108.11
37	U	312	KC1	CAB-C3B-C2B	-2.34	120.82	128.43
34	S	306	DD6	C25-C26-C27	-2.34	120.07	126.61
35	U	303	A86	C21-C20-C15	2.34	130.90	123.35
36	a	816	CLA	C3A-C2A-C1A	2.34	104.84	101.34
36	f	803	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
36	P	314	CLA	CMA-C3A-C4A	-2.34	105.49	111.77
36	N	308	CLA	C3C-C4C-NC	2.34	113.42	110.43
35	E	302	A86	O4-C38-O5	-2.34	118.48	122.99
36	P	314	CLA	C1-C2-C3	2.34	130.03	126.20
37	Q	311	KC1	CGD-CBD-CAD	-2.34	103.28	110.85
36	W	212	CLA	CMB-C2B-C3B	2.34	132.05	126.55
36	F	316	CLA	CHB-C4A-NA	2.34	127.77	124.40
36	R	310	CLA	CHB-C1B-NB	2.34	127.55	124.05
35	D	302	A86	O4-C38-O5	-2.34	118.48	122.99
36	a	830	CLA	C3A-C2A-C1A	2.34	104.84	101.34
35	Q	316	A86	C41-C32-C31	-2.34	108.38	110.47
36	R	313	CLA	CHB-C4A-NA	2.34	127.77	124.40
36	W	209	CLA	CMB-C2B-C1B	-2.33	121.86	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	301	A86	C12-C11-C13	2.33	119.78	116.00
37	O	315	KC1	CGD-CBD-CAD	-2.33	103.29	110.85
35	W	202	A86	C36-C31-C32	2.33	122.01	119.70
36	T	309	CLA	O2D-CGD-CBD	2.33	115.31	111.23
34	K	305	DD6	C3-C4-C5	-2.33	118.74	123.52
34	P	305	DD6	O1-C20-C21	-2.33	112.44	115.05
36	I	306	CLA	C3D-C4D-ND	2.33	113.78	109.99
36	b	825	CLA	CHA-C1A-NA	-2.33	121.11	126.39
36	b	819	CLA	C3B-C4B-NB	-2.33	108.45	110.53
36	H	309	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
37	U	312	KC1	O2D-CGD-O1D	-2.33	119.31	123.85
36	N	319	CLA	C4C-C3C-C2C	2.33	110.29	106.89
35	H	301	A86	C-C1-C24	2.33	121.65	118.09
36	W	214	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
36	S	315	CLA	CMC-C2C-C1C	-2.33	121.39	125.03
36	S	312	CLA	CED-O2D-CGD	2.33	121.20	115.92
44	l	207	BCR	C15-C14-C13	-2.33	124.01	127.28
36	J	312	CLA	O1D-CGD-CBD	2.33	129.12	124.52
35	W	202	A86	C28-C27-C29	2.33	124.12	118.94
36	C	214	CLA	CHB-C4A-NA	2.33	127.76	124.40
36	V	306	CLA	CMB-C2B-C3B	2.33	132.03	126.55
34	R	307	DD6	C3-C4-C5	-2.33	118.75	123.52
36	T	314	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
36	C	205	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
36	X	308	CLA	O2A-CGA-CBA	2.33	118.94	111.83
36	I	308	CLA	CMB-C2B-C1B	2.33	128.97	125.42
35	I	302	A86	C7-C6-C8	2.33	121.65	118.09
36	X	312	CLA	C3B-C4B-NB	-2.33	108.45	110.53
35	T	305	A86	C28-C27-C26	-2.33	119.04	122.82
35	X	314	A86	C9-C8-C6	-2.33	119.98	126.36
36	V	307	CLA	CHB-C4A-NA	2.33	127.76	124.40
35	O	305	A86	O1-C20-C19	-2.33	111.31	113.49
35	T	303	A86	C36-C31-C32	-2.33	117.39	119.70
44	h	201	BCR	C33-C5-C6	-2.33	121.94	124.48
36	a	823	CLA	C4D-C3D-CAD	-2.33	105.58	108.11
36	W	210	CLA	C1D-ND-C4D	2.33	107.94	106.31
34	D	305	DD6	C25-C26-C27	-2.33	120.10	126.61
37	Q	313	KC1	CGD-CBD-CAD	-2.33	103.31	110.85
36	l	202	CLA	CHB-C4A-NA	2.33	127.76	124.40
34	C	201	DD6	C37-C36-C31	-2.33	119.81	124.16
36	A	310	CLA	CMB-C2B-C3B	2.33	132.02	126.55
36	E	315	CLA	CHD-C1D-C2D	2.33	130.32	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	R	304	A86	C36-C31-C32	-2.32	117.39	119.70
35	J	302	A86	O4-C38-O5	-2.32	118.50	122.99
36	b	817	CLA	C2A-C3A-C4A	2.32	105.62	101.87
41	R	323	LHG	C5-O7-C7	-2.32	112.23	117.80
35	I	304	A86	O-C13-C11	-2.32	116.03	121.04
35	O	305	A86	C33-C32-C31	2.32	111.47	109.21
34	M	303	DD6	C25-C26-C27	-2.32	120.11	126.61
36	J	317	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
36	R	321	CLA	CHB-C1B-NB	2.32	127.53	124.05
36	R	320	CLA	CAC-C3C-C4C	2.32	127.81	124.79
37	O	313	KC1	CGD-CBD-CAD	-2.32	103.33	110.85
34	Q	302	DD6	O1-C20-C21	-2.32	112.45	115.05
44	a	846	BCR	C7-C8-C9	-2.32	122.80	126.23
34	D	303	DD6	C9-C10-C11	-2.32	124.02	127.28
36	i	102	CLA	CAA-CBA-CGA	-2.32	106.62	113.21
37	P	315	KC1	CGD-CBD-CAD	-2.32	103.33	110.85
36	P	302	CLA	CHB-C4A-NA	2.32	127.75	124.40
36	b	812	CLA	C3B-C4B-NB	-2.32	108.46	110.53
36	G	307	CLA	CHD-C4C-C3C	-2.32	121.39	124.77
35	M	302	A86	C23-C16-C22	-2.32	104.00	107.37
36	A	306	CLA	C1D-ND-C4D	-2.32	104.68	106.31
37	J	314	KC1	CHD-C1D-C2D	2.32	134.16	127.43
35	O	302	A86	C25-C24-C1	-2.32	120.00	126.36
36	R	314	CLA	C3B-C4B-NB	-2.32	108.46	110.53
36	b	825	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
36	U	308	CLA	C1-C2-C3	-2.32	122.40	126.20
35	F	306	A86	C10-C9-C8	-2.32	116.48	123.20
36	E	313	CLA	C3C-C4C-NC	2.32	113.40	110.43
34	G	303	DD6	C28-C27-C26	-2.32	119.68	124.18
35	J	303	A86	C9-C10-C11	-2.32	120.08	126.64
36	N	310	CLA	CHC-C1C-NC	2.32	127.80	124.31
36	D	308	CLA	O2A-CGA-CBA	2.32	118.90	111.83
35	P	303	A86	C25-C24-C1	-2.32	120.01	126.36
34	K	305	DD6	C25-C26-C27	-2.32	120.13	126.61
37	P	317	KC1	CBB-CAB-C3B	-2.32	115.95	127.53
37	L	317	KC1	C1C-C2C-C3C	-2.32	104.54	106.98
36	l	204	CLA	C3D-C4D-ND	2.32	113.75	109.99
36	l	202	CLA	O1D-CGD-CBD	2.32	129.09	124.52
36	b	807	CLA	CMB-C2B-C3B	2.32	132.00	126.55
36	F	309	CLA	CHB-C4A-NA	2.32	127.74	124.40
36	L	309	CLA	CHB-C4A-NA	2.32	127.74	124.40
35	X	303	A86	O-C13-C11	-2.32	116.05	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	b	845	BCR	C1-C6-C5	-2.32	119.47	122.64
35	L	319	A86	C25-C24-C1	-2.32	120.01	126.36
35	T	304	A86	C10-C9-C8	-2.32	116.49	123.20
35	S	304	A86	C26-C25-C24	-2.32	116.49	123.20
36	a	824	CLA	CHB-C4A-NA	2.31	127.74	124.40
35	T	306	A86	C25-C24-C1	-2.31	120.02	126.36
34	A	303	DD6	C28-C27-C26	-2.31	119.69	124.18
35	F	306	A86	O1-C15-C20	-2.31	57.49	59.45
36	W	206	CLA	CMB-C2B-C3B	2.31	131.99	126.55
37	G	308	KC1	CAC-C3C-C4C	2.31	127.80	124.79
34	R	308	DD6	C37-C36-C31	-2.31	119.83	124.16
36	a	816	CLA	C3D-C4D-ND	2.31	113.75	109.99
37	P	317	KC1	C1C-C2C-C3C	-2.31	104.55	106.98
36	I	310	CLA	C3B-C4B-NB	-2.31	108.47	110.53
36	b	828	CLA	C3B-C4B-NB	-2.31	108.47	110.53
36	H	307	CLA	CHC-C1C-NC	2.31	127.79	124.31
36	G	319	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
36	W	216	CLA	O1A-CGA-CBA	2.31	130.42	123.09
36	E	313	CLA	CHD-C1D-ND	-2.31	121.55	124.80
37	K	314	KC1	CMA-C3A-C2A	-2.31	122.83	128.43
34	K	305	DD6	C28-C27-C26	-2.31	119.69	124.18
35	A	316	A86	C41-C32-C31	-2.31	108.41	110.47
36	H	312	CLA	C4-C3-C5	2.31	119.24	115.23
36	a	826	CLA	CMB-C2B-C3B	2.31	131.98	126.55
36	b	833	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
36	F	311	CLA	C3A-C2A-C1A	2.31	104.80	101.34
35	S	308	A86	C9-C10-C11	-2.31	120.12	126.64
36	P	309	CLA	CMB-C2B-C3B	2.31	131.98	126.55
35	P	307	A86	O4-C38-O5	-2.31	118.54	122.99
36	K	308	CLA	CMB-C2B-C3B	2.31	131.98	126.55
36	b	810	CLA	C3B-C4B-NB	-2.31	108.47	110.53
35	J	305	A86	C41-C32-C31	-2.31	108.41	110.47
44	i	101	BCR	C28-C27-C26	-2.31	109.94	114.06
36	Q	306	CLA	CMB-C2B-C3B	2.31	131.97	126.55
44	m	101	BCR	C15-C16-C17	-2.31	118.80	123.52
36	L	316	CLA	O2D-CGD-CBD	2.31	115.26	111.23
34	L	305	DD6	O1-C20-C19	2.31	115.65	113.49
36	a	817	CLA	C2A-C1A-CHA	2.31	127.87	123.87
36	K	309	CLA	CHB-C4A-NA	2.31	127.73	124.40
36	S	314	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
36	E	308	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
35	V	302	A86	C36-C31-C32	-2.30	117.41	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	M	317	KC1	C1D-CHD-C4C	-2.30	120.83	126.25
36	D	307	CLA	C3B-C4B-NB	-2.30	108.47	110.53
36	h	203	CLA	C3B-C4B-NB	-2.30	108.47	110.53
34	D	303	DD6	C21-C20-C15	-2.30	118.51	122.30
35	O	305	A86	C21-C20-C15	2.30	130.79	123.35
42	L	321	LMG	C8-O7-C10	-2.30	112.28	117.80
36	R	311	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	W	218	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	b	819	CLA	CHD-C1D-C2D	2.30	130.28	125.49
36	A	310	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	C	212	CLA	CMB-C2B-C3B	2.30	131.97	126.55
36	E	310	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	E	311	CLA	CHB-C4A-NA	2.30	127.72	124.40
44	a	845	BCR	C24-C23-C22	-2.30	122.83	126.23
35	W	203	A86	C36-C31-C32	-2.30	117.41	119.70
35	F	301	A86	O4-C38-O5	-2.30	118.55	122.99
36	a	810	CLA	C1-O2A-CGA	2.30	122.22	116.65
35	R	302	A86	C4-C3-C2	-2.30	118.81	123.52
36	b	808	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
36	L	313	CLA	C3B-C4B-NB	-2.30	108.48	110.53
36	Q	314	CLA	CHB-C1B-NB	2.30	127.50	124.05
36	a	813	CLA	CHC-C4B-NB	2.30	127.50	124.05
34	S	307	DD6	C37-C36-C31	-2.30	119.86	124.16
44	l	207	BCR	C29-C30-C25	2.30	113.78	110.44
36	J	311	CLA	CHA-C1A-NA	-2.30	121.19	126.39
35	P	306	A86	C26-C25-C24	-2.30	116.54	123.20
36	a	832	CLA	C3A-C2A-C1A	2.30	104.78	101.34
36	R	321	CLA	C3B-C4B-NB	-2.30	108.48	110.53
35	Q	316	A86	O1-C20-C21	-2.30	112.48	115.05
34	B	304	DD6	C21-C20-C15	-2.30	118.52	122.30
35	U	304	A86	C-C1-C2	-2.30	119.09	122.82
36	B	309	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
36	a	817	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
34	J	304	DD6	C37-C36-C35	2.30	118.64	114.42
36	b	806	CLA	CAC-C3C-C4C	2.30	127.78	124.79
36	j	101	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
35	Q	301	A86	C33-C32-C31	2.30	111.44	109.21
34	A	303	DD6	C37-C36-C35	2.30	118.64	114.42
35	N	305	A86	O1-C20-C21	-2.30	112.48	115.05
35	K	306	A86	C21-C20-C19	2.30	116.82	114.24
34	E	303	DD6	C9-C8-C6	-2.30	120.07	126.36
36	X	308	CLA	C2A-C3A-C4A	-2.29	98.16	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	X	301	A86	O-C13-C11	-2.29	116.10	121.04
37	G	317	KC1	CHD-C1D-C2D	2.29	134.09	127.43
36	K	310	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
35	T	305	A86	C25-C24-C1	-2.29	120.07	126.36
35	R	301	A86	C9-C8-C6	-2.29	120.08	126.36
35	M	305	A86	C40-C32-C31	-2.29	108.42	110.47
36	G	313	CLA	CMB-C2B-C3B	2.29	131.94	126.55
35	K	303	A86	C9-C10-C11	-2.29	120.16	126.64
36	F	310	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
36	Q	314	CLA	CHB-C4A-NA	2.29	127.71	124.40
36	b	815	CLA	CHB-C4A-NA	2.29	127.71	124.40
35	L	307	A86	C3-C4-C5	-2.29	118.83	123.52
36	l	205	CLA	C2C-C1C-NC	2.29	112.39	109.98
35	F	302	A86	C40-C32-C31	-2.29	108.42	110.47
34	H	302	DD6	C10-C9-C8	-2.29	116.56	123.20
35	h	202	A86	O4-C38-O5	-2.29	118.57	122.99
36	R	316	CLA	CMC-C2C-C3C	2.29	132.34	126.15
36	J	310	CLA	CMB-C2B-C3B	2.29	131.93	126.55
36	I	311	CLA	C3B-C4B-NB	-2.29	108.49	110.53
42	h	206	LMG	C8-O7-C10	-2.29	112.32	117.80
36	V	314	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
41	j	104	LHG	C5-O7-C7	-2.29	112.32	117.80
41	G	301	LHG	C27-C26-C25	-2.29	102.80	114.37
36	R	312	CLA	CHB-C1B-NB	2.29	127.48	124.05
36	P	314	CLA	C4D-CHA-C1A	2.29	123.97	121.24
36	U	313	CLA	CHA-C1A-NA	-2.29	121.21	126.39
37	M	313	KC1	C1D-CHD-C4C	-2.29	120.87	126.25
36	B	305	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
36	L	313	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
41	a	842	LHG	C11-C10-C9	-2.29	102.81	114.37
44	f	806	BCR	C40-C30-C25	2.29	113.83	110.24
36	L	309	CLA	CMB-C2B-C3B	2.29	131.93	126.55
35	U	303	A86	C9-C10-C11	-2.29	120.18	126.64
36	H	312	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
36	S	309	CLA	CHB-C4A-NA	2.28	127.70	124.40
36	D	313	CLA	C3A-C2A-C1A	2.28	104.76	101.34
36	R	319	CLA	CAC-C3C-C4C	-2.28	121.82	124.79
36	O	307	CLA	CMB-C2B-C3B	2.28	131.92	126.55
36	l	205	CLA	C3A-C2A-C1A	2.28	104.76	101.34
36	f	804	CLA	CHD-C1D-C2D	2.28	130.24	125.49
36	H	307	CLA	CHD-C4C-C3C	2.28	128.10	124.77
36	K	311	CLA	C2A-C1A-CHA	2.28	127.83	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	810	CLA	O2D-CGD-CBD	2.28	115.22	111.23
36	U	310	CLA	CMC-C2C-C3C	2.28	132.32	126.15
35	X	314	A86	C4-C3-C2	-2.28	118.85	123.52
36	a	828	CLA	C3B-C4B-NB	-2.28	108.49	110.53
41	G	301	LHG	C20-C19-C18	-2.28	102.83	114.37
35	K	303	A86	C3-C2-C1	-2.28	124.08	127.28
35	W	203	A86	C41-C32-C31	2.28	112.51	110.47
37	G	317	KC1	C3A-C4A-NA	2.28	113.27	110.45
36	b	813	CLA	CAB-C3B-C2B	2.28	129.59	123.53
37	G	308	KC1	CAD-C3D-C2D	-2.28	139.46	144.26
36	V	308	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
36	N	315	CLA	CHB-C1B-C2B	-2.28	120.81	127.43
35	O	301	A86	C41-C32-C31	-2.28	108.43	110.47
35	I	301	A86	O1-C15-C20	-2.28	57.52	59.45
36	a	804	CLA	CAA-CBA-CGA	-2.28	106.74	113.21
35	T	302	A86	C23-C16-C17	-2.28	104.97	108.97
35	S	303	A86	C36-C31-C32	-2.28	117.44	119.70
42	V	316	LMG	C8-O7-C10	-2.28	112.35	117.80
36	b	822	CLA	O1D-CGD-CBD	2.28	129.01	124.52
38	b	804	SQD	O9-S-C6	2.28	110.15	106.76
36	N	315	CLA	CHB-C1B-NB	2.28	127.46	124.05
36	C	212	CLA	CAC-C3C-C2C	-2.28	123.38	127.56
36	V	314	CLA	C2B-C1B-NB	2.28	112.69	110.33
36	a	825	CLA	CHB-C4A-NA	2.28	127.68	124.40
36	b	841	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
35	G	306	A86	O1-C15-C20	-2.28	57.52	59.45
36	C	208	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
36	b	815	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
36	C	207	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
36	Q	310	CLA	C4D-CHA-C1A	2.27	123.96	121.24
36	F	316	CLA	CMA-C3A-C2A	-2.27	111.02	116.23
35	T	301	A86	O4-C38-O5	-2.27	118.60	122.99
36	D	316	CLA	C3B-C4B-NB	-2.27	108.50	110.53
35	O	303	A86	C33-C32-C31	2.27	111.42	109.21
34	D	305	DD6	C28-C27-C26	-2.27	119.77	124.18
34	S	306	DD6	C37-C36-C35	2.27	118.60	114.42
34	R	308	DD6	O1-C20-C21	-2.27	112.51	115.05
37	N	314	KC1	CED-O2D-CGD	2.27	121.07	115.92
36	F	317	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
36	H	308	CLA	C1-C2-C3	-2.27	122.47	126.20
37	L	317	KC1	O1D-CGD-CBD	-2.27	120.03	124.52
44	a	847	BCR	C2-C1-C6	2.27	113.74	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	304	A86	O4-C38-O5	-2.27	118.60	122.99
36	a	832	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
35	I	301	A86	C9-C10-C11	-2.27	120.22	126.64
37	V	312	KC1	CAA-CBA-CGA	-2.27	115.50	127.05
35	h	204	A86	C34-O4-C38	-2.27	113.83	117.85
35	P	304	A86	C33-C32-C31	2.27	111.42	109.21
36	U	313	CLA	CAA-C2A-C1A	2.27	117.42	111.81
35	O	301	A86	O1-C15-C20	-2.27	57.53	59.45
36	U	310	CLA	CBC-CAC-C3C	2.27	118.57	112.42
36	P	319	CLA	O2D-CGD-CBD	2.27	115.20	111.23
36	a	828	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
34	J	304	DD6	C28-C27-C26	-2.27	119.78	124.18
40	C	215	DGD	C2G-O2G-C1B	-2.27	112.37	117.80
36	B	311	CLA	CBC-CAC-C3C	2.27	118.57	112.42
36	b	819	CLA	CHD-C1D-ND	-2.27	121.61	124.80
35	X	303	A86	C4-C3-C2	-2.27	118.88	123.52
36	G	311	CLA	C2D-C1D-ND	-2.27	107.88	110.13
36	D	315	CLA	C3B-C4B-NB	-2.27	108.51	110.53
36	K	310	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
34	H	303	DD6	C25-C26-C27	-2.27	120.27	126.61
36	E	315	CLA	CHB-C1B-C2B	-2.27	120.85	127.43
37	F	308	KC1	CAB-C3B-C2B	2.27	135.80	128.43
35	X	301	A86	O-C13-C14	-2.27	117.12	121.76
34	B	304	DD6	C9-C8-C6	-2.27	120.15	126.36
35	E	302	A86	C9-C8-C6	-2.27	120.15	126.36
36	a	801	CLA	CHA-C4D-ND	2.27	137.22	132.55
36	X	308	CLA	CHB-C4A-NA	2.27	127.67	124.40
44	h	201	BCR	C16-C15-C14	-2.26	118.89	123.52
34	S	306	DD6	C25-C24-C1	-2.26	120.15	126.36
34	D	304	DD6	C25-C26-C27	-2.26	120.28	126.61
36	R	319	CLA	C3B-C4B-NB	-2.26	108.51	110.53
36	O	312	CLA	C4D-CHA-C1A	2.26	123.94	121.24
36	X	313	CLA	C3A-C2A-C1A	2.26	104.73	101.34
36	W	215	CLA	CHA-C1A-NA	-2.26	121.27	126.39
36	C	209	CLA	CHB-C4A-NA	2.26	127.67	124.40
34	a	849	DD6	C37-C36-C35	2.26	118.58	114.42
34	S	306	DD6	C28-C27-C26	-2.26	119.79	124.18
36	D	308	CLA	CHB-C4A-NA	2.26	127.66	124.40
36	H	307	CLA	CMB-C2B-C3B	2.26	131.87	126.55
36	V	314	CLA	CHB-C1B-NB	2.26	127.44	124.05
34	M	303	DD6	C28-C27-C26	-2.26	119.79	124.18
36	l	204	CLA	CHB-C4A-NA	2.26	127.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	A	306	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
36	N	317	CLA	CHA-C1A-NA	-2.26	121.28	126.39
36	a	841	CLA	CAA-CBA-CGA	-2.26	106.79	113.21
36	A	306	CLA	C3D-C4D-ND	2.26	113.66	109.99
37	S	316	KC1	C1C-C2C-C3C	-2.26	104.61	106.98
36	b	841	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
34	D	303	DD6	C37-C36-C31	-2.26	119.94	124.16
36	T	311	CLA	CHD-C1D-ND	-2.26	121.62	124.80
36	j	101	CLA	CHB-C4A-NA	2.26	127.66	124.40
36	b	821	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
36	D	307	CLA	C4-C3-C5	2.26	119.15	115.23
36	G	319	CLA	C5-C3-C4	2.26	119.78	114.59
36	E	314	CLA	C3B-C4B-NB	-2.26	108.52	110.53
36	W	210	CLA	C3B-C4B-NB	-2.26	108.52	110.53
34	A	301	DD6	C21-C20-C15	-2.26	118.59	122.30
36	b	812	CLA	C2D-C1D-ND	-2.26	107.89	110.13
36	A	307	CLA	O2D-CGD-CBD	2.25	115.17	111.23
35	S	308	A86	C41-C32-C31	-2.25	108.45	110.47
35	K	306	A86	C9-C10-C11	-2.25	120.27	126.64
35	I	302	A86	C36-C31-C32	-2.25	117.46	119.70
35	X	302	A86	C36-C31-C32	-2.25	117.46	119.70
36	U	308	CLA	C3A-C2A-C1A	2.25	104.72	101.34
36	O	311	CLA	C3B-C4B-NB	-2.25	108.52	110.53
36	a	824	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
36	M	310	CLA	C2B-C1B-NB	-2.25	107.99	110.33
36	N	318	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
36	a	839	CLA	O2D-CGD-CBD	2.25	115.17	111.23
35	J	306	A86	C3-C4-C5	-2.25	118.91	123.52
36	P	314	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
35	X	314	A86	C33-C32-C31	-2.25	107.02	109.21
35	S	301	A86	C9-C8-C6	-2.25	120.19	126.36
36	b	835	CLA	O2A-CGA-O1A	-2.25	117.54	123.33
35	M	304	A86	C40-C32-C31	-2.25	108.46	110.47
35	L	304	A86	C10-C9-C8	-2.25	116.68	123.20
34	P	305	DD6	O1-C15-C14	-2.25	110.43	116.88
35	R	302	A86	O4-C34-C35	-2.25	101.88	107.64
36	A	310	CLA	C3B-C4B-NB	-2.25	108.52	110.53
36	a	829	CLA	O2D-CGD-CBD	2.25	115.16	111.23
35	N	306	A86	C25-C24-C1	-2.25	120.19	126.36
35	U	303	A86	C12-C11-C13	2.25	119.65	116.00
35	N	301	A86	C9-C8-C6	-2.25	120.19	126.36
35	C	203	A86	C36-C31-C32	-2.25	117.46	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	I	309	CLA	CBC-CAC-C3C	2.25	118.52	112.42
36	A	308	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
36	b	809	CLA	CHB-C4A-NA	2.25	127.64	124.40
44	j	107	BCR	C1-C6-C5	-2.25	119.56	122.64
44	h	201	BCR	C40-C30-C39	-2.25	102.19	108.63
36	T	314	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
35	N	302	A86	C3-C2-C1	-2.25	124.12	127.28
36	O	309	CLA	C1-C2-C3	-2.25	122.51	126.20
35	J	305	A86	O1-C15-C20	-2.25	57.55	59.45
34	R	307	DD6	C28-C27-C26	-2.25	119.82	124.18
36	V	306	CLA	CAA-C2A-C3A	-2.25	106.93	113.00
44	b	847	BCR	C2-C3-C4	2.25	116.22	111.28
37	P	317	KC1	CMB-C2B-C1B	2.25	128.69	124.73
35	U	303	A86	C9-C8-C6	-2.25	120.20	126.36
35	N	303	A86	C36-C31-C32	-2.25	117.47	119.70
36	H	315	CLA	CAC-C3C-C2C	2.25	131.68	127.56
35	T	302	A86	C9-C8-C6	-2.25	120.21	126.36
35	R	304	A86	O-C13-C11	-2.25	116.21	121.04
36	a	806	CLA	CMB-C2B-C1B	2.24	128.84	125.42
36	W	218	CLA	CMC-C2C-C1C	-2.24	121.53	125.03
36	P	311	CLA	C1-C2-C3	-2.24	122.52	126.20
44	l	207	BCR	C24-C23-C22	-2.24	122.92	126.23
36	a	837	CLA	O2D-CGD-CBD	2.24	115.15	111.23
36	C	209	CLA	O2D-CGD-CBD	2.24	115.15	111.23
36	W	211	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
35	P	304	A86	C12-C11-C13	2.24	119.64	116.00
36	D	309	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
41	a	850	LHG	C5-O7-C7	-2.24	112.43	117.80
35	M	301	A86	C33-C32-C31	-2.24	107.03	109.21
36	a	826	CLA	C6-C5-C3	2.24	118.93	113.47
35	P	307	A86	O1-C15-C20	-2.24	57.55	59.45
36	i	102	CLA	C3B-C4B-NB	-2.24	108.53	110.53
36	G	319	CLA	CMC-C2C-C1C	2.24	128.53	125.03
35	I	302	A86	C3-C4-C5	-2.24	118.94	123.52
36	S	309	CLA	O2D-CGD-CBD	2.24	115.14	111.23
35	M	305	A86	C3-C4-C5	-2.24	118.94	123.52
35	S	308	A86	O4-C38-O5	-2.24	118.67	122.99
35	T	306	A86	C7-C6-C8	2.24	121.51	118.09
35	I	302	A86	C9-C10-C11	-2.24	120.31	126.64
35	I	301	A86	C12-C11-C13	2.24	119.63	116.00
35	X	301	A86	C3-C4-C5	-2.24	118.94	123.52
36	N	308	CLA	CAA-C2A-C3A	-2.24	106.95	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	R	314	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
34	E	301	DD6	C21-C20-C15	-2.24	118.62	122.30
36	L	320	CLA	C3B-C4B-NB	-2.24	108.53	110.53
41	F	318	LHG	C18-C17-C16	-2.24	103.06	114.37
36	S	310	CLA	C3A-C2A-C1A	2.24	104.69	101.34
36	N	311	CLA	CBA-CAA-C2A	-2.24	107.14	113.79
36	a	818	CLA	CHC-C1C-NC	2.24	127.68	124.31
36	j	102	CLA	C3A-C2A-C1A	2.24	104.69	101.34
34	B	304	DD6	C15-C14-C13	-2.24	121.27	125.99
34	H	302	DD6	C28-C27-C26	-2.23	119.84	124.18
35	P	306	A86	C41-C32-C31	-2.23	108.47	110.47
36	S	309	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
36	C	210	CLA	CAA-C2A-C1A	2.23	119.29	111.97
44	j	107	BCR	C24-C23-C22	-2.23	122.93	126.23
36	B	311	CLA	CHA-C4D-ND	2.23	137.16	132.55
35	O	303	A86	C12-C11-C13	2.23	119.62	116.00
36	l	201	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
36	a	818	CLA	C3B-C4B-NB	-2.23	108.54	110.53
36	a	817	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
37	X	311	KC1	C4D-CHA-C1A	-2.23	115.65	122.45
35	T	307	A86	C23-C16-C22	-2.23	104.13	107.37
34	Q	302	DD6	C9-C8-C6	-2.23	120.25	126.36
36	H	315	CLA	CAA-CBA-CGA	-2.23	106.87	113.21
36	I	305	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
36	f	802	CLA	C2A-C1A-CHA	2.23	127.74	123.87
37	W	217	KC1	C4D-CHA-C1A	-2.23	115.66	122.45
35	Q	301	A86	C12-C11-C13	2.23	119.62	116.00
35	L	301	A86	C9-C10-C11	-2.23	120.33	126.64
36	a	838	CLA	CMD-C2D-C3D	2.23	132.80	127.69
36	b	831	CLA	CHB-C4A-NA	2.23	127.62	124.40
36	b	806	CLA	CHC-C1C-NC	2.23	127.67	124.31
35	F	305	A86	O4-C38-O5	-2.23	118.69	122.99
35	M	305	A86	C9-C8-C6	-2.23	120.25	126.36
35	S	302	A86	C3-C2-C1	-2.23	124.15	127.28
36	D	316	CLA	CHD-C4C-C3C	2.23	128.02	124.77
36	T	311	CLA	C1-C2-C3	-2.23	122.55	126.20
36	N	319	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
36	b	805	CLA	CHA-C1A-NA	-2.23	121.35	126.39
37	F	315	KC1	C1D-CHD-C4C	-2.23	121.01	126.25
35	J	306	A86	C26-C25-C24	-2.23	116.75	123.20
36	Q	314	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
36	b	832	CLA	O2A-CGA-O1A	-2.23	118.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	812	CLA	CMB-C2B-C3B	2.23	131.79	126.55
36	X	307	CLA	C2A-C1A-CHA	2.23	127.73	123.87
36	H	308	CLA	CHB-C4A-NA	2.23	127.61	124.40
42	m	102	LMG	C8-O7-C10	-2.23	112.47	117.80
36	J	313	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
36	b	824	CLA	CMB-C2B-C1B	2.23	128.81	125.42
36	C	207	CLA	CMC-C2C-C1C	2.23	128.51	125.03
36	P	301	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
36	C	206	CLA	C3B-C4B-NB	-2.22	108.54	110.53
34	S	307	DD6	C10-C9-C8	-2.22	116.75	123.20
36	P	302	CLA	CBA-CAA-C2A	-2.22	108.69	113.41
36	H	310	CLA	CMD-C2D-C3D	2.22	132.79	127.69
34	a	849	DD6	C9-C8-C6	-2.22	120.27	126.36
36	R	322	CLA	CHB-C4A-NA	2.22	127.61	124.40
35	S	304	A86	C35-C34-C33	-2.22	105.89	109.89
36	a	841	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
35	E	305	A86	C26-C25-C24	-2.22	116.76	123.20
36	V	314	CLA	CHD-C4C-C3C	-2.22	121.53	124.77
36	b	820	CLA	CHB-C4A-NA	2.22	127.61	124.40
36	V	313	CLA	CHB-C4A-NA	2.22	127.61	124.40
44	f	806	BCR	C30-C25-C26	-2.22	119.60	122.64
36	S	319	CLA	CHA-C1A-NA	-2.22	121.36	126.39
44	a	845	BCR	C1-C6-C5	-2.22	119.60	122.64
34	P	305	DD6	C9-C8-C6	-2.22	120.27	126.36
36	b	824	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
36	L	311	CLA	O2D-CGD-CBD	2.22	115.11	111.23
36	S	312	CLA	CHB-C1B-NB	2.22	127.38	124.05
35	T	306	A86	C4-C3-C2	-2.22	118.97	123.52
35	W	203	A86	C3-C4-C5	-2.22	118.97	123.52
37	G	317	KC1	CAD-C3D-C2D	-2.22	139.59	144.26
36	b	813	CLA	CMB-C2B-C3B	2.22	129.43	123.53
36	b	805	CLA	C6-C5-C3	2.22	118.88	113.47
36	b	801	CLA	CAA-CBA-CGA	-2.22	106.91	113.21
35	K	303	A86	C40-C32-C31	2.22	112.46	110.47
36	b	809	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
35	B	303	A86	C41-C32-C40	2.22	114.98	108.63
35	F	304	A86	C3-C4-C5	-2.22	118.98	123.52
36	A	313	CLA	O1D-CGD-CBD	2.22	128.89	124.52
35	N	302	A86	C26-C25-C24	-2.22	116.77	123.20
36	S	311	CLA	CHA-C4D-ND	2.22	137.12	132.55
36	R	312	CLA	CED-O2D-CGD	-2.22	110.88	115.92
35	X	304	A86	C21-C20-C19	-2.22	111.75	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	303	A86	C9-C10-C11	-2.22	120.37	126.64
36	b	827	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
36	N	308	CLA	CHC-C1C-C2C	2.22	133.25	126.95
36	P	313	CLA	C3B-C4B-NB	-2.22	108.55	110.53
36	R	310	CLA	CHB-C4A-NA	2.22	127.60	124.40
35	H	304	A86	C9-C8-C6	-2.22	120.28	126.36
42	J	319	LMG	C8-O7-C10	-2.22	112.49	117.80
35	J	301	A86	C19-C18-C17	-2.22	106.65	110.79
36	a	807	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
35	J	305	A86	C19-C18-C17	-2.22	106.65	110.79
44	f	801	BCR	C40-C30-C25	2.21	113.72	110.24
34	G	303	DD6	C10-C9-C8	-2.21	116.78	123.20
36	E	315	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
35	F	307	A86	C7-C6-C8	2.21	121.47	118.09
36	B	305	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
44	i	103	BCR	C15-C14-C13	-2.21	124.17	127.28
35	N	305	A86	C28-C27-C26	-2.21	119.23	122.82
36	C	207	CLA	C3D-C4D-ND	2.21	113.58	109.99
36	I	312	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
35	T	301	A86	C9-C10-C11	-2.21	120.39	126.64
36	W	212	CLA	CHB-C1B-NB	2.21	127.37	124.05
35	G	305	A86	C33-C32-C31	2.21	111.36	109.21
36	N	315	CLA	CHA-C1A-NA	-2.21	121.38	126.39
44	i	103	BCR	C27-C26-C25	2.21	125.69	122.70
36	a	837	CLA	C2A-C1A-CHA	2.21	127.70	123.87
34	E	301	DD6	C37-C36-C35	2.21	118.48	114.42
36	D	307	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
44	b	846	BCR	C29-C30-C25	2.21	113.65	110.44
35	G	306	A86	C19-C18-C17	-2.21	106.66	110.79
36	B	311	CLA	C2D-C1D-ND	-2.21	107.94	110.13
37	T	315	KC1	C1A-NA-C4A	2.21	107.69	106.68
35	E	307	A86	O4-C38-O5	-2.21	118.73	122.99
36	b	806	CLA	C3C-C4C-NC	-2.21	107.60	110.43
36	T	308	CLA	C3B-C4B-NB	-2.21	108.56	110.53
36	a	802	CLA	C3B-C4B-NB	-2.21	108.56	110.53
37	S	316	KC1	O2D-CGD-O1D	-2.21	119.55	123.85
34	L	305	DD6	C28-C27-C26	-2.21	119.89	124.18
44	b	843	BCR	C30-C25-C26	-2.21	119.62	122.64
44	l	207	BCR	C28-C27-C26	-2.21	110.12	114.06
35	W	203	A86	C25-C24-C1	-2.21	120.31	126.36
36	E	313	CLA	CED-O2D-CGD	2.21	120.92	115.92
35	F	305	A86	C33-C32-C31	2.21	111.36	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Q	308	CLA	C1-C2-C3	-2.21	122.58	126.20
36	b	841	CLA	C2A-C1A-CHA	2.21	127.70	123.87
36	W	211	CLA	C3B-C4B-NB	-2.21	108.56	110.53
35	A	316	A86	O1-C15-C20	-2.21	57.58	59.45
34	K	304	DD6	C37-C36-C31	-2.21	120.03	124.16
36	a	816	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
35	S	302	A86	C26-C25-C24	-2.21	116.81	123.20
35	S	305	A86	C9-C8-C6	-2.21	120.31	126.36
36	T	311	CLA	C2C-C1C-NC	-2.21	107.67	109.98
35	E	305	A86	O1-C15-C20	-2.21	57.58	59.45
36	G	311	CLA	C4-C3-C5	2.21	119.06	115.23
35	L	319	A86	C33-C32-C31	-2.20	107.07	109.21
37	J	314	KC1	O2D-CGD-O1D	-2.20	119.56	123.85
36	H	317	CLA	CAC-C3C-C4C	2.20	127.66	124.79
35	F	305	A86	O-C13-C14	-2.20	117.24	121.76
37	H	313	KC1	CMD-C2D-C1D	-2.20	122.06	125.42
36	D	313	CLA	CBA-CAA-C2A	2.20	120.35	113.79
35	F	304	A86	C26-C25-C24	-2.20	116.82	123.20
36	J	315	CLA	CMA-C3A-C2A	-2.20	111.18	116.23
36	S	318	CLA	C2A-C1A-CHA	2.20	127.69	123.87
36	X	307	CLA	CHB-C4A-NA	2.20	127.58	124.40
35	P	307	A86	C3-C4-C5	-2.20	119.01	123.52
34	J	304	DD6	C25-C26-C27	-2.20	120.45	126.61
35	P	304	A86	C3-C4-C5	-2.20	119.01	123.52
35	Q	316	A86	C28-C27-C26	-2.20	119.25	122.82
44	f	806	BCR	C38-C26-C27	-2.20	108.90	113.60
35	L	304	A86	C9-C10-C11	-2.20	120.42	126.64
36	f	804	CLA	C2A-C3A-C4A	2.20	105.42	101.87
37	P	317	KC1	CBC-CAC-C3C	-2.20	106.45	112.42
36	B	307	CLA	CHA-C1A-NA	-2.20	121.41	126.39
36	R	321	CLA	C1-C2-C3	-2.20	122.59	126.20
36	b	827	CLA	CHA-C4D-ND	2.20	137.09	132.55
36	W	218	CLA	O1D-CGD-CBD	2.20	128.86	124.52
36	V	309	CLA	CHA-C1A-NA	-2.20	121.41	126.39
35	N	303	A86	C34-O4-C38	2.20	121.73	117.85
36	a	803	CLA	O2D-CGD-CBD	2.20	115.07	111.23
36	b	806	CLA	C1-C2-C3	-2.20	122.59	126.20
37	J	314	KC1	C1C-C2C-C3C	-2.20	104.67	106.98
36	U	306	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
36	b	816	CLA	CHB-C4A-NA	2.20	127.57	124.40
37	P	317	KC1	C4B-C3B-C2B	-2.20	104.91	106.81
35	S	304	A86	C21-C20-C15	2.20	130.45	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	303	DD6	C25-C24-C1	-2.20	120.34	126.36
37	T	315	KC1	C2B-C1B-NB	2.20	112.30	110.13
35	R	301	A86	C4-C3-C2	-2.20	119.02	123.52
36	W	212	CLA	CHD-C1D-C2D	2.20	130.06	125.49
36	N	313	CLA	C4D-CHA-C1A	2.20	123.86	121.24
36	J	312	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
36	P	316	CLA	C3B-C4B-NB	-2.20	108.57	110.53
36	E	310	CLA	CAA-C2A-C3A	-2.20	107.07	113.00
35	N	306	A86	C4-C3-C2	-2.19	119.03	123.52
35	O	303	A86	C3-C4-C5	-2.19	119.03	123.52
36	L	308	CLA	CMB-C2B-C3B	2.19	131.71	126.55
35	L	304	A86	C29-C30-C31	-2.19	175.07	177.66
35	U	304	A86	O1-C15-C20	-2.19	57.59	59.45
35	W	202	A86	C19-C18-C17	-2.19	106.69	110.79
35	M	304	A86	C7-C6-C5	-2.19	119.27	122.82
35	E	307	A86	C19-C18-C17	-2.19	106.69	110.79
34	P	305	DD6	C25-C26-C27	-2.19	120.48	126.61
36	K	312	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
36	U	309	CLA	CHA-C1A-NA	-2.19	121.43	126.39
35	C	204	A86	C9-C8-C6	-2.19	120.36	126.36
42	j	105	LMG	C8-O7-C10	-2.19	112.56	117.80
34	A	303	DD6	C25-C26-C27	-2.19	120.49	126.61
36	b	807	CLA	O2A-CGA-O1A	-2.19	117.70	123.33
35	V	302	A86	O2-C18-C17	-2.19	105.27	109.75
36	N	319	CLA	C3A-C2A-C1A	2.19	104.62	101.34
36	J	311	CLA	C2A-C1A-CHA	2.19	127.67	123.87
36	V	306	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
35	E	305	A86	C19-C18-C17	-2.19	106.70	110.79
36	b	827	CLA	CHB-C1B-NB	2.19	127.33	124.05
35	A	316	A86	C26-C25-C24	-2.19	116.86	123.20
36	T	308	CLA	CAC-C3C-C2C	-2.19	123.54	127.56
35	A	316	A86	C9-C8-C6	-2.19	120.36	126.36
36	D	309	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
36	X	313	CLA	C2A-C3A-C4A	2.19	105.40	101.87
35	P	303	A86	C33-C32-C31	-2.19	107.09	109.21
36	a	824	CLA	CMC-C2C-C3C	2.19	132.06	126.15
35	F	304	A86	O1-C15-C20	-2.19	57.60	59.45
36	F	310	CLA	CAC-C3C-C4C	2.18	127.63	124.79
36	M	309	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
35	F	301	A86	C12-C11-C13	2.18	119.54	116.00
35	I	301	A86	C9-C8-C6	-2.18	120.37	126.36
35	N	306	A86	C9-C8-C6	-2.18	120.38	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	831	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
36	H	312	CLA	O1D-CGD-CBD	2.18	128.82	124.52
36	D	316	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
36	I	314	CLA	CHB-C4A-NA	2.18	127.55	124.40
36	b	819	CLA	C3C-C4C-NC	-2.18	107.63	110.43
35	U	302	A86	C3-C2-C1	-2.18	124.22	127.28
36	I	307	CLA	C2A-C1A-CHA	2.18	127.66	123.87
34	A	301	DD6	O1-C20-C19	-2.18	111.45	113.49
36	H	307	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
36	Q	312	CLA	C3B-C4B-NB	-2.18	108.58	110.53
35	E	307	A86	O1-C15-C20	-2.18	57.60	59.45
36	U	306	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
35	Q	301	A86	C3-C4-C5	-2.18	119.06	123.52
41	a	842	LHG	C27-C26-C25	-2.18	103.35	114.37
36	E	308	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
36	B	309	CLA	CHB-C4A-NA	2.18	127.55	124.40
37	M	318	KC1	CAB-C3B-C4B	2.18	130.02	124.82
36	X	307	CLA	CED-O2D-CGD	2.18	120.86	115.92
36	U	309	CLA	C3B-C4B-NB	-2.18	108.58	110.53
37	B	310	KC1	C1C-C2C-C3C	-2.18	104.69	106.98
36	T	313	CLA	CAC-C3C-C4C	2.18	127.62	124.79
44	b	847	BCR	C15-C16-C17	-2.18	119.06	123.52
36	J	316	CLA	C3B-C4B-NB	-2.18	108.59	110.53
35	S	303	A86	C34-O4-C38	2.18	121.69	117.85
36	E	313	CLA	CHB-C1B-NB	-2.18	120.78	124.05
36	J	307	CLA	C2A-C1A-CHA	2.18	127.64	123.87
34	E	301	DD6	C28-C27-C26	-2.18	119.96	124.18
36	j	102	CLA	C2A-C1A-CHA	2.18	127.64	123.87
36	G	313	CLA	C16-C15-C13	-2.18	108.73	115.97
35	P	304	A86	O1-C20-C21	-2.18	112.62	115.05
36	b	826	CLA	C2A-C1A-CHA	2.18	127.64	123.87
36	U	306	CLA	C2A-C3A-C4A	2.17	105.38	101.87
36	a	826	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
36	A	310	CLA	C1-C2-C3	-2.17	122.63	126.20
36	S	312	CLA	CHB-C4A-NA	2.17	127.54	124.40
34	E	306	DD6	C28-C27-C26	-2.17	119.96	124.18
36	F	311	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
36	Q	310	CLA	C4-C3-C5	-2.17	111.45	115.23
35	Q	316	A86	C25-C26-C27	-2.17	124.23	127.28
36	l	204	CLA	C1C-C2C-C3C	-2.17	104.69	106.98
37	K	314	KC1	CAA-CBA-CGA	-2.17	116.00	127.05
35	O	319	A86	C28-C27-C26	-2.17	119.30	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	K	305	DD6	C25-C24-C1	-2.17	120.41	126.36
35	N	304	A86	O-C13-C11	-2.17	116.36	121.04
36	H	310	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
34	W	205	DD6	C25-C24-C1	-2.17	120.41	126.36
37	M	313	KC1	CAD-C3D-C2D	-2.17	139.69	144.26
36	H	310	CLA	C3D-C2D-C1D	2.17	108.79	105.83
36	R	320	CLA	CHD-C1D-C2D	2.17	130.00	125.49
36	U	311	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
36	K	309	CLA	O1D-CGD-CBD	2.17	128.80	124.52
36	B	307	CLA	CAA-C2A-C1A	2.17	119.08	111.97
36	a	806	CLA	C3C-C4C-NC	2.17	113.21	110.43
36	b	819	CLA	C2A-C1A-CHA	2.17	127.63	123.87
34	W	204	DD6	C28-C27-C26	-2.17	119.97	124.18
37	P	317	KC1	CAA-CBA-CGA	-2.17	116.02	127.05
35	R	301	A86	C9-C10-C11	-2.17	120.51	126.64
36	V	305	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
36	a	828	CLA	O2D-CGD-CBD	2.17	115.02	111.23
44	i	103	BCR	C37-C22-C21	-2.17	119.30	122.82
35	O	305	A86	C26-C25-C24	-2.17	116.92	123.20
35	H	304	A86	C40-C32-C31	-2.17	108.53	110.47
36	H	308	CLA	CHA-C1A-NA	-2.17	121.48	126.39
36	b	805	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
36	P	318	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
36	L	309	CLA	O1D-CGD-CBD	2.17	128.79	124.52
35	N	304	A86	O4-C38-O5	-2.17	118.81	122.99
35	H	304	A86	C19-C18-C17	-2.17	106.74	110.79
36	H	312	CLA	CAA-C2A-C1A	2.17	119.07	111.97
37	T	310	KC1	C3B-C2B-C1B	-2.17	105.00	107.05
37	M	313	KC1	C2A-C1A-CHA	-2.17	120.07	128.96
36	a	822	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
36	S	310	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
36	B	308	CLA	CHD-C4C-NC	2.16	127.59	124.23
35	F	305	A86	C28-C27-C26	-2.16	119.31	122.82
36	b	839	CLA	O2D-CGD-CBD	2.16	115.01	111.23
34	D	303	DD6	C25-C26-C27	-2.16	120.56	126.61
37	W	213	KC1	C2A-C1A-NA	2.16	112.81	109.34
36	X	315	CLA	CHA-C1A-NA	-2.16	121.49	126.39
44	j	107	BCR	C30-C25-C26	-2.16	119.68	122.64
35	O	302	A86	C33-C32-C31	-2.16	107.11	109.21
35	X	305	A86	O4-C38-O5	-2.16	118.82	122.99
36	b	838	CLA	CHB-C4A-NA	2.16	127.52	124.40
35	S	304	A86	C3-C4-C5	-2.16	119.10	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	E	304	DD6	C28-C27-C26	-2.16	119.98	124.18
35	C	203	A86	O1-C15-C20	-2.16	57.62	59.45
34	B	302	DD6	C-C1-C2	-2.16	119.31	122.82
35	S	304	A86	O1-C20-C19	-2.16	111.47	113.49
36	a	818	CLA	C1-C2-C3	-2.16	122.66	126.20
36	b	840	CLA	O2D-CGD-CBD	2.16	115.01	111.23
36	E	316	CLA	CMC-C2C-C3C	2.16	131.99	126.15
36	V	311	CLA	C2A-C1A-CHA	2.16	127.61	123.87
36	S	310	CLA	CHB-C4A-NA	2.16	127.51	124.40
36	R	315	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
36	V	310	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
36	V	313	CLA	CHA-C1A-NA	-2.16	121.51	126.39
36	S	313	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
36	X	310	CLA	C2A-C1A-CHA	2.15	127.59	123.86
36	D	310	CLA	O2D-CGD-CBD	2.15	115.00	111.23
36	a	820	CLA	O2D-CGD-CBD	2.15	115.00	111.23
35	X	305	A86	C4-C3-C2	-2.15	119.11	123.52
36	L	311	CLA	CHB-C1B-NB	2.15	127.28	124.05
35	W	203	A86	C21-C20-C19	-2.15	111.82	114.24
35	Q	304	A86	C9-C8-C6	-2.15	120.46	126.36
41	l	208	LHG	C5-O7-C7	-2.15	112.64	117.80
36	G	310	CLA	CHB-C4A-NA	2.15	127.51	124.40
44	a	847	BCR	C31-C1-C6	2.15	113.62	110.24
35	J	305	A86	C9-C8-C6	-2.15	120.46	126.36
36	H	315	CLA	CHA-C1A-NA	-2.15	121.52	126.39
34	B	302	DD6	C37-C36-C31	-2.15	120.14	124.16
36	a	829	CLA	C3B-C4B-NB	-2.15	108.61	110.53
35	I	302	A86	C4-C3-C2	-2.15	119.12	123.52
36	P	311	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
36	b	802	CLA	CHB-C1B-NB	2.15	127.28	124.05
36	G	315	CLA	C3D-C4D-ND	2.15	113.48	109.99
36	J	310	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
36	T	314	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
44	b	847	BCR	C10-C11-C12	-2.15	116.97	123.20
35	I	304	A86	C25-C24-C1	-2.15	120.47	126.36
36	L	308	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
36	O	314	CLA	C3B-C4B-NB	-2.15	108.61	110.53
35	C	203	A86	C10-C9-C8	-2.15	116.97	123.20
36	C	207	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
34	B	304	DD6	C28-C27-C26	-2.15	120.01	124.18
36	W	210	CLA	C3A-C2A-C1A	2.15	104.56	101.34
34	S	307	DD6	C7-C6-C8	2.15	121.37	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Q	301	A86	O1-C20-C21	-2.15	112.65	115.05
36	L	308	CLA	C4B-CHC-C1C	2.15	131.30	126.25
35	O	303	A86	O1-C20-C21	-2.15	112.65	115.05
37	F	308	KC1	C2D-C1D-ND	-2.15	108.10	110.33
36	O	310	CLA	O2D-CGD-CBD	2.15	114.98	111.23
36	l	205	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
36	b	830	CLA	C6-C7-C8	-2.15	108.83	115.97
35	C	203	A86	C41-C32-C31	-2.15	108.55	110.47
36	U	311	CLA	CMD-C2D-C1D	-2.15	120.95	124.73
36	i	102	CLA	C2A-C1A-CHA	2.15	127.59	123.87
36	T	314	CLA	CMB-C2B-C3B	2.15	131.60	126.55
36	a	824	CLA	C16-C15-C13	-2.14	108.84	115.97
36	Q	309	CLA	O2D-CGD-CBD	2.14	114.98	111.23
36	K	310	CLA	CMC-C2C-C1C	2.14	128.38	125.03
37	M	313	KC1	C3A-C4A-NA	2.14	113.10	110.45
36	I	307	CLA	CAA-C2A-C3A	-2.14	107.20	113.00
36	I	306	CLA	C3B-C2B-C1B	-2.14	104.64	107.17
35	V	301	A86	C19-C18-C17	-2.14	106.78	110.79
36	Q	308	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
36	H	308	CLA	CMB-C2B-C3B	2.14	131.59	126.55
35	S	301	A86	C40-C32-C33	2.14	119.21	109.06
36	R	314	CLA	C3A-C2A-C1A	2.14	104.55	101.34
36	b	823	CLA	CMB-C2B-C3B	2.14	131.59	126.55
36	V	305	CLA	CHD-C1D-C2D	2.14	129.94	125.49
36	W	216	CLA	C2C-C1C-NC	2.14	112.23	109.98
36	R	319	CLA	C3A-C2A-C1A	2.14	104.55	101.34
37	D	314	KC1	O2D-CGD-O1D	-2.14	119.68	123.85
35	U	304	A86	C40-C32-C31	-2.14	108.56	110.47
34	A	304	DD6	C25-C24-C1	-2.14	120.49	126.36
36	D	306	CLA	C3B-C4B-NB	-2.14	108.62	110.53
36	a	836	CLA	C3A-C2A-C1A	2.14	104.55	101.34
35	W	203	A86	O1-C20-C19	-2.14	111.48	113.49
36	a	831	CLA	CHA-C1A-NA	-2.14	121.55	126.39
36	J	309	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
36	b	813	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
36	S	319	CLA	C2A-C1A-CHA	2.14	127.58	123.87
35	N	305	A86	C25-C26-C27	-2.14	124.28	127.28
36	R	312	CLA	C2A-C1A-CHA	2.14	127.58	123.87
36	C	210	CLA	CHA-C1A-NA	-2.14	121.55	126.39
36	G	311	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
36	S	320	CLA	C2A-C1A-CHA	2.14	127.58	123.87
35	J	301	A86	C9-C10-C11	-2.14	120.59	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	P	312	CLA	O2D-CGD-CBD	2.14	114.97	111.23
35	I	301	A86	C19-C18-C17	-2.14	106.79	110.79
36	N	310	CLA	C4D-C3D-CAD	2.14	110.43	108.11
37	T	315	KC1	CAA-CBA-CGA	-2.14	116.18	127.05
34	D	304	DD6	C25-C24-C1	-2.14	120.50	126.36
36	D	308	CLA	CMB-C2B-C3B	2.14	131.58	126.55
36	a	809	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
36	a	804	CLA	C1-C2-C3	2.14	129.70	126.20
35	X	314	A86	O1-C15-C20	-2.14	57.64	59.45
40	L	302	DGD	O2G-C1B-O1B	-2.14	118.71	123.70
36	G	309	CLA	C4D-CHA-C1A	-2.14	118.70	121.24
44	l	207	BCR	C31-C1-C6	2.14	113.59	110.24
35	N	301	A86	C40-C32-C33	2.14	119.18	109.06
35	F	307	A86	C21-C20-C19	-2.14	111.84	114.24
36	l	204	CLA	CHC-C1C-C2C	-2.14	120.88	126.95
35	G	305	A86	C40-C32-C31	-2.14	108.56	110.47
36	C	209	CLA	C3A-C2A-C1A	2.14	104.54	101.34
36	V	308	CLA	CMB-C2B-C3B	2.13	131.57	126.55
36	O	316	CLA	C2A-C3A-C4A	2.13	105.32	101.87
35	T	301	A86	C25-C24-C1	-2.13	120.51	126.36
36	b	832	CLA	O2D-CGD-CBD	2.13	114.96	111.23
35	B	301	A86	O1-C15-C20	-2.13	57.64	59.45
35	K	303	A86	C26-C25-C24	-2.13	117.02	123.20
34	P	305	DD6	C28-C27-C26	-2.13	120.04	124.18
36	K	308	CLA	CHB-C4A-NA	2.13	127.48	124.40
39	a	851	LMT	C1B-O1B-C4'	-2.13	112.92	117.98
35	D	302	A86	C19-C18-C17	-2.13	106.80	110.79
36	L	314	CLA	O2A-CGA-CBA	2.13	118.34	111.83
35	T	303	A86	C9-C8-C6	-2.13	120.52	126.36
35	T	302	A86	C33-C32-C31	-2.13	107.14	109.21
36	A	307	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
36	a	829	CLA	CHB-C4A-NA	2.13	127.48	124.40
40	b	849	DGD	O3D-C3D-C4D	-2.13	105.35	110.38
36	a	848	CLA	C4-C3-C2	-2.13	118.16	123.63
37	G	318	KC1	C2D-C1D-ND	-2.13	108.12	110.33
36	P	312	CLA	CAA-C2A-C1A	2.13	118.95	111.97
44	h	201	BCR	C24-C23-C22	-2.13	123.08	126.23
36	D	315	CLA	C2A-C1A-CHA	2.13	127.55	123.86
36	T	311	CLA	C11-C12-C13	-2.13	108.89	115.97
34	G	303	DD6	C12-C11-C13	2.13	121.34	118.09
36	D	309	CLA	C4B-C3B-C2B	-2.13	104.66	107.30
35	H	301	A86	C23-C16-C22	-2.13	104.28	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	E	303	DD6	C37-C36-C35	2.13	118.33	114.42
37	G	308	KC1	O2D-CGD-O1D	-2.13	119.71	123.85
35	N	303	A86	C33-C32-C31	-2.13	107.14	109.21
36	N	319	CLA	CHB-C1B-NB	2.13	127.24	124.05
36	S	320	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
34	j	103	DD6	C32-C33-C34	-2.13	108.93	113.59
36	b	824	CLA	CED-O2D-CGD	2.13	120.74	115.92
35	h	204	A86	O4-C38-O5	-2.13	118.89	122.99
34	D	305	DD6	C21-C20-C15	-2.13	118.80	122.30
36	O	316	CLA	C4-C3-C5	2.13	118.92	115.23
36	R	313	CLA	CMB-C2B-C3B	2.13	131.55	126.55
36	O	309	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
36	Q	309	CLA	CAA-C2A-C1A	2.13	118.94	111.97
35	B	303	A86	C23-C16-C22	2.12	110.46	107.37
36	b	828	CLA	CMB-C2B-C1B	-2.12	122.18	125.42
36	D	312	CLA	O1D-CGD-CBD	2.12	128.71	124.52
36	b	817	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
36	G	311	CLA	CHB-C4A-NA	2.12	127.47	124.40
35	K	303	A86	C34-O4-C38	2.12	121.60	117.85
36	I	305	CLA	C14-C13-C15	2.12	124.82	111.59
36	K	309	CLA	C4-C3-C5	2.12	118.91	115.23
36	a	809	CLA	O2D-CGD-CBD	2.12	114.94	111.23
36	f	804	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
36	b	830	CLA	CHA-C4D-ND	2.12	136.93	132.55
36	J	307	CLA	C4-C3-C5	2.12	118.91	115.23
36	W	210	CLA	C2D-C1D-ND	-2.12	108.03	110.13
36	b	825	CLA	C3B-C4B-NB	-2.12	108.64	110.53
44	l	203	BCR	C29-C30-C25	2.12	113.52	110.44
36	W	209	CLA	CMB-C2B-C3B	2.12	131.54	126.55
34	D	301	DD6	C25-C24-C1	-2.12	120.54	126.36
36	P	311	CLA	CBC-CAC-C3C	2.12	118.17	112.42
35	R	309	A86	C26-C25-C24	-2.12	117.05	123.20
36	E	311	CLA	C3B-C4B-NB	-2.12	108.64	110.53
37	T	315	KC1	O2D-CGD-O1D	-2.12	119.72	123.85
35	J	306	A86	C10-C9-C8	-2.12	117.06	123.20
36	a	835	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
36	f	802	CLA	CHD-C1D-ND	-2.12	121.82	124.80
36	R	321	CLA	O2D-CGD-CBD	2.12	114.94	111.23
36	F	317	CLA	C3C-C4C-NC	2.12	113.14	110.43
34	L	305	DD6	C7-C6-C8	2.12	121.33	118.09
36	O	309	CLA	CBC-CAC-C3C	2.12	118.16	112.42
36	O	310	CLA	CAA-C2A-C1A	2.12	118.92	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	207	CLA	C1-O2A-CGA	2.12	121.78	116.65
44	h	201	BCR	C11-C10-C9	-2.12	124.31	127.28
34	S	307	DD6	C12-C11-C13	2.12	121.32	118.09
37	W	217	KC1	C3A-C4A-NA	2.12	113.07	110.45
36	b	809	CLA	O1D-CGD-CBD	2.12	128.70	124.52
36	O	316	CLA	CHA-C4D-ND	-2.12	128.18	132.55
36	R	310	CLA	CMB-C2B-C3B	2.12	131.53	126.55
36	N	308	CLA	C1D-ND-C4D	-2.12	104.83	106.31
44	h	201	BCR	C7-C8-C9	-2.12	123.10	126.23
36	C	205	CLA	O2D-CGD-CBD	2.12	114.93	111.23
44	l	203	BCR	C31-C1-C6	2.12	113.56	110.24
34	D	303	DD6	C25-C24-C1	-2.12	120.56	126.36
35	B	303	A86	C19-C18-C17	-2.12	106.83	110.79
35	J	305	A86	C4-C3-C2	-2.12	119.19	123.52
35	L	301	A86	O1-C15-C20	-2.12	57.66	59.45
44	l	203	BCR	C24-C23-C22	-2.12	123.11	126.23
35	L	301	A86	C19-C18-C17	-2.12	106.83	110.79
37	X	311	KC1	C3A-C4A-NA	2.12	113.07	110.45
36	b	815	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
36	a	817	CLA	CAA-C2A-C3A	-2.11	107.28	113.00
36	Q	308	CLA	CBC-CAC-C3C	2.11	118.15	112.42
36	K	311	CLA	CHA-C1A-NA	-2.11	121.60	126.39
35	R	306	A86	C9-C10-C11	-2.11	120.66	126.64
35	E	305	A86	C10-C9-C8	-2.11	117.08	123.20
35	F	302	A86	O1-C15-C20	-2.11	57.66	59.45
35	R	301	A86	C41-C32-C31	2.11	112.36	110.47
36	E	312	CLA	CMB-C2B-C3B	2.11	131.52	126.55
36	P	319	CLA	CHB-C1B-NB	2.11	127.22	124.05
36	O	308	CLA	C1-C2-C3	-2.11	122.74	126.20
36	E	312	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
35	K	306	A86	C9-C8-C6	-2.11	120.57	126.36
36	F	314	CLA	C2A-C1A-CHA	2.11	127.53	123.87
34	J	304	DD6	C10-C9-C8	-2.11	117.08	123.20
36	a	848	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
36	b	839	CLA	C3A-C2A-C1A	2.11	104.50	101.34
34	E	306	DD6	C25-C26-C27	-2.11	120.71	126.61
41	G	301	LHG	C18-C17-C16	-2.11	103.70	114.37
35	L	301	A86	C9-C8-C6	-2.11	120.58	126.36
36	a	838	CLA	O2D-CGD-CBD	2.11	114.92	111.23
36	f	803	CLA	C4B-C3B-C2B	-2.11	104.68	107.30
34	J	304	DD6	C3-C4-C5	-2.11	119.20	123.52
37	X	311	KC1	C1D-CHD-C4C	-2.11	121.29	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	819	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
36	T	312	CLA	C3A-C2A-C1A	2.11	104.50	101.34
36	b	805	CLA	CHA-C4D-ND	2.11	136.90	132.55
36	J	309	CLA	CHB-C4A-NA	2.11	127.44	124.40
35	G	305	A86	C36-C31-C32	2.11	121.79	119.70
36	E	314	CLA	CHD-C4C-NC	2.11	127.50	124.23
36	a	832	CLA	CHD-C1D-ND	-2.11	121.84	124.80
36	W	212	CLA	C3D-C4D-ND	2.11	113.41	109.99
34	j	103	DD6	C28-C27-C26	-2.11	120.09	124.18
36	b	808	CLA	O1D-CGD-CBD	2.11	128.68	124.52
34	R	307	DD6	C37-C36-C31	-2.11	120.22	124.16
34	a	849	DD6	C4-C3-C2	-2.11	119.21	123.52
37	D	314	KC1	CMB-C2B-C1B	2.11	128.44	124.73
34	Q	302	DD6	C28-C27-C26	-2.11	120.09	124.18
36	b	826	CLA	C1D-ND-C4D	2.11	107.79	106.31
36	b	828	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
35	J	301	A86	C41-C32-C31	-2.11	108.59	110.47
34	D	303	DD6	C8-C6-C5	-2.11	115.70	119.01
37	P	315	KC1	CBA-CAA-C2A	2.11	133.91	125.45
36	S	313	CLA	CMB-C2B-C3B	2.11	131.50	126.55
36	b	805	CLA	C2A-C1A-CHA	2.11	127.52	123.87
41	f	808	LHG	C5-O7-C7	-2.11	112.76	117.80
37	J	314	KC1	C2B-C1B-NB	2.10	112.21	110.13
36	D	310	CLA	C3A-C2A-C1A	2.10	104.49	101.34
36	F	312	CLA	C3A-C2A-C1A	2.10	104.49	101.34
36	a	830	CLA	C1D-ND-C4D	2.10	107.79	106.31
36	W	201	CLA	O2D-CGD-CBD	2.10	114.91	111.23
34	G	303	DD6	C32-C33-C34	-2.10	108.98	113.59
35	N	320	A86	C9-C8-C6	-2.10	120.60	126.36
36	X	306	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
36	b	841	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
44	l	207	BCR	C27-C26-C25	2.10	125.54	122.70
36	b	840	CLA	CAC-C3C-C2C	-2.10	123.70	127.56
36	L	314	CLA	C2A-C1A-CHA	2.10	127.51	123.87
36	b	824	CLA	CHB-C1B-NB	-2.10	120.90	124.05
37	O	313	KC1	CBA-CAA-C2A	2.10	133.89	125.45
36	F	310	CLA	CMB-C2B-C3B	2.10	131.49	126.55
36	M	311	CLA	CHB-C4A-NA	2.10	127.43	124.40
36	a	831	CLA	CHB-C4A-NA	2.10	127.43	124.40
35	M	301	A86	C19-C18-C17	-2.10	106.86	110.79
34	C	201	DD6	C25-C24-C1	-2.10	120.61	126.36
36	b	828	CLA	O1D-CGD-CBD	2.10	128.66	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	E	310	CLA	CMD-C2D-C3D	2.10	132.50	127.69
35	S	308	A86	C4-C3-C2	-2.10	119.22	123.52
36	W	209	CLA	CHA-C1A-NA	-2.10	121.64	126.39
36	Q	312	CLA	CHC-C4B-NB	2.10	127.20	124.05
36	I	306	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
36	K	312	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
35	T	301	A86	O1-C15-C20	-2.10	57.67	59.45
36	K	308	CLA	CAC-C3C-C4C	2.10	127.52	124.79
37	Q	313	KC1	CBA-CAA-C2A	2.10	133.88	125.45
36	K	311	CLA	O2A-CGA-O1A	-2.10	116.94	123.20
35	M	301	A86	C25-C24-C1	-2.10	120.61	126.36
36	T	312	CLA	CAC-C3C-C4C	2.10	127.52	124.79
36	I	311	CLA	C1-C2-C3	-2.10	122.76	126.20
36	a	831	CLA	CMB-C2B-C3B	2.10	131.48	126.55
36	R	318	CLA	CMA-C3A-C2A	-2.10	111.42	116.23
36	N	310	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
44	b	847	BCR	C4-C5-C6	2.10	125.54	122.70
44	b	846	BCR	C35-C13-C14	-2.10	119.42	122.82
35	R	306	A86	C12-C11-C13	2.10	119.40	116.00
36	S	312	CLA	C1-C2-C3	-2.10	122.76	126.20
36	a	829	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
36	O	316	CLA	C2A-C1A-CHA	-2.09	120.23	123.87
36	F	310	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
37	W	217	KC1	C1D-CHD-C4C	-2.09	121.32	126.25
35	U	302	A86	O1-C20-C19	-2.09	111.53	113.49
35	O	319	A86	C40-C32-C31	2.09	112.34	110.47
36	B	309	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
36	P	310	CLA	C1-C2-C3	-2.09	122.77	126.20
35	U	302	A86	C36-C31-C32	-2.09	117.62	119.70
40	b	849	DGD	C3D-C4D-C5D	-2.09	106.44	110.23
36	C	207	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
34	O	304	DD6	C12-C11-C10	-2.09	119.43	122.82
35	S	303	A86	C33-C32-C31	-2.09	107.18	109.21
36	b	841	CLA	C4D-CHA-C1A	2.09	123.74	121.24
35	F	305	A86	C3-C4-C5	-2.09	119.24	123.52
35	J	306	A86	O1-C15-C20	-2.09	57.68	59.45
35	D	302	A86	O1-C15-C20	-2.09	57.68	59.45
36	a	824	CLA	CBA-CAA-C2A	2.09	120.02	113.79
34	K	305	DD6	C32-C33-C34	-2.09	109.01	113.59
34	H	302	DD6	C25-C26-C27	-2.09	120.76	126.61
35	V	302	A86	C9-C10-C11	-2.09	120.73	126.64
35	F	306	A86	C3-C4-C5	-2.09	119.24	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	819	CLA	C3D-C4D-ND	2.09	113.39	109.99
36	J	311	CLA	CHA-C4D-ND	2.09	136.86	132.55
36	O	312	CLA	C2A-C1A-CHA	2.09	125.95	122.71
44	f	801	BCR	C38-C26-C27	-2.09	109.14	113.60
35	T	303	A86	C4-C3-C2	-2.09	119.24	123.52
35	W	202	A86	C23-C16-C22	-2.09	104.33	107.37
44	h	201	BCR	C21-C20-C19	-2.09	117.14	123.20
36	T	312	CLA	CHA-C1A-NA	-2.09	121.66	126.39
36	a	813	CLA	O2A-CGA-O1A	-2.09	117.96	123.33
36	T	313	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
35	V	301	A86	O1-C15-C20	-2.09	57.68	59.45
44	a	844	BCR	C30-C25-C26	-2.09	119.78	122.64
36	P	316	CLA	CHC-C4B-NB	2.09	127.18	124.05
36	a	820	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
36	R	320	CLA	CHA-C4D-ND	2.09	136.86	132.55
35	X	303	A86	C23-C16-C17	-2.09	105.30	108.97
44	b	843	BCR	C16-C15-C14	-2.09	119.25	123.52
36	a	826	CLA	C3A-C2A-C1A	2.09	104.47	101.34
36	U	306	CLA	CMC-C2C-C1C	2.09	128.29	125.03
36	V	313	CLA	O2D-CGD-CBD	2.09	114.88	111.23
36	b	819	CLA	C2D-C1D-ND	-2.09	108.06	110.13
35	D	302	A86	C26-C25-C24	-2.09	117.16	123.20
35	V	302	A86	C23-C16-C17	-2.09	105.30	108.97
37	Q	311	KC1	CBA-CAA-C2A	2.09	133.83	125.45
36	a	835	CLA	CBA-CAA-C2A	-2.09	107.59	113.79
34	D	303	DD6	C28-C27-C26	-2.08	120.13	124.18
35	X	303	A86	C9-C10-C11	-2.08	120.75	126.64
35	J	303	A86	C10-C9-C8	-2.08	117.16	123.20
36	K	307	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
37	G	317	KC1	CAA-CBA-CGA	-2.08	116.45	127.05
36	A	306	CLA	C4B-C3B-C2B	-2.08	104.71	107.30
36	a	826	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
34	j	103	DD6	C21-C20-C15	-2.08	118.87	122.30
36	M	306	CLA	C1D-ND-C4D	2.08	107.77	106.31
36	X	309	CLA	C1D-ND-C4D	-2.08	104.85	106.31
35	H	301	A86	C34-O4-C38	-2.08	114.17	117.85
35	L	307	A86	C33-C32-C31	-2.08	107.19	109.21
37	O	315	KC1	CBA-CAA-C2A	2.08	133.82	125.45
36	a	817	CLA	C3A-C2A-C1A	2.08	104.46	101.34
36	O	309	CLA	CMB-C2B-C3B	2.08	131.45	126.55
34	S	307	DD6	C25-C26-C27	-2.08	120.79	126.61
36	J	309	CLA	CMB-C2B-C1B	-2.08	122.25	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	J	307	CLA	CHA-C1A-NA	-2.08	121.68	126.39
36	b	840	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
36	a	823	CLA	C3A-C2A-C1A	2.08	104.46	101.34
36	D	307	CLA	CGD-CBD-CAD	2.08	117.58	110.85
36	b	835	CLA	C2A-C1A-CHA	2.08	127.48	123.87
35	Q	316	A86	C10-C9-C8	-2.08	117.17	123.20
36	L	309	CLA	CAA-C2A-C3A	-2.08	107.38	113.00
34	D	301	DD6	C10-C9-C8	-2.08	117.17	123.20
36	R	312	CLA	C3A-C2A-C1A	2.08	104.45	101.34
36	b	833	CLA	C4-C3-C5	2.08	118.84	115.23
36	S	319	CLA	CAA-C2A-C1A	2.08	118.79	111.97
36	a	829	CLA	O1D-CGD-CBD	2.08	128.62	124.52
36	O	316	CLA	CAC-C3C-C4C	2.08	127.50	124.79
35	L	306	A86	C3-C4-C5	-2.08	119.27	123.52
36	b	830	CLA	CAA-C2A-C3A	-2.08	107.38	113.00
36	b	841	CLA	CMB-C2B-C3B	2.08	131.44	126.55
44	f	806	BCR	C35-C13-C14	-2.08	119.45	122.82
35	B	301	A86	C25-C26-C27	-2.08	124.36	127.28
36	a	824	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
35	V	302	A86	C9-C8-C6	-2.08	120.66	126.36
40	b	849	DGD	O5E-C6E-C5E	-2.08	104.26	111.33
42	D	320	LMG	C8-O7-C10	-2.08	112.82	117.80
36	F	317	CLA	C1D-ND-C4D	-2.08	104.85	106.31
36	a	806	CLA	C2A-C3A-C4A	2.08	105.22	101.87
35	R	301	A86	C40-C32-C33	2.08	118.90	109.06
36	O	314	CLA	CHC-C4B-NB	2.08	127.16	124.05
36	H	310	CLA	CGD-CBD-CAD	2.08	117.57	110.85
36	Q	310	CLA	CBA-CAA-C2A	2.08	119.97	113.79
39	G	322	LMT	C1B-O1B-C4'	-2.08	113.06	117.98
40	b	849	DGD	C7A-C6A-C5A	-2.08	103.88	114.37
34	F	303	DD6	C12-C11-C10	-2.08	119.45	122.82
35	K	301	A86	C41-C32-C31	-2.07	108.61	110.47
34	O	304	DD6	C7-C6-C5	-2.07	119.45	122.82
35	S	308	A86	C19-C18-C17	-2.07	106.91	110.79
35	M	305	A86	C9-C10-C11	-2.07	120.78	126.64
35	N	306	A86	C9-C10-C11	-2.07	120.78	126.64
36	W	215	CLA	C2A-C1A-CHA	2.07	127.47	123.87
34	B	304	DD6	C4-C3-C2	-2.07	119.28	123.52
36	R	319	CLA	C2A-C1A-CHA	2.07	127.47	123.87
36	b	812	CLA	C6-C7-C8	-2.07	109.08	115.97
34	M	303	DD6	C10-C9-C8	-2.07	117.19	123.20
37	G	317	KC1	C1C-C2C-C3C	-2.07	104.80	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	j	101	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
34	D	303	DD6	C14-C13-C11	-2.07	122.31	125.53
36	K	310	CLA	CHD-C4C-C3C	-2.07	121.75	124.77
35	J	303	A86	C9-C8-C6	-2.07	120.68	126.36
40	b	849	DGD	CBB-CAB-C9B	-2.07	103.90	114.37
35	N	305	A86	C10-C9-C8	-2.07	117.20	123.20
35	A	302	A86	O4-C38-C39	2.07	114.78	111.09
35	L	319	A86	C4-C3-C2	-2.07	119.28	123.52
36	a	819	CLA	C3B-C4B-NB	-2.07	108.68	110.53
37	N	314	KC1	O2D-CGD-O1D	-2.07	119.82	123.85
36	R	320	CLA	CHA-C1A-NA	-2.07	121.70	126.39
36	b	820	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
36	a	817	CLA	CHA-C1A-NA	-2.07	121.71	126.39
37	M	317	KC1	CAA-CBA-CGA	-2.07	116.53	127.05
44	b	845	BCR	C15-C16-C17	-2.07	119.29	123.52
36	D	316	CLA	C3C-C4C-NC	-2.07	107.78	110.43
36	b	812	CLA	O2D-CGD-CBD	2.07	114.85	111.23
36	U	311	CLA	CMC-C2C-C1C	2.07	128.26	125.03
35	K	302	A86	C3-C4-C5	-2.07	119.29	123.52
36	W	209	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
36	P	311	CLA	CMB-C2B-C3B	2.07	131.41	126.55
36	R	311	CLA	CMB-C2B-C3B	2.07	131.41	126.55
35	V	301	A86	C25-C24-C1	-2.07	120.70	126.36
35	K	303	A86	C12-C11-C13	2.07	119.35	116.00
35	T	303	A86	O4-C34-C35	-2.07	102.35	107.64
36	T	309	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
36	Q	308	CLA	CMB-C2B-C3B	2.07	131.41	126.55
36	f	804	CLA	CHC-C1C-C2C	-2.07	121.08	126.95
34	H	302	DD6	O1-C20-C19	2.06	115.43	113.49
44	b	847	BCR	C38-C26-C27	-2.06	109.19	113.60
36	C	211	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
35	O	302	A86	C4-C3-C2	-2.06	119.30	123.52
35	F	302	A86	C4-C3-C2	-2.06	119.30	123.52
36	P	301	CLA	O2A-CGA-CBA	2.06	118.13	111.83
36	l	204	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
36	D	310	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
36	A	314	CLA	C3B-C4B-NB	-2.06	108.69	110.53
44	l	207	BCR	C30-C25-C26	-2.06	119.82	122.64
36	a	802	CLA	C2B-C1B-NB	-2.06	108.19	110.33
36	D	316	CLA	C2D-C1D-ND	-2.06	108.08	110.13
35	V	302	A86	C26-C25-C24	-2.06	117.22	123.20
36	B	311	CLA	O2A-CGA-O1A	-2.06	118.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	J	308	CLA	CMD-C2D-C1D	2.06	128.36	124.73
36	H	307	CLA	CHD-C1D-C2D	2.06	129.78	125.49
36	E	315	CLA	C4D-CHA-C1A	-2.06	118.78	121.24
36	V	307	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
35	I	304	A86	O1-C20-C19	-2.06	111.56	113.49
36	D	317	CLA	C1-C2-C3	-2.06	122.82	126.20
34	S	307	DD6	C-C1-C2	-2.06	119.48	122.82
34	E	303	DD6	C4-C3-C2	-2.06	119.30	123.52
36	P	310	CLA	C11-C12-C13	-2.06	109.12	115.97
36	f	805	CLA	O1D-CGD-CBD	2.06	128.58	124.52
36	G	311	CLA	CMA-C3A-C2A	-2.06	106.02	113.98
37	B	310	KC1	C4D-CHA-C1A	-2.06	116.17	122.45
35	P	303	A86	C4-C3-C2	-2.06	119.30	123.52
36	B	309	CLA	C4D-CHA-C1A	-2.06	118.79	121.24
36	Q	310	CLA	C2B-C1B-NB	-2.06	108.19	110.33
36	a	804	CLA	C1D-ND-C4D	2.06	107.76	106.31
36	S	311	CLA	C2A-C1A-CHA	2.06	127.44	123.87
44	f	806	BCR	C1-C6-C5	-2.06	119.82	122.64
36	l	201	CLA	CHD-C1D-ND	-2.06	121.91	124.80
35	S	308	A86	O1-C15-C20	-2.06	57.71	59.45
36	W	210	CLA	CAC-C3C-C4C	2.06	127.47	124.79
36	A	306	CLA	C2A-C3A-C4A	2.06	105.19	101.87
36	a	834	CLA	C2A-C1A-CHA	2.06	127.44	123.87
35	h	204	A86	C-C1-C2	-2.06	119.48	122.82
35	G	302	A86	C25-C26-C27	-2.06	124.39	127.28
36	b	806	CLA	CHB-C1B-NB	2.06	127.14	124.05
36	U	310	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
37	P	317	KC1	C2A-C3A-C4A	2.06	107.96	106.41
36	a	817	CLA	C6-C7-C8	-2.06	109.13	115.97
35	T	301	A86	C9-C8-C6	-2.06	120.72	126.36
42	E	318	LMG	O1-C1-C2	2.06	111.40	108.27
36	A	308	CLA	C3A-C2A-C1A	2.06	104.42	101.34
36	P	314	CLA	C6-C7-C8	-2.06	109.13	115.97
36	l	206	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
36	h	203	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
36	I	305	CLA	CMB-C2B-C3B	2.06	131.39	126.55
35	G	306	A86	C3-C2-C1	-2.06	124.39	127.28
36	O	314	CLA	O1D-CGD-CBD	2.06	128.57	124.52
36	b	840	CLA	C11-C12-C13	-2.06	109.13	115.97
36	L	320	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
35	N	304	A86	C12-C11-C13	2.06	119.33	116.00
36	Q	312	CLA	O1D-CGD-CBD	2.06	128.57	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	813	CLA	C2A-C3A-C4A	2.06	105.19	101.87
36	O	316	CLA	C1-O2A-CGA	2.06	121.62	116.65
36	O	311	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
36	U	311	CLA	C2A-C1A-CHA	2.05	127.43	123.87
36	a	808	CLA	CHA-C1A-NA	-2.05	121.74	126.39
36	N	310	CLA	CMA-C3A-C2A	-2.05	111.52	116.23
37	N	314	KC1	CAC-C3C-C2C	2.05	131.33	127.56
36	b	831	CLA	CMB-C2B-C3B	2.05	131.38	126.55
35	X	304	A86	C4-C3-C2	-2.05	119.32	123.52
36	D	315	CLA	CBC-CAC-C3C	2.05	117.99	112.42
36	H	305	CLA	O2D-CGD-CBD	2.05	114.82	111.23
36	O	309	CLA	O2D-CGD-CBD	2.05	114.82	111.23
36	E	316	CLA	CMC-C2C-C1C	-2.05	121.83	125.03
35	W	202	A86	O-C13-C11	-2.05	116.62	121.04
36	T	311	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
36	B	306	CLA	CAC-C3C-C4C	2.05	127.46	124.79
36	T	316	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
35	M	302	A86	C40-C32-C31	-2.05	108.64	110.47
36	A	306	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
34	L	305	DD6	C21-C20-C15	-2.05	118.92	122.30
36	C	205	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
36	K	313	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
36	V	306	CLA	C2A-C1A-CHA	2.05	127.43	123.87
36	a	806	CLA	CHD-C1D-ND	-2.05	121.92	124.80
34	R	308	DD6	C12-C11-C10	-2.05	119.49	122.82
36	K	313	CLA	CHA-C4D-ND	2.05	136.78	132.55
36	D	307	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
36	S	317	CLA	CMA-C3A-C2A	-2.05	111.53	116.23
36	N	309	CLA	C3A-C2A-C1A	2.05	104.41	101.34
36	b	807	CLA	C2A-C1A-CHA	2.05	127.42	123.87
35	O	305	A86	C4-C3-C2	-2.05	119.32	123.52
36	a	802	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
34	G	303	DD6	C37-C36-C35	2.05	118.19	114.42
36	N	308	CLA	C4C-C3C-C2C	-2.05	103.91	106.89
36	Q	308	CLA	O2D-CGD-CBD	2.05	114.81	111.23
34	D	304	DD6	C15-C14-C13	-2.05	121.66	125.99
36	l	201	CLA	C4-C3-C5	2.05	118.78	115.23
36	P	316	CLA	O1D-CGD-CBD	2.05	128.56	124.52
36	a	814	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
35	K	302	A86	C26-C25-C24	-2.05	117.27	123.20
34	W	204	DD6	C37-C36-C31	-2.05	120.33	124.16
36	R	312	CLA	CMB-C2B-C3B	2.05	131.37	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	l	207	BCR	C1-C6-C5	-2.05	119.84	122.64
35	R	305	A86	C21-C20-C15	2.05	129.96	123.35
36	b	817	CLA	C1C-C2C-C3C	2.05	109.13	106.98
36	b	840	CLA	C1-C2-C3	-2.05	122.84	126.20
35	A	316	A86	C9-C10-C11	-2.05	120.86	126.64
36	G	310	CLA	O1D-CGD-CBD	2.04	128.55	124.52
35	T	303	A86	C21-C20-C15	-2.04	116.75	123.35
42	J	319	LMG	O7-C10-O9	-2.04	118.92	123.70
36	b	822	CLA	CED-O2D-CGD	2.04	120.55	115.92
36	b	801	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
36	b	828	CLA	C16-C15-C13	-2.04	109.17	115.97
36	P	314	CLA	C2B-C1B-NB	-2.04	108.21	110.33
35	J	301	A86	C9-C8-C6	-2.04	120.76	126.36
36	S	312	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
36	b	817	CLA	C6-C5-C3	-2.04	108.49	113.47
36	X	309	CLA	O2D-CGD-O1D	-2.04	119.44	124.08
35	J	302	A86	C7-C6-C5	-2.04	119.51	122.82
36	D	311	CLA	O2A-CGA-O1A	-2.04	117.10	123.20
36	W	208	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
36	M	306	CLA	O2D-CGD-CBD	2.04	114.80	111.23
36	V	305	CLA	CHB-C4A-NA	2.04	127.35	124.40
36	a	834	CLA	O1D-CGD-CBD	2.04	128.54	124.52
34	A	301	DD6	C25-C24-C1	-2.04	120.77	126.36
36	H	312	CLA	C2A-C1A-CHA	2.04	127.41	123.87
36	a	807	CLA	C2A-C1A-CHA	2.04	127.41	123.87
35	M	304	A86	O1-C15-C20	-2.04	57.72	59.45
36	X	307	CLA	CMB-C2B-C3B	2.04	131.35	126.55
36	a	808	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
35	G	304	A86	C4-C5-C6	-2.04	124.42	127.28
35	H	304	A86	C7-C6-C5	-2.04	119.51	122.82
35	F	305	A86	C-C1-C24	2.04	121.20	118.09
35	F	301	A86	C33-C32-C31	-2.04	107.23	109.21
35	F	304	A86	C10-C9-C8	-2.04	117.29	123.20
35	J	305	A86	C40-C32-C31	-2.04	108.65	110.47
36	U	305	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
35	P	307	A86	C40-C32-C31	-2.04	108.65	110.47
35	W	202	A86	C7-C6-C8	2.04	121.20	118.09
36	b	801	CLA	CHA-C1A-NA	-2.04	121.77	126.39
36	b	818	CLA	CHA-C1A-NA	-2.04	121.77	126.39
35	X	301	A86	C40-C32-C33	2.04	118.72	109.06
36	a	818	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
34	H	303	DD6	C21-C20-C15	-2.04	118.95	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	203	A86	C4-C3-C2	-2.04	119.35	123.52
34	R	307	DD6	O1-C20-C19	2.04	115.40	113.49
40	b	849	DGD	CAB-C9B-C8B	-2.04	104.07	114.37
36	L	311	CLA	C1-C2-C3	-2.04	122.86	126.20
37	L	315	KC1	C1C-C2C-C3C	-2.04	104.84	106.98
36	b	835	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
36	S	321	CLA	C3A-C2A-C1A	2.04	104.39	101.34
35	R	302	A86	C21-C20-C19	2.04	116.53	114.24
35	E	307	A86	C40-C32-C31	-2.04	108.65	110.47
35	h	202	A86	C-C1-C24	2.04	121.20	118.09
35	R	304	A86	O5-C38-C39	-2.04	117.56	124.77
34	j	103	DD6	C37-C36-C35	2.04	118.16	114.42
41	O	317	LHG	O7-C7-O9	-2.03	118.95	123.70
35	V	302	A86	C4-C3-C2	-2.03	119.36	123.52
41	a	843	LHG	C5-O7-C7	-2.03	112.93	117.80
44	j	107	BCR	C28-C27-C26	-2.03	110.43	114.06
35	J	303	A86	C33-C32-C31	-2.03	107.23	109.21
44	b	843	BCR	C1-C6-C5	-2.03	119.86	122.64
36	b	826	CLA	C2D-C1D-ND	-2.03	108.11	110.13
36	W	215	CLA	CHB-C4A-NA	2.03	127.33	124.40
34	I	303	DD6	C10-C9-C8	-2.03	117.31	123.20
35	C	202	A86	O-C13-C11	-2.03	116.66	121.04
36	a	812	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
36	b	813	CLA	CHB-C4A-NA	2.03	127.33	124.40
36	a	804	CLA	C1-O2A-CGA	2.03	121.57	116.65
37	U	312	KC1	C1C-C2C-C3C	-2.03	104.84	106.98
36	W	214	CLA	CHA-C1A-NA	-2.03	121.79	126.39
34	M	303	DD6	C14-C13-C11	-2.03	122.38	125.53
35	J	301	A86	C21-C20-C15	2.03	129.91	123.35
36	a	805	CLA	C2A-C1A-CHA	2.03	127.39	123.87
35	U	304	A86	C4-C3-C2	-2.03	119.36	123.52
36	I	306	CLA	C3C-C4C-NC	2.03	113.03	110.43
36	R	312	CLA	C1-C2-C3	-2.03	122.87	126.20
36	b	836	CLA	C2A-C3A-C4A	2.03	105.15	101.87
34	E	301	DD6	C15-C14-C13	-2.03	121.70	125.99
36	A	308	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
36	I	307	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
36	P	313	CLA	O1D-CGD-CBD	2.03	128.52	124.52
36	X	306	CLA	O2D-CGD-CBD	2.03	114.78	111.23
35	G	306	A86	C12-C11-C10	-2.03	118.74	123.67
36	P	313	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
36	A	307	CLA	CMB-C2B-C3B	2.03	131.32	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	L	311	CLA	CHA-C1A-NA	-2.03	121.80	126.39
36	P	311	CLA	O2D-CGD-CBD	2.03	114.78	111.23
36	b	830	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
36	b	841	CLA	C16-C15-C13	-2.03	109.22	115.97
36	H	316	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
34	H	302	DD6	C3-C4-C5	-2.03	119.37	123.52
36	N	317	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
36	E	311	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
36	l	204	CLA	C2A-C3A-C4A	2.03	105.14	101.87
35	K	302	A86	C19-C18-C17	-2.03	107.00	110.79
36	F	314	CLA	CHA-C1A-NA	-2.03	121.80	126.39
36	U	310	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
35	E	302	A86	C4-C3-C2	-2.03	119.37	123.52
36	X	310	CLA	CHA-C4D-ND	2.03	136.73	132.55
36	N	317	CLA	O1D-CGD-CBD	2.03	128.52	124.52
36	b	831	CLA	C2D-C1D-ND	-2.03	108.12	110.13
35	J	303	A86	O-C13-C11	-2.03	116.68	121.04
35	K	303	A86	C23-C16-C22	-2.03	104.43	107.37
44	f	806	BCR	C33-C5-C6	-2.03	122.27	124.48
34	R	307	DD6	C9-C8-C6	-2.03	120.81	126.36
42	D	320	LMG	O7-C10-O9	-2.03	118.97	123.70
37	T	310	KC1	CAB-C3B-C4B	2.03	129.66	124.82
36	L	320	CLA	O1D-CGD-CBD	2.03	128.51	124.52
37	T	310	KC1	O1D-CGD-CBD	-2.03	120.52	124.52
36	J	317	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
35	X	304	A86	C41-C32-C31	2.02	112.28	110.47
37	J	314	KC1	C1D-CHD-C4C	-2.02	121.49	126.25
36	b	827	CLA	CHA-C1A-NA	-2.02	121.81	126.39
36	V	314	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
36	P	301	CLA	C1-C2-C3	2.02	129.51	126.20
42	E	319	LMG	O7-C10-O9	-2.02	118.97	123.70
37	T	315	KC1	C3D-C4D-ND	-2.02	107.38	110.20
36	T	314	CLA	C2A-C1A-CHA	2.02	127.38	123.87
35	U	304	A86	C9-C10-C11	-2.02	120.92	126.64
35	F	306	A86	C33-C32-C31	-2.02	107.25	109.21
36	H	308	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
36	S	309	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
35	M	304	A86	C41-C32-C31	-2.02	108.66	110.47
36	X	308	CLA	CHD-C4C-C3C	2.02	127.72	124.77
36	C	208	CLA	C4-C3-C5	2.02	118.74	115.23
36	R	316	CLA	O2D-CGD-CBD	2.02	114.77	111.23
35	T	303	A86	C3-C4-C5	-2.02	119.38	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	G	318	KC1	C2B-C1B-NB	2.02	112.13	110.13
36	D	308	CLA	CHB-C1B-NB	2.02	127.08	124.05
36	X	309	CLA	CBA-CAA-C2A	-2.02	107.78	113.79
34	D	305	DD6	O1-C20-C21	-2.02	112.79	115.05
36	E	315	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
44	l	207	BCR	C15-C16-C17	-2.02	119.38	123.52
44	i	101	BCR	C39-C30-C25	2.02	113.41	110.24
37	X	311	KC1	C2B-C1B-NB	2.02	112.13	110.13
36	b	828	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
41	O	318	LHG	O8-C23-O10	-2.02	118.58	123.63
35	U	304	A86	O4-C38-O5	-2.02	119.09	122.99
36	I	313	CLA	CMA-C3A-C2A	-2.02	111.60	116.23
36	V	310	CLA	C3B-C4B-NB	-2.02	108.73	110.53
36	A	311	CLA	O1D-CGD-CBD	2.02	128.50	124.52
37	L	317	KC1	C4D-CHA-C1A	-2.02	116.30	122.45
36	a	833	CLA	C2A-C1A-CHA	2.02	127.37	123.87
34	E	303	DD6	C28-C27-C26	-2.02	120.26	124.18
36	S	310	CLA	CMB-C2B-C3B	2.02	131.30	126.55
36	l	205	CLA	C2A-C1A-CHA	2.02	127.37	123.87
36	U	311	CLA	CMD-C2D-C3D	2.02	132.32	127.69
44	b	846	BCR	C30-C25-C26	-2.02	119.88	122.64
36	M	307	CLA	CHB-C1B-NB	2.02	127.07	124.05
36	a	848	CLA	CAC-C3C-C4C	2.02	127.41	124.79
36	l	205	CLA	C1-O2A-CGA	2.02	121.53	116.65
36	b	812	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
37	L	315	KC1	C1D-CHD-C4C	-2.02	121.51	126.25
36	b	827	CLA	O2D-CGD-CBD	2.01	114.75	111.23
35	R	305	A86	O1-C20-C19	-2.01	111.60	113.49
36	L	314	CLA	C3B-C4B-NB	-2.01	108.73	110.53
35	U	304	A86	C19-C18-C17	-2.01	107.02	110.79
36	X	306	CLA	CHA-C4D-ND	2.01	136.70	132.55
36	X	307	CLA	CBA-CAA-C2A	2.01	119.78	113.79
36	b	815	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
36	H	307	CLA	CHA-C1A-NA	-2.01	121.83	126.39
36	S	320	CLA	CHA-C1A-NA	-2.01	121.83	126.39
35	V	301	A86	C4-C3-C2	-2.01	119.40	123.52
36	b	828	CLA	CMB-C2B-C3B	2.01	131.28	126.55
35	G	305	A86	C4-C3-C2	-2.01	119.40	123.52
44	j	107	BCR	C27-C26-C25	2.01	125.42	122.70
35	X	301	A86	C10-C9-C8	-2.01	117.37	123.20
34	j	103	DD6	C25-C26-C27	-2.01	120.98	126.61
36	I	306	CLA	CHC-C1C-C2C	-2.01	121.23	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	O	302	A86	C40-C32-C33	2.01	118.59	109.06
36	b	822	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
36	U	306	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
36	R	321	CLA	CMA-C3A-C2A	-2.01	106.21	113.98
35	P	303	A86	C40-C32-C33	2.01	118.58	109.06
36	j	101	CLA	O1D-CGD-CBD	2.01	128.48	124.52
35	Q	304	A86	C28-C27-C26	-2.01	119.56	122.82
36	b	805	CLA	CMD-C2D-C1D	-2.01	121.19	124.73
36	S	319	CLA	O2D-CGD-CBD	2.01	114.74	111.23
44	a	844	BCR	C11-C10-C9	-2.01	124.46	127.28
36	J	316	CLA	CHD-C4C-C3C	2.01	127.70	124.77
35	T	306	A86	C10-C9-C8	-2.01	117.38	123.20
36	a	828	CLA	C1-C2-C3	-2.01	122.91	126.20
36	f	803	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
35	H	304	A86	O1-C15-C20	-2.01	57.75	59.45
36	W	210	CLA	CHB-C1B-NB	2.01	127.06	124.05
36	N	310	CLA	CHA-C4D-ND	2.01	136.69	132.55
34	A	304	DD6	C15-C14-C13	-2.01	121.75	125.99
42	h	206	LMG	O7-C10-O9	-2.01	119.01	123.70
35	h	204	A86	C25-C24-C1	-2.01	120.86	126.36
36	a	837	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
36	H	314	CLA	CMA-C3A-C2A	-2.01	111.62	116.23
36	a	848	CLA	CHB-C4A-NA	2.01	127.30	124.40
35	T	303	A86	O4-C34-C33	2.01	112.78	107.64
36	a	816	CLA	CAC-C3C-C4C	2.01	127.40	124.79
35	V	304	A86	C33-C32-C31	-2.01	107.26	109.21
36	f	803	CLA	CHB-C4A-NA	2.01	127.30	124.40
36	b	830	CLA	CHD-C1D-C2D	2.01	129.66	125.49
41	F	319	LHG	O7-C7-O9	-2.01	119.01	123.70
41	l	208	LHG	O7-C7-O9	-2.01	119.01	123.70
35	C	204	A86	O1-C15-C20	-2.01	57.75	59.45
36	b	822	CLA	C2A-C1A-CHA	2.01	127.35	123.87
34	E	304	DD6	C21-C20-C15	-2.01	119.00	122.30
34	L	305	DD6	C-C1-C2	-2.01	119.57	122.82
35	V	304	A86	C34-O4-C38	2.01	121.39	117.85
36	a	802	CLA	C2A-C1A-CHA	2.01	127.35	123.87
35	U	304	A86	C8-C6-C5	2.01	122.16	119.01
36	D	311	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
36	O	311	CLA	O1D-CGD-CBD	2.01	128.47	124.52
35	F	304	A86	C41-C32-C31	-2.01	108.68	110.47
36	D	307	CLA	CMC-C2C-C3C	2.01	131.57	126.15
35	L	319	A86	C40-C32-C33	2.00	118.56	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	212	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
36	a	811	CLA	CHB-C1B-NB	2.00	127.06	124.05
36	C	211	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
44	a	846	BCR	C30-C25-C26	-2.00	119.90	122.64
37	M	313	KC1	CAA-CBA-CGA	-2.00	116.86	127.05
34	F	303	DD6	C37-C36-C31	-2.00	120.41	124.16
36	b	830	CLA	C3C-C4C-NC	-2.00	107.86	110.43
36	A	313	CLA	C2A-C1A-CHA	2.00	127.33	123.86
36	L	310	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
36	K	309	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
36	W	214	CLA	CHA-C4D-ND	2.00	136.68	132.55
35	B	301	A86	C40-C32-C31	-2.00	108.68	110.47
36	b	833	CLA	CBA-CAA-C2A	2.00	119.75	113.79
36	a	827	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
36	M	307	CLA	O2D-CGD-CBD	2.00	114.73	111.23
44	b	845	BCR	C21-C20-C19	-2.00	117.40	123.20
35	R	301	A86	C12-C11-C13	2.00	119.25	116.00
35	N	320	A86	C28-C27-C26	-2.00	119.57	122.82
36	a	827	CLA	C3A-C2A-C1A	2.00	104.34	101.34
36	O	308	CLA	CHA-C1A-NA	-2.00	121.86	126.39
36	T	308	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
36	M	311	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
36	V	310	CLA	O2D-CGD-CBD	2.00	114.73	111.23
36	K	311	CLA	CMA-C3A-C4A	-2.00	106.40	111.77
36	N	312	CLA	O1D-CGD-CBD	2.00	128.46	124.52

All (321) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	A	305	CLA	ND
36	A	306	CLA	ND
36	A	306	CLA	C8
36	A	307	CLA	ND
36	A	308	CLA	ND
36	A	309	CLA	ND
36	A	310	CLA	ND
36	A	311	CLA	ND
36	A	313	CLA	ND
36	A	314	CLA	ND
36	B	305	CLA	ND
36	B	306	CLA	ND
36	B	307	CLA	ND

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Mol	Chain	Res	Type	Atom
36	B	308	CLA	ND
36	B	309	CLA	ND
36	B	311	CLA	ND
36	C	205	CLA	ND
36	C	206	CLA	ND
36	C	207	CLA	C8
36	C	208	CLA	ND
36	C	209	CLA	ND
36	C	210	CLA	ND
36	C	211	CLA	ND
36	C	212	CLA	ND
36	C	214	CLA	ND
36	D	306	CLA	ND
36	D	307	CLA	ND
36	D	308	CLA	ND
36	D	309	CLA	ND
36	D	309	CLA	C8
36	D	310	CLA	ND
36	D	312	CLA	ND
36	D	313	CLA	ND
36	D	315	CLA	ND
36	D	316	CLA	ND
36	D	317	CLA	ND
36	E	308	CLA	ND
36	E	311	CLA	ND
36	E	312	CLA	ND
36	E	313	CLA	ND
36	E	313	CLA	C8
36	E	314	CLA	ND
36	E	315	CLA	ND
36	E	315	CLA	C8
36	E	316	CLA	ND
36	E	317	CLA	ND
36	F	309	CLA	ND
36	F	310	CLA	ND
36	F	311	CLA	ND
36	F	312	CLA	ND
36	F	313	CLA	ND
36	F	314	CLA	ND
36	F	316	CLA	ND
36	F	317	CLA	ND
36	F	317	CLA	C8

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Mol	Chain	Res	Type	Atom
36	G	309	CLA	ND
36	G	310	CLA	ND
36	G	311	CLA	ND
36	G	312	CLA	ND
36	G	313	CLA	ND
36	G	314	CLA	ND
36	G	315	CLA	ND
36	G	315	CLA	C8
36	G	316	CLA	ND
36	G	319	CLA	ND
36	H	305	CLA	ND
36	H	306	CLA	ND
36	H	307	CLA	ND
36	H	308	CLA	ND
36	H	309	CLA	ND
36	H	310	CLA	ND
36	H	311	CLA	ND
36	H	312	CLA	ND
36	H	314	CLA	ND
36	H	315	CLA	ND
36	H	316	CLA	ND
36	H	317	CLA	ND
36	H	318	CLA	ND
36	I	305	CLA	ND
36	I	305	CLA	C13
36	I	306	CLA	ND
36	I	306	CLA	C8
36	I	307	CLA	ND
36	I	308	CLA	C8
36	I	309	CLA	ND
36	I	310	CLA	ND
36	I	311	CLA	ND
36	I	312	CLA	ND
36	I	313	CLA	ND
36	I	314	CLA	ND
36	J	307	CLA	ND
36	J	309	CLA	ND
36	J	310	CLA	ND
36	J	311	CLA	ND
36	J	312	CLA	ND
36	J	313	CLA	ND
36	J	315	CLA	ND

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Mol	Chain	Res	Type	Atom
36	J	316	CLA	ND
36	J	317	CLA	ND
36	K	307	CLA	ND
36	K	307	CLA	C8
36	K	308	CLA	ND
36	K	309	CLA	ND
36	K	310	CLA	ND
36	K	310	CLA	C8
36	K	311	CLA	ND
36	K	312	CLA	ND
36	K	313	CLA	ND
36	K	315	CLA	ND
36	K	316	CLA	ND
36	L	308	CLA	ND
36	L	308	CLA	C8
36	L	309	CLA	ND
36	L	310	CLA	ND
36	L	311	CLA	ND
36	L	313	CLA	ND
36	L	314	CLA	ND
36	L	316	CLA	ND
36	L	320	CLA	ND
36	M	306	CLA	ND
36	M	307	CLA	ND
36	M	308	CLA	ND
36	M	309	CLA	ND
36	M	310	CLA	ND
36	M	311	CLA	ND
36	M	312	CLA	ND
36	M	314	CLA	ND
36	M	316	CLA	ND
36	N	307	CLA	ND
36	N	308	CLA	ND
36	N	309	CLA	ND
36	N	310	CLA	ND
36	N	311	CLA	ND
36	N	312	CLA	ND
36	N	313	CLA	ND
36	N	316	CLA	ND
36	N	317	CLA	ND
36	N	318	CLA	ND
36	N	319	CLA	ND

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Mol	Chain	Res	Type	Atom
36	O	306	CLA	ND
36	O	307	CLA	ND
36	O	308	CLA	ND
36	O	309	CLA	ND
36	O	310	CLA	ND
36	O	311	CLA	ND
36	O	314	CLA	ND
36	O	316	CLA	C8
36	P	301	CLA	ND
36	P	308	CLA	ND
36	P	309	CLA	ND
36	P	310	CLA	ND
36	P	311	CLA	ND
36	P	312	CLA	ND
36	P	313	CLA	ND
36	P	316	CLA	ND
36	P	318	CLA	ND
36	P	319	CLA	ND
36	Q	305	CLA	ND
36	Q	306	CLA	ND
36	Q	307	CLA	ND
36	Q	308	CLA	ND
36	Q	309	CLA	ND
36	Q	312	CLA	ND
36	Q	314	CLA	ND
36	R	310	CLA	ND
36	R	311	CLA	ND
36	R	312	CLA	ND
36	R	313	CLA	ND
36	R	314	CLA	ND
36	R	315	CLA	ND
36	R	316	CLA	ND
36	R	318	CLA	ND
36	R	319	CLA	ND
36	R	320	CLA	ND
36	R	322	CLA	ND
36	S	309	CLA	ND
36	S	310	CLA	ND
36	S	311	CLA	ND
36	S	313	CLA	ND
36	S	315	CLA	ND
36	S	317	CLA	ND

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Mol	Chain	Res	Type	Atom
36	S	318	CLA	ND
36	S	319	CLA	ND
36	T	308	CLA	ND
36	T	309	CLA	ND
36	T	311	CLA	ND
36	T	312	CLA	ND
36	T	313	CLA	ND
36	T	314	CLA	ND
36	T	316	CLA	ND
36	W	201	CLA	ND
36	W	206	CLA	ND
36	W	207	CLA	ND
36	W	208	CLA	ND
36	W	209	CLA	ND
36	W	210	CLA	ND
36	W	211	CLA	ND
36	W	215	CLA	ND
36	W	216	CLA	ND
36	W	218	CLA	ND
36	X	306	CLA	ND
36	X	308	CLA	ND
36	X	310	CLA	ND
36	X	312	CLA	ND
36	a	801	CLA	ND
36	a	802	CLA	ND
36	a	802	CLA	C8
36	a	803	CLA	ND
36	a	804	CLA	ND
36	a	805	CLA	ND
36	a	806	CLA	ND
36	a	806	CLA	C8
36	a	807	CLA	ND
36	a	808	CLA	ND
36	a	809	CLA	ND
36	a	810	CLA	ND
36	a	811	CLA	ND
36	a	812	CLA	ND
36	a	813	CLA	ND
36	a	814	CLA	ND
36	a	815	CLA	ND
36	a	816	CLA	C8
36	a	817	CLA	ND

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Mol	Chain	Res	Type	Atom
36	a	818	CLA	ND
36	a	819	CLA	ND
36	a	820	CLA	ND
36	a	821	CLA	ND
36	a	822	CLA	ND
36	a	823	CLA	ND
36	a	823	CLA	C8
36	a	824	CLA	ND
36	a	825	CLA	ND
36	a	825	CLA	C8
36	a	826	CLA	ND
36	a	827	CLA	ND
36	a	828	CLA	ND
36	a	829	CLA	ND
36	a	831	CLA	ND
36	a	832	CLA	ND
36	a	833	CLA	ND
36	a	834	CLA	ND
36	a	835	CLA	ND
36	a	836	CLA	ND
36	a	837	CLA	ND
36	a	838	CLA	ND
36	a	839	CLA	ND
36	a	841	CLA	ND
36	a	848	CLA	ND
36	a	848	CLA	C8
36	b	801	CLA	ND
36	b	802	CLA	ND
36	b	805	CLA	ND
36	b	806	CLA	ND
36	b	807	CLA	ND
36	b	808	CLA	ND
36	b	809	CLA	ND
36	b	810	CLA	ND
36	b	811	CLA	ND
36	b	812	CLA	ND
36	b	813	CLA	ND
36	b	814	CLA	ND
36	b	815	CLA	ND
36	b	816	CLA	ND
36	b	816	CLA	C8
36	b	817	CLA	ND

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Mol	Chain	Res	Type	Atom
36	b	817	CLA	C8
36	b	819	CLA	ND
36	b	820	CLA	ND
36	b	821	CLA	ND
36	b	822	CLA	ND
36	b	823	CLA	ND
36	b	824	CLA	ND
36	b	825	CLA	ND
36	b	826	CLA	ND
36	b	827	CLA	ND
36	b	828	CLA	ND
36	b	829	CLA	ND
36	b	830	CLA	ND
36	b	831	CLA	ND
36	b	832	CLA	ND
36	b	833	CLA	ND
36	b	834	CLA	ND
36	b	835	CLA	ND
36	b	836	CLA	C8
36	b	837	CLA	ND
36	b	838	CLA	ND
36	b	839	CLA	ND
36	b	840	CLA	ND
36	b	841	CLA	ND
36	f	802	CLA	ND
36	f	803	CLA	ND
36	f	803	CLA	C8
36	f	804	CLA	ND
36	f	804	CLA	C8
36	f	805	CLA	ND
36	i	102	CLA	ND
36	j	101	CLA	ND
36	j	102	CLA	C8
36	j	106	CLA	ND
36	l	201	CLA	ND
36	l	202	CLA	ND
36	l	205	CLA	ND
36	l	205	CLA	C8
36	l	206	CLA	ND
36	h	203	CLA	ND
36	U	305	CLA	ND
36	U	306	CLA	C8

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Mol	Chain	Res	Type	Atom
36	U	307	CLA	ND
36	U	308	CLA	ND
36	U	310	CLA	ND
36	U	311	CLA	ND
36	U	313	CLA	ND
36	V	305	CLA	ND
36	V	306	CLA	ND
36	V	307	CLA	ND
36	V	308	CLA	ND
36	V	309	CLA	ND
36	V	310	CLA	ND
36	V	311	CLA	ND
36	V	313	CLA	ND
36	V	314	CLA	C8

All (5875) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	301	DD6	C10-C11-C13-C14
34	A	301	DD6	C13-C14-C15-C20
34	A	301	DD6	C13-C14-C15-O1
34	A	303	DD6	C10-C11-C13-C14
34	A	303	DD6	C12-C11-C13-C14
34	A	303	DD6	C13-C14-C15-C16
34	A	303	DD6	C13-C14-C15-C20
34	A	303	DD6	C13-C14-C15-O1
34	A	304	DD6	C10-C11-C13-C14
34	A	304	DD6	C12-C11-C13-C14
34	A	304	DD6	C13-C14-C15-C20
34	A	304	DD6	C13-C14-C15-O1
34	B	302	DD6	C10-C11-C13-C14
34	B	302	DD6	C12-C11-C13-C14
34	B	302	DD6	C13-C14-C15-O1
34	C	201	DD6	C13-C14-C15-C16
34	C	201	DD6	C13-C14-C15-C20
34	C	201	DD6	C13-C14-C15-O1
34	C	201	DD6	C5-C6-C8-C9
34	C	201	DD6	C7-C6-C8-C9
34	D	301	DD6	C10-C11-C13-C14
34	D	301	DD6	C13-C14-C15-C16
34	D	301	DD6	C13-C14-C15-C20
34	D	301	DD6	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
34	D	301	DD6	C5-C6-C8-C9
34	D	303	DD6	C-C1-C2-C3
34	D	303	DD6	C2-C1-C24-C25
34	D	303	DD6	C13-C14-C15-O1
34	D	304	DD6	C13-C14-C15-C20
34	D	304	DD6	C5-C6-C8-C9
34	D	304	DD6	C7-C6-C8-C9
34	E	301	DD6	C13-C14-C15-C16
34	E	303	DD6	C10-C11-C13-C14
34	E	303	DD6	C13-C14-C15-C16
34	E	303	DD6	C13-C14-C15-C20
34	E	303	DD6	C5-C6-C8-C9
34	E	304	DD6	C13-C14-C15-C20
34	F	303	DD6	C10-C11-C13-C14
34	F	303	DD6	C12-C11-C13-C14
34	F	303	DD6	C13-C14-C15-C16
34	F	303	DD6	C13-C14-C15-C20
34	F	303	DD6	C13-C14-C15-O1
34	G	303	DD6	C13-C14-C15-C20
34	H	302	DD6	C13-C14-C15-O1
34	H	303	DD6	C10-C11-C13-C14
34	H	303	DD6	C12-C11-C13-C14
34	H	303	DD6	C13-C14-C15-C20
34	H	303	DD6	C13-C14-C15-O1
34	H	303	DD6	C5-C6-C8-C9
34	H	303	DD6	C7-C6-C8-C9
34	I	303	DD6	C10-C11-C13-C14
34	I	303	DD6	C12-C11-C13-C14
34	I	303	DD6	C13-C14-C15-C20
34	J	304	DD6	C10-C11-C13-C14
34	J	304	DD6	C13-C14-C15-O1
34	L	305	DD6	C10-C11-C13-C14
34	L	305	DD6	C12-C11-C13-C14
34	L	305	DD6	C13-C14-C15-C20
34	M	303	DD6	C10-C11-C13-C14
34	O	304	DD6	C10-C11-C13-C14
34	O	304	DD6	C12-C11-C13-C14
34	O	304	DD6	C13-C14-C15-O1
34	O	304	DD6	C5-C6-C8-C9
34	O	304	DD6	C7-C6-C8-C9
34	Q	302	DD6	C2-C1-C24-C25
34	Q	302	DD6	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
34	R	307	DD6	C2-C1-C24-C25
34	R	307	DD6	C10-C11-C13-C14
34	R	307	DD6	C12-C11-C13-C14
34	R	307	DD6	C13-C14-C15-C20
34	R	307	DD6	C5-C6-C8-C9
34	R	307	DD6	C7-C6-C8-C9
34	R	308	DD6	C2-C1-C24-C25
34	R	308	DD6	C11-C10-C9-C8
34	R	308	DD6	C13-C14-C15-O1
34	S	306	DD6	C13-C14-C15-O1
34	S	306	DD6	C5-C6-C8-C9
34	S	306	DD6	C7-C6-C8-C9
34	W	204	DD6	C-C1-C24-C25
34	W	204	DD6	C2-C1-C24-C25
34	W	204	DD6	C10-C11-C13-C14
34	W	204	DD6	C12-C11-C13-C14
34	W	204	DD6	C13-C14-C15-C16
34	W	205	DD6	C13-C14-C15-C20
34	W	205	DD6	C5-C6-C8-C9
34	a	849	DD6	C13-C14-C15-C20
34	j	103	DD6	C10-C11-C13-C14
34	j	103	DD6	C12-C11-C13-C14
34	j	103	DD6	C13-C14-C15-C20
35	A	316	A86	C13-C14-C15-C16
35	A	316	A86	C13-C14-C15-O1
35	A	316	A86	C26-C27-C29-C30
35	A	316	A86	C39-C38-O4-C34
35	B	303	A86	C11-C10-C9-C8
35	B	303	A86	C10-C11-C13-C14
35	B	303	A86	C12-C11-C13-C14
35	B	303	A86	O-C13-C14-C15
35	B	303	A86	C11-C13-C14-C15
35	C	203	A86	C2-C1-C24-C25
35	C	203	A86	C33-C34-O4-C38
35	C	203	A86	C39-C38-O4-C34
35	C	203	A86	O5-C38-O4-C34
35	C	204	A86	O-C13-C14-C15
35	C	204	A86	C28-C27-C29-C30
35	D	302	A86	C35-C34-O4-C38
35	D	302	A86	C39-C38-O4-C34
35	D	302	A86	C5-C6-C8-C9
35	E	302	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
35	E	305	A86	C39-C38-O4-C34
35	E	305	A86	O5-C38-O4-C34
35	E	305	A86	C5-C6-C8-C9
35	E	307	A86	C13-C14-C15-O1
35	F	301	A86	C-C1-C24-C25
35	F	301	A86	C2-C1-C24-C25
35	F	302	A86	C35-C34-O4-C38
35	F	302	A86	C39-C38-O4-C34
35	F	304	A86	C13-C14-C15-O1
35	F	304	A86	O5-C38-O4-C34
35	G	302	A86	C2-C1-C24-C25
35	G	302	A86	C39-C38-O4-C34
35	G	304	A86	C10-C11-C13-C14
35	G	304	A86	C12-C11-C13-C14
35	G	304	A86	C13-C14-C15-C20
35	G	305	A86	C39-C38-O4-C34
35	G	305	A86	O5-C38-O4-C34
35	G	306	A86	C39-C38-O4-C34
35	H	304	A86	C-C1-C24-C25
35	H	304	A86	C2-C1-C24-C25
35	H	304	A86	C24-C25-C26-C27
35	H	304	A86	C26-C27-C29-C30
35	H	304	A86	C33-C34-O4-C38
35	H	304	A86	C39-C38-O4-C34
35	H	304	A86	O5-C38-O4-C34
35	I	301	A86	C2-C1-C24-C25
35	I	301	A86	C24-C25-C26-C27
35	I	301	A86	C5-C6-C8-C9
35	J	301	A86	C-C1-C24-C25
35	J	301	A86	C13-C14-C15-C20
35	J	301	A86	C13-C14-C15-O1
35	J	302	A86	C13-C14-C15-O1
35	J	305	A86	C35-C34-O4-C38
35	J	305	A86	C5-C6-C8-C9
35	J	305	A86	C7-C6-C8-C9
35	J	306	A86	C2-C1-C24-C25
35	J	306	A86	C12-C11-C13-C14
35	J	306	A86	C13-C14-C15-O1
35	J	306	A86	C33-C34-O4-C38
35	J	306	A86	C39-C38-O4-C34
35	K	301	A86	C-C1-C24-C25
35	K	301	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
35	K	301	A86	C13-C14-C15-O1
35	K	301	A86	O5-C38-O4-C34
35	K	302	A86	C10-C11-C13-C14
35	K	302	A86	C12-C11-C13-C14
35	K	306	A86	C10-C11-C13-C14
35	K	306	A86	C12-C11-C13-O
35	K	306	A86	C12-C11-C13-C14
35	L	301	A86	C2-C1-C24-C25
35	L	301	A86	C39-C38-O4-C34
35	L	306	A86	C-C1-C24-C25
35	L	306	A86	C2-C1-C24-C25
35	L	306	A86	C10-C11-C13-O
35	L	306	A86	C12-C11-C13-O
35	L	307	A86	C2-C1-C24-C25
35	L	307	A86	C11-C10-C9-C8
35	L	307	A86	C5-C6-C8-C9
35	L	307	A86	C7-C6-C8-C9
35	L	319	A86	C10-C11-C13-C14
35	L	319	A86	C12-C11-C13-C14
35	M	301	A86	C10-C11-C13-C14
35	M	301	A86	C12-C11-C13-C14
35	M	302	A86	C12-C11-C13-O
35	M	304	A86	C-C1-C24-C25
35	M	304	A86	C2-C1-C24-C25
35	M	304	A86	C39-C38-O4-C34
35	M	304	A86	C5-C6-C8-C9
35	M	304	A86	C7-C6-C8-C9
35	M	305	A86	C10-C11-C13-C14
35	M	305	A86	C12-C11-C13-C14
35	N	301	A86	C12-C11-C13-C14
35	N	301	A86	C13-C14-C15-C20
35	N	304	A86	C-C1-C24-C25
35	N	304	A86	C2-C1-C24-C25
35	N	304	A86	C33-C34-O4-C38
35	N	304	A86	C5-C6-C8-C9
35	N	304	A86	C7-C6-C8-C9
35	N	305	A86	C39-C38-O4-C34
35	N	306	A86	C10-C11-C13-O
35	N	306	A86	C10-C11-C13-C14
35	N	306	A86	C12-C11-C13-O
35	N	306	A86	C12-C11-C13-C14
35	N	320	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
35	N	320	A86	C12-C11-C13-C14
35	O	301	A86	C5-C6-C8-C9
35	O	301	A86	C7-C6-C8-C9
35	O	302	A86	C10-C11-C13-C14
35	O	302	A86	C12-C11-C13-C14
35	O	305	A86	C39-C38-O4-C34
35	O	305	A86	O5-C38-O4-C34
35	O	305	A86	C5-C6-C8-C9
35	O	305	A86	C7-C6-C8-C9
35	O	319	A86	C11-C10-C9-C8
35	O	319	A86	C10-C11-C13-C14
35	O	319	A86	C12-C11-C13-O
35	P	303	A86	C10-C11-C13-C14
35	P	303	A86	C12-C11-C13-C14
35	P	306	A86	C39-C38-O4-C34
35	Q	303	A86	C2-C1-C24-C25
35	Q	303	A86	C39-C38-O4-C34
35	Q	303	A86	O5-C38-O4-C34
35	Q	304	A86	C10-C11-C13-C14
35	Q	304	A86	C12-C11-C13-O
35	Q	304	A86	C12-C11-C13-C14
35	Q	316	A86	C39-C38-O4-C34
35	R	305	A86	C2-C1-C24-C25
35	R	306	A86	C10-C11-C13-C14
35	R	306	A86	C12-C11-C13-C14
35	R	309	A86	C10-C11-C13-C14
35	R	309	A86	C12-C11-C13-C14
35	S	301	A86	C12-C11-C13-C14
35	S	301	A86	C13-C14-C15-C20
35	S	304	A86	C-C1-C24-C25
35	S	304	A86	C2-C1-C24-C25
35	S	304	A86	C13-C14-C15-C16
35	S	304	A86	C33-C34-O4-C38
35	S	304	A86	C39-C38-O4-C34
35	S	305	A86	C10-C11-C13-C14
35	S	305	A86	C12-C11-C13-O
35	S	305	A86	C12-C11-C13-C14
35	S	305	A86	C13-C14-C15-C20
35	S	308	A86	C-C1-C24-C25
35	S	308	A86	C28-C27-C29-C30
35	W	202	A86	C12-C11-C13-C14
35	X	301	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
35	X	301	A86	C12-C11-C13-C14
35	X	314	A86	O5-C38-O4-C34
35	h	202	A86	C13-C14-C15-O1
35	U	303	A86	C-C1-C24-C25
35	U	303	A86	C2-C1-C24-C25
35	U	303	A86	C11-C10-C9-C8
35	U	303	A86	C13-C14-C15-C16
35	U	303	A86	C39-C38-O4-C34
35	U	303	A86	C5-C6-C8-C9
35	U	304	A86	C-C1-C24-C25
35	U	304	A86	C2-C1-C24-C25
35	U	304	A86	C12-C11-C13-C14
35	U	304	A86	C13-C14-C15-C16
35	U	304	A86	C13-C14-C15-O1
35	U	304	A86	C1-C2-C3-C4
35	V	301	A86	C2-C1-C24-C25
35	V	301	A86	C13-C14-C15-C16
35	V	301	A86	C13-C14-C15-C20
35	V	301	A86	C13-C14-C15-O1
35	V	301	A86	C39-C38-O4-C34
35	V	304	A86	C13-C14-C15-C20
36	A	305	CLA	C4B-C3B-CAB-CBB
36	A	306	CLA	C1A-C2A-CAA-CBA
36	A	309	CLA	CBA-CGA-O2A-C1
36	A	309	CLA	C4B-C3B-CAB-CBB
36	A	309	CLA	CBD-CGD-O2D-CED
36	A	311	CLA	C1A-C2A-CAA-CBA
36	A	311	CLA	C3A-C2A-CAA-CBA
36	A	314	CLA	C1A-C2A-CAA-CBA
36	A	314	CLA	C3A-C2A-CAA-CBA
36	A	314	CLA	C4B-C3B-CAB-CBB
36	B	308	CLA	CBD-CGD-O2D-CED
36	B	308	CLA	C4-C3-C5-C6
36	B	311	CLA	CHA-CBD-CGD-O1D
36	B	311	CLA	CHA-CBD-CGD-O2D
36	C	206	CLA	C11-C10-C8-C7
36	C	207	CLA	C11-C12-C13-C14
36	C	208	CLA	C2B-C3B-CAB-CBB
36	C	208	CLA	C4B-C3B-CAB-CBB
36	C	208	CLA	CHA-CBD-CGD-O1D
36	C	208	CLA	CHA-CBD-CGD-O2D
36	C	210	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	C	210	CLA	CBA-CGA-O2A-C1
36	C	210	CLA	C2B-C3B-CAB-CBB
36	C	210	CLA	C4B-C3B-CAB-CBB
36	D	306	CLA	C4B-C3B-CAB-CBB
36	D	307	CLA	C1A-C2A-CAA-CBA
36	D	308	CLA	C11-C10-C8-C7
36	D	309	CLA	C2B-C3B-CAB-CBB
36	D	309	CLA	C4B-C3B-CAB-CBB
36	D	309	CLA	CBD-CGD-O2D-CED
36	D	311	CLA	C2B-C3B-CAB-CBB
36	D	311	CLA	C4B-C3B-CAB-CBB
36	D	311	CLA	CBD-CGD-O2D-CED
36	D	312	CLA	CBD-CGD-O2D-CED
36	D	316	CLA	C2B-C3B-CAB-CBB
36	D	316	CLA	C4B-C3B-CAB-CBB
36	D	316	CLA	CBD-CGD-O2D-CED
36	D	316	CLA	O1D-CGD-O2D-CED
36	E	308	CLA	C4B-C3B-CAB-CBB
36	E	312	CLA	C1A-C2A-CAA-CBA
36	E	316	CLA	C1A-C2A-CAA-CBA
36	E	316	CLA	C3A-C2A-CAA-CBA
36	E	317	CLA	C3A-C2A-CAA-CBA
36	E	317	CLA	C2B-C3B-CAB-CBB
36	E	317	CLA	C4B-C3B-CAB-CBB
36	E	317	CLA	CHA-CBD-CGD-O2D
36	F	314	CLA	C1A-C2A-CAA-CBA
36	F	314	CLA	C3A-C2A-CAA-CBA
36	F	314	CLA	C6-C7-C8-C10
36	F	317	CLA	C1A-C2A-CAA-CBA
36	G	314	CLA	C2B-C3B-CAB-CBB
36	G	314	CLA	C4B-C3B-CAB-CBB
36	G	315	CLA	CBA-CGA-O2A-C1
36	G	315	CLA	O1A-CGA-O2A-C1
36	G	315	CLA	CBD-CGD-O2D-CED
36	G	316	CLA	C2B-C3B-CAB-CBB
36	G	316	CLA	C4B-C3B-CAB-CBB
36	G	316	CLA	CBD-CGD-O2D-CED
36	H	307	CLA	CBA-CGA-O2A-C1
36	H	307	CLA	O1A-CGA-O2A-C1
36	H	308	CLA	CAD-CBD-CGD-O1D
36	H	308	CLA	CAD-CBD-CGD-O2D
36	H	309	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
36	H	310	CLA	CBA-CGA-O2A-C1
36	H	310	CLA	O1A-CGA-O2A-C1
36	H	310	CLA	C4B-C3B-CAB-CBB
36	H	312	CLA	C1A-C2A-CAA-CBA
36	H	315	CLA	CHA-CBD-CGD-O1D
36	H	315	CLA	CHA-CBD-CGD-O2D
36	H	316	CLA	C4B-C3B-CAB-CBB
36	H	316	CLA	C6-C7-C8-C9
36	H	317	CLA	CBD-CGD-O2D-CED
36	H	318	CLA	CBD-CGD-O2D-CED
36	I	305	CLA	C6-C7-C8-C9
36	I	308	CLA	CAD-CBD-CGD-O1D
36	I	308	CLA	CAD-CBD-CGD-O2D
36	I	309	CLA	C2B-C3B-CAB-CBB
36	I	309	CLA	C4B-C3B-CAB-CBB
36	I	313	CLA	CBD-CGD-O2D-CED
36	I	314	CLA	C4B-C3B-CAB-CBB
36	J	311	CLA	CBA-CGA-O2A-C1
36	J	311	CLA	O1A-CGA-O2A-C1
36	J	311	CLA	C4B-C3B-CAB-CBB
36	J	312	CLA	CBD-CGD-O2D-CED
36	J	313	CLA	C2B-C3B-CAB-CBB
36	J	313	CLA	C4B-C3B-CAB-CBB
36	J	316	CLA	C4B-C3B-CAB-CBB
36	J	316	CLA	CBD-CGD-O2D-CED
36	J	317	CLA	C2B-C3B-CAB-CBB
36	J	317	CLA	C4B-C3B-CAB-CBB
36	K	307	CLA	C1A-C2A-CAA-CBA
36	K	307	CLA	C3A-C2A-CAA-CBA
36	K	307	CLA	CBD-CGD-O2D-CED
36	K	309	CLA	C2B-C3B-CAB-CBB
36	K	309	CLA	C4B-C3B-CAB-CBB
36	K	316	CLA	C2B-C3B-CAB-CBB
36	K	316	CLA	C4B-C3B-CAB-CBB
36	L	308	CLA	C1A-C2A-CAA-CBA
36	L	308	CLA	C3A-C2A-CAA-CBA
36	L	308	CLA	C2B-C3B-CAB-CBB
36	L	308	CLA	C4B-C3B-CAB-CBB
36	L	312	CLA	C3A-C2A-CAA-CBA
36	L	312	CLA	C2B-C3B-CAB-CBB
36	L	312	CLA	C4B-C3B-CAB-CBB
36	L	312	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	L	312	CLA	O1D-CGD-O2D-CED
36	L	314	CLA	C1A-C2A-CAA-CBA
36	M	306	CLA	C2B-C3B-CAB-CBB
36	M	306	CLA	C4B-C3B-CAB-CBB
36	M	307	CLA	CBA-CGA-O2A-C1
36	M	307	CLA	O1A-CGA-O2A-C1
36	M	308	CLA	C2B-C3B-CAB-CBB
36	M	308	CLA	C4B-C3B-CAB-CBB
36	M	309	CLA	CBD-CGD-O2D-CED
36	M	310	CLA	C3A-C2A-CAA-CBA
36	M	310	CLA	CBA-CGA-O2A-C1
36	M	310	CLA	O1A-CGA-O2A-C1
36	M	310	CLA	C2B-C3B-CAB-CBB
36	M	310	CLA	C4B-C3B-CAB-CBB
36	M	315	CLA	C4B-C3B-CAB-CBB
36	M	316	CLA	C1A-C2A-CAA-CBA
36	M	316	CLA	C3A-C2A-CAA-CBA
36	M	316	CLA	CBD-CGD-O2D-CED
36	N	308	CLA	CBD-CGD-O2D-CED
36	N	309	CLA	C2-C3-C5-C6
36	N	311	CLA	C3A-C2A-CAA-CBA
36	N	311	CLA	C2B-C3B-CAB-CBB
36	N	311	CLA	C4B-C3B-CAB-CBB
36	N	316	CLA	C4B-C3B-CAB-CBB
36	N	317	CLA	C2B-C3B-CAB-CBB
36	N	317	CLA	C4B-C3B-CAB-CBB
36	N	317	CLA	CBD-CGD-O2D-CED
36	N	318	CLA	C4B-C3B-CAB-CBB
36	N	319	CLA	CAD-CBD-CGD-O1D
36	N	319	CLA	CBD-CGD-O2D-CED
36	O	306	CLA	C2B-C3B-CAB-CBB
36	O	306	CLA	C4B-C3B-CAB-CBB
36	O	310	CLA	C1A-C2A-CAA-CBA
36	O	310	CLA	CBA-CGA-O2A-C1
36	O	310	CLA	O1A-CGA-O2A-C1
36	O	310	CLA	C4B-C3B-CAB-CBB
36	O	310	CLA	CBD-CGD-O2D-CED
36	O	316	CLA	C1A-C2A-CAA-CBA
36	O	316	CLA	C3A-C2A-CAA-CBA
36	P	302	CLA	C1A-C2A-CAA-CBA
36	P	302	CLA	C3A-C2A-CAA-CBA
36	P	308	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	P	308	CLA	C4B-C3B-CAB-CBB
36	P	312	CLA	C1A-C2A-CAA-CBA
36	P	312	CLA	CBA-CGA-O2A-C1
36	P	312	CLA	O1A-CGA-O2A-C1
36	P	312	CLA	C4B-C3B-CAB-CBB
36	P	312	CLA	CBD-CGD-O2D-CED
36	P	314	CLA	C1A-C2A-CAA-CBA
36	P	314	CLA	C3A-C2A-CAA-CBA
36	P	318	CLA	C1A-C2A-CAA-CBA
36	Q	305	CLA	C2B-C3B-CAB-CBB
36	Q	305	CLA	C4B-C3B-CAB-CBB
36	Q	309	CLA	C1A-C2A-CAA-CBA
36	Q	309	CLA	CBA-CGA-O2A-C1
36	Q	309	CLA	O1A-CGA-O2A-C1
36	Q	309	CLA	C4B-C3B-CAB-CBB
36	Q	309	CLA	CBD-CGD-O2D-CED
36	Q	314	CLA	CHA-CBD-CGD-O1D
36	Q	314	CLA	CHA-CBD-CGD-O2D
36	Q	314	CLA	CBD-CGD-O2D-CED
36	R	311	CLA	CBD-CGD-O2D-CED
36	R	314	CLA	C3A-C2A-CAA-CBA
36	R	314	CLA	CBA-CGA-O2A-C1
36	R	314	CLA	C4B-C3B-CAB-CBB
36	R	316	CLA	C1A-C2A-CAA-CBA
36	R	318	CLA	CBD-CGD-O2D-CED
36	R	321	CLA	CHA-CBD-CGD-O2D
36	R	322	CLA	C1A-C2A-CAA-CBA
36	R	322	CLA	CBD-CGD-O2D-CED
36	S	310	CLA	CBD-CGD-O2D-CED
36	S	310	CLA	O2A-C1-C2-C3
36	S	311	CLA	CBD-CGD-O2D-CED
36	S	312	CLA	CAD-CBD-CGD-O1D
36	S	312	CLA	CAD-CBD-CGD-O2D
36	S	312	CLA	CBD-CGD-O2D-CED
36	S	313	CLA	C3A-C2A-CAA-CBA
36	S	313	CLA	CBA-CGA-O2A-C1
36	S	314	CLA	C1A-C2A-CAA-CBA
36	S	314	CLA	C2B-C3B-CAB-CBB
36	S	314	CLA	C4B-C3B-CAB-CBB
36	S	314	CLA	CBD-CGD-O2D-CED
36	S	314	CLA	O1D-CGD-O2D-CED
36	S	314	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	S	314	CLA	C4-C3-C5-C6
36	S	315	CLA	C2B-C3B-CAB-CBB
36	S	315	CLA	C4B-C3B-CAB-CBB
36	S	318	CLA	C1A-C2A-CAA-CBA
36	S	318	CLA	C3A-C2A-CAA-CBA
36	S	318	CLA	C4B-C3B-CAB-CBB
36	S	319	CLA	C2B-C3B-CAB-CBB
36	S	319	CLA	C4B-C3B-CAB-CBB
36	S	320	CLA	C1A-C2A-CAA-CBA
36	S	321	CLA	C1A-C2A-CAA-CBA
36	S	321	CLA	C2B-C3B-CAB-CBB
36	S	321	CLA	C4B-C3B-CAB-CBB
36	T	308	CLA	C2B-C3B-CAB-CBB
36	T	308	CLA	C4B-C3B-CAB-CBB
36	T	308	CLA	CBD-CGD-O2D-CED
36	T	312	CLA	C1A-C2A-CAA-CBA
36	T	312	CLA	C4B-C3B-CAB-CBB
36	T	314	CLA	C1A-C2A-CAA-CBA
36	W	208	CLA	C2B-C3B-CAB-CBB
36	W	208	CLA	C4B-C3B-CAB-CBB
36	W	209	CLA	CHA-CBD-CGD-O1D
36	W	209	CLA	CHA-CBD-CGD-O2D
36	W	210	CLA	C3A-C2A-CAA-CBA
36	W	210	CLA	C2B-C3B-CAB-CBB
36	W	210	CLA	C4B-C3B-CAB-CBB
36	W	212	CLA	C1A-C2A-CAA-CBA
36	W	214	CLA	C4B-C3B-CAB-CBB
36	W	215	CLA	C2B-C3B-CAB-CBB
36	W	215	CLA	C4B-C3B-CAB-CBB
36	W	216	CLA	C4B-C3B-CAB-CBB
36	X	307	CLA	CBD-CGD-O2D-CED
36	X	308	CLA	C1A-C2A-CAA-CBA
36	X	308	CLA	C4B-C3B-CAB-CBB
36	X	309	CLA	C1A-C2A-CAA-CBA
36	X	310	CLA	C2B-C3B-CAB-CBB
36	X	310	CLA	C4B-C3B-CAB-CBB
36	X	310	CLA	CBD-CGD-O2D-CED
36	X	312	CLA	CBD-CGD-O2D-CED
36	X	313	CLA	C1A-C2A-CAA-CBA
36	X	313	CLA	C3A-C2A-CAA-CBA
36	X	313	CLA	CBD-CGD-O2D-CED
36	a	803	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	a	803	CLA	CBA-CGA-O2A-C1
36	a	804	CLA	CAD-CBD-CGD-O1D
36	a	804	CLA	CAD-CBD-CGD-O2D
36	a	805	CLA	C1A-C2A-CAA-CBA
36	a	805	CLA	C3A-C2A-CAA-CBA
36	a	806	CLA	C2B-C3B-CAB-CBB
36	a	806	CLA	C4B-C3B-CAB-CBB
36	a	807	CLA	C3A-C2A-CAA-CBA
36	a	807	CLA	CHA-CBD-CGD-O2D
36	a	810	CLA	C2B-C3B-CAB-CBB
36	a	810	CLA	C4B-C3B-CAB-CBB
36	a	812	CLA	C11-C10-C8-C9
36	a	816	CLA	C1A-C2A-CAA-CBA
36	a	816	CLA	C3A-C2A-CAA-CBA
36	a	816	CLA	CHA-CBD-CGD-O1D
36	a	816	CLA	CHA-CBD-CGD-O2D
36	a	817	CLA	C3A-C2A-CAA-CBA
36	a	817	CLA	C4B-C3B-CAB-CBB
36	a	818	CLA	C1A-C2A-CAA-CBA
36	a	818	CLA	C3A-C2A-CAA-CBA
36	a	821	CLA	C1A-C2A-CAA-CBA
36	a	821	CLA	C3A-C2A-CAA-CBA
36	a	822	CLA	C2-C3-C5-C6
36	a	823	CLA	C2B-C3B-CAB-CBB
36	a	824	CLA	CHA-CBD-CGD-O1D
36	a	824	CLA	CHA-CBD-CGD-O2D
36	a	825	CLA	C3A-C2A-CAA-CBA
36	a	825	CLA	C11-C10-C8-C9
36	a	827	CLA	C11-C12-C13-C14
36	a	829	CLA	CHA-CBD-CGD-O1D
36	a	829	CLA	CHA-CBD-CGD-O2D
36	a	830	CLA	C1A-C2A-CAA-CBA
36	a	830	CLA	C3A-C2A-CAA-CBA
36	a	832	CLA	C2B-C3B-CAB-CBB
36	a	832	CLA	C4B-C3B-CAB-CBB
36	a	832	CLA	CHA-CBD-CGD-O1D
36	a	832	CLA	CHA-CBD-CGD-O2D
36	a	833	CLA	C4B-C3B-CAB-CBB
36	a	834	CLA	C4B-C3B-CAB-CBB
36	a	836	CLA	CBD-CGD-O2D-CED
36	a	841	CLA	C3A-C2A-CAA-CBA
36	a	848	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	a	848	CLA	C2-C3-C5-C6
36	a	848	CLA	C4-C3-C5-C6
36	b	808	CLA	C1A-C2A-CAA-CBA
36	b	808	CLA	C3A-C2A-CAA-CBA
36	b	809	CLA	C6-C7-C8-C9
36	b	810	CLA	C2B-C3B-CAB-CBB
36	b	810	CLA	C4B-C3B-CAB-CBB
36	b	811	CLA	CHA-CBD-CGD-O1D
36	b	811	CLA	CHA-CBD-CGD-O2D
36	b	816	CLA	C1A-C2A-CAA-CBA
36	b	816	CLA	C3A-C2A-CAA-CBA
36	b	817	CLA	CHA-CBD-CGD-O1D
36	b	817	CLA	CHA-CBD-CGD-O2D
36	b	819	CLA	C2B-C3B-CAB-CBB
36	b	819	CLA	C4B-C3B-CAB-CBB
36	b	820	CLA	C3A-C2A-CAA-CBA
36	b	821	CLA	C2B-C3B-CAB-CBB
36	b	821	CLA	C4B-C3B-CAB-CBB
36	b	822	CLA	C2B-C3B-CAB-CBB
36	b	822	CLA	C4B-C3B-CAB-CBB
36	b	824	CLA	C1A-C2A-CAA-CBA
36	b	824	CLA	C2B-C3B-CAB-CBB
36	b	824	CLA	C4B-C3B-CAB-CBB
36	b	824	CLA	C4-C3-C5-C6
36	b	825	CLA	CHA-CBD-CGD-O1D
36	b	825	CLA	CHA-CBD-CGD-O2D
36	b	826	CLA	CBD-CGD-O2D-CED
36	b	826	CLA	C11-C10-C8-C9
36	b	827	CLA	C1A-C2A-CAA-CBA
36	b	828	CLA	C1A-C2A-CAA-CBA
36	b	828	CLA	C3A-C2A-CAA-CBA
36	b	829	CLA	C1A-C2A-CAA-CBA
36	b	829	CLA	C3A-C2A-CAA-CBA
36	b	831	CLA	C1A-C2A-CAA-CBA
36	b	831	CLA	C3A-C2A-CAA-CBA
36	b	836	CLA	C4-C3-C5-C6
36	f	803	CLA	C11-C10-C8-C9
36	f	804	CLA	CBD-CGD-O2D-CED
36	i	102	CLA	C1A-C2A-CAA-CBA
36	i	102	CLA	C3A-C2A-CAA-CBA
36	i	102	CLA	CAD-CBD-CGD-O1D
36	i	102	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
36	i	102	CLA	CBD-CGD-O2D-CED
36	j	106	CLA	CAD-CBD-CGD-O1D
36	j	106	CLA	CAD-CBD-CGD-O2D
36	l	202	CLA	C1A-C2A-CAA-CBA
36	l	204	CLA	C3A-C2A-CAA-CBA
36	h	203	CLA	C1A-C2A-CAA-CBA
36	U	307	CLA	C4B-C3B-CAB-CBB
36	U	309	CLA	C1A-C2A-CAA-CBA
36	U	309	CLA	CBA-CGA-O2A-C1
36	U	309	CLA	C2B-C3B-CAB-CBB
36	U	309	CLA	C4B-C3B-CAB-CBB
36	U	310	CLA	CBD-CGD-O2D-CED
36	U	311	CLA	C3A-C2A-CAA-CBA
36	V	305	CLA	C4B-C3B-CAB-CBB
36	V	306	CLA	CBD-CGD-O2D-CED
36	V	309	CLA	C3A-C2A-CAA-CBA
36	V	311	CLA	C1A-C2A-CAA-CBA
36	V	313	CLA	C1A-C2A-CAA-CBA
36	V	313	CLA	CBD-CGD-O2D-CED
36	V	314	CLA	C1A-C2A-CAA-CBA
36	V	314	CLA	CBD-CGD-O2D-CED
37	C	213	KC1	C3A-C2A-CAA-CBA
37	D	314	KC1	C3A-C2A-CAA-CBA
37	F	308	KC1	C2B-C3B-CAB-CBB
37	F	308	KC1	C4B-C3B-CAB-CBB
37	F	315	KC1	CBD-CGD-O2D-CED
37	G	317	KC1	C3A-C2A-CAA-CBA
37	G	317	KC1	CBD-CGD-O2D-CED
37	G	318	KC1	CHA-CBD-CGD-O2D
37	H	313	KC1	C3A-C2A-CAA-CBA
37	K	314	KC1	C1A-C2A-CAA-CBA
37	K	314	KC1	C3A-C2A-CAA-CBA
37	L	315	KC1	C3A-C2A-CAA-CBA
37	M	313	KC1	CBD-CGD-O2D-CED
37	M	318	KC1	C3A-C2A-CAA-CBA
37	M	318	KC1	C2B-C3B-CAB-CBB
37	M	318	KC1	CBD-CGD-O2D-CED
37	N	314	KC1	C3A-C2A-CAA-CBA
37	P	317	KC1	C3A-C2A-CAA-CBA
37	S	316	KC1	C1A-C2A-CAA-CBA
37	S	316	KC1	C3A-C2A-CAA-CBA
37	T	315	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	T	315	KC1	CAA-CBA-CGA-O2A
37	W	213	KC1	C3A-C2A-CAA-CBA
37	W	217	KC1	C2B-C3B-CAB-CBB
37	W	217	KC1	C4B-C3B-CAB-CBB
37	X	311	KC1	C3A-C2A-CAA-CBA
37	U	312	KC1	C1A-C2A-CAA-CBA
37	U	312	KC1	C3A-C2A-CAA-CBA
37	V	312	KC1	C1A-C2A-CAA-CBA
37	V	312	KC1	C3A-C2A-CAA-CBA
38	b	804	SQD	C2-C1-O6-C44
38	b	804	SQD	O5-C1-O6-C44
38	b	804	SQD	O5-C5-C6-S
39	B	312	LMT	O5'-C1'-O1'-C1
39	E	323	LMT	O5'-C1'-O1'-C1
39	E	323	LMT	C2-C1-O1'-C1'
39	F	320	LMT	O5'-C1'-O1'-C1
39	F	321	LMT	C3'-C4'-O1B-C1B
39	G	322	LMT	C2-C1-O1'-C1'
39	G	323	LMT	C2-C1-O1'-C1'
39	I	317	LMT	O5'-C1'-O1'-C1
39	K	318	LMT	O5'-C1'-O1'-C1
39	L	318	LMT	C2'-C1'-O1'-C1
39	P	320	LMT	O5'-C1'-O1'-C1
39	P	320	LMT	C2-C1-O1'-C1'
39	P	321	LMT	C2'-C1'-O1'-C1
39	P	321	LMT	O5'-C1'-O1'-C1
39	a	853	LMT	O5'-C1'-O1'-C1
39	a	854	LMT	C2'-C1'-O1'-C1
39	a	854	LMT	O5'-C1'-O1'-C1
39	b	848	LMT	C2'-C1'-O1'-C1
39	b	848	LMT	O5'-C1'-O1'-C1
39	b	848	LMT	C2-C1-O1'-C1'
39	f	807	LMT	O5'-C1'-O1'-C1
39	h	205	LMT	C2-C1-O1'-C1'
40	C	215	DGD	C2B-C1B-O2G-C2G
40	L	302	DGD	O1A-C1A-O1G-C1G
40	b	849	DGD	O2G-C2G-C3G-O3G
41	D	318	LHG	C3-O3-P-O5
41	D	318	LHG	C3-O3-P-O6
41	D	318	LHG	O9-C7-O7-C5
41	D	318	LHG	C8-C7-O7-C5
41	D	319	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
41	D	319	LHG	C3-O3-P-O5
41	D	319	LHG	C8-C7-O7-C5
41	E	322	LHG	C4-O6-P-O3
41	E	322	LHG	C4-O6-P-O4
41	E	322	LHG	C4-O6-P-O5
41	F	319	LHG	C3-O3-P-O4
41	F	319	LHG	C3-O3-P-O6
41	F	319	LHG	C4-O6-P-O5
41	F	319	LHG	C8-C7-O7-C5
41	G	301	LHG	C1-C2-C3-O3
41	G	301	LHG	C4-O6-P-O3
41	G	301	LHG	C4-O6-P-O5
41	G	321	LHG	C3-O3-P-O4
41	G	321	LHG	C3-O3-P-O6
41	G	321	LHG	C4-O6-P-O3
41	G	321	LHG	C4-O6-P-O5
41	I	316	LHG	C1-C2-C3-O3
41	I	316	LHG	C4-O6-P-O3
41	I	316	LHG	C4-O6-P-O4
41	O	317	LHG	C1-C2-C3-O3
41	O	317	LHG	C3-O3-P-O5
41	O	317	LHG	C3-O3-P-O6
41	O	317	LHG	C4-O6-P-O5
41	O	318	LHG	O1-C1-C2-O2
41	O	318	LHG	O1-C1-C2-C3
41	O	318	LHG	C3-O3-P-O4
41	O	318	LHG	C3-O3-P-O6
41	Q	315	LHG	C1-C2-C3-O3
41	Q	315	LHG	C3-O3-P-O5
41	Q	315	LHG	C4-O6-P-O5
41	Q	315	LHG	C5-C4-O6-P
41	Q	315	LHG	C8-C7-O7-C5
41	R	323	LHG	O1-C1-C2-O2
41	R	323	LHG	O1-C1-C2-C3
41	R	323	LHG	C4-O6-P-O5
41	R	323	LHG	O9-C7-O7-C5
41	a	842	LHG	O1-C1-C2-C3
41	a	842	LHG	C3-O3-P-O5
41	a	842	LHG	C4-O6-P-O4
41	a	843	LHG	C3-O3-P-O5
41	a	850	LHG	C3-O3-P-O5
41	a	850	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
41	a	850	LHG	O9-C7-O7-C5
41	a	850	LHG	C8-C7-O7-C5
41	b	850	LHG	C4-O6-P-O3
41	b	850	LHG	C4-O6-P-O4
41	b	850	LHG	C4-O6-P-O5
41	b	850	LHG	O9-C7-O7-C5
41	b	850	LHG	C8-C7-O7-C5
41	f	808	LHG	C1-C2-C3-O3
41	f	808	LHG	C2-C3-O3-P
41	f	809	LHG	C2-C3-O3-P
41	f	809	LHG	C3-O3-P-O4
41	f	809	LHG	C4-O6-P-O3
41	f	809	LHG	C4-O6-P-O4
41	f	809	LHG	C4-O6-P-O5
41	i	104	LHG	C2-C3-O3-P
41	i	104	LHG	C4-O6-P-O3
41	i	104	LHG	C4-O6-P-O4
41	i	104	LHG	C4-O6-P-O5
41	i	104	LHG	O10-C23-O8-C6
41	i	104	LHG	C24-C23-O8-C6
41	j	104	LHG	C3-O3-P-O5
41	j	104	LHG	C4-O6-P-O3
41	l	208	LHG	C4-O6-P-O3
41	l	208	LHG	C4-O6-P-O4
41	l	208	LHG	C8-C7-O7-C5
42	D	320	LMG	C11-C10-O7-C8
42	D	321	LMG	O6-C1-O1-C7
42	E	318	LMG	O6-C1-O1-C7
42	E	319	LMG	C11-C10-O7-C8
42	G	324	LMG	O10-C28-O8-C9
42	G	324	LMG	C29-C28-O8-C9
42	I	315	LMG	C11-C10-O7-C8
42	J	318	LMG	O9-C10-O7-C8
42	J	319	LMG	O9-C10-O7-C8
42	a	852	LMG	C11-C10-O7-C8
42	j	105	LMG	O6-C1-O1-C7
42	j	105	LMG	O10-C28-O8-C9
42	j	105	LMG	C29-C28-O8-C9
42	m	102	LMG	C11-C10-O7-C8
42	h	206	LMG	C2-C1-O1-C7
42	h	206	LMG	O6-C1-O1-C7
42	h	206	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
42	h	206	LMG	C29-C28-O8-C9
42	V	315	LMG	O9-C10-O7-C8
43	a	840	PQN	C21-C22-C23-C24
44	a	845	BCR	C7-C8-C9-C10
44	a	845	BCR	C7-C8-C9-C34
44	a	845	BCR	C21-C22-C23-C24
44	a	846	BCR	C7-C8-C9-C10
44	a	847	BCR	C21-C22-C23-C24
44	b	843	BCR	C7-C8-C9-C10
44	b	843	BCR	C37-C22-C23-C24
44	b	844	BCR	C11-C10-C9-C8
44	b	844	BCR	C21-C22-C23-C24
44	b	844	BCR	C37-C22-C23-C24
44	f	801	BCR	C7-C8-C9-C34
44	f	801	BCR	C21-C22-C23-C24
44	f	801	BCR	C37-C22-C23-C24
44	f	806	BCR	C7-C8-C9-C34
44	f	806	BCR	C35-C13-C14-C15
44	i	103	BCR	C21-C22-C23-C24
44	i	103	BCR	C23-C24-C25-C26
44	i	103	BCR	C23-C24-C25-C30
44	j	107	BCR	C7-C8-C9-C10
44	j	107	BCR	C7-C8-C9-C34
44	l	203	BCR	C11-C10-C9-C8
44	l	203	BCR	C21-C22-C23-C24
44	l	203	BCR	C37-C22-C23-C24
44	l	207	BCR	C7-C8-C9-C10
44	m	101	BCR	C7-C8-C9-C10
44	m	101	BCR	C7-C8-C9-C34
44	m	101	BCR	C20-C21-C22-C37
44	h	201	BCR	C7-C8-C9-C10
44	h	201	BCR	C22-C23-C24-C25
36	L	308	CLA	C4C-C3C-CAC-CBC
36	a	819	CLA	C4C-C3C-CAC-CBC
36	a	824	CLA	C4C-C3C-CAC-CBC
37	G	318	KC1	C4C-C3C-CAC-CBC
36	G	314	CLA	O1D-CGD-O2D-CED
36	G	316	CLA	O1D-CGD-O2D-CED
36	H	316	CLA	O1D-CGD-O2D-CED
36	K	307	CLA	O1D-CGD-O2D-CED
36	N	312	CLA	O1D-CGD-O2D-CED
36	Q	314	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	W	212	CLA	O1D-CGD-O2D-CED
36	X	310	CLA	O1D-CGD-O2D-CED
36	a	848	CLA	O1D-CGD-O2D-CED
36	h	203	CLA	O1D-CGD-O2D-CED
36	V	306	CLA	O1D-CGD-O2D-CED
37	F	315	KC1	O1D-CGD-O2D-CED
35	A	302	A86	C39-C38-O4-C34
35	B	303	A86	C39-C38-O4-C34
35	F	307	A86	C39-C38-O4-C34
35	G	302	A86	O5-C38-O4-C34
35	G	306	A86	O5-C38-O4-C34
35	I	302	A86	C39-C38-O4-C34
35	J	301	A86	C39-C38-O4-C34
35	J	302	A86	C39-C38-O4-C34
35	J	303	A86	C39-C38-O4-C34
35	K	301	A86	C39-C38-O4-C34
35	K	303	A86	C39-C38-O4-C34
35	K	306	A86	C39-C38-O4-C34
35	L	304	A86	C39-C38-O4-C34
35	L	306	A86	C39-C38-O4-C34
35	M	302	A86	C39-C38-O4-C34
35	M	304	A86	O5-C38-O4-C34
35	M	305	A86	C39-C38-O4-C34
35	N	302	A86	C39-C38-O4-C34
35	N	305	A86	O5-C38-O4-C34
35	N	306	A86	C39-C38-O4-C34
35	N	320	A86	C39-C38-O4-C34
35	O	303	A86	C39-C38-O4-C34
35	O	319	A86	C39-C38-O4-C34
35	P	304	A86	C39-C38-O4-C34
35	P	306	A86	O5-C38-O4-C34
35	Q	301	A86	C39-C38-O4-C34
35	Q	304	A86	C39-C38-O4-C34
35	Q	316	A86	O5-C38-O4-C34
35	R	302	A86	C39-C38-O4-C34
35	R	306	A86	C39-C38-O4-C34
35	R	309	A86	C39-C38-O4-C34
35	S	302	A86	C39-C38-O4-C34
35	S	305	A86	C39-C38-O4-C34
35	T	302	A86	C39-C38-O4-C34
35	T	306	A86	C39-C38-O4-C34
35	T	307	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	W	203	A86	C39-C38-O4-C34
35	X	302	A86	C39-C38-O4-C34
35	X	305	A86	C39-C38-O4-C34
35	X	314	A86	C39-C38-O4-C34
35	h	202	A86	C39-C38-O4-C34
35	U	302	A86	C39-C38-O4-C34
35	U	303	A86	O5-C38-O4-C34
35	V	302	A86	C39-C38-O4-C34
35	V	304	A86	C39-C38-O4-C34
39	K	317	LMT	C2B-C1B-O1B-C4'
36	R	316	CLA	C4C-C3C-CAC-CBC
36	R	319	CLA	C4C-C3C-CAC-CBC
37	F	308	KC1	C4C-C3C-CAC-CBC
36	K	310	CLA	C2C-C3C-CAC-CBC
36	L	308	CLA	C2C-C3C-CAC-CBC
36	B	308	CLA	O1D-CGD-O2D-CED
36	B	309	CLA	O1D-CGD-O2D-CED
36	D	309	CLA	O1D-CGD-O2D-CED
36	N	317	CLA	O1D-CGD-O2D-CED
36	O	310	CLA	O1D-CGD-O2D-CED
36	P	312	CLA	O1D-CGD-O2D-CED
36	P	319	CLA	O1D-CGD-O2D-CED
36	Q	309	CLA	O1D-CGD-O2D-CED
36	R	322	CLA	O1D-CGD-O2D-CED
36	W	209	CLA	O1D-CGD-O2D-CED
36	X	315	CLA	O1D-CGD-O2D-CED
36	b	826	CLA	O1D-CGD-O2D-CED
36	i	102	CLA	O1D-CGD-O2D-CED
36	V	308	CLA	O1D-CGD-O2D-CED
36	V	314	CLA	O1D-CGD-O2D-CED
37	M	318	KC1	O1D-CGD-O2D-CED
35	A	316	A86	O5-C38-O4-C34
35	B	301	A86	C39-C38-O4-C34
35	C	204	A86	C39-C38-O4-C34
35	D	302	A86	O5-C38-O4-C34
35	F	301	A86	C39-C38-O4-C34
35	F	302	A86	O5-C38-O4-C34
35	F	305	A86	C39-C38-O4-C34
35	I	301	A86	C39-C38-O4-C34
35	J	305	A86	C39-C38-O4-C34
35	J	306	A86	O5-C38-O4-C34
35	N	304	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	R	304	A86	C39-C38-O4-C34
35	S	304	A86	O5-C38-O4-C34
35	V	301	A86	O5-C38-O4-C34
36	A	307	CLA	CBD-CGD-O2D-CED
36	A	313	CLA	CBD-CGD-O2D-CED
36	B	306	CLA	CBD-CGD-O2D-CED
36	B	309	CLA	CBD-CGD-O2D-CED
36	B	311	CLA	CBD-CGD-O2D-CED
36	D	313	CLA	CBD-CGD-O2D-CED
36	G	309	CLA	CBD-CGD-O2D-CED
36	G	313	CLA	CBD-CGD-O2D-CED
36	G	314	CLA	CBD-CGD-O2D-CED
36	H	305	CLA	CBD-CGD-O2D-CED
36	H	312	CLA	CBD-CGD-O2D-CED
36	H	316	CLA	CBD-CGD-O2D-CED
36	J	315	CLA	CBD-CGD-O2D-CED
36	K	309	CLA	CBD-CGD-O2D-CED
36	K	310	CLA	CBD-CGD-O2D-CED
36	L	311	CLA	CBD-CGD-O2D-CED
36	L	314	CLA	CBD-CGD-O2D-CED
36	M	312	CLA	CBD-CGD-O2D-CED
36	M	314	CLA	CBD-CGD-O2D-CED
36	M	315	CLA	CBD-CGD-O2D-CED
36	N	312	CLA	CBD-CGD-O2D-CED
36	N	318	CLA	CBD-CGD-O2D-CED
36	O	309	CLA	CBD-CGD-O2D-CED
36	P	311	CLA	CBD-CGD-O2D-CED
36	P	318	CLA	CBD-CGD-O2D-CED
36	P	319	CLA	CBD-CGD-O2D-CED
36	Q	308	CLA	CBD-CGD-O2D-CED
36	R	313	CLA	CBD-CGD-O2D-CED
36	S	315	CLA	CBD-CGD-O2D-CED
36	S	318	CLA	CBD-CGD-O2D-CED
36	S	321	CLA	CBD-CGD-O2D-CED
36	T	309	CLA	CBD-CGD-O2D-CED
36	T	313	CLA	CBD-CGD-O2D-CED
36	W	209	CLA	CBD-CGD-O2D-CED
36	W	212	CLA	CBD-CGD-O2D-CED
36	W	214	CLA	CBD-CGD-O2D-CED
36	X	308	CLA	CBD-CGD-O2D-CED
36	X	315	CLA	CBD-CGD-O2D-CED
36	a	817	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	b	840	CLA	CBD-CGD-O2D-CED
36	j	106	CLA	CBD-CGD-O2D-CED
36	h	203	CLA	CBD-CGD-O2D-CED
36	U	308	CLA	CBD-CGD-O2D-CED
36	U	311	CLA	CBD-CGD-O2D-CED
36	U	313	CLA	CBD-CGD-O2D-CED
36	V	308	CLA	CBD-CGD-O2D-CED
36	V	311	CLA	CBD-CGD-O2D-CED
36	A	306	CLA	O1A-CGA-O2A-C1
36	D	307	CLA	O1A-CGA-O2A-C1
36	D	308	CLA	O1A-CGA-O2A-C1
36	H	311	CLA	O1A-CGA-O2A-C1
36	I	310	CLA	O1A-CGA-O2A-C1
36	a	803	CLA	O1A-CGA-O2A-C1
41	G	301	LHG	O10-C23-O8-C6
42	E	319	LMG	O10-C28-O8-C9
42	J	318	LMG	O10-C28-O8-C9
36	A	309	CLA	O1A-CGA-O2A-C1
36	C	210	CLA	O1A-CGA-O2A-C1
36	R	314	CLA	O1A-CGA-O2A-C1
36	S	313	CLA	O1A-CGA-O2A-C1
36	W	210	CLA	O1A-CGA-O2A-C1
36	U	309	CLA	O1A-CGA-O2A-C1
39	G	322	LMT	C5'-C4'-O1B-C1B
36	E	316	CLA	C4C-C3C-CAC-CBC
37	T	310	KC1	C4C-C3C-CAC-CBC
36	X	308	CLA	C2C-C3C-CAC-CBC
36	a	824	CLA	C2C-C3C-CAC-CBC
37	G	318	KC1	C2C-C3C-CAC-CBC
37	G	317	KC1	O1D-CGD-O2D-CED
35	F	304	A86	C39-C38-O4-C34
35	P	307	A86	C39-C38-O4-C34
36	O	316	CLA	C15-C16-C17-C18
36	j	102	CLA	C8-C10-C11-C12
39	L	318	LMT	C2B-C1B-O1B-C4'
35	A	316	A86	C35-C34-O4-C38
35	C	204	A86	C33-C34-O4-C38
35	G	302	A86	C35-C34-O4-C38
35	O	305	A86	C35-C34-O4-C38
35	S	308	A86	C35-C34-O4-C38
35	U	303	A86	C33-C34-O4-C38
35	V	301	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
36	K	311	CLA	CBA-CGA-O2A-C1
36	W	210	CLA	CBA-CGA-O2A-C1
36	K	310	CLA	C4C-C3C-CAC-CBC
36	M	308	CLA	C4C-C3C-CAC-CBC
36	a	819	CLA	C2C-C3C-CAC-CBC
37	F	308	KC1	C2C-C3C-CAC-CBC
36	B	311	CLA	O1D-CGD-O2D-CED
36	H	312	CLA	O1D-CGD-O2D-CED
36	K	310	CLA	O1D-CGD-O2D-CED
36	W	214	CLA	O1D-CGD-O2D-CED
36	U	308	CLA	O1D-CGD-O2D-CED
36	U	313	CLA	O1D-CGD-O2D-CED
36	A	306	CLA	CBA-CGA-O2A-C1
36	D	307	CLA	CBA-CGA-O2A-C1
36	D	308	CLA	CBA-CGA-O2A-C1
40	L	302	DGD	C2A-C1A-O1G-C1G
42	E	319	LMG	C29-C28-O8-C9
42	J	318	LMG	C29-C28-O8-C9
35	L	301	A86	O5-C38-O4-C34
36	F	312	CLA	CBD-CGD-O2D-CED
36	b	835	CLA	CBD-CGD-O2D-CED
36	V	307	CLA	CBD-CGD-O2D-CED
36	A	310	CLA	O1A-CGA-O2A-C1
36	B	308	CLA	O1A-CGA-O2A-C1
36	D	312	CLA	O1A-CGA-O2A-C1
36	F	314	CLA	O1A-CGA-O2A-C1
36	G	311	CLA	O1A-CGA-O2A-C1
36	G	312	CLA	O1A-CGA-O2A-C1
36	G	319	CLA	O1A-CGA-O2A-C1
36	J	307	CLA	O1A-CGA-O2A-C1
36	L	309	CLA	O1A-CGA-O2A-C1
36	L	313	CLA	O1A-CGA-O2A-C1
36	N	312	CLA	O1A-CGA-O2A-C1
36	O	308	CLA	O1A-CGA-O2A-C1
36	P	310	CLA	O1A-CGA-O2A-C1
36	Q	307	CLA	O1A-CGA-O2A-C1
36	R	311	CLA	O1A-CGA-O2A-C1
36	T	309	CLA	O1A-CGA-O2A-C1
36	T	313	CLA	O1A-CGA-O2A-C1
36	W	207	CLA	O1A-CGA-O2A-C1
36	a	804	CLA	O1A-CGA-O2A-C1
36	a	816	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	a	818	CLA	O1A-CGA-O2A-C1
36	a	839	CLA	O1A-CGA-O2A-C1
36	b	834	CLA	O1A-CGA-O2A-C1
36	f	804	CLA	O1A-CGA-O2A-C1
36	V	306	CLA	O1A-CGA-O2A-C1
41	a	850	LHG	O10-C23-O8-C6
41	f	809	LHG	O10-C23-O8-C6
42	D	321	LMG	O10-C28-O8-C9
42	a	852	LMG	O10-C28-O8-C9
42	m	102	LMG	O10-C28-O8-C9
36	b	817	CLA	C8-C10-C11-C12
36	G	315	CLA	O1D-CGD-O2D-CED
36	I	313	CLA	O1D-CGD-O2D-CED
36	L	311	CLA	O1D-CGD-O2D-CED
36	M	316	CLA	O1D-CGD-O2D-CED
36	N	308	CLA	O1D-CGD-O2D-CED
36	R	318	CLA	O1D-CGD-O2D-CED
36	S	310	CLA	O1D-CGD-O2D-CED
36	S	312	CLA	O1D-CGD-O2D-CED
36	X	308	CLA	O1D-CGD-O2D-CED
36	X	313	CLA	O1D-CGD-O2D-CED
36	U	310	CLA	O1D-CGD-O2D-CED
37	K	314	KC1	CAA-CBA-CGA-O1A
37	K	314	KC1	CAA-CBA-CGA-O2A
37	R	317	KC1	CAA-CBA-CGA-O1A
37	R	317	KC1	CAA-CBA-CGA-O2A
37	S	316	KC1	CAA-CBA-CGA-O1A
37	T	315	KC1	CAA-CBA-CGA-O1A
39	a	851	LMT	C3'-C4'-O1B-C1B
37	E	309	KC1	C4C-C3C-CAC-CBC
36	E	316	CLA	C2C-C3C-CAC-CBC
37	E	309	KC1	C2C-C3C-CAC-CBC
36	D	311	CLA	O1D-CGD-O2D-CED
36	D	312	CLA	O1D-CGD-O2D-CED
36	H	318	CLA	O1D-CGD-O2D-CED
36	J	312	CLA	O1D-CGD-O2D-CED
36	J	316	CLA	O1D-CGD-O2D-CED
36	N	319	CLA	O1D-CGD-O2D-CED
36	S	311	CLA	O1D-CGD-O2D-CED
36	T	308	CLA	O1D-CGD-O2D-CED
36	X	307	CLA	O1D-CGD-O2D-CED
36	X	312	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	f	804	CLA	O1D-CGD-O2D-CED
37	M	313	KC1	O1D-CGD-O2D-CED
35	A	302	A86	O5-C38-O4-C34
35	C	202	A86	C39-C38-O4-C34
35	G	304	A86	C39-C38-O4-C34
35	I	302	A86	O5-C38-O4-C34
35	J	301	A86	O5-C38-O4-C34
35	J	302	A86	O5-C38-O4-C34
35	J	303	A86	O5-C38-O4-C34
35	K	303	A86	O5-C38-O4-C34
35	M	302	A86	O5-C38-O4-C34
35	M	305	A86	O5-C38-O4-C34
35	N	302	A86	O5-C38-O4-C34
35	N	306	A86	O5-C38-O4-C34
35	N	320	A86	O5-C38-O4-C34
35	O	319	A86	O5-C38-O4-C34
35	Q	304	A86	O5-C38-O4-C34
35	R	302	A86	O5-C38-O4-C34
35	R	306	A86	O5-C38-O4-C34
35	S	302	A86	O5-C38-O4-C34
35	T	302	A86	O5-C38-O4-C34
35	W	203	A86	O5-C38-O4-C34
35	V	302	A86	O5-C38-O4-C34
36	I	306	CLA	C8-C10-C11-C12
36	O	308	CLA	C5-C6-C7-C8
36	A	311	CLA	CBD-CGD-O2D-CED
36	K	313	CLA	CBD-CGD-O2D-CED
36	M	308	CLA	CBD-CGD-O2D-CED
36	T	311	CLA	CBD-CGD-O2D-CED
36	a	827	CLA	CBD-CGD-O2D-CED
36	R	319	CLA	C2C-C3C-CAC-CBC
36	T	311	CLA	C2C-C3C-CAC-CBC
37	T	310	KC1	C2C-C3C-CAC-CBC
38	b	804	SQD	O49-C7-O47-C45
40	C	215	DGD	O1B-C1B-O2G-C2G
40	L	302	DGD	O1B-C1B-O2G-C2G
41	D	319	LHG	O9-C7-O7-C5
41	F	319	LHG	O9-C7-O7-C5
41	Q	315	LHG	O9-C7-O7-C5
41	l	208	LHG	O9-C7-O7-C5
42	D	320	LMG	O9-C10-O7-C8
42	E	319	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
42	I	315	LMG	O9-C10-O7-C8
42	a	852	LMG	O9-C10-O7-C8
42	m	102	LMG	O9-C10-O7-C8
36	R	311	CLA	O1D-CGD-O2D-CED
35	R	309	A86	C35-C34-O4-C38
35	B	303	A86	O5-C38-O4-C34
35	K	306	A86	O5-C38-O4-C34
35	L	304	A86	O5-C38-O4-C34
35	L	306	A86	O5-C38-O4-C34
35	R	305	A86	C39-C38-O4-C34
35	S	305	A86	O5-C38-O4-C34
35	T	306	A86	O5-C38-O4-C34
35	X	302	A86	O5-C38-O4-C34
35	X	305	A86	O5-C38-O4-C34
35	U	302	A86	O5-C38-O4-C34
35	V	304	A86	O5-C38-O4-C34
36	X	309	CLA	O1A-CGA-O2A-C1
36	A	306	CLA	C3-C5-C6-C7
36	A	314	CLA	C3-C5-C6-C7
36	B	305	CLA	C3-C5-C6-C7
36	C	208	CLA	C3-C5-C6-C7
36	C	211	CLA	C3-C5-C6-C7
36	C	212	CLA	C3-C5-C6-C7
36	D	307	CLA	C3-C5-C6-C7
36	D	313	CLA	C3-C5-C6-C7
36	E	315	CLA	C3-C5-C6-C7
36	E	316	CLA	C3-C5-C6-C7
36	G	313	CLA	C3-C5-C6-C7
36	H	308	CLA	C3-C5-C6-C7
36	I	306	CLA	C3-C5-C6-C7
36	I	308	CLA	C3-C5-C6-C7
36	J	313	CLA	C3-C5-C6-C7
36	K	307	CLA	C3-C5-C6-C7
36	K	308	CLA	C3-C5-C6-C7
36	K	313	CLA	C3-C5-C6-C7
36	M	307	CLA	C3-C5-C6-C7
36	O	306	CLA	C3-C5-C6-C7
36	P	301	CLA	C3-C5-C6-C7
36	P	308	CLA	C3-C5-C6-C7
36	P	314	CLA	C3-C5-C6-C7
36	Q	305	CLA	C3-C5-C6-C7
36	Q	310	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	S	310	CLA	C3-C5-C6-C7
36	W	207	CLA	C3-C5-C6-C7
36	W	211	CLA	C3-C5-C6-C7
36	a	829	CLA	C3-C5-C6-C7
36	b	811	CLA	C3-C5-C6-C7
36	b	816	CLA	C3-C5-C6-C7
36	b	819	CLA	C3-C5-C6-C7
36	j	101	CLA	C3-C5-C6-C7
36	U	310	CLA	C3-C5-C6-C7
36	A	309	CLA	O1D-CGD-O2D-CED
36	H	317	CLA	O1D-CGD-O2D-CED
36	H	311	CLA	CBA-CGA-O2A-C1
36	I	307	CLA	CBA-CGA-O2A-C1
36	I	310	CLA	CBA-CGA-O2A-C1
36	J	307	CLA	CBA-CGA-O2A-C1
36	L	313	CLA	CBA-CGA-O2A-C1
36	M	311	CLA	CBA-CGA-O2A-C1
36	N	312	CLA	CBA-CGA-O2A-C1
36	O	308	CLA	CBA-CGA-O2A-C1
36	P	310	CLA	CBA-CGA-O2A-C1
36	Q	307	CLA	CBA-CGA-O2A-C1
36	R	311	CLA	CBA-CGA-O2A-C1
36	S	310	CLA	CBA-CGA-O2A-C1
36	T	309	CLA	CBA-CGA-O2A-C1
36	W	207	CLA	CBA-CGA-O2A-C1
36	f	804	CLA	CBA-CGA-O2A-C1
36	V	306	CLA	CBA-CGA-O2A-C1
41	F	319	LHG	C24-C23-O8-C6
41	G	301	LHG	C24-C23-O8-C6
41	a	850	LHG	C24-C23-O8-C6
41	f	808	LHG	C24-C23-O8-C6
41	f	809	LHG	C24-C23-O8-C6
42	D	321	LMG	C29-C28-O8-C9
42	a	852	LMG	C29-C28-O8-C9
42	m	102	LMG	C29-C28-O8-C9
35	F	307	A86	O5-C38-O4-C34
35	O	303	A86	O5-C38-O4-C34
35	P	304	A86	O5-C38-O4-C34
35	Q	301	A86	O5-C38-O4-C34
35	R	309	A86	O5-C38-O4-C34
35	T	307	A86	O5-C38-O4-C34
35	h	202	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
39	G	323	LMT	C3'-C4'-O1B-C1B
36	A	305	CLA	CBD-CGD-O2D-CED
36	A	306	CLA	CBD-CGD-O2D-CED
36	A	308	CLA	CBD-CGD-O2D-CED
36	A	314	CLA	CBD-CGD-O2D-CED
36	B	305	CLA	CBD-CGD-O2D-CED
36	C	212	CLA	CBD-CGD-O2D-CED
36	C	214	CLA	CBD-CGD-O2D-CED
36	E	315	CLA	CBD-CGD-O2D-CED
36	G	319	CLA	CBD-CGD-O2D-CED
36	H	314	CLA	CBD-CGD-O2D-CED
36	J	310	CLA	CBD-CGD-O2D-CED
36	K	315	CLA	CBD-CGD-O2D-CED
36	N	309	CLA	CBD-CGD-O2D-CED
36	O	316	CLA	CBD-CGD-O2D-CED
36	R	310	CLA	CBD-CGD-O2D-CED
36	R	312	CLA	CBD-CGD-O2D-CED
36	S	317	CLA	CBD-CGD-O2D-CED
36	W	210	CLA	CBD-CGD-O2D-CED
36	W	216	CLA	CBD-CGD-O2D-CED
36	a	802	CLA	CBD-CGD-O2D-CED
36	a	808	CLA	CBD-CGD-O2D-CED
36	a	809	CLA	CBD-CGD-O2D-CED
36	a	828	CLA	CBD-CGD-O2D-CED
36	a	832	CLA	CBD-CGD-O2D-CED
36	a	837	CLA	CBD-CGD-O2D-CED
36	a	838	CLA	CBD-CGD-O2D-CED
36	b	805	CLA	CBD-CGD-O2D-CED
36	b	806	CLA	CBD-CGD-O2D-CED
36	b	824	CLA	CBD-CGD-O2D-CED
36	b	828	CLA	CBD-CGD-O2D-CED
36	l	206	CLA	CBD-CGD-O2D-CED
37	H	313	KC1	CBD-CGD-O2D-CED
38	b	804	SQD	C8-C7-O47-C45
40	L	302	DGD	C2B-C1B-O2G-C2G
41	R	323	LHG	C8-C7-O7-C5
42	J	318	LMG	C11-C10-O7-C8
42	J	319	LMG	C11-C10-O7-C8
36	W	218	CLA	C2C-C3C-CAC-CBC
39	B	312	LMT	O5B-C1B-O1B-C4'
36	A	307	CLA	O1D-CGD-O2D-CED
36	K	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	M	309	CLA	O1D-CGD-O2D-CED
36	a	836	CLA	O1D-CGD-O2D-CED
36	K	312	CLA	O1A-CGA-O2A-C1
39	K	317	LMT	C5'-C4'-O1B-C1B
36	B	306	CLA	O1A-CGA-O2A-C1
36	R	316	CLA	C2C-C3C-CAC-CBC
37	V	312	KC1	C2C-C3C-CAC-CBC
36	G	309	CLA	O1D-CGD-O2D-CED
36	V	313	CLA	O1D-CGD-O2D-CED
35	F	305	A86	O5-C38-O4-C34
37	C	213	KC1	CAA-CBA-CGA-O1A
37	C	213	KC1	CAA-CBA-CGA-O2A
37	S	316	KC1	CAA-CBA-CGA-O2A
37	T	310	KC1	CAA-CBA-CGA-O1A
37	T	310	KC1	CAA-CBA-CGA-O2A
37	V	312	KC1	CAA-CBA-CGA-O1A
39	I	318	LMT	O5B-C1B-O1B-C4'
39	a	851	LMT	O5B-C1B-O1B-C4'
36	B	311	CLA	C4-C3-C5-C6
36	C	206	CLA	C4-C3-C5-C6
36	C	208	CLA	C4-C3-C5-C6
36	D	307	CLA	C4-C3-C5-C6
36	E	314	CLA	C4-C3-C5-C6
36	F	309	CLA	C4-C3-C5-C6
36	F	314	CLA	C4-C3-C5-C6
36	G	311	CLA	C4-C3-C5-C6
36	G	315	CLA	C4-C3-C5-C6
36	H	316	CLA	C4-C3-C5-C6
36	J	307	CLA	C4-C3-C5-C6
36	L	308	CLA	C4-C3-C5-C6
36	L	309	CLA	C4-C3-C5-C6
36	O	307	CLA	C4-C3-C5-C6
36	P	309	CLA	C4-C3-C5-C6
36	Q	306	CLA	C4-C3-C5-C6
36	R	310	CLA	C4-C3-C5-C6
36	R	311	CLA	C4-C3-C5-C6
36	W	206	CLA	C4-C3-C5-C6
36	a	823	CLA	C4-C3-C5-C6
36	a	836	CLA	C4-C3-C5-C6
36	b	817	CLA	C4-C3-C5-C6
36	b	818	CLA	C4-C3-C5-C6
36	f	804	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	j	101	CLA	C4-C3-C5-C6
36	h	203	CLA	C4-C3-C5-C6
36	U	310	CLA	C4-C3-C5-C6
36	B	308	CLA	C2-C3-C5-C6
36	B	311	CLA	C2-C3-C5-C6
36	C	206	CLA	C2-C3-C5-C6
36	C	208	CLA	C2-C3-C5-C6
36	D	307	CLA	C2-C3-C5-C6
36	F	309	CLA	C2-C3-C5-C6
36	F	314	CLA	C2-C3-C5-C6
36	G	311	CLA	C2-C3-C5-C6
36	G	315	CLA	C2-C3-C5-C6
36	H	316	CLA	C2-C3-C5-C6
36	J	307	CLA	C2-C3-C5-C6
36	L	308	CLA	C2-C3-C5-C6
36	R	310	CLA	C2-C3-C5-C6
36	W	206	CLA	C2-C3-C5-C6
36	a	836	CLA	C2-C3-C5-C6
36	b	818	CLA	C2-C3-C5-C6
36	b	824	CLA	C2-C3-C5-C6
36	b	836	CLA	C2-C3-C5-C6
36	f	804	CLA	C2-C3-C5-C6
36	h	203	CLA	C2-C3-C5-C6
36	U	310	CLA	C2-C3-C5-C6
38	A	315	SQD	C24-C23-O48-C46
36	B	306	CLA	CBA-CGA-O2A-C1
36	I	309	CLA	CBA-CGA-O2A-C1
36	X	309	CLA	CBA-CGA-O2A-C1
36	H	315	CLA	C4C-C3C-CAC-CBC
36	N	307	CLA	CBD-CGD-O2D-CED
36	b	818	CLA	CBD-CGD-O2D-CED
36	U	305	CLA	CBD-CGD-O2D-CED
36	B	306	CLA	O1D-CGD-O2D-CED
36	F	313	CLA	C3-C5-C6-C7
36	G	313	CLA	C2A-CAA-CBA-CGA
36	K	311	CLA	C2A-CAA-CBA-CGA
36	a	834	CLA	C2A-CAA-CBA-CGA
36	b	832	CLA	C2A-CAA-CBA-CGA
36	A	311	CLA	C3-C5-C6-C7
36	C	207	CLA	C3-C5-C6-C7
36	F	314	CLA	C3-C5-C6-C7
36	L	313	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	M	306	CLA	C3-C5-C6-C7
36	P	319	CLA	C3-C5-C6-C7
36	R	310	CLA	C3-C5-C6-C7
36	R	311	CLA	C3-C5-C6-C7
36	R	312	CLA	C3-C5-C6-C7
36	S	312	CLA	C3-C5-C6-C7
36	a	806	CLA	C3-C5-C6-C7
36	a	812	CLA	C3-C5-C6-C7
36	b	812	CLA	C3-C5-C6-C7
36	b	824	CLA	C3-C5-C6-C7
36	j	102	CLA	C3-C5-C6-C7
36	A	310	CLA	CBA-CGA-O2A-C1
36	B	308	CLA	CBA-CGA-O2A-C1
36	D	312	CLA	CBA-CGA-O2A-C1
36	D	317	CLA	CBA-CGA-O2A-C1
36	E	313	CLA	CBA-CGA-O2A-C1
36	F	312	CLA	CBA-CGA-O2A-C1
36	F	314	CLA	CBA-CGA-O2A-C1
36	G	311	CLA	CBA-CGA-O2A-C1
36	G	312	CLA	CBA-CGA-O2A-C1
36	G	316	CLA	CBA-CGA-O2A-C1
36	G	319	CLA	CBA-CGA-O2A-C1
36	L	309	CLA	CBA-CGA-O2A-C1
36	M	312	CLA	CBA-CGA-O2A-C1
36	N	308	CLA	CBA-CGA-O2A-C1
36	P	314	CLA	CBA-CGA-O2A-C1
36	S	320	CLA	CBA-CGA-O2A-C1
36	T	313	CLA	CBA-CGA-O2A-C1
36	a	804	CLA	CBA-CGA-O2A-C1
36	a	816	CLA	CBA-CGA-O2A-C1
36	a	818	CLA	CBA-CGA-O2A-C1
36	a	839	CLA	CBA-CGA-O2A-C1
36	b	833	CLA	CBA-CGA-O2A-C1
36	b	834	CLA	CBA-CGA-O2A-C1
36	U	306	CLA	CBA-CGA-O2A-C1
40	C	215	DGD	C2A-C1A-O1G-C1G
41	Q	315	LHG	C24-C23-O8-C6
42	G	325	LMG	C29-C28-O8-C9
35	I	301	A86	O5-C38-O4-C34
35	R	304	A86	O5-C38-O4-C34
39	I	317	LMT	C4'-C5'-C6'-O6'
40	C	215	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
35	F	301	A86	O5-C38-O4-C34
36	S	320	CLA	CBD-CGD-O2D-CED
39	F	320	LMT	O5'-C5'-C6'-O6'
39	G	322	LMT	O5B-C5B-C6B-O6B
42	j	105	LMG	C4-C5-C6-O5
34	Q	302	DD6	C3-C4-C5-C6
34	R	307	DD6	C1-C2-C3-C4
34	j	103	DD6	C11-C10-C9-C8
35	S	308	A86	C3-C4-C5-C6
35	U	301	A86	C24-C25-C26-C27
35	U	303	A86	C3-C4-C5-C6
35	V	301	A86	C3-C4-C5-C6
36	B	305	CLA	O1A-CGA-O2A-C1
36	C	211	CLA	O1A-CGA-O2A-C1
36	D	317	CLA	O1A-CGA-O2A-C1
36	E	313	CLA	O1A-CGA-O2A-C1
36	F	312	CLA	O1A-CGA-O2A-C1
36	I	307	CLA	O1A-CGA-O2A-C1
36	J	312	CLA	O1A-CGA-O2A-C1
36	M	311	CLA	O1A-CGA-O2A-C1
36	N	308	CLA	O1A-CGA-O2A-C1
36	O	316	CLA	O1A-CGA-O2A-C1
36	P	314	CLA	O1A-CGA-O2A-C1
36	Q	310	CLA	O1A-CGA-O2A-C1
36	S	310	CLA	O1A-CGA-O2A-C1
36	S	320	CLA	O1A-CGA-O2A-C1
36	W	211	CLA	O1A-CGA-O2A-C1
36	b	820	CLA	O1A-CGA-O2A-C1
36	b	833	CLA	O1A-CGA-O2A-C1
36	U	306	CLA	O1A-CGA-O2A-C1
36	V	310	CLA	O1A-CGA-O2A-C1
41	F	319	LHG	O10-C23-O8-C6
41	G	321	LHG	O10-C23-O8-C6
41	f	808	LHG	O10-C23-O8-C6
36	M	308	CLA	C2C-C3C-CAC-CBC
36	K	311	CLA	O1A-CGA-O2A-C1
36	X	308	CLA	C4C-C3C-CAC-CBC
36	H	305	CLA	O1D-CGD-O2D-CED
36	a	817	CLA	O1D-CGD-O2D-CED
35	L	307	A86	C39-C38-O4-C34
35	T	303	A86	C39-C38-O4-C34
37	V	312	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	E	314	CLA	C3-C5-C6-C7
36	F	310	CLA	C3-C5-C6-C7
36	L	310	CLA	C3-C5-C6-C7
36	L	320	CLA	C3-C5-C6-C7
36	O	311	CLA	C3-C5-C6-C7
36	P	313	CLA	C3-C5-C6-C7
36	W	206	CLA	C3-C5-C6-C7
36	a	839	CLA	C3-C5-C6-C7
36	b	805	CLA	C3-C5-C6-C7
36	l	205	CLA	C3-C5-C6-C7
36	U	311	CLA	C3-C5-C6-C7
36	V	306	CLA	C3-C5-C6-C7
36	D	308	CLA	CBD-CGD-O2D-CED
36	H	315	CLA	C2C-C3C-CAC-CBC
39	B	312	LMT	C2B-C1B-O1B-C4'
41	G	301	LHG	O2-C2-C3-O3
41	I	316	LHG	O2-C2-C3-O3
41	O	318	LHG	O2-C2-C3-O3
41	Q	315	LHG	O2-C2-C3-O3
41	a	843	LHG	O2-C2-C3-O3
41	j	104	LHG	O2-C2-C3-O3
41	l	208	LHG	O2-C2-C3-O3
36	G	313	CLA	O1D-CGD-O2D-CED
36	L	314	CLA	O1D-CGD-O2D-CED
36	M	312	CLA	O1D-CGD-O2D-CED
36	M	314	CLA	O1D-CGD-O2D-CED
36	P	318	CLA	O1D-CGD-O2D-CED
36	S	315	CLA	O1D-CGD-O2D-CED
36	j	106	CLA	O1D-CGD-O2D-CED
36	U	311	CLA	O1D-CGD-O2D-CED
36	B	305	CLA	CBA-CGA-O2A-C1
36	C	211	CLA	CBA-CGA-O2A-C1
36	J	312	CLA	CBA-CGA-O2A-C1
36	K	312	CLA	CBA-CGA-O2A-C1
36	K	313	CLA	CBA-CGA-O2A-C1
36	Q	310	CLA	CBA-CGA-O2A-C1
36	X	306	CLA	CBA-CGA-O2A-C1
36	V	310	CLA	CBA-CGA-O2A-C1
41	G	321	LHG	C24-C23-O8-C6
42	D	320	LMG	C29-C28-O8-C9
42	V	315	LMG	C29-C28-O8-C9
35	X	301	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
36	G	316	CLA	O1A-CGA-O2A-C1
38	b	804	SQD	O10-C23-O48-C46
42	D	320	LMG	O10-C28-O8-C9
42	G	325	LMG	O10-C28-O8-C9
36	A	313	CLA	O1D-CGD-O2D-CED
36	V	311	CLA	O1D-CGD-O2D-CED
35	C	202	A86	O5-C38-O4-C34
35	G	304	A86	O5-C38-O4-C34
35	H	301	A86	O5-C38-O4-C34
35	I	304	A86	C39-C38-O4-C34
35	I	304	A86	O5-C38-O4-C34
35	K	302	A86	C39-C38-O4-C34
35	K	302	A86	O5-C38-O4-C34
35	L	307	A86	O5-C38-O4-C34
35	L	319	A86	C39-C38-O4-C34
35	L	319	A86	O5-C38-O4-C34
35	M	301	A86	C39-C38-O4-C34
35	M	301	A86	O5-C38-O4-C34
35	N	301	A86	C39-C38-O4-C34
35	N	301	A86	O5-C38-O4-C34
35	N	303	A86	C39-C38-O4-C34
35	N	303	A86	O5-C38-O4-C34
35	O	302	A86	C39-C38-O4-C34
35	O	302	A86	O5-C38-O4-C34
35	P	303	A86	C39-C38-O4-C34
35	P	303	A86	O5-C38-O4-C34
35	R	301	A86	C39-C38-O4-C34
35	R	301	A86	O5-C38-O4-C34
35	R	303	A86	C39-C38-O4-C34
35	R	303	A86	O5-C38-O4-C34
35	S	301	A86	C39-C38-O4-C34
35	S	301	A86	O5-C38-O4-C34
35	S	303	A86	C39-C38-O4-C34
35	S	303	A86	O5-C38-O4-C34
35	T	303	A86	O5-C38-O4-C34
35	T	305	A86	C39-C38-O4-C34
35	T	305	A86	O5-C38-O4-C34
35	W	202	A86	C39-C38-O4-C34
35	W	202	A86	O5-C38-O4-C34
35	X	301	A86	O5-C38-O4-C34
35	X	303	A86	C39-C38-O4-C34
35	X	303	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	X	304	A86	C39-C38-O4-C34
35	X	304	A86	O5-C38-O4-C34
35	U	301	A86	C39-C38-O4-C34
35	U	301	A86	O5-C38-O4-C34
35	V	303	A86	C39-C38-O4-C34
35	V	303	A86	O5-C38-O4-C34
39	a	851	LMT	O5'-C5'-C6'-O6'
39	U	315	LMT	O5'-C5'-C6'-O6'
42	J	319	LMG	O6-C5-C6-O5
39	K	317	LMT	C4B-C5B-C6B-O6B
36	D	307	CLA	CBD-CGD-O2D-CED
36	a	820	CLA	CBD-CGD-O2D-CED
36	a	830	CLA	CBD-CGD-O2D-CED
41	f	809	LHG	C8-C7-O7-C5
35	X	305	A86	C35-C34-O4-C38
36	D	311	CLA	CBA-CGA-O2A-C1
36	N	311	CLA	CBA-CGA-O2A-C1
36	J	316	CLA	C2C-C3C-CAC-CBC
39	B	313	LMT	O5B-C1B-O1B-C4'
39	a	854	LMT	C3'-C4'-O1B-C1B
39	B	313	LMT	O5'-C5'-C6'-O6'
39	I	318	LMT	O5'-C5'-C6'-O6'
39	K	318	LMT	O5'-C5'-C6'-O6'
39	a	851	LMT	O5B-C5B-C6B-O6B
42	G	325	LMG	O6-C5-C6-O5
42	J	318	LMG	O6-C5-C6-O5
42	L	321	LMG	O6-C5-C6-O5
36	b	836	CLA	C2C-C3C-CAC-CBC
36	J	315	CLA	O1D-CGD-O2D-CED
36	E	310	CLA	C3-C5-C6-C7
36	O	308	CLA	C3-C5-C6-C7
36	T	309	CLA	C3-C5-C6-C7
36	a	803	CLA	C3-C5-C6-C7
36	b	820	CLA	C3-C5-C6-C7
36	b	825	CLA	C3-C5-C6-C7
41	b	850	LHG	C5-C6-O8-C23
36	O	312	CLA	CBD-CGD-O2D-CED
36	O	314	CLA	CBD-CGD-O2D-CED
36	P	314	CLA	CBD-CGD-O2D-CED
36	P	316	CLA	CBD-CGD-O2D-CED
36	Q	310	CLA	CBD-CGD-O2D-CED
36	Q	312	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	W	206	CLA	CBD-CGD-O2D-CED
36	X	306	CLA	CBD-CGD-O2D-CED
36	a	815	CLA	CBD-CGD-O2D-CED
36	a	829	CLA	CBD-CGD-O2D-CED
36	b	808	CLA	CBD-CGD-O2D-CED
36	b	816	CLA	CBD-CGD-O2D-CED
36	l	202	CLA	CBD-CGD-O2D-CED
39	I	317	LMT	O5'-C5'-C6'-O6'
39	L	318	LMT	O5'-C5'-C6'-O6'
40	b	849	DGD	O6E-C5E-C6E-O5E
39	F	320	LMT	C4'-C5'-C6'-O6'
42	E	319	LMG	C4-C5-C6-O5
36	M	315	CLA	O1D-CGD-O2D-CED
36	O	309	CLA	O1D-CGD-O2D-CED
36	P	311	CLA	O1D-CGD-O2D-CED
36	Q	308	CLA	O1D-CGD-O2D-CED
36	S	318	CLA	O1D-CGD-O2D-CED
36	O	316	CLA	CBA-CGA-O2A-C1
36	W	211	CLA	CBA-CGA-O2A-C1
36	b	817	CLA	CBA-CGA-O2A-C1
36	b	820	CLA	CBA-CGA-O2A-C1
38	b	804	SQD	C24-C23-O48-C46
36	D	308	CLA	C4-C3-C5-C6
36	E	313	CLA	C4-C3-C5-C6
36	K	307	CLA	C4-C3-C5-C6
36	K	309	CLA	C4-C3-C5-C6
36	L	314	CLA	C4-C3-C5-C6
36	M	306	CLA	C4-C3-C5-C6
36	a	811	CLA	C4-C3-C5-C6
36	l	201	CLA	C4-C3-C5-C6
36	E	313	CLA	C2-C3-C5-C6
36	E	314	CLA	C2-C3-C5-C6
36	K	307	CLA	C2-C3-C5-C6
36	K	309	CLA	C2-C3-C5-C6
36	L	314	CLA	C2-C3-C5-C6
36	M	306	CLA	C2-C3-C5-C6
36	O	316	CLA	C2-C3-C5-C6
36	R	311	CLA	C2-C3-C5-C6
36	a	811	CLA	C2-C3-C5-C6
36	a	823	CLA	C2-C3-C5-C6
36	l	201	CLA	C2-C3-C5-C6
36	E	314	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	M	312	CLA	O1A-CGA-O2A-C1
36	X	306	CLA	O1A-CGA-O2A-C1
40	C	215	DGD	O1A-C1A-O1G-C1G
41	Q	315	LHG	O10-C23-O8-C6
41	f	809	LHG	O9-C7-O7-C5
39	B	312	LMT	O5'-C5'-C6'-O6'
39	F	321	LMT	O5B-C5B-C6B-O6B
42	D	320	LMG	O6-C5-C6-O5
42	V	315	LMG	O6-C5-C6-O5
42	V	316	LMG	O6-C5-C6-O5
36	N	318	CLA	O1D-CGD-O2D-CED
42	J	318	LMG	C4-C5-C6-O5
35	L	304	A86	C35-C34-O4-C38
41	D	318	LHG	C31-C32-C33-C34
36	b	837	CLA	CBD-CGD-O2D-CED
36	I	309	CLA	O1A-CGA-O2A-C1
36	T	309	CLA	O1D-CGD-O2D-CED
36	K	313	CLA	C5-C6-C7-C8
41	E	322	LHG	C2-C3-O3-P
41	Q	315	LHG	C2-C3-O3-P
41	j	104	LHG	C2-C3-O3-P
39	G	322	LMT	C4B-C5B-C6B-O6B
36	S	321	CLA	C3-C5-C6-C7
36	a	828	CLA	C2A-CAA-CBA-CGA
36	f	802	CLA	C2A-CAA-CBA-CGA
39	U	315	LMT	O5B-C1B-O1B-C4'
36	R	313	CLA	O1D-CGD-O2D-CED
36	S	321	CLA	O1D-CGD-O2D-CED
36	T	313	CLA	O1D-CGD-O2D-CED
36	K	313	CLA	O1A-CGA-O2A-C1
36	b	817	CLA	O1A-CGA-O2A-C1
42	V	315	LMG	O10-C28-O8-C9
39	E	321	LMT	O5'-C1'-O1'-C1
39	G	322	LMT	O5'-C1'-O1'-C1
39	I	318	LMT	O5'-C1'-O1'-C1
39	L	318	LMT	O5'-C1'-O1'-C1
40	C	215	DGD	O6D-C1D-O3G-C3G
40	L	302	DGD	O6D-C1D-O3G-C3G
42	D	320	LMG	O6-C1-O1-C7
42	E	319	LMG	O6-C1-O1-C7
42	G	324	LMG	O6-C1-O1-C7
42	V	316	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
42	E	319	LMG	O6-C5-C6-O5
36	F	312	CLA	O1D-CGD-O2D-CED
36	E	314	CLA	CBA-CGA-O2A-C1
36	N	318	CLA	CBA-CGA-O2A-C1
42	D	320	LMG	C23-C24-C25-C26
36	C	205	CLA	CBD-CGD-O2D-CED
36	J	309	CLA	CBD-CGD-O2D-CED
36	K	311	CLA	CBD-CGD-O2D-CED
36	M	307	CLA	CBD-CGD-O2D-CED
36	N	316	CLA	CBD-CGD-O2D-CED
36	P	302	CLA	CBD-CGD-O2D-CED
36	R	316	CLA	CBD-CGD-O2D-CED
36	R	321	CLA	CBD-CGD-O2D-CED
36	S	319	CLA	CBD-CGD-O2D-CED
36	T	312	CLA	CBD-CGD-O2D-CED
36	b	815	CLA	CBD-CGD-O2D-CED
37	T	315	KC1	CBD-CGD-O2D-CED
37	U	312	KC1	CBD-CGD-O2D-CED
39	F	321	LMT	O5'-C5'-C6'-O6'
41	f	808	LHG	C24-C25-C26-C27
36	R	316	CLA	CBA-CGA-O2A-C1
36	N	316	CLA	C13-C15-C16-C17
35	J	305	A86	O5-C38-O4-C34
35	N	304	A86	O5-C38-O4-C34
35	S	308	A86	C39-C38-O4-C34
37	B	310	KC1	CAA-CBA-CGA-O1A
37	G	317	KC1	CAA-CBA-CGA-O1A
37	G	318	KC1	CAA-CBA-CGA-O2A
37	H	313	KC1	CAA-CBA-CGA-O2A
41	a	842	LHG	C28-C29-C30-C31
39	B	313	LMT	O5B-C5B-C6B-O6B
39	K	317	LMT	O5B-C5B-C6B-O6B
40	L	302	DGD	O6E-C5E-C6E-O5E
42	a	852	LMG	O6-C5-C6-O5
42	j	105	LMG	O6-C5-C6-O5
36	a	802	CLA	O1D-CGD-O2D-CED
36	a	827	CLA	O1D-CGD-O2D-CED
36	b	828	CLA	O1D-CGD-O2D-CED
36	b	840	CLA	O1D-CGD-O2D-CED
36	V	307	CLA	O1D-CGD-O2D-CED
39	G	323	LMT	C4B-C5B-C6B-O6B
41	D	319	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
41	a	850	LHG	C28-C29-C30-C31
41	i	104	LHG	C12-C13-C14-C15
36	J	308	CLA	CBD-CGD-O2D-CED
36	R	315	CLA	CBD-CGD-O2D-CED
41	F	318	LHG	C8-C7-O7-C5
36	W	218	CLA	C4C-C3C-CAC-CBC
36	D	313	CLA	O1D-CGD-O2D-CED
35	C	204	A86	O5-C38-O4-C34
39	U	315	LMT	C4'-C5'-C6'-O6'
40	C	215	DGD	C4B-C5B-C6B-C7B
41	D	319	LHG	C34-C35-C36-C37
41	E	322	LHG	C18-C19-C20-C21
42	J	318	LMG	C23-C24-C25-C26
34	D	303	DD6	C1-C2-C3-C4
34	D	303	DD6	C3-C4-C5-C6
34	L	305	DD6	C24-C25-C26-C27
34	W	204	DD6	C24-C25-C26-C27
35	N	304	A86	C11-C10-C9-C8
35	U	303	A86	C1-C2-C3-C4
36	H	308	CLA	O1A-CGA-O2A-C1
36	A	311	CLA	O1D-CGD-O2D-CED
36	A	314	CLA	CBA-CGA-O2A-C1
36	D	316	CLA	CBA-CGA-O2A-C1
36	E	308	CLA	CBA-CGA-O2A-C1
36	H	308	CLA	CBA-CGA-O2A-C1
36	I	305	CLA	CBA-CGA-O2A-C1
36	K	308	CLA	CBA-CGA-O2A-C1
36	M	306	CLA	CBA-CGA-O2A-C1
36	O	306	CLA	CBA-CGA-O2A-C1
36	P	308	CLA	CBA-CGA-O2A-C1
36	Q	305	CLA	CBA-CGA-O2A-C1
36	R	312	CLA	CBA-CGA-O2A-C1
36	a	822	CLA	CBA-CGA-O2A-C1
36	a	836	CLA	CBA-CGA-O2A-C1
36	b	824	CLA	CBA-CGA-O2A-C1
36	b	831	CLA	CBA-CGA-O2A-C1
36	b	840	CLA	CBA-CGA-O2A-C1
36	l	202	CLA	CBA-CGA-O2A-C1
36	l	204	CLA	CBA-CGA-O2A-C1
36	U	305	CLA	CBA-CGA-O2A-C1
41	I	316	LHG	C24-C23-O8-C6
39	I	317	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
42	E	318	LMG	C15-C16-C17-C18
42	G	325	LMG	C14-C15-C16-C17
42	j	105	LMG	C19-C20-C21-C22
35	B	303	A86	C35-C34-O4-C38
35	F	305	A86	C35-C34-O4-C38
35	N	302	A86	C35-C34-O4-C38
35	S	302	A86	C35-C34-O4-C38
35	T	303	A86	C35-C34-O4-C38
35	W	202	A86	C33-C34-O4-C38
35	V	303	A86	C33-C34-O4-C38
36	a	824	CLA	C8-C10-C11-C12
36	L	308	CLA	CBD-CGD-O2D-CED
42	a	852	LMG	C4-C5-C6-O5
41	G	321	LHG	C11-C10-C9-C8
41	Q	315	LHG	C11-C10-C9-C8
41	a	850	LHG	C11-C10-C9-C8
41	a	850	LHG	C30-C31-C32-C33
41	b	850	LHG	C11-C10-C9-C8
41	j	104	LHG	C11-C10-C9-C8
41	j	104	LHG	C17-C18-C19-C20
42	E	318	LMG	C20-C21-C22-C23
42	I	315	LMG	C13-C14-C15-C16
36	A	308	CLA	O1D-CGD-O2D-CED
36	M	308	CLA	O1D-CGD-O2D-CED
36	S	317	CLA	O1D-CGD-O2D-CED
36	T	311	CLA	O1D-CGD-O2D-CED
36	W	216	CLA	O1D-CGD-O2D-CED
36	b	806	CLA	O1D-CGD-O2D-CED
36	b	835	CLA	O1D-CGD-O2D-CED
37	H	313	KC1	O1D-CGD-O2D-CED
41	a	850	LHG	C10-C11-C12-C13
39	F	321	LMT	C4'-C5'-C6'-O6'
39	U	315	LMT	C4B-C5B-C6B-O6B
36	a	822	CLA	O1A-CGA-O2A-C1
36	K	313	CLA	O1D-CGD-O2D-CED
40	C	215	DGD	C2B-C3B-C4B-C5B
41	Q	315	LHG	C28-C29-C30-C31
42	I	315	LMG	C36-C37-C38-C39
37	F	308	KC1	CAA-CBA-CGA-O2A
37	H	313	KC1	CAA-CBA-CGA-O1A
37	J	314	KC1	CAA-CBA-CGA-O1A
37	M	313	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
37	W	213	KC1	CAA-CBA-CGA-O2A
36	A	306	CLA	C4-C3-C5-C6
36	C	212	CLA	C4-C3-C5-C6
36	E	315	CLA	C4-C3-C5-C6
36	O	316	CLA	C4-C3-C5-C6
36	b	833	CLA	C4-C3-C5-C6
36	A	306	CLA	C2-C3-C5-C6
36	C	212	CLA	C2-C3-C5-C6
36	D	308	CLA	C2-C3-C5-C6
36	E	315	CLA	C2-C3-C5-C6
36	L	309	CLA	C2-C3-C5-C6
36	O	307	CLA	C2-C3-C5-C6
36	P	309	CLA	C2-C3-C5-C6
36	Q	306	CLA	C2-C3-C5-C6
36	b	817	CLA	C2-C3-C5-C6
36	b	833	CLA	C2-C3-C5-C6
36	j	101	CLA	C2-C3-C5-C6
39	U	315	LMT	C2B-C1B-O1B-C4'
36	J	312	CLA	C3-C5-C6-C7
36	a	816	CLA	C3-C5-C6-C7
36	l	201	CLA	C3-C5-C6-C7
36	B	305	CLA	C14-C13-C15-C16
36	C	206	CLA	C6-C7-C8-C9
36	C	207	CLA	C11-C10-C8-C9
36	C	208	CLA	C6-C7-C8-C9
36	C	212	CLA	C14-C13-C15-C16
36	D	307	CLA	C11-C10-C8-C9
36	D	308	CLA	C6-C7-C8-C9
36	E	311	CLA	C11-C10-C8-C9
36	E	315	CLA	C11-C12-C13-C14
36	E	315	CLA	C14-C13-C15-C16
36	E	316	CLA	C6-C7-C8-C9
36	F	317	CLA	C6-C7-C8-C9
36	G	309	CLA	C11-C12-C13-C14
36	G	309	CLA	C14-C13-C15-C16
36	G	313	CLA	C11-C12-C13-C14
36	H	315	CLA	C6-C7-C8-C9
36	I	306	CLA	C11-C12-C13-C14
36	I	308	CLA	C11-C10-C8-C9
36	I	308	CLA	C11-C12-C13-C14
36	J	309	CLA	C11-C12-C13-C14
36	J	313	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
36	K	310	CLA	C6-C7-C8-C9
36	K	313	CLA	C11-C12-C13-C14
36	L	309	CLA	C6-C7-C8-C9
36	M	311	CLA	C11-C12-C13-C14
36	N	308	CLA	C14-C13-C15-C16
36	O	309	CLA	C6-C7-C8-C9
36	O	316	CLA	C11-C10-C8-C9
36	P	301	CLA	C6-C7-C8-C9
36	P	301	CLA	C11-C12-C13-C14
36	P	311	CLA	C6-C7-C8-C9
36	Q	308	CLA	C6-C7-C8-C9
36	Q	310	CLA	C11-C10-C8-C9
36	S	310	CLA	C6-C7-C8-C9
36	T	309	CLA	C6-C7-C8-C9
36	T	314	CLA	C6-C7-C8-C9
36	W	207	CLA	C6-C7-C8-C9
36	a	806	CLA	C11-C10-C8-C9
36	a	825	CLA	C11-C12-C13-C14
36	a	831	CLA	C11-C10-C8-C9
36	a	839	CLA	C11-C10-C8-C9
36	a	839	CLA	C14-C13-C15-C16
36	b	816	CLA	C11-C10-C8-C9
36	b	817	CLA	C6-C7-C8-C9
36	b	821	CLA	C6-C7-C8-C9
36	i	102	CLA	C6-C7-C8-C9
36	l	205	CLA	C11-C10-C8-C9
36	h	203	CLA	C6-C7-C8-C9
36	U	305	CLA	C6-C7-C8-C9
36	V	306	CLA	C6-C7-C8-C9
36	V	314	CLA	C11-C12-C13-C14
43	b	842	PQN	C24-C23-C25-C26
39	a	853	LMT	C4B-C5B-C6B-O6B
40	L	302	DGD	C4E-C5E-C6E-O5E
36	a	828	CLA	O1D-CGD-O2D-CED
35	B	301	A86	O5-C38-O4-C34
39	E	321	LMT	C2'-C1'-O1'-C1
39	G	322	LMT	C2'-C1'-O1'-C1
39	I	318	LMT	C2'-C1'-O1'-C1
39	P	320	LMT	C2'-C1'-O1'-C1
39	a	851	LMT	C2'-C1'-O1'-C1
39	a	853	LMT	C2'-C1'-O1'-C1
40	C	215	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
40	L	302	DGD	C2D-C1D-O3G-C3G
42	D	320	LMG	C2-C1-O1-C7
42	D	321	LMG	C2-C1-O1-C7
42	E	318	LMG	C2-C1-O1-C7
42	E	319	LMG	C2-C1-O1-C7
42	V	316	LMG	C2-C1-O1-C7
41	E	322	LHG	C14-C15-C16-C17
41	b	850	LHG	C10-C11-C12-C13
37	N	314	KC1	C2C-C3C-CAC-CBC
35	S	305	A86	C35-C34-O4-C38
36	D	311	CLA	O1A-CGA-O2A-C1
36	B	307	CLA	CBA-CGA-O2A-C1
41	F	319	LHG	O2-C2-C3-O3
41	O	317	LHG	O2-C2-C3-O3
41	a	850	LHG	O2-C2-C3-O3
41	f	808	LHG	O2-C2-C3-O3
36	C	212	CLA	O1D-CGD-O2D-CED
36	J	310	CLA	O1D-CGD-O2D-CED
42	a	852	LMG	C15-C16-C17-C18
35	P	307	A86	O5-C38-O4-C34
36	A	314	CLA	O1A-CGA-O2A-C1
36	K	308	CLA	O1A-CGA-O2A-C1
36	R	312	CLA	O1A-CGA-O2A-C1
36	b	824	CLA	O1A-CGA-O2A-C1
39	B	313	LMT	C4B-C5B-C6B-O6B
39	F	321	LMT	C4B-C5B-C6B-O6B
41	R	323	LHG	C30-C31-C32-C33
36	a	834	CLA	CBD-CGD-O2D-CED
36	a	808	CLA	O1D-CGD-O2D-CED
36	a	832	CLA	O1D-CGD-O2D-CED
36	a	837	CLA	O1D-CGD-O2D-CED
34	A	301	DD6	C12-C11-C13-C14
34	C	201	DD6	C12-C11-C13-C14
34	D	301	DD6	C12-C11-C13-C14
34	D	301	DD6	C7-C6-C8-C9
34	D	303	DD6	C-C1-C24-C25
34	D	303	DD6	C12-C11-C13-C14
34	E	303	DD6	C12-C11-C13-C14
34	E	303	DD6	C7-C6-C8-C9
34	E	306	DD6	C12-C11-C13-C14
34	G	303	DD6	C12-C11-C13-C14
34	J	304	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
34	L	305	DD6	C-C1-C24-C25
34	M	303	DD6	C12-C11-C13-C14
34	Q	302	DD6	C-C1-C24-C25
34	R	307	DD6	C-C1-C24-C25
34	R	308	DD6	C-C1-C24-C25
34	R	308	DD6	C12-C11-C13-C14
34	R	308	DD6	C7-C6-C8-C9
34	S	307	DD6	C-C1-C24-C25
34	W	205	DD6	C7-C6-C8-C9
34	a	849	DD6	C7-C6-C8-C9
34	j	103	DD6	C7-C6-C8-C9
35	C	203	A86	C-C1-C24-C25
35	D	302	A86	C7-C6-C8-C9
35	E	305	A86	C7-C6-C8-C9
35	G	302	A86	C-C1-C24-C25
35	I	301	A86	C-C1-C24-C25
35	I	301	A86	C7-C6-C8-C9
35	J	306	A86	C-C1-C24-C25
35	L	301	A86	C-C1-C24-C25
35	L	307	A86	C-C1-C24-C25
35	O	305	A86	C-C1-C24-C25
35	Q	303	A86	C-C1-C24-C25
35	R	305	A86	C-C1-C24-C25
35	U	303	A86	C7-C6-C8-C9
35	V	301	A86	C-C1-C24-C25
44	a	844	BCR	C7-C8-C9-C34
44	a	846	BCR	C7-C8-C9-C34
44	a	847	BCR	C37-C22-C23-C24
44	b	843	BCR	C7-C8-C9-C34
44	b	846	BCR	C7-C8-C9-C34
44	f	806	BCR	C37-C22-C23-C24
44	i	103	BCR	C7-C8-C9-C34
44	h	201	BCR	C7-C8-C9-C34
39	G	323	LMT	O5B-C5B-C6B-O6B
34	C	201	DD6	C10-C11-C13-C14
34	D	303	DD6	C10-C11-C13-C14
34	E	306	DD6	C10-C11-C13-C14
34	G	303	DD6	C10-C11-C13-C14
34	L	305	DD6	C2-C1-C24-C25
34	R	308	DD6	C5-C6-C8-C9
34	j	103	DD6	C5-C6-C8-C9
35	J	301	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
35	O	305	A86	C2-C1-C24-C25
35	S	308	A86	C2-C1-C24-C25
44	b	846	BCR	C7-C8-C9-C10
36	F	311	CLA	C3-C5-C6-C7
36	a	821	CLA	C2A-CAA-CBA-CGA
38	b	804	SQD	C23-C24-C25-C26
41	F	318	LHG	C23-C24-C25-C26
42	a	852	LMG	C28-C29-C30-C31
36	b	824	CLA	O1D-CGD-O2D-CED
36	D	316	CLA	O1A-CGA-O2A-C1
36	I	305	CLA	O1A-CGA-O2A-C1
36	b	831	CLA	O1A-CGA-O2A-C1
36	U	305	CLA	O1A-CGA-O2A-C1
36	R	315	CLA	C3-C5-C6-C7
41	O	317	LHG	C8-C7-O7-C5
35	H	301	A86	C35-C34-O4-C38
35	O	301	A86	C39-C38-O4-C34
37	B	310	KC1	CAA-CBA-CGA-O2A
37	D	314	KC1	CAA-CBA-CGA-O2A
37	E	309	KC1	CAA-CBA-CGA-O1A
37	E	309	KC1	CAA-CBA-CGA-O2A
37	G	308	KC1	CAA-CBA-CGA-O1A
37	G	308	KC1	CAA-CBA-CGA-O2A
37	G	317	KC1	CAA-CBA-CGA-O2A
37	G	318	KC1	CAA-CBA-CGA-O1A
37	J	314	KC1	CAA-CBA-CGA-O2A
37	M	313	KC1	CAA-CBA-CGA-O2A
37	N	314	KC1	CAA-CBA-CGA-O2A
37	W	213	KC1	CAA-CBA-CGA-O1A
36	a	823	CLA	C2C-C3C-CAC-CBC
36	O	316	CLA	O1D-CGD-O2D-CED
36	a	809	CLA	O1D-CGD-O2D-CED
36	R	310	CLA	CBA-CGA-O2A-C1
36	h	203	CLA	CBA-CGA-O2A-C1
41	b	850	LHG	C24-C23-O8-C6
36	G	309	CLA	C13-C15-C16-C17
36	S	320	CLA	C13-C15-C16-C17
36	a	820	CLA	C5-C6-C7-C8
42	I	315	LMG	C10-C11-C12-C13
42	j	105	LMG	C10-C11-C12-C13
36	a	804	CLA	C2-C1-O2A-CGA
38	A	315	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
36	A	305	CLA	O1D-CGD-O2D-CED
36	A	314	CLA	O1D-CGD-O2D-CED
36	B	305	CLA	O1D-CGD-O2D-CED
36	H	314	CLA	O1D-CGD-O2D-CED
36	l	206	CLA	O1D-CGD-O2D-CED
39	B	313	LMT	C4'-C5'-C6'-O6'
39	K	318	LMT	C4'-C5'-C6'-O6'
42	G	325	LMG	C4-C5-C6-O5
41	Q	315	LHG	C25-C26-C27-C28
42	D	321	LMG	C13-C14-C15-C16
36	A	307	CLA	C10-C11-C12-C13
36	D	308	CLA	C5-C6-C7-C8
36	F	309	CLA	C13-C15-C16-C17
36	H	316	CLA	C5-C6-C7-C8
36	P	301	CLA	C5-C6-C7-C8
36	P	311	CLA	C8-C10-C11-C12
36	Q	308	CLA	C8-C10-C11-C12
36	a	810	CLA	C8-C10-C11-C12
36	a	812	CLA	C10-C11-C12-C13
36	b	809	CLA	C10-C11-C12-C13
36	b	837	CLA	C13-C15-C16-C17
36	U	306	CLA	C13-C15-C16-C17
36	V	313	CLA	C8-C10-C11-C12
36	V	311	CLA	C3-C5-C6-C7
42	J	319	LMG	C4-C5-C6-O5
41	G	320	LHG	C23-C24-C25-C26
35	T	302	A86	C35-C34-O4-C38
36	O	306	CLA	O1A-CGA-O2A-C1
36	L	309	CLA	C5-C6-C7-C8
36	U	311	CLA	C5-C6-C7-C8
36	W	218	CLA	CBD-CGD-O2D-CED
36	a	811	CLA	CBD-CGD-O2D-CED
41	j	104	LHG	C11-C12-C13-C14
36	A	306	CLA	C2C-C3C-CAC-CBC
36	H	315	CLA	C12-C13-C15-C16
36	J	308	CLA	C6-C7-C8-C10
36	K	309	CLA	C11-C10-C8-C7
36	N	316	CLA	C11-C12-C13-C15
36	P	301	CLA	C11-C10-C8-C7
36	a	801	CLA	C12-C13-C15-C16
36	b	809	CLA	C11-C10-C8-C7
36	b	820	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
36	l	201	CLA	C11-C12-C13-C15
36	l	205	CLA	C12-C13-C15-C16
36	S	309	CLA	CBA-CGA-O2A-C1
36	V	314	CLA	CBA-CGA-O2A-C1
41	O	317	LHG	C24-C23-O8-C6
39	I	318	LMT	O1'-C1-C2-C3
37	D	314	KC1	CAA-CBA-CGA-O1A
37	F	308	KC1	CAA-CBA-CGA-O1A
37	N	314	KC1	CAA-CBA-CGA-O1A
36	C	212	CLA	C2C-C3C-CAC-CBC
39	L	303	LMT	O5'-C5'-C6'-O6'
39	b	848	LMT	O5B-C5B-C6B-O6B
36	J	313	CLA	C5-C6-C7-C8
36	O	309	CLA	C8-C10-C11-C12
36	V	308	CLA	C10-C11-C12-C13
36	R	310	CLA	O1D-CGD-O2D-CED
41	E	322	LHG	C23-C24-C25-C26
41	G	321	LHG	C7-C8-C9-C10
42	L	321	LMG	C10-C11-C12-C13
34	F	303	DD6	C11-C10-C9-C8
34	R	307	DD6	C11-C10-C9-C8
35	M	304	A86	C11-C10-C9-C8
35	M	304	A86	C1-C2-C3-C4
35	M	304	A86	C24-C25-C26-C27
35	M	304	A86	C3-C4-C5-C6
35	U	303	A86	C24-C25-C26-C27
39	G	323	LMT	O1'-C1-C2-C3
39	P	321	LMT	O1'-C1-C2-C3
36	N	311	CLA	O1A-CGA-O2A-C1
42	D	321	LMG	C4-C5-C6-O5
36	K	310	CLA	C3-C5-C6-C7
36	f	804	CLA	C3-C5-C6-C7
35	E	302	A86	C33-C34-O4-C38
35	N	306	A86	C35-C34-O4-C38
35	R	306	A86	C35-C34-O4-C38
36	F	309	CLA	C15-C16-C17-C18
36	I	311	CLA	C15-C16-C17-C18
36	O	307	CLA	C8-C10-C11-C12
36	P	309	CLA	C8-C10-C11-C12
36	Q	306	CLA	C8-C10-C11-C12
36	Q	314	CLA	C10-C11-C12-C13
36	a	829	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	b	837	CLA	C5-C6-C7-C8
36	a	838	CLA	O1D-CGD-O2D-CED
38	b	804	SQD	C7-C8-C9-C10
41	a	842	LHG	C7-C8-C9-C10
41	a	850	LHG	C23-C24-C25-C26
41	f	808	LHG	C23-C24-C25-C26
42	D	321	LMG	C10-C11-C12-C13
36	M	306	CLA	O1A-CGA-O2A-C1
36	P	308	CLA	O1A-CGA-O2A-C1
36	Q	305	CLA	O1A-CGA-O2A-C1
36	b	840	CLA	O1A-CGA-O2A-C1
36	l	202	CLA	O1A-CGA-O2A-C1
36	l	204	CLA	O1A-CGA-O2A-C1
36	C	214	CLA	O1D-CGD-O2D-CED
36	G	319	CLA	O1D-CGD-O2D-CED
36	K	315	CLA	O1D-CGD-O2D-CED
36	A	314	CLA	C15-C16-C17-C18
36	C	207	CLA	C13-C15-C16-C17
36	C	212	CLA	C13-C15-C16-C17
36	F	314	CLA	C15-C16-C17-C18
36	H	308	CLA	C10-C11-C12-C13
36	H	308	CLA	C15-C16-C17-C18
36	H	309	CLA	C13-C15-C16-C17
36	H	316	CLA	C15-C16-C17-C18
36	K	308	CLA	C15-C16-C17-C18
36	K	310	CLA	C5-C6-C7-C8
36	L	308	CLA	C5-C6-C7-C8
36	L	320	CLA	C10-C11-C12-C13
36	M	309	CLA	C15-C16-C17-C18
36	M	311	CLA	C10-C11-C12-C13
36	O	307	CLA	C10-C11-C12-C13
36	P	309	CLA	C10-C11-C12-C13
36	P	310	CLA	C5-C6-C7-C8
36	P	313	CLA	C10-C11-C12-C13
36	Q	306	CLA	C10-C11-C12-C13
36	R	311	CLA	C13-C15-C16-C17
36	R	311	CLA	C15-C16-C17-C18
36	R	312	CLA	C8-C10-C11-C12
36	R	321	CLA	C13-C15-C16-C17
36	R	321	CLA	C15-C16-C17-C18
36	S	314	CLA	C10-C11-C12-C13
36	T	309	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	W	207	CLA	C5-C6-C7-C8
36	a	807	CLA	C5-C6-C7-C8
36	a	820	CLA	C13-C15-C16-C17
36	b	802	CLA	C8-C10-C11-C12
36	b	808	CLA	C15-C16-C17-C18
36	b	815	CLA	C8-C10-C11-C12
36	V	308	CLA	C15-C16-C17-C18
36	V	313	CLA	C5-C6-C7-C8
37	V	312	KC1	C4C-C3C-CAC-CBC
36	G	319	CLA	C2A-CAA-CBA-CGA
36	H	316	CLA	C2A-CAA-CBA-CGA
36	I	312	CLA	C3-C5-C6-C7
36	a	807	CLA	C2A-CAA-CBA-CGA
36	a	819	CLA	C2A-CAA-CBA-CGA
36	a	823	CLA	C2A-CAA-CBA-CGA
36	b	816	CLA	C2A-CAA-CBA-CGA
36	b	834	CLA	C2A-CAA-CBA-CGA
36	b	839	CLA	C2A-CAA-CBA-CGA
36	l	206	CLA	C2A-CAA-CBA-CGA
36	E	315	CLA	O1D-CGD-O2D-CED
36	S	320	CLA	O1D-CGD-O2D-CED
36	B	308	CLA	C13-C15-C16-C17
36	C	211	CLA	C10-C11-C12-C13
36	D	307	CLA	C8-C10-C11-C12
36	D	310	CLA	C15-C16-C17-C18
36	E	311	CLA	C5-C6-C7-C8
36	E	315	CLA	C5-C6-C7-C8
36	G	313	CLA	C10-C11-C12-C13
36	J	308	CLA	C8-C10-C11-C12
36	L	311	CLA	C10-C11-C12-C13
36	L	313	CLA	C10-C11-C12-C13
36	M	307	CLA	C15-C16-C17-C18
36	O	316	CLA	C5-C6-C7-C8
36	Q	314	CLA	C13-C15-C16-C17
36	S	310	CLA	C13-C15-C16-C17
36	S	319	CLA	C8-C10-C11-C12
36	T	314	CLA	C5-C6-C7-C8
36	a	802	CLA	C13-C15-C16-C17
36	a	827	CLA	C10-C11-C12-C13
36	a	831	CLA	C5-C6-C7-C8
36	b	820	CLA	C5-C6-C7-C8
36	b	825	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	b	826	CLA	C10-C11-C12-C13
36	l	201	CLA	C8-C10-C11-C12
43	b	842	PQN	C15-C16-C17-C18
35	F	307	A86	C33-C34-O4-C38
35	I	302	A86	C35-C34-O4-C38
35	N	301	A86	C33-C34-O4-C38
35	N	320	A86	C35-C34-O4-C38
35	O	319	A86	C35-C34-O4-C38
35	Q	304	A86	C35-C34-O4-C38
35	S	301	A86	C33-C34-O4-C38
39	L	303	LMT	C4'-C5'-C6'-O6'
40	C	215	DGD	C1A-C2A-C3A-C4A
40	L	302	DGD	C1B-C2B-C3B-C4B
41	D	318	LHG	C23-C24-C25-C26
41	G	321	LHG	C23-C24-C25-C26
41	f	809	LHG	C7-C8-C9-C10
42	I	315	LMG	C28-C29-C30-C31
42	a	852	LMG	C10-C11-C12-C13
42	V	315	LMG	C28-C29-C30-C31
36	W	210	CLA	O1D-CGD-O2D-CED
36	b	805	CLA	O1D-CGD-O2D-CED
36	E	308	CLA	O1A-CGA-O2A-C1
36	N	318	CLA	O1A-CGA-O2A-C1
41	I	316	LHG	O10-C23-O8-C6
36	T	313	CLA	C3-C5-C6-C7
36	a	820	CLA	C3-C5-C6-C7
35	R	305	A86	O5-C38-O4-C34
39	a	851	LMT	O5'-C1'-O1'-C1
40	L	302	DGD	O6E-C1E-O5D-C6D
41	D	319	LHG	C12-C13-C14-C15
41	a	850	LHG	C17-C18-C19-C20
42	V	315	LMG	C32-C33-C34-C35
39	U	315	LMT	O5B-C5B-C6B-O6B
39	G	322	LMT	O1'-C1-C2-C3
36	A	306	CLA	O1D-CGD-O2D-CED
36	D	308	CLA	O1D-CGD-O2D-CED
36	R	312	CLA	O1D-CGD-O2D-CED
36	b	818	CLA	O1D-CGD-O2D-CED
36	A	308	CLA	C10-C11-C12-C13
36	B	305	CLA	C10-C11-C12-C13
36	B	305	CLA	C13-C15-C16-C17
36	B	305	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	C	208	CLA	C5-C6-C7-C8
36	E	311	CLA	C13-C15-C16-C17
36	H	308	CLA	C5-C6-C7-C8
36	H	315	CLA	C10-C11-C12-C13
36	I	310	CLA	C13-C15-C16-C17
36	J	313	CLA	C13-C15-C16-C17
36	O	307	CLA	C5-C6-C7-C8
36	O	316	CLA	C10-C11-C12-C13
36	P	309	CLA	C5-C6-C7-C8
36	Q	306	CLA	C5-C6-C7-C8
36	R	313	CLA	C10-C11-C12-C13
36	R	315	CLA	C13-C15-C16-C17
36	W	212	CLA	C15-C16-C17-C18
36	a	802	CLA	C15-C16-C17-C18
36	a	817	CLA	C8-C10-C11-C12
36	a	825	CLA	C5-C6-C7-C8
36	a	825	CLA	C8-C10-C11-C12
36	a	839	CLA	C15-C16-C17-C18
36	b	808	CLA	C10-C11-C12-C13
36	b	809	CLA	C5-C6-C7-C8
36	b	815	CLA	C10-C11-C12-C13
36	b	841	CLA	C15-C16-C17-C18
36	l	201	CLA	C10-C11-C12-C13
36	h	203	CLA	C15-C16-C17-C18
36	U	310	CLA	C13-C15-C16-C17
36	U	311	CLA	C8-C10-C11-C12
36	V	308	CLA	C8-C10-C11-C12
36	V	314	CLA	C15-C16-C17-C18
42	j	105	LMG	C15-C16-C17-C18
41	R	323	LHG	O2-C2-C3-O3
41	i	104	LHG	O2-C2-C3-O3
41	D	319	LHG	C24-C23-O8-C6
36	H	310	CLA	CBD-CGD-O2D-CED
39	G	323	LMT	C4'-C5'-C6'-O6'
36	W	209	CLA	C8-C10-C11-C12
40	C	215	DGD	C1B-C2B-C3B-C4B
41	G	301	LHG	C23-C24-C25-C26
42	L	321	LMG	C28-C29-C30-C31
42	h	206	LMG	C10-C11-C12-C13
36	C	208	CLA	C8-C10-C11-C12
36	H	311	CLA	C10-C11-C12-C13
36	I	311	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	K	316	CLA	C13-C15-C16-C17
36	b	811	CLA	C13-C15-C16-C17
36	b	830	CLA	C10-C11-C12-C13
42	D	321	LMG	C31-C32-C33-C34
35	M	302	A86	C35-C34-O4-C38
35	O	303	A86	C35-C34-O4-C38
35	P	304	A86	C35-C34-O4-C38
35	Q	301	A86	C35-C34-O4-C38
39	G	323	LMT	O5'-C5'-C6'-O6'
39	I	318	LMT	C4'-C5'-C6'-O6'
36	K	309	CLA	C3-C5-C6-C7
36	O	316	CLA	C3-C5-C6-C7
36	U	306	CLA	C3-C5-C6-C7
36	N	307	CLA	O1D-CGD-O2D-CED
36	N	309	CLA	O1D-CGD-O2D-CED
36	U	305	CLA	O1D-CGD-O2D-CED
36	G	309	CLA	C10-C11-C12-C13
36	H	309	CLA	C15-C16-C17-C18
36	H	316	CLA	C13-C15-C16-C17
36	I	308	CLA	C13-C15-C16-C17
36	K	307	CLA	C10-C11-C12-C13
36	a	809	CLA	C5-C6-C7-C8
36	j	101	CLA	C5-C6-C7-C8
36	V	314	CLA	C13-C15-C16-C17
37	L	317	KC1	CAA-CBA-CGA-O2A
36	a	816	CLA	CBD-CGD-O2D-CED
36	R	310	CLA	O1A-CGA-O2A-C1
36	a	836	CLA	O1A-CGA-O2A-C1
39	I	318	LMT	C4B-C5B-C6B-O6B
41	F	319	LHG	C23-C24-C25-C26
42	J	319	LMG	C28-C29-C30-C31
36	X	306	CLA	O1D-CGD-O2D-CED
39	L	303	LMT	O1'-C1-C2-C3
36	A	314	CLA	C13-C15-C16-C17
36	F	310	CLA	C5-C6-C7-C8
36	H	312	CLA	C8-C10-C11-C12
36	b	806	CLA	C13-C15-C16-C17
36	b	839	CLA	C5-C6-C7-C8
36	h	203	CLA	C8-C10-C11-C12
36	U	310	CLA	C15-C16-C17-C18
36	V	308	CLA	C13-C15-C16-C17
36	H	316	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	V	305	CLA	CBA-CGA-O2A-C1
36	D	316	CLA	C2C-C3C-CAC-CBC
36	C	211	CLA	CBD-CGD-O2D-CED
36	h	203	CLA	O1A-CGA-O2A-C1
41	b	850	LHG	O10-C23-O8-C6
41	a	850	LHG	C7-C8-C9-C10
42	V	315	LMG	C4-C5-C6-O5
36	S	314	CLA	C13-C15-C16-C17
36	T	311	CLA	C8-C10-C11-C12
36	H	306	CLA	C3-C5-C6-C7
36	a	827	CLA	C13-C15-C16-C17
40	b	849	DGD	C4E-C5E-C6E-O5E
42	L	321	LMG	C4-C5-C6-O5
36	E	308	CLA	CBD-CGD-O2D-CED
40	C	215	DGD	C6B-C7B-C8B-C9B
34	E	306	DD6	C24-C25-C26-C27
34	Q	302	DD6	C1-C2-C3-C4
36	B	308	CLA	C8-C10-C11-C12
41	F	318	LHG	O9-C7-O7-C5
41	O	317	LHG	O9-C7-O7-C5
41	F	319	LHG	C1-C2-C3-O3
41	R	323	LHG	C1-C2-C3-O3
41	i	104	LHG	C1-C2-C3-O3
36	B	308	CLA	C2A-CAA-CBA-CGA
36	L	312	CLA	C2A-CAA-CBA-CGA
36	S	321	CLA	C2A-CAA-CBA-CGA
36	b	825	CLA	C2A-CAA-CBA-CGA
36	W	212	CLA	CBA-CGA-O2A-C1
41	E	322	LHG	C24-C23-O8-C6
42	a	852	LMG	C22-C23-C24-C25
35	R	301	A86	C33-C34-O4-C38
35	T	306	A86	C35-C34-O4-C38
35	X	302	A86	C35-C34-O4-C38
36	A	306	CLA	C8-C10-C11-C12
36	F	312	CLA	C8-C10-C11-C12
36	F	312	CLA	C10-C11-C12-C13
36	I	308	CLA	C8-C10-C11-C12
36	K	316	CLA	C8-C10-C11-C12
36	L	320	CLA	C5-C6-C7-C8
36	O	309	CLA	C15-C16-C17-C18
36	O	311	CLA	C5-C6-C7-C8
36	P	311	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	P	313	CLA	C5-C6-C7-C8
36	Q	308	CLA	C15-C16-C17-C18
36	R	310	CLA	C5-C6-C7-C8
36	R	312	CLA	C13-C15-C16-C17
36	S	310	CLA	C5-C6-C7-C8
36	W	212	CLA	C5-C6-C7-C8
36	a	831	CLA	C8-C10-C11-C12
36	a	839	CLA	C13-C15-C16-C17
36	b	805	CLA	C8-C10-C11-C12
36	b	815	CLA	C15-C16-C17-C18
36	b	820	CLA	C10-C11-C12-C13
36	b	826	CLA	C13-C15-C16-C17
36	f	804	CLA	C13-C15-C16-C17
36	j	102	CLA	C13-C15-C16-C17
36	l	201	CLA	C5-C6-C7-C8
36	U	306	CLA	C8-C10-C11-C12
36	V	311	CLA	C15-C16-C17-C18
43	a	840	PQN	C20-C21-C22-C23
36	b	812	CLA	CBD-CGD-O2D-CED
36	V	310	CLA	CBD-CGD-O2D-CED
36	A	308	CLA	C8-C10-C11-C12
36	E	311	CLA	C8-C10-C11-C12
36	K	307	CLA	C8-C10-C11-C12
36	N	316	CLA	C10-C11-C12-C13
36	O	308	CLA	C13-C15-C16-C17
36	T	309	CLA	C5-C6-C7-C8
36	a	810	CLA	C10-C11-C12-C13
36	a	812	CLA	C8-C10-C11-C12
36	l	201	CLA	C13-C15-C16-C17
36	U	311	CLA	C10-C11-C12-C13
39	I	317	LMT	C4B-C5B-C6B-O6B
39	a	851	LMT	C4'-C5'-C6'-O6'
36	D	307	CLA	C5-C6-C7-C8
36	E	316	CLA	C5-C6-C7-C8
36	O	316	CLA	C13-C15-C16-C17
36	P	310	CLA	C13-C15-C16-C17
36	a	817	CLA	C10-C11-C12-C13
36	a	836	CLA	C13-C15-C16-C17
36	b	819	CLA	C5-C6-C7-C8
36	b	820	CLA	C8-C10-C11-C12
36	b	827	CLA	C10-C11-C12-C13
36	V	306	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	V	311	CLA	C5-C6-C7-C8
36	V	311	CLA	C13-C15-C16-C17
36	V	314	CLA	C5-C6-C7-C8
43	a	840	PQN	C25-C26-C27-C28
35	L	306	A86	C33-C34-O4-C38
36	C	207	CLA	CBA-CGA-O2A-C1
36	K	309	CLA	CBA-CGA-O2A-C1
37	M	318	KC1	CAA-CBA-CGA-O2A
36	F	313	CLA	C4-C3-C5-C6
36	S	312	CLA	C4-C3-C5-C6
36	Q	312	CLA	O1D-CGD-O2D-CED
36	b	836	CLA	C4C-C3C-CAC-CBC
36	l	205	CLA	C8-C10-C11-C12
36	D	308	CLA	C2C-C3C-CAC-CBC
36	D	312	CLA	C3-C5-C6-C7
35	T	301	A86	C39-C38-O4-C34
36	R	312	CLA	C11-C12-C13-C14
36	O	314	CLA	O1D-CGD-O2D-CED
36	P	316	CLA	O1D-CGD-O2D-CED
36	a	815	CLA	O1D-CGD-O2D-CED
36	a	820	CLA	O1D-CGD-O2D-CED
36	b	808	CLA	O1D-CGD-O2D-CED
42	D	320	LMG	C15-C16-C17-C18
36	W	215	CLA	O2A-C1-C2-C3
38	A	315	SQD	C2-C1-O6-C44
39	B	313	LMT	C2'-C1'-O1'-C1
39	E	320	LMT	C2'-C1'-O1'-C1
39	E	323	LMT	C2'-C1'-O1'-C1
39	K	318	LMT	C2'-C1'-O1'-C1
39	U	314	LMT	C2'-C1'-O1'-C1
40	L	302	DGD	C2E-C1E-O5D-C6D
36	L	308	CLA	C8-C10-C11-C12
36	W	207	CLA	C15-C16-C17-C18
36	V	305	CLA	C10-C11-C12-C13
39	h	205	LMT	O5B-C5B-C6B-O6B
41	I	316	LHG	C7-C8-C9-C10
39	a	851	LMT	C4B-C5B-C6B-O6B
35	J	303	A86	C35-C34-O4-C38
36	L	320	CLA	CBA-CGA-O2A-C1
36	O	311	CLA	CBA-CGA-O2A-C1
36	P	313	CLA	CBA-CGA-O2A-C1
39	I	318	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
36	a	826	CLA	C16-C17-C18-C20
36	l	201	CLA	C16-C17-C18-C20
36	A	306	CLA	C10-C11-C12-C13
36	f	802	CLA	C15-C16-C17-C18
44	a	845	BCR	C20-C21-C22-C37
44	b	844	BCR	C11-C10-C9-C34
44	l	203	BCR	C11-C10-C9-C34
44	l	203	BCR	C20-C21-C22-C37
41	D	319	LHG	C23-C24-C25-C26
42	E	319	LMG	C28-C29-C30-C31
39	a	853	LMT	O5B-C5B-C6B-O6B
42	D	321	LMG	O6-C5-C6-O5
35	H	301	A86	C39-C38-O4-C34
36	a	829	CLA	O1D-CGD-O2D-CED
36	P	314	CLA	C10-C11-C12-C13
36	a	825	CLA	C10-C11-C12-C13
36	j	102	CLA	C10-C11-C12-C13
34	B	304	DD6	C12-C11-C13-C14
34	D	301	DD6	C-C1-C24-C25
34	D	304	DD6	C12-C11-C13-C14
34	W	205	DD6	C12-C11-C13-C14
34	a	849	DD6	C12-C11-C13-C14
35	D	302	A86	C-C1-C24-C25
44	a	846	BCR	C37-C22-C23-C24
44	b	845	BCR	C7-C8-C9-C34
44	b	847	BCR	C7-C8-C9-C34
44	i	103	BCR	C37-C22-C23-C24
36	a	814	CLA	C2C-C3C-CAC-CBC
39	a	854	LMT	C5'-C4'-O1B-C1B
34	B	304	DD6	C10-C11-C13-C14
34	D	304	DD6	C10-C11-C13-C14
34	R	308	DD6	C10-C11-C13-C14
34	S	307	DD6	C2-C1-C24-C25
34	W	205	DD6	C10-C11-C13-C14
34	a	849	DD6	C5-C6-C8-C9
35	B	303	A86	C5-C6-C8-C9
35	D	302	A86	C2-C1-C24-C25
36	S	309	CLA	O1A-CGA-O2A-C1
36	V	314	CLA	O1A-CGA-O2A-C1
35	M	305	A86	C35-C34-O4-C38
36	C	208	CLA	C2A-CAA-CBA-CGA
36	D	317	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	F	317	CLA	C2A-CAA-CBA-CGA
36	J	311	CLA	C2A-CAA-CBA-CGA
36	O	308	CLA	C2A-CAA-CBA-CGA
36	P	310	CLA	C2A-CAA-CBA-CGA
36	P	319	CLA	C2A-CAA-CBA-CGA
36	Q	307	CLA	C2A-CAA-CBA-CGA
36	R	312	CLA	C2A-CAA-CBA-CGA
36	R	322	CLA	C2A-CAA-CBA-CGA
36	a	808	CLA	C2A-CAA-CBA-CGA
36	D	312	CLA	C13-C15-C16-C17
36	E	312	CLA	C10-C11-C12-C13
36	R	310	CLA	C8-C10-C11-C12
36	a	832	CLA	C5-C6-C7-C8
36	b	837	CLA	C15-C16-C17-C18
41	D	318	LHG	O1-C1-C2-C3
41	F	319	LHG	O1-C1-C2-C3
41	G	320	LHG	O1-C1-C2-C3
41	a	850	LHG	O1-C1-C2-C3
41	b	850	LHG	O1-C1-C2-C3
41	f	808	LHG	O1-C1-C2-C3
41	l	208	LHG	O1-C1-C2-C3
36	a	830	CLA	O1D-CGD-O2D-CED
36	A	307	CLA	C11-C12-C13-C15
36	A	311	CLA	C16-C17-C18-C20
36	B	311	CLA	C6-C7-C8-C9
36	O	308	CLA	C16-C17-C18-C19
36	b	810	CLA	C16-C17-C18-C20
36	j	101	CLA	C16-C17-C18-C20
41	G	320	LHG	C15-C16-C17-C18
39	U	315	LMT	O1'-C1-C2-C3
36	V	305	CLA	O1A-CGA-O2A-C1
41	O	317	LHG	O10-C23-O8-C6
36	E	313	CLA	C3-C5-C6-C7
36	F	309	CLA	C3-C5-C6-C7
36	H	316	CLA	C3-C5-C6-C7
36	a	827	CLA	C3-C5-C6-C7
36	a	836	CLA	C3-C5-C6-C7
36	f	803	CLA	C3-C5-C6-C7
39	P	321	LMT	O5'-C5'-C6'-O6'
36	a	807	CLA	C8-C10-C11-C12
44	f	806	BCR	C11-C10-C9-C8
44	f	806	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
44	l	203	BCR	C20-C21-C22-C23
44	h	201	BCR	C20-C21-C22-C23
38	A	315	SQD	O5-C1-O6-C44
39	B	313	LMT	O5'-C1'-O1'-C1
39	E	320	LMT	O5'-C1'-O1'-C1
35	B	301	A86	C33-C34-O4-C38
35	I	304	A86	C33-C34-O4-C38
35	X	301	A86	C33-C34-O4-C38
35	X	303	A86	C33-C34-O4-C38
35	U	302	A86	C35-C34-O4-C38
37	L	317	KC1	CAA-CBA-CGA-O1A
37	M	317	KC1	CAA-CBA-CGA-O1A
37	M	318	KC1	CAA-CBA-CGA-O1A
36	l	205	CLA	C15-C16-C17-C18
36	b	837	CLA	O1D-CGD-O2D-CED
36	O	312	CLA	O1D-CGD-O2D-CED
36	P	314	CLA	O1D-CGD-O2D-CED
36	Q	310	CLA	O1D-CGD-O2D-CED
36	b	816	CLA	O1D-CGD-O2D-CED
36	A	311	CLA	CBA-CGA-O2A-C1
36	T	314	CLA	CBA-CGA-O2A-C1
36	a	805	CLA	CBA-CGA-O2A-C1
36	f	805	CLA	CBA-CGA-O2A-C1
36	l	201	CLA	CBA-CGA-O2A-C1
36	U	310	CLA	CBA-CGA-O2A-C1
39	I	318	LMT	C1-C2-C3-C4
36	H	308	CLA	C8-C10-C11-C12
36	O	311	CLA	CBD-CGD-O2D-CED
36	P	313	CLA	CBD-CGD-O2D-CED
41	R	323	LHG	C23-C24-C25-C26
40	C	215	DGD	O6E-C5E-C6E-O5E
36	K	312	CLA	C3-C5-C6-C7
36	K	307	CLA	C2-C1-O2A-CGA
36	b	824	CLA	C2-C1-O2A-CGA
36	A	307	CLA	C11-C12-C13-C14
36	B	305	CLA	C16-C17-C18-C20
36	B	311	CLA	C6-C7-C8-C10
36	G	313	CLA	C16-C17-C18-C20
36	H	316	CLA	C16-C17-C18-C19
36	H	316	CLA	C16-C17-C18-C20
36	O	308	CLA	C16-C17-C18-C20
36	R	315	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
36	a	807	CLA	C16-C17-C18-C20
36	a	828	CLA	C16-C17-C18-C19
36	b	820	CLA	C11-C12-C13-C14
36	b	821	CLA	C16-C17-C18-C20
36	U	306	CLA	C16-C17-C18-C20
36	U	310	CLA	C16-C17-C18-C19
36	U	310	CLA	C16-C17-C18-C20
36	V	311	CLA	C16-C17-C18-C20
36	I	305	CLA	C5-C6-C7-C8
35	B	301	A86	C35-C34-O4-C38
36	l	202	CLA	O1D-CGD-O2D-CED
39	a	851	LMT	C2-C3-C4-C5
41	G	321	LHG	C30-C31-C32-C33
41	O	318	LHG	C13-C14-C15-C16
41	a	842	LHG	C24-C25-C26-C27
41	a	850	LHG	C15-C16-C17-C18
41	f	808	LHG	C25-C26-C27-C28
42	G	325	LMG	C19-C20-C21-C22
36	L	320	CLA	CBD-CGD-O2D-CED
38	b	804	SQD	C28-C29-C30-C31
39	F	321	LMT	C5-C6-C7-C8
39	a	851	LMT	C11-C10-C9-C8
41	F	319	LHG	C16-C17-C18-C19
41	R	323	LHG	C27-C28-C29-C30
41	a	850	LHG	C32-C33-C34-C35
41	i	104	LHG	C15-C16-C17-C18
42	D	321	LMG	C30-C31-C32-C33
42	L	321	LMG	C13-C14-C15-C16
42	V	315	LMG	C15-C16-C17-C18
36	R	316	CLA	O1D-CGD-O2D-CED
39	L	303	LMT	O5B-C5B-C6B-O6B
36	S	310	CLA	C15-C16-C17-C18
36	G	315	CLA	C11-C10-C8-C9
38	b	804	SQD	C11-C10-C9-C8
39	B	312	LMT	C11-C10-C9-C8
39	E	320	LMT	C6-C7-C8-C9
39	G	322	LMT	C2-C3-C4-C5
40	C	215	DGD	C3A-C4A-C5A-C6A
41	F	319	LHG	C17-C18-C19-C20
41	Q	315	LHG	C34-C35-C36-C37
41	l	208	LHG	C30-C31-C32-C33
42	E	318	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
42	G	325	LMG	C33-C34-C35-C36
42	I	315	LMG	C40-C41-C42-C43
42	J	318	LMG	C21-C22-C23-C24
42	j	105	LMG	C40-C41-C42-C43
36	H	316	CLA	O1A-CGA-O2A-C1
41	D	319	LHG	O10-C23-O8-C6
36	D	313	CLA	CBA-CGA-O2A-C1
36	T	308	CLA	CBA-CGA-O2A-C1
36	a	810	CLA	CBA-CGA-O2A-C1
36	l	206	CLA	CBA-CGA-O2A-C1
39	G	322	LMT	C1-C2-C3-C4
39	E	323	LMT	C5-C6-C7-C8
40	b	849	DGD	C3A-C4A-C5A-C6A
41	E	322	LHG	C9-C10-C11-C12
41	G	321	LHG	C15-C16-C17-C18
41	G	321	LHG	C29-C30-C31-C32
41	Q	315	LHG	C13-C14-C15-C16
41	f	809	LHG	C9-C10-C11-C12
41	j	104	LHG	C12-C13-C14-C15
41	l	208	LHG	C11-C10-C9-C8
42	E	318	LMG	C14-C15-C16-C17
42	E	319	LMG	C12-C13-C14-C15
42	G	324	LMG	C13-C14-C15-C16
42	I	315	LMG	C11-C12-C13-C14
42	J	318	LMG	C22-C23-C24-C25
42	j	105	LMG	C16-C17-C18-C19
42	h	206	LMG	C23-C24-C25-C26
42	V	316	LMG	C17-C18-C19-C20
39	U	315	LMT	C2-C1-O1'-C1'
41	D	318	LHG	O1-C1-C2-O2
41	D	319	LHG	O1-C1-C2-O2
41	G	320	LHG	O1-C1-C2-O2
41	a	842	LHG	O1-C1-C2-O2
41	l	208	LHG	O1-C1-C2-O2
39	U	314	LMT	C3-C4-C5-C6
41	G	301	LHG	C17-C18-C19-C20
41	i	104	LHG	C28-C29-C30-C31
41	l	208	LHG	C10-C11-C12-C13
42	h	206	LMG	C11-C12-C13-C14
42	V	316	LMG	C15-C16-C17-C18
36	M	307	CLA	O1D-CGD-O2D-CED
36	P	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	S	319	CLA	O1D-CGD-O2D-CED
36	W	206	CLA	O1D-CGD-O2D-CED
36	a	832	CLA	C13-C15-C16-C17
36	A	313	CLA	C4B-C3B-CAB-CBB
36	B	306	CLA	C4B-C3B-CAB-CBB
36	B	307	CLA	C4B-C3B-CAB-CBB
36	C	206	CLA	C4B-C3B-CAB-CBB
36	C	209	CLA	C4B-C3B-CAB-CBB
36	C	214	CLA	C4B-C3B-CAB-CBB
36	D	312	CLA	C4B-C3B-CAB-CBB
36	D	317	CLA	C4B-C3B-CAB-CBB
36	H	306	CLA	C4B-C3B-CAB-CBB
36	H	317	CLA	C4B-C3B-CAB-CBB
36	K	311	CLA	C4B-C3B-CAB-CBB
36	M	314	CLA	C4B-C3B-CAB-CBB
36	N	307	CLA	C4B-C3B-CAB-CBB
36	O	314	CLA	C4B-C3B-CAB-CBB
36	O	316	CLA	C4B-C3B-CAB-CBB
36	P	316	CLA	C4B-C3B-CAB-CBB
36	Q	312	CLA	C4B-C3B-CAB-CBB
36	R	310	CLA	C4B-C3B-CAB-CBB
36	R	312	CLA	C4B-C3B-CAB-CBB
36	R	315	CLA	C4B-C3B-CAB-CBB
36	R	319	CLA	C4B-C3B-CAB-CBB
36	R	320	CLA	C4B-C3B-CAB-CBB
36	R	322	CLA	C4B-C3B-CAB-CBB
36	S	311	CLA	C4B-C3B-CAB-CBB
36	S	317	CLA	C4B-C3B-CAB-CBB
36	S	320	CLA	C4B-C3B-CAB-CBB
36	T	316	CLA	C4B-C3B-CAB-CBB
36	W	211	CLA	C4B-C3B-CAB-CBB
36	X	306	CLA	C4B-C3B-CAB-CBB
36	X	309	CLA	C4B-C3B-CAB-CBB
36	X	313	CLA	C4B-C3B-CAB-CBB
36	a	804	CLA	C4B-C3B-CAB-CBB
36	a	808	CLA	C4B-C3B-CAB-CBB
36	a	814	CLA	C4B-C3B-CAB-CBB
36	a	823	CLA	C4B-C3B-CAB-CBB
36	b	808	CLA	C4B-C3B-CAB-CBB
36	b	811	CLA	C4B-C3B-CAB-CBB
36	b	829	CLA	C4B-C3B-CAB-CBB
36	b	835	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	b	839	CLA	C4B-C3B-CAB-CBB
36	j	106	CLA	C4B-C3B-CAB-CBB
36	l	202	CLA	C4B-C3B-CAB-CBB
36	U	305	CLA	C4B-C3B-CAB-CBB
36	U	313	CLA	C4B-C3B-CAB-CBB
36	V	309	CLA	C4B-C3B-CAB-CBB
42	J	319	LMG	C10-C11-C12-C13
35	K	303	A86	C35-C34-O4-C38
39	h	205	LMT	C4-C5-C6-C7
40	b	849	DGD	C4A-C5A-C6A-C7A
41	G	321	LHG	C28-C29-C30-C31
41	Q	315	LHG	C32-C33-C34-C35
42	G	325	LMG	C40-C41-C42-C43
36	G	313	CLA	C16-C17-C18-C19
36	H	312	CLA	C16-C17-C18-C20
36	P	319	CLA	C11-C12-C13-C14
36	P	319	CLA	C11-C12-C13-C15
36	Q	314	CLA	C16-C17-C18-C20
36	R	315	CLA	C16-C17-C18-C19
36	a	807	CLA	C16-C17-C18-C19
36	b	825	CLA	C16-C17-C18-C20
36	J	309	CLA	O1D-CGD-O2D-CED
36	b	815	CLA	O1D-CGD-O2D-CED
39	E	323	LMT	C11-C10-C9-C8
41	D	318	LHG	C12-C13-C14-C15
42	j	105	LMG	C17-C18-C19-C20
36	C	212	CLA	C5-C6-C7-C8
36	D	310	CLA	C8-C10-C11-C12
36	D	313	CLA	C8-C10-C11-C12
36	H	309	CLA	C10-C11-C12-C13
36	H	311	CLA	C13-C15-C16-C17
36	R	311	CLA	C8-C10-C11-C12
36	a	805	CLA	C8-C10-C11-C12
36	b	815	CLA	C13-C15-C16-C17
42	D	321	LMG	C11-C10-O7-C8
42	L	321	LMG	C11-C10-O7-C8
41	F	318	LHG	C12-C13-C14-C15
41	G	301	LHG	C27-C28-C29-C30
36	G	309	CLA	C6-C7-C8-C10
36	I	305	CLA	C11-C12-C13-C15
36	I	311	CLA	C6-C7-C8-C10
36	J	307	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
36	L	311	CLA	C12-C13-C15-C16
36	l	202	CLA	C11-C12-C13-C15
41	E	322	LHG	C16-C17-C18-C19
41	G	301	LHG	C29-C30-C31-C32
36	M	307	CLA	C13-C15-C16-C17
36	b	808	CLA	C13-C15-C16-C17
36	b	809	CLA	C15-C16-C17-C18
36	b	812	CLA	C8-C10-C11-C12
36	b	821	CLA	C15-C16-C17-C18
36	V	313	CLA	C10-C11-C12-C13
39	G	323	LMT	C1-C2-C3-C4
40	b	849	DGD	C4B-C5B-C6B-C7B
41	D	319	LHG	C10-C11-C12-C13
41	G	320	LHG	C25-C26-C27-C28
41	O	317	LHG	C26-C27-C28-C29
41	b	850	LHG	C12-C13-C14-C15
42	G	324	LMG	C12-C13-C14-C15
36	W	212	CLA	O1A-CGA-O2A-C1
36	b	809	CLA	C3-C5-C6-C7
36	B	307	CLA	C3A-C2A-CAA-CBA
36	C	210	CLA	C3A-C2A-CAA-CBA
36	E	312	CLA	C3A-C2A-CAA-CBA
36	F	310	CLA	C3A-C2A-CAA-CBA
36	F	312	CLA	C3A-C2A-CAA-CBA
36	F	317	CLA	C3A-C2A-CAA-CBA
36	G	307	CLA	C3A-C2A-CAA-CBA
36	H	312	CLA	C3A-C2A-CAA-CBA
36	I	309	CLA	C3A-C2A-CAA-CBA
36	M	312	CLA	C3A-C2A-CAA-CBA
36	O	310	CLA	C3A-C2A-CAA-CBA
36	P	312	CLA	C3A-C2A-CAA-CBA
36	Q	309	CLA	C3A-C2A-CAA-CBA
36	Q	310	CLA	C3A-C2A-CAA-CBA
36	S	314	CLA	C3A-C2A-CAA-CBA
36	S	320	CLA	C3A-C2A-CAA-CBA
36	T	312	CLA	C3A-C2A-CAA-CBA
36	X	309	CLA	C3A-C2A-CAA-CBA
36	a	831	CLA	C3A-C2A-CAA-CBA
36	a	832	CLA	C4-C3-C5-C6
36	b	801	CLA	C3A-C2A-CAA-CBA
36	b	815	CLA	C3A-C2A-CAA-CBA
36	b	827	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	f	805	CLA	C3A-C2A-CAA-CBA
36	h	203	CLA	C3A-C2A-CAA-CBA
36	U	309	CLA	C3A-C2A-CAA-CBA
36	V	311	CLA	C3A-C2A-CAA-CBA
35	L	319	A86	C33-C34-O4-C38
35	O	302	A86	C33-C34-O4-C38
35	P	303	A86	C33-C34-O4-C38
36	N	316	CLA	O1D-CGD-O2D-CED
39	G	323	LMT	C3-C4-C5-C6
41	b	850	LHG	C15-C16-C17-C18
37	N	314	KC1	C4C-C3C-CAC-CBC
36	b	809	CLA	CBD-CGD-O2D-CED
36	J	316	CLA	CBA-CGA-O2A-C1
39	b	848	LMT	O1'-C1-C2-C3
39	K	318	LMT	C7-C8-C9-C10
36	I	306	CLA	C5-C6-C7-C8
36	I	311	CLA	C13-C15-C16-C17
36	J	310	CLA	C8-C10-C11-C12
36	M	309	CLA	C10-C11-C12-C13
36	W	211	CLA	C10-C11-C12-C13
36	l	205	CLA	C13-C15-C16-C17
36	h	203	CLA	C10-C11-C12-C13
36	U	306	CLA	C5-C6-C7-C8
37	U	312	KC1	O1D-CGD-O2D-CED
34	R	308	DD6	C3-C4-C5-C6
34	S	307	DD6	C24-C25-C26-C27
35	I	301	A86	C11-C10-C9-C8
35	O	305	A86	C3-C4-C5-C6
36	A	311	CLA	C16-C17-C18-C19
36	I	306	CLA	C16-C17-C18-C19
36	Q	314	CLA	C16-C17-C18-C19
36	a	826	CLA	C16-C17-C18-C19
36	b	810	CLA	C16-C17-C18-C19
36	b	825	CLA	C16-C17-C18-C19
36	U	311	CLA	C16-C17-C18-C20
42	I	315	LMG	O6-C5-C6-O5
39	B	312	LMT	C1-C2-C3-C4
39	U	315	LMT	C1-C2-C3-C4
36	C	207	CLA	O1A-CGA-O2A-C1
36	K	309	CLA	O1A-CGA-O2A-C1
41	E	322	LHG	O10-C23-O8-C6
39	U	315	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
41	G	301	LHG	C12-C13-C14-C15
41	I	316	LHG	C27-C28-C29-C30
41	b	850	LHG	C29-C30-C31-C32
42	J	318	LMG	C39-C40-C41-C42
42	h	206	LMG	C21-C22-C23-C24
36	Q	306	CLA	CBD-CGD-O2D-CED
41	F	319	LHG	C9-C10-C11-C12
41	f	808	LHG	C12-C13-C14-C15
41	i	104	LHG	C25-C26-C27-C28
42	E	318	LMG	C11-C12-C13-C14
41	G	320	LHG	C1-C2-C3-O3
36	H	318	CLA	CBA-CGA-O2A-C1
36	J	309	CLA	CBA-CGA-O2A-C1
36	L	308	CLA	CBA-CGA-O2A-C1
36	N	307	CLA	CBA-CGA-O2A-C1
42	V	316	LMG	C29-C28-O8-C9
39	L	318	LMT	C1-C2-C3-C4
41	R	323	LHG	C4-C5-C6-O8
39	F	321	LMT	C3-C4-C5-C6
41	D	318	LHG	C25-C26-C27-C28
41	O	317	LHG	C16-C17-C18-C19
41	R	323	LHG	C34-C35-C36-C37
41	b	850	LHG	C28-C29-C30-C31
42	j	105	LMG	C35-C36-C37-C38
36	H	317	CLA	C3-C5-C6-C7
36	b	833	CLA	C3-C5-C6-C7
35	N	320	A86	C33-C34-O4-C38
35	Q	304	A86	C33-C34-O4-C38
36	b	805	CLA	C13-C15-C16-C17
39	E	321	LMT	C5-C6-C7-C8
39	a	854	LMT	C7-C8-C9-C10
39	b	848	LMT	C5-C6-C7-C8
39	U	314	LMT	C4-C5-C6-C7
39	U	314	LMT	C5-C6-C7-C8
41	D	319	LHG	C31-C32-C33-C34
41	I	316	LHG	C12-C13-C14-C15
41	I	316	LHG	C16-C17-C18-C19
41	f	809	LHG	C33-C34-C35-C36
41	l	208	LHG	C15-C16-C17-C18
42	G	324	LMG	C36-C37-C38-C39
42	G	325	LMG	C18-C19-C20-C21
42	a	852	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
36	A	311	CLA	O1A-CGA-O2A-C1
36	L	320	CLA	O1A-CGA-O2A-C1
36	O	311	CLA	O1A-CGA-O2A-C1
36	P	313	CLA	O1A-CGA-O2A-C1
36	U	310	CLA	O1A-CGA-O2A-C1
42	D	320	LMG	C4-C5-C6-O5
39	P	320	LMT	C6-C7-C8-C9
41	E	322	LHG	C11-C10-C9-C8
41	F	318	LHG	C10-C11-C12-C13
42	J	319	LMG	C15-C16-C17-C18
42	h	206	LMG	C17-C18-C19-C20
36	D	307	CLA	O1D-CGD-O2D-CED
36	K	311	CLA	O1D-CGD-O2D-CED
36	R	315	CLA	O1D-CGD-O2D-CED
36	R	321	CLA	O1D-CGD-O2D-CED
39	E	321	LMT	C3-C4-C5-C6
41	G	321	LHG	C33-C34-C35-C36
41	i	104	LHG	C14-C15-C16-C17
42	D	320	LMG	C20-C21-C22-C23
42	G	325	LMG	C11-C12-C13-C14
42	G	325	LMG	C38-C39-C40-C41
39	E	323	LMT	O5'-C5'-C6'-O6'
36	R	313	CLA	C15-C16-C17-C18
36	C	205	CLA	O1D-CGD-O2D-CED
36	T	312	CLA	O1D-CGD-O2D-CED
39	G	323	LMT	C4-C5-C6-C7
39	a	854	LMT	C6-C7-C8-C9
41	D	319	LHG	C25-C26-C27-C28
41	O	317	LHG	C18-C19-C20-C21
41	l	208	LHG	C33-C34-C35-C36
42	I	315	LMG	C41-C42-C43-C44
36	B	305	CLA	C16-C17-C18-C19
36	b	840	CLA	C16-C17-C18-C20
36	V	311	CLA	C16-C17-C18-C19
41	i	104	LHG	C7-C8-C9-C10
42	j	105	LMG	C28-C29-C30-C31
36	f	805	CLA	O1A-CGA-O2A-C1
36	A	305	CLA	C2B-C3B-CAB-CBB
36	A	309	CLA	C2B-C3B-CAB-CBB
36	A	314	CLA	C2B-C3B-CAB-CBB
36	B	307	CLA	C2B-C3B-CAB-CBB
36	C	206	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	D	306	CLA	C2B-C3B-CAB-CBB
36	D	317	CLA	C2B-C3B-CAB-CBB
36	E	308	CLA	C2B-C3B-CAB-CBB
36	H	310	CLA	C2B-C3B-CAB-CBB
36	H	316	CLA	C2B-C3B-CAB-CBB
36	H	317	CLA	C2B-C3B-CAB-CBB
36	I	314	CLA	C2B-C3B-CAB-CBB
36	J	311	CLA	C2B-C3B-CAB-CBB
36	J	316	CLA	C2B-C3B-CAB-CBB
36	K	311	CLA	C2B-C3B-CAB-CBB
36	M	315	CLA	C2B-C3B-CAB-CBB
36	N	316	CLA	C2B-C3B-CAB-CBB
36	N	318	CLA	C2B-C3B-CAB-CBB
36	O	310	CLA	C2B-C3B-CAB-CBB
36	P	312	CLA	C2B-C3B-CAB-CBB
36	Q	309	CLA	C2B-C3B-CAB-CBB
36	R	310	CLA	C2B-C3B-CAB-CBB
36	R	314	CLA	C2B-C3B-CAB-CBB
36	R	319	CLA	C2B-C3B-CAB-CBB
36	R	320	CLA	C2B-C3B-CAB-CBB
36	S	311	CLA	C2B-C3B-CAB-CBB
36	S	318	CLA	C2B-C3B-CAB-CBB
36	T	312	CLA	C2B-C3B-CAB-CBB
36	T	316	CLA	C2B-C3B-CAB-CBB
36	W	214	CLA	C2B-C3B-CAB-CBB
36	W	216	CLA	C2B-C3B-CAB-CBB
36	a	804	CLA	C2B-C3B-CAB-CBB
36	a	808	CLA	C2B-C3B-CAB-CBB
36	a	817	CLA	C2B-C3B-CAB-CBB
36	a	833	CLA	C2B-C3B-CAB-CBB
36	a	834	CLA	C2B-C3B-CAB-CBB
36	b	829	CLA	C2B-C3B-CAB-CBB
36	b	835	CLA	C2B-C3B-CAB-CBB
36	b	839	CLA	C2B-C3B-CAB-CBB
36	j	106	CLA	C2B-C3B-CAB-CBB
36	l	202	CLA	C2B-C3B-CAB-CBB
36	U	307	CLA	C2B-C3B-CAB-CBB
36	V	305	CLA	C2B-C3B-CAB-CBB
44	a	847	BCR	C23-C24-C25-C26
44	a	847	BCR	C23-C24-C25-C30
44	b	846	BCR	C1-C6-C7-C8
44	h	201	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
44	h	201	BCR	C5-C6-C7-C8
39	F	321	LMT	C4-C5-C6-C7
41	O	318	LHG	C16-C17-C18-C19
41	a	850	LHG	C13-C14-C15-C16
42	D	320	LMG	C21-C22-C23-C24
42	m	102	LMG	C12-C13-C14-C15
36	O	307	CLA	CBD-CGD-O2D-CED
36	P	309	CLA	CBD-CGD-O2D-CED
36	b	801	CLA	CBD-CGD-O2D-CED
36	b	833	CLA	CBD-CGD-O2D-CED
36	U	306	CLA	CBD-CGD-O2D-CED
41	f	808	LHG	C8-C7-O7-C5
36	B	307	CLA	O1A-CGA-O2A-C1
36	R	316	CLA	O1A-CGA-O2A-C1
39	L	318	LMT	C4'-C5'-C6'-O6'
36	I	311	CLA	C5-C6-C7-C8
36	T	313	CLA	C15-C16-C17-C18
36	b	834	CLA	C15-C16-C17-C18
35	K	306	A86	C35-C34-O4-C38
41	G	321	LHG	C2-C3-O3-P
39	I	317	LMT	C9-C10-C11-C12
42	h	206	LMG	C24-C25-C26-C27
36	F	312	CLA	C3-C5-C6-C7
36	P	310	CLA	C3-C5-C6-C7
41	D	318	LHG	C27-C28-C29-C30
41	f	809	LHG	C24-C25-C26-C27
42	G	324	LMG	C38-C39-C40-C41
42	I	315	LMG	C30-C31-C32-C33
41	G	321	LHG	C10-C11-C12-C13
42	G	325	LMG	C16-C17-C18-C19
42	G	325	LMG	C21-C22-C23-C24
42	V	315	LMG	C16-C17-C18-C19
42	V	316	LMG	C18-C19-C20-C21
36	A	309	CLA	C2A-CAA-CBA-CGA
36	D	311	CLA	C2A-CAA-CBA-CGA
36	E	316	CLA	C2A-CAA-CBA-CGA
36	P	301	CLA	C2A-CAA-CBA-CGA
36	a	848	CLA	C2A-CAA-CBA-CGA
41	l	208	LHG	C23-C24-C25-C26
36	T	314	CLA	C10-C11-C12-C13
39	U	315	LMT	C7-C8-C9-C10
42	J	318	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
42	j	105	LMG	C14-C15-C16-C17
36	J	309	CLA	O1A-CGA-O2A-C1
36	T	308	CLA	O1A-CGA-O2A-C1
36	T	314	CLA	O1A-CGA-O2A-C1
36	l	201	CLA	O1A-CGA-O2A-C1
39	L	318	LMT	O5B-C5B-C6B-O6B
39	a	851	LMT	C5-C6-C7-C8
41	O	317	LHG	C25-C26-C27-C28
41	a	842	LHG	C29-C30-C31-C32
42	I	315	LMG	C15-C16-C17-C18
39	B	313	LMT	C5'-C4'-O1B-C1B
41	a	842	LHG	O9-C7-O7-C5
42	D	321	LMG	O9-C10-O7-C8
42	L	321	LMG	O9-C10-O7-C8
36	I	305	CLA	C12-C13-C15-C16
36	D	317	CLA	C4-C3-C5-C6
36	a	828	CLA	C4-C3-C5-C6
39	F	320	LMT	C7-C8-C9-C10
40	C	215	DGD	C8B-C9B-CAB-CBB
40	b	849	DGD	C6A-C7A-C8A-C9A
44	m	101	BCR	C18-C19-C20-C21
36	F	313	CLA	C2-C3-C5-C6
36	S	312	CLA	C2-C3-C5-C6
36	a	832	CLA	C2-C3-C5-C6
39	B	313	LMT	C6-C7-C8-C9
39	L	303	LMT	C3-C4-C5-C6
39	P	321	LMT	C2-C3-C4-C5
39	P	321	LMT	C3-C4-C5-C6
41	D	319	LHG	C11-C12-C13-C14
41	O	318	LHG	C32-C33-C34-C35
41	l	208	LHG	C28-C29-C30-C31
42	G	324	LMG	C18-C19-C20-C21
36	C	206	CLA	CBA-CGA-O2A-C1
36	F	309	CLA	CBA-CGA-O2A-C1
36	P	319	CLA	CBA-CGA-O2A-C1
36	a	809	CLA	CBA-CGA-O2A-C1
36	a	823	CLA	CBA-CGA-O2A-C1
36	a	848	CLA	CBA-CGA-O2A-C1
36	j	101	CLA	CBA-CGA-O2A-C1
42	E	318	LMG	C29-C28-O8-C9
39	G	323	LMT	O5B-C1B-O1B-C4'
41	O	317	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
36	M	307	CLA	C6-C7-C8-C9
36	R	310	CLA	C6-C7-C8-C9
36	V	311	CLA	C6-C7-C8-C9
39	U	314	LMT	C7-C8-C9-C10
41	F	318	LHG	C16-C17-C18-C19
41	G	301	LHG	C32-C33-C34-C35
41	O	318	LHG	C24-C25-C26-C27
41	f	809	LHG	C10-C11-C12-C13
42	j	105	LMG	C31-C32-C33-C34
42	V	315	LMG	C29-C30-C31-C32
36	A	308	CLA	C5-C6-C7-C8
36	b	816	CLA	C10-C11-C12-C13
36	i	102	CLA	C5-C6-C7-C8
36	R	314	CLA	C2C-C3C-CAC-CBC
39	P	321	LMT	C4-C5-C6-C7
41	D	318	LHG	C17-C18-C19-C20
41	D	319	LHG	C11-C10-C9-C8
41	I	316	LHG	C14-C15-C16-C17
41	I	316	LHG	C18-C19-C20-C21
41	Q	315	LHG	C27-C28-C29-C30
41	R	323	LHG	C17-C18-C19-C20
39	U	314	LMT	O5'-C1'-O1'-C1
41	a	843	LHG	C11-C10-C9-C8
42	j	105	LMG	C11-C12-C13-C14
39	U	314	LMT	O1'-C1-C2-C3
39	F	320	LMT	C2'-C1'-O1'-C1
39	f	807	LMT	C2'-C1'-O1'-C1
42	L	321	LMG	C2-C1-O1-C7
36	B	308	CLA	C10-C11-C12-C13
36	L	308	CLA	C10-C11-C12-C13
36	W	209	CLA	C5-C6-C7-C8
36	a	816	CLA	C8-C10-C11-C12
36	b	805	CLA	C15-C16-C17-C18
36	i	102	CLA	C13-C15-C16-C17
36	a	805	CLA	O1A-CGA-O2A-C1
39	B	313	LMT	C4-C5-C6-C7
39	G	323	LMT	C5-C6-C7-C8
39	G	323	LMT	C11-C10-C9-C8
40	b	849	DGD	C2A-C3A-C4A-C5A
42	a	852	LMG	C35-C36-C37-C38
39	L	318	LMT	C4-C5-C6-C7
40	b	849	DGD	CEB-CFB-CGB-CHB

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Mol	Chain	Res	Type	Atoms
41	F	319	LHG	C18-C19-C20-C21
41	j	104	LHG	C34-C35-C36-C37
41	l	208	LHG	C31-C32-C33-C34
40	C	215	DGD	O6D-C5D-C6D-O5D
35	S	308	A86	O5-C38-O4-C34
37	M	317	KC1	CAA-CBA-CGA-O2A
39	a	853	LMT	C4-C5-C6-C7
41	I	316	LHG	C24-C25-C26-C27
41	Q	315	LHG	C14-C15-C16-C17
42	J	318	LMG	C38-C39-C40-C41
42	h	206	LMG	C12-C13-C14-C15
36	G	309	CLA	C5-C6-C7-C8
36	O	316	CLA	C8-C10-C11-C12
36	a	805	CLA	C3-C5-C6-C7
36	E	315	CLA	CBA-CGA-O2A-C1
36	H	312	CLA	CBA-CGA-O2A-C1
35	J	301	A86	C24-C25-C26-C27
35	R	305	A86	C11-C10-C9-C8
41	j	104	LHG	C35-C36-C37-C38
36	b	821	CLA	C16-C17-C18-C19
41	I	316	LHG	C8-C7-O7-C5
41	a	843	LHG	C8-C7-O7-C5
41	i	104	LHG	C8-C7-O7-C5
42	E	318	LMG	C11-C10-O7-C8
42	G	325	LMG	C11-C10-O7-C8
42	V	315	LMG	C11-C10-O7-C8
36	l	206	CLA	O1A-CGA-O2A-C1
41	O	318	LHG	C23-C24-C25-C26
42	G	325	LMG	C42-C43-C44-C45
39	B	313	LMT	C5-C6-C7-C8
40	C	215	DGD	C9B-CAB-CBB-CCB
40	L	302	DGD	C2B-C3B-C4B-C5B
41	b	850	LHG	C17-C18-C19-C20
39	B	313	LMT	C3'-C4'-O1B-C1B
39	b	851	LMT	C1-C2-C3-C4
36	K	308	CLA	C8-C10-C11-C12
36	b	830	CLA	C8-C10-C11-C12
36	j	102	CLA	C15-C16-C17-C18
41	f	808	LHG	O9-C7-O7-C5
42	E	318	LMG	O9-C10-O7-C8
40	b	849	DGD	C3B-C4B-C5B-C6B
42	G	324	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
42	J	319	LMG	C11-C12-C13-C14
40	C	215	DGD	C5A-C6A-C7A-C8A
42	G	324	LMG	C17-C18-C19-C20
42	V	315	LMG	C22-C23-C24-C25
35	R	302	A86	C35-C34-O4-C38
35	W	203	A86	C35-C34-O4-C38
36	H	318	CLA	O1A-CGA-O2A-C1
36	L	308	CLA	O1A-CGA-O2A-C1
36	N	307	CLA	O1A-CGA-O2A-C1
36	B	308	CLA	C5-C6-C7-C8
36	C	208	CLA	C13-C15-C16-C17
36	b	829	CLA	C5-C6-C7-C8
34	E	304	DD6	C12-C11-C13-C14
34	K	304	DD6	C7-C6-C8-C9
34	P	305	DD6	C-C1-C24-C25
35	B	303	A86	C7-C6-C8-C9
35	F	302	A86	C7-C6-C8-C9
44	a	845	BCR	C37-C22-C23-C24
41	D	318	LHG	C11-C12-C13-C14
42	D	321	LMG	C28-C29-C30-C31
42	E	318	LMG	C28-C29-C30-C31
36	I	307	CLA	C5-C6-C7-C8
39	a	851	LMT	C7-C8-C9-C10
42	G	324	LMG	C8-C7-O1-C1
36	C	212	CLA	C8-C10-C11-C12
36	E	312	CLA	C2A-CAA-CBA-CGA
36	M	315	CLA	C2A-CAA-CBA-CGA
36	V	305	CLA	C2A-CAA-CBA-CGA
37	A	312	KC1	CAA-CBA-CGA-O2A
36	F	312	CLA	C16-C17-C18-C19
36	a	828	CLA	C16-C17-C18-C20
36	b	840	CLA	C16-C17-C18-C19
36	j	101	CLA	C16-C17-C18-C19
36	l	201	CLA	C16-C17-C18-C19
36	U	311	CLA	C16-C17-C18-C19
36	E	317	CLA	CBD-CGD-O2D-CED
39	U	314	LMT	C2-C3-C4-C5
42	G	325	LMG	C37-C38-C39-C40
42	m	102	LMG	C29-C30-C31-C32
36	I	312	CLA	C4-C3-C5-C6
36	T	309	CLA	C4-C3-C5-C6
36	a	829	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	V	306	CLA	C4-C3-C5-C6
36	D	313	CLA	O1A-CGA-O2A-C1
37	P	317	KC1	C2B-C3B-CAB-CBB
37	S	316	KC1	C2B-C3B-CAB-CBB
37	T	310	KC1	C2B-C3B-CAB-CBB
39	a	851	LMT	C4-C5-C6-C7
42	V	315	LMG	C20-C21-C22-C23
42	V	316	LMG	C32-C33-C34-C35
36	H	310	CLA	O1D-CGD-O2D-CED
35	E	302	A86	C35-C34-O4-C38
36	A	310	CLA	C15-C16-C17-C18
36	I	310	CLA	C10-C11-C12-C13
36	a	839	CLA	C5-C6-C7-C8
36	V	306	CLA	C15-C16-C17-C18
41	O	317	LHG	C13-C14-C15-C16
41	f	809	LHG	C29-C30-C31-C32
39	K	317	LMT	O1'-C1-C2-C3
39	E	323	LMT	C1-C2-C3-C4
36	a	810	CLA	C13-C15-C16-C17
36	f	805	CLA	CBD-CGD-O2D-CED
41	a	850	LHG	C16-C17-C18-C19
42	E	319	LMG	C13-C14-C15-C16
36	a	810	CLA	O1A-CGA-O2A-C1
42	V	316	LMG	O10-C28-O8-C9
36	a	837	CLA	C3-C5-C6-C7
36	E	311	CLA	C10-C11-C12-C13
36	L	314	CLA	C5-C6-C7-C8
36	O	307	CLA	C13-C15-C16-C17
36	P	309	CLA	C13-C15-C16-C17
36	Q	306	CLA	C13-C15-C16-C17
36	a	831	CLA	C13-C15-C16-C17
36	b	841	CLA	C13-C15-C16-C17
39	b	848	LMT	C4-C5-C6-C7
42	J	318	LMG	C29-C30-C31-C32
36	b	840	CLA	C2C-C3C-CAC-CBC
39	a	854	LMT	O1'-C1-C2-C3
39	K	317	LMT	C4-C5-C6-C7
41	f	809	LHG	C30-C31-C32-C33
42	E	318	LMG	C17-C18-C19-C20
42	G	325	LMG	C13-C14-C15-C16
41	i	104	LHG	O9-C7-O7-C5
41	D	318	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
41	i	104	LHG	C13-C14-C15-C16
36	G	313	CLA	C13-C15-C16-C17
36	K	308	CLA	C13-C15-C16-C17
36	M	309	CLA	C8-C10-C11-C12
36	M	311	CLA	C5-C6-C7-C8
36	a	828	CLA	C13-C15-C16-C17
36	b	816	CLA	C5-C6-C7-C8
36	b	829	CLA	C8-C10-C11-C12
36	V	313	CLA	C15-C16-C17-C18
37	F	315	KC1	C4B-C3B-CAB-CBB
37	M	318	KC1	C4B-C3B-CAB-CBB
37	R	317	KC1	C4B-C3B-CAB-CBB
35	C	202	A86	C33-C34-O4-C38
38	b	804	SQD	C13-C14-C15-C16
39	I	317	LMT	C5-C6-C7-C8
39	P	321	LMT	C5-C6-C7-C8
41	j	104	LHG	C24-C25-C26-C27
36	j	101	CLA	O1A-CGA-O2A-C1
37	T	315	KC1	O1D-CGD-O2D-CED
42	I	315	LMG	C31-C32-C33-C34
42	J	318	LMG	C33-C34-C35-C36
42	V	316	LMG	C28-C29-C30-C31
36	a	804	CLA	C13-C15-C16-C17
36	a	805	CLA	C5-C6-C7-C8
36	N	317	CLA	C5-C6-C7-C8
41	E	322	LHG	C31-C32-C33-C34
41	f	808	LHG	C11-C12-C13-C14
42	j	105	LMG	C18-C19-C20-C21
36	G	315	CLA	C3-C5-C6-C7
36	i	102	CLA	C3-C5-C6-C7
41	D	319	LHG	C30-C31-C32-C33
36	E	312	CLA	CBA-CGA-O2A-C1
36	J	317	CLA	CBA-CGA-O2A-C1
36	f	802	CLA	CBA-CGA-O2A-C1
41	a	842	LHG	C24-C23-O8-C6
39	E	323	LMT	C2-C3-C4-C5
39	K	318	LMT	C5-C6-C7-C8
39	K	318	LMT	C6-C7-C8-C9
40	L	302	DGD	C2A-C3A-C4A-C5A
41	R	323	LHG	C16-C17-C18-C19
42	E	318	LMG	C19-C20-C21-C22
42	J	319	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
36	E	310	CLA	C13-C15-C16-C17
36	H	306	CLA	C8-C10-C11-C12
41	D	318	LHG	C9-C10-C11-C12
41	j	104	LHG	C27-C28-C29-C30
42	E	319	LMG	C11-C12-C13-C14
39	K	317	LMT	C2-C3-C4-C5
42	I	315	LMG	C14-C15-C16-C17
42	V	316	LMG	C14-C15-C16-C17
36	F	317	CLA	C2-C1-O2A-CGA
36	F	312	CLA	C16-C17-C18-C20
36	H	315	CLA	C16-C17-C18-C20
36	l	202	CLA	C16-C17-C18-C19
36	U	306	CLA	C16-C17-C18-C19
41	D	319	LHG	C2-C3-O3-P
41	Q	315	LHG	C24-C25-C26-C27
41	a	843	LHG	C9-C10-C11-C12
42	D	320	LMG	C32-C33-C34-C35
36	b	814	CLA	C3-C5-C6-C7
36	a	818	CLA	C2-C3-C5-C6
36	a	828	CLA	C2-C3-C5-C6
42	G	325	LMG	O9-C10-O7-C8
41	j	104	LHG	C1-C2-C3-O3
41	l	208	LHG	C1-C2-C3-O3
41	E	322	LHG	O2-C2-C3-O3
41	I	316	LHG	C11-C12-C13-C14
36	C	209	CLA	C2A-CAA-CBA-CGA
36	D	308	CLA	C2A-CAA-CBA-CGA
36	M	307	CLA	C2A-CAA-CBA-CGA
36	T	309	CLA	C2A-CAA-CBA-CGA
36	b	801	CLA	C2A-CAA-CBA-CGA
36	b	806	CLA	C2A-CAA-CBA-CGA
36	b	829	CLA	C2A-CAA-CBA-CGA
36	V	306	CLA	C2A-CAA-CBA-CGA
36	V	313	CLA	C2A-CAA-CBA-CGA
36	F	310	CLA	CBD-CGD-O2D-CED
36	j	101	CLA	CBD-CGD-O2D-CED
36	a	811	CLA	O1D-CGD-O2D-CED
39	a	851	LMT	C6-C7-C8-C9
41	D	318	LHG	C29-C30-C31-C32
41	O	318	LHG	C33-C34-C35-C36
41	f	808	LHG	C34-C35-C36-C37
41	j	104	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
42	E	319	LMG	C32-C33-C34-C35
36	G	319	CLA	C2C-C3C-CAC-CBC
36	L	308	CLA	O1D-CGD-O2D-CED
41	E	322	LHG	C25-C26-C27-C28
41	G	321	LHG	C27-C28-C29-C30
41	j	104	LHG	C31-C32-C33-C34
36	P	314	CLA	C8-C10-C11-C12
36	F	309	CLA	O1A-CGA-O2A-C1
42	E	318	LMG	O10-C28-O8-C9
39	G	323	LMT	C2-C3-C4-C5
41	R	323	LHG	C31-C32-C33-C34
39	I	317	LMT	O5B-C1B-O1B-C4'
41	D	319	LHG	C27-C28-C29-C30
36	B	305	CLA	C1A-C2A-CAA-CBA
36	B	307	CLA	C1A-C2A-CAA-CBA
36	C	212	CLA	C1A-C2A-CAA-CBA
36	D	316	CLA	C1A-C2A-CAA-CBA
36	D	317	CLA	C1A-C2A-CAA-CBA
36	E	317	CLA	C1A-C2A-CAA-CBA
36	F	310	CLA	C1A-C2A-CAA-CBA
36	F	312	CLA	C1A-C2A-CAA-CBA
36	F	313	CLA	C1A-C2A-CAA-CBA
36	G	307	CLA	C1A-C2A-CAA-CBA
36	G	313	CLA	C1A-C2A-CAA-CBA
36	H	311	CLA	C1A-C2A-CAA-CBA
36	I	309	CLA	C1A-C2A-CAA-CBA
36	L	312	CLA	C1A-C2A-CAA-CBA
36	M	310	CLA	C1A-C2A-CAA-CBA
36	M	311	CLA	C1A-C2A-CAA-CBA
36	N	308	CLA	C1A-C2A-CAA-CBA
36	N	311	CLA	C1A-C2A-CAA-CBA
36	N	312	CLA	C1A-C2A-CAA-CBA
36	P	319	CLA	C1A-C2A-CAA-CBA
36	Q	310	CLA	C1A-C2A-CAA-CBA
36	Q	314	CLA	C1A-C2A-CAA-CBA
36	R	311	CLA	C1A-C2A-CAA-CBA
36	R	314	CLA	C1A-C2A-CAA-CBA
36	S	309	CLA	C1A-C2A-CAA-CBA
36	S	310	CLA	C1A-C2A-CAA-CBA
36	S	313	CLA	C1A-C2A-CAA-CBA
36	T	309	CLA	C1A-C2A-CAA-CBA
36	W	210	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	W	218	CLA	C1A-C2A-CAA-CBA
36	X	307	CLA	C1A-C2A-CAA-CBA
36	a	807	CLA	C1A-C2A-CAA-CBA
36	a	809	CLA	C1A-C2A-CAA-CBA
36	a	810	CLA	C1A-C2A-CAA-CBA
36	a	817	CLA	C1A-C2A-CAA-CBA
36	a	823	CLA	C1A-C2A-CAA-CBA
36	a	825	CLA	C1A-C2A-CAA-CBA
36	a	831	CLA	C1A-C2A-CAA-CBA
36	a	832	CLA	C1A-C2A-CAA-CBA
36	a	841	CLA	C1A-C2A-CAA-CBA
36	b	801	CLA	C1A-C2A-CAA-CBA
36	b	815	CLA	C1A-C2A-CAA-CBA
36	b	820	CLA	C1A-C2A-CAA-CBA
36	b	822	CLA	C1A-C2A-CAA-CBA
36	b	823	CLA	C1A-C2A-CAA-CBA
36	b	832	CLA	C1A-C2A-CAA-CBA
36	b	838	CLA	C1A-C2A-CAA-CBA
36	f	805	CLA	C1A-C2A-CAA-CBA
36	l	204	CLA	C1A-C2A-CAA-CBA
36	l	206	CLA	C1A-C2A-CAA-CBA
36	U	311	CLA	C1A-C2A-CAA-CBA
36	V	305	CLA	C1A-C2A-CAA-CBA
36	V	309	CLA	C1A-C2A-CAA-CBA
35	W	202	A86	C35-C34-O4-C38
35	U	303	A86	C35-C34-O4-C38
36	K	309	CLA	C8-C10-C11-C12
36	K	310	CLA	C10-C11-C12-C13
42	L	321	LMG	O6-C1-O1-C7
39	E	323	LMT	C6-C7-C8-C9
39	K	317	LMT	C3-C4-C5-C6
41	b	850	LHG	C11-C12-C13-C14
42	G	324	LMG	C19-C20-C21-C22
42	J	319	LMG	C17-C18-C19-C20
35	O	301	A86	O5-C38-O4-C34
36	a	823	CLA	O1A-CGA-O2A-C1
36	a	848	CLA	O1A-CGA-O2A-C1
36	U	310	CLA	C4C-C3C-CAC-CBC
41	I	316	LHG	C11-C10-C9-C8
41	f	808	LHG	C33-C34-C35-C36
42	D	321	LMG	C15-C16-C17-C18
36	K	312	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	V	306	CLA	C13-C15-C16-C17
41	O	317	LHG	O6-C4-C5-C6
40	b	849	DGD	C8A-C9A-CAA-CBA
41	a	842	LHG	C11-C10-C9-C8
41	f	808	LHG	C27-C28-C29-C30
42	E	319	LMG	C31-C32-C33-C34
42	G	325	LMG	C17-C18-C19-C20
36	R	321	CLA	C3-C5-C6-C7
36	A	306	CLA	C6-C7-C8-C10
36	A	311	CLA	C11-C12-C13-C15
36	B	305	CLA	C11-C10-C8-C7
36	C	212	CLA	C6-C7-C8-C10
36	C	212	CLA	C12-C13-C15-C16
36	E	313	CLA	C6-C7-C8-C10
36	E	316	CLA	C6-C7-C8-C10
36	F	312	CLA	C12-C13-C15-C16
36	G	309	CLA	C11-C10-C8-C7
36	G	313	CLA	C11-C12-C13-C15
36	H	312	CLA	C11-C12-C13-C15
36	I	306	CLA	C11-C12-C13-C15
36	I	308	CLA	C11-C10-C8-C7
36	I	308	CLA	C11-C12-C13-C15
36	J	312	CLA	C12-C13-C15-C16
36	L	313	CLA	C12-C13-C15-C16
36	L	314	CLA	C11-C12-C13-C15
36	M	311	CLA	C11-C12-C13-C15
36	N	307	CLA	C11-C12-C13-C15
36	N	308	CLA	C11-C12-C13-C15
36	O	307	CLA	C12-C13-C15-C16
36	O	316	CLA	C12-C13-C15-C16
36	P	301	CLA	C6-C7-C8-C10
36	P	309	CLA	C12-C13-C15-C16
36	Q	306	CLA	C12-C13-C15-C16
36	S	310	CLA	C6-C7-C8-C10
36	T	308	CLA	C11-C12-C13-C15
36	a	812	CLA	C6-C7-C8-C10
36	a	812	CLA	C11-C10-C8-C7
36	a	824	CLA	C11-C10-C8-C7
36	a	828	CLA	C12-C13-C15-C16
36	a	839	CLA	C11-C10-C8-C7
36	a	839	CLA	C11-C12-C13-C15
36	a	839	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
36	b	802	CLA	C11-C10-C8-C7
36	b	805	CLA	C6-C7-C8-C10
36	b	809	CLA	C12-C13-C15-C16
36	b	827	CLA	C6-C7-C8-C10
36	b	827	CLA	C11-C12-C13-C15
36	f	803	CLA	C11-C10-C8-C7
36	i	102	CLA	C6-C7-C8-C10
36	j	102	CLA	C12-C13-C15-C16
36	h	203	CLA	C6-C7-C8-C10
36	h	203	CLA	C11-C12-C13-C15
36	V	305	CLA	C11-C10-C8-C7
36	Q	310	CLA	C16-C17-C18-C20
36	J	313	CLA	C15-C16-C17-C18
36	W	212	CLA	C8-C10-C11-C12
36	P	319	CLA	O1A-CGA-O2A-C1
36	b	816	CLA	CBA-CGA-O2A-C1
41	F	319	LHG	C24-C25-C26-C27
42	E	319	LMG	C29-C30-C31-C32
36	D	306	CLA	C2C-C3C-CAC-CBC
36	R	313	CLA	C5-C6-C7-C8
42	m	102	LMG	C10-C11-C12-C13
36	U	306	CLA	C4-C3-C5-C6
36	I	312	CLA	C2-C3-C5-C6
36	a	829	CLA	C2-C3-C5-C6
36	a	837	CLA	C2-C3-C5-C6
36	U	306	CLA	C2-C3-C5-C6
36	U	308	CLA	C2-C3-C5-C6
36	V	313	CLA	C2-C3-C5-C6
39	U	315	LMT	C6-C7-C8-C9
41	F	318	LHG	C11-C10-C9-C8
41	a	850	LHG	C12-C13-C14-C15
36	C	206	CLA	O1A-CGA-O2A-C1
42	E	318	LMG	C31-C32-C33-C34
42	a	852	LMG	C32-C33-C34-C35
36	a	823	CLA	C4C-C3C-CAC-CBC
36	F	312	CLA	C13-C15-C16-C17
36	L	320	CLA	C8-C10-C11-C12
36	O	311	CLA	C8-C10-C11-C12
36	P	313	CLA	C8-C10-C11-C12
36	W	206	CLA	C10-C11-C12-C13
36	G	311	CLA	C3-C5-C6-C7
36	P	314	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	a	839	CLA	C2A-CAA-CBA-CGA
36	b	820	CLA	C2A-CAA-CBA-CGA
36	b	828	CLA	C2A-CAA-CBA-CGA
36	A	311	CLA	C14-C13-C15-C16
36	B	305	CLA	C11-C10-C8-C9
36	C	206	CLA	C11-C12-C13-C14
36	C	211	CLA	C14-C13-C15-C16
36	F	309	CLA	C6-C7-C8-C9
36	F	312	CLA	C6-C7-C8-C9
36	H	308	CLA	C6-C7-C8-C9
36	H	311	CLA	C14-C13-C15-C16
36	I	306	CLA	C6-C7-C8-C9
36	I	308	CLA	C6-C7-C8-C9
36	J	308	CLA	C11-C10-C8-C9
36	J	313	CLA	C11-C10-C8-C9
36	L	308	CLA	C11-C10-C8-C9
36	L	314	CLA	C11-C12-C13-C14
36	N	307	CLA	C11-C12-C13-C14
36	R	310	CLA	C11-C12-C13-C14
36	T	308	CLA	C11-C12-C13-C14
36	T	314	CLA	C11-C12-C13-C14
36	W	206	CLA	C11-C12-C13-C14
36	a	801	CLA	C14-C13-C15-C16
36	a	802	CLA	C6-C7-C8-C9
36	a	824	CLA	C11-C10-C8-C9
36	a	839	CLA	C11-C12-C13-C14
36	b	805	CLA	C6-C7-C8-C9
36	b	815	CLA	C11-C10-C8-C9
36	b	827	CLA	C11-C12-C13-C14
36	j	101	CLA	C11-C12-C13-C14
36	h	203	CLA	C11-C12-C13-C14
36	U	311	CLA	C11-C10-C8-C9
36	V	306	CLA	C11-C12-C13-C14
43	b	842	PQN	C21-C22-C23-C24
41	I	316	LHG	C26-C27-C28-C29
41	a	842	LHG	C12-C13-C14-C15
42	E	319	LMG	C33-C34-C35-C36
42	V	316	LMG	C22-C23-C24-C25
36	R	315	CLA	CBA-CGA-O2A-C1
36	a	826	CLA	CBA-CGA-O2A-C1
41	O	318	LHG	C24-C23-O8-C6
36	J	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	W	218	CLA	O1D-CGD-O2D-CED
41	F	318	LHG	C11-C12-C13-C14
41	a	842	LHG	C16-C17-C18-C19
39	P	320	LMT	O1'-C1-C2-C3
36	J	316	CLA	C4C-C3C-CAC-CBC
39	E	320	LMT	O5B-C1B-O1B-C4'
37	A	312	KC1	CAA-CBA-CGA-O1A
40	b	849	DGD	C1G-C2G-C3G-O3G
41	F	319	LHG	C4-C5-C6-O8
41	G	301	LHG	C4-C5-C6-O8
41	G	320	LHG	C4-C5-C6-O8
41	O	318	LHG	C4-C5-C6-O8
42	D	320	LMG	C7-C8-C9-O8
42	L	321	LMG	C7-C8-C9-O8
42	V	315	LMG	C7-C8-C9-O8
40	L	302	DGD	C4B-C5B-C6B-C7B
40	b	849	DGD	C5A-C6A-C7A-C8A
41	a	850	LHG	C25-C26-C27-C28
41	f	808	LHG	C14-C15-C16-C17
35	R	303	A86	C33-C34-O4-C38
35	V	304	A86	C35-C34-O4-C38
39	G	322	LMT	O5B-C1B-O1B-C4'
42	m	102	LMG	C30-C31-C32-C33
43	b	842	PQN	C20-C21-C22-C23
39	G	322	LMT	C6-C7-C8-C9
41	I	316	LHG	C32-C33-C34-C35
41	R	323	LHG	C11-C10-C9-C8
42	G	324	LMG	C29-C30-C31-C32
42	j	105	LMG	C41-C42-C43-C44
36	C	212	CLA	CBA-CGA-O2A-C1
36	E	311	CLA	CBA-CGA-O2A-C1
36	X	307	CLA	CBA-CGA-O2A-C1
42	E	318	LMG	C10-C11-C12-C13
42	E	319	LMG	C10-C11-C12-C13
39	E	323	LMT	O5B-C5B-C6B-O6B
39	a	854	LMT	O5'-C5'-C6'-O6'
39	f	807	LMT	O5'-C5'-C6'-O6'
36	H	315	CLA	C16-C17-C18-C19
36	Q	310	CLA	C16-C17-C18-C19
40	C	215	DGD	CAB-CBB-CCB-CDB
41	E	322	LHG	C29-C30-C31-C32
41	O	318	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
42	I	315	LMG	C23-C24-C25-C26
42	j	105	LMG	C30-C31-C32-C33
41	j	104	LHG	C18-C19-C20-C21
41	l	208	LHG	C25-C26-C27-C28
40	b	849	DGD	CAB-CBB-CCB-CDB
36	N	312	CLA	C2-C1-O2A-CGA
44	b	843	BCR	C20-C21-C22-C37
44	i	103	BCR	C11-C10-C9-C34
36	A	314	CLA	C10-C11-C12-C13
36	H	311	CLA	C15-C16-C17-C18
41	E	322	LHG	C7-C8-C9-C10
36	E	315	CLA	O1A-CGA-O2A-C1
36	H	312	CLA	O1A-CGA-O2A-C1
36	J	317	CLA	O1A-CGA-O2A-C1
36	a	809	CLA	O1A-CGA-O2A-C1
36	f	802	CLA	O1A-CGA-O2A-C1
40	b	849	DGD	C2B-C3B-C4B-C5B
41	D	318	LHG	C11-C10-C9-C8
41	Q	315	LHG	C17-C18-C19-C20
41	j	104	LHG	C33-C34-C35-C36
36	a	818	CLA	C4-C3-C5-C6
36	a	837	CLA	C4-C3-C5-C6
36	V	313	CLA	C4-C3-C5-C6
36	P	314	CLA	C2-C3-C5-C6
36	a	804	CLA	C2-C3-C5-C6
41	l	208	LHG	C14-C15-C16-C17
36	B	305	CLA	C5-C6-C7-C8
36	K	313	CLA	C10-C11-C12-C13
44	l	207	BCR	C7-C8-C9-C34
41	I	316	LHG	O9-C7-O7-C5
40	C	215	DGD	C2A-C3A-C4A-C5A
41	f	808	LHG	C30-C31-C32-C33
41	j	104	LHG	C10-C11-C12-C13
42	h	206	LMG	O6-C5-C6-O5
36	A	306	CLA	C4C-C3C-CAC-CBC
36	E	312	CLA	O1A-CGA-O2A-C1
36	E	315	CLA	C15-C16-C17-C18
36	N	308	CLA	C15-C16-C17-C18
41	O	317	LHG	C11-C10-C9-C8
42	L	321	LMG	C11-C12-C13-C14
42	a	852	LMG	C37-C38-C39-C40
36	a	834	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	A	314	CLA	C2A-CAA-CBA-CGA
36	S	309	CLA	C2A-CAA-CBA-CGA
41	I	316	LHG	C34-C35-C36-C37
39	E	320	LMT	C4B-C5B-C6B-O6B
36	R	311	CLA	C5-C6-C7-C8
36	S	320	CLA	C8-C10-C11-C12
36	b	815	CLA	C5-C6-C7-C8
38	b	804	SQD	C14-C15-C16-C17
42	L	321	LMG	C12-C13-C14-C15
41	D	319	LHG	C7-C8-C9-C10
41	F	319	LHG	C7-C8-C9-C10
41	D	318	LHG	C13-C14-C15-C16
42	D	320	LMG	C29-C30-C31-C32
42	V	316	LMG	C11-C12-C13-C14
36	b	836	CLA	CBA-CGA-O2A-C1
36	M	307	CLA	O2A-C1-C2-C3
36	O	316	CLA	O2A-C1-C2-C3
36	P	314	CLA	O2A-C1-C2-C3
36	Q	314	CLA	O2A-C1-C2-C3
38	b	804	SQD	C46-C45-O47-C7
41	D	318	LHG	C6-C5-O7-C7
41	O	317	LHG	C6-C5-O7-C7
42	D	321	LMG	C9-C8-O7-C10
42	a	852	LMG	C39-C40-C41-C42
44	b	846	BCR	C10-C11-C12-C13
36	a	828	CLA	C8-C10-C11-C12
36	a	829	CLA	C8-C10-C11-C12
36	U	306	CLA	C15-C16-C17-C18
41	i	104	LHG	C32-C33-C34-C35
41	l	208	LHG	C9-C10-C11-C12
42	E	318	LMG	C32-C33-C34-C35
42	a	852	LMG	C18-C19-C20-C21
34	S	307	DD6	C11-C10-C9-C8
39	B	312	LMT	C4'-C5'-C6'-O6'
42	V	316	LMG	C4-C5-C6-O5
36	b	816	CLA	O1A-CGA-O2A-C1
36	a	831	CLA	C3-C5-C6-C7
44	f	801	BCR	C11-C10-C9-C8
41	O	318	LHG	C25-C26-C27-C28
41	E	322	LHG	C1-C2-C3-O3
39	h	205	LMT	O5'-C1'-O1'-C1
39	K	318	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
42	G	324	LMG	C37-C38-C39-C40
36	C	209	CLA	CBA-CGA-O2A-C1
36	F	317	CLA	CBA-CGA-O2A-C1
36	b	829	CLA	CBA-CGA-O2A-C1
36	j	102	CLA	CBA-CGA-O2A-C1
36	a	826	CLA	O1A-CGA-O2A-C1
35	F	307	A86	C35-C34-O4-C38
40	L	302	DGD	C4A-C5A-C6A-C7A
42	V	316	LMG	C24-C25-C26-C27
41	b	850	LHG	C32-C33-C34-C35
41	f	808	LHG	C28-C29-C30-C31
42	I	315	LMG	C22-C23-C24-C25
42	a	852	LMG	C20-C21-C22-C23
42	h	206	LMG	C22-C23-C24-C25
36	a	804	CLA	C4-C3-C5-C6
36	U	308	CLA	C4-C3-C5-C6
41	D	319	LHG	C35-C36-C37-C38
42	D	321	LMG	C29-C30-C31-C32
36	A	308	CLA	C16-C17-C18-C19
36	l	205	CLA	C16-C17-C18-C20
39	G	323	LMT	C5'-C4'-O1B-C1B
42	I	315	LMG	C34-C35-C36-C37
42	J	318	LMG	C11-C12-C13-C14
42	J	319	LMG	C13-C14-C15-C16
39	a	854	LMT	C9-C10-C11-C12
42	E	318	LMG	C21-C22-C23-C24
42	m	102	LMG	C32-C33-C34-C35
39	G	322	LMT	C7-C8-C9-C10
41	Q	315	LHG	C15-C16-C17-C18
41	a	850	LHG	C29-C30-C31-C32
42	J	319	LMG	C22-C23-C24-C25
42	h	206	LMG	C30-C31-C32-C33
39	E	320	LMT	C1-C2-C3-C4
42	G	325	LMG	O1-C7-C8-O7
40	C	215	DGD	C6A-C7A-C8A-C9A
41	j	104	LHG	C19-C20-C21-C22
41	f	808	LHG	C29-C30-C31-C32
36	a	807	CLA	CBA-CGA-O2A-C1
36	U	311	CLA	CBA-CGA-O2A-C1
39	K	318	LMT	C11-C10-C9-C8
41	R	323	LHG	C14-C15-C16-C17
42	G	325	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
42	J	319	LMG	C18-C19-C20-C21
39	L	303	LMT	C4-C5-C6-C7
36	C	206	CLA	C3-C5-C6-C7
36	K	316	CLA	C3-C5-C6-C7
36	b	810	CLA	C3-C5-C6-C7
36	h	203	CLA	C3-C5-C6-C7
40	C	215	DGD	C4A-C5A-C6A-C7A
41	l	208	LHG	C19-C20-C21-C22
36	V	310	CLA	O1D-CGD-O2D-CED
37	G	308	KC1	C2C-C3C-CAC-CBC
36	i	102	CLA	C2-C1-O2A-CGA
40	L	302	DGD	C7B-C8B-C9B-CAB
36	a	816	CLA	C2C-C3C-CAC-CBC
36	E	315	CLA	C8-C10-C11-C12
41	D	319	LHG	C33-C34-C35-C36
41	R	323	LHG	C15-C16-C17-C18
41	l	208	LHG	C18-C19-C20-C21
42	a	852	LMG	C31-C32-C33-C34
42	j	105	LMG	C20-C21-C22-C23
42	j	105	LMG	C36-C37-C38-C39
42	V	315	LMG	C18-C19-C20-C21
39	E	323	LMT	C9-C10-C11-C12
41	D	319	LHG	C19-C20-C21-C22
41	f	809	LHG	C12-C13-C14-C15
36	a	824	CLA	CBD-CGD-O2D-CED
41	i	104	LHG	C35-C36-C37-C38
42	D	321	LMG	C16-C17-C18-C19
41	f	809	LHG	C25-C26-C27-C28
36	A	310	CLA	C3-C5-C6-C7
39	a	854	LMT	C5-C6-C7-C8
42	G	325	LMG	C29-C30-C31-C32
36	a	816	CLA	O1D-CGD-O2D-CED
39	P	320	LMT	C11-C10-C9-C8
36	D	313	CLA	C15-C16-C17-C18
36	P	301	CLA	C8-C10-C11-C12
36	A	308	CLA	C16-C17-C18-C20
36	b	813	CLA	C6-C7-C8-C9
36	b	823	CLA	C6-C7-C8-C9
36	b	823	CLA	C6-C7-C8-C10
36	P	314	CLA	C4-C3-C5-C6
36	Q	314	CLA	C4-C3-C5-C6
36	l	202	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	b	805	CLA	C2-C3-C5-C6
36	b	817	CLA	C10-C11-C12-C13
41	a	850	LHG	C24-C25-C26-C27
41	D	318	LHG	C24-C23-O8-C6
41	j	104	LHG	C24-C23-O8-C6
36	A	310	CLA	C10-C11-C12-C13
36	I	308	CLA	C15-C16-C17-C18
39	G	323	LMT	C9-C10-C11-C12
39	L	318	LMT	C5-C6-C7-C8
41	G	301	LHG	C35-C36-C37-C38
41	O	317	LHG	C9-C10-C11-C12
36	C	211	CLA	O1D-CGD-O2D-CED
39	L	303	LMT	C2-C3-C4-C5
41	a	843	LHG	O9-C7-O7-C5
34	D	305	DD6	C27-C29-C30-C31
39	B	313	LMT	C2-C1-O1'-C1'
39	F	321	LMT	C2-C1-O1'-C1'
39	K	318	LMT	C2-C1-O1'-C1'
41	f	808	LHG	O1-C1-C2-O2
36	A	306	CLA	C6-C7-C8-C9
36	A	311	CLA	C11-C12-C13-C14
36	C	212	CLA	C6-C7-C8-C9
36	E	313	CLA	C6-C7-C8-C9
36	F	312	CLA	C14-C13-C15-C16
36	F	314	CLA	C6-C7-C8-C9
36	G	309	CLA	C11-C10-C8-C9
36	G	310	CLA	C11-C12-C13-C14
36	H	312	CLA	C11-C12-C13-C14
36	H	312	CLA	C14-C13-C15-C16
36	H	315	CLA	C14-C13-C15-C16
36	J	312	CLA	C14-C13-C15-C16
36	J	313	CLA	C6-C7-C8-C9
36	L	311	CLA	C14-C13-C15-C16
36	L	313	CLA	C14-C13-C15-C16
36	O	307	CLA	C11-C10-C8-C9
36	O	307	CLA	C14-C13-C15-C16
36	O	316	CLA	C11-C12-C13-C14
36	O	316	CLA	C14-C13-C15-C16
36	P	309	CLA	C11-C10-C8-C9
36	P	309	CLA	C14-C13-C15-C16
36	Q	306	CLA	C11-C10-C8-C9
36	Q	306	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
36	W	211	CLA	C14-C13-C15-C16
36	W	212	CLA	C11-C12-C13-C14
36	a	802	CLA	C14-C13-C15-C16
36	a	805	CLA	C11-C12-C13-C14
36	a	817	CLA	C11-C10-C8-C9
36	a	818	CLA	C11-C12-C13-C14
36	a	826	CLA	C11-C12-C13-C14
36	a	828	CLA	C14-C13-C15-C16
36	a	829	CLA	C6-C7-C8-C9
36	a	831	CLA	C6-C7-C8-C9
36	a	831	CLA	C11-C12-C13-C14
36	b	802	CLA	C11-C10-C8-C9
36	b	805	CLA	C11-C10-C8-C9
36	b	806	CLA	C11-C10-C8-C9
36	b	809	CLA	C11-C10-C8-C9
36	b	809	CLA	C14-C13-C15-C16
36	f	802	CLA	C14-C13-C15-C16
36	i	102	CLA	C14-C13-C15-C16
36	j	102	CLA	C14-C13-C15-C16
36	l	205	CLA	C14-C13-C15-C16
36	U	305	CLA	C11-C12-C13-C14
36	U	306	CLA	C6-C7-C8-C9
42	a	852	LMG	C33-C34-C35-C36
36	S	312	CLA	C10-C11-C12-C13
43	b	842	PQN	C23-C25-C26-C27
41	O	317	LHG	C2-C3-O3-P
41	R	323	LHG	C2-C3-O3-P
36	A	311	CLA	C4B-C3B-CAB-CBB
36	C	211	CLA	C4B-C3B-CAB-CBB
36	D	307	CLA	C4B-C3B-CAB-CBB
36	E	316	CLA	C4B-C3B-CAB-CBB
36	F	311	CLA	C4B-C3B-CAB-CBB
36	F	314	CLA	C4B-C3B-CAB-CBB
36	F	316	CLA	C4B-C3B-CAB-CBB
36	G	312	CLA	C4B-C3B-CAB-CBB
36	H	309	CLA	C4B-C3B-CAB-CBB
36	I	313	CLA	C4B-C3B-CAB-CBB
36	L	316	CLA	C4B-C3B-CAB-CBB
36	M	309	CLA	C4B-C3B-CAB-CBB
36	M	312	CLA	C4B-C3B-CAB-CBB
36	M	316	CLA	C4B-C3B-CAB-CBB
36	N	308	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	N	319	CLA	C4B-C3B-CAB-CBB
36	O	308	CLA	C4B-C3B-CAB-CBB
36	P	301	CLA	C4B-C3B-CAB-CBB
36	P	310	CLA	C4B-C3B-CAB-CBB
36	P	319	CLA	C4B-C3B-CAB-CBB
36	Q	307	CLA	C4B-C3B-CAB-CBB
36	S	309	CLA	C4B-C3B-CAB-CBB
36	W	201	CLA	C4B-C3B-CAB-CBB
36	W	207	CLA	C4B-C3B-CAB-CBB
36	a	801	CLA	C4B-C3B-CAB-CBB
36	a	805	CLA	C4B-C3B-CAB-CBB
36	a	809	CLA	C4B-C3B-CAB-CBB
36	a	819	CLA	C4B-C3B-CAB-CBB
36	b	805	CLA	C4B-C3B-CAB-CBB
36	b	809	CLA	C4B-C3B-CAB-CBB
36	b	814	CLA	C4B-C3B-CAB-CBB
36	b	831	CLA	C4B-C3B-CAB-CBB
36	b	833	CLA	C4B-C3B-CAB-CBB
36	U	308	CLA	C4B-C3B-CAB-CBB
36	V	307	CLA	C4B-C3B-CAB-CBB
36	V	313	CLA	C4B-C3B-CAB-CBB
35	V	302	A86	C35-C34-O4-C38
36	a	807	CLA	C15-C16-C17-C18
36	W	208	CLA	CBD-CGD-O2D-CED
36	T	311	CLA	C16-C17-C18-C19
39	F	320	LMT	C3-C4-C5-C6
36	b	826	CLA	CBA-CGA-O2A-C1
36	b	841	CLA	CBA-CGA-O2A-C1
36	O	311	CLA	C10-C11-C12-C13
36	B	309	CLA	C3-C5-C6-C7
35	T	301	A86	O5-C38-O4-C34
41	D	319	LHG	C24-C25-C26-C27
41	I	316	LHG	C15-C16-C17-C18
42	m	102	LMG	C11-C12-C13-C14
36	N	308	CLA	C3-C5-C6-C7
36	a	801	CLA	C3-C5-C6-C7
36	b	821	CLA	C3-C5-C6-C7
36	b	823	CLA	C3-C5-C6-C7
39	B	313	LMT	C9-C10-C11-C12
39	F	321	LMT	C7-C8-C9-C10
39	h	205	LMT	C9-C10-C11-C12
41	E	322	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
41	G	301	LHG	O6-C4-C5-C6
41	Q	315	LHG	O6-C4-C5-C6
41	i	104	LHG	O6-C4-C5-C6
41	Q	315	LHG	C35-C36-C37-C38
41	a	850	LHG	C33-C34-C35-C36
41	f	808	LHG	C35-C36-C37-C38
42	J	318	LMG	C42-C43-C44-C45
35	K	302	A86	C35-C34-O4-C38
35	T	305	A86	C35-C34-O4-C38
36	A	311	CLA	C6-C7-C8-C10
36	A	311	CLA	C11-C10-C8-C7
36	A	314	CLA	C11-C12-C13-C15
36	B	305	CLA	C12-C13-C15-C16
36	C	206	CLA	C11-C12-C13-C15
36	C	207	CLA	C11-C12-C13-C15
36	C	208	CLA	C12-C13-C15-C16
36	C	211	CLA	C12-C13-C15-C16
36	E	315	CLA	C12-C13-C15-C16
36	F	312	CLA	C6-C7-C8-C10
36	G	310	CLA	C11-C12-C13-C15
36	H	311	CLA	C12-C13-C15-C16
36	H	315	CLA	C6-C7-C8-C10
36	H	316	CLA	C6-C7-C8-C10
36	I	305	CLA	C6-C7-C8-C10
36	I	306	CLA	C6-C7-C8-C10
36	I	308	CLA	C6-C7-C8-C10
36	J	313	CLA	C11-C10-C8-C7
36	K	312	CLA	C12-C13-C15-C16
36	L	308	CLA	C11-C10-C8-C7
36	O	308	CLA	C6-C7-C8-C10
36	O	316	CLA	C11-C10-C8-C7
36	O	316	CLA	C11-C12-C13-C15
36	Q	306	CLA	C11-C10-C8-C7
36	Q	314	CLA	C12-C13-C15-C16
36	R	310	CLA	C11-C12-C13-C15
36	R	313	CLA	C12-C13-C15-C16
36	T	314	CLA	C11-C12-C13-C15
36	W	206	CLA	C11-C12-C13-C15
36	W	211	CLA	C12-C13-C15-C16
36	W	212	CLA	C11-C12-C13-C15
36	a	802	CLA	C6-C7-C8-C10
36	a	805	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
36	a	816	CLA	C11-C12-C13-C15
36	a	818	CLA	C11-C12-C13-C15
36	a	825	CLA	C11-C10-C8-C7
36	a	825	CLA	C11-C12-C13-C15
36	a	826	CLA	C11-C12-C13-C15
36	a	831	CLA	C6-C7-C8-C10
36	a	831	CLA	C11-C12-C13-C15
36	b	805	CLA	C11-C10-C8-C7
36	b	806	CLA	C11-C10-C8-C7
36	b	821	CLA	C11-C10-C8-C7
36	b	826	CLA	C6-C7-C8-C10
36	b	826	CLA	C11-C10-C8-C7
36	f	802	CLA	C12-C13-C15-C16
36	i	102	CLA	C12-C13-C15-C16
36	j	101	CLA	C6-C7-C8-C10
36	j	101	CLA	C11-C12-C13-C15
36	U	305	CLA	C11-C12-C13-C15
36	U	306	CLA	C6-C7-C8-C10
36	U	311	CLA	C11-C10-C8-C7
36	V	306	CLA	C11-C12-C13-C15
36	V	314	CLA	C11-C12-C13-C15
43	a	840	PQN	C17-C18-C20-C21
43	a	840	PQN	C21-C22-C23-C25
43	b	842	PQN	C21-C22-C23-C25
36	G	315	CLA	C5-C6-C7-C8
36	l	201	CLA	C15-C16-C17-C18
36	R	315	CLA	O1A-CGA-O2A-C1
41	a	843	LHG	C7-C8-C9-C10
39	K	317	LMT	C5-C6-C7-C8
42	J	318	LMG	C24-C25-C26-C27
39	b	848	LMT	C9-C10-C11-C12
40	C	215	DGD	CFB-CGB-CHB-CIB
41	a	843	LHG	C10-C11-C12-C13
39	P	321	LMT	C7-C8-C9-C10
36	X	307	CLA	O1A-CGA-O2A-C1
36	D	310	CLA	C4-C3-C5-C6
36	P	319	CLA	C3A-C2A-CAA-CBA
36	R	316	CLA	C3A-C2A-CAA-CBA
36	a	803	CLA	C3A-C2A-CAA-CBA
36	b	814	CLA	C3A-C2A-CAA-CBA
36	b	832	CLA	C3A-C2A-CAA-CBA
36	V	308	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	V	313	CLA	C3A-C2A-CAA-CBA
36	V	314	CLA	C3A-C2A-CAA-CBA
36	L	314	CLA	C13-C15-C16-C17
41	F	319	LHG	C14-C15-C16-C17
42	I	315	LMG	O6-C1-O1-C7
39	b	851	LMT	C4-C5-C6-C7
42	I	315	LMG	C21-C22-C23-C24
36	C	212	CLA	O1A-CGA-O2A-C1
36	A	311	CLA	C10-C11-C12-C13
36	I	310	CLA	C15-C16-C17-C18
41	E	322	LHG	C5-C6-O8-C23
36	b	819	CLA	C11-C12-C13-C14
39	b	851	LMT	C6-C7-C8-C9
41	f	808	LHG	C31-C32-C33-C34
34	A	301	DD6	C24-C25-C26-C27
34	M	303	DD6	C24-C25-C26-C27
34	R	308	DD6	C1-C2-C3-C4
35	S	304	A86	C11-C10-C9-C8
35	S	308	A86	C11-C10-C9-C8
36	b	813	CLA	C6-C7-C8-C10
36	U	310	CLA	C2C-C3C-CAC-CBC
39	I	317	LMT	O5B-C5B-C6B-O6B
41	a	850	LHG	C26-C27-C28-C29
41	b	850	LHG	C33-C34-C35-C36
35	N	303	A86	C35-C34-O4-C38
35	S	303	A86	C35-C34-O4-C38
36	a	822	CLA	C4-C3-C5-C6
36	E	311	CLA	O1A-CGA-O2A-C1
36	b	836	CLA	O1A-CGA-O2A-C1
36	E	308	CLA	O1D-CGD-O2D-CED
36	b	812	CLA	O1D-CGD-O2D-CED
34	a	849	DD6	C10-C11-C13-C14
40	C	215	DGD	C7B-C8B-C9B-CAB
42	a	852	LMG	C40-C41-C42-C43
36	O	310	CLA	C2A-CAA-CBA-CGA
36	P	312	CLA	C2A-CAA-CBA-CGA
36	Q	309	CLA	C2A-CAA-CBA-CGA
35	A	316	A86	C12-C11-C13-O
35	B	301	A86	C12-C11-C13-O
35	B	303	A86	C12-C11-C13-O
35	C	202	A86	C12-C11-C13-O
35	F	305	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
35	F	307	A86	C12-C11-C13-O
35	G	304	A86	C12-C11-C13-O
35	H	301	A86	C12-C11-C13-O
35	I	302	A86	C12-C11-C13-O
35	I	304	A86	C12-C11-C13-O
35	J	303	A86	C12-C11-C13-O
35	K	302	A86	C12-C11-C13-O
35	K	303	A86	C12-C11-C13-O
35	L	319	A86	C12-C11-C13-O
35	M	301	A86	C12-C11-C13-O
35	M	304	A86	C12-C11-C13-O
35	M	305	A86	C12-C11-C13-O
35	N	301	A86	C12-C11-C13-O
35	N	302	A86	C12-C11-C13-O
35	N	320	A86	C12-C11-C13-O
35	O	302	A86	C12-C11-C13-O
35	O	303	A86	C12-C11-C13-O
35	O	305	A86	C12-C11-C13-O
35	P	303	A86	C12-C11-C13-O
35	P	304	A86	C12-C11-C13-O
35	Q	301	A86	C12-C11-C13-O
35	Q	303	A86	C12-C11-C13-O
35	R	301	A86	C12-C11-C13-O
35	R	302	A86	C12-C11-C13-O
35	R	303	A86	C12-C11-C13-O
35	R	304	A86	C12-C11-C13-O
35	R	306	A86	C12-C11-C13-O
35	R	309	A86	C12-C11-C13-O
35	S	301	A86	C12-C11-C13-O
35	S	302	A86	C12-C11-C13-O
35	T	302	A86	C12-C11-C13-O
35	T	303	A86	C12-C11-C13-O
35	T	306	A86	C12-C11-C13-O
35	T	307	A86	C12-C11-C13-O
35	W	202	A86	C12-C11-C13-O
35	W	203	A86	C12-C11-C13-O
35	X	301	A86	C12-C11-C13-O
35	X	302	A86	C12-C11-C13-O
35	X	303	A86	C12-C11-C13-O
35	X	305	A86	C12-C11-C13-O
35	U	302	A86	C12-C11-C13-O
35	U	304	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
35	V	303	A86	C12-C11-C13-O
35	V	304	A86	C12-C11-C13-O
42	G	324	LMG	C7-C8-C9-O8
42	J	318	LMG	O1-C7-C8-C9
42	j	105	LMG	O1-C7-C8-C9
41	j	104	LHG	C9-C10-C11-C12
42	V	315	LMG	C33-C34-C35-C36
35	G	304	A86	C35-C34-O4-C38
35	M	301	A86	C35-C34-O4-C38
36	a	830	CLA	C2C-C3C-CAC-CBC
36	b	840	CLA	C8-C10-C11-C12
39	a	854	LMT	C3-C4-C5-C6
41	j	104	LHG	C13-C14-C15-C16
39	E	321	LMT	C4-C5-C6-C7
39	U	315	LMT	C4-C5-C6-C7
42	I	315	LMG	C19-C20-C21-C22
39	U	314	LMT	C1-C2-C3-C4
36	I	306	CLA	C10-C11-C12-C13
36	R	315	CLA	C15-C16-C17-C18
36	a	831	CLA	C15-C16-C17-C18
42	G	324	LMG	C33-C34-C35-C36
36	H	308	CLA	C4-C3-C5-C6
36	H	309	CLA	C4-C3-C5-C6
36	J	310	CLA	C4-C3-C5-C6
36	b	805	CLA	C4-C3-C5-C6
36	b	834	CLA	C4-C3-C5-C6
41	F	319	LHG	C19-C20-C21-C22
39	E	320	LMT	C7-C8-C9-C10
42	V	316	LMG	C31-C32-C33-C34
36	b	834	CLA	C2-C3-C5-C6
42	a	852	LMG	C36-C37-C38-C39
35	A	316	A86	C10-C11-C13-O
35	B	301	A86	C10-C11-C13-O
35	B	303	A86	C10-C11-C13-O
35	C	202	A86	C10-C11-C13-O
35	F	305	A86	C10-C11-C13-O
35	F	307	A86	C10-C11-C13-O
35	G	304	A86	C10-C11-C13-O
35	H	301	A86	C10-C11-C13-O
35	I	302	A86	C10-C11-C13-O
35	I	304	A86	C10-C11-C13-O
35	J	303	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
35	K	302	A86	C10-C11-C13-O
35	K	303	A86	C10-C11-C13-O
35	K	306	A86	C10-C11-C13-O
35	L	304	A86	C10-C11-C13-O
35	L	319	A86	C10-C11-C13-O
35	M	301	A86	C10-C11-C13-O
35	M	302	A86	C10-C11-C13-O
35	M	304	A86	C10-C11-C13-O
35	M	305	A86	C10-C11-C13-O
35	N	301	A86	C10-C11-C13-O
35	N	302	A86	C10-C11-C13-O
35	N	303	A86	C10-C11-C13-O
35	N	320	A86	C10-C11-C13-O
35	O	302	A86	C10-C11-C13-O
35	O	303	A86	C10-C11-C13-O
35	O	305	A86	C10-C11-C13-O
35	O	319	A86	C10-C11-C13-O
35	P	303	A86	C10-C11-C13-O
35	P	304	A86	C10-C11-C13-O
35	Q	301	A86	C10-C11-C13-O
35	Q	303	A86	C10-C11-C13-O
35	Q	304	A86	C10-C11-C13-O
35	R	301	A86	C10-C11-C13-O
35	R	302	A86	C10-C11-C13-O
35	R	303	A86	C10-C11-C13-O
35	R	304	A86	C10-C11-C13-O
35	R	306	A86	C10-C11-C13-O
35	R	309	A86	C10-C11-C13-O
35	S	301	A86	C10-C11-C13-O
35	S	302	A86	C10-C11-C13-O
35	S	303	A86	C10-C11-C13-O
35	S	305	A86	C10-C11-C13-O
35	T	302	A86	C10-C11-C13-O
35	T	303	A86	C10-C11-C13-O
35	T	305	A86	C10-C11-C13-O
35	T	306	A86	C10-C11-C13-O
35	T	307	A86	C10-C11-C13-O
35	W	202	A86	C10-C11-C13-O
35	W	203	A86	C10-C11-C13-O
35	X	301	A86	C10-C11-C13-O
35	X	302	A86	C10-C11-C13-O
35	X	303	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
35	X	304	A86	C10-C11-C13-O
35	X	305	A86	C10-C11-C13-O
35	U	302	A86	C10-C11-C13-O
35	U	304	A86	C10-C11-C13-O
35	V	302	A86	C10-C11-C13-O
35	V	303	A86	C10-C11-C13-O
35	V	304	A86	C10-C11-C13-O
36	L	320	CLA	O1D-CGD-O2D-CED
36	P	313	CLA	O1D-CGD-O2D-CED
36	a	808	CLA	C16-C17-C18-C20
41	j	104	LHG	C23-C24-C25-C26
36	L	309	CLA	C13-C15-C16-C17
41	F	319	LHG	O6-C4-C5-O7
41	a	850	LHG	O6-C4-C5-O7
41	i	104	LHG	O6-C4-C5-O7
39	E	321	LMT	C2-C3-C4-C5
42	J	319	LMG	C19-C20-C21-C22
36	O	311	CLA	O1D-CGD-O2D-CED
36	M	316	CLA	C2B-C3B-CAB-CBB
36	a	814	CLA	C2B-C3B-CAB-CBB
36	V	307	CLA	C2B-C3B-CAB-CBB
44	a	846	BCR	C1-C6-C7-C8
44	a	847	BCR	C1-C6-C7-C8
44	b	843	BCR	C1-C6-C7-C8
44	b	846	BCR	C5-C6-C7-C8
44	b	846	BCR	C23-C24-C25-C30
44	f	806	BCR	C1-C6-C7-C8
44	i	103	BCR	C1-C6-C7-C8
44	l	203	BCR	C1-C6-C7-C8
44	l	203	BCR	C23-C24-C25-C30
44	m	101	BCR	C23-C24-C25-C30
44	h	201	BCR	C23-C24-C25-C30
41	G	320	LHG	O2-C2-C3-O3
36	C	209	CLA	C10-C11-C12-C13
36	I	306	CLA	C13-C15-C16-C17
43	a	840	PQN	C23-C25-C26-C27
35	S	301	A86	C35-C34-O4-C38
41	O	317	LHG	C5-C4-O6-P
36	F	310	CLA	C11-C10-C8-C9
41	G	301	LHG	C19-C20-C21-C22
36	a	837	CLA	C10-C11-C12-C13
36	b	828	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	b	840	CLA	C15-C16-C17-C18
36	a	825	CLA	CBD-CGD-O2D-CED
41	D	318	LHG	C32-C33-C34-C35
36	b	833	CLA	O1D-CGD-O2D-CED
41	a	850	LHG	C18-C19-C20-C21
41	j	104	LHG	C28-C29-C30-C31
42	I	315	LMG	C12-C13-C14-C15
39	b	848	LMT	C4B-C5B-C6B-O6B
36	H	309	CLA	C16-C17-C18-C20
36	H	312	CLA	C16-C17-C18-C19
36	I	306	CLA	C16-C17-C18-C20
36	T	311	CLA	C16-C17-C18-C20
36	l	205	CLA	C16-C17-C18-C19
36	R	315	CLA	C2A-CAA-CBA-CGA
36	a	817	CLA	C2A-CAA-CBA-CGA
36	J	312	CLA	C15-C16-C17-C18
38	b	804	SQD	O47-C45-C46-O48
41	F	319	LHG	O7-C5-C6-O8
41	f	809	LHG	O7-C5-C6-O8
42	E	319	LMG	O1-C7-C8-O7
42	G	324	LMG	O1-C7-C8-O7
42	I	315	LMG	O7-C8-C9-O8
42	J	318	LMG	O1-C7-C8-O7
42	h	206	LMG	O7-C8-C9-O8
41	G	321	LHG	C17-C18-C19-C20
35	N	301	A86	C35-C34-O4-C38
35	R	303	A86	C35-C34-O4-C38
41	E	322	LHG	C26-C27-C28-C29
36	B	311	CLA	C3-C5-C6-C7
36	F	309	CLA	C5-C6-C7-C8
36	f	804	CLA	C15-C16-C17-C18
42	j	105	LMG	C39-C40-C41-C42
36	K	307	CLA	C12-C13-C15-C16
36	C	209	CLA	O1A-CGA-O2A-C1
36	j	102	CLA	O1A-CGA-O2A-C1
36	b	809	CLA	O1D-CGD-O2D-CED
41	O	317	LHG	C17-C18-C19-C20
36	H	312	CLA	C5-C6-C7-C8
36	W	207	CLA	C13-C15-C16-C17
36	D	310	CLA	C2-C3-C5-C6
36	H	309	CLA	C2-C3-C5-C6
36	J	310	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	l	202	CLA	C2-C3-C5-C6
36	V	308	CLA	C2-C3-C5-C6
41	E	322	LHG	C19-C20-C21-C22
39	a	853	LMT	C1-C2-C3-C4
39	I	318	LMT	C3-C4-C5-C6
41	f	808	LHG	C11-C10-C9-C8
39	L	318	LMT	O5B-C1B-O1B-C4'
35	R	301	A86	C35-C34-O4-C38
39	a	853	LMT	C3-C4-C5-C6
41	O	318	LHG	C28-C29-C30-C31
41	Q	315	LHG	C12-C13-C14-C15
41	a	842	LHG	C34-C35-C36-C37
41	f	809	LHG	C27-C28-C29-C30
42	G	325	LMG	C41-C42-C43-C44
36	b	825	CLA	C13-C15-C16-C17
41	O	318	LHG	C7-C8-C9-C10
36	O	307	CLA	O1D-CGD-O2D-CED
36	P	309	CLA	O1D-CGD-O2D-CED
36	W	201	CLA	CBD-CGD-O2D-CED
36	A	314	CLA	C11-C12-C13-C14
36	H	307	CLA	C11-C10-C8-C9
36	K	312	CLA	C14-C13-C15-C16
36	N	308	CLA	C11-C12-C13-C14
36	N	316	CLA	C6-C7-C8-C9
36	Q	314	CLA	C14-C13-C15-C16
36	b	826	CLA	C6-C7-C8-C9
36	j	101	CLA	C6-C7-C8-C9
36	U	311	CLA	C11-C12-C13-C14
36	V	308	CLA	C14-C13-C15-C16
36	Q	306	CLA	O1D-CGD-O2D-CED
36	C	207	CLA	C5-C6-C7-C8
36	L	309	CLA	C15-C16-C17-C18
36	f	805	CLA	O1D-CGD-O2D-CED
44	b	847	BCR	C6-C7-C8-C9
39	a	854	LMT	C4-C5-C6-C7
41	D	319	LHG	C32-C33-C34-C35
39	U	314	LMT	C9-C10-C11-C12
39	b	851	LMT	C7-C8-C9-C10
42	J	318	LMG	C20-C21-C22-C23
42	j	105	LMG	C2-C1-O1-C7
36	G	311	CLA	C8-C10-C11-C12
36	f	803	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	N	310	CLA	C4C-C3C-CAC-CBC
42	G	324	LMG	C24-C25-C26-C27
41	i	104	LHG	C34-C35-C36-C37
36	a	801	CLA	C8-C10-C11-C12
41	G	321	LHG	C13-C14-C15-C16
36	a	807	CLA	O1A-CGA-O2A-C1
41	Q	315	LHG	O1-C1-C2-O2
41	b	850	LHG	O1-C1-C2-O2
36	J	308	CLA	C3-C5-C6-C7
36	W	209	CLA	CBA-CGA-O2A-C1
36	f	805	CLA	C4-C3-C5-C6
35	G	302	A86	C11-C10-C9-C8
41	I	316	LHG	C19-C20-C21-C22
36	A	314	CLA	C16-C17-C18-C20
36	a	820	CLA	C16-C17-C18-C19
36	b	820	CLA	C11-C12-C13-C15
36	J	316	CLA	O1A-CGA-O2A-C1
36	H	312	CLA	C15-C16-C17-C18
36	L	314	CLA	C15-C16-C17-C18
36	f	802	CLA	C13-C15-C16-C17
36	b	829	CLA	O1A-CGA-O2A-C1
36	G	311	CLA	C4C-C3C-CAC-CBC
36	f	803	CLA	C2C-C3C-CAC-CBC
36	E	317	CLA	O1D-CGD-O2D-CED
41	l	208	LHG	C32-C33-C34-C35
39	L	303	LMT	C9-C10-C11-C12
41	O	318	LHG	C1-C2-C3-O3
41	a	843	LHG	C1-C2-C3-O3
39	U	315	LMT	C3-C4-C5-C6
44	a	844	BCR	C20-C21-C22-C37
44	b	846	BCR	C11-C10-C9-C34
41	R	323	LHG	C19-C20-C21-C22
36	G	312	CLA	C3-C5-C6-C7
36	V	307	CLA	CBA-CGA-O2A-C1
36	T	313	CLA	C13-C15-C16-C17
36	b	821	CLA	C13-C15-C16-C17
42	J	318	LMG	C15-C16-C17-C18
41	O	318	LHG	O6-C4-C5-C6
41	b	850	LHG	O6-C4-C5-C6
36	H	309	CLA	C16-C17-C18-C19
36	l	202	CLA	C16-C17-C18-C20
39	I	317	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
35	J	302	A86	C35-C34-O4-C38
39	b	848	LMT	C2-C3-C4-C5
36	V	307	CLA	O1A-CGA-O2A-C1
36	M	309	CLA	C5-C6-C7-C8
36	R	310	CLA	C10-C11-C12-C13
34	Q	302	DD6	C12-C11-C13-C14
44	b	847	BCR	C11-C12-C13-C35
42	G	324	LMG	C42-C43-C44-C45
41	i	104	LHG	C11-C10-C9-C8
42	E	319	LMG	C14-C15-C16-C17
42	J	319	LMG	C20-C21-C22-C23
36	B	305	CLA	C11-C12-C13-C15
36	H	307	CLA	C11-C10-C8-C7
36	I	311	CLA	C11-C10-C8-C7
36	K	310	CLA	C11-C12-C13-C15
36	L	309	CLA	C6-C7-C8-C10
36	N	316	CLA	C6-C7-C8-C10
36	O	307	CLA	C11-C10-C8-C7
36	P	309	CLA	C11-C10-C8-C7
36	P	310	CLA	C12-C13-C15-C16
36	S	310	CLA	C11-C12-C13-C15
36	T	314	CLA	C12-C13-C15-C16
36	a	817	CLA	C6-C7-C8-C10
36	a	827	CLA	C11-C12-C13-C15
36	a	831	CLA	C11-C10-C8-C7
36	a	848	CLA	C11-C10-C8-C7
36	b	809	CLA	C6-C7-C8-C10
36	b	828	CLA	C12-C13-C15-C16
36	b	837	CLA	C12-C13-C15-C16
36	l	205	CLA	C11-C10-C8-C7
36	U	311	CLA	C11-C12-C13-C15
36	V	306	CLA	C6-C7-C8-C10
36	V	308	CLA	C6-C7-C8-C10
36	V	308	CLA	C12-C13-C15-C16
36	V	311	CLA	C12-C13-C15-C16
43	b	842	PQN	C22-C23-C25-C26
41	i	104	LHG	C26-C27-C28-C29
36	J	307	CLA	C3-C5-C6-C7
36	L	308	CLA	C3-C5-C6-C7
36	a	802	CLA	C10-C11-C12-C13
36	a	828	CLA	C15-C16-C17-C18
34	E	304	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
34	Q	302	DD6	C10-C11-C13-C14
35	C	204	A86	C2-C1-C24-C25
36	T	311	CLA	CBA-CGA-O2A-C1
41	G	321	LHG	C31-C32-C33-C34
38	b	804	SQD	C45-C44-O6-C1
40	C	215	DGD	C2G-C3G-O3G-C1D
40	L	302	DGD	C2G-C3G-O3G-C1D
42	D	321	LMG	C8-C7-O1-C1
42	I	315	LMG	C8-C7-O1-C1
35	X	301	A86	C35-C34-O4-C38
36	U	306	CLA	O1D-CGD-O2D-CED
36	W	207	CLA	C2A-CAA-CBA-CGA
36	a	812	CLA	C2A-CAA-CBA-CGA
36	F	317	CLA	C11-C10-C8-C9
36	K	307	CLA	C14-C13-C15-C16
36	a	839	CLA	C16-C17-C18-C20
42	V	316	LMG	C11-C10-O7-C8
36	H	315	CLA	C4-C3-C5-C6
36	R	322	CLA	C4-C3-C5-C6
36	a	820	CLA	C4-C3-C5-C6
36	b	841	CLA	O1A-CGA-O2A-C1
41	D	318	LHG	O10-C23-O8-C6
41	j	104	LHG	O10-C23-O8-C6
36	T	309	CLA	C2-C3-C5-C6
36	f	805	CLA	C2-C3-C5-C6
37	L	315	KC1	C2B-C3B-CAB-CBB
42	a	852	LMG	C12-C13-C14-C15
39	U	315	LMT	C9-C10-C11-C12
41	b	850	LHG	C13-C14-C15-C16
42	D	320	LMG	C33-C34-C35-C36
39	G	322	LMT	C2B-C1B-O1B-C4'
39	a	851	LMT	C5'-C4'-O1B-C1B
36	R	314	CLA	CBD-CGD-O2D-CED
36	U	310	CLA	C8-C10-C11-C12
36	I	308	CLA	O2A-C1-C2-C3
36	W	207	CLA	O2A-C1-C2-C3
36	a	804	CLA	O2A-C1-C2-C3
40	C	215	DGD	C1G-C2G-O2G-C1B
41	Q	315	LHG	C4-C5-O7-C7
41	a	842	LHG	C6-C5-O7-C7
41	l	208	LHG	C6-C5-O7-C7
42	a	852	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
36	F	317	CLA	O1A-CGA-O2A-C1
36	b	826	CLA	O1A-CGA-O2A-C1
36	G	310	CLA	C8-C10-C11-C12
36	G	311	CLA	C13-C15-C16-C17
34	D	303	DD6	C11-C10-C9-C8
35	J	301	A86	C11-C10-C9-C8
35	V	301	A86	C1-C2-C3-C4
39	F	320	LMT	O5B-C5B-C6B-O6B
36	b	841	CLA	CBD-CGD-O2D-CED
41	F	319	LHG	C12-C13-C14-C15
36	a	839	CLA	C16-C17-C18-C19
41	i	104	LHG	C33-C34-C35-C36
36	O	309	CLA	C3-C5-C6-C7
36	P	311	CLA	C3-C5-C6-C7
36	Q	308	CLA	C3-C5-C6-C7
39	U	315	LMT	C5-C6-C7-C8
41	F	319	LHG	C10-C11-C12-C13
36	H	309	CLA	C8-C10-C11-C12
40	b	849	DGD	O1B-C1B-O2G-C2G
41	G	301	LHG	O9-C7-O7-C5
41	F	318	LHG	O6-C4-C5-O7
41	G	301	LHG	O6-C4-C5-O7
41	Q	315	LHG	O6-C4-C5-O7
42	V	315	LMG	C17-C18-C19-C20
39	a	853	LMT	C6-C7-C8-C9
42	j	105	LMG	C21-C22-C23-C24
36	j	101	CLA	O1D-CGD-O2D-CED
41	f	809	LHG	C26-C27-C28-C29
41	O	317	LHG	C4-C5-C6-O8
42	D	321	LMG	C7-C8-C9-O8
42	G	325	LMG	O1-C7-C8-C9
42	h	206	LMG	C7-C8-C9-O8
42	D	320	LMG	C10-C11-C12-C13
36	S	312	CLA	C8-C10-C11-C12
39	E	321	LMT	C3'-C4'-O1B-C1B
37	B	310	KC1	C4B-C3B-CAB-CBB
37	C	213	KC1	C4B-C3B-CAB-CBB
37	E	309	KC1	C4B-C3B-CAB-CBB
37	G	308	KC1	C4B-C3B-CAB-CBB
37	J	314	KC1	C4B-C3B-CAB-CBB
37	K	314	KC1	C4B-C3B-CAB-CBB
37	L	315	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	L	317	KC1	C4B-C3B-CAB-CBB
37	N	314	KC1	C4B-C3B-CAB-CBB
37	O	313	KC1	C4B-C3B-CAB-CBB
37	O	315	KC1	C4B-C3B-CAB-CBB
37	P	315	KC1	C4B-C3B-CAB-CBB
37	Q	311	KC1	C4B-C3B-CAB-CBB
37	Q	313	KC1	C4B-C3B-CAB-CBB
37	S	316	KC1	C4B-C3B-CAB-CBB
37	T	315	KC1	C4B-C3B-CAB-CBB
37	W	213	KC1	C4B-C3B-CAB-CBB
36	b	801	CLA	O1D-CGD-O2D-CED
36	b	806	CLA	C3-C5-C6-C7
42	G	324	LMG	C11-C12-C13-C14
42	G	324	LMG	C41-C42-C43-C44
36	Q	310	CLA	C4-C3-C5-C6
36	X	306	CLA	C2A-CAA-CBA-CGA
36	I	311	CLA	CBD-CGD-O2D-CED
36	D	317	CLA	C2-C3-C5-C6
35	H	304	A86	C28-C27-C29-C30
35	I	301	A86	C28-C27-C29-C30
35	J	301	A86	C28-C27-C29-C30
35	U	303	A86	C28-C27-C29-C30
39	f	807	LMT	C1-C2-C3-C4
36	U	311	CLA	O1A-CGA-O2A-C1
39	L	318	LMT	O1'-C1-C2-C3
40	C	215	DGD	O1G-C1G-C2G-O2G
41	G	301	LHG	O7-C5-C6-O8
41	G	321	LHG	O7-C5-C6-O8
41	O	317	LHG	O7-C5-C6-O8
41	O	318	LHG	O7-C5-C6-O8
41	R	323	LHG	O7-C5-C6-O8
42	G	324	LMG	O7-C8-C9-O8
42	L	321	LMG	O7-C8-C9-O8
42	j	105	LMG	O1-C7-C8-O7
42	V	315	LMG	O1-C7-C8-O7
42	V	315	LMG	O7-C8-C9-O8
36	b	802	CLA	C15-C16-C17-C18
36	b	834	CLA	C10-C11-C12-C13
36	H	316	CLA	C14-C13-C15-C16
36	K	310	CLA	C11-C12-C13-C14
36	M	311	CLA	C14-C13-C15-C16
36	P	314	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
36	S	309	CLA	C11-C12-C13-C14
36	T	314	CLA	C14-C13-C15-C16
36	X	306	CLA	C11-C12-C13-C14
36	a	829	CLA	C11-C10-C8-C9
36	a	837	CLA	C11-C10-C8-C9
36	b	827	CLA	C6-C7-C8-C9
36	U	311	CLA	C6-C7-C8-C9
36	a	808	CLA	C16-C17-C18-C19
42	a	852	LMG	C38-C39-C40-C41
41	a	850	LHG	C19-C20-C21-C22
39	B	312	LMT	C6-C7-C8-C9
42	j	105	LMG	C12-C13-C14-C15
42	j	105	LMG	C32-C33-C34-C35
36	W	209	CLA	O1A-CGA-O2A-C1
36	E	313	CLA	C15-C16-C17-C18
36	b	840	CLA	C10-C11-C12-C13
35	C	204	A86	C13-C14-C15-O1
35	F	302	A86	C13-C14-C15-O1
35	L	301	A86	C13-C14-C15-O1
41	F	318	LHG	C9-C10-C11-C12
36	b	819	CLA	C10-C11-C12-C13
41	a	842	LHG	C27-C28-C29-C30
41	j	104	LHG	C29-C30-C31-C32
35	L	306	A86	C35-C34-O4-C38
36	I	311	CLA	C8-C10-C11-C12
36	V	310	CLA	C3-C5-C6-C7
41	i	104	LHG	C27-C28-C29-C30
36	D	309	CLA	C2-C1-O2A-CGA
36	O	316	CLA	C16-C17-C18-C19
36	a	816	CLA	C16-C17-C18-C19
36	a	820	CLA	C16-C17-C18-C20
36	a	804	CLA	C15-C16-C17-C18
41	E	322	LHG	C5-C4-O6-P
39	b	851	LMT	C2-C3-C4-C5
42	G	325	LMG	C22-C23-C24-C25
41	f	808	LHG	C16-C17-C18-C19
42	V	316	LMG	C12-C13-C14-C15
36	F	314	CLA	C2A-CAA-CBA-CGA
42	V	315	LMG	C31-C32-C33-C34
36	M	312	CLA	C4C-C3C-CAC-CBC
36	O	308	CLA	C10-C11-C12-C13
41	F	319	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
42	J	318	LMG	C32-C33-C34-C35
42	J	319	LMG	C23-C24-C25-C26
39	h	205	LMT	C6-C7-C8-C9
41	R	323	LHG	C13-C14-C15-C16
36	W	207	CLA	CBD-CGD-O2D-CED
36	b	840	CLA	C3-C5-C6-C7
36	f	802	CLA	C3-C5-C6-C7
39	U	314	LMT	C6-C7-C8-C9
36	a	814	CLA	C4C-C3C-CAC-CBC
41	O	317	LHG	C12-C13-C14-C15
39	b	851	LMT	C2-C1-O1'-C1'
36	I	307	CLA	C3-C5-C6-C7
43	b	842	PQN	C13-C15-C16-C17
41	I	316	LHG	C9-C10-C11-C12
34	W	205	DD6	C-C1-C24-C25
44	b	845	BCR	C37-C22-C23-C24
35	P	306	A86	O-C13-C14-C15
35	S	304	A86	O-C13-C14-C15
35	T	301	A86	O-C13-C14-C15
35	U	303	A86	O-C13-C14-C15
36	A	307	CLA	C1A-C2A-CAA-CBA
36	C	206	CLA	C1A-C2A-CAA-CBA
36	E	313	CLA	C4B-C3B-CAB-CBB
36	E	314	CLA	C1A-C2A-CAA-CBA
36	H	318	CLA	C4B-C3B-CAB-CBB
36	L	310	CLA	C4B-C3B-CAB-CBB
36	O	312	CLA	C4B-C3B-CAB-CBB
36	P	314	CLA	C4B-C3B-CAB-CBB
36	Q	310	CLA	C4B-C3B-CAB-CBB
36	T	313	CLA	C1A-C2A-CAA-CBA
36	a	827	CLA	C1A-C2A-CAA-CBA
36	a	838	CLA	C4B-C3B-CAB-CBB
36	b	802	CLA	C4B-C3B-CAB-CBB
36	b	813	CLA	C1A-C2A-CAA-CBA
36	b	835	CLA	C1A-C2A-CAA-CBA
36	F	310	CLA	O1D-CGD-O2D-CED
36	S	319	CLA	C4-C3-C5-C6
36	a	827	CLA	C4-C3-C5-C6
36	b	802	CLA	C4-C3-C5-C6
36	b	828	CLA	C4-C3-C5-C6
36	f	803	CLA	C4-C3-C5-C6
44	i	103	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
44	l	207	BCR	C6-C7-C8-C9
36	a	820	CLA	C2-C3-C5-C6
36	V	306	CLA	C2-C3-C5-C6
34	D	301	DD6	C2-C1-C24-C25
34	P	305	DD6	C2-C1-C24-C25
35	F	302	A86	C5-C6-C8-C9
35	S	308	A86	C24-C25-C26-C27
40	C	215	DGD	CBB-CCB-CDB-CEB
36	C	207	CLA	CBD-CGD-O2D-CED
36	T	311	CLA	O1A-CGA-O2A-C1
36	B	309	CLA	C2A-CAA-CBA-CGA
36	J	313	CLA	C2A-CAA-CBA-CGA
42	h	206	LMG	C14-C15-C16-C17
42	j	105	LMG	C42-C43-C44-C45
36	E	315	CLA	C13-C15-C16-C17
36	U	311	CLA	C15-C16-C17-C18
41	D	318	LHG	O6-C4-C5-C6
41	l	208	LHG	O6-C4-C5-C6
39	E	321	LMT	C7-C8-C9-C10
41	O	318	LHG	O9-C7-O7-C5
38	A	315	SQD	C5-C6-S-O9
36	P	301	CLA	C10-C11-C12-C13
38	b	804	SQD	C10-C11-C12-C13
42	G	324	LMG	C40-C41-C42-C43
36	A	314	CLA	C12-C13-C15-C16
36	C	208	CLA	C6-C7-C8-C10
36	C	208	CLA	C11-C10-C8-C7
36	E	311	CLA	C12-C13-C15-C16
36	E	315	CLA	C11-C12-C13-C15
36	E	316	CLA	C12-C13-C15-C16
36	F	309	CLA	C11-C12-C13-C15
36	J	309	CLA	C11-C12-C13-C15
36	K	310	CLA	C6-C7-C8-C10
36	L	308	CLA	C11-C12-C13-C15
36	N	308	CLA	C12-C13-C15-C16
36	P	314	CLA	C6-C7-C8-C10
36	Q	310	CLA	C11-C10-C8-C7
36	Q	314	CLA	C11-C12-C13-C15
36	T	309	CLA	C6-C7-C8-C10
36	W	209	CLA	C6-C7-C8-C10
36	a	804	CLA	C6-C7-C8-C10
36	a	810	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
36	a	825	CLA	C6-C7-C8-C10
36	a	832	CLA	C6-C7-C8-C10
36	b	808	CLA	C11-C12-C13-C15
36	b	810	CLA	C11-C10-C8-C7
36	b	815	CLA	C6-C7-C8-C10
36	b	820	CLA	C6-C7-C8-C10
36	f	803	CLA	C6-C7-C8-C10
36	U	306	CLA	C11-C10-C8-C7
36	U	308	CLA	C6-C7-C8-C10
36	V	305	CLA	C6-C7-C8-C10
36	T	309	CLA	C16-C17-C18-C19
42	D	320	LMG	C24-C25-C26-C27
42	I	315	LMG	C33-C34-C35-C36
36	J	313	CLA	CBD-CGD-O2D-CED
41	b	850	LHG	O2-C2-C3-O3
35	P	303	A86	C35-C34-O4-C38
35	T	307	A86	C35-C34-O4-C38
41	D	318	LHG	C26-C27-C28-C29
36	I	311	CLA	CBA-CGA-O2A-C1
36	S	321	CLA	CBA-CGA-O2A-C1
42	D	320	LMG	C14-C15-C16-C17
36	a	802	CLA	C8-C10-C11-C12
39	I	318	LMT	C5-C6-C7-C8
39	B	313	LMT	C3-C4-C5-C6
36	W	208	CLA	O1D-CGD-O2D-CED
36	Q	314	CLA	C5-C6-C7-C8
41	D	318	LHG	C5-C4-O6-P
41	G	321	LHG	C5-C4-O6-P
40	C	215	DGD	CEB-CFB-CGB-CHB
36	R	321	CLA	C3A-C2A-CAA-CBA
36	C	207	CLA	C16-C17-C18-C19
35	L	319	A86	C35-C34-O4-C38
42	h	206	LMG	O9-C10-O7-C8
42	V	316	LMG	O9-C10-O7-C8
41	O	318	LHG	O6-C4-C5-O7
41	b	850	LHG	O6-C4-C5-O7
41	l	208	LHG	O6-C4-C5-O7
36	G	312	CLA	C10-C11-C12-C13
39	B	312	LMT	C9-C10-C11-C12
42	m	102	LMG	C16-C17-C18-C19
39	L	303	LMT	C5-C6-C7-C8
36	C	212	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
38	A	315	SQD	C8-C7-O47-C45
42	h	206	LMG	C11-C10-O7-C8
36	K	307	CLA	C2A-CAA-CBA-CGA
36	S	314	CLA	C2A-CAA-CBA-CGA
36	A	311	CLA	C6-C7-C8-C9
36	C	208	CLA	C14-C13-C15-C16
36	K	309	CLA	C11-C10-C8-C9
36	L	314	CLA	C14-C13-C15-C16
36	N	316	CLA	C11-C12-C13-C14
36	P	310	CLA	C14-C13-C15-C16
36	R	313	CLA	C14-C13-C15-C16
36	S	310	CLA	C11-C12-C13-C14
36	a	817	CLA	C6-C7-C8-C9
36	a	848	CLA	C11-C10-C8-C9
36	b	821	CLA	C11-C10-C8-C9
36	b	828	CLA	C14-C13-C15-C16
36	b	837	CLA	C14-C13-C15-C16
36	V	308	CLA	C6-C7-C8-C9
36	V	311	CLA	C14-C13-C15-C16
43	a	840	PQN	C19-C18-C20-C21
36	b	806	CLA	C15-C16-C17-C18
34	W	204	DD6	C1-C2-C3-C4
34	j	103	DD6	C24-C25-C26-C27
35	K	301	A86	C24-C25-C26-C27
35	X	314	A86	C24-C25-C26-C27
36	a	824	CLA	O1D-CGD-O2D-CED
35	C	204	A86	C26-C27-C29-C30
35	I	301	A86	C26-C27-C29-C30
35	S	308	A86	C26-C27-C29-C30
36	A	305	CLA	C1-C2-C3-C4
36	E	308	CLA	C1-C2-C3-C4
36	X	309	CLA	CAD-CBD-CGD-O1D
36	a	821	CLA	C1-C2-C3-C4
36	b	832	CLA	C1-C2-C3-C4
37	C	213	KC1	C1A-C2A-CAA-CBA
37	D	314	KC1	C1A-C2A-CAA-CBA
37	G	317	KC1	C1A-C2A-CAA-CBA
37	H	313	KC1	C1A-C2A-CAA-CBA
37	L	315	KC1	C1A-C2A-CAA-CBA
37	M	317	KC1	C1A-C2A-CAA-CBA
37	P	317	KC1	C1A-C2A-CAA-CBA
37	T	315	KC1	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	X	311	KC1	C1A-C2A-CAA-CBA
41	G	301	LHG	C33-C34-C35-C36
41	a	842	LHG	C9-C10-C11-C12
42	G	324	LMG	C14-C15-C16-C17
42	E	318	LMG	C36-C37-C38-C39
42	V	316	LMG	C13-C14-C15-C16
36	b	806	CLA	C8-C10-C11-C12
35	O	302	A86	C35-C34-O4-C38
40	C	215	DGD	CCB-CDB-CEB-CFB
41	D	319	LHG	C29-C30-C31-C32
39	B	312	LMT	C4B-C5B-C6B-O6B
41	D	319	LHG	O7-C5-C6-O8
41	l	208	LHG	O7-C5-C6-O8
42	D	320	LMG	O1-C7-C8-O7
42	D	321	LMG	O7-C8-C9-O8
42	I	315	LMG	O1-C7-C8-O7
39	b	848	LMT	C6-C7-C8-C9
41	O	317	LHG	C24-C25-C26-C27
36	E	316	CLA	C13-C15-C16-C17
42	G	324	LMG	C28-C29-C30-C31
36	K	316	CLA	C16-C17-C18-C20
38	A	315	SQD	C44-C45-C46-O48
38	b	804	SQD	C44-C45-C46-O48
41	l	208	LHG	C4-C5-C6-O8
42	I	315	LMG	C7-C8-C9-O8
42	V	315	LMG	O1-C7-C8-C9
36	a	810	CLA	C4-C3-C5-C6
39	K	317	LMT	C3'-C4'-O1B-C1B
42	G	324	LMG	C39-C40-C41-C42
36	T	309	CLA	C13-C15-C16-C17
36	b	828	CLA	CAA-CBA-CGA-O2A
36	Q	310	CLA	C2-C3-C5-C6
42	E	318	LMG	O6-C5-C6-O5
35	A	302	A86	C13-C14-C15-C20
35	A	316	A86	C13-C14-C15-C20
35	C	202	A86	C13-C14-C15-C20
35	F	305	A86	C13-C14-C15-C20
35	I	304	A86	C13-C14-C15-C20
35	K	302	A86	C13-C14-C15-C20
35	L	304	A86	C13-C14-C15-C20
35	L	319	A86	C13-C14-C15-C20
35	M	301	A86	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
35	M	305	A86	C13-C14-C15-C20
35	N	306	A86	C13-C14-C15-C20
35	N	320	A86	C13-C14-C15-C20
35	O	302	A86	C13-C14-C15-C20
35	P	303	A86	C13-C14-C15-C20
35	Q	304	A86	C13-C14-C15-C20
35	R	301	A86	C13-C14-C15-C20
35	R	304	A86	C13-C14-C15-C20
35	R	306	A86	C13-C14-C15-C20
35	R	309	A86	C13-C14-C15-C20
35	T	305	A86	C13-C14-C15-C20
35	T	307	A86	C13-C14-C15-C20
35	W	202	A86	C13-C14-C15-C20
35	X	303	A86	C13-C14-C15-C20
35	X	305	A86	C13-C14-C15-C20
35	U	302	A86	C13-C14-C15-C20
36	A	308	CLA	CAD-CBD-CGD-O2D
36	B	309	CLA	CAD-CBD-CGD-O2D
36	C	209	CLA	CAD-CBD-CGD-O2D
36	E	312	CLA	CAD-CBD-CGD-O2D
36	F	311	CLA	CAD-CBD-CGD-O2D
36	G	311	CLA	CAD-CBD-CGD-O2D
36	N	319	CLA	CAD-CBD-CGD-O2D
36	O	309	CLA	CAD-CBD-CGD-O2D
36	O	316	CLA	CAD-CBD-CGD-O2D
36	P	311	CLA	CAD-CBD-CGD-O2D
36	Q	308	CLA	CAD-CBD-CGD-O2D
36	R	313	CLA	CAD-CBD-CGD-O2D
36	X	308	CLA	CAD-CBD-CGD-O2D
36	V	314	CLA	CAD-CBD-CGD-O2D
36	C	212	CLA	C15-C16-C17-C18
42	j	105	LMG	C13-C14-C15-C16
36	N	317	CLA	C6-C7-C8-C9
36	C	208	CLA	CBA-CGA-O2A-C1
36	H	309	CLA	CBA-CGA-O2A-C1
39	U	315	LMT	O5'-C1'-O1'-C1
35	K	306	A86	C33-C34-O4-C38
38	b	804	SQD	C11-C12-C13-C14
41	j	104	LHG	C26-C27-C28-C29
36	H	312	CLA	C13-C15-C16-C17
41	O	318	LHG	C10-C11-C12-C13
36	Q	314	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	B	302	DD6	C11-C10-C9-C8
35	A	302	A86	C10-C11-C13-C14
35	B	301	A86	C10-C11-C13-C14
35	C	202	A86	C10-C11-C13-C14
35	C	204	A86	C10-C11-C13-C14
35	F	305	A86	C10-C11-C13-C14
35	F	307	A86	C10-C11-C13-C14
35	I	302	A86	C10-C11-C13-C14
35	I	304	A86	C10-C11-C13-C14
35	J	303	A86	C10-C11-C13-C14
35	L	304	A86	C10-C11-C13-C14
35	L	306	A86	C10-C11-C13-C14
35	M	302	A86	C10-C11-C13-C14
35	N	301	A86	C10-C11-C13-C14
35	N	302	A86	C10-C11-C13-C14
35	O	303	A86	C10-C11-C13-C14
35	O	305	A86	C10-C11-C13-C14
35	P	304	A86	C10-C11-C13-C14
35	Q	301	A86	C10-C11-C13-C14
35	Q	303	A86	C10-C11-C13-C14
35	R	301	A86	C10-C11-C13-C14
35	R	302	A86	C10-C11-C13-C14
35	R	303	A86	C10-C11-C13-C14
35	R	304	A86	C10-C11-C13-C14
35	S	301	A86	C10-C11-C13-C14
35	S	302	A86	C10-C11-C13-C14
35	T	302	A86	C10-C11-C13-C14
35	T	303	A86	C10-C11-C13-C14
35	T	305	A86	C10-C11-C13-C14
35	T	306	A86	C10-C11-C13-C14
35	T	307	A86	C10-C11-C13-C14
35	W	202	A86	C10-C11-C13-C14
35	W	203	A86	C10-C11-C13-C14
35	X	302	A86	C10-C11-C13-C14
35	X	303	A86	C10-C11-C13-C14
35	X	304	A86	C10-C11-C13-C14
35	X	305	A86	C10-C11-C13-C14
35	U	302	A86	C10-C11-C13-C14
35	V	303	A86	C10-C11-C13-C14
35	V	304	A86	C10-C11-C13-C14
36	A	308	CLA	CAD-CBD-CGD-O1D
36	B	309	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
36	C	209	CLA	CAD-CBD-CGD-O1D
36	E	312	CLA	CAD-CBD-CGD-O1D
36	E	317	CLA	CHA-CBD-CGD-O1D
36	F	311	CLA	CAD-CBD-CGD-O1D
36	G	307	CLA	CHA-CBD-CGD-O2D
36	G	307	CLA	CAD-CBD-CGD-O2D
36	G	311	CLA	CAD-CBD-CGD-O1D
36	H	308	CLA	CHA-CBD-CGD-O2D
36	H	309	CLA	CHA-CBD-CGD-O1D
36	O	309	CLA	CAD-CBD-CGD-O1D
36	O	316	CLA	CAD-CBD-CGD-O1D
36	P	311	CLA	CAD-CBD-CGD-O1D
36	Q	308	CLA	CAD-CBD-CGD-O1D
36	R	313	CLA	CAD-CBD-CGD-O1D
36	R	321	CLA	CHA-CBD-CGD-O1D
36	X	308	CLA	CAD-CBD-CGD-O1D
36	a	807	CLA	CHA-CBD-CGD-O1D
36	b	823	CLA	CHA-CBD-CGD-O1D
36	b	830	CLA	CHA-CBD-CGD-O1D
36	b	830	CLA	CHA-CBD-CGD-O2D
36	j	102	CLA	CHA-CBD-CGD-O1D
36	j	102	CLA	CHA-CBD-CGD-O2D
36	l	204	CLA	CHA-CBD-CGD-O1D
36	l	204	CLA	CHA-CBD-CGD-O2D
36	V	314	CLA	CAD-CBD-CGD-O1D
37	G	318	KC1	CHA-CBD-CGD-O1D
37	W	217	KC1	CAD-CBD-CGD-O1D
41	D	318	LHG	C3-O3-P-O4
41	D	319	LHG	C3-O3-P-O4
41	D	319	LHG	C3-O3-P-O6
41	F	319	LHG	C3-O3-P-O5
41	F	319	LHG	C4-O6-P-O3
41	F	319	LHG	C4-O6-P-O4
41	G	320	LHG	C3-O3-P-O5
41	G	320	LHG	C4-O6-P-O5
41	G	321	LHG	C4-O6-P-O4
41	I	316	LHG	C3-O3-P-O5
41	O	317	LHG	C3-O3-P-O4
41	O	317	LHG	C4-O6-P-O3
41	Q	315	LHG	C4-O6-P-O3
41	a	842	LHG	C4-O6-P-O3
41	a	850	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
41	f	808	LHG	C4-O6-P-O5
41	f	809	LHG	C3-O3-P-O5
41	f	809	LHG	C3-O3-P-O6
41	j	104	LHG	C4-O6-P-O5
41	l	208	LHG	C4-O6-P-O5
36	H	317	CLA	C8-C10-C11-C12
40	b	849	DGD	C1B-C2B-C3B-C4B
39	G	322	LMT	C3-C4-C5-C6
36	A	313	CLA	C2B-C3B-CAB-CBB
36	B	306	CLA	C2B-C3B-CAB-CBB
36	C	209	CLA	C2B-C3B-CAB-CBB
36	C	214	CLA	C2B-C3B-CAB-CBB
36	D	312	CLA	C2B-C3B-CAB-CBB
36	E	313	CLA	C2B-C3B-CAB-CBB
36	H	306	CLA	C2B-C3B-CAB-CBB
36	L	310	CLA	C2B-C3B-CAB-CBB
36	M	312	CLA	C2B-C3B-CAB-CBB
36	M	314	CLA	C2B-C3B-CAB-CBB
36	N	307	CLA	C2B-C3B-CAB-CBB
36	N	308	CLA	C2B-C3B-CAB-CBB
36	O	312	CLA	C2B-C3B-CAB-CBB
36	O	314	CLA	C2B-C3B-CAB-CBB
36	P	314	CLA	C2B-C3B-CAB-CBB
36	P	316	CLA	C2B-C3B-CAB-CBB
36	P	319	CLA	C2B-C3B-CAB-CBB
36	Q	310	CLA	C2B-C3B-CAB-CBB
36	Q	312	CLA	C2B-C3B-CAB-CBB
36	R	312	CLA	C2B-C3B-CAB-CBB
36	R	315	CLA	C2B-C3B-CAB-CBB
36	R	322	CLA	C2B-C3B-CAB-CBB
36	S	317	CLA	C2B-C3B-CAB-CBB
36	S	320	CLA	C2B-C3B-CAB-CBB
36	W	201	CLA	C2B-C3B-CAB-CBB
36	W	211	CLA	C2B-C3B-CAB-CBB
36	X	306	CLA	C2B-C3B-CAB-CBB
36	X	308	CLA	C2B-C3B-CAB-CBB
36	X	309	CLA	C2B-C3B-CAB-CBB
36	a	805	CLA	C2B-C3B-CAB-CBB
36	a	830	CLA	C2B-C3B-CAB-CBB
36	a	838	CLA	C2B-C3B-CAB-CBB
36	b	808	CLA	C2B-C3B-CAB-CBB
36	b	811	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	b	814	CLA	C2B-C3B-CAB-CBB
36	b	833	CLA	C2B-C3B-CAB-CBB
36	U	305	CLA	C2B-C3B-CAB-CBB
36	U	308	CLA	C2B-C3B-CAB-CBB
36	U	313	CLA	C2B-C3B-CAB-CBB
36	V	309	CLA	C2B-C3B-CAB-CBB
39	F	320	LMT	C6-C7-C8-C9
41	f	809	LHG	C34-C35-C36-C37
36	H	315	CLA	C2-C3-C5-C6
42	E	318	LMG	C29-C30-C31-C32
36	U	306	CLA	C10-C11-C12-C13
35	I	304	A86	C35-C34-O4-C38
34	F	303	DD6	C7-C6-C8-C9
34	S	307	DD6	C7-C6-C8-C9
41	I	316	LHG	C2-C3-O3-P
44	b	847	BCR	C37-C22-C23-C24
41	R	323	LHG	C32-C33-C34-C35
39	I	317	LMT	C2B-C1B-O1B-C4'
36	b	801	CLA	C15-C16-C17-C18
36	C	207	CLA	C16-C17-C18-C20
42	V	315	LMG	C10-C11-C12-C13
41	I	316	LHG	C35-C36-C37-C38
36	I	311	CLA	O1A-CGA-O2A-C1
36	E	312	CLA	C5-C6-C7-C8
36	J	312	CLA	C10-C11-C12-C13
42	V	316	LMG	C33-C34-C35-C36
35	A	302	A86	C12-C11-C13-C14
35	B	301	A86	C12-C11-C13-C14
35	C	202	A86	C12-C11-C13-C14
35	C	204	A86	C12-C11-C13-C14
35	F	305	A86	C12-C11-C13-C14
35	I	302	A86	C12-C11-C13-C14
35	I	304	A86	C12-C11-C13-C14
35	J	303	A86	C12-C11-C13-C14
35	L	306	A86	C12-C11-C13-C14
35	M	302	A86	C12-C11-C13-C14
35	O	305	A86	C12-C11-C13-C14
35	O	319	A86	C12-C11-C13-C14
35	Q	303	A86	C12-C11-C13-C14
35	R	301	A86	C12-C11-C13-C14
35	R	304	A86	C12-C11-C13-C14
35	T	302	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
35	T	307	A86	C12-C11-C13-C14
35	X	303	A86	C12-C11-C13-C14
35	X	305	A86	C12-C11-C13-C14
35	U	301	A86	C12-C11-C13-C14
35	U	302	A86	C12-C11-C13-C14
35	V	303	A86	C12-C11-C13-C14
35	V	304	A86	C12-C11-C13-C14
41	F	318	LHG	C4-O6-P-O5
41	E	322	LHG	C28-C29-C30-C31
41	R	323	LHG	C33-C34-C35-C36
42	D	321	LMG	C12-C13-C14-C15
42	J	318	LMG	C37-C38-C39-C40
42	m	102	LMG	C13-C14-C15-C16
36	T	311	CLA	C13-C15-C16-C17
36	a	836	CLA	C15-C16-C17-C18
36	A	306	CLA	C12-C13-C15-C16
36	l	204	CLA	O2A-C1-C2-C3
37	G	308	KC1	C4C-C3C-CAC-CBC
42	D	320	LMG	C9-C8-O7-C10
42	I	315	LMG	C9-C8-O7-C10
36	a	808	CLA	C15-C16-C17-C18
39	P	321	LMT	C4'-C5'-C6'-O6'
39	E	321	LMT	O5'-C5'-C6'-O6'
42	G	324	LMG	O6-C5-C6-O5
42	I	315	LMG	C37-C38-C39-C40
34	S	306	DD6	C11-C10-C9-C8
39	P	320	LMT	C4'-C5'-C6'-O6'
41	F	318	LHG	O6-C4-C5-C6
41	a	850	LHG	O6-C4-C5-C6
38	b	804	SQD	C26-C27-C28-C29
41	G	301	LHG	C24-C25-C26-C27
42	D	320	LMG	C30-C31-C32-C33
42	J	318	LMG	C14-C15-C16-C17
36	K	307	CLA	CBA-CGA-O2A-C1
36	a	830	CLA	CBA-CGA-O2A-C1
36	A	311	CLA	C11-C10-C8-C9
36	B	305	CLA	C11-C12-C13-C14
36	D	312	CLA	C11-C10-C8-C9
36	D	312	CLA	C14-C13-C15-C16
36	E	316	CLA	C14-C13-C15-C16
36	F	309	CLA	C11-C12-C13-C14
36	I	305	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	K	307	CLA	C11-C12-C13-C14
36	L	314	CLA	C6-C7-C8-C9
36	O	308	CLA	C6-C7-C8-C9
36	O	309	CLA	C14-C13-C15-C16
36	P	311	CLA	C14-C13-C15-C16
36	Q	308	CLA	C14-C13-C15-C16
36	a	808	CLA	C14-C13-C15-C16
36	a	810	CLA	C11-C12-C13-C14
36	a	816	CLA	C11-C12-C13-C14
36	a	832	CLA	C6-C7-C8-C9
36	b	820	CLA	C11-C10-C8-C9
36	D	317	CLA	O1D-CGD-O2D-CED
42	h	206	LMG	C29-C30-C31-C32
36	C	209	CLA	C11-C12-C13-C15
36	E	311	CLA	C11-C10-C8-C7
36	H	308	CLA	C11-C12-C13-C15
36	L	320	CLA	C12-C13-C15-C16
36	O	309	CLA	C12-C13-C15-C16
36	P	311	CLA	C12-C13-C15-C16
36	Q	308	CLA	C12-C13-C15-C16
36	R	312	CLA	C6-C7-C8-C10
36	S	309	CLA	C11-C12-C13-C15
36	X	306	CLA	C11-C12-C13-C15
36	a	806	CLA	C11-C10-C8-C7
36	a	832	CLA	C11-C12-C13-C15
36	b	816	CLA	C11-C10-C8-C7
36	l	201	CLA	C6-C7-C8-C10
41	b	850	LHG	C31-C32-C33-C34
36	a	837	CLA	C13-C15-C16-C17
44	i	103	BCR	C20-C21-C22-C23
41	l	208	LHG	C7-C8-C9-C10
39	B	312	LMT	C5-C6-C7-C8
36	K	307	CLA	O1A-CGA-O2A-C1
36	G	311	CLA	C2C-C3C-CAC-CBC
39	I	318	LMT	C3'-C4'-O1B-C1B
41	a	850	LHG	C1-C2-C3-O3
41	O	317	LHG	O6-C4-C5-O7
39	L	303	LMT	O5'-C1'-O1'-C1
36	a	818	CLA	C16-C17-C18-C20
36	M	307	CLA	C5-C6-C7-C8
36	M	312	CLA	C2C-C3C-CAC-CBC
38	b	804	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
36	D	310	CLA	C16-C17-C18-C19
36	G	310	CLA	C16-C17-C18-C19
36	G	310	CLA	C16-C17-C18-C20
36	L	314	CLA	C16-C17-C18-C20
36	a	830	CLA	O1A-CGA-O2A-C1
38	A	315	SQD	O49-C7-O47-C45
36	a	817	CLA	C13-C15-C16-C17
39	a	854	LMT	C2-C3-C4-C5
41	O	318	LHG	C11-C12-C13-C14
41	G	320	LHG	O7-C5-C6-O8
42	D	320	LMG	O7-C8-C9-O8
41	D	318	LHG	O2-C2-C3-O3
39	I	317	LMT	C4-C5-C6-C7
41	l	208	LHG	C24-C25-C26-C27
41	O	317	LHG	C7-C8-C9-C10
34	D	304	DD6	C11-C10-C9-C8
35	E	307	A86	C11-C10-C9-C8
36	V	314	CLA	C2C-C3C-CAC-CBC
36	a	816	CLA	C16-C17-C18-C20
36	W	201	CLA	O1D-CGD-O2D-CED
36	a	817	CLA	CAA-CBA-CGA-O2A
36	G	311	CLA	C2A-CAA-CBA-CGA
36	I	308	CLA	C2A-CAA-CBA-CGA
36	K	308	CLA	C2A-CAA-CBA-CGA
36	a	825	CLA	O1D-CGD-O2D-CED
36	D	307	CLA	C4C-C3C-CAC-CBC
36	M	309	CLA	C16-C17-C18-C20
42	L	321	LMG	O7-C10-C11-C12
41	j	104	LHG	C15-C16-C17-C18
36	C	206	CLA	C8-C10-C11-C12
42	G	325	LMG	C24-C25-C26-C27
36	W	211	CLA	C13-C15-C16-C17
34	D	305	DD6	C7-C6-C8-C9
35	F	302	A86	C-C1-C24-C25
34	K	304	DD6	C5-C6-C8-C9
36	C	207	CLA	O1D-CGD-O2D-CED
38	b	804	SQD	O48-C23-C24-C25
36	T	311	CLA	C4C-C3C-CAC-CBC
36	C	208	CLA	O1A-CGA-O2A-C1
42	h	206	LMG	C20-C21-C22-C23
36	B	311	CLA	C2A-CAA-CBA-CGA
36	K	313	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	T	311	CLA	C2A-CAA-CBA-CGA
36	a	811	CLA	C2A-CAA-CBA-CGA
36	a	816	CLA	C2A-CAA-CBA-CGA
36	b	807	CLA	C2A-CAA-CBA-CGA
34	D	301	DD6	C24-C25-C26-C27
34	R	307	DD6	C3-C4-C5-C6
35	B	301	A86	C11-C10-C9-C8
36	O	316	CLA	C16-C17-C18-C20
36	a	806	CLA	CBD-CGD-O2D-CED
42	J	319	LMG	O6-C1-O1-C7
39	a	853	LMT	C5-C6-C7-C8
36	b	811	CLA	C4-C3-C5-C6
36	b	815	CLA	C4-C3-C5-C6
36	S	319	CLA	C2-C3-C5-C6
36	a	827	CLA	C2-C3-C5-C6
36	b	802	CLA	C2-C3-C5-C6
36	a	825	CLA	C15-C16-C17-C18
36	b	816	CLA	C8-C10-C11-C12
41	l	208	LHG	C34-C35-C36-C37
36	S	321	CLA	O1A-CGA-O2A-C1
35	R	304	A86	C33-C34-O4-C38
35	S	308	A86	C33-C34-O4-C38
42	E	318	LMG	C30-C31-C32-C33
35	L	307	A86	C13-C14-C15-C16
35	O	305	A86	C13-C14-C15-C16
39	B	312	LMT	C2-C1-O1'-C1'
39	K	317	LMT	C2-C1-O1'-C1'
39	a	853	LMT	C2-C1-O1'-C1'
41	F	319	LHG	O1-C1-C2-O2
41	a	842	LHG	C1-C2-C3-O3
36	E	311	CLA	C16-C17-C18-C20
36	a	818	CLA	C16-C17-C18-C19
36	A	310	CLA	C14-C13-C15-C16
36	I	311	CLA	C6-C7-C8-C9
36	a	838	CLA	C14-C13-C15-C16
40	b	849	DGD	C9B-CAB-CBB-CCB
36	b	828	CLA	CBA-CGA-O2A-C1
36	V	308	CLA	CBA-CGA-O2A-C1
41	G	320	LHG	C24-C23-O8-C6
39	P	320	LMT	C1-C2-C3-C4
36	F	312	CLA	C4B-C3B-CAB-CBB
36	J	309	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	O	309	CLA	C4B-C3B-CAB-CBB
36	P	311	CLA	C4B-C3B-CAB-CBB
36	Q	308	CLA	C4B-C3B-CAB-CBB
36	S	310	CLA	C4B-C3B-CAB-CBB
36	j	101	CLA	C4B-C3B-CAB-CBB
36	U	310	CLA	C4B-C3B-CAB-CBB
39	h	205	LMT	C5-C6-C7-C8
41	G	301	LHG	C28-C29-C30-C31
36	U	311	CLA	C13-C15-C16-C17
36	A	314	CLA	C16-C17-C18-C19
36	P	310	CLA	C16-C17-C18-C20
42	G	324	LMG	C35-C36-C37-C38
36	a	848	CLA	C5-C6-C7-C8
36	V	310	CLA	C10-C11-C12-C13
36	N	307	CLA	C2A-CAA-CBA-CGA
36	I	306	CLA	C4-C3-C5-C6
36	N	316	CLA	C4-C3-C5-C6
36	b	828	CLA	C2-C3-C5-C6
36	Q	314	CLA	C3-C5-C6-C7
42	m	102	LMG	C28-C29-C30-C31
36	K	316	CLA	O1A-CGA-O2A-C1
36	D	307	CLA	C2C-C3C-CAC-CBC
37	P	317	KC1	C4B-C3B-CAB-CBB
37	T	310	KC1	C4B-C3B-CAB-CBB
39	G	322	LMT	C3'-C4'-O1B-C1B
39	I	318	LMT	C11-C10-C9-C8
36	I	311	CLA	O1D-CGD-O2D-CED
39	I	317	LMT	C3-C4-C5-C6
36	A	308	CLA	C12-C13-C15-C16
36	C	207	CLA	C12-C13-C15-C16
36	C	212	CLA	C11-C10-C8-C7
36	G	309	CLA	C12-C13-C15-C16
36	K	307	CLA	C11-C10-C8-C7
36	T	314	CLA	C6-C7-C8-C10
36	a	820	CLA	C11-C10-C8-C7
36	f	802	CLA	C6-C7-C8-C10
36	H	309	CLA	O1A-CGA-O2A-C1
36	D	317	CLA	CBD-CGD-O2D-CED
41	f	809	LHG	C28-C29-C30-C31
36	V	314	CLA	C4C-C3C-CAC-CBC
39	I	318	LMT	C7-C8-C9-C10
41	G	320	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
39	U	314	LMT	C5'-C4'-O1B-C1B
39	I	318	LMT	C6-C7-C8-C9
36	G	311	CLA	C10-C11-C12-C13
42	J	319	LMG	O7-C8-C9-O8
36	A	306	CLA	C3A-C2A-CAA-CBA
36	N	317	CLA	C4-C3-C5-C6
36	P	301	CLA	C3A-C2A-CAA-CBA
36	T	314	CLA	C3A-C2A-CAA-CBA
36	W	212	CLA	C3A-C2A-CAA-CBA
36	a	827	CLA	C3A-C2A-CAA-CBA
36	b	806	CLA	C4-C3-C5-C6
36	l	202	CLA	C3A-C2A-CAA-CBA
35	T	307	A86	C33-C34-O4-C38
42	h	206	LMG	C15-C16-C17-C18
36	f	803	CLA	C2-C3-C5-C6
41	a	842	LHG	C10-C11-C12-C13
35	C	203	A86	C25-C26-C27-C28
35	G	306	A86	C-C1-C2-C3
35	G	306	A86	C4-C5-C6-C7
35	U	301	A86	C4-C5-C6-C7
35	U	304	A86	C25-C26-C27-C28
44	b	845	BCR	C20-C21-C22-C37
36	i	102	CLA	O1A-CGA-O2A-C1
36	N	308	CLA	C13-C15-C16-C17
36	L	310	CLA	C6-C7-C8-C9
42	J	318	LMG	C18-C19-C20-C21
35	X	304	A86	C35-C34-O4-C38
36	A	306	CLA	C14-C13-C15-C16
36	V	314	CLA	C8-C10-C11-C12
42	h	206	LMG	C31-C32-C33-C34
40	b	849	DGD	C6B-C7B-C8B-C9B
34	A	301	DD6	C11-C10-C9-C8
34	S	306	DD6	C24-C25-C26-C27
35	E	305	A86	C24-C25-C26-C27
35	J	305	A86	C24-C25-C26-C27
36	B	308	CLA	C2-C1-O2A-CGA
36	G	319	CLA	C2-C1-O2A-CGA
36	T	314	CLA	C2-C1-O2A-CGA
36	b	802	CLA	C2-C1-O2A-CGA
36	b	816	CLA	C2-C1-O2A-CGA
41	O	317	LHG	C11-C12-C13-C14
36	V	306	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	R	321	CLA	C10-C11-C12-C13
36	U	310	CLA	C10-C11-C12-C13
44	m	101	BCR	C37-C22-C23-C24
40	L	302	DGD	C3A-C4A-C5A-C6A
39	U	314	LMT	C3'-C4'-O1B-C1B
36	B	308	CLA	C15-C16-C17-C18
36	K	310	CLA	C13-C15-C16-C17
41	E	322	LHG	C27-C28-C29-C30
36	W	207	CLA	O1D-CGD-O2D-CED
34	S	307	DD6	C5-C6-C8-C9
36	I	310	CLA	C4-C3-C5-C6
36	H	312	CLA	CAA-CBA-CGA-O2A
36	F	313	CLA	C2A-CAA-CBA-CGA
36	U	308	CLA	C2A-CAA-CBA-CGA
36	U	311	CLA	C2A-CAA-CBA-CGA
39	h	205	LMT	C5'-C4'-O1B-C1B
36	D	306	CLA	CAA-CBA-CGA-O1A
41	l	208	LHG	C12-C13-C14-C15
35	A	302	A86	C12-C11-C13-O
35	T	305	A86	C12-C11-C13-O
35	X	304	A86	C12-C11-C13-O
35	V	302	A86	C12-C11-C13-O
42	I	315	LMG	C29-C30-C31-C32
39	B	313	LMT	C1-C2-C3-C4
36	B	311	CLA	C5-C6-C7-C8
35	J	302	A86	C33-C34-O4-C38
36	V	308	CLA	O1A-CGA-O2A-C1
36	A	308	CLA	C14-C13-C15-C16
36	F	314	CLA	C11-C10-C8-C9
36	H	309	CLA	C11-C12-C13-C14
36	I	310	CLA	C14-C13-C15-C16
36	K	307	CLA	C11-C10-C8-C9
36	K	310	CLA	C14-C13-C15-C16
36	N	308	CLA	C6-C7-C8-C9
36	a	801	CLA	C11-C12-C13-C14
36	a	805	CLA	C11-C10-C8-C9
36	b	811	CLA	C14-C13-C15-C16
36	b	825	CLA	C6-C7-C8-C9
36	b	825	CLA	C14-C13-C15-C16
36	f	802	CLA	C6-C7-C8-C9
36	U	306	CLA	C11-C10-C8-C9
36	V	314	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
39	F	320	LMT	C3'-C4'-O1B-C1B
36	a	848	CLA	C16-C17-C18-C19
36	L	311	CLA	C8-C10-C11-C12
36	L	313	CLA	C15-C16-C17-C18
39	F	320	LMT	C5-C6-C7-C8
41	l	208	LHG	C13-C14-C15-C16
36	A	307	CLA	C8-C10-C11-C12
39	a	854	LMT	O5B-C1B-O1B-C4'
39	I	318	LMT	C5'-C4'-O1B-C1B
36	a	808	CLA	C3-C5-C6-C7
35	X	303	A86	C35-C34-O4-C38
35	V	303	A86	C35-C34-O4-C38
41	F	319	LHG	C26-C27-C28-C29
42	I	315	LMG	C39-C40-C41-C42
36	I	305	CLA	C4-C3-C5-C6
36	K	316	CLA	C4-C3-C5-C6
36	W	209	CLA	C4-C3-C5-C6
39	E	320	LMT	O5B-C5B-C6B-O6B
36	V	314	CLA	CAA-CBA-CGA-O2A
36	N	317	CLA	C2-C3-C5-C6
36	W	218	CLA	C2A-CAA-CBA-CGA
39	h	205	LMT	C2-C3-C4-C5
42	G	324	LMG	C34-C35-C36-C37
42	J	319	LMG	C2-C1-O1-C7
36	C	206	CLA	C10-C11-C12-C13
36	D	306	CLA	CAA-CBA-CGA-O2A
36	F	309	CLA	C2A-CAA-CBA-CGA
36	L	311	CLA	C2A-CAA-CBA-CGA
36	Q	306	CLA	C2A-CAA-CBA-CGA
36	R	313	CLA	C2A-CAA-CBA-CGA
39	F	320	LMT	C1-C2-C3-C4
36	S	313	CLA	C2C-C3C-CAC-CBC
41	i	104	LHG	C10-C11-C12-C13
36	P	301	CLA	CAA-CBA-CGA-O2A
35	A	302	A86	C10-C11-C13-O
35	C	203	A86	C25-C26-C27-C29
35	G	306	A86	C24-C1-C2-C3
35	G	306	A86	C4-C5-C6-C8
35	U	301	A86	C10-C11-C13-O
35	U	301	A86	C4-C5-C6-C8
35	U	304	A86	C25-C26-C27-C29
36	I	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	M	312	CLA	C1A-C2A-CAA-CBA
36	W	211	CLA	C1A-C2A-CAA-CBA
36	a	812	CLA	C1A-C2A-CAA-CBA
36	a	833	CLA	C1A-C2A-CAA-CBA
36	a	835	CLA	C1A-C2A-CAA-CBA
36	b	814	CLA	C1A-C2A-CAA-CBA
36	b	830	CLA	C1A-C2A-CAA-CBA
36	j	102	CLA	C1A-C2A-CAA-CBA
36	K	316	CLA	CBA-CGA-O2A-C1
40	b	849	DGD	C7B-C8B-C9B-CAB
41	b	850	LHG	C16-C17-C18-C19
39	E	320	LMT	C9-C10-C11-C12
36	A	311	CLA	C2B-C3B-CAB-CBB
36	D	307	CLA	C2B-C3B-CAB-CBB
36	F	311	CLA	C2B-C3B-CAB-CBB
36	F	312	CLA	C2B-C3B-CAB-CBB
36	F	313	CLA	C2B-C3B-CAB-CBB
36	F	316	CLA	C2B-C3B-CAB-CBB
36	G	312	CLA	C2B-C3B-CAB-CBB
36	G	313	CLA	C2B-C3B-CAB-CBB
36	H	309	CLA	C2B-C3B-CAB-CBB
36	H	318	CLA	C2B-C3B-CAB-CBB
36	J	308	CLA	C2B-C3B-CAB-CBB
36	J	309	CLA	C2B-C3B-CAB-CBB
36	K	310	CLA	C2B-C3B-CAB-CBB
36	L	316	CLA	C2B-C3B-CAB-CBB
36	N	312	CLA	C2B-C3B-CAB-CBB
36	O	309	CLA	C2B-C3B-CAB-CBB
36	P	311	CLA	C2B-C3B-CAB-CBB
36	Q	308	CLA	C2B-C3B-CAB-CBB
36	S	310	CLA	C2B-C3B-CAB-CBB
36	T	311	CLA	C2B-C3B-CAB-CBB
36	W	209	CLA	C2B-C3B-CAB-CBB
36	a	809	CLA	C2B-C3B-CAB-CBB
36	a	819	CLA	C2B-C3B-CAB-CBB
36	b	820	CLA	C2B-C3B-CAB-CBB
36	j	101	CLA	C2B-C3B-CAB-CBB
36	V	313	CLA	C2B-C3B-CAB-CBB
44	a	844	BCR	C1-C6-C7-C8
44	a	844	BCR	C23-C24-C25-C30
44	a	846	BCR	C5-C6-C7-C8
44	a	847	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
44	b	843	BCR	C5-C6-C7-C8
44	b	843	BCR	C23-C24-C25-C30
44	b	844	BCR	C1-C6-C7-C8
44	b	844	BCR	C5-C6-C7-C8
44	b	846	BCR	C23-C24-C25-C26
44	b	847	BCR	C1-C6-C7-C8
44	b	847	BCR	C5-C6-C7-C8
44	f	806	BCR	C5-C6-C7-C8
44	i	103	BCR	C5-C6-C7-C8
44	l	203	BCR	C5-C6-C7-C8
44	l	203	BCR	C23-C24-C25-C26
44	m	101	BCR	C23-C24-C25-C26
44	h	201	BCR	C23-C24-C25-C26
41	F	318	LHG	C24-C25-C26-C27
39	f	807	LMT	C6-C7-C8-C9
39	h	205	LMT	C3'-C4'-O1B-C1B
36	D	308	CLA	C4C-C3C-CAC-CBC
36	E	312	CLA	C4-C3-C5-C6
36	H	317	CLA	C4-C3-C5-C6
36	O	309	CLA	C4-C3-C5-C6
36	P	311	CLA	C4-C3-C5-C6
36	Q	308	CLA	C4-C3-C5-C6
36	a	805	CLA	C4-C3-C5-C6
41	R	323	LHG	O6-C4-C5-C6
36	R	322	CLA	C2-C3-C5-C6
36	b	806	CLA	C2-C3-C5-C6
36	b	811	CLA	C2-C3-C5-C6
36	b	815	CLA	C2-C3-C5-C6
42	m	102	LMG	C15-C16-C17-C18
36	A	310	CLA	C12-C13-C15-C16
36	C	211	CLA	C6-C7-C8-C10
36	D	312	CLA	C11-C10-C8-C7
36	D	312	CLA	C12-C13-C15-C16
36	F	312	CLA	C11-C10-C8-C7
36	F	317	CLA	C6-C7-C8-C10
36	Q	310	CLA	C12-C13-C15-C16
36	a	801	CLA	C11-C12-C13-C15
36	a	807	CLA	C12-C13-C15-C16
36	a	810	CLA	C6-C7-C8-C10
36	a	829	CLA	C11-C10-C8-C7
36	a	838	CLA	C12-C13-C15-C16
36	b	821	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
36	h	203	CLA	C11-C10-C8-C7
36	U	310	CLA	C12-C13-C15-C16
39	E	320	LMT	C11-C10-C9-C8
36	E	310	CLA	C16-C17-C18-C20
36	F	314	CLA	C16-C17-C18-C20
36	E	310	CLA	C2A-CAA-CBA-CGA
36	L	309	CLA	C2A-CAA-CBA-CGA
36	O	307	CLA	C2A-CAA-CBA-CGA
36	P	309	CLA	C2A-CAA-CBA-CGA
36	W	209	CLA	C2A-CAA-CBA-CGA
36	a	802	CLA	C2A-CAA-CBA-CGA
36	b	810	CLA	C2A-CAA-CBA-CGA
42	E	319	LMG	C15-C16-C17-C18
36	f	804	CLA	C5-C6-C7-C8
41	j	104	LHG	O7-C5-C6-O8
42	V	316	LMG	O7-C8-C9-O8
42	j	105	LMG	C38-C39-C40-C41
41	l	208	LHG	C29-C30-C31-C32
39	E	320	LMT	C4-C5-C6-C7
36	A	310	CLA	C16-C17-C18-C20
41	a	842	LHG	C26-C27-C28-C29
41	G	321	LHG	C5-C6-O8-C23
36	D	307	CLA	C12-C13-C15-C16
36	F	310	CLA	C11-C10-C8-C7
36	F	317	CLA	C11-C10-C8-C7
36	G	315	CLA	C11-C10-C8-C7
36	b	811	CLA	C10-C11-C12-C13
36	V	308	CLA	C5-C6-C7-C8
36	H	308	CLA	C2-C3-C5-C6
36	I	306	CLA	C2-C3-C5-C6
36	K	316	CLA	C2-C3-C5-C6
36	N	316	CLA	C2-C3-C5-C6
36	Q	314	CLA	C2-C3-C5-C6
36	W	209	CLA	C2-C3-C5-C6
36	H	315	CLA	C8-C10-C11-C12
36	j	101	CLA	C10-C11-C12-C13
34	W	205	DD6	C2-C1-C24-C25
39	b	848	LMT	C11-C10-C9-C8
36	A	314	CLA	C14-C13-C15-C16
36	C	207	CLA	C14-C13-C15-C16
36	F	312	CLA	C11-C12-C13-C14
36	J	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	M	309	CLA	C11-C12-C13-C14
36	a	810	CLA	C11-C10-C8-C9
36	b	811	CLA	C11-C10-C8-C9
42	a	852	LMG	C11-C12-C13-C14
34	J	304	DD6	C1-C2-C3-C4
41	j	104	LHG	C14-C15-C16-C17
36	l	205	CLA	C10-C11-C12-C13
36	M	309	CLA	C16-C17-C18-C19
36	D	316	CLA	C4C-C3C-CAC-CBC
41	Q	315	LHG	C31-C32-C33-C34
41	a	842	LHG	C11-C12-C13-C14
41	O	317	LHG	C14-C15-C16-C17
36	b	815	CLA	C4C-C3C-CAC-CBC
36	B	305	CLA	C4-C3-C5-C6
36	L	311	CLA	C4-C3-C5-C6
36	b	801	CLA	C4-C3-C5-C6
36	a	838	CLA	C8-C10-C11-C12
36	O	309	CLA	C10-C11-C12-C13
36	P	311	CLA	C10-C11-C12-C13
36	Q	308	CLA	C10-C11-C12-C13
36	a	827	CLA	C5-C6-C7-C8
36	l	205	CLA	C5-C6-C7-C8
41	I	316	LHG	C17-C18-C19-C20
36	a	826	CLA	C13-C15-C16-C17
42	E	318	LMG	C16-C17-C18-C19
40	C	215	DGD	O1G-C1G-C2G-C3G
40	L	302	DGD	C1G-C2G-C3G-O3G
41	D	319	LHG	C4-C5-C6-O8
41	G	321	LHG	C4-C5-C6-O8
42	D	320	LMG	O1-C7-C8-C9
42	I	315	LMG	O1-C7-C8-C9
42	J	319	LMG	C12-C13-C14-C15
39	K	318	LMT	C9-C10-C11-C12
36	Q	314	CLA	C2A-CAA-CBA-CGA
36	b	831	CLA	C2A-CAA-CBA-CGA
36	V	308	CLA	C2A-CAA-CBA-CGA
42	G	325	LMG	C30-C31-C32-C33
36	E	311	CLA	C16-C17-C18-C19
37	T	310	KC1	O1D-CGD-O2D-CED
36	C	206	CLA	C5-C6-C7-C8
36	K	313	CLA	C15-C16-C17-C18
34	D	304	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
41	E	322	LHG	O1-C1-C2-O2
41	f	809	LHG	O6-C4-C5-O7
36	P	301	CLA	C4-C3-C5-C6
35	J	301	A86	C3-C4-C5-C6
36	H	318	CLA	CAA-CBA-CGA-O2A
36	i	102	CLA	C16-C17-C18-C20
36	f	803	CLA	C15-C16-C17-C18
37	T	310	KC1	CBD-CGD-O2D-CED
36	C	205	CLA	C4B-C3B-CAB-CBB
36	F	313	CLA	C4B-C3B-CAB-CBB
36	G	313	CLA	C4B-C3B-CAB-CBB
36	J	308	CLA	C4B-C3B-CAB-CBB
36	K	310	CLA	C4B-C3B-CAB-CBB
36	N	312	CLA	C4B-C3B-CAB-CBB
36	R	313	CLA	C4B-C3B-CAB-CBB
36	T	309	CLA	C4B-C3B-CAB-CBB
36	W	209	CLA	C4B-C3B-CAB-CBB
36	a	830	CLA	C4B-C3B-CAB-CBB
36	N	317	CLA	O1A-CGA-O2A-C1
41	a	842	LHG	O10-C23-O8-C6
36	a	806	CLA	O1D-CGD-O2D-CED
39	G	322	LMT	C11-C10-C9-C8
41	O	318	LHG	C35-C36-C37-C38
36	B	309	CLA	CAA-CBA-CGA-O2A
36	a	806	CLA	C10-C11-C12-C13
39	a	854	LMT	C2B-C1B-O1B-C4'
36	b	830	CLA	C16-C17-C18-C20
42	I	315	LMG	C4-C5-C6-O5
36	J	313	CLA	O1D-CGD-O2D-CED
36	H	309	CLA	C2A-CAA-CBA-CGA
36	W	208	CLA	CAA-CBA-CGA-O2A
36	b	807	CLA	CAA-CBA-CGA-O1A
36	b	807	CLA	CAA-CBA-CGA-O2A
42	V	316	LMG	C29-C30-C31-C32
41	F	319	LHG	O6-C4-C5-C6
36	j	102	CLA	C16-C17-C18-C19
41	a	850	LHG	O7-C5-C6-O8
36	R	319	CLA	CAA-CBA-CGA-O2A
36	R	320	CLA	CAA-CBA-CGA-O2A
41	F	318	LHG	C15-C16-C17-C18
36	L	311	CLA	C2-C3-C5-C6
36	b	801	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	L	309	CLA	C3-C5-C6-C7
41	G	320	LHG	C19-C20-C21-C22
39	K	317	LMT	O5'-C1'-O1'-C1
36	R	314	CLA	O1D-CGD-O2D-CED
36	L	311	CLA	C5-C6-C7-C8
36	P	301	CLA	C13-C15-C16-C17
36	a	826	CLA	C5-C6-C7-C8
41	G	301	LHG	C2-C3-O3-P
41	D	318	LHG	C24-C25-C26-C27
36	H	309	CLA	C11-C12-C13-C15
36	H	317	CLA	C6-C7-C8-C10
36	I	310	CLA	C12-C13-C15-C16
36	K	313	CLA	C11-C12-C13-C15
36	S	312	CLA	C6-C7-C8-C10
36	b	811	CLA	C11-C10-C8-C7
36	b	825	CLA	C12-C13-C15-C16
36	U	305	CLA	C6-C7-C8-C10
39	G	322	LMT	C4-C5-C6-C7
34	E	301	DD6	C24-C25-C26-C27
39	U	314	LMT	C4B-C5B-C6B-O6B
44	b	843	BCR	C21-C22-C23-C24
36	P	308	CLA	O1D-CGD-O2D-CED
36	G	311	CLA	C11-C12-C13-C14
36	I	308	CLA	C14-C13-C15-C16
36	J	307	CLA	C6-C7-C8-C9
36	J	310	CLA	C11-C12-C13-C14
36	L	308	CLA	C11-C12-C13-C14
36	M	311	CLA	C11-C10-C8-C9
36	O	308	CLA	C11-C10-C8-C9
36	Q	314	CLA	C11-C12-C13-C14
36	S	312	CLA	C11-C10-C8-C9
36	a	804	CLA	C6-C7-C8-C9
36	a	812	CLA	C6-C7-C8-C9
36	a	836	CLA	C6-C7-C8-C9
42	L	321	LMG	C29-C30-C31-C32
38	A	315	SQD	C5-C6-S-O8
42	E	318	LMG	C8-C7-O1-C1
36	E	312	CLA	C8-C10-C11-C12
36	D	309	CLA	C2A-CAA-CBA-CGA
36	J	310	CLA	C2A-CAA-CBA-CGA
36	K	309	CLA	C2A-CAA-CBA-CGA
36	S	313	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	D	316	CLA	C2-C1-O2A-CGA
36	E	308	CLA	C2-C1-O2A-CGA
36	H	306	CLA	C2-C1-O2A-CGA
36	Q	314	CLA	C2-C1-O2A-CGA
36	a	830	CLA	C2-C1-O2A-CGA
36	a	838	CLA	C2-C1-O2A-CGA
36	A	308	CLA	C3-C5-C6-C7
36	D	307	CLA	C14-C13-C15-C16
36	F	314	CLA	C16-C17-C18-C19
39	b	851	LMT	C9-C10-C11-C12
36	M	306	CLA	C5-C6-C7-C8
36	D	307	CLA	C3A-C2A-CAA-CBA
36	G	309	CLA	C4-C3-C5-C6
36	G	315	CLA	C3A-C2A-CAA-CBA
36	L	314	CLA	C3A-C2A-CAA-CBA
36	O	309	CLA	C3A-C2A-CAA-CBA
36	P	311	CLA	C3A-C2A-CAA-CBA
36	P	318	CLA	C3A-C2A-CAA-CBA
36	Q	308	CLA	C3A-C2A-CAA-CBA
36	S	321	CLA	C3A-C2A-CAA-CBA
36	a	812	CLA	C3A-C2A-CAA-CBA
36	b	824	CLA	C3A-C2A-CAA-CBA
37	M	318	KC1	C2C-C3C-CAC-CBC
36	a	810	CLA	C2-C3-C5-C6
36	a	816	CLA	C15-C16-C17-C18
39	F	320	LMT	C5'-C4'-O1B-C1B
36	G	319	CLA	C4C-C3C-CAC-CBC
36	E	315	CLA	C16-C17-C18-C19
36	a	801	CLA	C16-C17-C18-C20
36	Q	305	CLA	O1D-CGD-O2D-CED
36	F	311	CLA	CBA-CGA-O2A-C1
38	b	804	SQD	C45-C46-O48-C23
36	a	816	CLA	C4C-C3C-CAC-CBC
41	G	321	LHG	C11-C12-C13-C14
36	b	808	CLA	CAA-CBA-CGA-O2A
36	W	208	CLA	CAA-CBA-CGA-O1A
39	K	317	LMT	C4'-C5'-C6'-O6'
36	O	306	CLA	O1D-CGD-O2D-CED
36	R	319	CLA	CAA-CBA-CGA-O1A
36	I	306	CLA	CBA-CGA-O2A-C1
36	a	817	CLA	CBA-CGA-O2A-C1
36	i	102	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
43	b	842	PQN	C18-C20-C21-C22
42	J	318	LMG	C17-C18-C19-C20
34	D	301	DD6	C13-C14-C15-O1
34	D	304	DD6	C13-C14-C15-O1
34	E	301	DD6	C13-C14-C15-O1
34	E	303	DD6	C13-C14-C15-O1
34	E	306	DD6	C13-C14-C15-O1
34	W	205	DD6	C13-C14-C15-O1
44	b	845	BCR	C20-C21-C22-C23
41	F	319	LHG	C2-C3-O3-P
41	O	318	LHG	C11-C10-C9-C8
41	f	809	LHG	C4-C5-C6-O8
42	E	319	LMG	O1-C7-C8-C9
42	G	324	LMG	O1-C7-C8-C9
36	I	306	CLA	O1A-CGA-O2A-C1
41	a	850	LHG	O1-C1-C2-O2
42	J	319	LMG	C24-C25-C26-C27
36	I	311	CLA	C4-C3-C5-C6
36	a	806	CLA	C4-C3-C5-C6
41	i	104	LHG	C16-C17-C18-C19
41	a	850	LHG	O7-C7-C8-C9
34	j	103	DD6	C3-C4-C5-C6
44	h	201	BCR	C19-C20-C21-C22
39	K	318	LMT	C4-C5-C6-C7
36	b	838	CLA	C2-C1-O2A-CGA
35	B	303	A86	C28-C27-C29-C30
35	M	304	A86	C28-C27-C29-C30
35	N	320	A86	C28-C27-C29-C30
35	Q	304	A86	C28-C27-C29-C30
41	G	321	LHG	C32-C33-C34-C35
36	C	207	CLA	C8-C10-C11-C12
36	R	312	CLA	C15-C16-C17-C18
36	a	823	CLA	CBD-CGD-O2D-CED
42	a	852	LMG	C16-C17-C18-C19
36	G	309	CLA	C6-C7-C8-C9
36	S	320	CLA	C6-C7-C8-C9
36	a	825	CLA	C6-C7-C8-C9
36	b	808	CLA	C11-C12-C13-C14
36	b	815	CLA	C6-C7-C8-C9
36	U	308	CLA	C6-C7-C8-C9
41	E	322	LHG	O7-C7-C8-C9
42	V	315	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
39	E	320	LMT	C2B-C1B-O1B-C4'
36	b	828	CLA	O1A-CGA-O2A-C1
35	A	302	A86	C33-C34-O4-C38
36	R	320	CLA	CAA-CBA-CGA-O1A
36	D	312	CLA	C15-C16-C17-C18
36	L	313	CLA	C13-C15-C16-C17
35	B	301	A86	C13-C14-C15-O1
35	G	305	A86	C13-C14-C15-O1
35	S	305	A86	C13-C14-C15-O1
35	S	308	A86	C13-C14-C15-O1
35	h	204	A86	C13-C14-C15-O1
36	I	309	CLA	CAA-CBA-CGA-O2A
36	a	802	CLA	C16-C17-C18-C20
36	E	312	CLA	C2-C3-C5-C6
36	a	805	CLA	C2-C3-C5-C6
36	A	314	CLA	C11-C10-C8-C7
36	C	206	CLA	C6-C7-C8-C10
36	C	207	CLA	C11-C10-C8-C7
36	D	307	CLA	C11-C10-C8-C7
36	D	308	CLA	C6-C7-C8-C10
36	E	316	CLA	C11-C10-C8-C7
36	G	311	CLA	C11-C12-C13-C15
36	H	306	CLA	C6-C7-C8-C10
36	H	317	CLA	C11-C10-C8-C7
36	I	308	CLA	C12-C13-C15-C16
36	J	307	CLA	C11-C12-C13-C15
36	J	313	CLA	C12-C13-C15-C16
36	L	311	CLA	C11-C12-C13-C15
36	M	309	CLA	C11-C12-C13-C15
36	N	316	CLA	C11-C10-C8-C7
36	O	316	CLA	C6-C7-C8-C10
36	P	301	CLA	C11-C12-C13-C15
36	P	319	CLA	C6-C7-C8-C10
36	S	312	CLA	C11-C10-C8-C7
36	W	207	CLA	C6-C7-C8-C10
36	a	805	CLA	C11-C10-C8-C7
36	a	805	CLA	C12-C13-C15-C16
36	a	810	CLA	C11-C10-C8-C7
36	a	826	CLA	C12-C13-C15-C16
36	a	836	CLA	C6-C7-C8-C10
36	U	306	CLA	C11-C12-C13-C15
41	O	318	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
36	C	205	CLA	C2B-C3B-CAB-CBB
36	C	211	CLA	C2B-C3B-CAB-CBB
36	C	212	CLA	C2B-C3B-CAB-CBB
36	E	316	CLA	C2B-C3B-CAB-CBB
36	F	314	CLA	C2B-C3B-CAB-CBB
36	I	310	CLA	C2B-C3B-CAB-CBB
36	I	313	CLA	C2B-C3B-CAB-CBB
36	J	307	CLA	C2B-C3B-CAB-CBB
36	M	309	CLA	C2B-C3B-CAB-CBB
36	N	319	CLA	C2B-C3B-CAB-CBB
36	O	308	CLA	C2B-C3B-CAB-CBB
36	O	316	CLA	C2B-C3B-CAB-CBB
36	P	301	CLA	C2B-C3B-CAB-CBB
36	P	310	CLA	C2B-C3B-CAB-CBB
36	Q	307	CLA	C2B-C3B-CAB-CBB
36	R	313	CLA	C2B-C3B-CAB-CBB
36	R	318	CLA	C2B-C3B-CAB-CBB
36	S	309	CLA	C2B-C3B-CAB-CBB
36	S	313	CLA	C2B-C3B-CAB-CBB
36	T	309	CLA	C2B-C3B-CAB-CBB
36	W	207	CLA	C2B-C3B-CAB-CBB
36	a	801	CLA	C2B-C3B-CAB-CBB
36	a	831	CLA	C2B-C3B-CAB-CBB
36	a	848	CLA	C2B-C3B-CAB-CBB
36	b	805	CLA	C2B-C3B-CAB-CBB
36	b	809	CLA	C2B-C3B-CAB-CBB
36	b	826	CLA	C2B-C3B-CAB-CBB
36	b	831	CLA	C2B-C3B-CAB-CBB
36	b	836	CLA	C2B-C3B-CAB-CBB
36	U	310	CLA	C2B-C3B-CAB-CBB
44	a	844	BCR	C5-C6-C7-C8
44	a	844	BCR	C23-C24-C25-C26
44	a	845	BCR	C23-C24-C25-C26
44	a	845	BCR	C23-C24-C25-C30
44	a	846	BCR	C23-C24-C25-C26
44	a	846	BCR	C23-C24-C25-C30
44	b	843	BCR	C23-C24-C25-C26
44	b	845	BCR	C5-C6-C7-C8
44	b	847	BCR	C23-C24-C25-C26
44	b	847	BCR	C23-C24-C25-C30
44	f	806	BCR	C23-C24-C25-C26
44	f	806	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
44	i	101	BCR	C5-C6-C7-C8
44	j	107	BCR	C23-C24-C25-C30
44	l	207	BCR	C5-C6-C7-C8
44	l	207	BCR	C23-C24-C25-C26
44	l	207	BCR	C23-C24-C25-C30
44	m	101	BCR	C1-C6-C7-C8
44	m	101	BCR	C5-C6-C7-C8
36	L	314	CLA	CAA-CBA-CGA-O2A
36	Q	310	CLA	CAA-CBA-CGA-O2A
36	b	841	CLA	CAA-CBA-CGA-O2A
36	A	310	CLA	C2-C1-O2A-CGA
36	P	319	CLA	C2-C1-O2A-CGA
36	W	215	CLA	C2-C1-O2A-CGA
36	a	808	CLA	C2-C1-O2A-CGA
36	b	806	CLA	C2-C1-O2A-CGA
36	b	827	CLA	C2-C1-O2A-CGA
36	b	833	CLA	C2-C1-O2A-CGA
36	U	305	CLA	C2-C1-O2A-CGA
36	F	312	CLA	CAA-CBA-CGA-O2A
36	f	802	CLA	CAA-CBA-CGA-O2A
36	P	308	CLA	CBD-CGD-O2D-CED
42	E	318	LMG	C35-C36-C37-C38
36	P	313	CLA	C16-C17-C18-C20
36	C	209	CLA	C4-C3-C5-C6
36	X	308	CLA	CAA-CBA-CGA-O2A
36	C	209	CLA	C2-C3-C5-C6
36	a	812	CLA	C15-C16-C17-C18
36	N	318	CLA	C2-C1-O2A-CGA
39	f	807	LMT	C2-C3-C4-C5
36	A	307	CLA	C2A-CAA-CBA-CGA
36	H	307	CLA	C2A-CAA-CBA-CGA
42	J	318	LMG	C41-C42-C43-C44
36	J	310	CLA	C15-C16-C17-C18
36	R	313	CLA	O1A-CGA-O2A-C1
36	L	311	CLA	CAA-CBA-CGA-O2A
36	a	804	CLA	CAA-CBA-CGA-O2A
36	D	310	CLA	C16-C17-C18-C20
36	a	823	CLA	O1D-CGD-O2D-CED
36	D	313	CLA	C13-C15-C16-C17
36	R	313	CLA	CBA-CGA-O2A-C1
36	M	312	CLA	CAA-CBA-CGA-O2A
36	a	801	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
38	A	315	SQD	C4-C5-C6-S
36	O	306	CLA	CBD-CGD-O2D-CED
36	a	841	CLA	C4-C3-C5-C6
36	b	829	CLA	C4-C3-C5-C6
43	b	842	PQN	C14-C13-C15-C16
36	K	307	CLA	CAA-CBA-CGA-O2A
36	T	309	CLA	CAA-CBA-CGA-O2A
36	U	308	CLA	CAA-CBA-CGA-O2A
36	I	310	CLA	C2-C3-C5-C6
36	a	841	CLA	C2-C3-C5-C6
36	Q	305	CLA	CBD-CGD-O2D-CED
36	E	314	CLA	C8-C10-C11-C12
36	I	308	CLA	C5-C6-C7-C8
36	D	310	CLA	C2A-CAA-CBA-CGA
36	F	311	CLA	C2A-CAA-CBA-CGA
41	f	808	LHG	C19-C20-C21-C22
36	b	806	CLA	CAA-CBA-CGA-O2A
42	G	324	LMG	C22-C23-C24-C25
39	I	318	LMT	C2-C1-O1'-C1'
41	f	809	LHG	O1-C1-C2-O2
36	K	316	CLA	C5-C6-C7-C8
36	C	208	CLA	C11-C10-C8-C9
36	E	311	CLA	C14-C13-C15-C16
36	E	314	CLA	C6-C7-C8-C9
36	H	311	CLA	C6-C7-C8-C9
36	J	310	CLA	C11-C10-C8-C9
36	K	308	CLA	C14-C13-C15-C16
36	Q	310	CLA	C14-C13-C15-C16
36	S	312	CLA	C6-C7-C8-C9
36	W	209	CLA	C6-C7-C8-C9
36	a	820	CLA	C11-C10-C8-C9
36	b	808	CLA	C6-C7-C8-C9
36	b	810	CLA	C11-C10-C8-C9
36	U	310	CLA	C14-C13-C15-C16
43	b	842	PQN	C19-C18-C20-C21
36	b	805	CLA	C5-C6-C7-C8
36	b	810	CLA	C15-C16-C17-C18
35	C	204	A86	C-C1-C24-C25
36	E	311	CLA	CAA-CBA-CGA-O2A
36	a	841	CLA	CAA-CBA-CGA-O2A
36	b	812	CLA	CAA-CBA-CGA-O2A
41	I	316	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	a	812	CLA	O1A-CGA-O2A-C1
36	b	825	CLA	O1A-CGA-O2A-C1
42	J	319	LMG	C7-C8-C9-O8
36	S	318	CLA	C4C-C3C-CAC-CBC
35	E	302	A86	O-C13-C14-C15
36	C	212	CLA	C4B-C3B-CAB-CBB
36	D	309	CLA	C1A-C2A-CAA-CBA
36	G	311	CLA	C1A-C2A-CAA-CBA
36	H	305	CLA	C1A-C2A-CAA-CBA
36	H	315	CLA	C4B-C3B-CAB-CBB
36	I	305	CLA	C1A-C2A-CAA-CBA
36	J	307	CLA	C4B-C3B-CAB-CBB
36	K	311	CLA	C1A-C2A-CAA-CBA
36	N	309	CLA	C1A-C2A-CAA-CBA
36	N	309	CLA	C4B-C3B-CAB-CBB
36	P	301	CLA	C1A-C2A-CAA-CBA
36	P	318	CLA	C4B-C3B-CAB-CBB
36	R	318	CLA	C4B-C3B-CAB-CBB
36	R	321	CLA	C1A-C2A-CAA-CBA
36	S	313	CLA	C4B-C3B-CAB-CBB
36	T	311	CLA	C4B-C3B-CAB-CBB
36	a	831	CLA	C4B-C3B-CAB-CBB
36	a	835	CLA	C4B-C3B-CAB-CBB
36	b	820	CLA	C4B-C3B-CAB-CBB
41	O	318	LHG	C31-C32-C33-C34
40	L	302	DGD	C1A-C2A-C3A-C4A
39	L	318	LMT	C4B-C5B-C6B-O6B
36	L	320	CLA	C4-C3-C5-C6
36	O	311	CLA	C4-C3-C5-C6
36	P	313	CLA	C4-C3-C5-C6
36	C	211	CLA	C15-C16-C17-C18
36	P	311	CLA	C4C-C3C-CAC-CBC
36	N	309	CLA	CAA-CBA-CGA-O2A
36	b	809	CLA	CAA-CBA-CGA-O2A
41	R	323	LHG	O7-C7-C8-C9
36	P	301	CLA	C2-C3-C5-C6
40	L	302	DGD	O1G-C1G-C2G-O2G
41	D	318	LHG	O7-C5-C6-O8
42	J	318	LMG	O7-C8-C9-O8
36	O	309	CLA	C4C-C3C-CAC-CBC
34	F	303	DD6	C5-C6-C8-C9
35	F	302	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
44	f	801	BCR	C7-C8-C9-C10
35	G	302	A86	C24-C25-C26-C27
35	G	305	A86	C11-C10-C9-C8
35	T	301	A86	C1-C2-C3-C4
36	Q	308	CLA	C4C-C3C-CAC-CBC
36	S	315	CLA	C4C-C3C-CAC-CBC
36	L	314	CLA	C16-C17-C18-C19
36	N	317	CLA	CBA-CGA-O2A-C1
41	O	318	LHG	C27-C28-C29-C30
36	P	318	CLA	CAA-CBA-CGA-O2A
41	G	301	LHG	C18-C19-C20-C21
36	a	817	CLA	O1A-CGA-O2A-C1
36	J	308	CLA	C2A-CAA-CBA-CGA
36	Q	310	CLA	C2A-CAA-CBA-CGA
36	b	840	CLA	C2A-CAA-CBA-CGA
36	f	805	CLA	C2A-CAA-CBA-CGA
39	K	317	LMT	C2'-C1'-O1'-C1
36	E	312	CLA	C4C-C3C-CAC-CBC
36	a	830	CLA	C4C-C3C-CAC-CBC
36	R	315	CLA	C5-C6-C7-C8
35	U	302	A86	C33-C34-O4-C38
40	b	849	DGD	C7A-C8A-C9A-CAA
36	M	309	CLA	CAA-CBA-CGA-O2A
36	a	824	CLA	CAA-CBA-CGA-O2A
36	V	305	CLA	C8-C10-C11-C12
37	L	315	KC1	CAA-CBA-CGA-O2A
36	P	318	CLA	C2-C3-C5-C6
38	A	315	SQD	C5-C6-S-O7
39	a	854	LMT	C11-C10-C9-C8
41	G	320	LHG	C18-C19-C20-C21
36	D	317	CLA	C2-C1-O2A-CGA
36	E	312	CLA	C2-C1-O2A-CGA
36	G	316	CLA	C2-C1-O2A-CGA
36	P	314	CLA	C2-C1-O2A-CGA
36	a	825	CLA	C2-C1-O2A-CGA
36	b	829	CLA	C2-C1-O2A-CGA
36	l	204	CLA	C2-C1-O2A-CGA
36	V	306	CLA	C2-C1-O2A-CGA
36	G	316	CLA	CAA-CBA-CGA-O2A
36	A	311	CLA	C12-C13-C15-C16
36	B	308	CLA	C6-C7-C8-C10
36	G	313	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
36	J	308	CLA	C11-C10-C8-C7
36	J	310	CLA	C11-C12-C13-C15
36	K	308	CLA	C11-C12-C13-C15
36	a	807	CLA	C6-C7-C8-C10
36	a	816	CLA	C12-C13-C15-C16
36	a	827	CLA	C6-C7-C8-C10
36	E	310	CLA	CBA-CGA-O2A-C1
36	H	317	CLA	C2-C3-C5-C6
36	a	818	CLA	C8-C10-C11-C12
39	B	312	LMT	C4-C5-C6-C7
39	E	320	LMT	C5-C6-C7-C8
36	F	311	CLA	O1A-CGA-O2A-C1
41	i	104	LHG	C29-C30-C31-C32
39	G	323	LMT	C2B-C1B-O1B-C4'
36	I	309	CLA	CAA-CBA-CGA-O1A
36	B	307	CLA	C2A-CAA-CBA-CGA
36	M	309	CLA	C2A-CAA-CBA-CGA
36	S	312	CLA	C2A-CAA-CBA-CGA
36	X	308	CLA	C2A-CAA-CBA-CGA
36	l	204	CLA	C2A-CAA-CBA-CGA
36	A	310	CLA	C13-C15-C16-C17
36	b	841	CLA	C16-C17-C18-C19
36	A	314	CLA	C8-C10-C11-C12
36	W	212	CLA	C10-C11-C12-C13
42	V	316	LMG	O8-C28-C29-C30
36	H	305	CLA	C3A-C2A-CAA-CBA
36	R	322	CLA	C3A-C2A-CAA-CBA
36	a	835	CLA	C3A-C2A-CAA-CBA
36	j	102	CLA	C3A-C2A-CAA-CBA
36	b	828	CLA	CAA-CBA-CGA-O1A
36	O	307	CLA	CBA-CGA-O2A-C1
36	P	309	CLA	CBA-CGA-O2A-C1
36	Q	306	CLA	CBA-CGA-O2A-C1
36	a	812	CLA	CBA-CGA-O2A-C1
37	J	314	KC1	C4C-C3C-CAC-CBC
36	W	207	CLA	CAA-CBA-CGA-O2A
35	A	302	A86	C35-C34-O4-C38
36	G	316	CLA	CAA-CBA-CGA-O1A
36	Q	310	CLA	CAA-CBA-CGA-O1A
36	C	206	CLA	C11-C10-C8-C9
36	C	211	CLA	C6-C7-C8-C9
36	C	212	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
36	D	308	CLA	C11-C10-C8-C9
36	I	311	CLA	C11-C10-C8-C9
36	J	308	CLA	C11-C12-C13-C14
36	O	316	CLA	C6-C7-C8-C9
36	P	314	CLA	C6-C7-C8-C9
36	a	810	CLA	C6-C7-C8-C9
36	a	816	CLA	C14-C13-C15-C16
36	a	828	CLA	C11-C12-C13-C14
36	a	832	CLA	C11-C12-C13-C14
36	b	820	CLA	C6-C7-C8-C9
36	f	803	CLA	C6-C7-C8-C9
36	V	305	CLA	C6-C7-C8-C9
36	O	309	CLA	CAA-CBA-CGA-O2A
36	P	311	CLA	CAA-CBA-CGA-O2A
36	Q	308	CLA	CAA-CBA-CGA-O2A
36	E	311	CLA	CAA-CBA-CGA-O1A
36	f	802	CLA	CAA-CBA-CGA-O1A
36	F	311	CLA	O1D-CGD-O2D-CED
36	F	310	CLA	C4-C3-C5-C6
36	b	830	CLA	C4-C3-C5-C6
36	M	312	CLA	CAA-CBA-CGA-O1A
36	U	308	CLA	CAA-CBA-CGA-O1A
41	E	322	LHG	O9-C7-C8-C9
41	R	323	LHG	O9-C7-C8-C9
36	b	822	CLA	O1D-CGD-O2D-CED
36	I	305	CLA	C2-C3-C5-C6
34	B	304	DD6	C13-C14-C15-C16
34	E	304	DD6	C13-C14-C15-C16
34	P	305	DD6	C13-C14-C15-C16
34	Q	302	DD6	C13-C14-C15-C16
34	R	307	DD6	C13-C14-C15-C16
34	R	308	DD6	C13-C14-C15-C16
34	a	849	DD6	C13-C14-C15-C16
35	M	304	A86	C26-C27-C29-C30
35	U	303	A86	C26-C27-C29-C30
36	N	309	CLA	C4-C3-C5-C6
37	F	308	KC1	C1A-C2A-CAA-CBA
37	G	308	KC1	C1A-C2A-CAA-CBA
37	G	318	KC1	C1A-C2A-CAA-CBA
37	M	313	KC1	C1A-C2A-CAA-CBA
37	M	317	KC1	C3A-C2A-CAA-CBA
37	M	318	KC1	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	N	314	KC1	C1A-C2A-CAA-CBA
37	W	213	KC1	C1A-C2A-CAA-CBA
38	A	315	SQD	O5-C5-C6-S
35	E	307	A86	C39-C38-O4-C34
36	a	824	CLA	CAA-CBA-CGA-O1A
36	a	841	CLA	CAA-CBA-CGA-O1A
41	O	318	LHG	C18-C19-C20-C21
44	i	103	BCR	C7-C8-C9-C10
41	I	316	LHG	O9-C7-C8-C9
42	V	315	LMG	O9-C10-C11-C12
41	Q	315	LHG	C19-C20-C21-C22
36	V	313	CLA	C13-C15-C16-C17
42	V	316	LMG	C8-C7-O1-C1
38	A	315	SQD	O47-C45-C46-O48
36	a	828	CLA	C3-C5-C6-C7
36	b	809	CLA	CAA-CBA-CGA-O1A
36	b	812	CLA	CAA-CBA-CGA-O1A
41	a	850	LHG	O9-C7-C8-C9
36	L	308	CLA	CAA-CBA-CGA-O2A
42	E	319	LMG	O8-C28-C29-C30
36	S	320	CLA	C5-C6-C7-C8
36	B	305	CLA	C2A-CAA-CBA-CGA
39	B	312	LMT	O1'-C1-C2-C3
36	b	836	CLA	C8-C10-C11-C12
35	L	304	A86	C12-C11-C13-O
35	N	303	A86	C12-C11-C13-O
35	S	303	A86	C12-C11-C13-O
35	U	301	A86	C12-C11-C13-O
36	R	315	CLA	C4-C3-C5-C6
36	a	805	CLA	C15-C16-C17-C18
36	a	806	CLA	C15-C16-C17-C18
36	a	826	CLA	C10-C11-C12-C13
36	b	834	CLA	C5-C6-C7-C8
36	P	314	CLA	CAA-CBA-CGA-O2A
36	H	305	CLA	O1A-CGA-O2A-C1
36	B	305	CLA	C2-C3-C5-C6
35	F	304	A86	C33-C34-O4-C38
35	F	301	A86	C11-C10-C9-C8
36	a	804	CLA	CAA-CBA-CGA-O1A
36	b	806	CLA	CAA-CBA-CGA-O1A
36	D	315	CLA	C4C-C3C-CAC-CBC
41	G	320	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
35	K	306	A86	C13-C14-C15-C20
35	X	301	A86	C13-C14-C15-C20
35	X	304	A86	C13-C14-C15-C20
36	A	310	CLA	CAD-CBD-CGD-O2D
36	D	315	CLA	CAD-CBD-CGD-O2D
36	E	311	CLA	CAD-CBD-CGD-O2D
36	G	316	CLA	CAD-CBD-CGD-O2D
36	J	317	CLA	CAD-CBD-CGD-O2D
36	K	307	CLA	CAD-CBD-CGD-O2D
36	L	316	CLA	CAD-CBD-CGD-O2D
36	N	312	CLA	CAD-CBD-CGD-O2D
36	X	313	CLA	CAD-CBD-CGD-O2D
36	a	831	CLA	CAD-CBD-CGD-O2D
36	b	833	CLA	CAD-CBD-CGD-O2D
37	W	217	KC1	CAD-CBD-CGD-O2D
36	l	204	CLA	C2C-C3C-CAC-CBC
36	L	314	CLA	C3-C5-C6-C7
36	K	307	CLA	CAA-CBA-CGA-O1A
36	L	311	CLA	CAA-CBA-CGA-O1A
36	M	309	CLA	CAA-CBA-CGA-O1A
35	I	301	A86	C35-C34-O4-C38
35	X	302	A86	C33-C34-O4-C38
44	b	845	BCR	C6-C7-C8-C9
36	E	311	CLA	C2-C1-O2A-CGA
36	F	309	CLA	C2-C1-O2A-CGA
36	F	313	CLA	C2-C1-O2A-CGA
36	H	312	CLA	C2-C1-O2A-CGA
36	M	307	CLA	C2-C1-O2A-CGA
36	a	806	CLA	C2-C1-O2A-CGA
36	B	311	CLA	CAA-CBA-CGA-O2A
36	b	816	CLA	CAA-CBA-CGA-O2A
41	a	850	LHG	C9-C10-C11-C12
36	T	309	CLA	CAA-CBA-CGA-O1A
41	F	318	LHG	O10-C23-C24-C25
36	P	319	CLA	C5-C6-C7-C8
36	S	310	CLA	C8-C10-C11-C12
36	b	802	CLA	C13-C15-C16-C17
37	J	314	KC1	C2C-C3C-CAC-CBC
41	Q	315	LHG	C30-C31-C32-C33
36	I	312	CLA	CAA-CBA-CGA-O2A
36	J	307	CLA	CAA-CBA-CGA-O2A
36	M	315	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
41	f	808	LHG	O8-C23-C24-C25
42	h	206	LMG	O7-C10-C11-C12
36	f	803	CLA	C13-C15-C16-C17
37	L	315	KC1	CAA-CBA-CGA-O1A
41	G	321	LHG	C26-C27-C28-C29
36	G	315	CLA	CAA-CBA-CGA-O2A
36	H	310	CLA	CAA-CBA-CGA-O2A
36	Q	314	CLA	CAA-CBA-CGA-O2A
36	S	312	CLA	CAA-CBA-CGA-O2A
36	b	819	CLA	CAA-CBA-CGA-O2A
36	N	309	CLA	CAA-CBA-CGA-O1A
36	P	318	CLA	CAA-CBA-CGA-O1A
35	T	306	A86	C33-C34-O4-C38

All (11) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	V	301	A86	C31-C32-C33-C34-C35-C36
35	J	302	A86	C31-C32-C33-C34-C35-C36
35	K	301	A86	C31-C32-C33-C34-C35-C36
35	G	306	A86	C31-C32-C33-C34-C35-C36
35	T	301	A86	C31-C32-C33-C34-C35-C36
35	X	314	A86	C31-C32-C33-C34-C35-C36
35	C	203	A86	C31-C32-C33-C34-C35-C36
35	h	202	A86	C31-C32-C33-C34-C35-C36
35	L	301	A86	C31-C32-C33-C34-C35-C36
35	L	307	A86	C31-C32-C33-C34-C35-C36
35	F	306	A86	C31-C32-C33-C34-C35-C36

498 monomers are involved in 2733 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	b	806	CLA	2	0
36	a	812	CLA	1	0
36	a	823	CLA	1	0
36	A	314	CLA	20	0
36	b	813	CLA	1	0
36	O	306	CLA	1	0
36	C	211	CLA	1	0
36	W	215	CLA	3	0
36	A	305	CLA	4	0
37	E	309	KC1	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	L	303	LMT	1	0
37	L	317	KC1	2	0
44	a	847	BCR	1	0
36	W	216	CLA	1	0
41	D	319	LHG	12	0
36	D	307	CLA	12	0
41	I	316	LHG	10	0
35	P	306	A86	4	0
36	M	309	CLA	8	0
36	a	838	CLA	1	0
36	P	314	CLA	5	0
35	X	302	A86	1	0
36	b	828	CLA	4	0
36	a	839	CLA	1	0
41	Q	315	LHG	19	0
35	R	305	A86	7	0
44	l	207	BCR	4	0
36	L	308	CLA	36	0
39	h	205	LMT	21	0
44	j	107	BCR	1	0
36	E	310	CLA	1	0
36	N	316	CLA	6	0
35	Q	316	A86	27	0
36	b	818	CLA	3	0
36	a	813	CLA	12	0
36	U	307	CLA	11	0
35	A	302	A86	1	0
36	M	310	CLA	1	0
35	C	204	A86	4	0
35	L	301	A86	5	0
36	a	841	CLA	3	0
36	B	305	CLA	3	0
36	E	313	CLA	7	0
36	a	801	CLA	6	0
34	A	304	DD6	2	0
36	M	316	CLA	3	0
44	b	843	BCR	6	0
36	M	311	CLA	3	0
34	R	308	DD6	5	0
36	H	308	CLA	19	0
35	I	301	A86	4	0
36	b	841	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	Q	305	CLA	4	0
44	h	201	BCR	4	0
36	I	307	CLA	6	0
36	G	316	CLA	3	0
35	H	304	A86	7	0
36	J	310	CLA	4	0
36	H	316	CLA	2	0
36	D	308	CLA	6	0
36	V	314	CLA	31	0
36	L	312	CLA	1	0
36	K	313	CLA	6	0
36	a	806	CLA	19	0
36	L	314	CLA	2	0
36	I	311	CLA	1	0
41	F	319	LHG	4	0
36	M	307	CLA	18	0
36	N	312	CLA	6	0
34	a	849	DD6	1	0
36	J	313	CLA	5	0
41	F	318	LHG	1	0
36	Q	306	CLA	3	0
35	C	203	A86	12	0
43	a	840	PQN	3	0
37	F	308	KC1	15	0
36	a	808	CLA	7	0
36	K	307	CLA	15	0
37	Q	311	KC1	8	0
36	R	311	CLA	1	0
36	S	320	CLA	2	0
41	G	320	LHG	14	0
34	R	307	DD6	11	0
35	W	203	A86	1	0
35	h	204	A86	4	0
44	m	101	BCR	11	0
41	j	104	LHG	14	0
36	M	312	CLA	3	0
36	a	833	CLA	2	0
35	S	302	A86	1	0
41	G	301	LHG	3	0
37	F	315	KC1	5	0
34	W	204	DD6	22	0
36	W	218	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	a	851	LMT	8	0
44	a	845	BCR	3	0
36	H	315	CLA	3	0
36	a	821	CLA	2	0
44	f	801	BCR	2	0
36	P	301	CLA	9	0
36	W	209	CLA	7	0
35	N	304	A86	14	0
41	E	322	LHG	24	0
36	Q	314	CLA	50	0
35	Q	304	A86	1	0
36	D	306	CLA	5	0
35	R	303	A86	1	0
36	O	309	CLA	8	0
35	M	304	A86	12	0
36	b	826	CLA	1	0
36	a	816	CLA	30	0
39	a	853	LMT	12	0
36	I	305	CLA	5	0
36	B	307	CLA	1	0
36	i	102	CLA	3	0
36	J	307	CLA	1	0
42	E	319	LMG	6	0
36	W	206	CLA	1	0
36	O	311	CLA	3	0
39	P	321	LMT	2	0
36	A	313	CLA	3	0
36	H	314	CLA	6	0
36	b	821	CLA	1	0
36	a	819	CLA	10	0
36	R	310	CLA	9	0
36	N	318	CLA	15	0
36	f	804	CLA	12	0
36	U	308	CLA	19	0
36	b	822	CLA	2	0
34	B	302	DD6	5	0
37	K	314	KC1	9	0
42	V	315	LMG	14	0
36	Q	307	CLA	5	0
36	J	311	CLA	3	0
36	C	210	CLA	6	0
36	I	306	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	E	314	CLA	4	0
36	b	819	CLA	3	0
36	a	836	CLA	6	0
34	E	306	DD6	4	0
34	K	305	DD6	4	0
36	A	310	CLA	1	0
36	N	319	CLA	14	0
36	a	835	CLA	1	0
36	V	308	CLA	12	0
36	L	310	CLA	1	0
36	N	309	CLA	6	0
36	F	313	CLA	6	0
37	Q	313	KC1	8	0
34	j	103	DD6	4	0
42	J	319	LMG	12	0
35	I	302	A86	17	0
36	J	309	CLA	2	0
36	B	311	CLA	7	0
36	a	832	CLA	3	0
36	I	308	CLA	29	0
41	D	318	LHG	16	0
36	D	317	CLA	1	0
39	G	322	LMT	10	0
34	D	303	DD6	5	0
37	M	313	KC1	1	0
36	I	309	CLA	17	0
35	S	304	A86	21	0
36	L	320	CLA	2	0
45	b	803	SF4	2	0
36	H	318	CLA	4	0
36	G	315	CLA	24	0
41	f	809	LHG	20	0
34	O	304	DD6	6	0
36	a	803	CLA	5	0
35	U	304	A86	15	0
36	C	208	CLA	5	0
36	D	312	CLA	2	0
36	T	313	CLA	13	0
34	A	303	DD6	4	0
39	U	315	LMT	17	0
36	D	315	CLA	1	0
36	U	311	CLA	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	L	305	DD6	25	0
36	a	817	CLA	3	0
36	N	308	CLA	4	0
42	a	852	LMG	20	0
35	V	301	A86	27	0
36	F	314	CLA	6	0
36	H	312	CLA	2	0
35	X	314	A86	24	0
34	D	304	DD6	2	0
34	W	205	DD6	23	0
44	i	103	BCR	5	0
36	a	811	CLA	3	0
34	D	301	DD6	12	0
41	a	850	LHG	15	0
42	h	206	LMG	7	0
36	f	802	CLA	4	0
35	L	307	A86	8	0
36	D	311	CLA	5	0
36	N	313	CLA	5	0
36	b	808	CLA	1	0
36	V	307	CLA	1	0
34	M	303	DD6	18	0
44	b	844	BCR	2	0
36	C	205	CLA	14	0
36	a	829	CLA	1	0
36	U	309	CLA	4	0
44	b	846	BCR	4	0
36	F	309	CLA	5	0
39	U	314	LMT	15	0
39	E	323	LMT	5	0
39	G	323	LMT	4	0
36	b	817	CLA	6	0
34	S	306	DD6	2	0
34	K	304	DD6	4	0
36	O	308	CLA	6	0
37	T	315	KC1	1	0
39	F	320	LMT	19	0
42	L	321	LMG	10	0
35	V	304	A86	6	0
36	K	309	CLA	6	0
36	V	306	CLA	22	0
38	A	315	SQD	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	J	302	A86	3	0
38	b	804	SQD	10	0
35	T	301	A86	2	0
36	S	321	CLA	7	0
36	b	811	CLA	1	0
41	b	850	LHG	18	0
36	J	308	CLA	8	0
36	h	203	CLA	11	0
35	T	306	A86	1	0
35	K	301	A86	4	0
36	G	309	CLA	4	0
36	l	204	CLA	6	0
37	A	312	KC1	4	0
36	G	311	CLA	11	0
35	A	316	A86	2	0
36	a	810	CLA	4	0
36	b	815	CLA	2	0
36	E	315	CLA	29	0
36	T	311	CLA	4	0
36	I	314	CLA	2	0
41	O	318	LHG	6	0
37	G	317	KC1	6	0
36	a	827	CLA	2	0
36	I	312	CLA	16	0
42	D	320	LMG	12	0
36	R	313	CLA	2	0
42	G	325	LMG	14	0
42	V	316	LMG	28	0
36	B	308	CLA	7	0
36	U	306	CLA	31	0
36	a	828	CLA	1	0
42	D	321	LMG	5	0
35	V	303	A86	13	0
35	O	301	A86	13	0
35	O	305	A86	13	0
36	a	826	CLA	2	0
36	W	201	CLA	1	0
35	X	305	A86	2	0
36	C	209	CLA	1	0
36	O	312	CLA	2	0
41	R	323	LHG	14	0
36	T	309	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	b	816	CLA	9	0
36	E	316	CLA	3	0
39	I	317	LMT	15	0
35	G	305	A86	3	0
36	D	310	CLA	1	0
36	S	315	CLA	15	0
34	P	305	DD6	6	0
36	f	805	CLA	20	0
36	V	305	CLA	32	0
34	E	301	DD6	4	0
37	S	316	KC1	4	0
36	H	310	CLA	9	0
36	J	315	CLA	3	0
36	D	313	CLA	3	0
36	W	212	CLA	23	0
41	i	104	LHG	28	0
36	a	834	CLA	2	0
36	b	814	CLA	2	0
36	A	309	CLA	6	0
36	b	837	CLA	2	0
36	C	212	CLA	6	0
36	P	313	CLA	7	0
35	P	307	A86	2	0
36	F	312	CLA	6	0
35	B	303	A86	8	0
42	J	318	LMG	24	0
36	E	311	CLA	6	0
36	G	307	CLA	12	0
36	b	809	CLA	2	0
44	f	806	BCR	1	0
36	H	317	CLA	1	0
36	b	824	CLA	4	0
37	B	310	KC1	2	0
40	L	302	DGD	20	0
44	l	203	BCR	1	0
36	I	310	CLA	4	0
35	B	301	A86	11	0
36	I	313	CLA	2	0
36	W	207	CLA	8	0
36	a	831	CLA	1	0
35	J	301	A86	14	0
36	Q	308	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	K	318	LMT	8	0
35	Q	303	A86	14	0
36	V	310	CLA	15	0
36	b	829	CLA	3	0
36	a	805	CLA	1	0
36	S	314	CLA	3	0
36	a	815	CLA	3	0
36	l	205	CLA	3	0
43	b	842	PQN	3	0
34	H	303	DD6	5	0
36	G	314	CLA	1	0
36	J	312	CLA	5	0
36	N	315	CLA	1	0
36	E	312	CLA	1	0
36	a	825	CLA	2	0
34	S	307	DD6	1	0
36	B	309	CLA	16	0
36	j	106	CLA	1	0
36	V	309	CLA	7	0
36	K	311	CLA	5	0
42	m	102	LMG	9	0
35	S	308	A86	5	0
36	V	311	CLA	16	0
36	b	805	CLA	2	0
36	b	823	CLA	11	0
35	N	302	A86	4	0
36	S	319	CLA	2	0
35	F	302	A86	2	0
36	a	822	CLA	3	0
36	M	315	CLA	2	0
35	U	303	A86	15	0
36	L	311	CLA	2	0
36	S	309	CLA	5	0
39	E	320	LMT	16	0
36	S	311	CLA	8	0
35	O	319	A86	1	0
39	b	848	LMT	5	0
40	C	215	DGD	19	0
36	W	211	CLA	1	0
36	D	309	CLA	10	0
36	T	308	CLA	3	0
41	f	808	LHG	23	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	N	317	CLA	3	0
36	P	316	CLA	4	0
36	a	830	CLA	4	0
36	a	848	CLA	10	0
37	V	312	KC1	1	0
36	A	307	CLA	3	0
36	H	307	CLA	10	0
36	T	316	CLA	1	0
37	T	310	KC1	17	0
36	b	833	CLA	8	0
36	R	322	CLA	1	0
36	b	838	CLA	1	0
36	l	202	CLA	8	0
44	i	101	BCR	4	0
36	G	319	CLA	4	0
35	K	303	A86	2	0
35	F	301	A86	10	0
37	P	315	KC1	2	0
35	N	303	A86	15	0
35	U	301	A86	1	0
34	Q	302	DD6	19	0
39	F	321	LMT	25	0
39	B	312	LMT	15	0
36	N	310	CLA	6	0
34	J	304	DD6	4	0
36	a	804	CLA	3	0
39	f	807	LMT	2	0
36	D	316	CLA	1	0
36	b	831	CLA	2	0
36	X	307	CLA	3	0
36	P	318	CLA	1	0
37	O	313	KC1	1	0
44	a	846	BCR	2	0
36	F	316	CLA	3	0
36	b	830	CLA	1	0
36	P	309	CLA	2	0
36	P	310	CLA	2	0
39	E	321	LMT	8	0
36	E	317	CLA	1	0
44	a	844	BCR	7	0
36	a	809	CLA	5	0
42	I	315	LMG	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	T	304	A86	5	0
36	A	311	CLA	3	0
36	O	316	CLA	22	0
36	K	310	CLA	21	0
35	T	303	A86	1	0
36	W	208	CLA	1	0
36	b	801	CLA	1	0
39	K	317	LMT	6	0
35	G	302	A86	2	0
39	I	318	LMT	7	0
36	K	316	CLA	3	0
36	T	314	CLA	1	0
36	b	840	CLA	3	0
36	E	308	CLA	3	0
36	P	319	CLA	13	0
36	U	305	CLA	3	0
35	L	304	A86	1	0
36	G	310	CLA	1	0
37	G	308	KC1	2	0
35	D	302	A86	6	0
36	a	818	CLA	3	0
36	V	313	CLA	12	0
36	X	315	CLA	24	0
35	E	305	A86	4	0
36	b	836	CLA	20	0
37	W	217	KC1	14	0
35	N	301	A86	2	0
36	H	305	CLA	2	0
35	N	305	A86	20	0
34	F	303	DD6	3	0
36	S	313	CLA	1	0
36	A	308	CLA	2	0
36	P	302	CLA	6	0
36	K	308	CLA	2	0
36	a	807	CLA	1	0
36	M	306	CLA	1	0
36	R	316	CLA	1	0
44	b	847	BCR	1	0
36	T	312	CLA	1	0
39	a	854	LMT	5	0
36	F	317	CLA	29	0
36	L	309	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	K	315	CLA	2	0
41	O	317	LHG	8	0
36	b	810	CLA	2	0
35	J	306	A86	6	0
36	X	308	CLA	4	0
40	b	849	DGD	4	0
36	j	101	CLA	11	0
41	a	843	LHG	5	0
36	R	320	CLA	7	0
35	N	306	A86	1	0
35	U	302	A86	4	0
36	C	206	CLA	3	0
36	f	803	CLA	3	0
34	E	303	DD6	4	0
34	G	303	DD6	2	0
39	B	313	LMT	5	0
34	H	302	DD6	1	0
44	b	845	BCR	1	0
36	C	207	CLA	7	0
36	R	321	CLA	2	0
39	P	320	LMT	6	0
36	a	824	CLA	2	0
36	P	308	CLA	1	0
36	U	310	CLA	15	0
36	b	807	CLA	4	0
36	Q	310	CLA	9	0
37	M	318	KC1	6	0
36	l	201	CLA	6	0
36	l	206	CLA	1	0
36	a	802	CLA	4	0
35	J	305	A86	6	0
42	G	324	LMG	17	0
34	A	301	DD6	8	0
36	b	820	CLA	6	0
36	X	310	CLA	3	0
36	F	311	CLA	2	0
34	C	201	DD6	4	0
36	R	314	CLA	3	0
35	h	202	A86	5	0
34	I	303	DD6	6	0
36	H	311	CLA	3	0
36	K	312	CLA	3	0

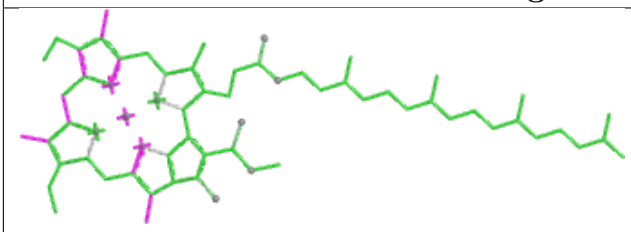
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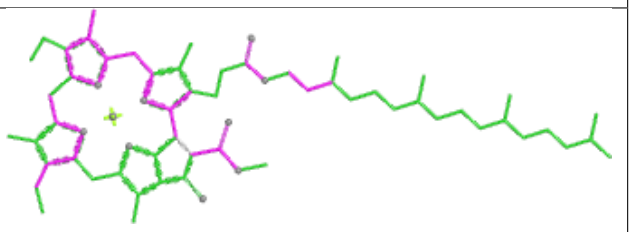
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	S	318	CLA	3	0
37	O	315	KC1	12	0
41	G	321	LHG	10	0
36	b	802	CLA	3	0
35	G	306	A86	4	0
36	X	309	CLA	2	0
36	A	306	CLA	17	0
36	b	834	CLA	3	0
42	j	105	LMG	26	0
42	E	318	LMG	19	0
36	U	313	CLA	1	0
36	J	317	CLA	1	0
41	l	208	LHG	17	0
36	b	825	CLA	3	0
36	b	839	CLA	1	0
36	G	313	CLA	18	0
37	L	315	KC1	9	0
35	R	304	A86	2	0
39	L	318	LMT	9	0
37	C	213	KC1	1	0
36	S	312	CLA	3	0
36	b	812	CLA	2	0
35	E	307	A86	14	0
39	b	851	LMT	20	0
34	B	304	DD6	10	0
36	j	102	CLA	19	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.

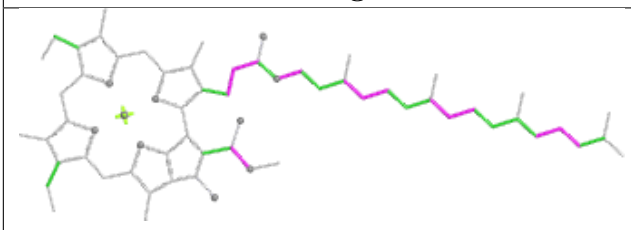
Ligand CLA b 806



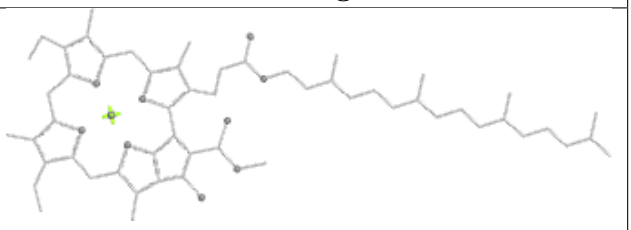
Bond lengths



Bond angles

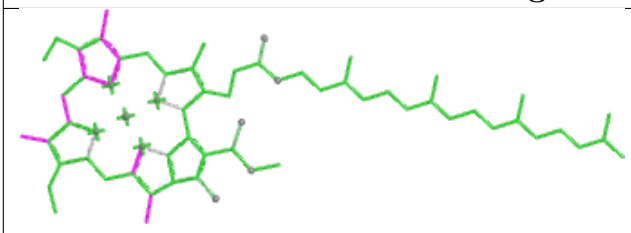


Torsions

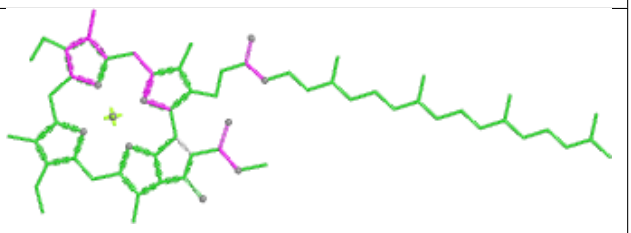


Rings

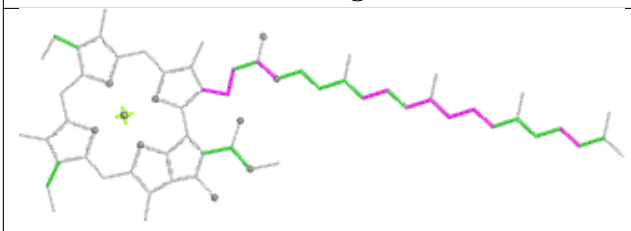
Ligand CLA a 812



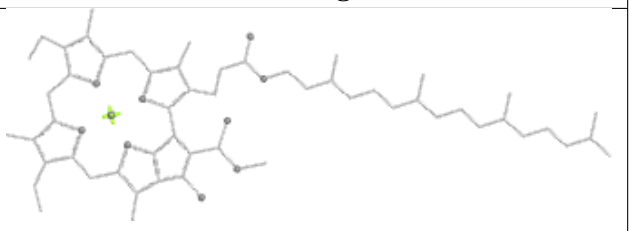
Bond lengths



Bond angles

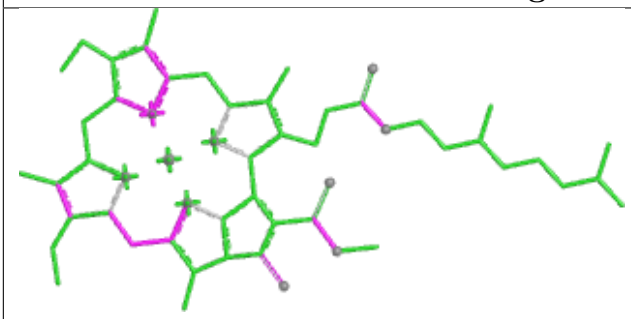


Torsions

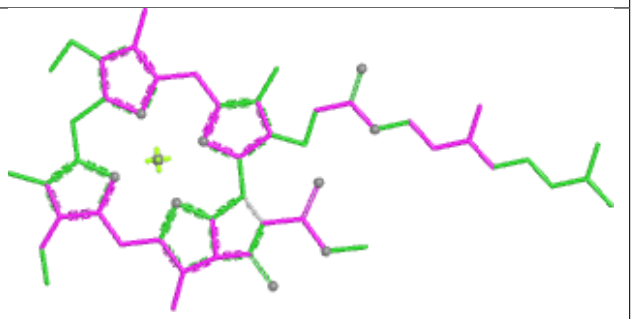


Rings

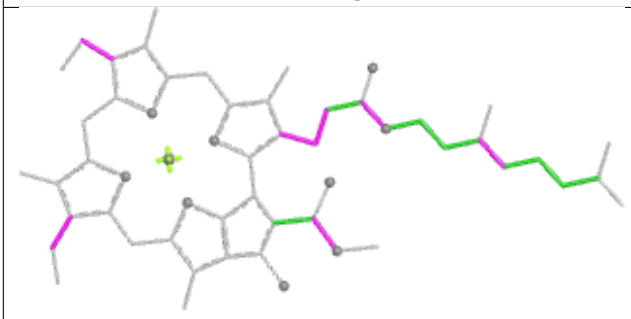
Ligand CLA a 823



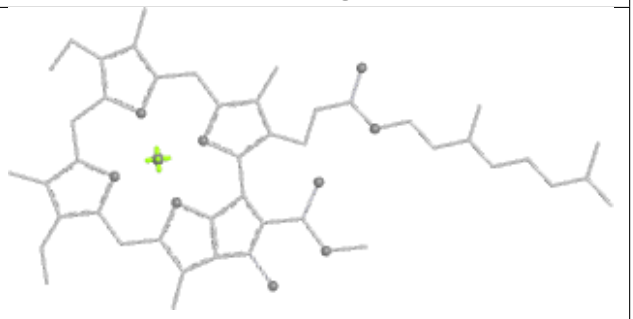
Bond lengths



Bond angles

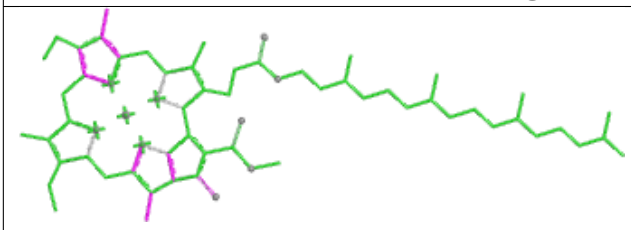


Torsions

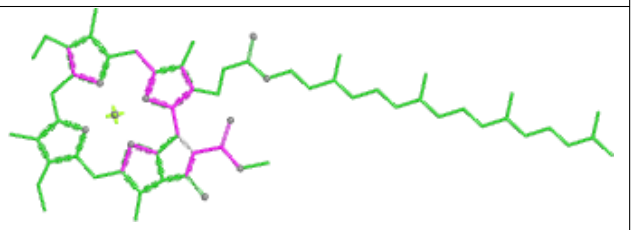


Rings

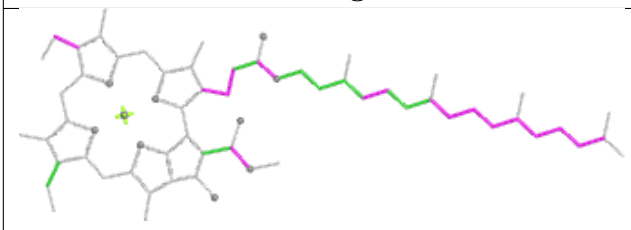
Ligand CLA A 314



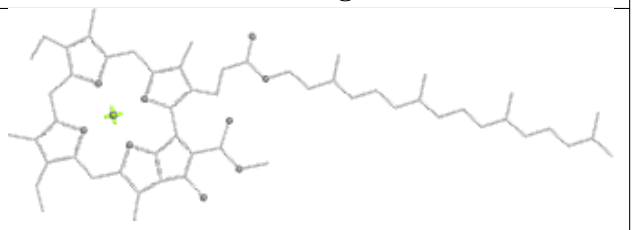
Bond lengths



Bond angles

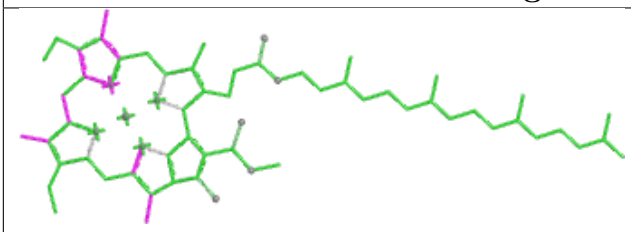


Torsions

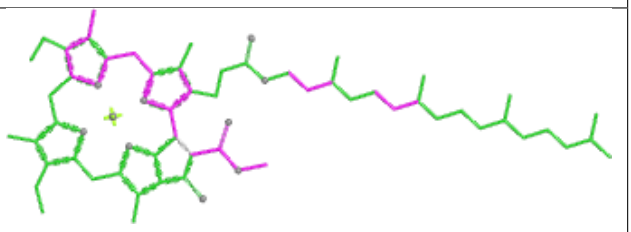


Rings

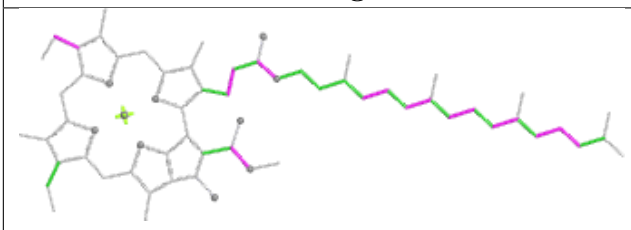
Ligand CLA R 312



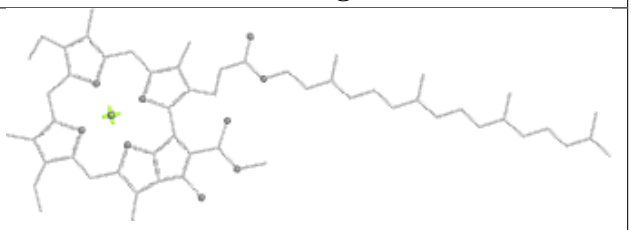
Bond lengths



Bond angles

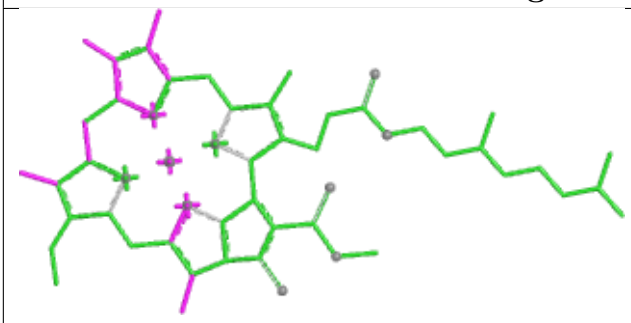


Torsions

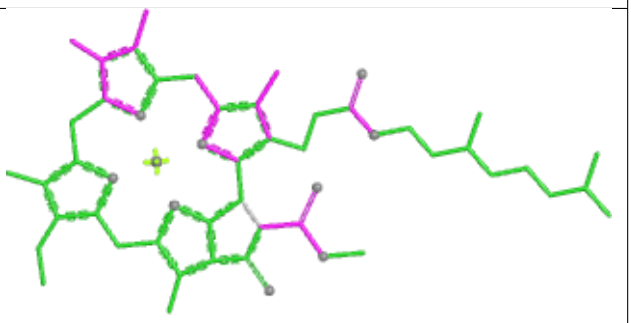


Rings

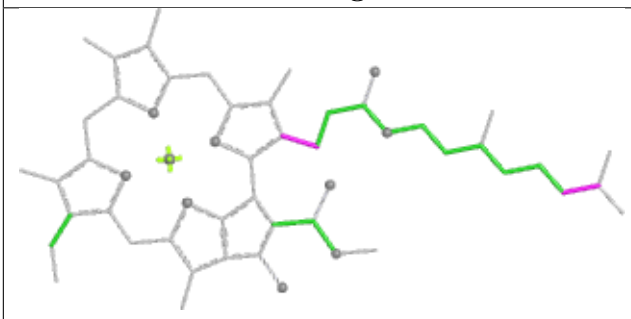
Ligand CLA b 813



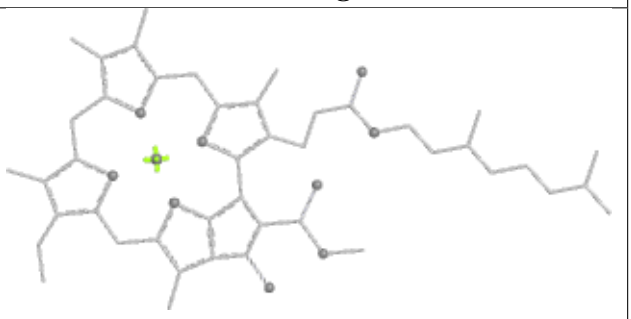
Bond lengths



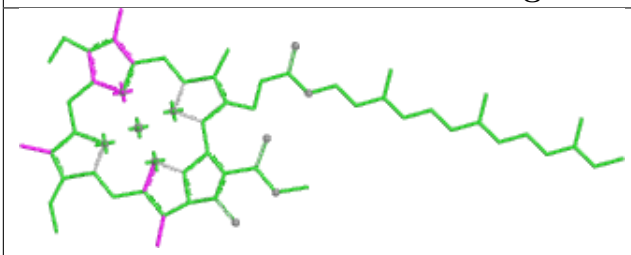
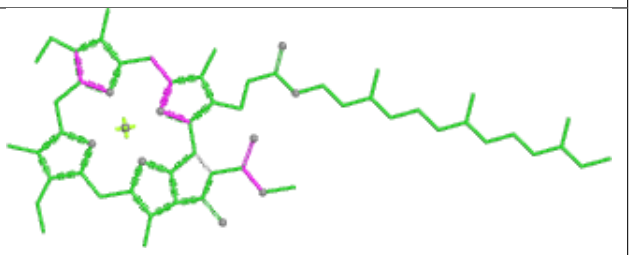
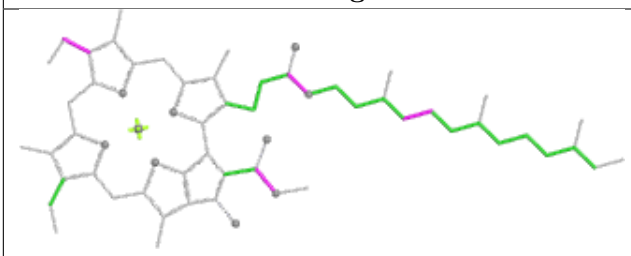
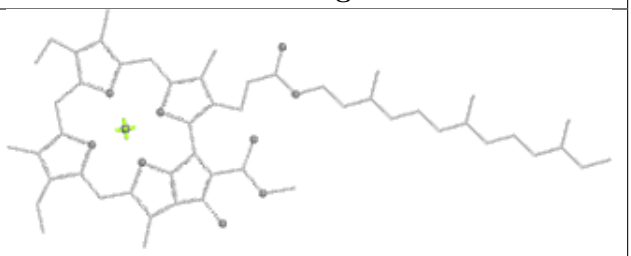
Bond angles

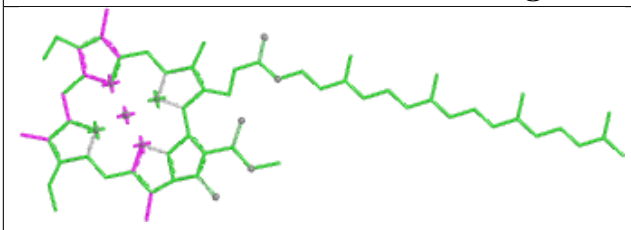
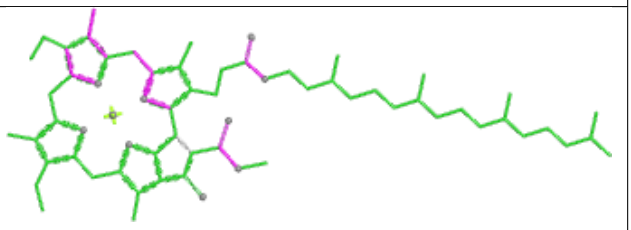
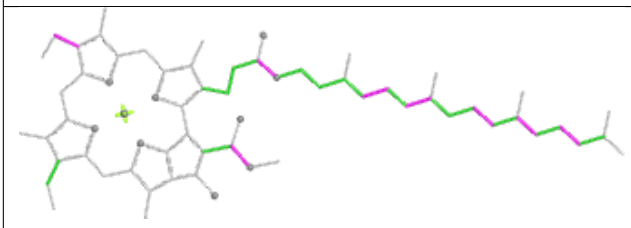
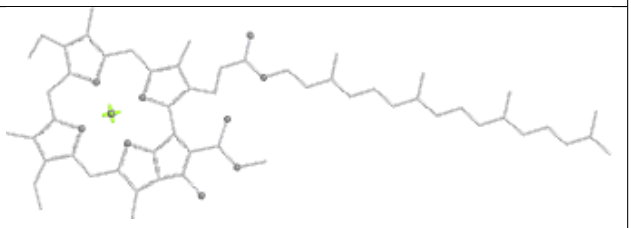


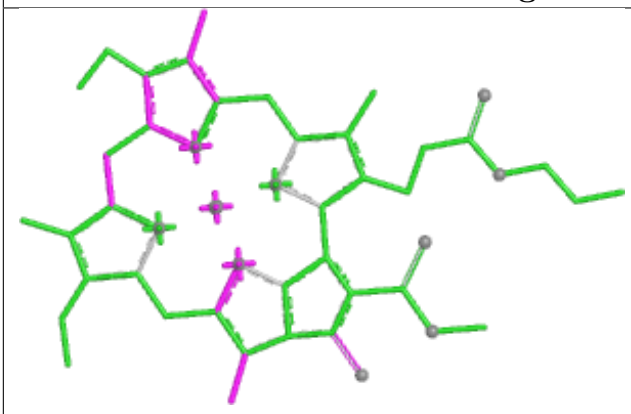
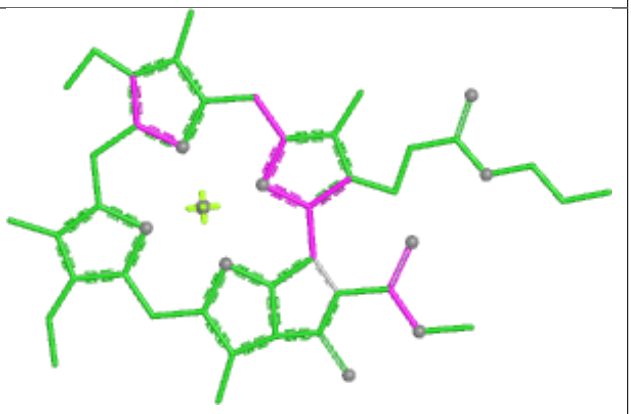
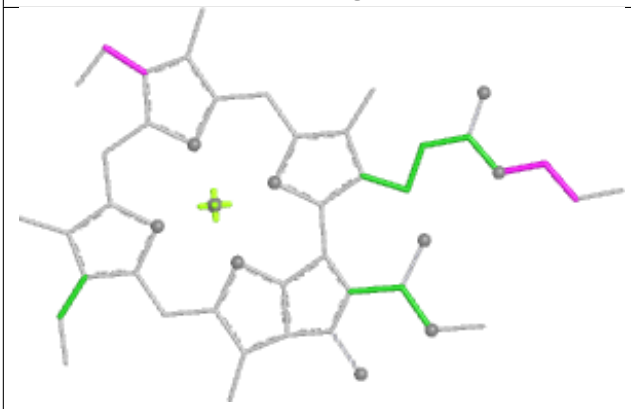
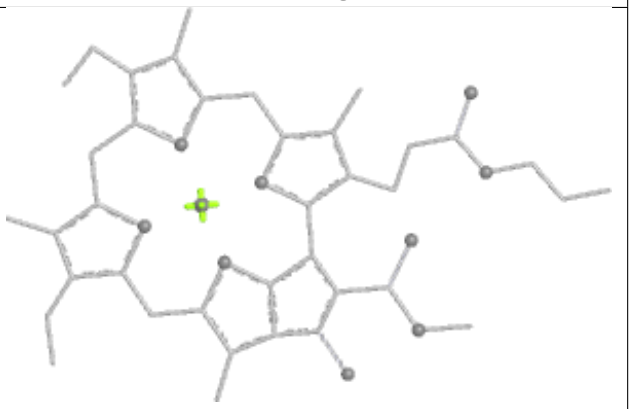
Torsions

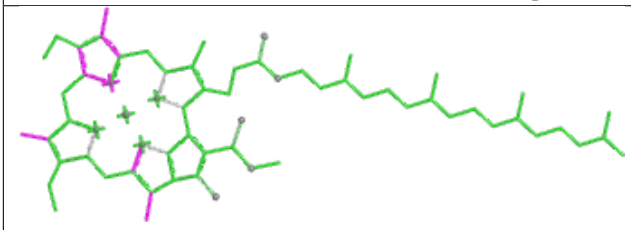
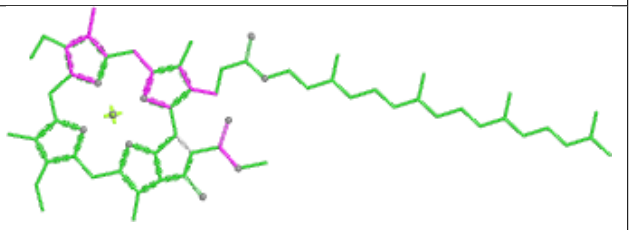
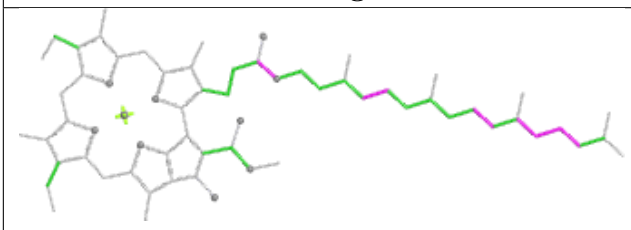
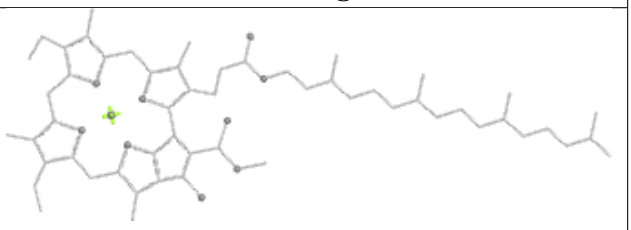


Rings

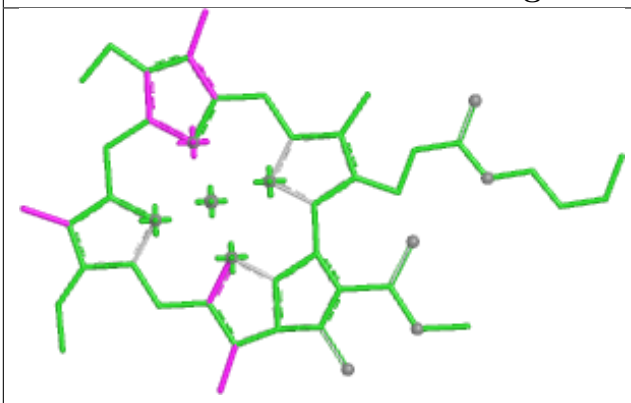
Ligand CLA O 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 211	
	
Bond lengths	Bond angles
	
Torsions	Rings

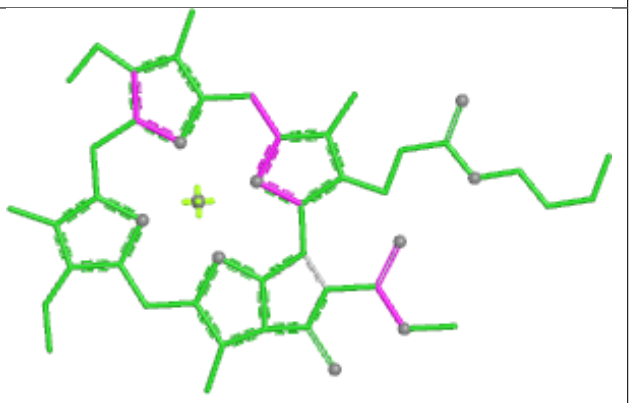
Ligand CLA W 215	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

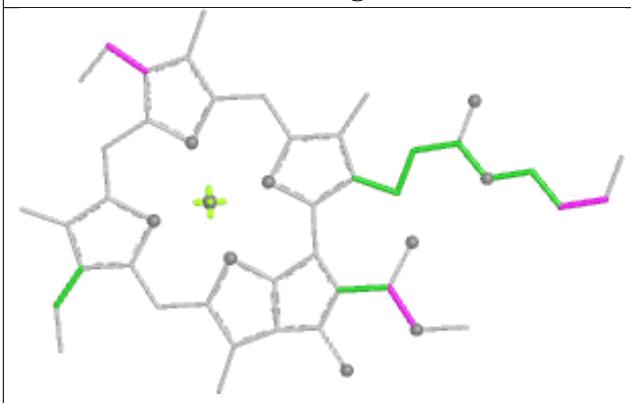
Ligand CLA A 305



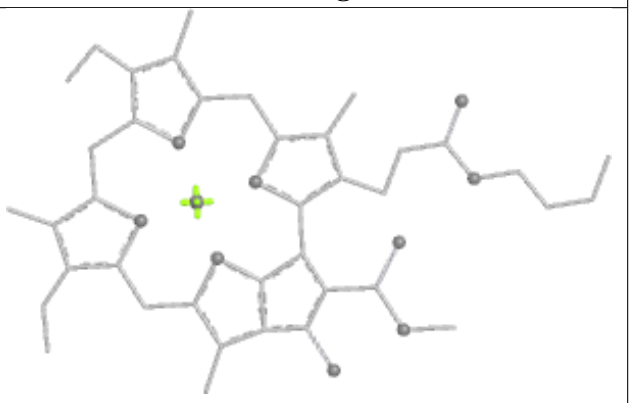
Bond lengths



Bond angles

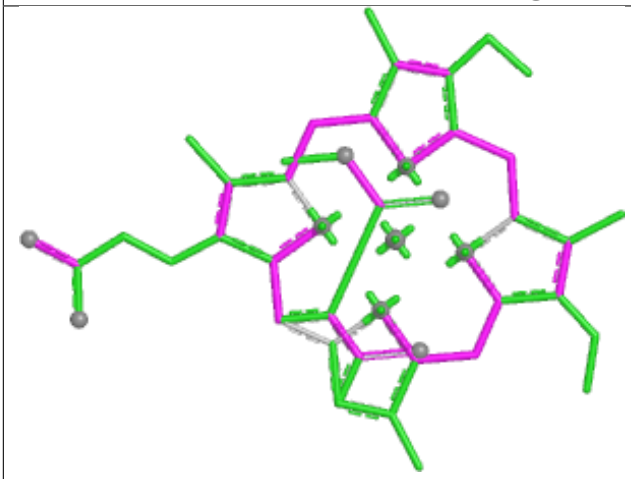


Torsions

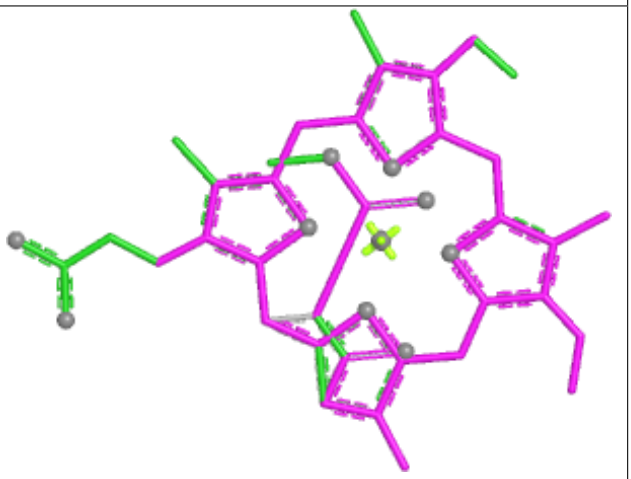


Rings

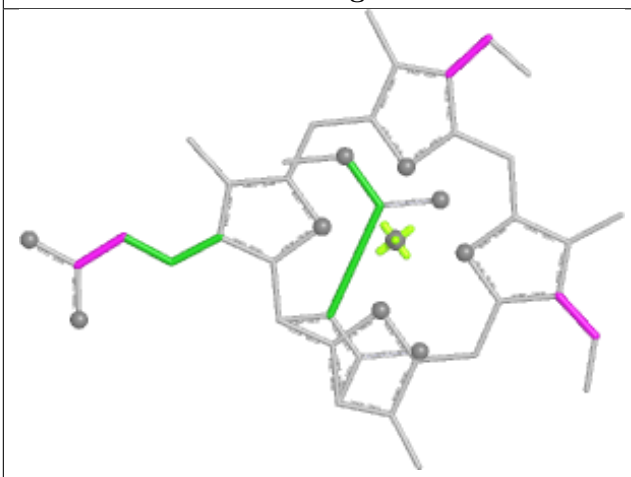
Ligand KC1 E 309



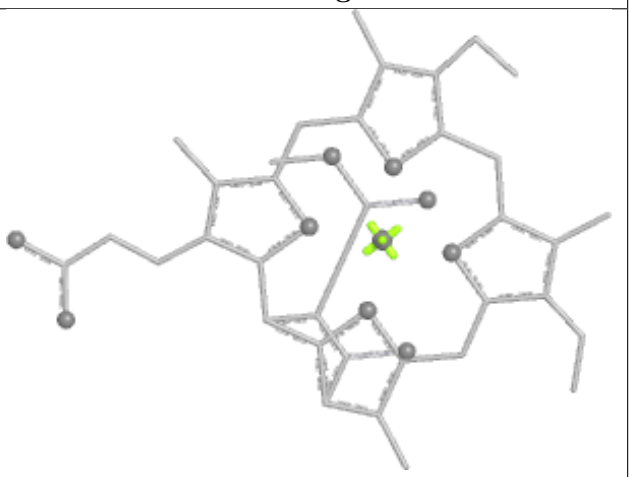
Bond lengths



Bond angles

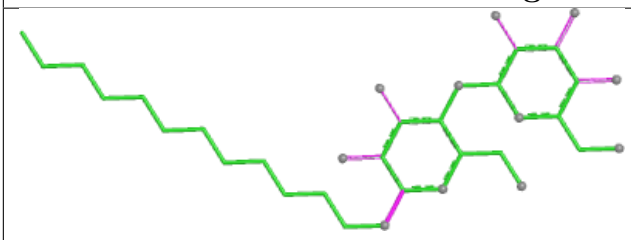


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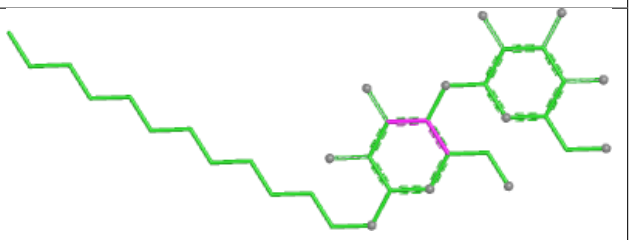


Rings

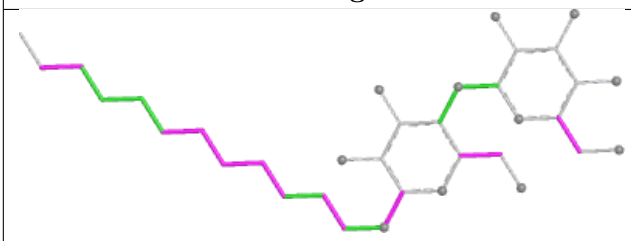
Ligand LMT L 303



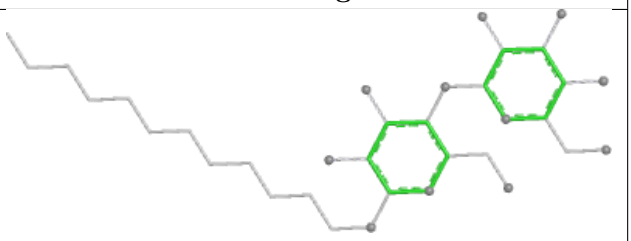
Bond lengths



Bond angles

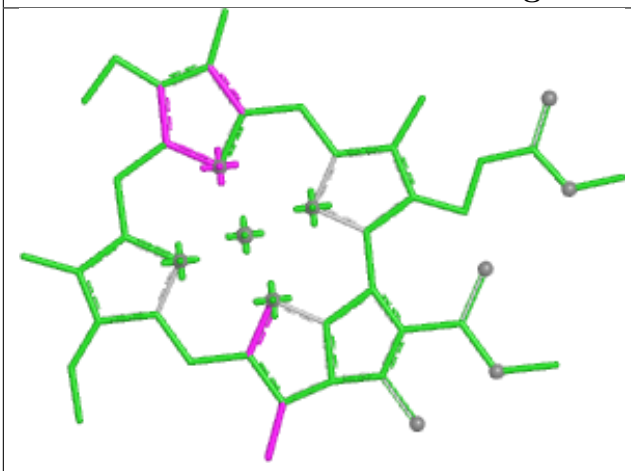


Torsions

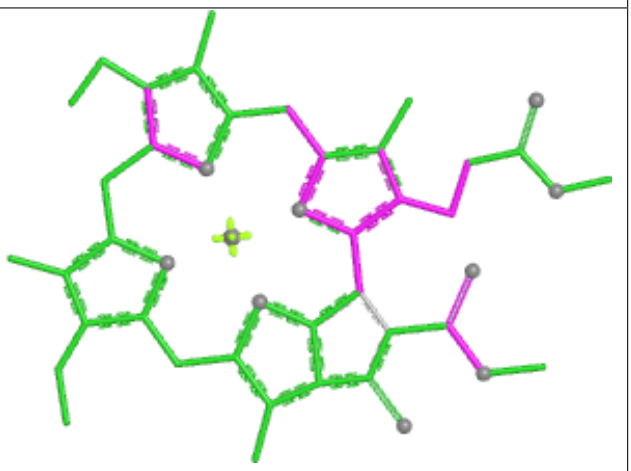


Rings

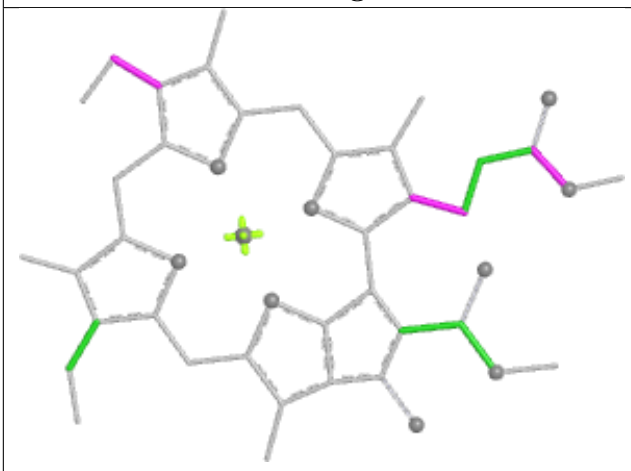
Ligand CLA N 311



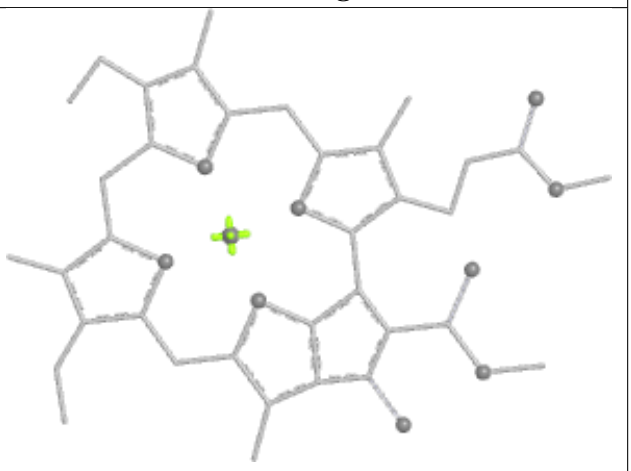
Bond lengths



Bond angles

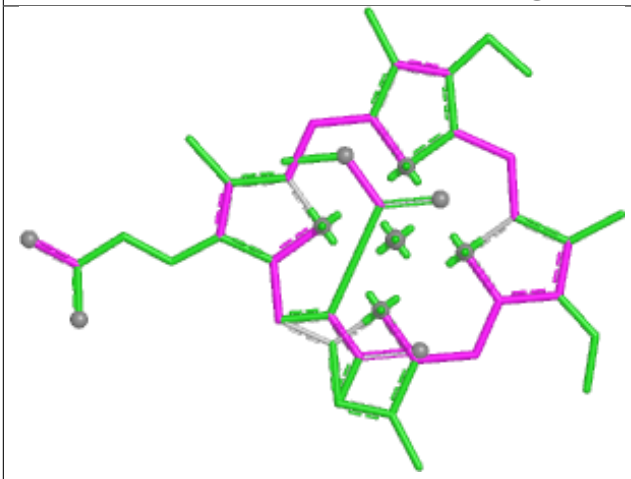


Torsions

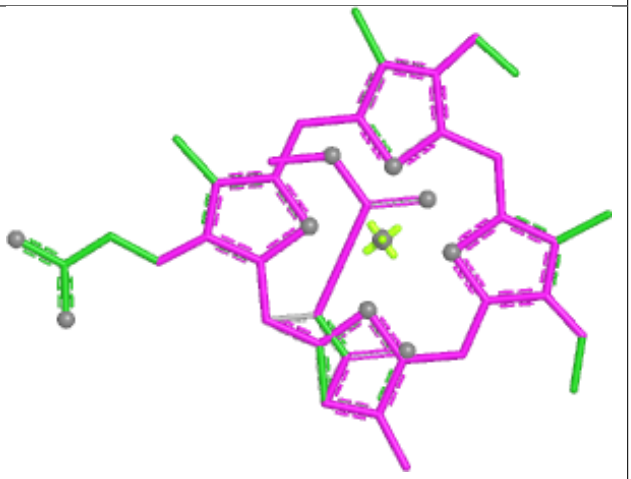


Rings

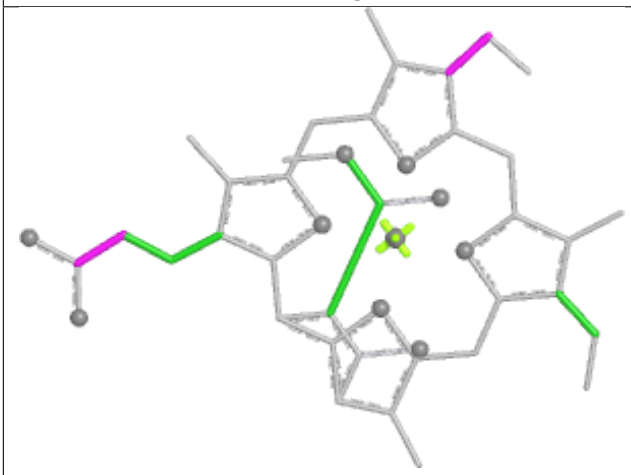
Ligand KC1 L 317



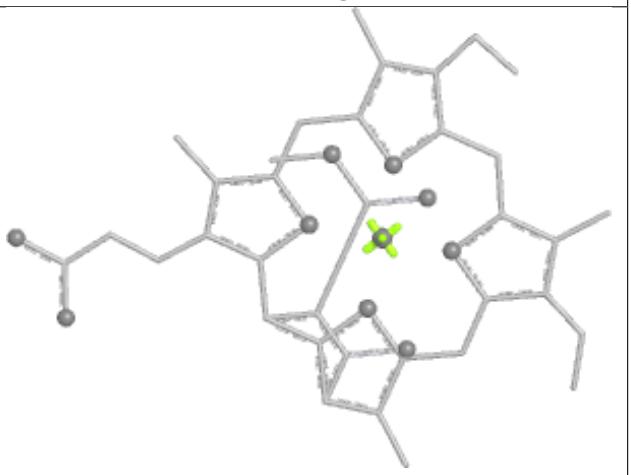
Bond lengths



Bond angles



Torsions

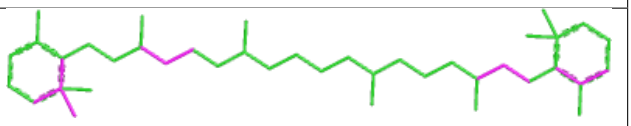


Rings

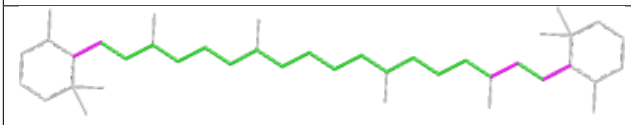
Ligand BCR a 847



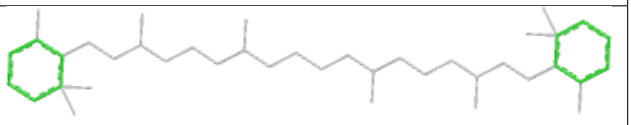
Bond lengths



Bond angles

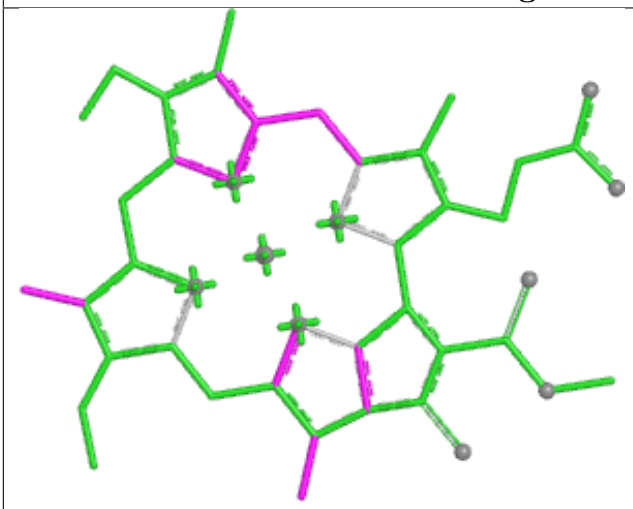


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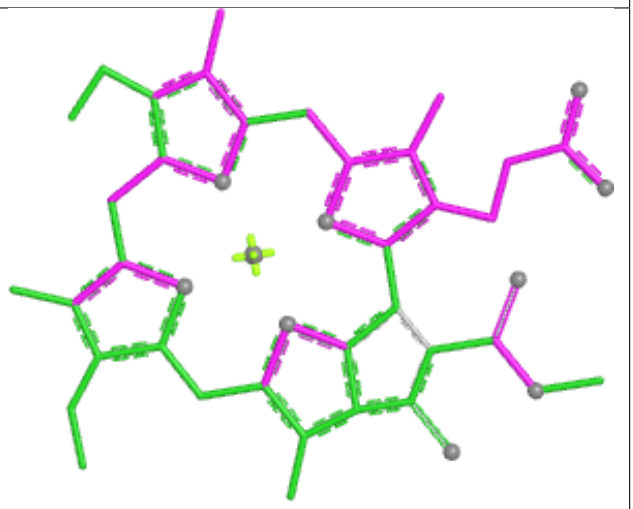


Rings

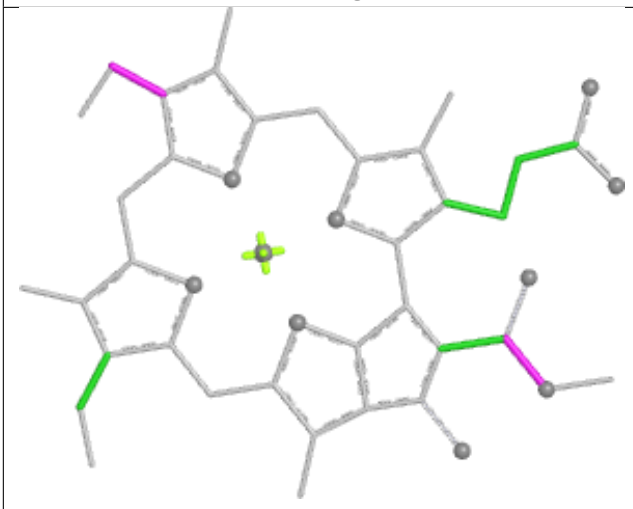
Ligand CLA W 216



Bond lengths



Bond angles

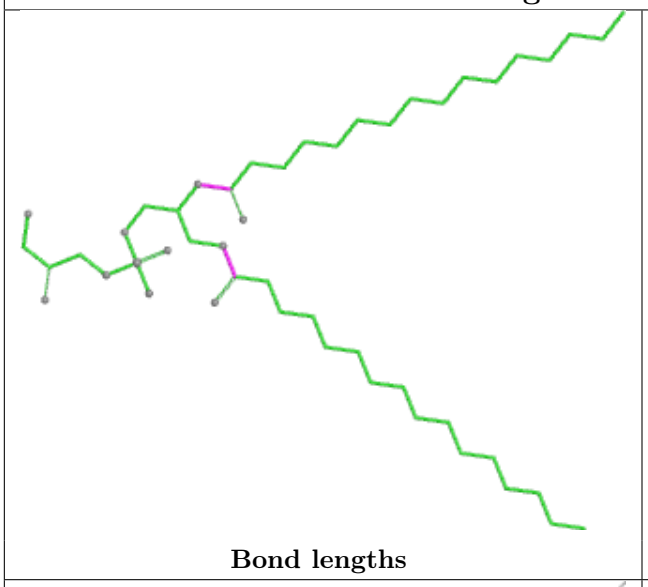


Torsions

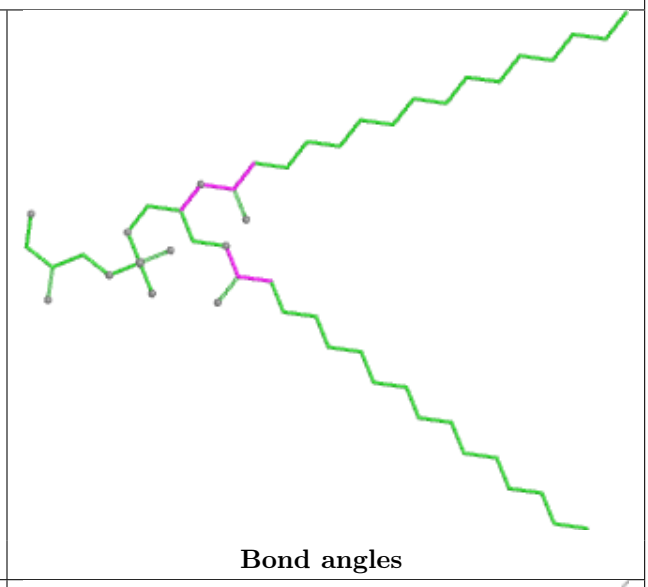


Rings

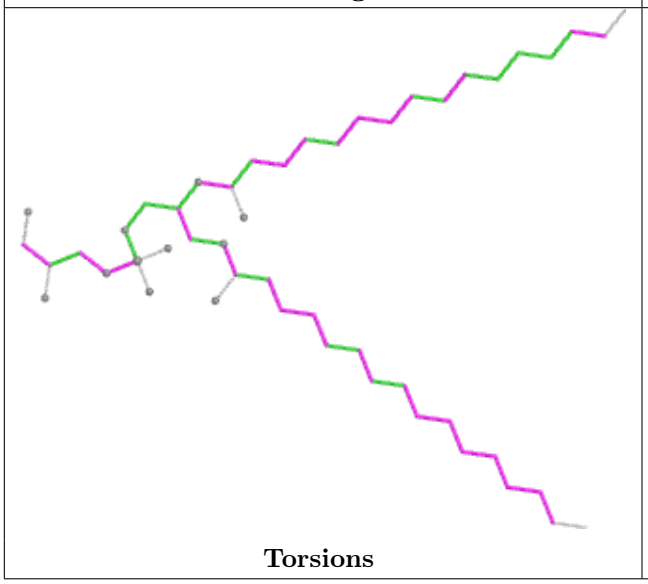
Ligand LHG D 319



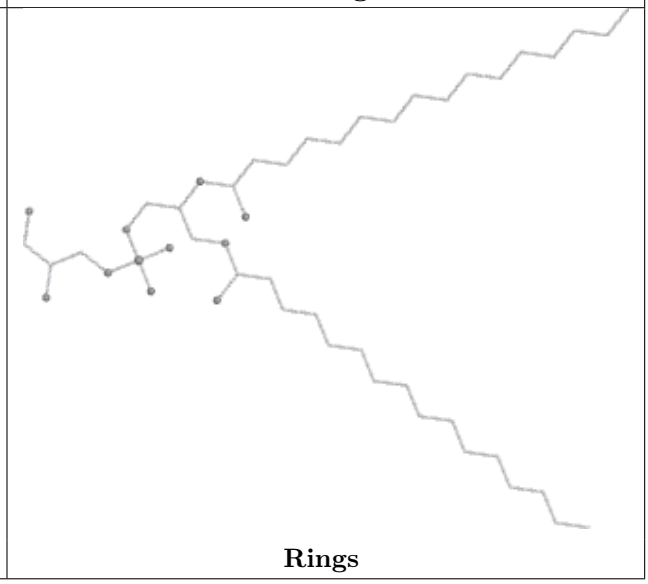
Bond lengths



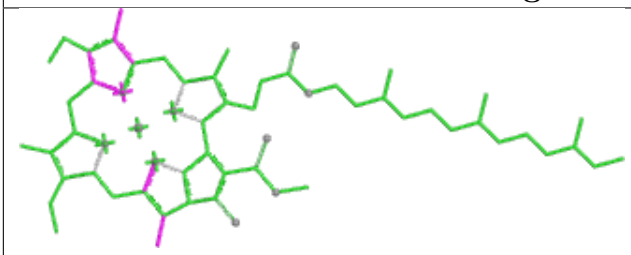
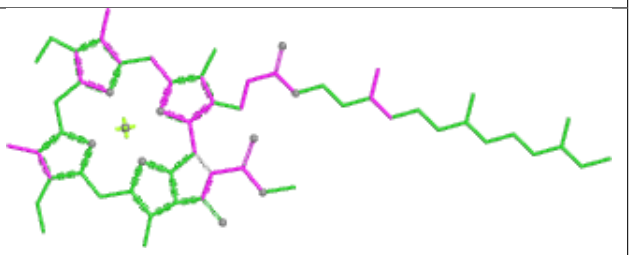
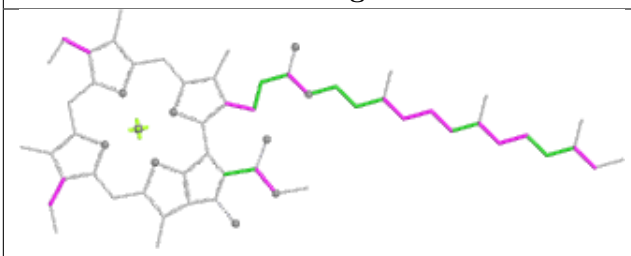
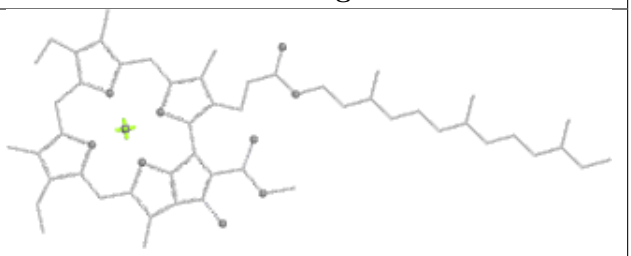
Bond angles

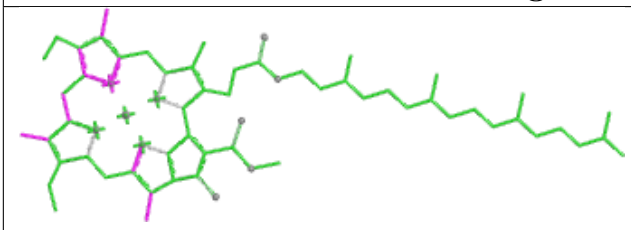
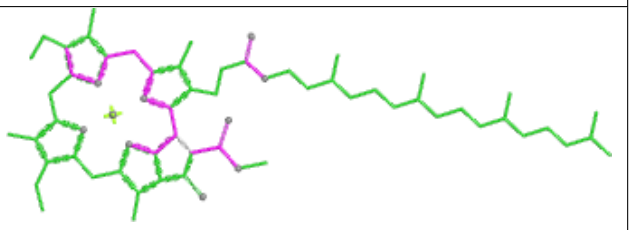
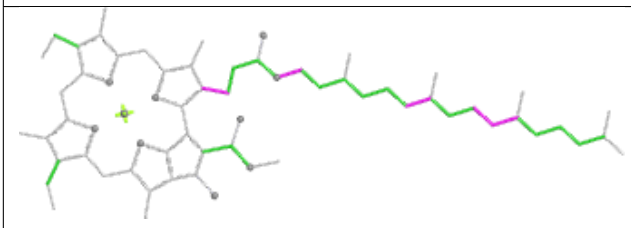
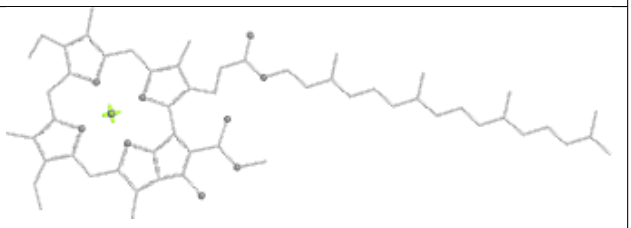


Torsions

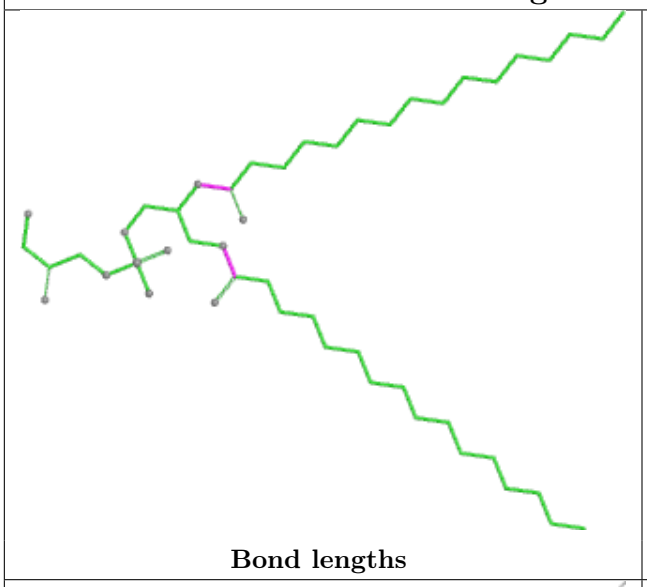


Rings

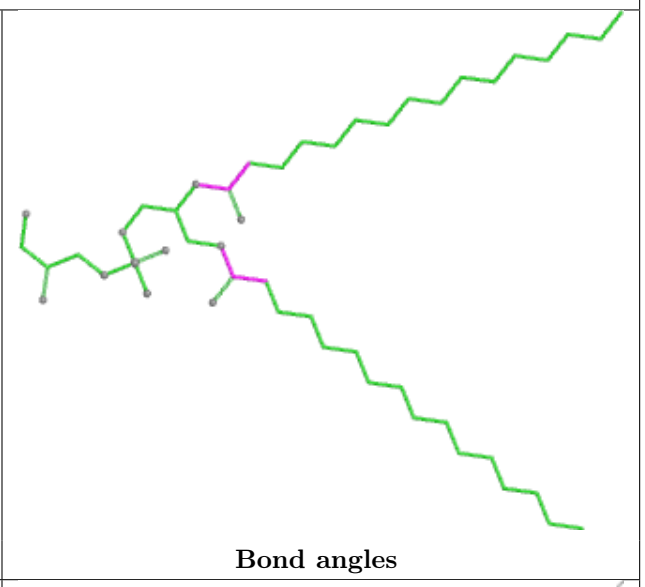
Ligand CLA D 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

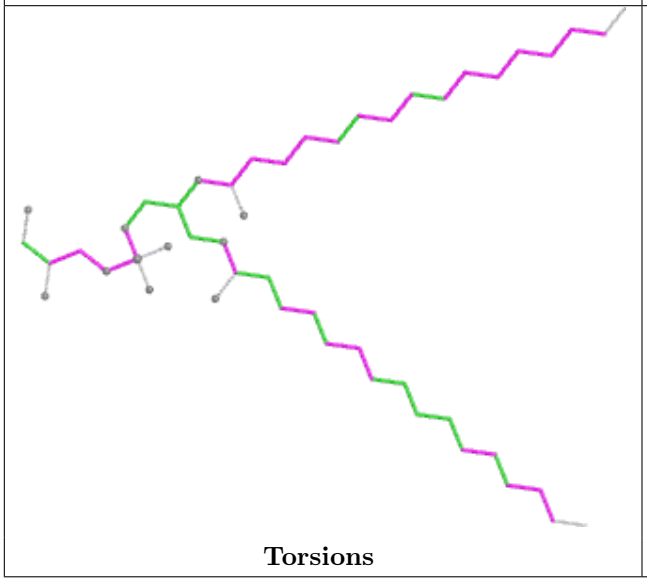
Ligand LHG I 316



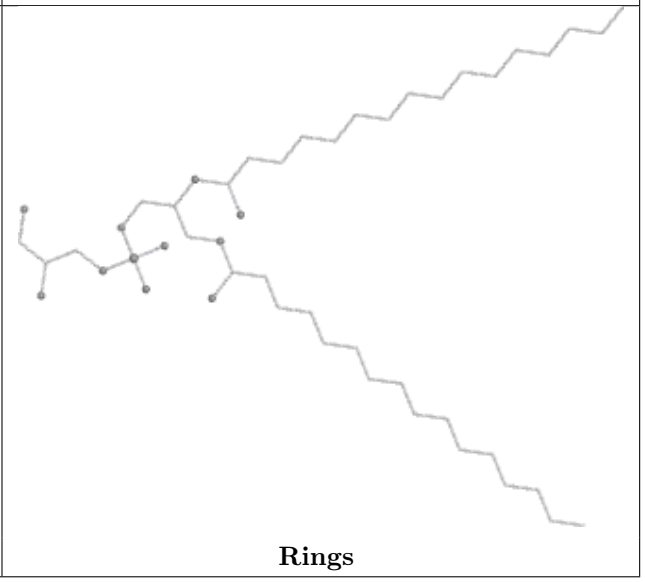
Bond lengths



Bond angles

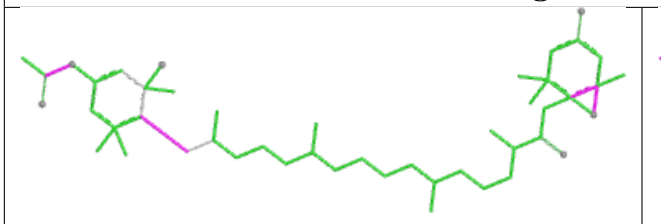


Torsions

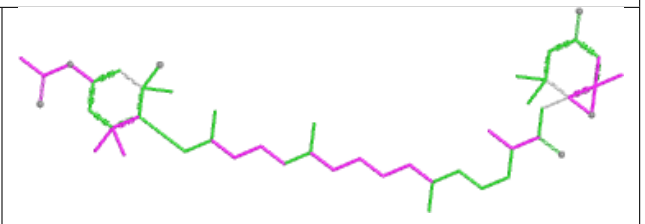


Rings

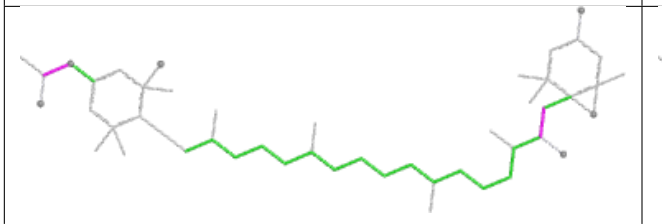
Ligand A86 P 306



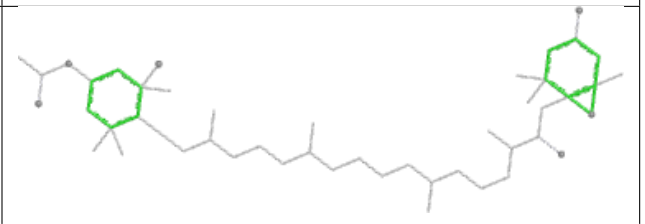
Bond lengths



Bond angles

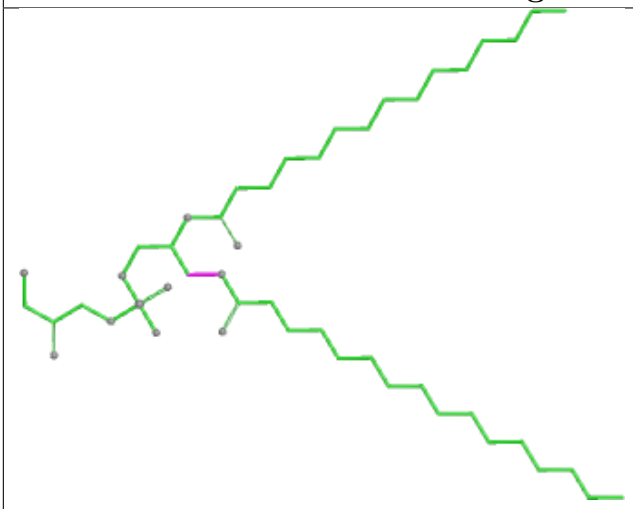


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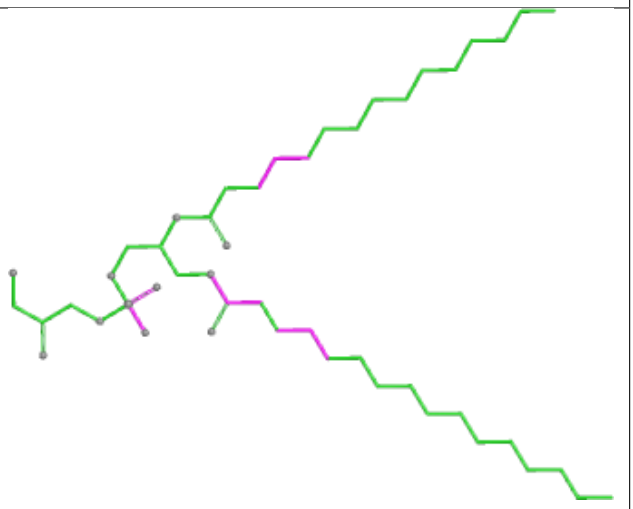


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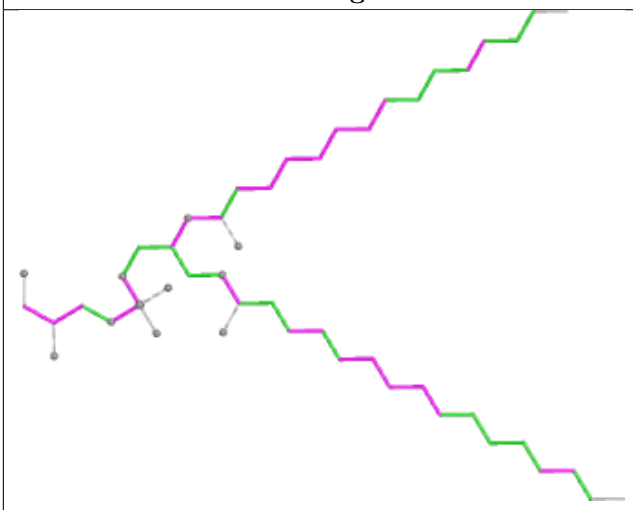
Ligand LHG a 842



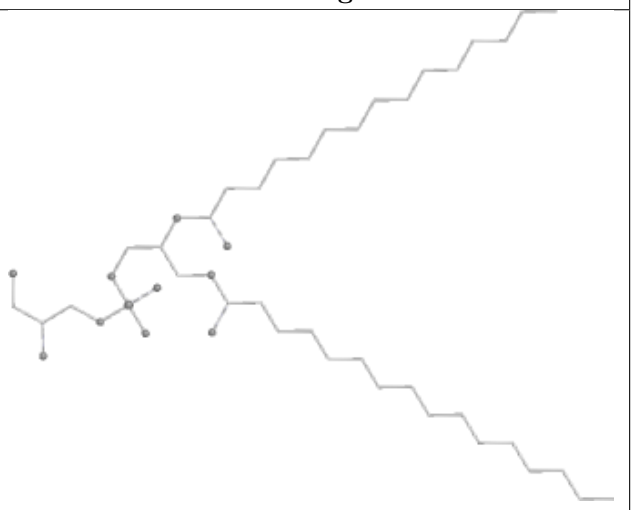
Bond lengths



Bond angles

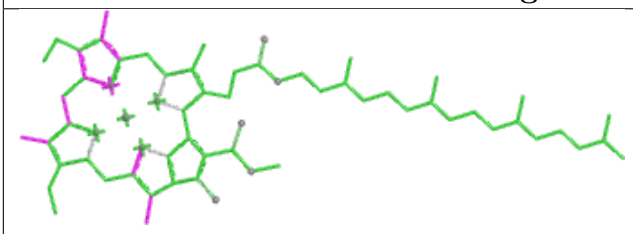


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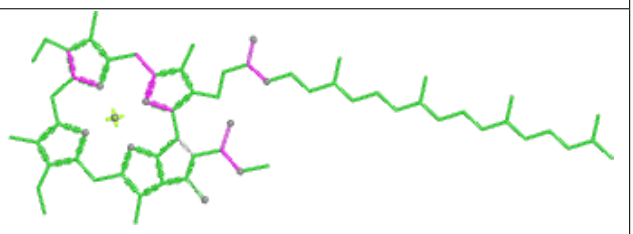


Rings

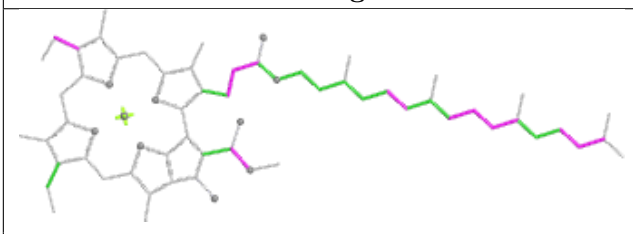
Ligand CLA M 309



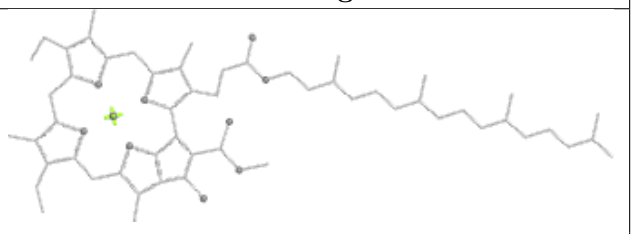
Bond lengths



Bond angles

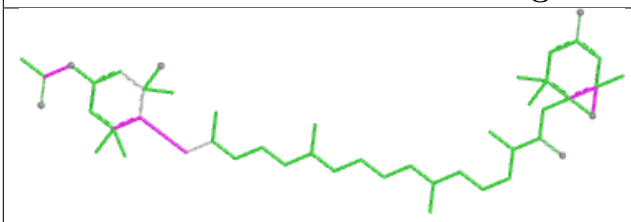


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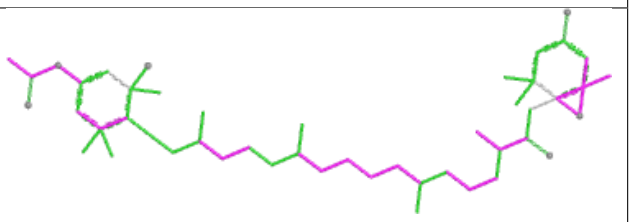


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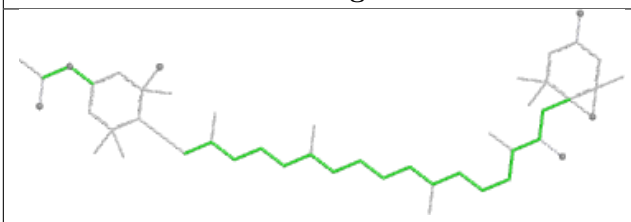
Ligand A86 F 306



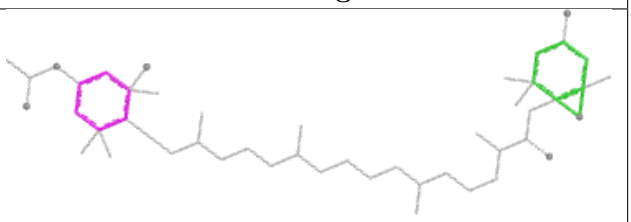
Bond lengths



Bond angles

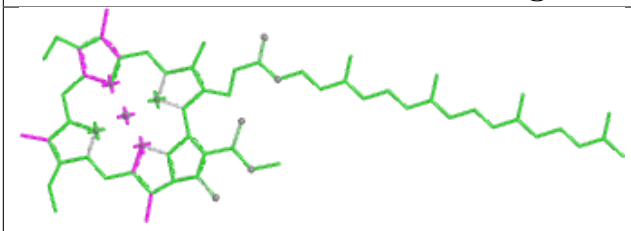


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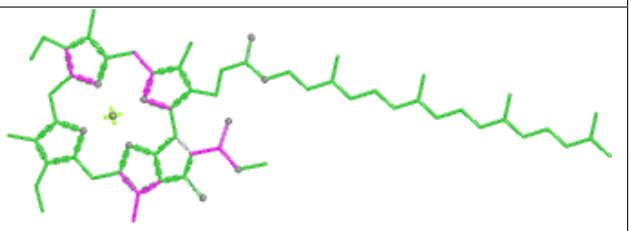


Rings

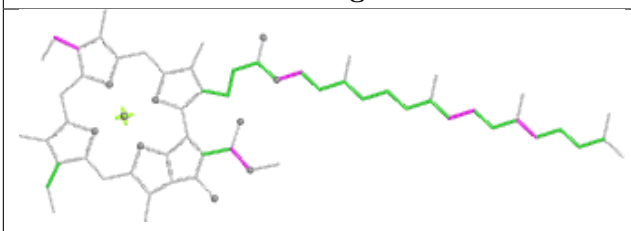
Ligand CLA a 838



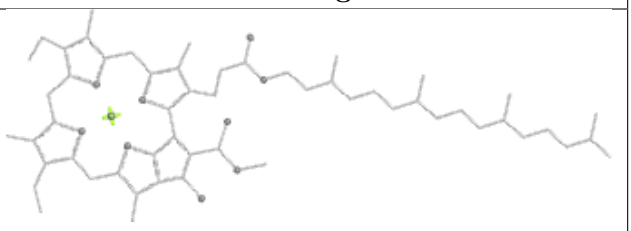
Bond lengths



Bond angles

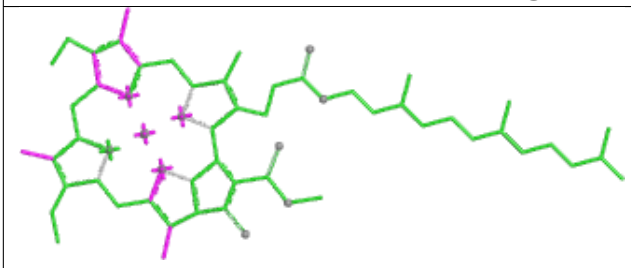


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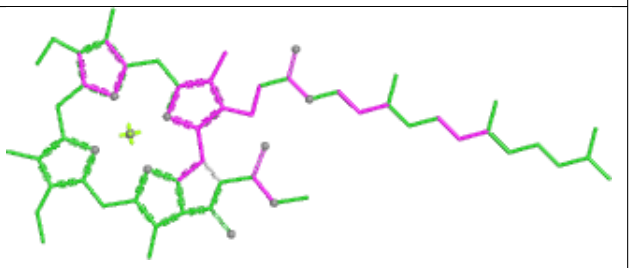


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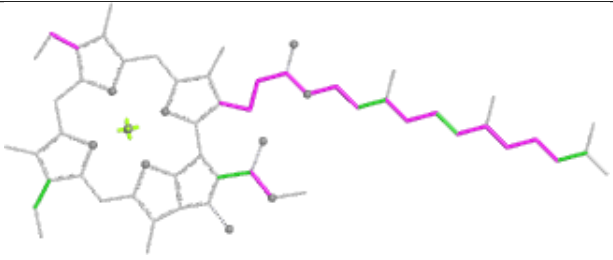
Ligand CLA P 314



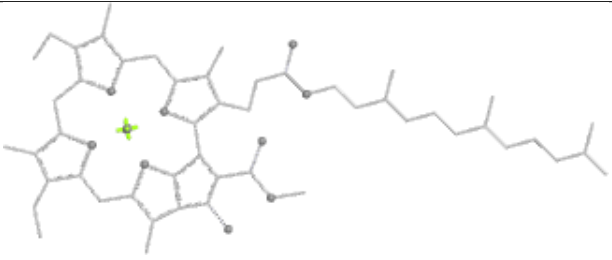
Bond lengths



Bond angles

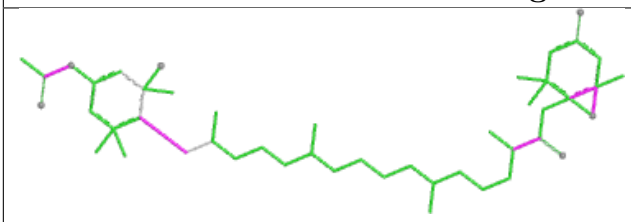


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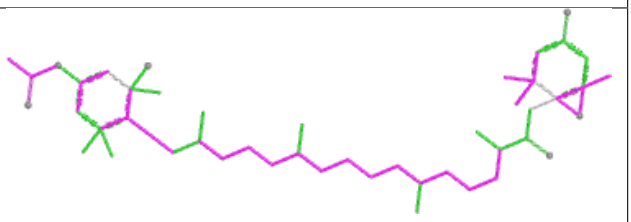


Rings

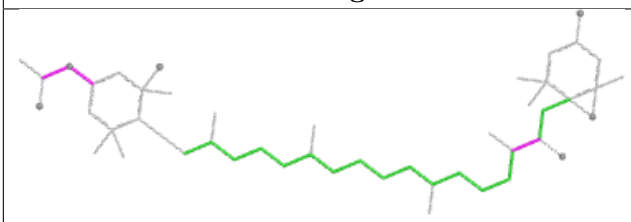
Ligand A86 X 302



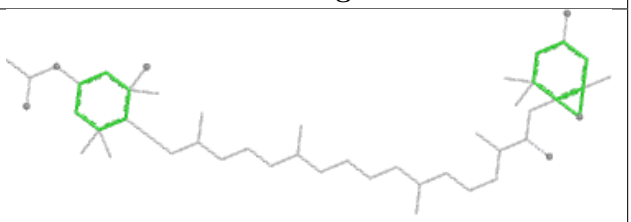
Bond lengths



Bond angles

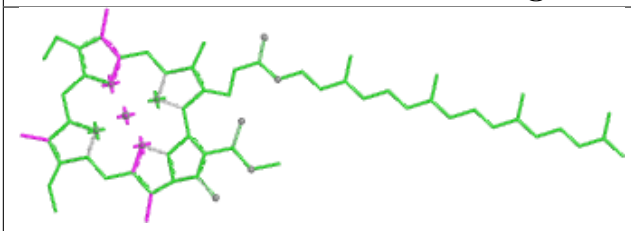


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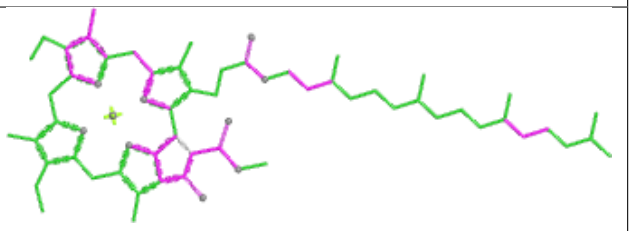


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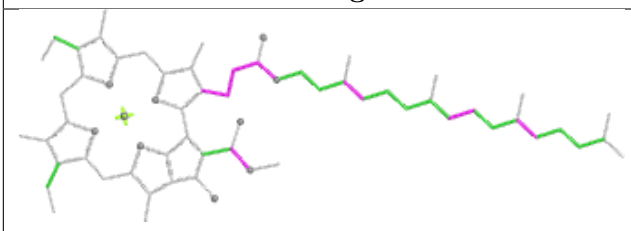
Ligand CLA b 828



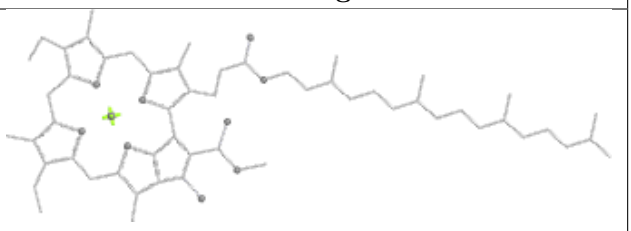
Bond lengths



Bond angles

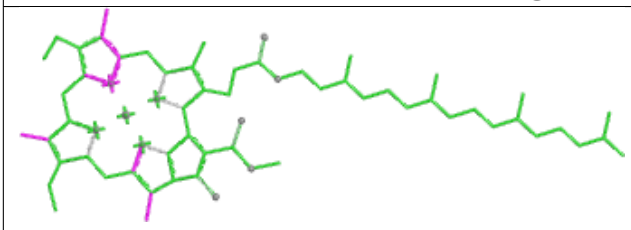


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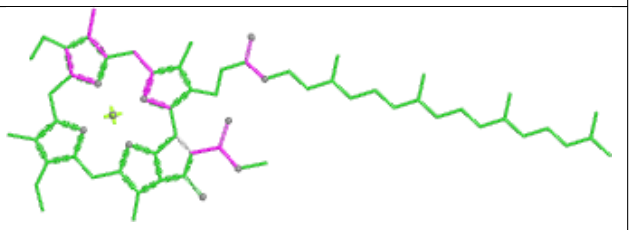


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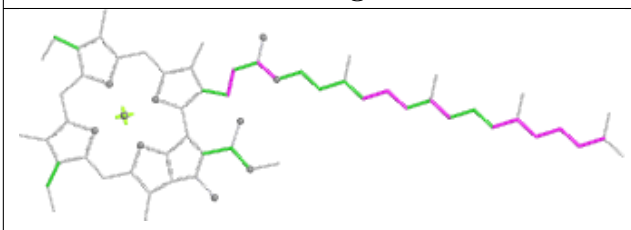
Ligand CLA a 839



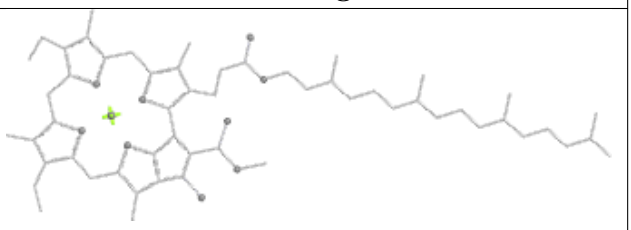
Bond lengths



Bond angles

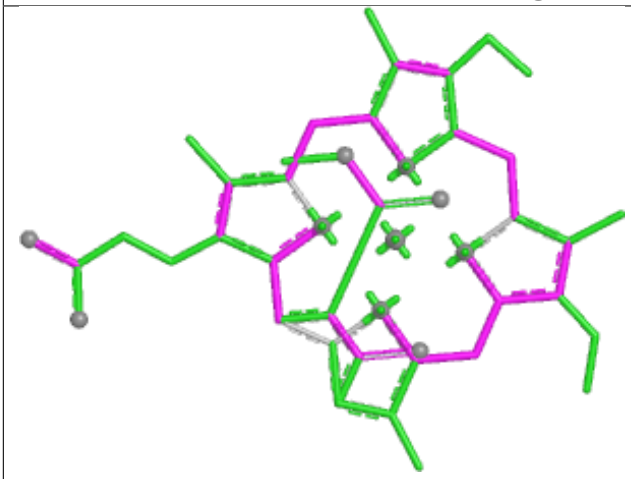


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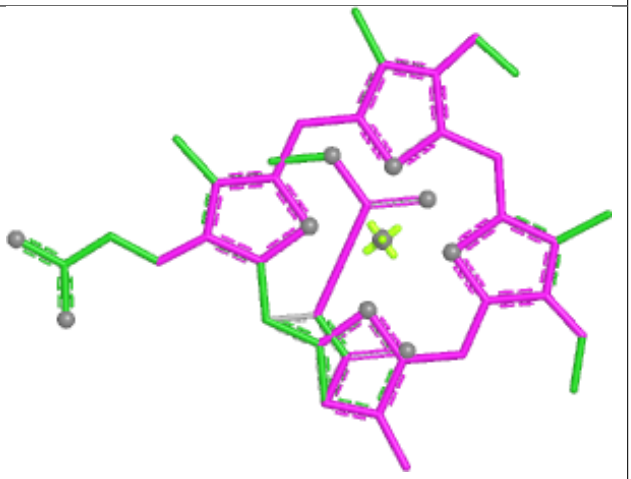


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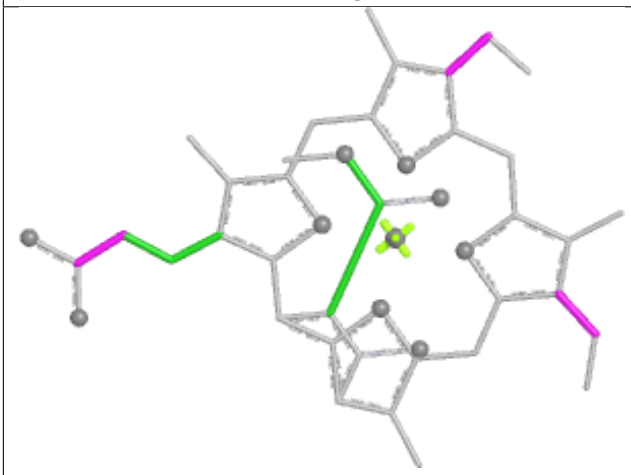
Ligand KC1 J 314



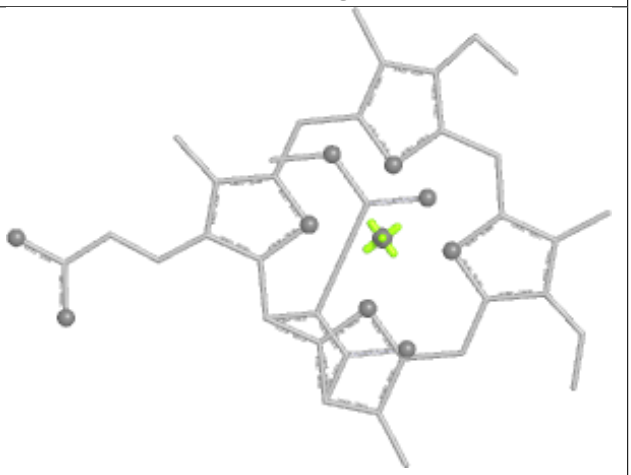
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Bond angles

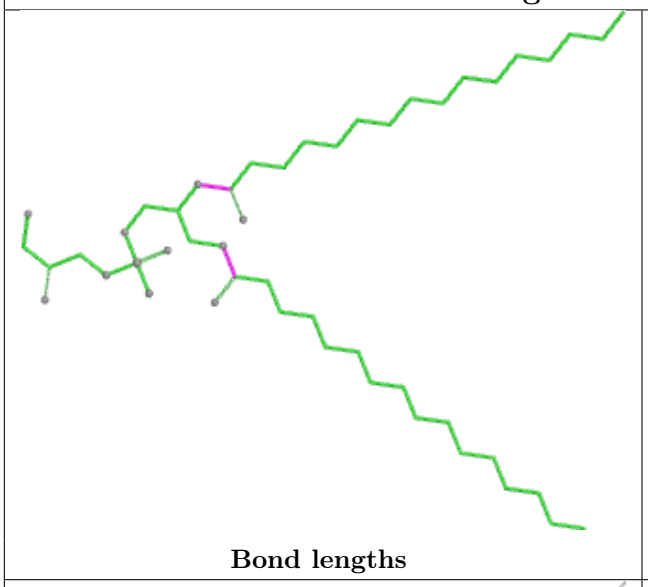


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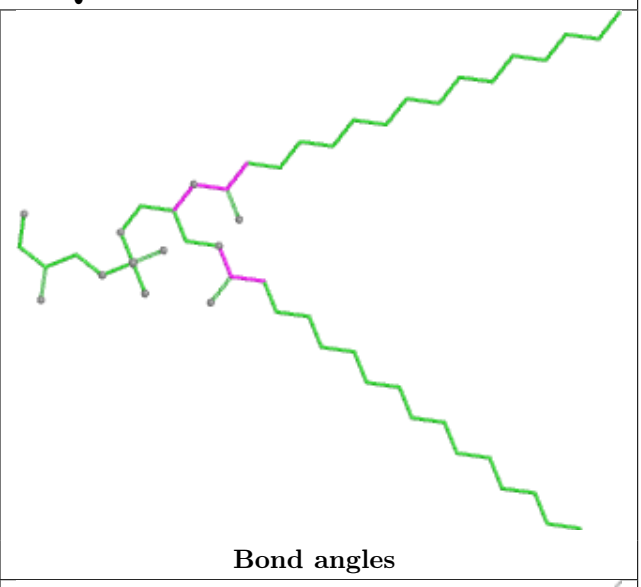


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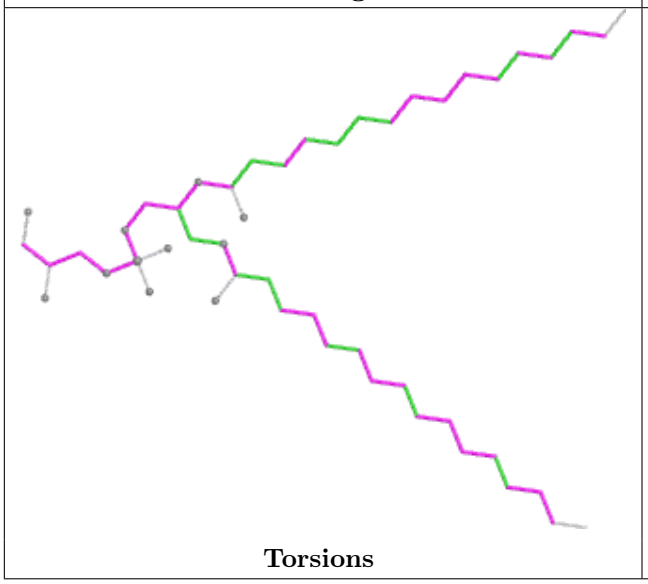
Ligand LHG Q 315



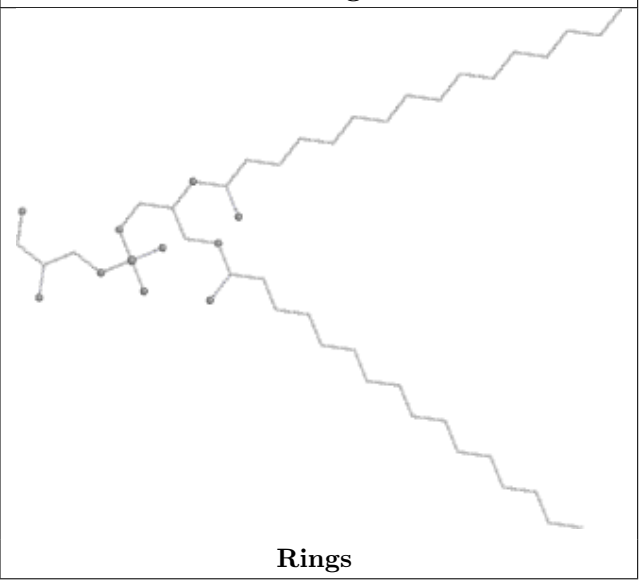
Bond lengths



Bond angles

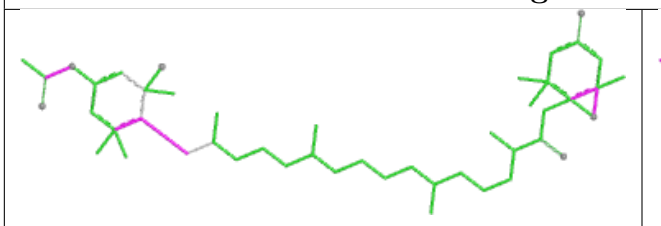


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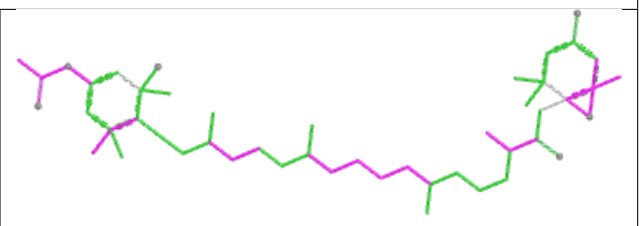


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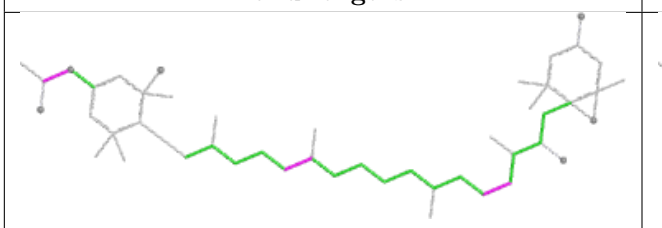
Ligand A86 R 305



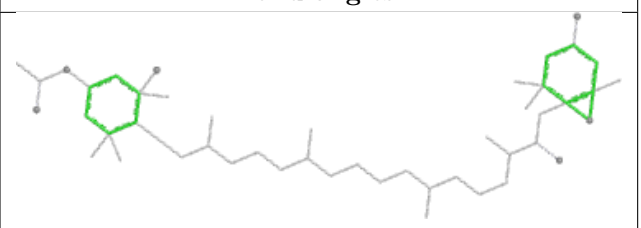
Bond lengths



Bond angles

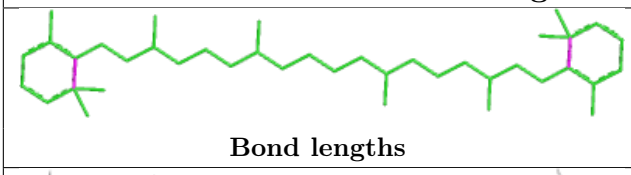


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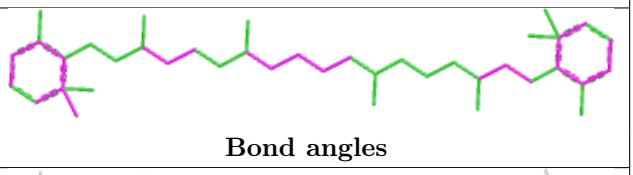


Rings

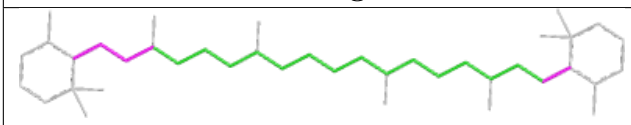
Ligand BCR l 207



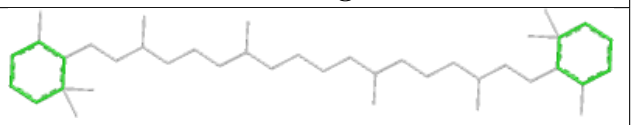
Bond lengths



Bond angles

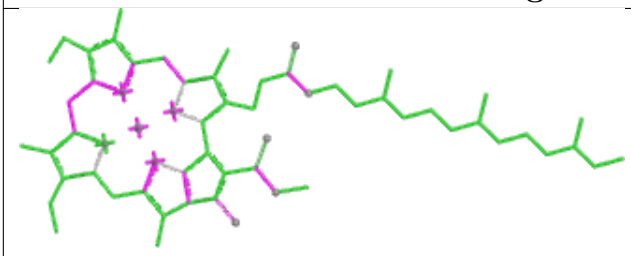


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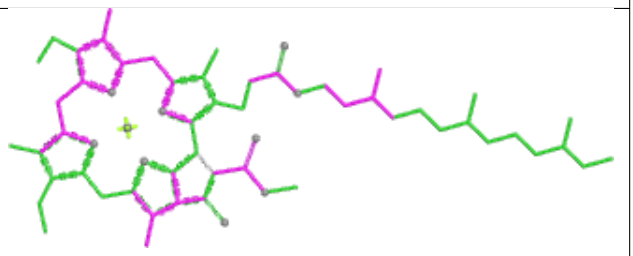


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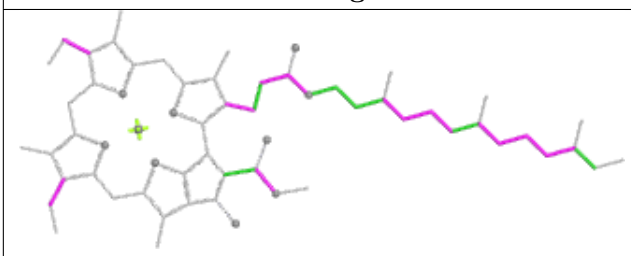
Ligand CLA L 308



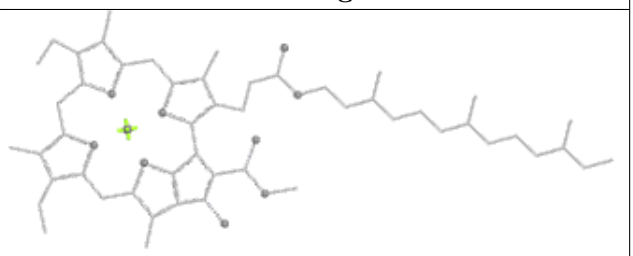
Bond lengths



Bond angles

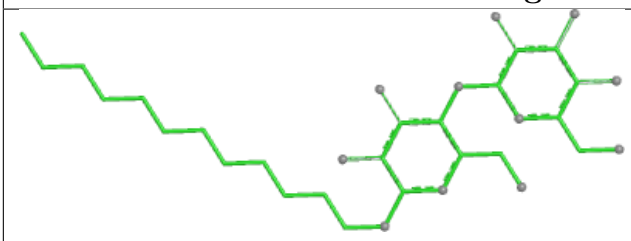


Torsions

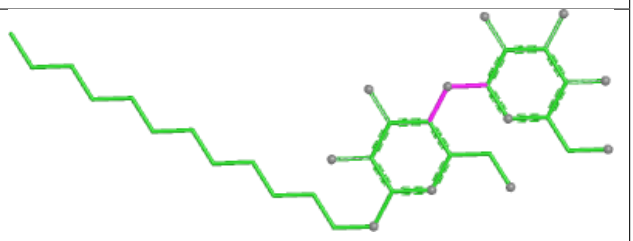


Rings

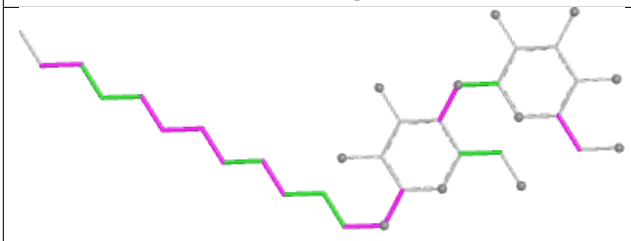
Ligand LMT h 205



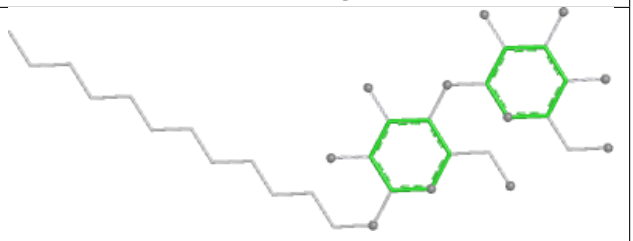
Bond lengths



Bond angles

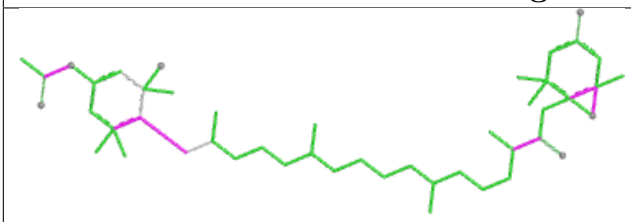


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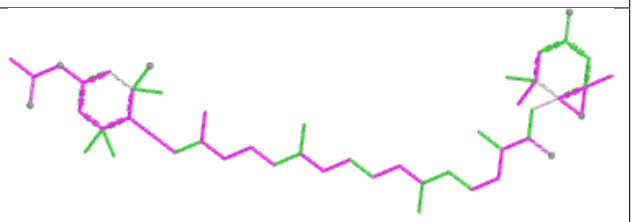


Rings

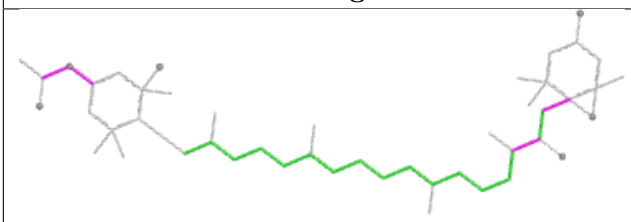
Ligand A86 C 202



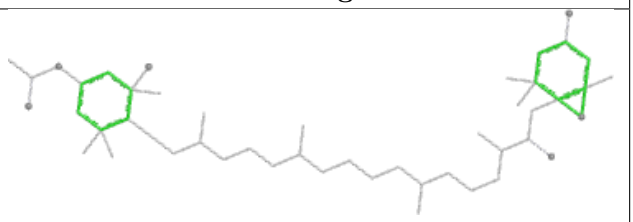
Bond lengths



Bond angles

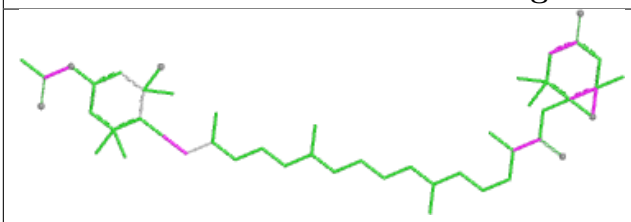


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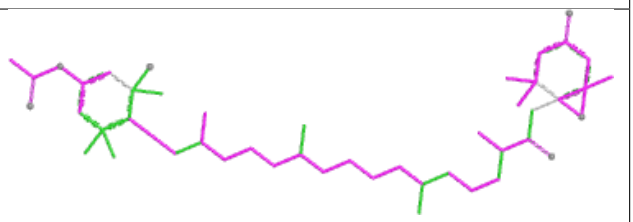


Rings

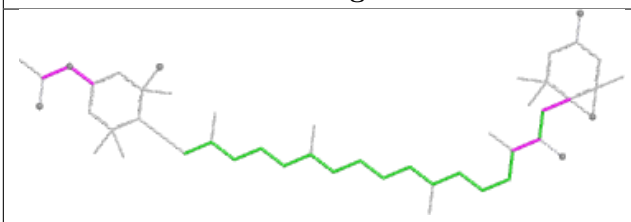
Ligand A86 T 305



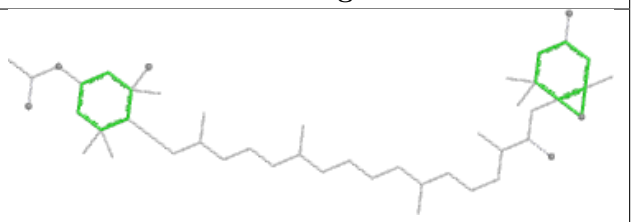
Bond lengths



Bond angles

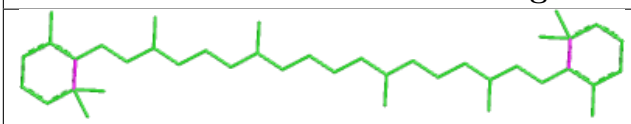


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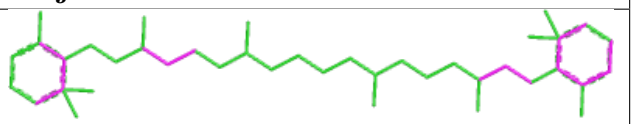


Rings

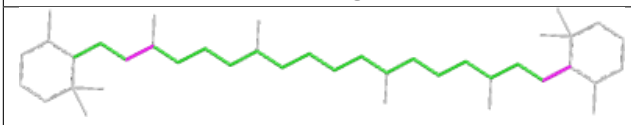
Ligand BCR j 107



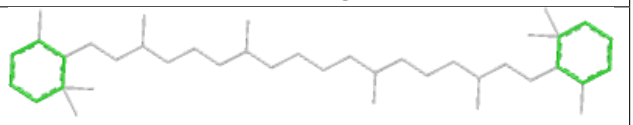
Bond lengths



Bond angles

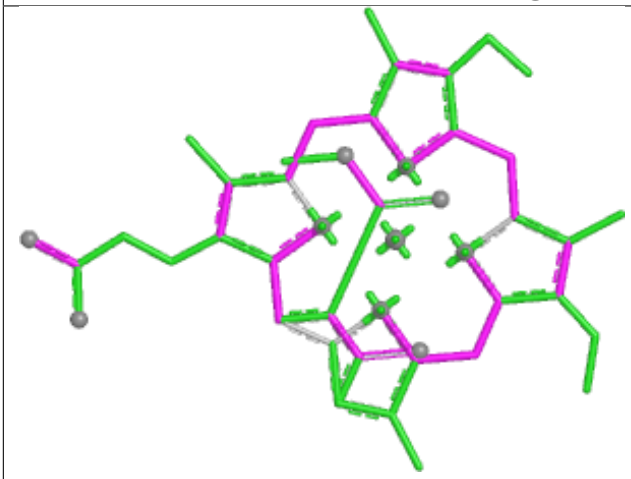


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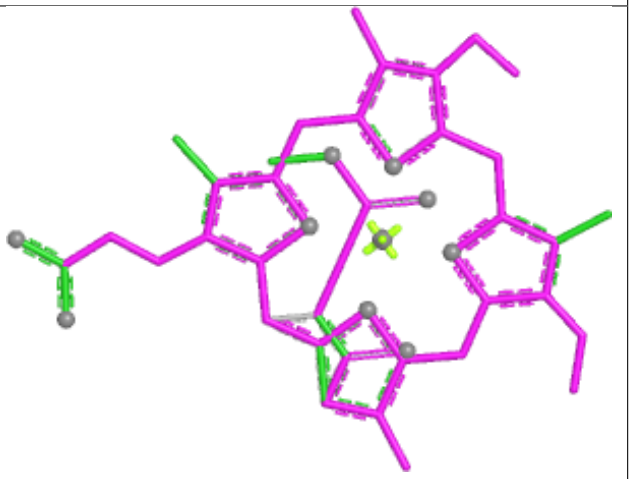


Rings

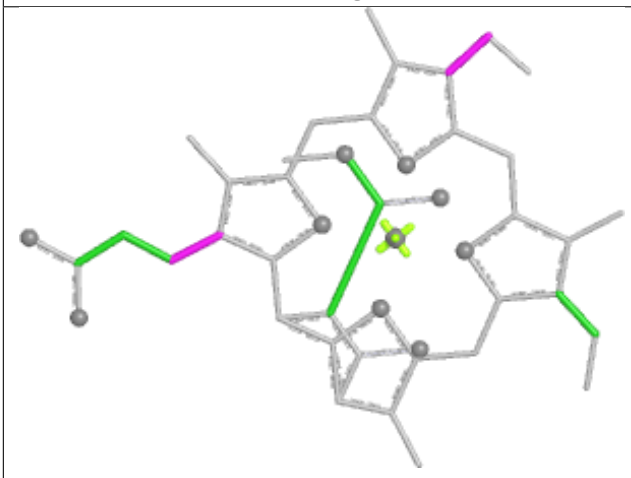
Ligand KC1 P 317



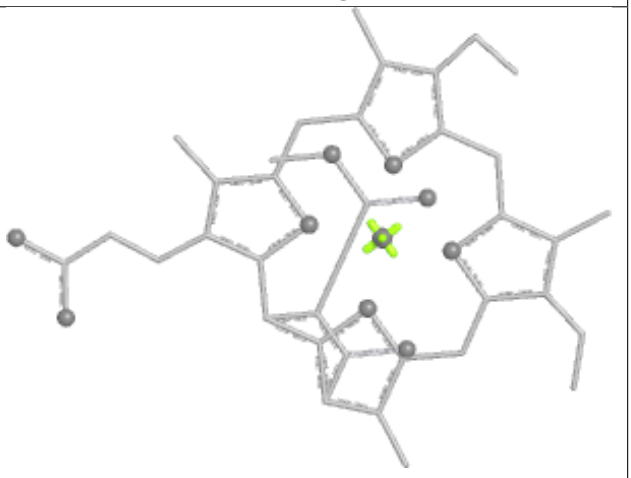
Bond lengths



Bond angles

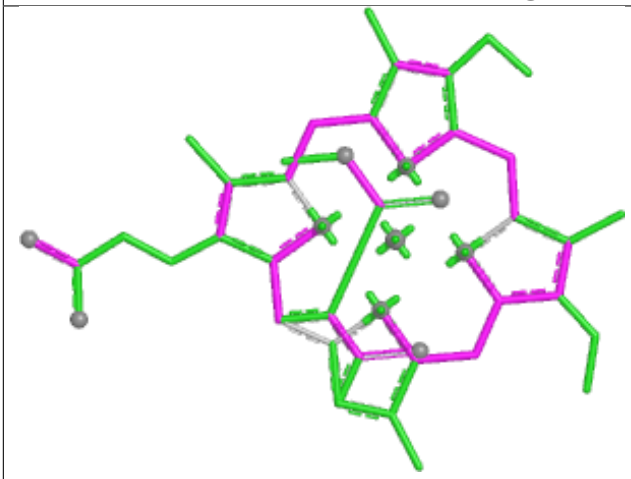


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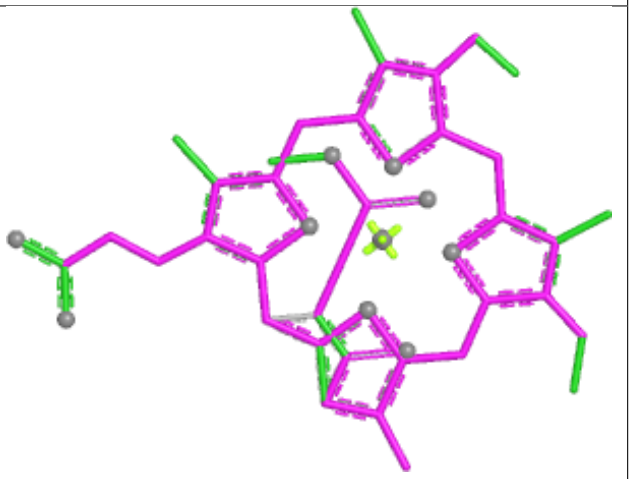


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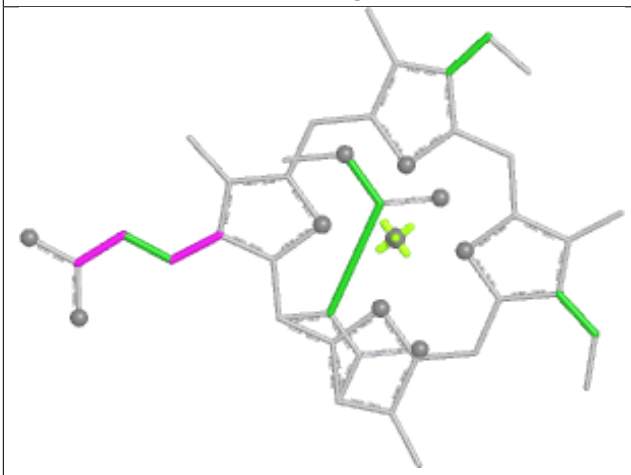
Ligand KC1 M 317



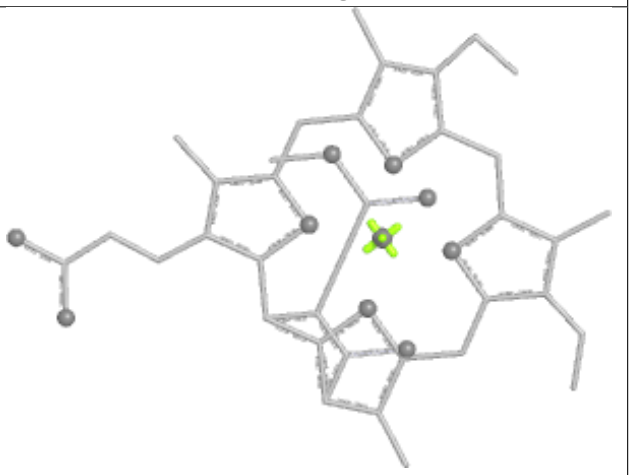
Bond lengths



Bond angles

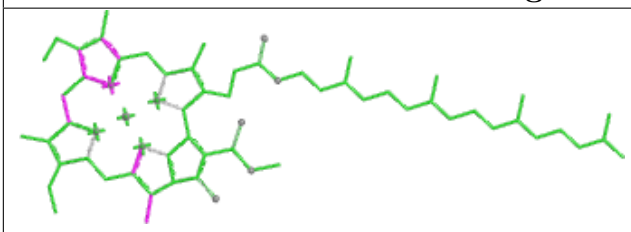


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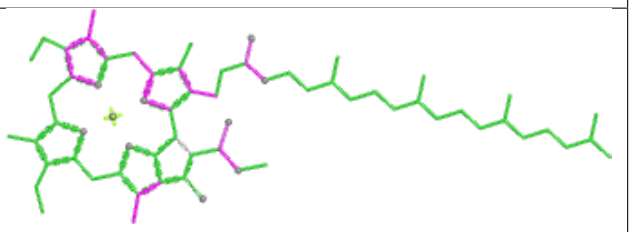


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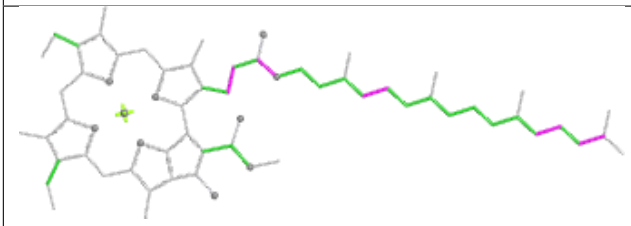
Ligand CLA E 310



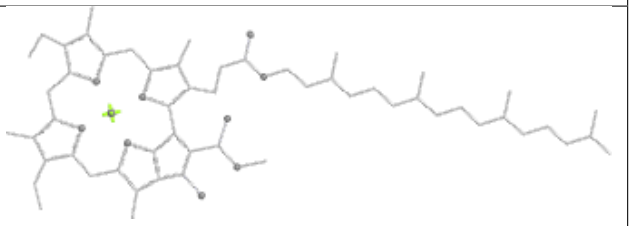
Bond lengths



Bond angles

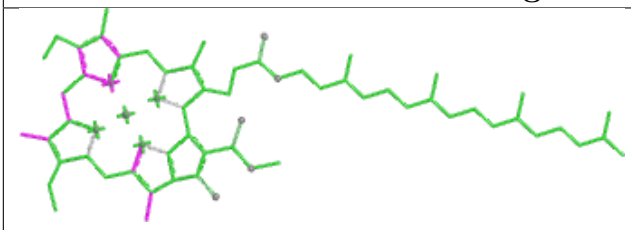


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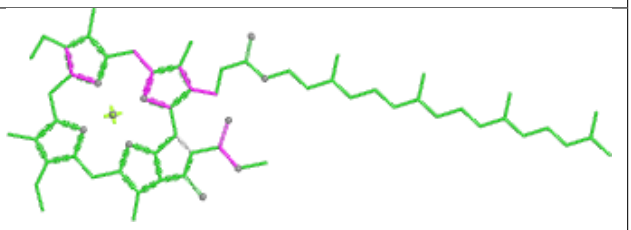


Rings

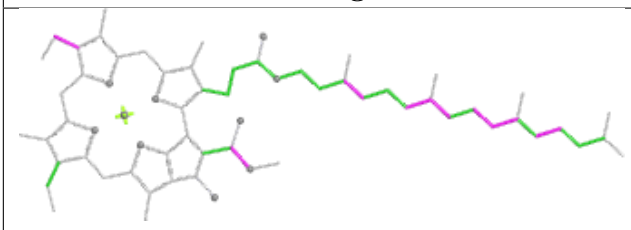
Ligand CLA N 316



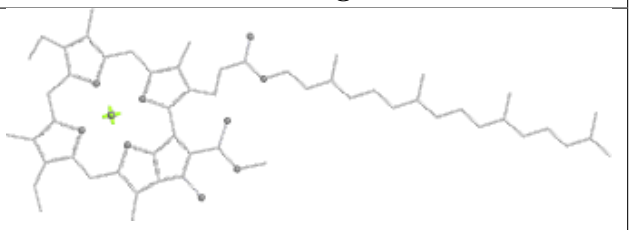
Bond lengths



Bond angles

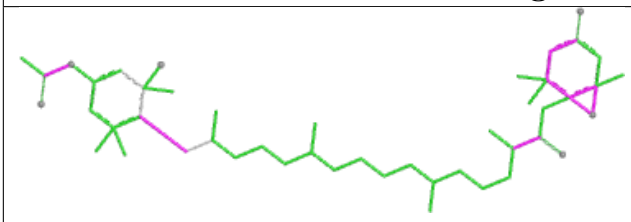


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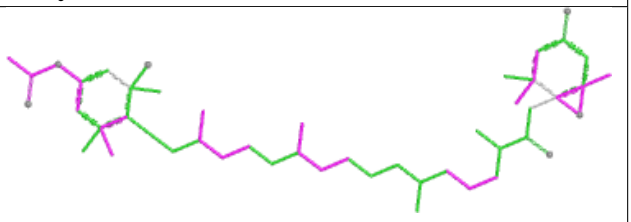


Rings

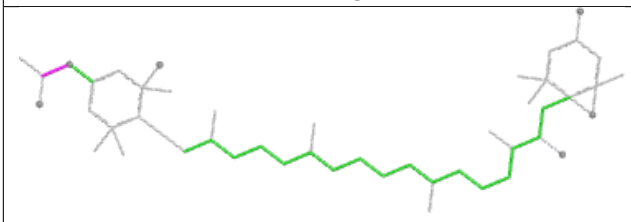
Ligand A86 Q 316



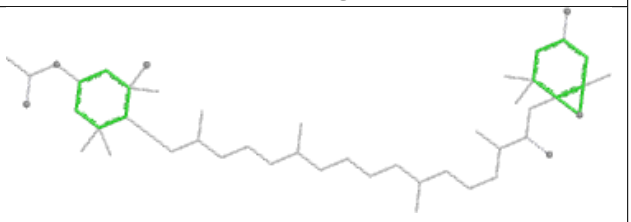
Bond lengths



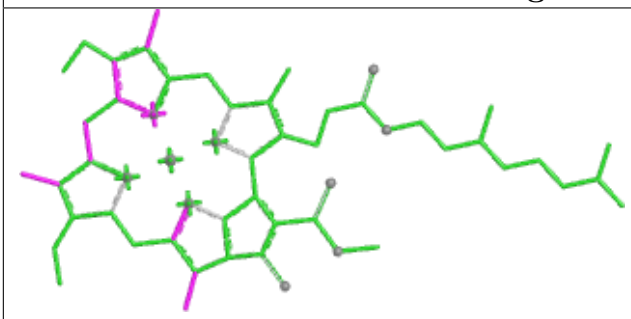
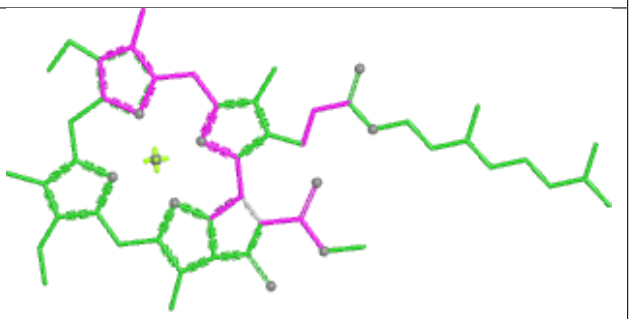
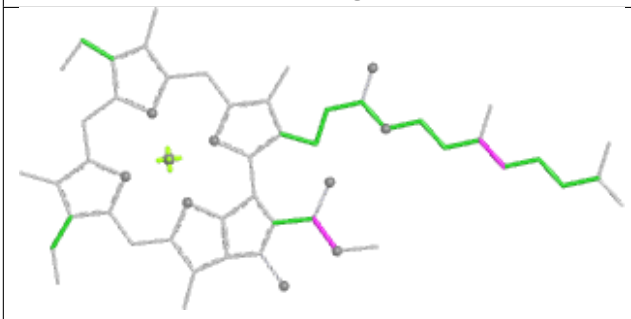
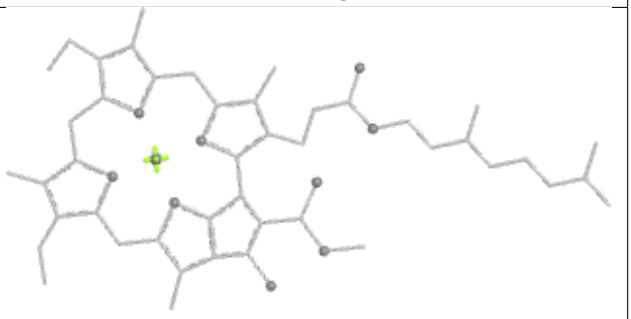
Bond angles

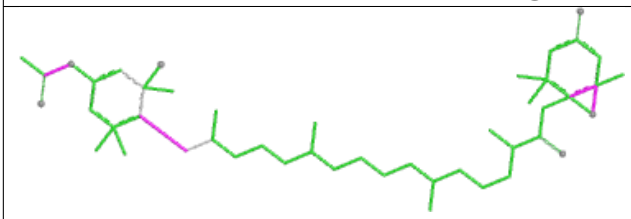
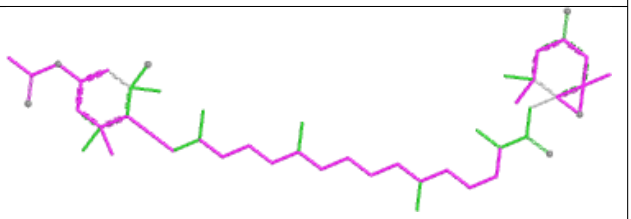
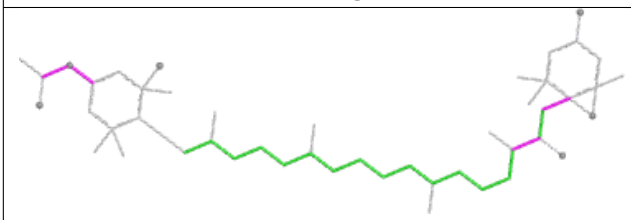
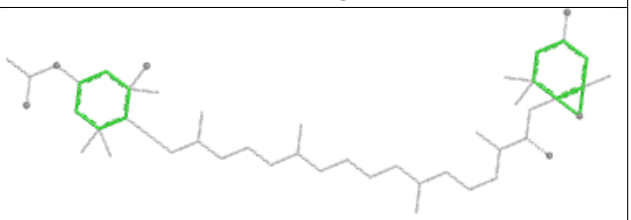


Torsions

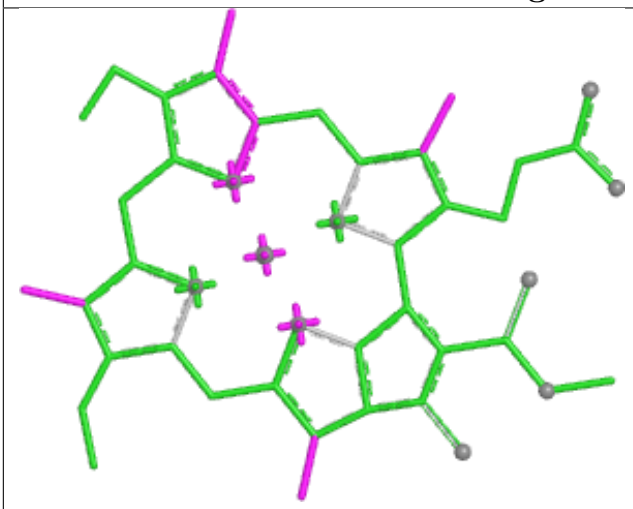


Rings

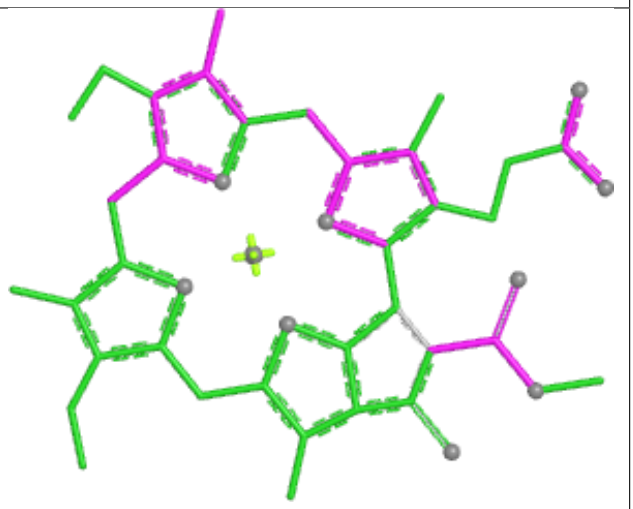
Ligand CLA b 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 M 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

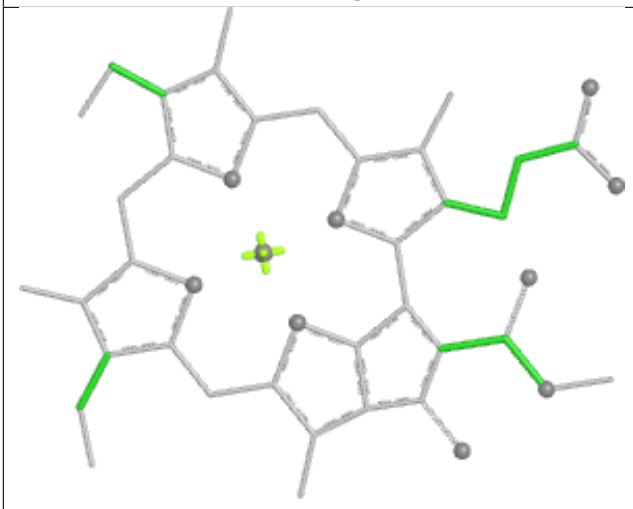
Ligand CLA a 813



Bond lengths



Bond angles

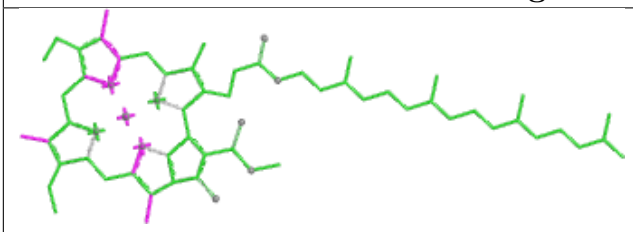


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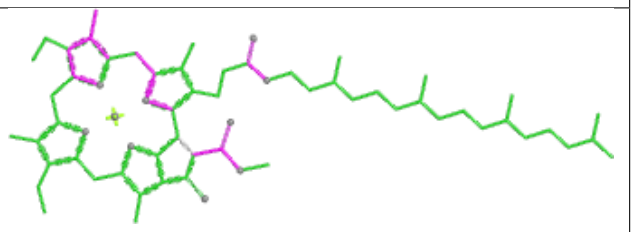


Rings

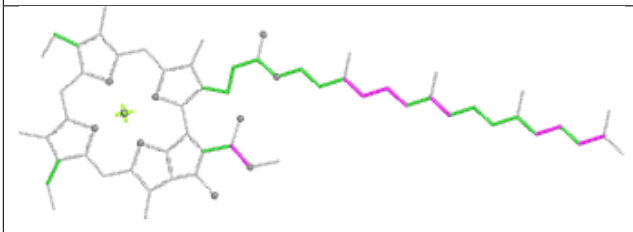
Ligand CLA a 820



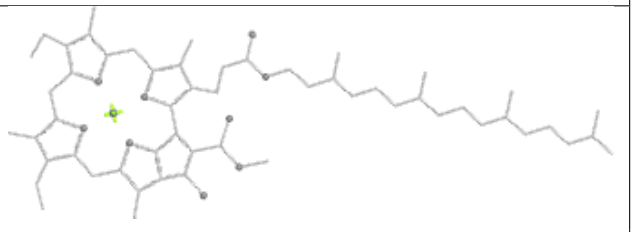
Bond lengths



Bond angles

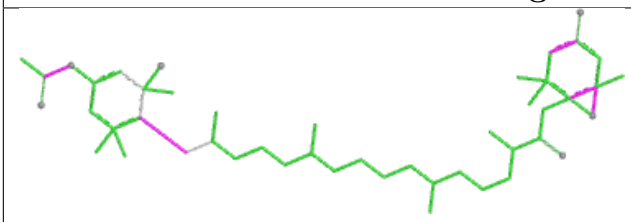


Torsions

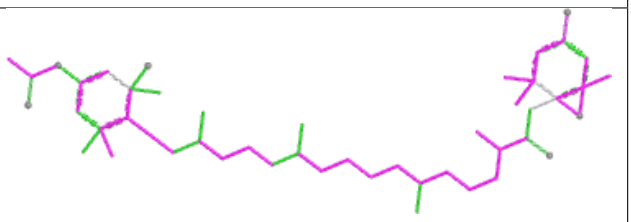


Rings

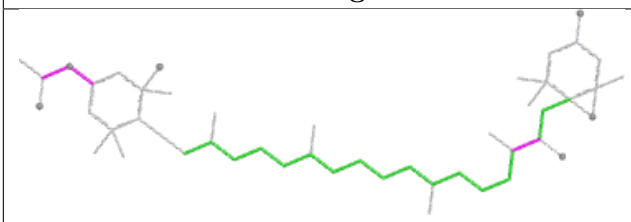
Ligand A86 V 302



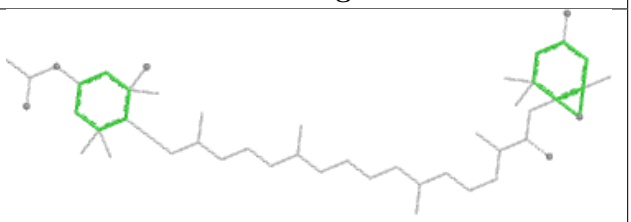
Bond lengths



Bond angles

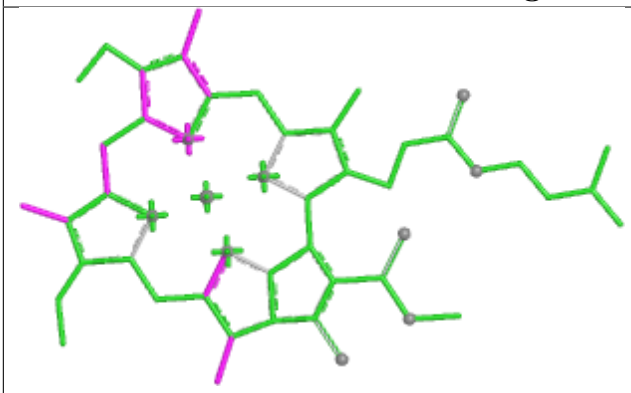


Torsions

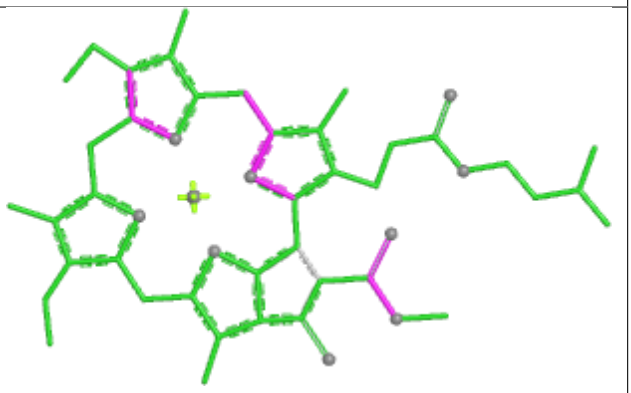


Rings

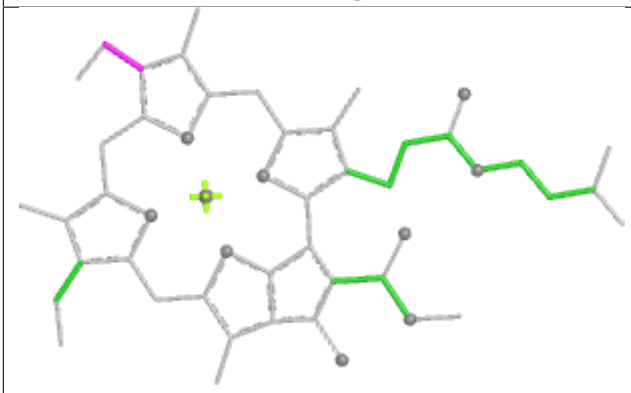
Ligand CLA U 307



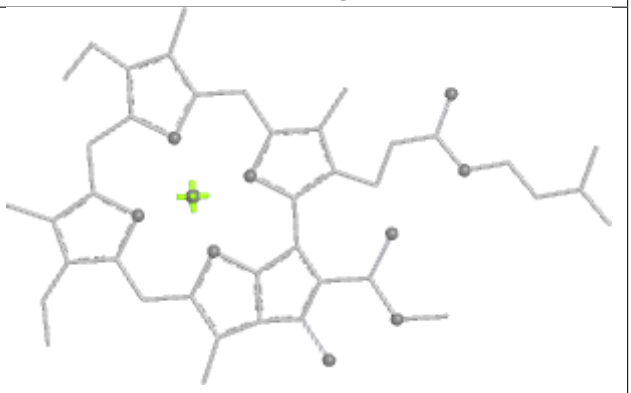
Bond lengths



Bond angles

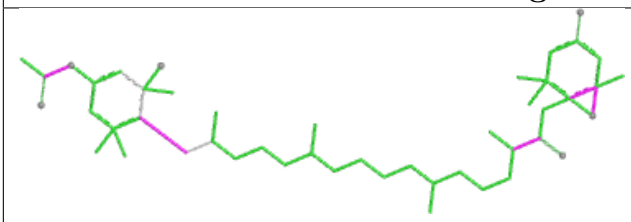


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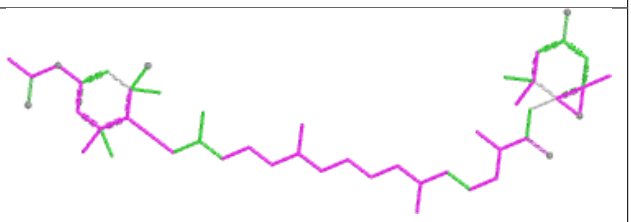


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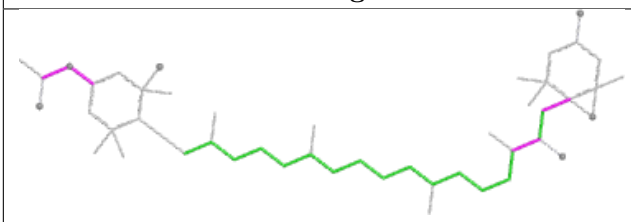
Ligand A86 A 302



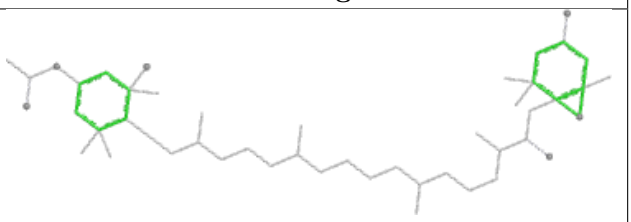
Bond lengths



Bond angles

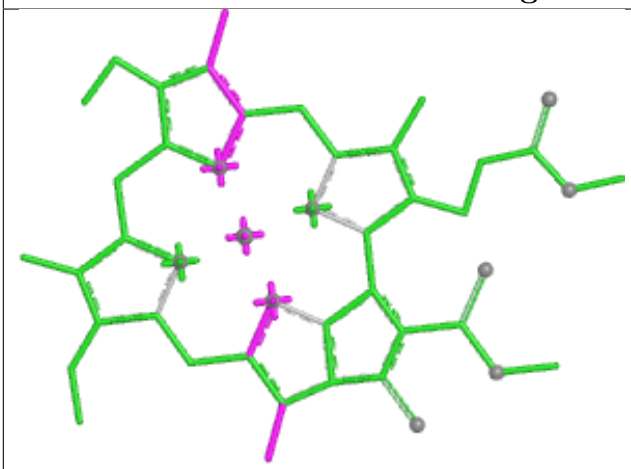


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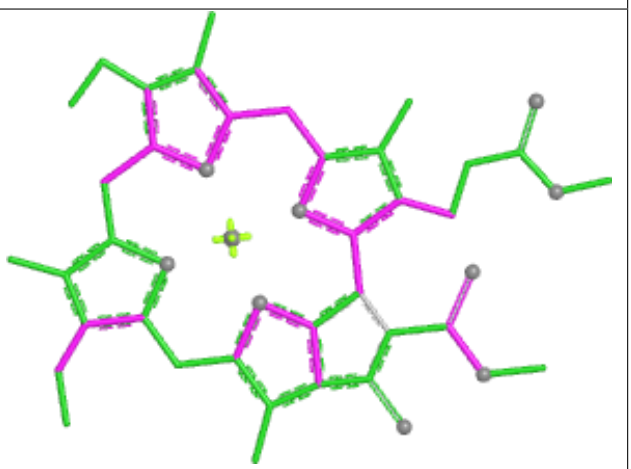


Rings

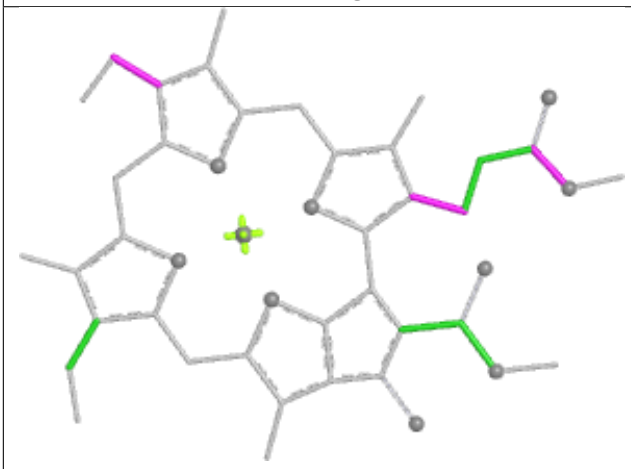
Ligand CLA M 310



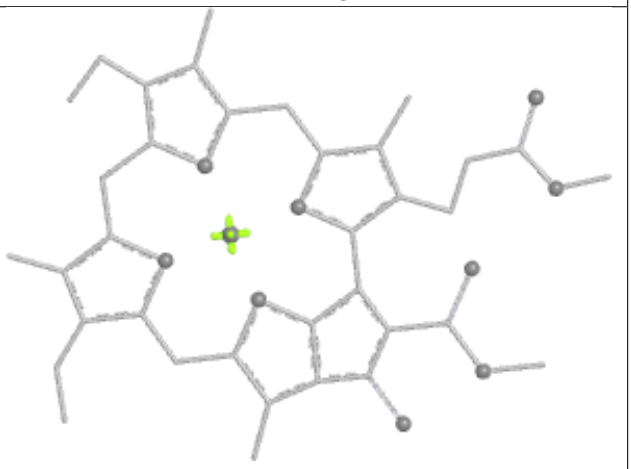
Bond lengths



Bond angles

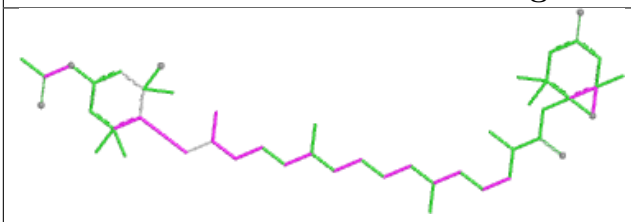


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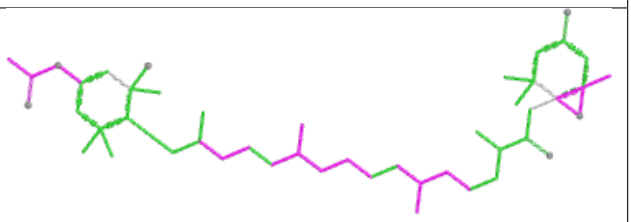


Rings

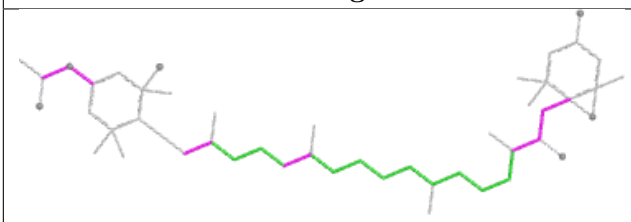
Ligand A86 C 204



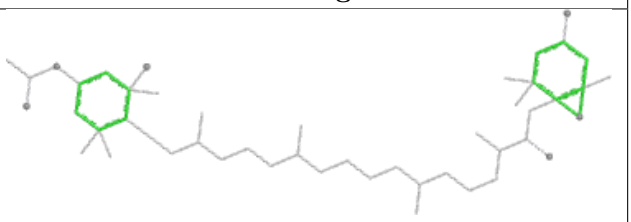
Bond lengths



Bond angles

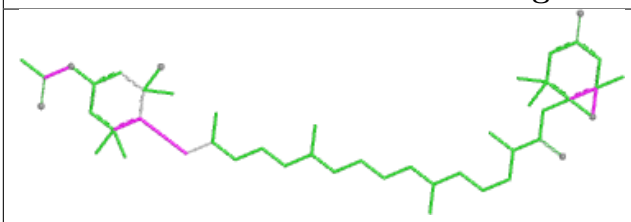


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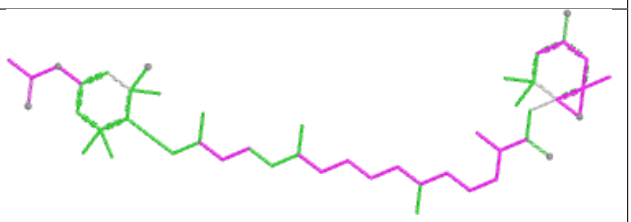


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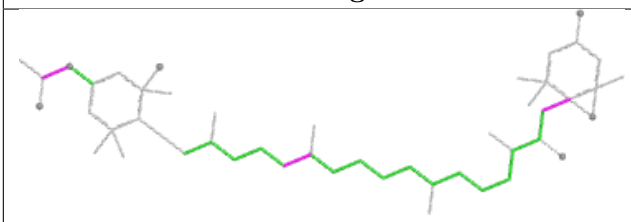
Ligand A86 L 301



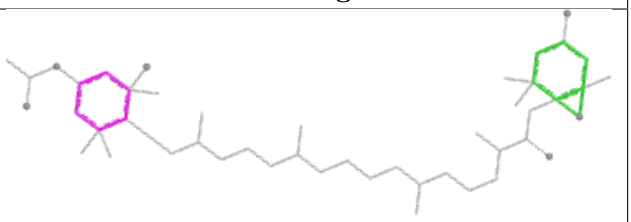
Bond lengths



Bond angles

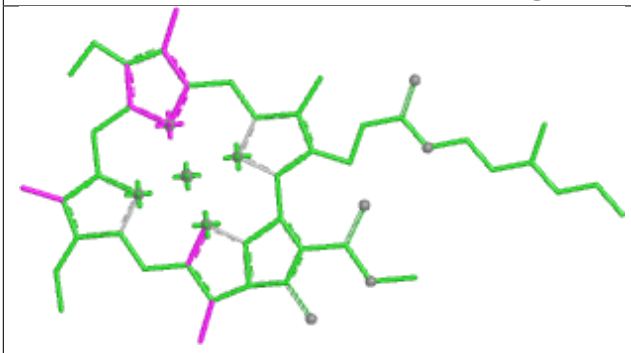


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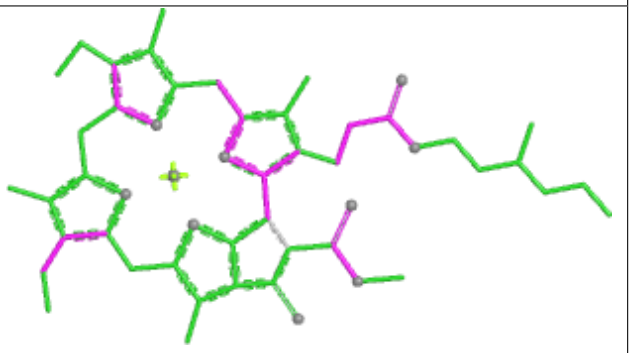


Rings

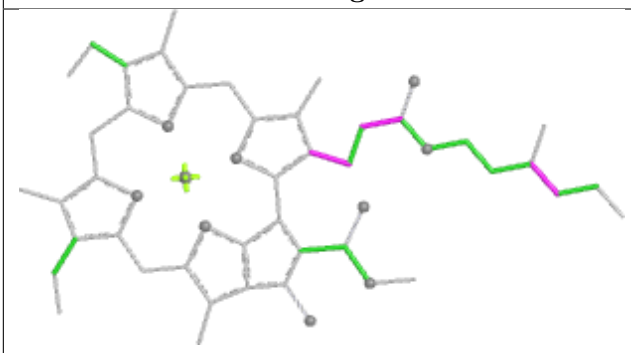
Ligand CLA a 841



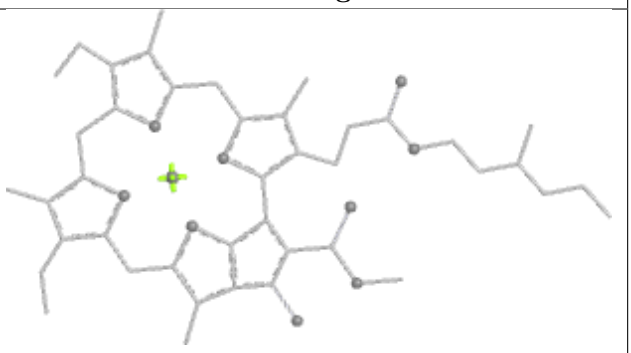
Bond lengths



Bond angles

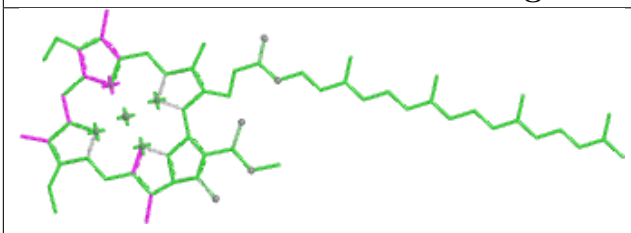


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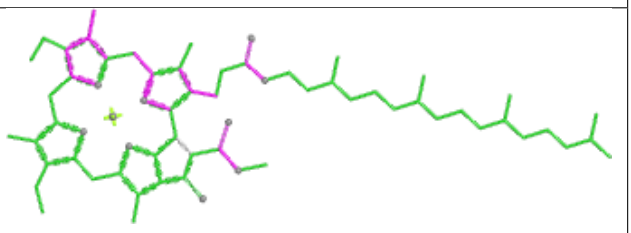


Rings

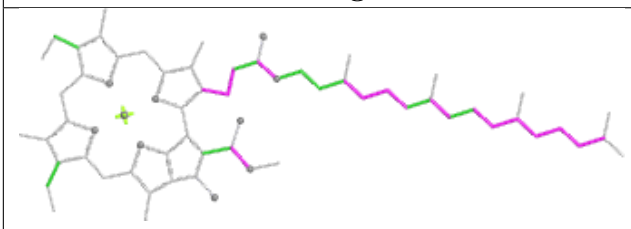
Ligand CLA B 305



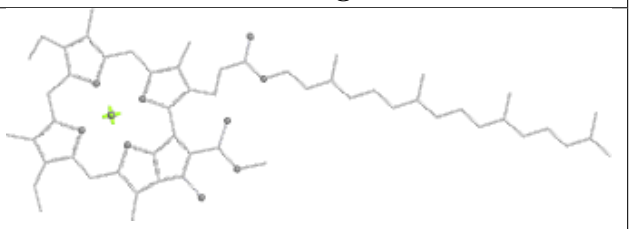
Bond lengths



Bond angles

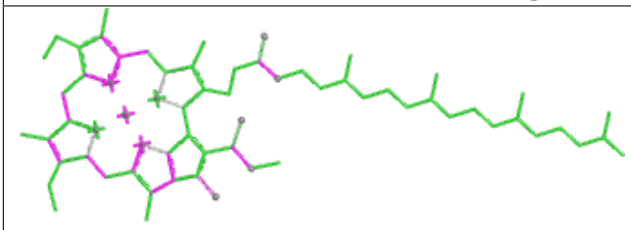


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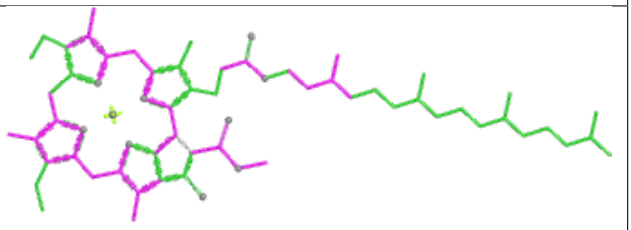


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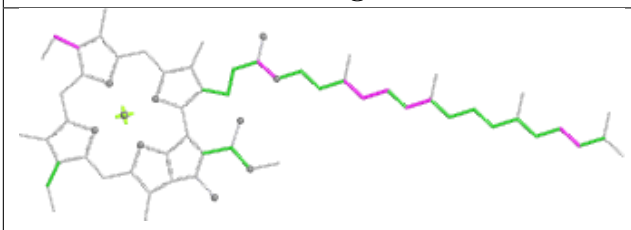
Ligand CLA E 313



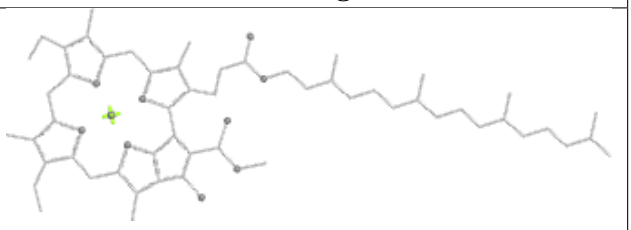
Bond lengths



Bond angles

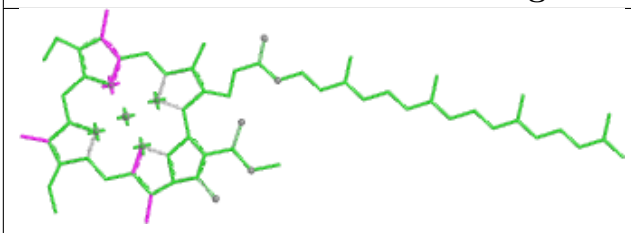


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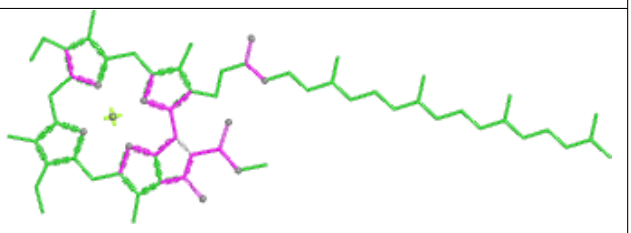


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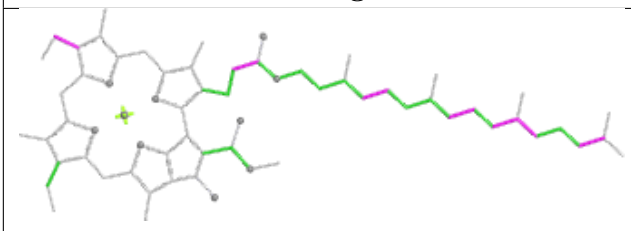
Ligand CLA a 801



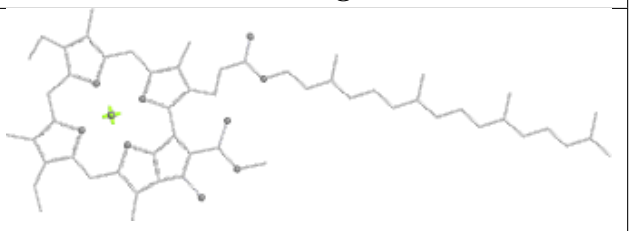
Bond lengths



Bond angles

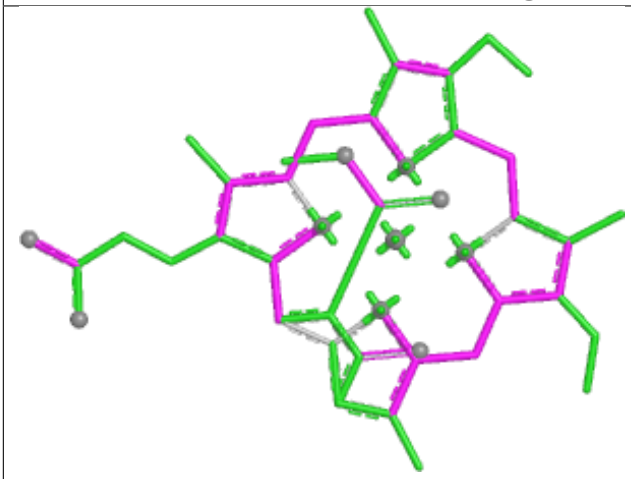


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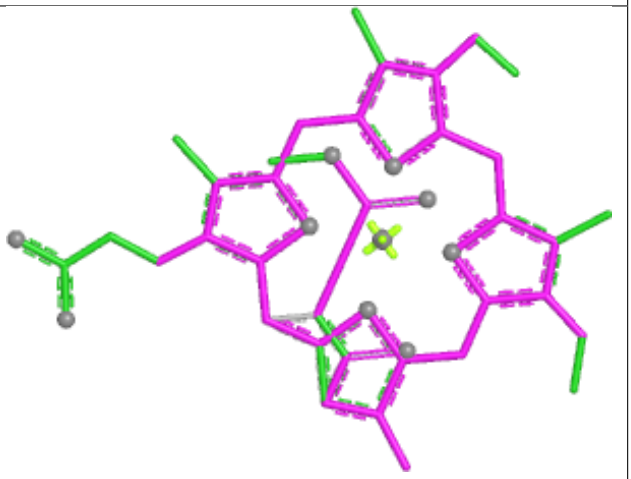


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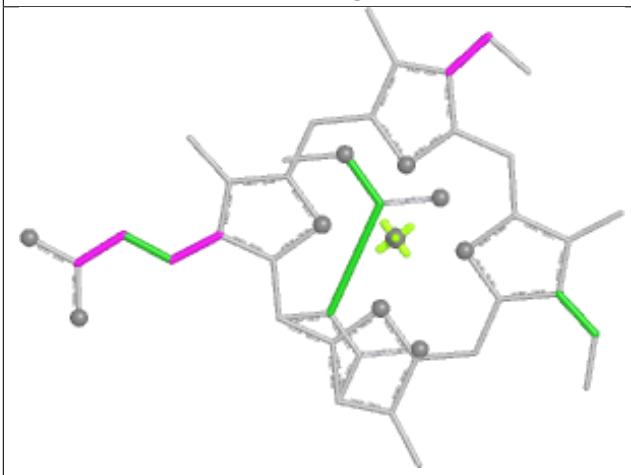
Ligand KC1 W 213



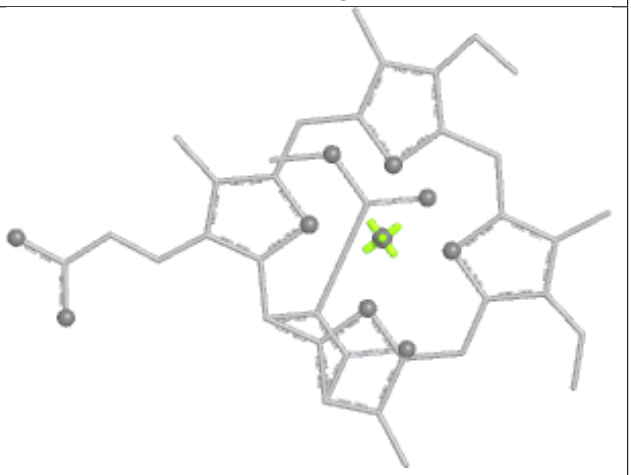
Bond lengths



Bond angles

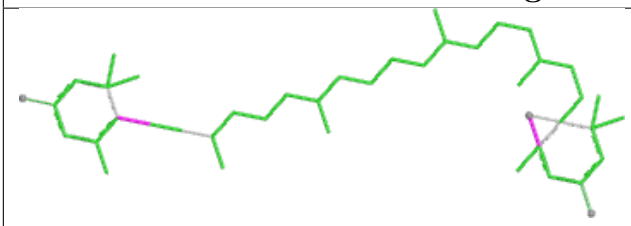


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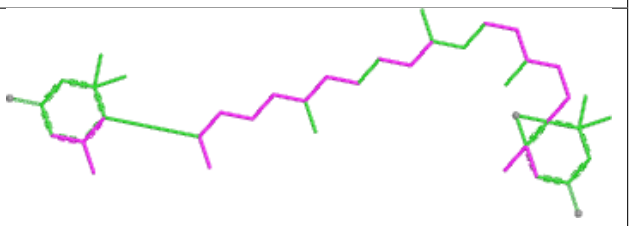


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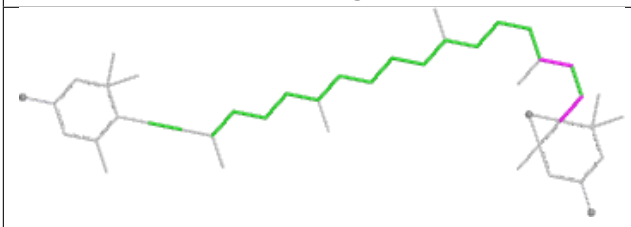
Ligand DD6 A 304



Bond lengths



Bond angles

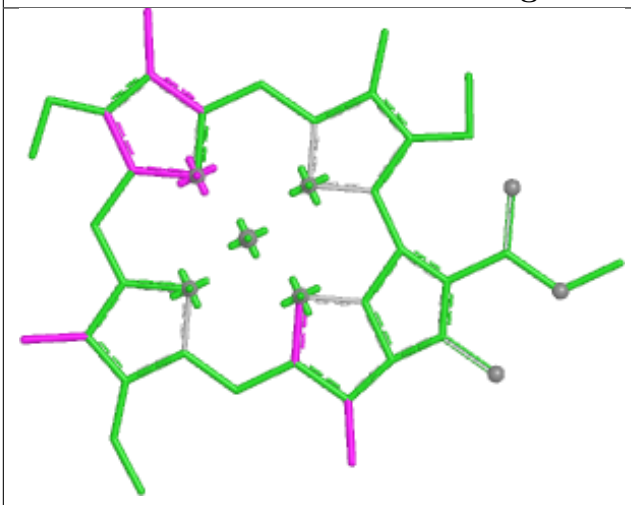


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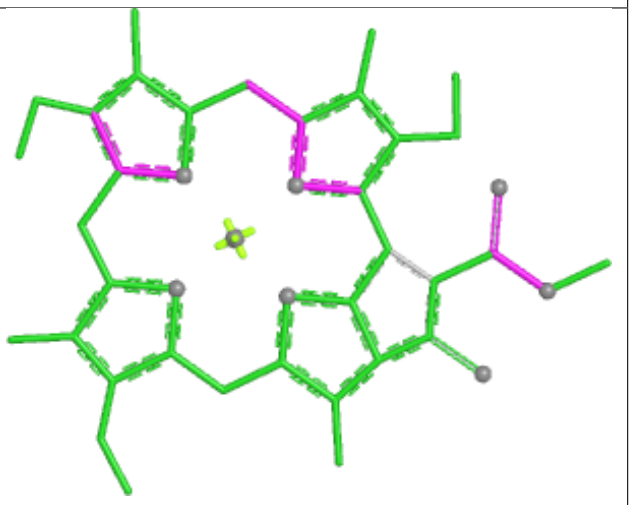


Rings

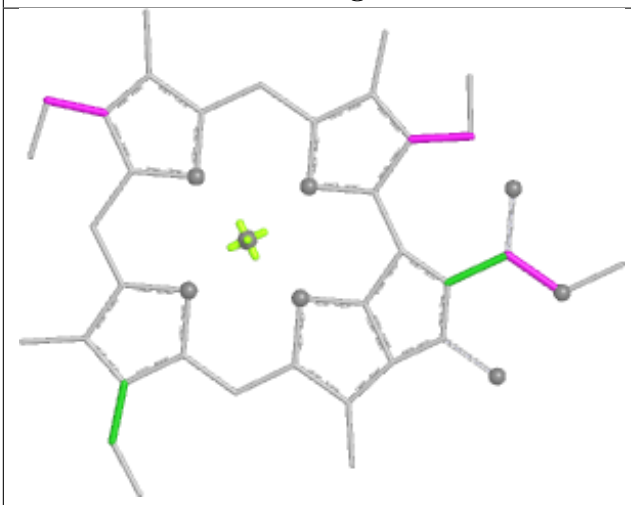
Ligand CLA M 316



Bond lengths



Bond angles

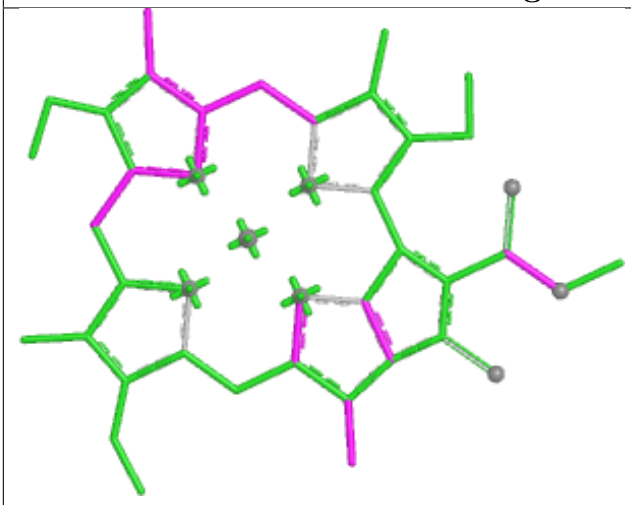


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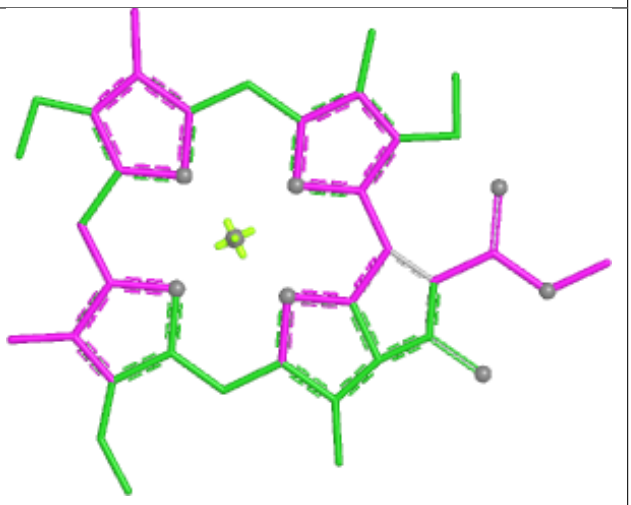


Rings

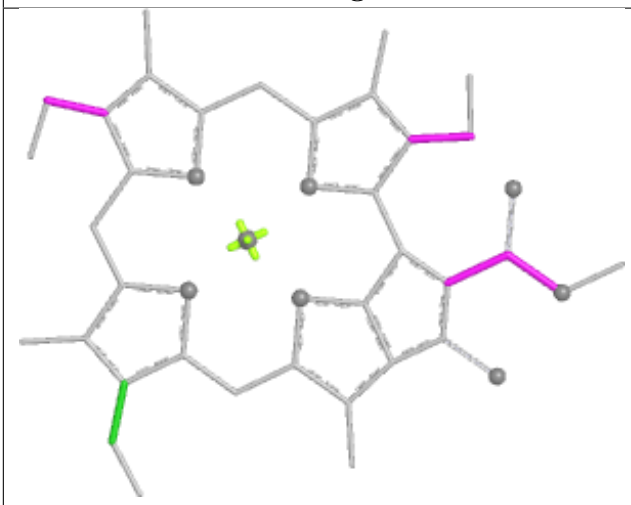
Ligand CLA X 313



Bond lengths



Bond angles



Torsions

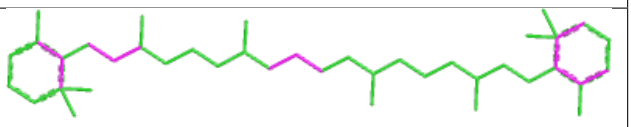


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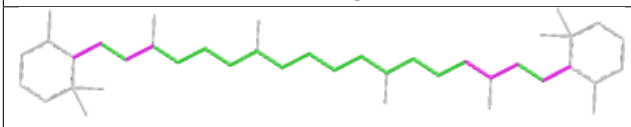
Ligand BCR b 843



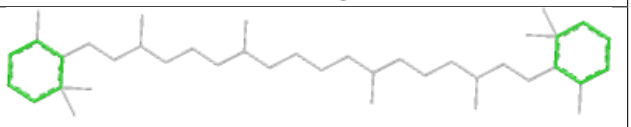
Bond lengths



Bond angles

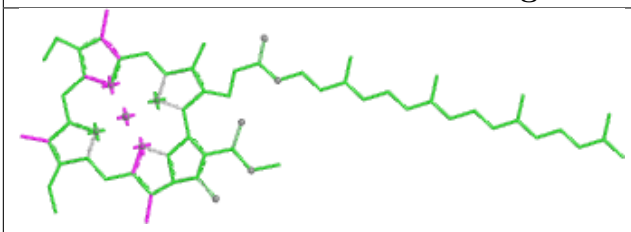


Torsions

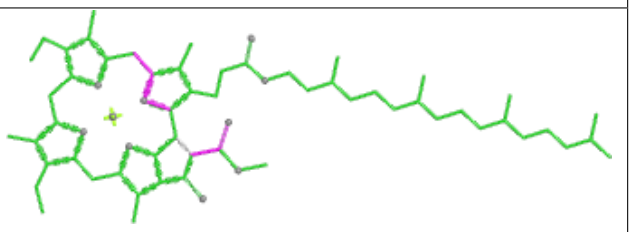


Rings

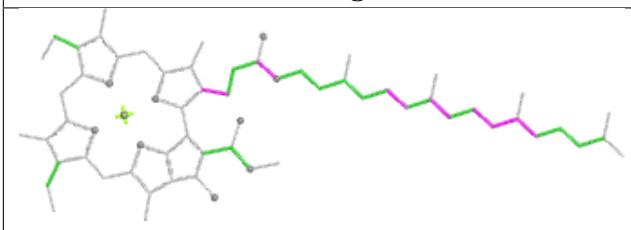
Ligand CLA M 311



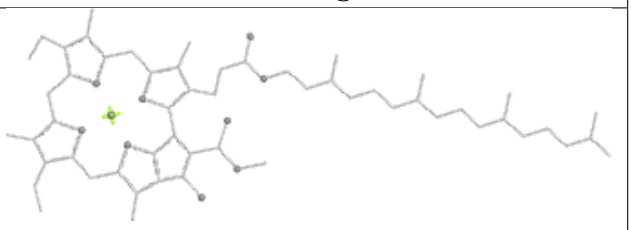
Bond lengths



Bond angles



Torsions

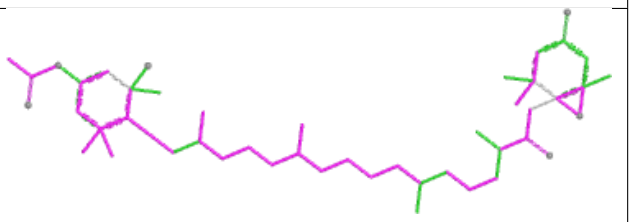


Rings

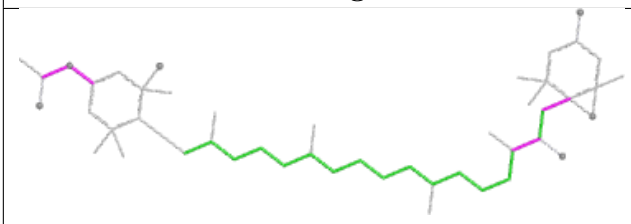
Ligand A86 F 305



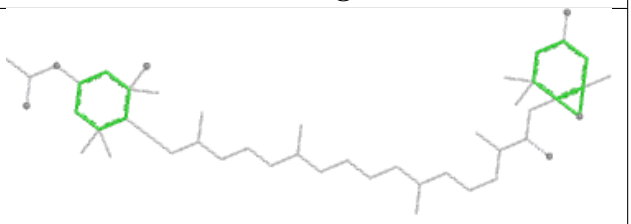
Bond lengths



Bond angles

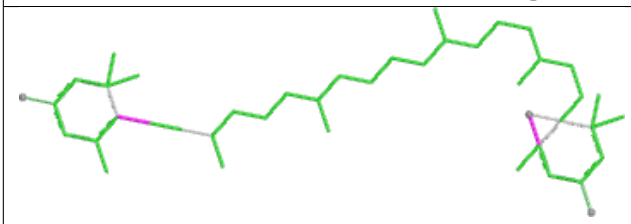


Torsions

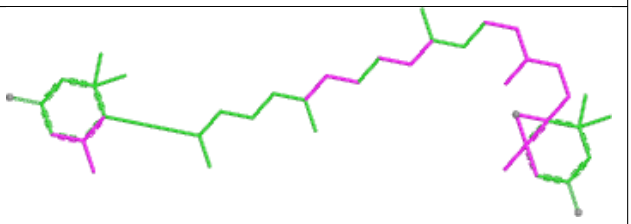


Rings

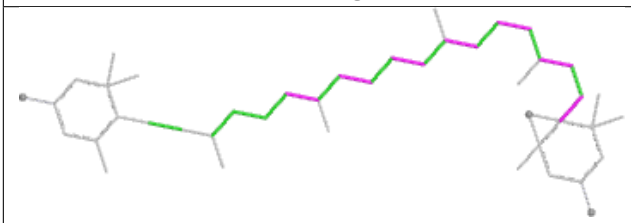
Ligand DD6 R 308



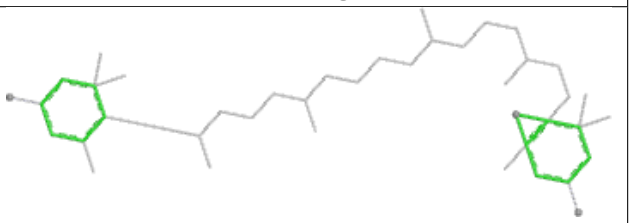
Bond lengths



Bond angles

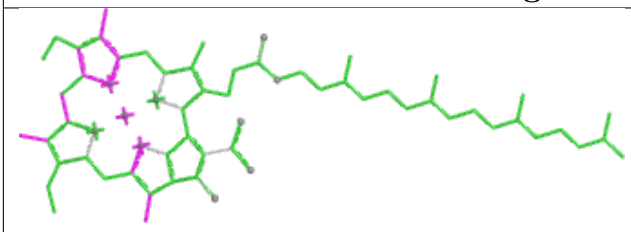


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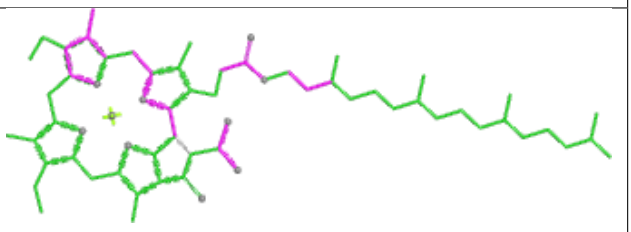


Rings

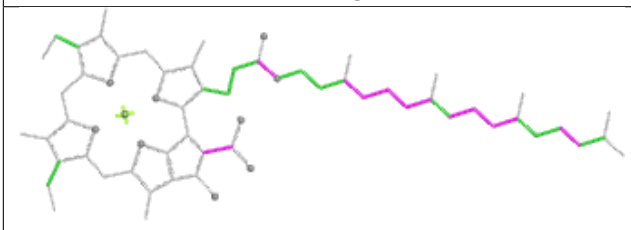
Ligand CLA H 308



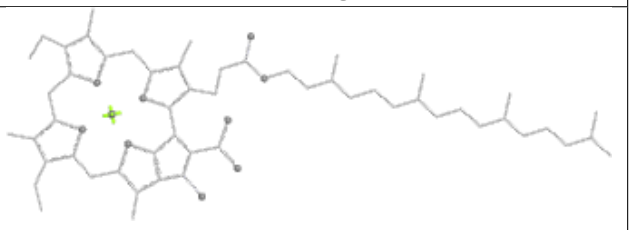
Bond lengths



Bond angles

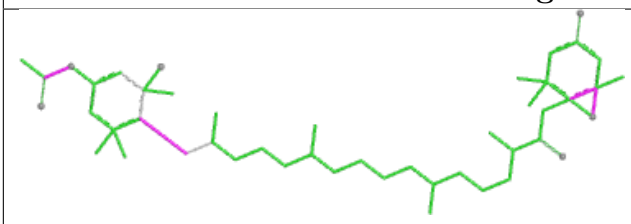


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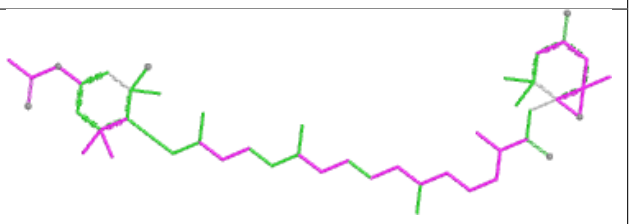


Rings

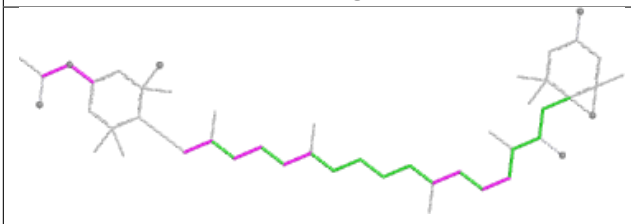
Ligand A86 I 301



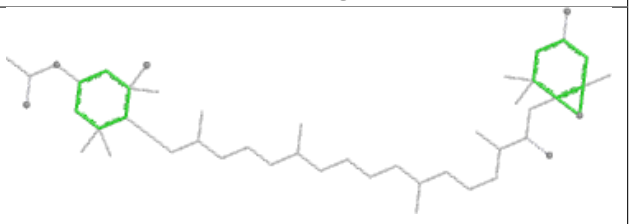
Bond lengths



Bond angles

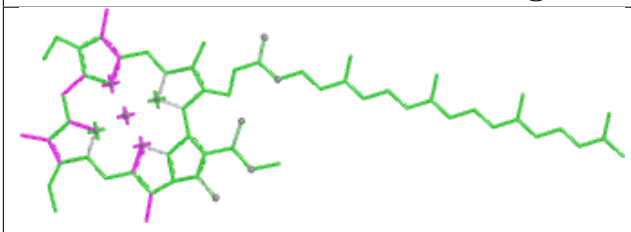


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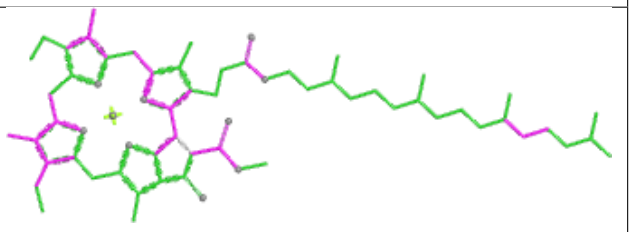


Rings

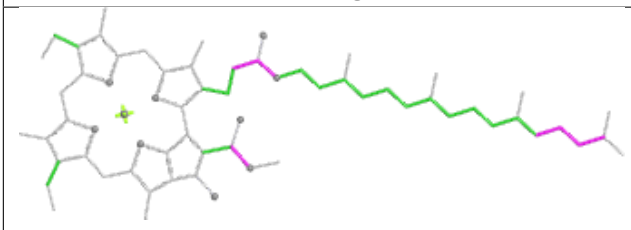
Ligand CLA b 841



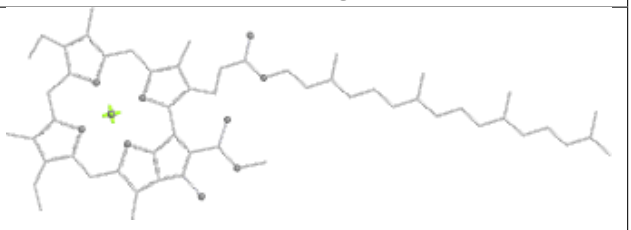
Bond lengths



Bond angles

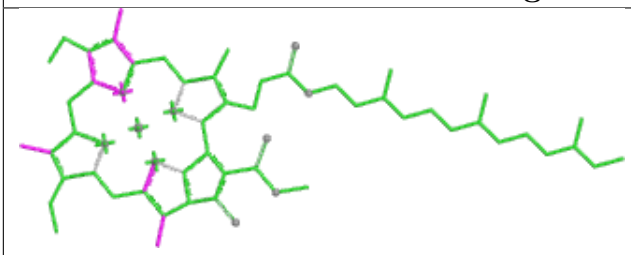


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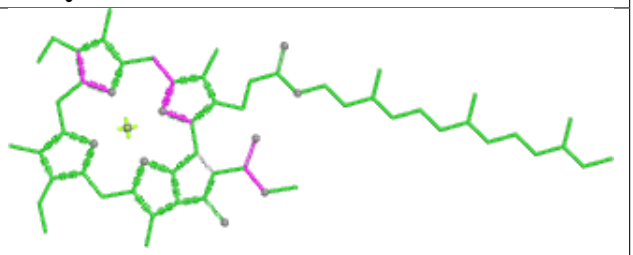


Rings

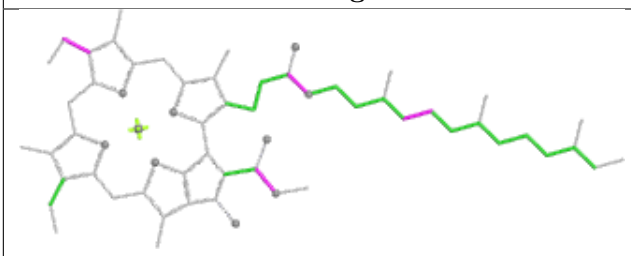
Ligand CLA Q 305



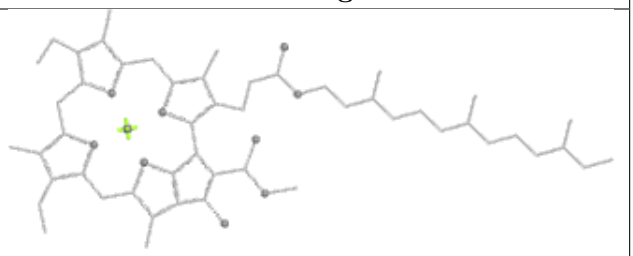
Bond lengths



Bond angles

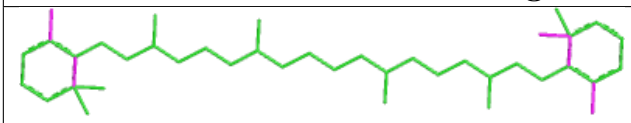


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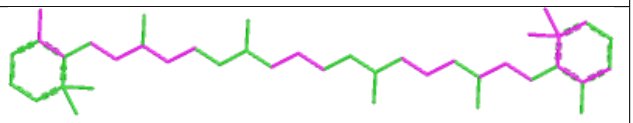


Rings

Ligand BCR h 201



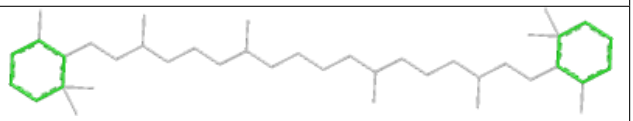
Bond lengths



Bond angles

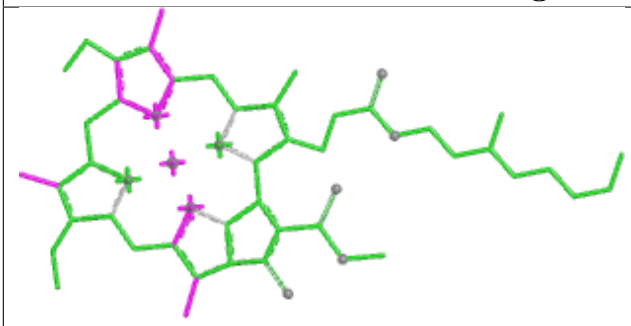


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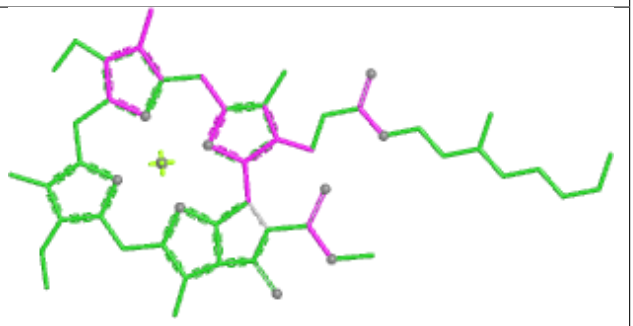


Rings

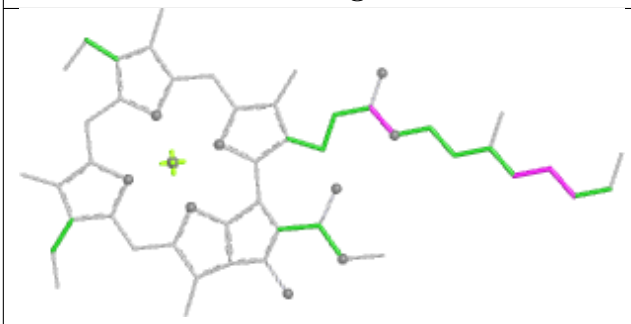
Ligand CLA I 307



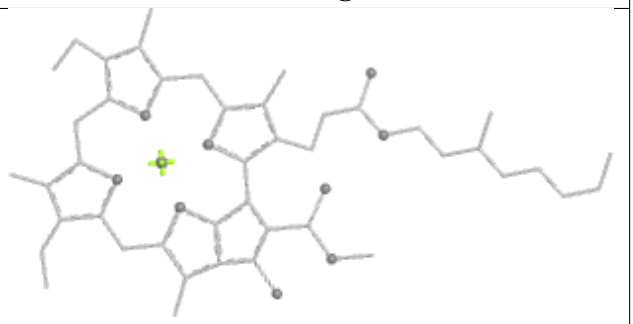
Bond lengths



Bond angles

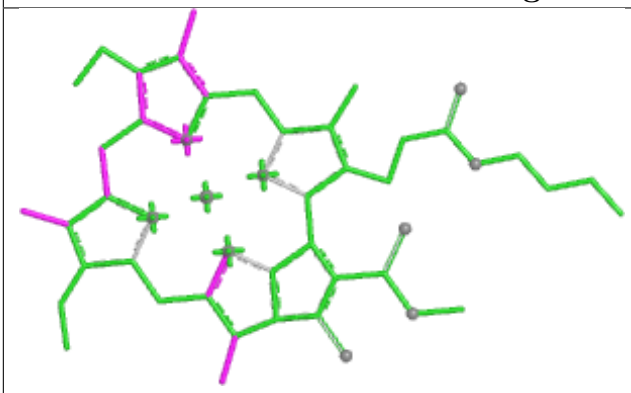


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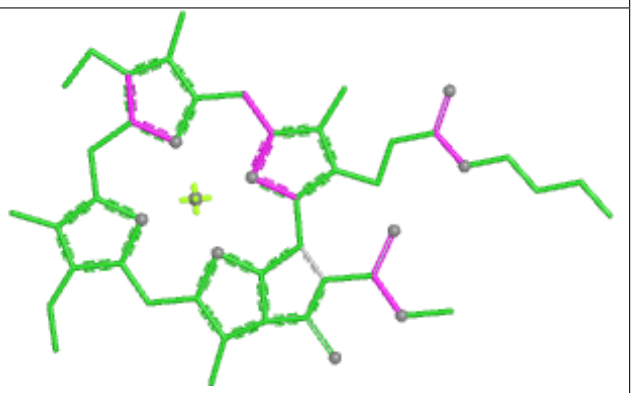


Rings

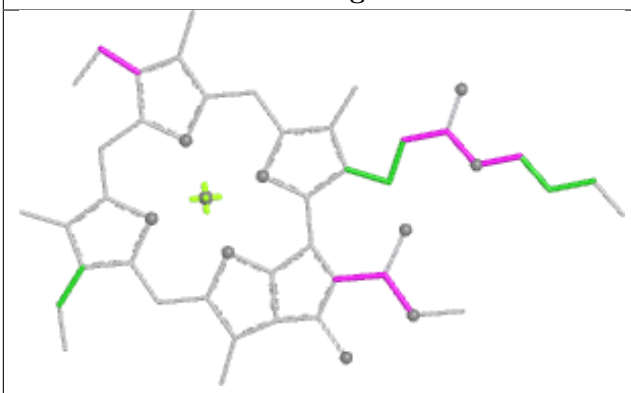
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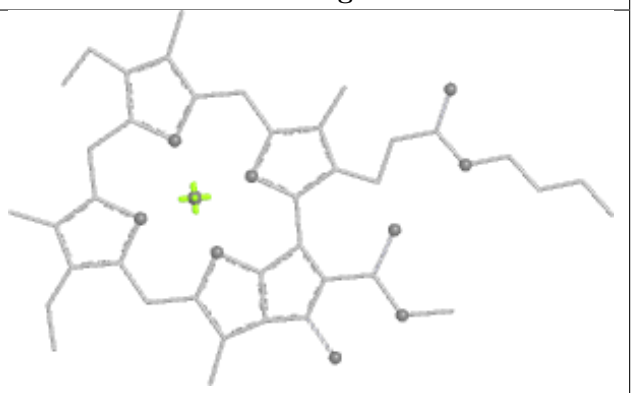
Bond lengths



Bond angles

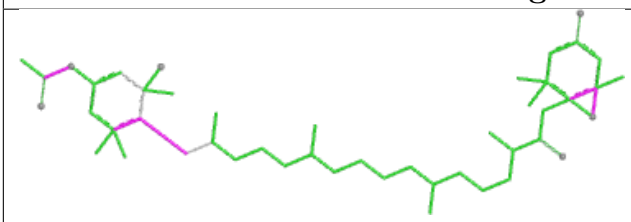


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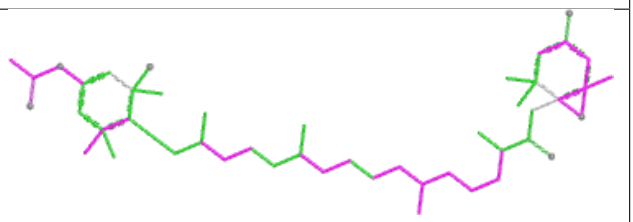


Rings

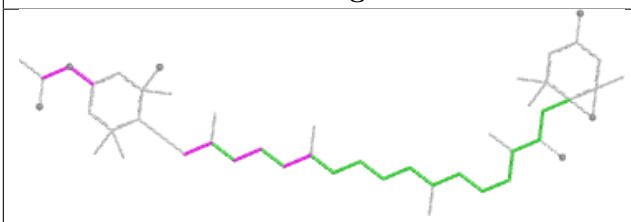
Ligand A86 H 304



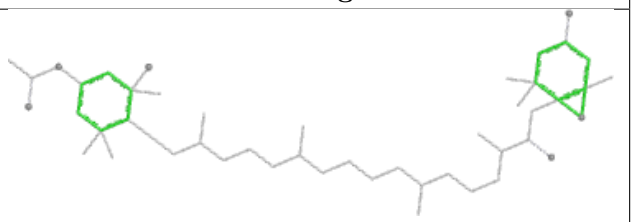
Bond lengths



Bond angles

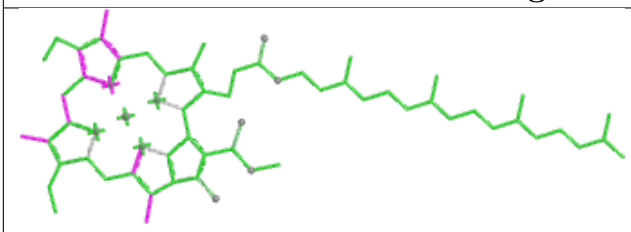


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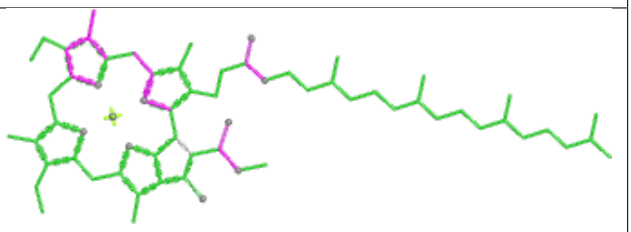


Rings

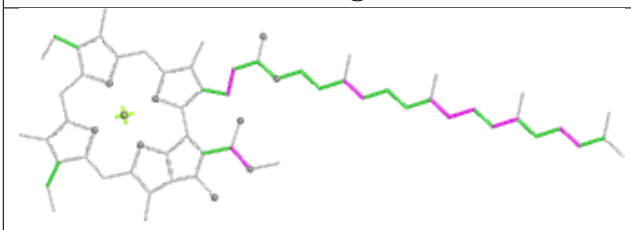
Ligand CLA J 310



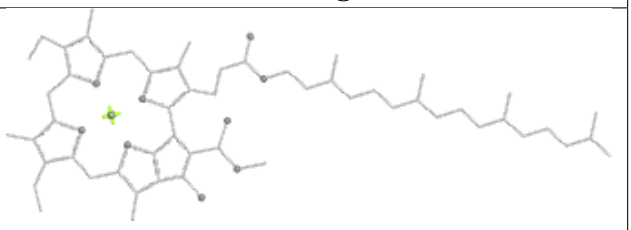
Bond lengths



Bond angles

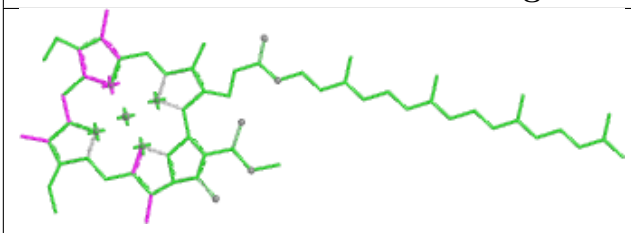


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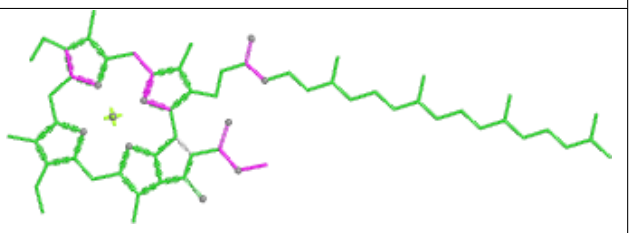


Rings

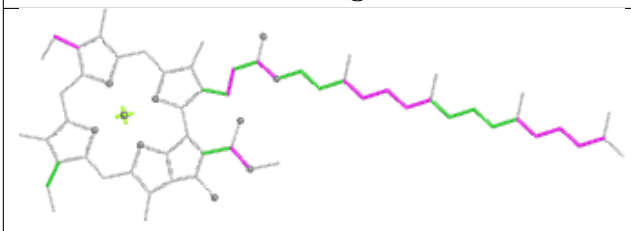
Ligand CLA H 316



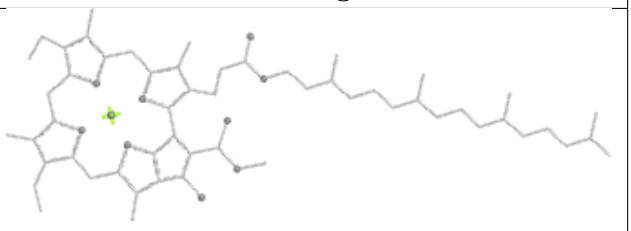
Bond lengths



Bond angles

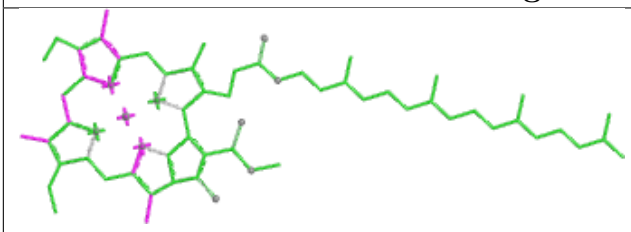


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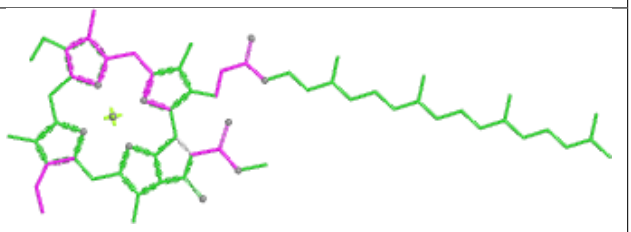


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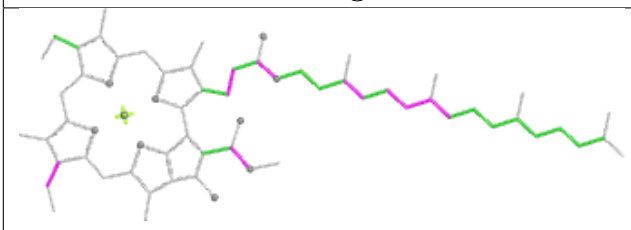
Ligand CLA D 308



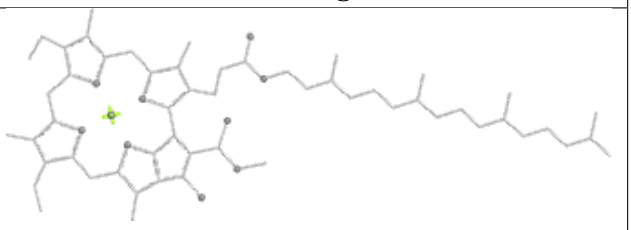
Bond lengths



Bond angles

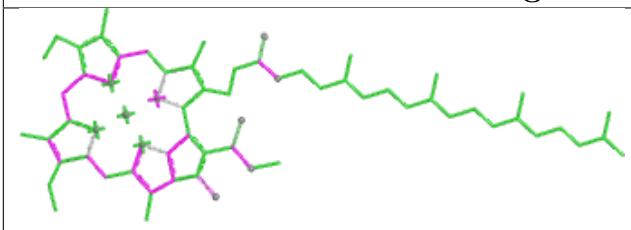


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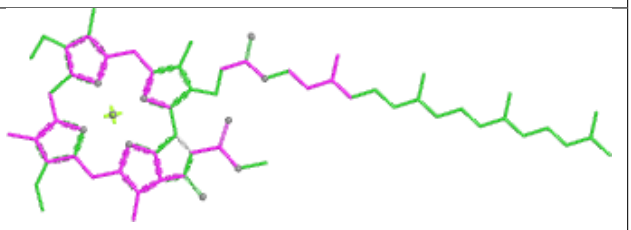


Rings

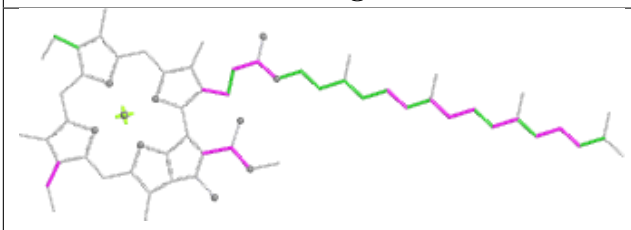
Ligand CLA V 314



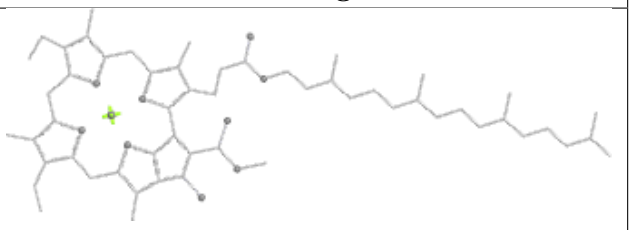
Bond lengths



Bond angles

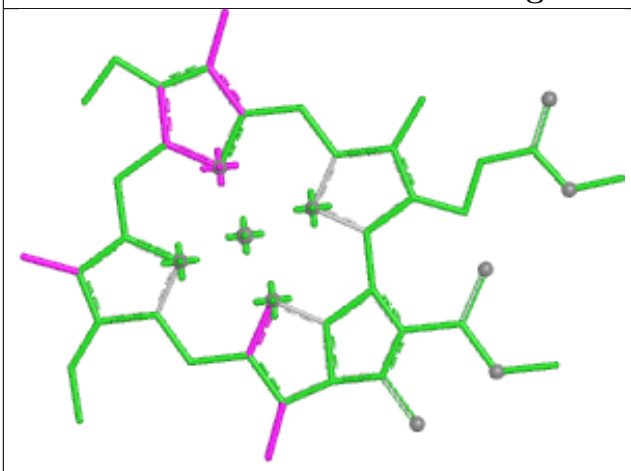


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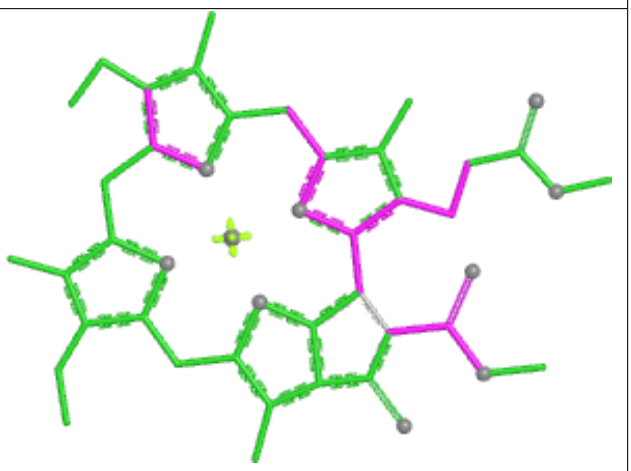


Rings

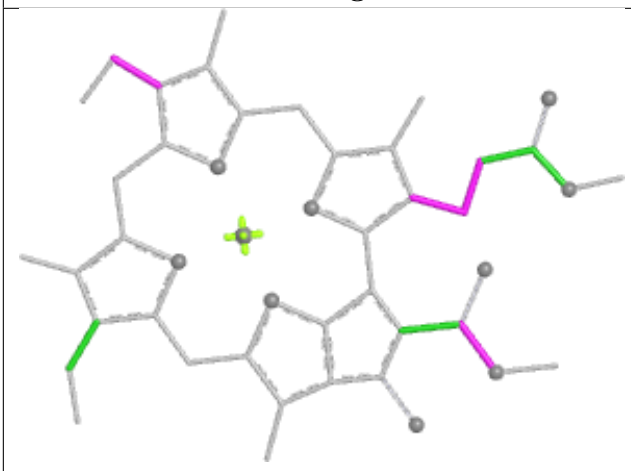
Ligand CLA L 312



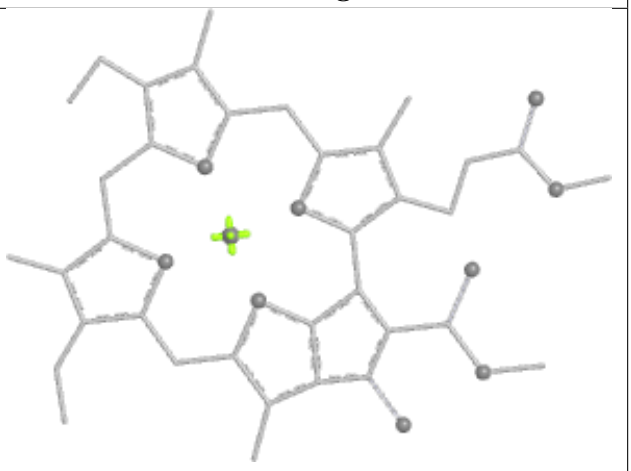
Bond lengths



Bond angles

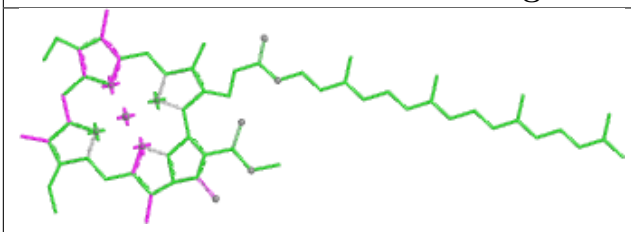


Torsions

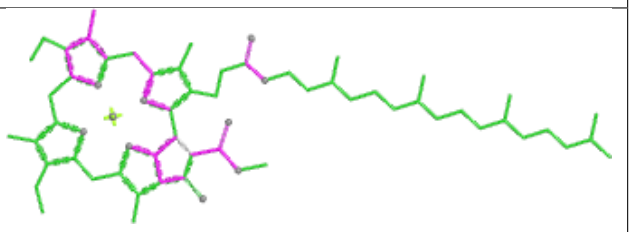


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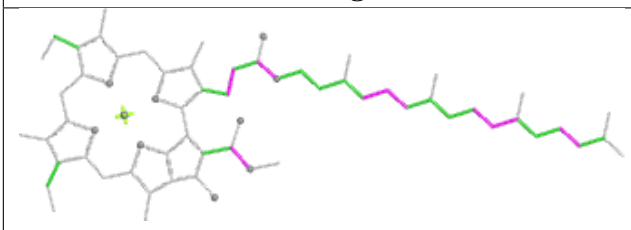
Ligand CLA K 313



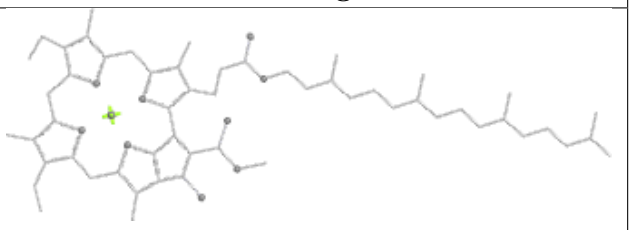
Bond lengths



Bond angles

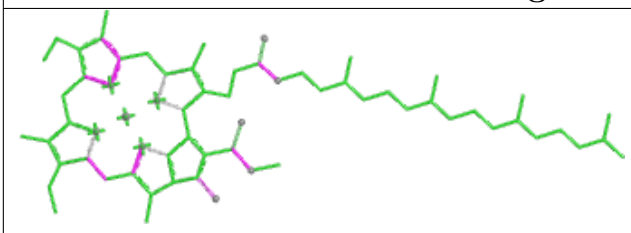


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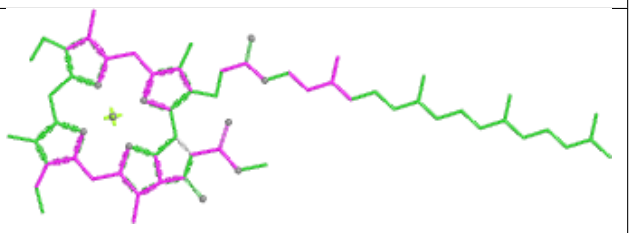


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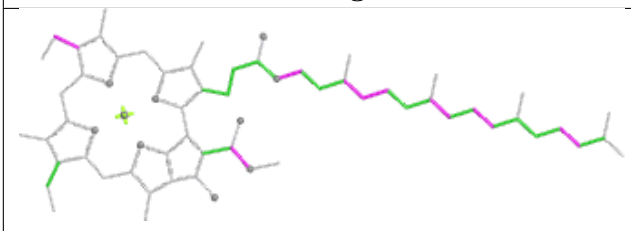
Ligand CLA a 806



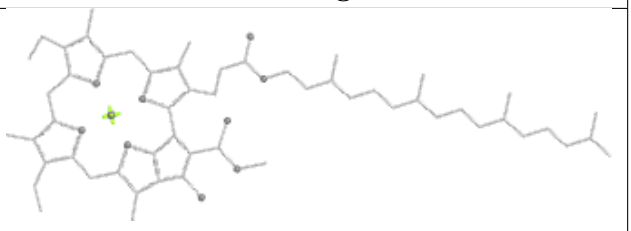
Bond lengths



Bond angles

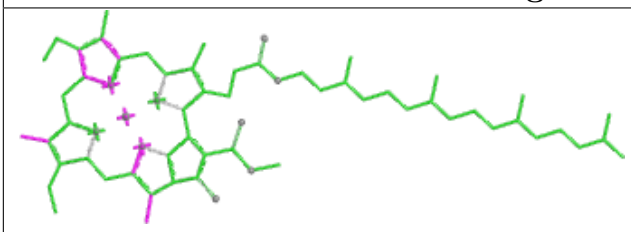


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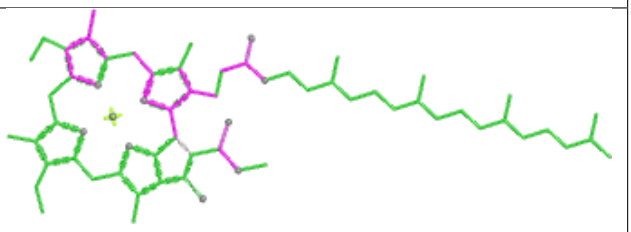


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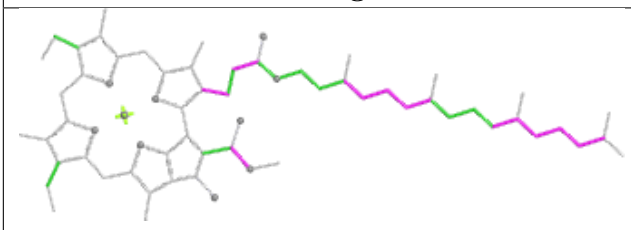
Ligand CLA L 314



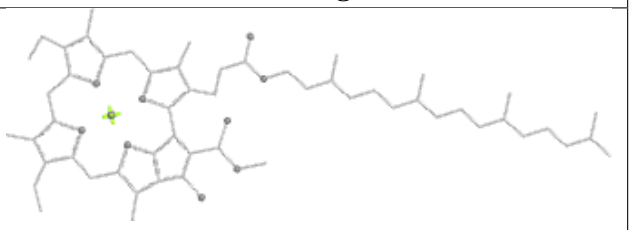
Bond lengths



Bond angles

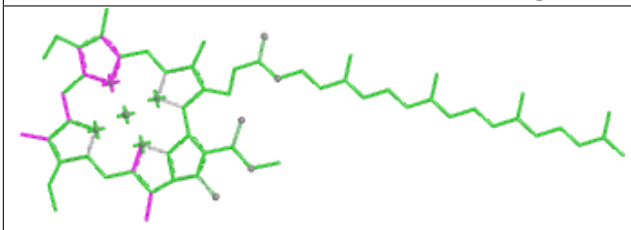


Torsions

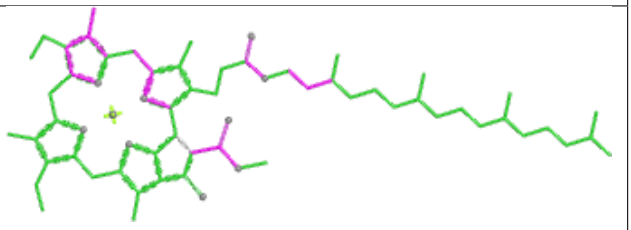


Rings

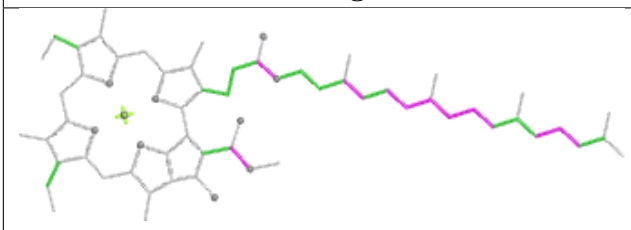
Ligand CLA I 311



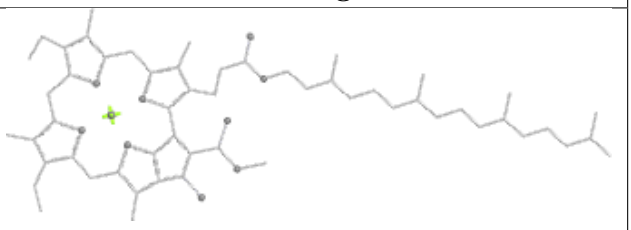
Bond lengths



Bond angles

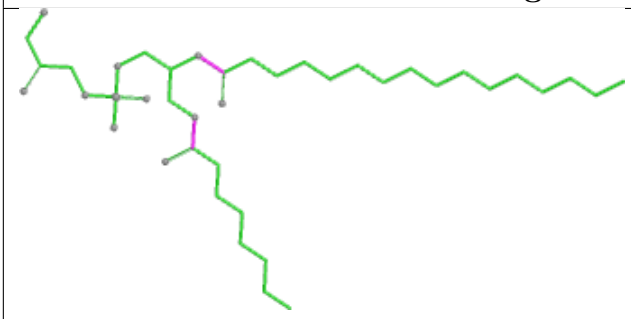


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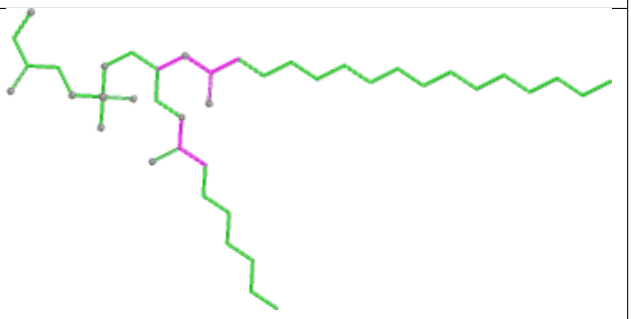


Rings

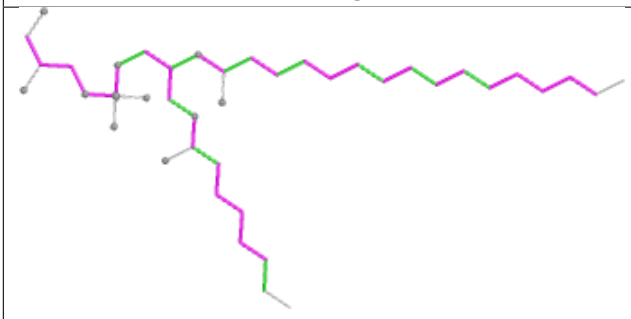
Ligand LHG F 319



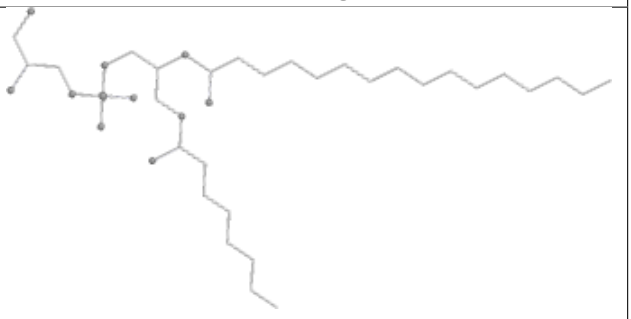
Bond lengths



Bond angles

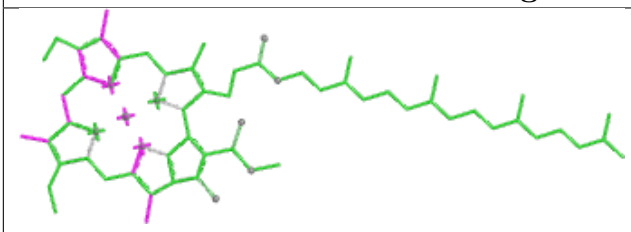


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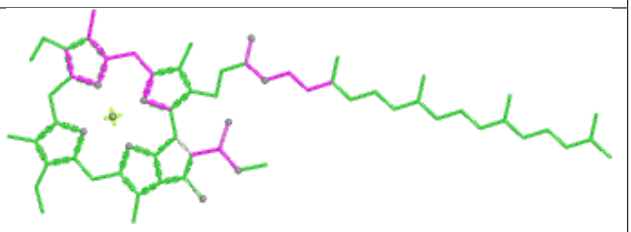


Rings

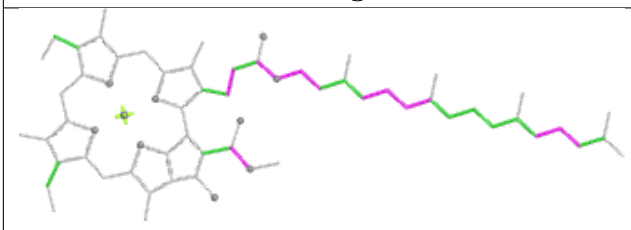
Ligand CLA M 307



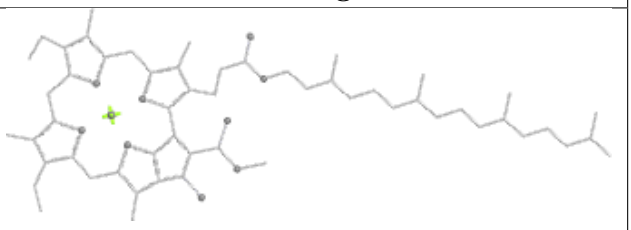
Bond lengths



Bond angles

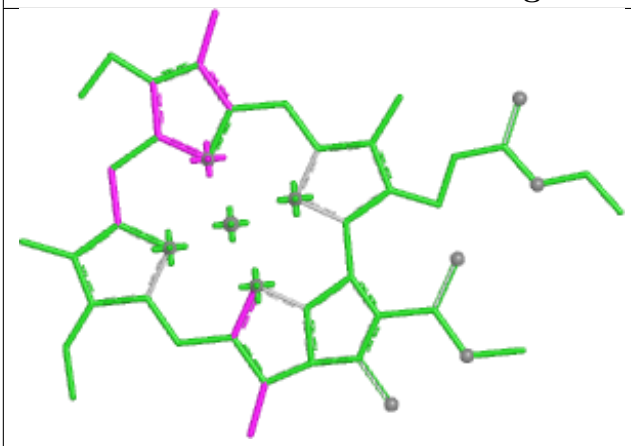


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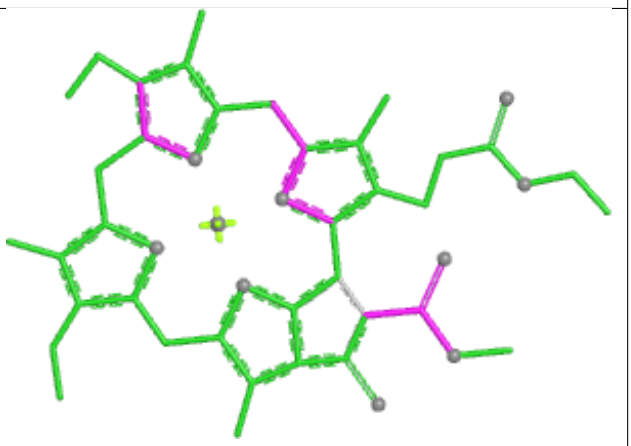


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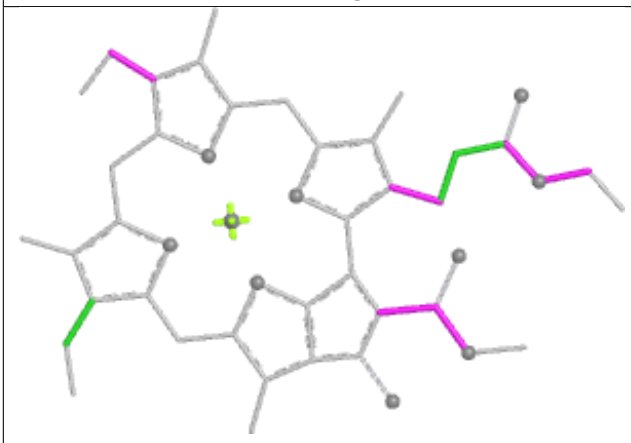
Ligand CLA N 312



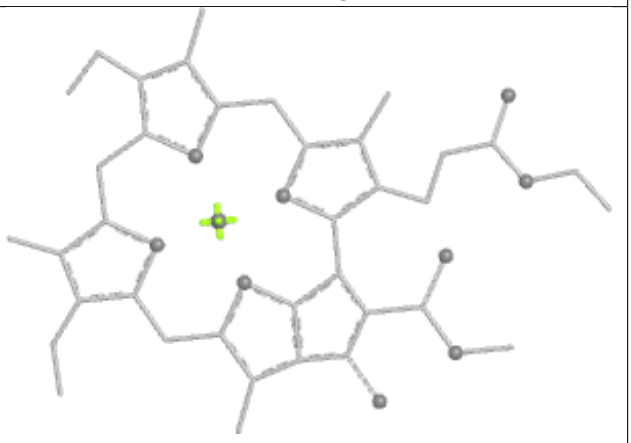
Bond lengths



Bond angles

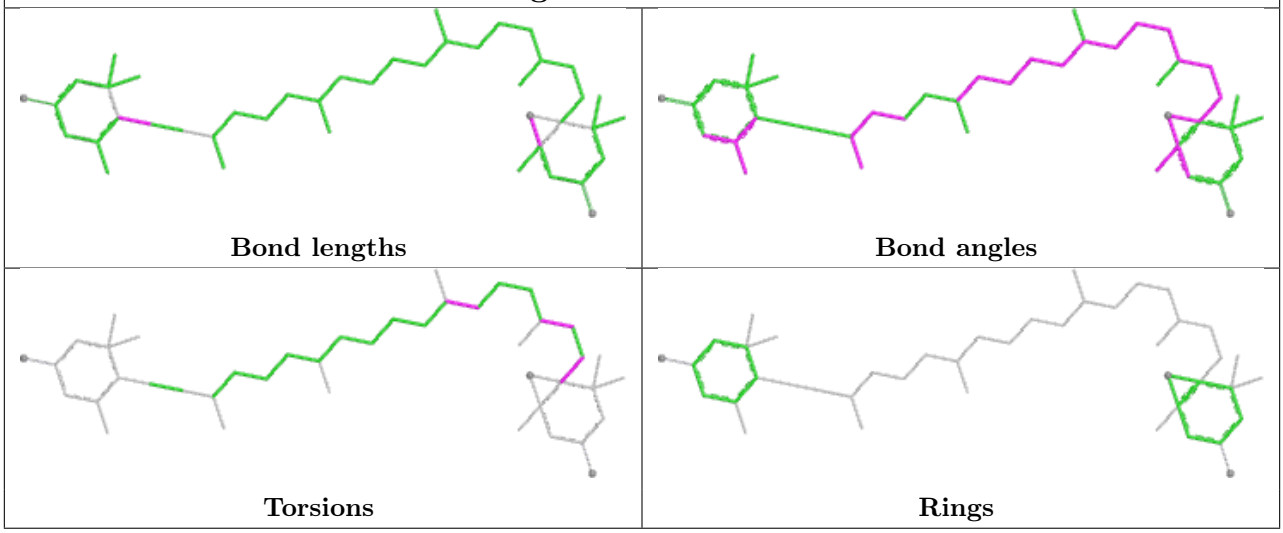


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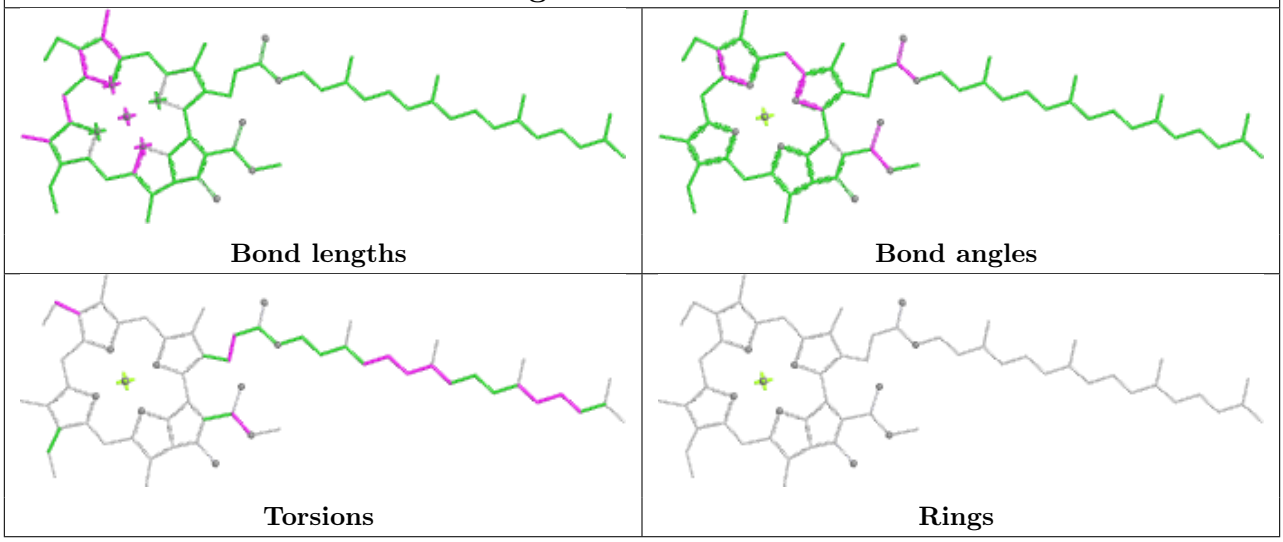


Rings

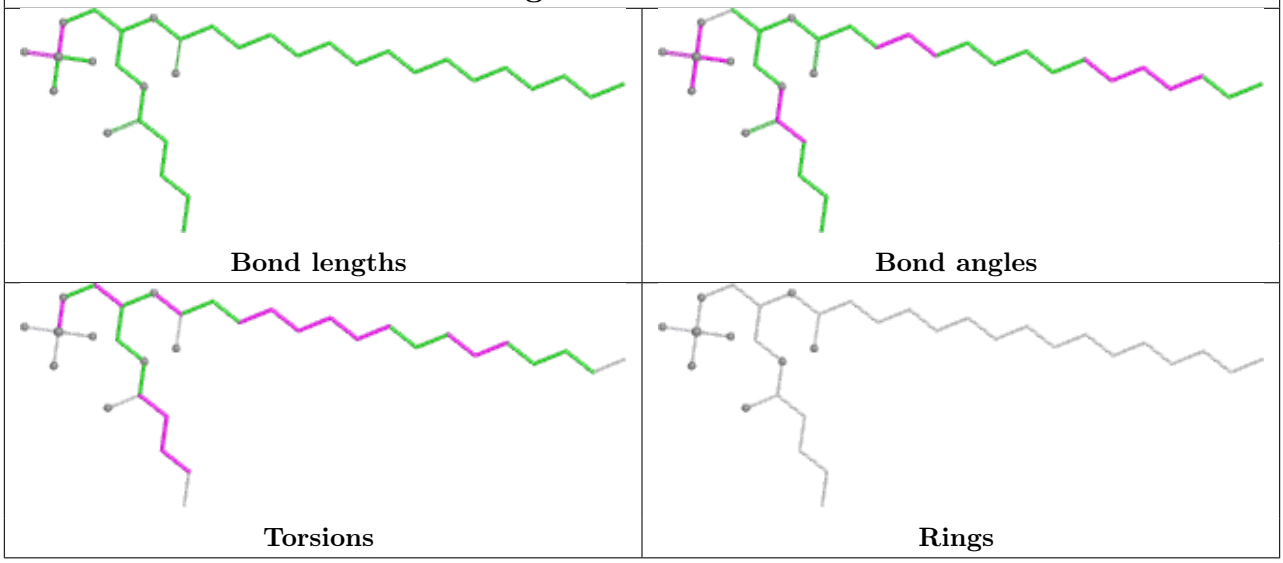
Ligand DD6 a 849



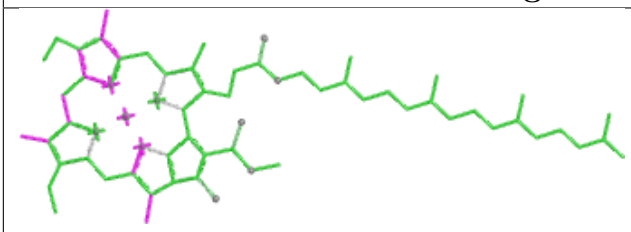
Ligand CLA J 313



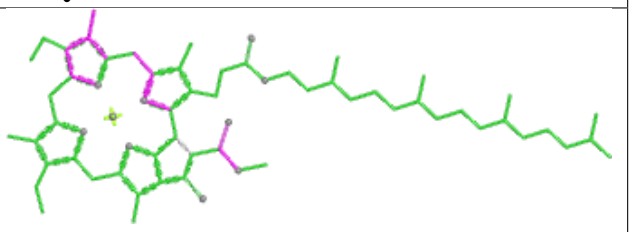
Ligand LHG F 318



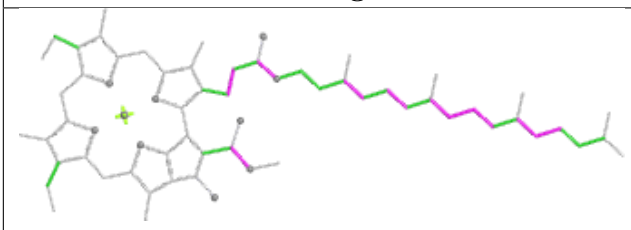
Ligand CLA Q 306



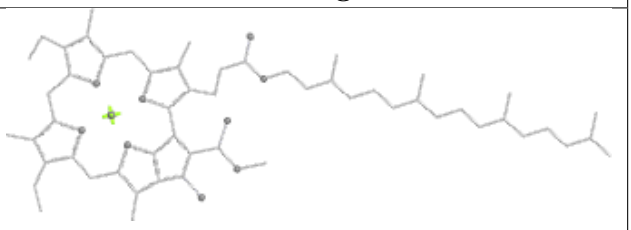
Bond lengths



Bond angles



Torsions

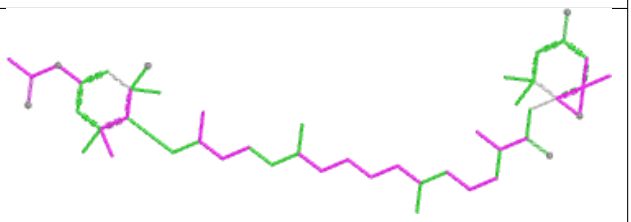


Rings

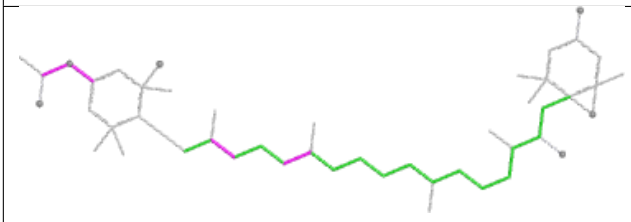
Ligand A86 C 203



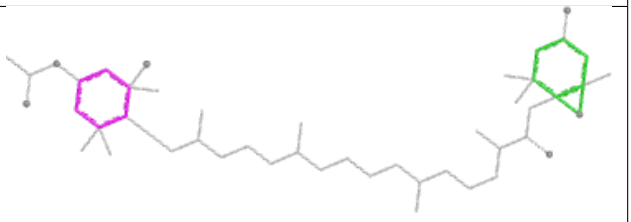
Bond lengths



Bond angles

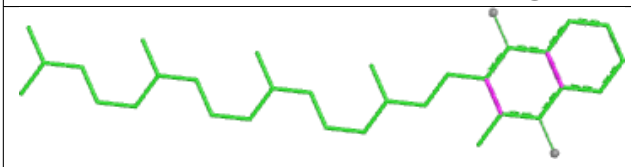


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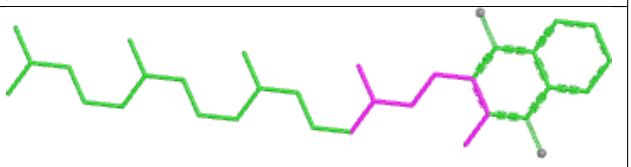


Rings

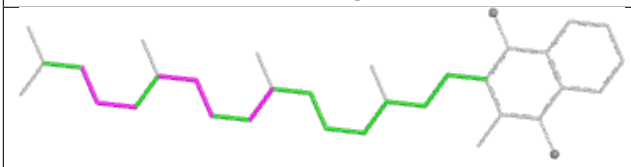
Ligand PQN a 840



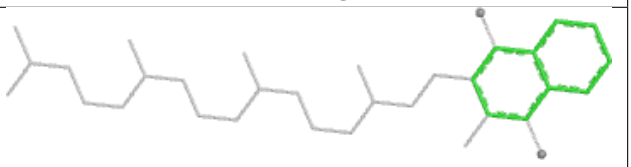
Bond lengths



Bond angles

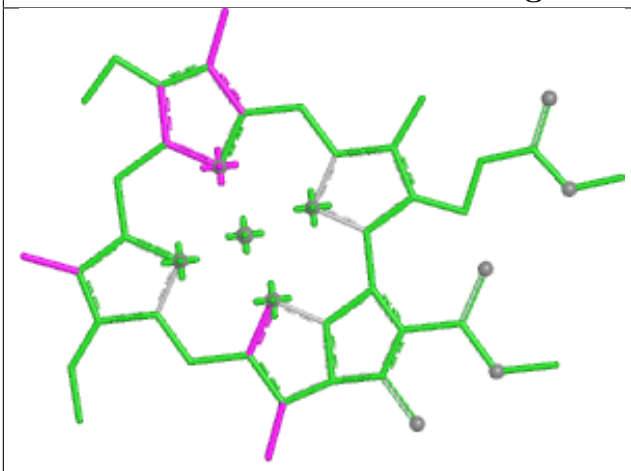


Torsions

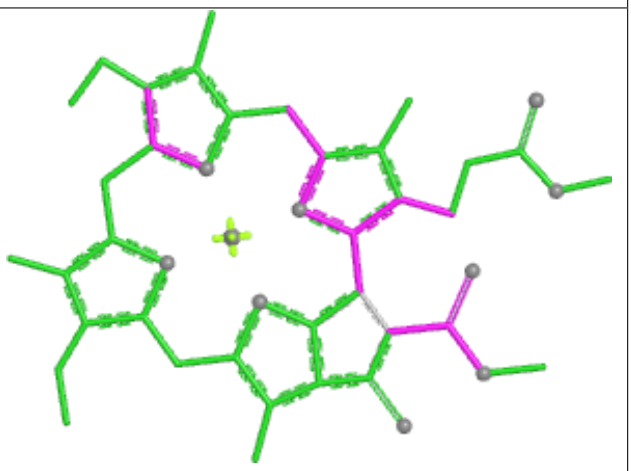


Rings

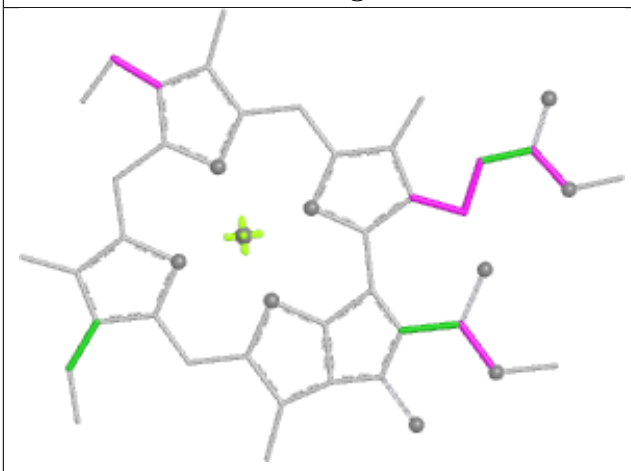
Ligand CLA P 312



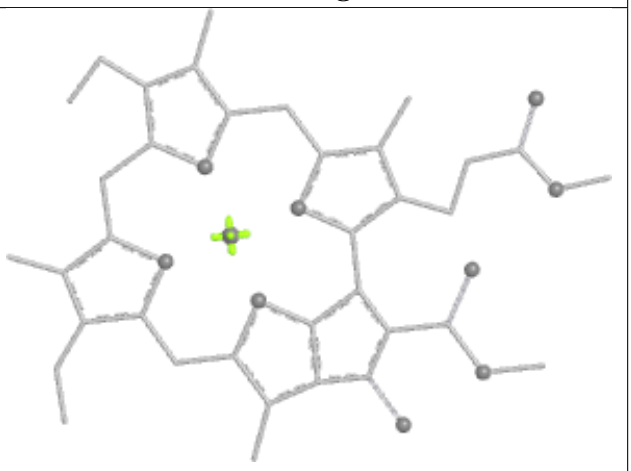
Bond lengths



Bond angles

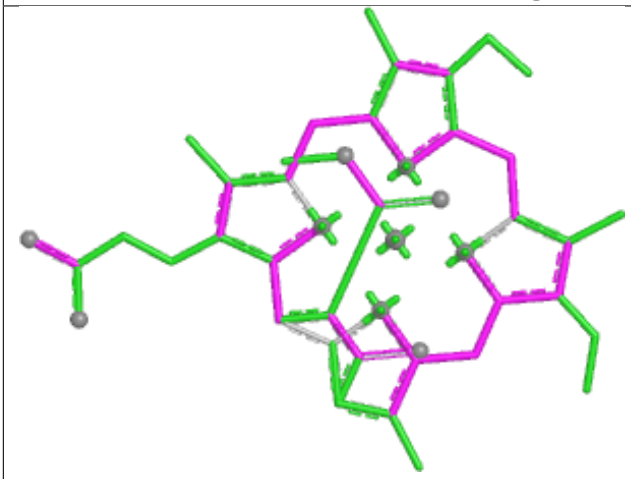


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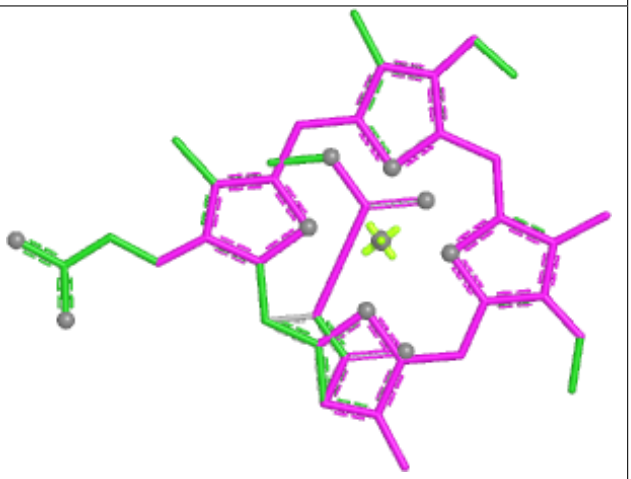


Rings

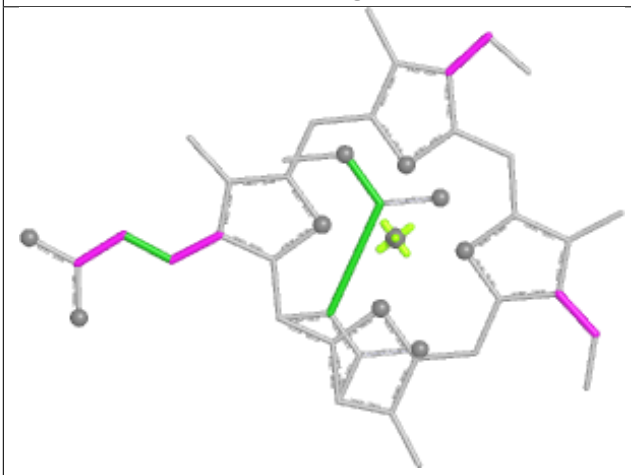
Ligand KC1 F 308



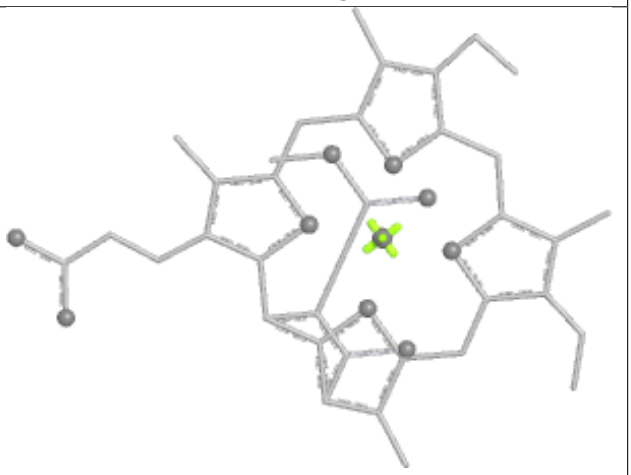
Bond lengths



Bond angles

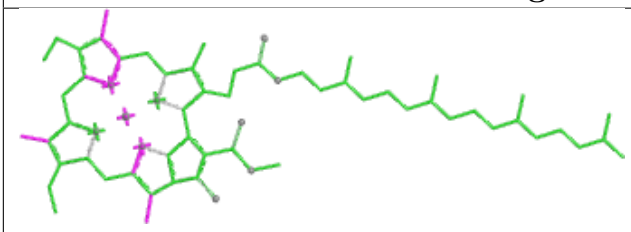


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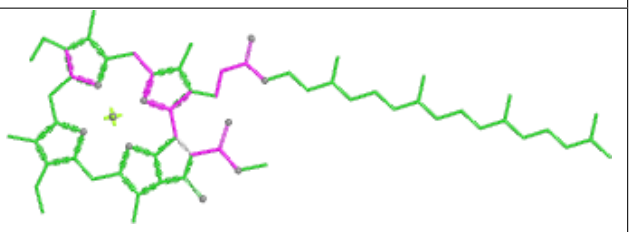


Rings

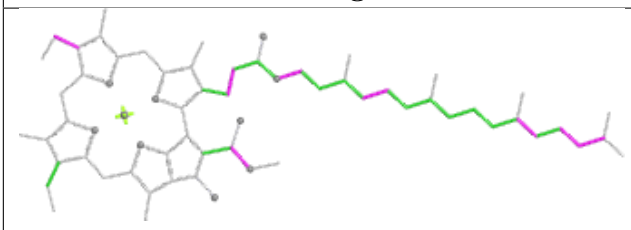
Ligand CLA a 808



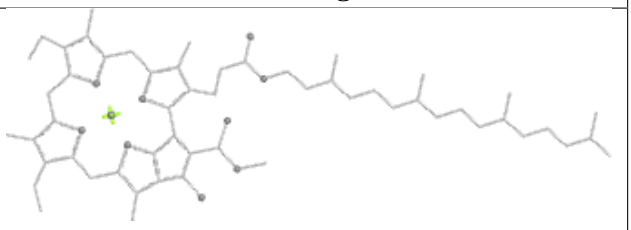
Bond lengths



Bond angles

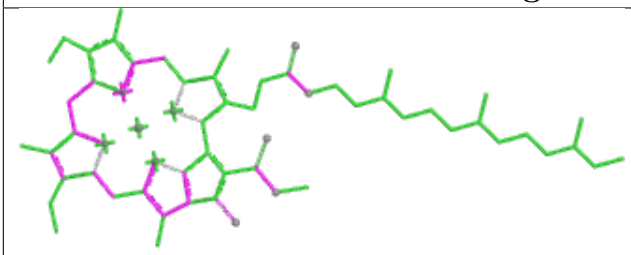


Torsions

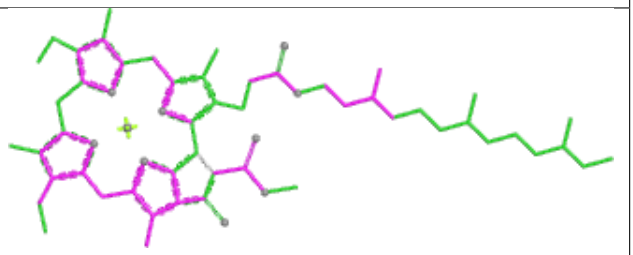


Rings

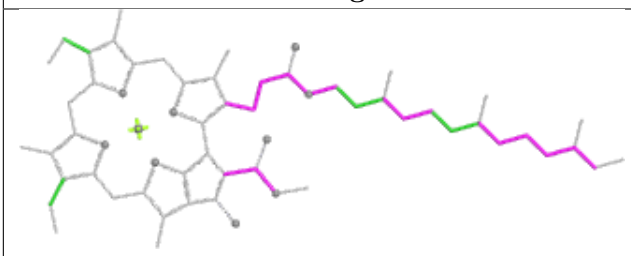
Ligand CLA K 307



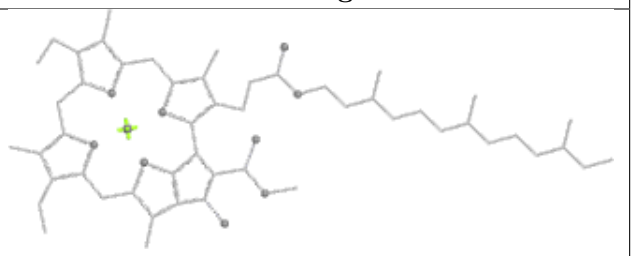
Bond lengths



Bond angles

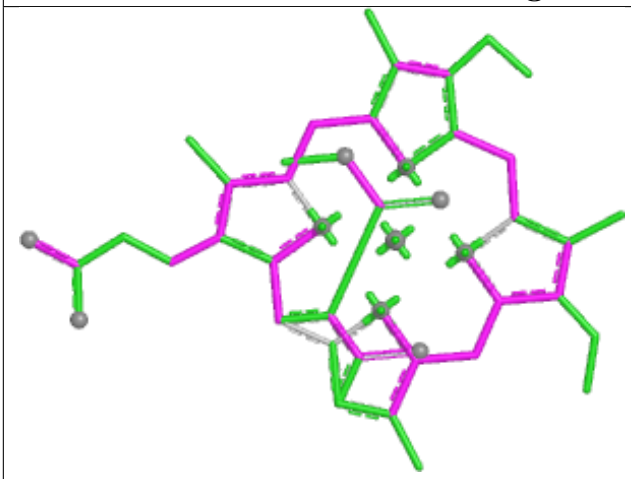


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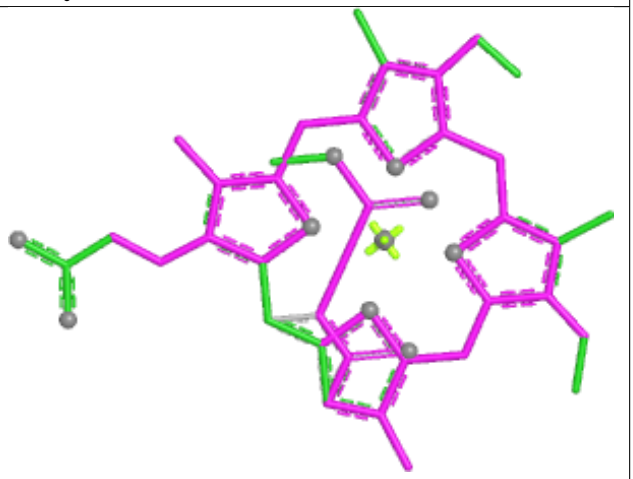


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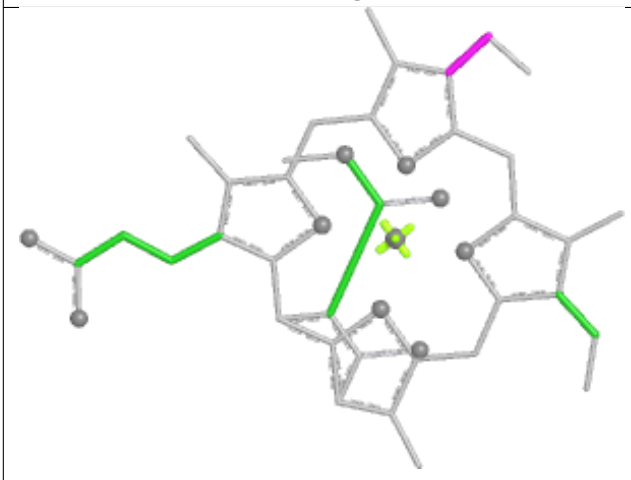
Ligand KC1 Q 311



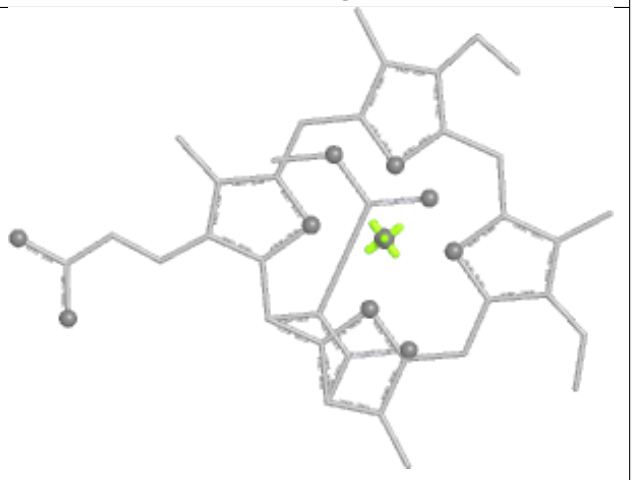
Bond lengths



Bond angles

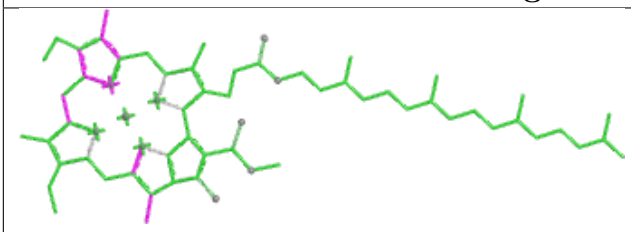


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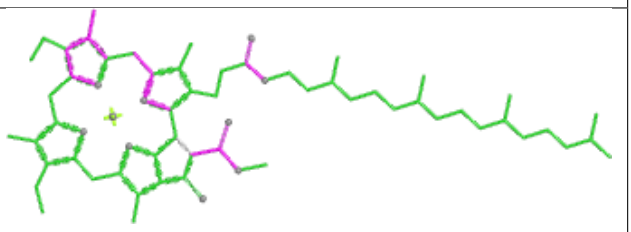


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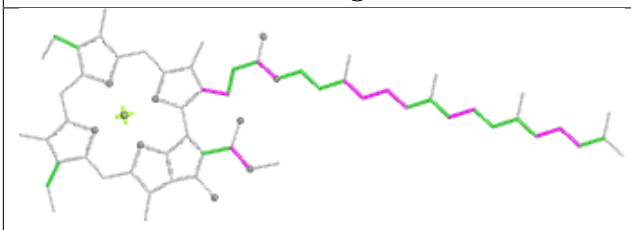
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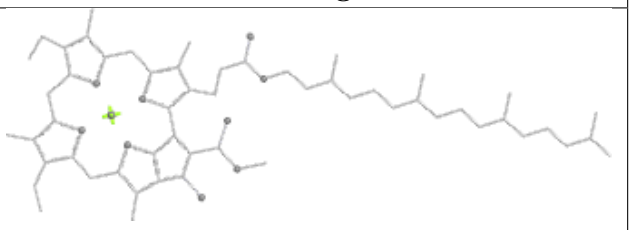
Bond lengths



Bond angles

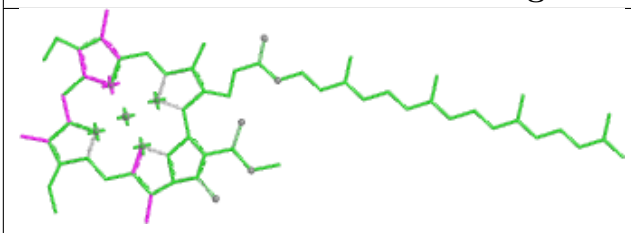


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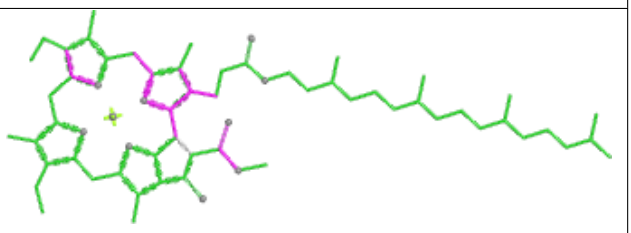


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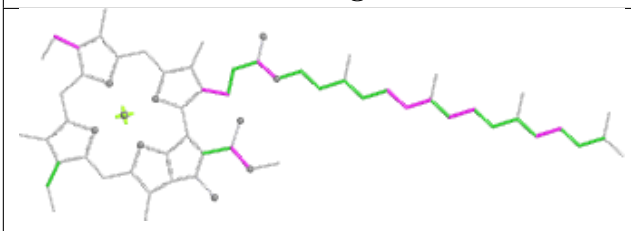
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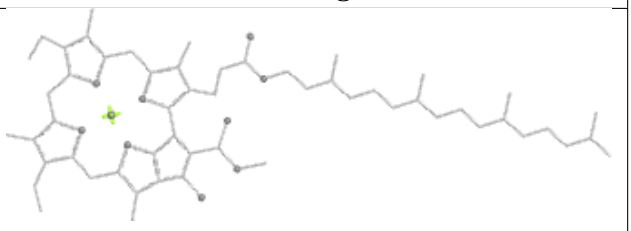
Bond lengths



Bond angles

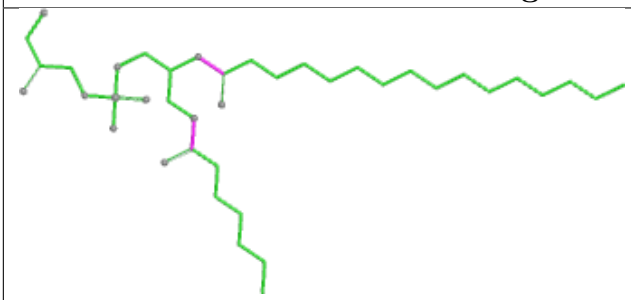


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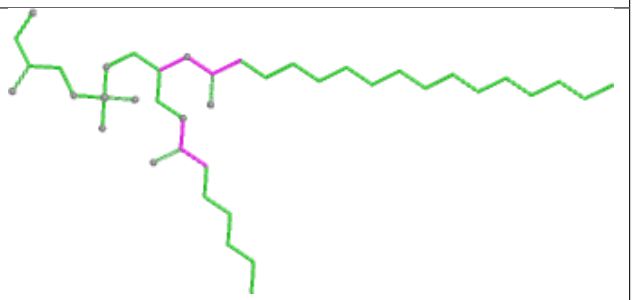


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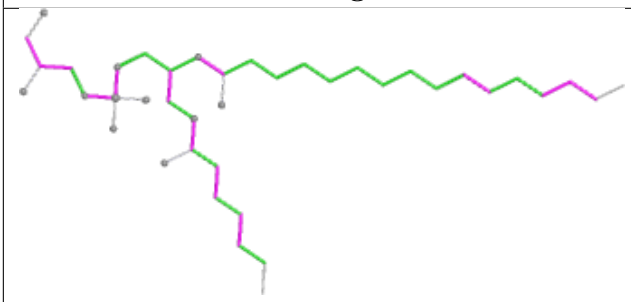
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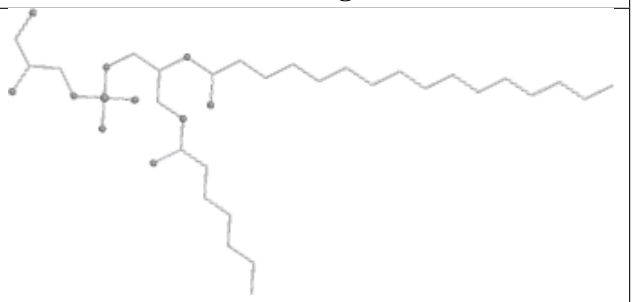
Bond lengths



Bond angles

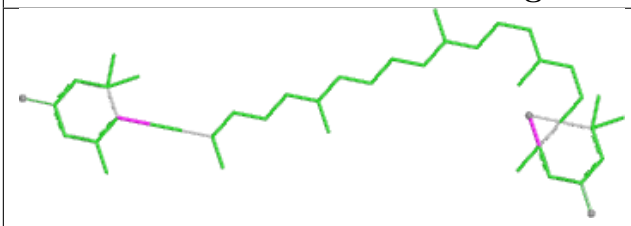


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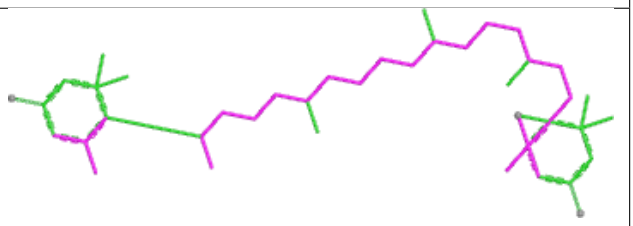


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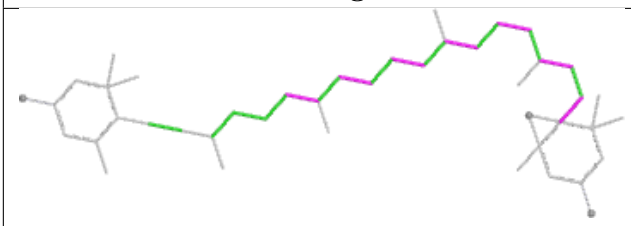
Ligand DD6 R 307



Bond lengths



Bond angles

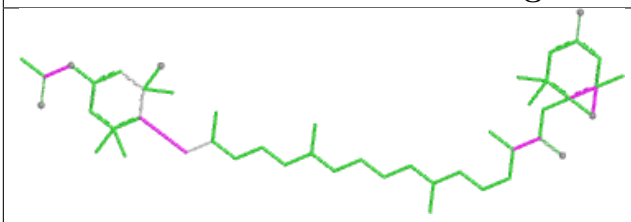


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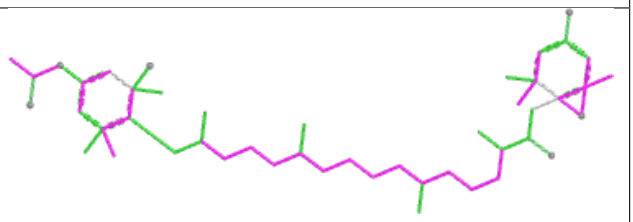


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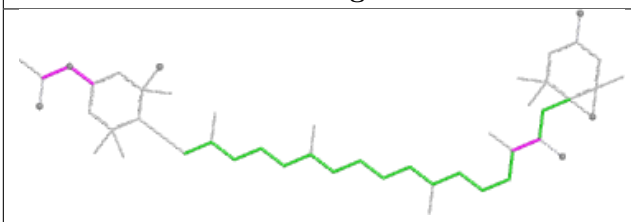
Ligand A86 W 203



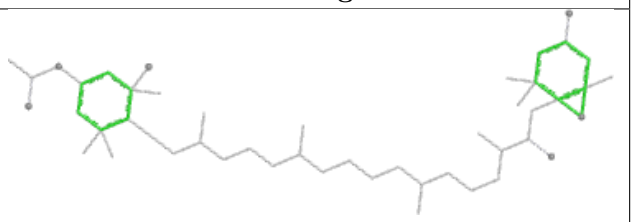
Bond lengths



Bond angles

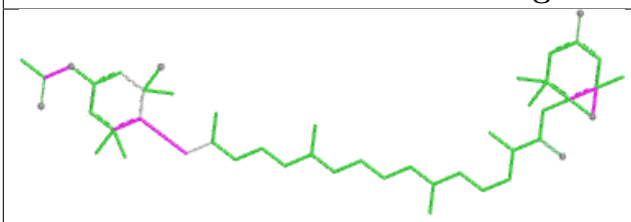


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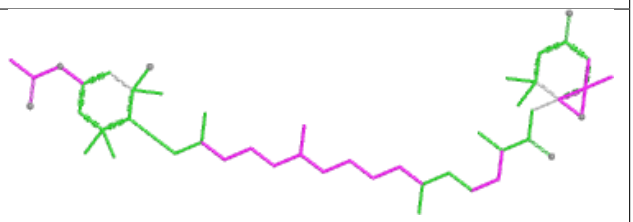


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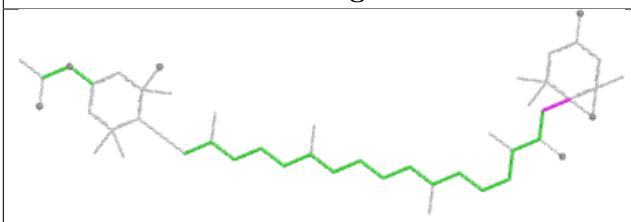
Ligand A86 h 204



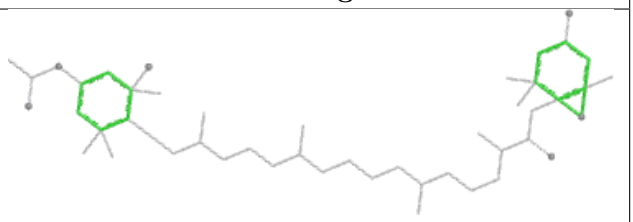
Bond lengths



Bond angles

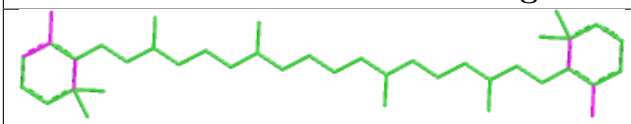


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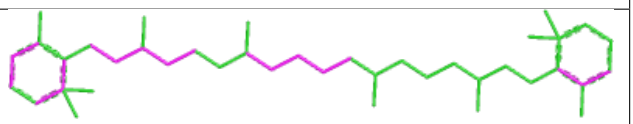


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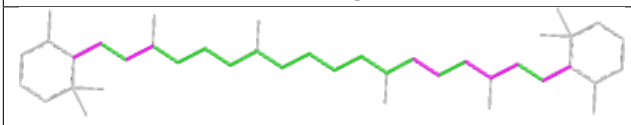
Ligand BCR m 101



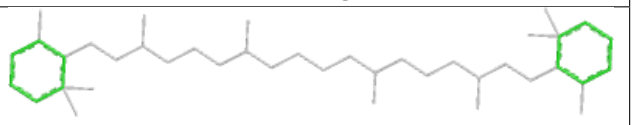
Bond lengths



Bond angles

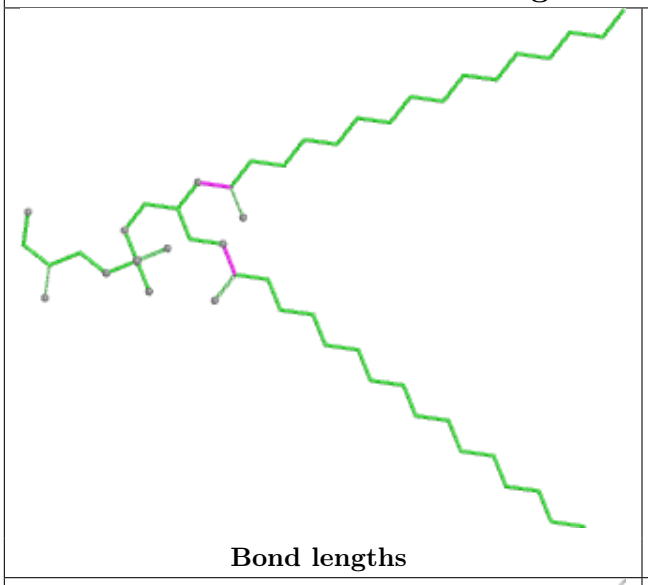


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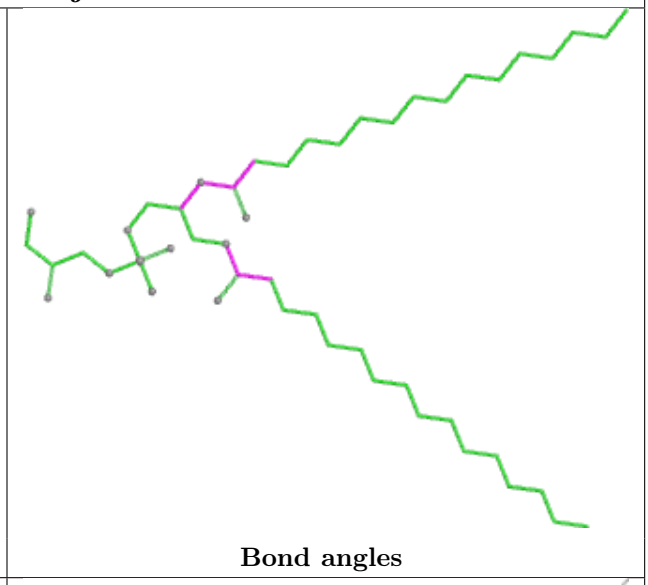


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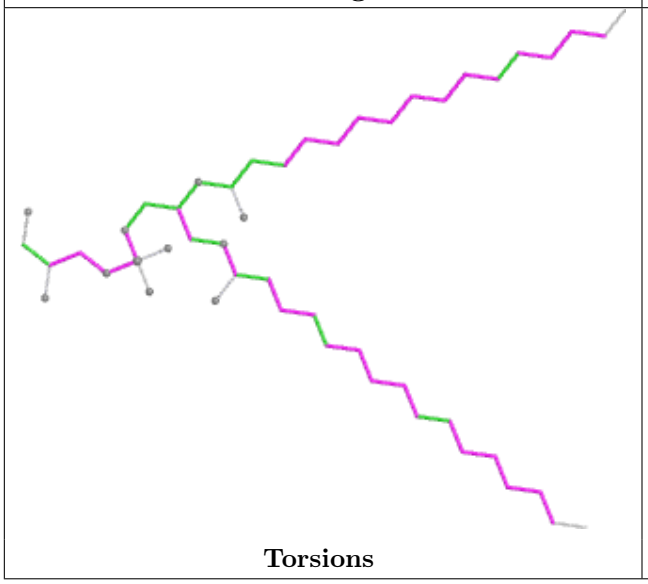
Ligand LHG j 104



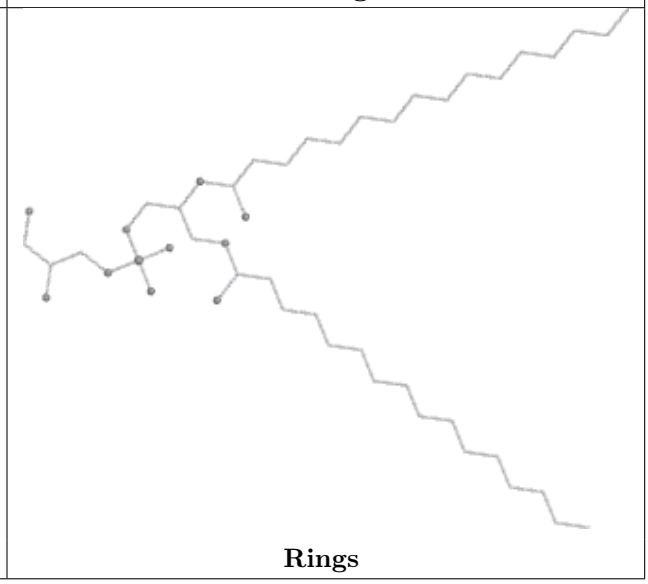
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Bond angles

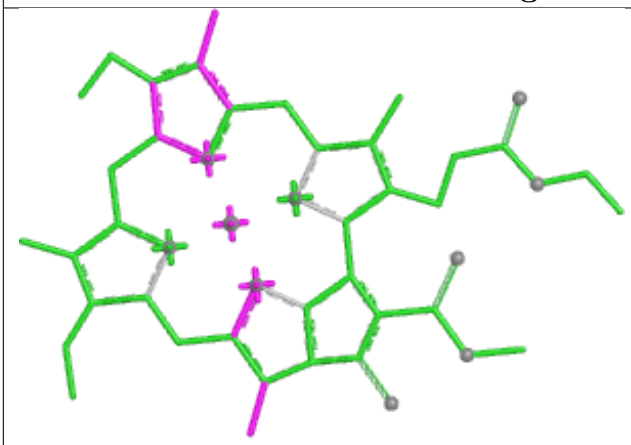


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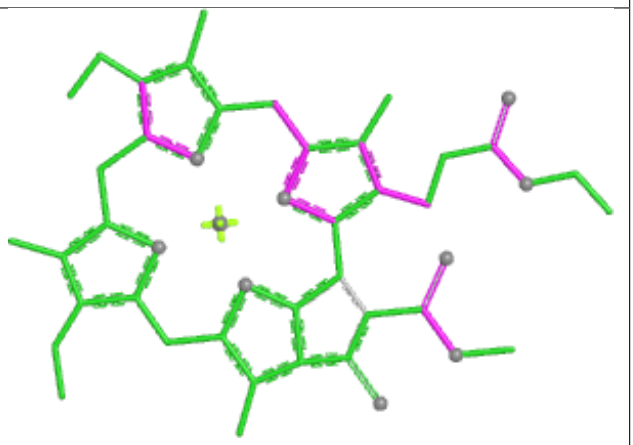


Rings

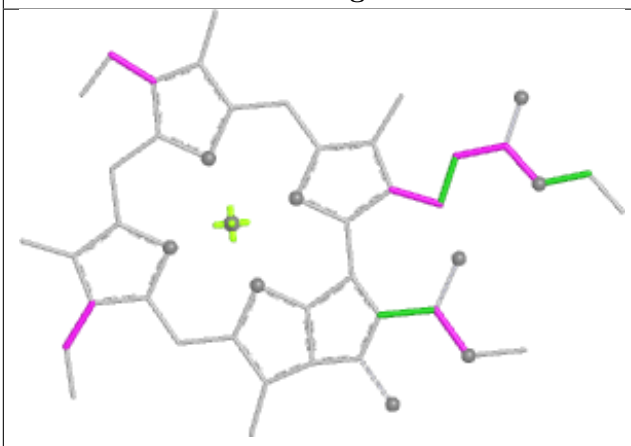
Ligand CLA M 312



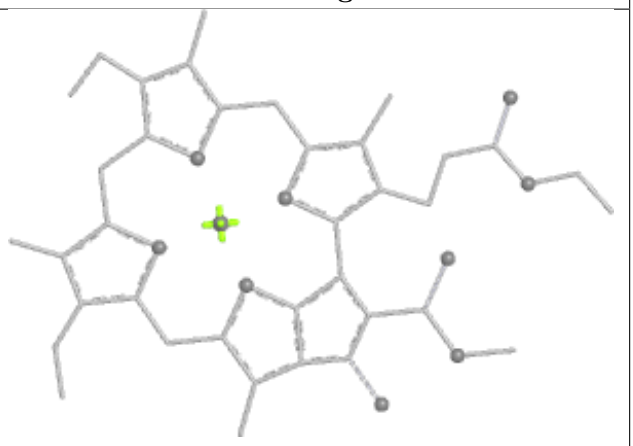
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Bond angles

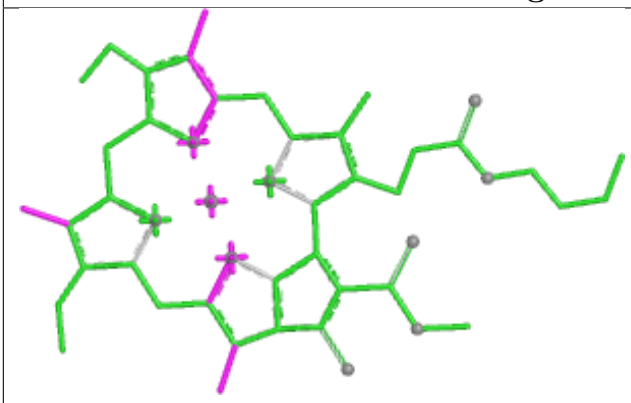


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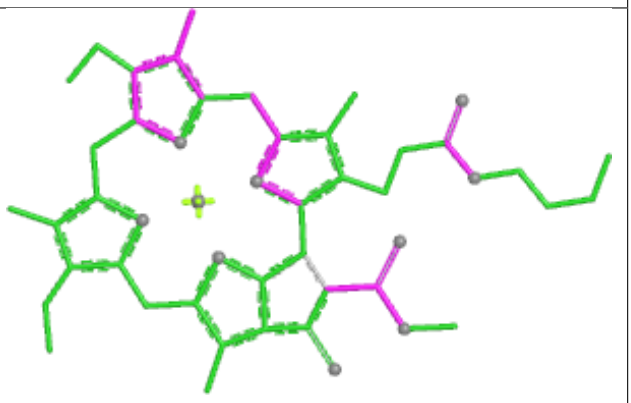


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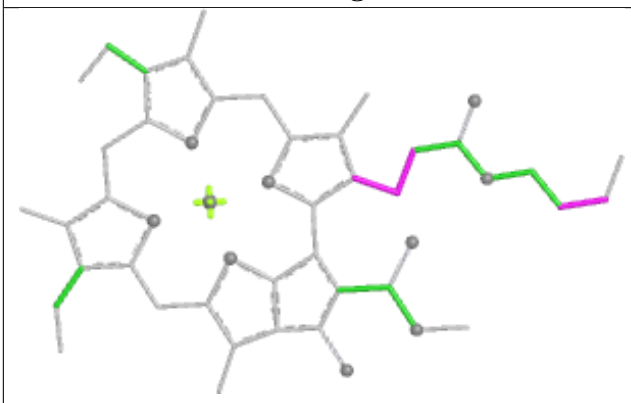
Ligand CLA b 832



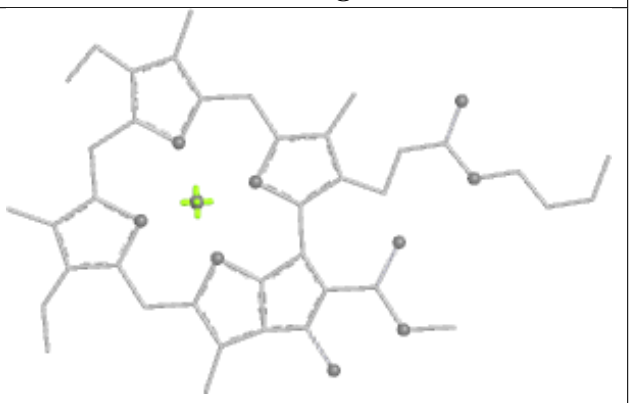
Bond lengths



Bond angles

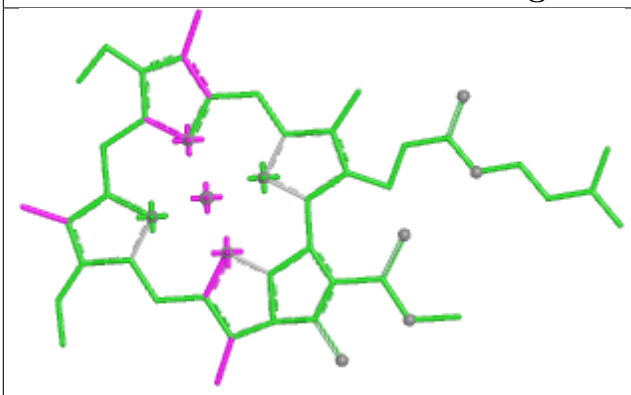


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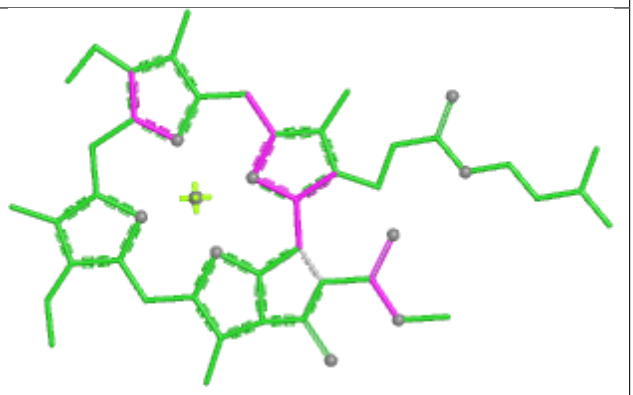


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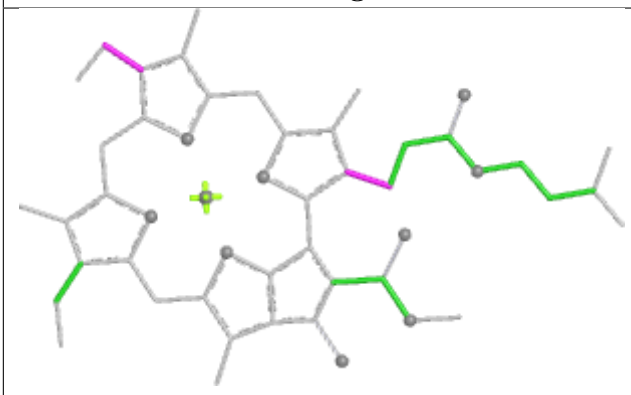
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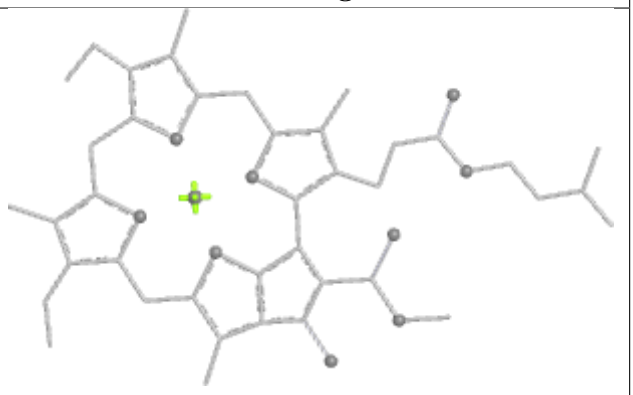
Bond lengths



Bond angles

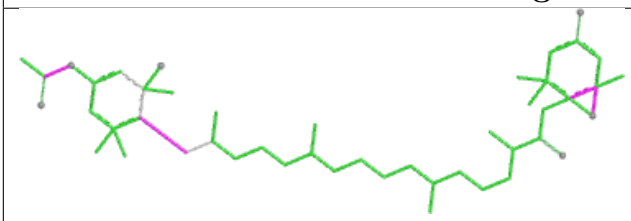


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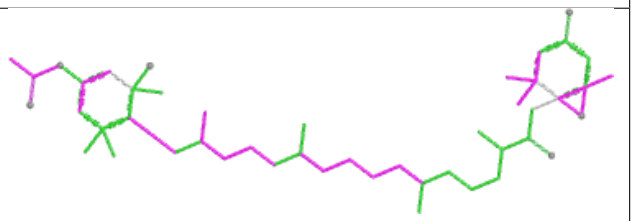


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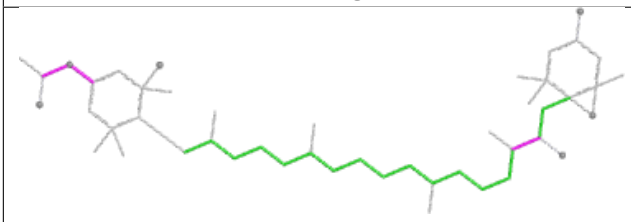
Ligand A86 S 302



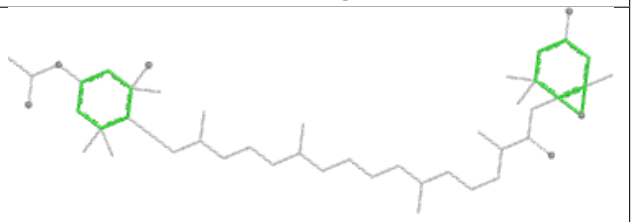
Bond lengths



Bond angles

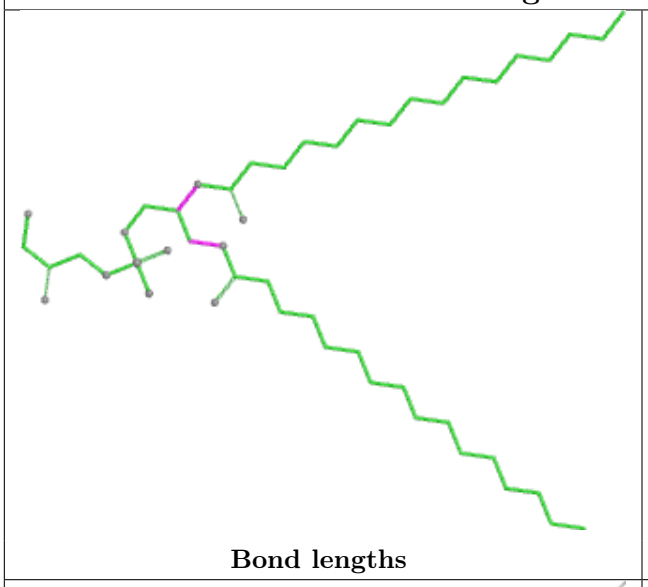


Torsions

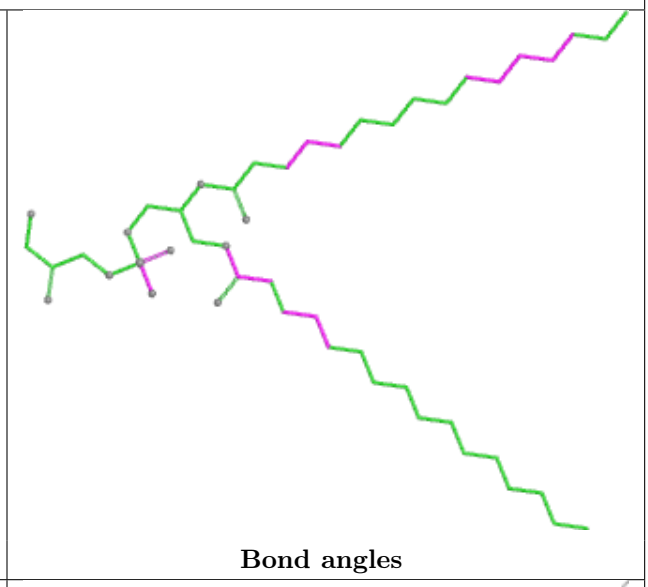


Rings

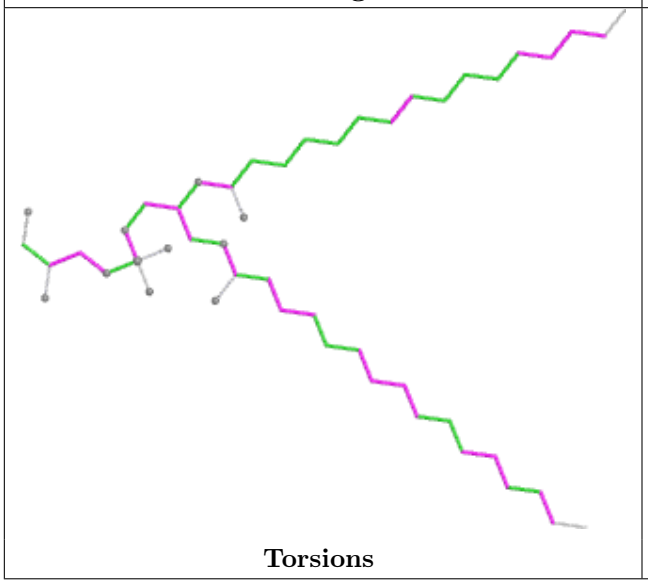
Ligand LHG G 301



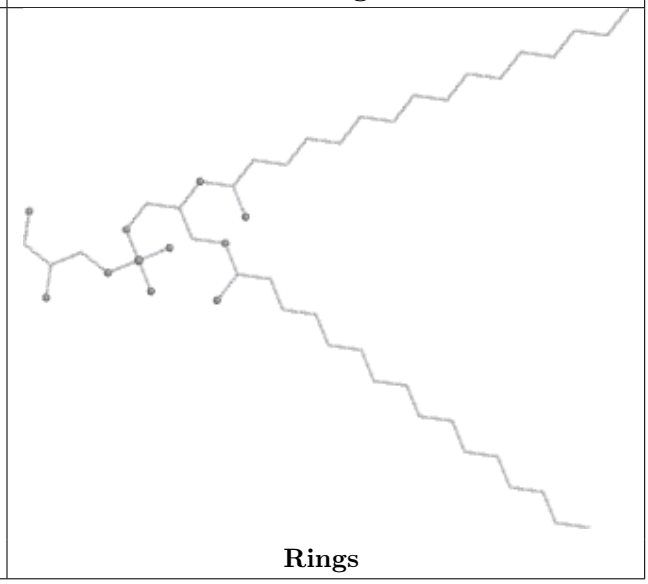
Bond lengths



Bond angles

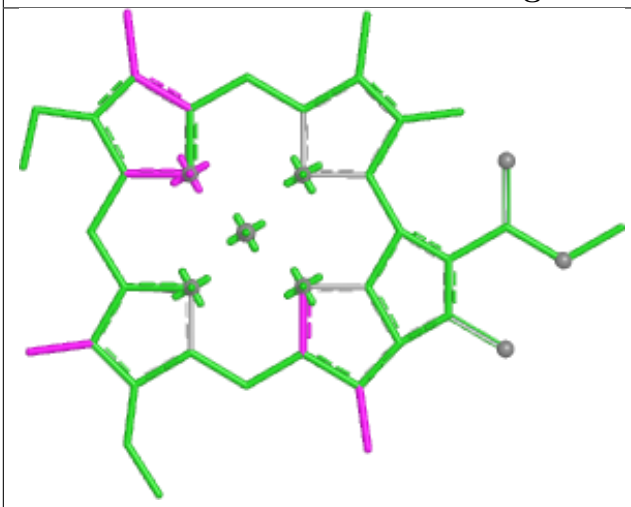


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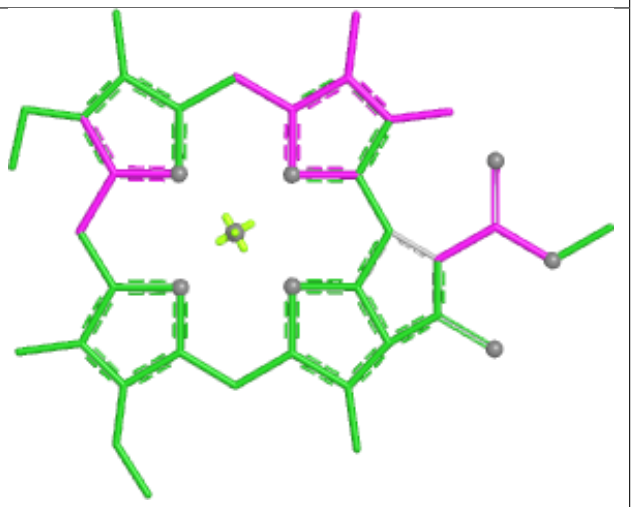


Rings

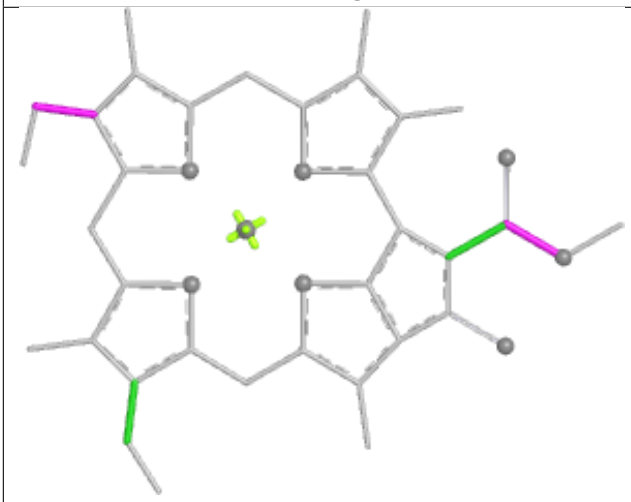
Ligand CLA O 314



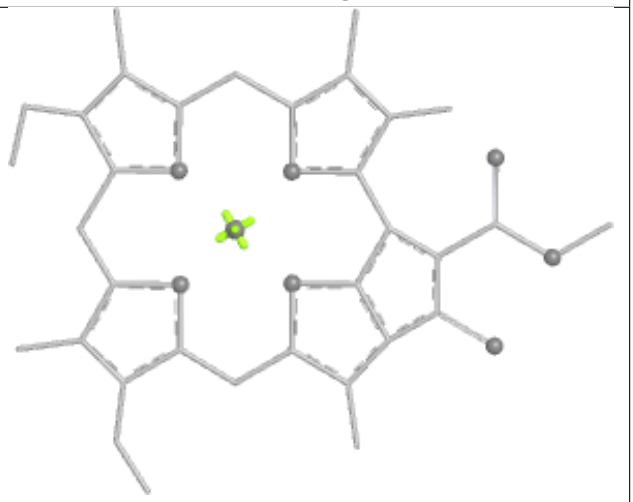
Bond lengths



Bond angles

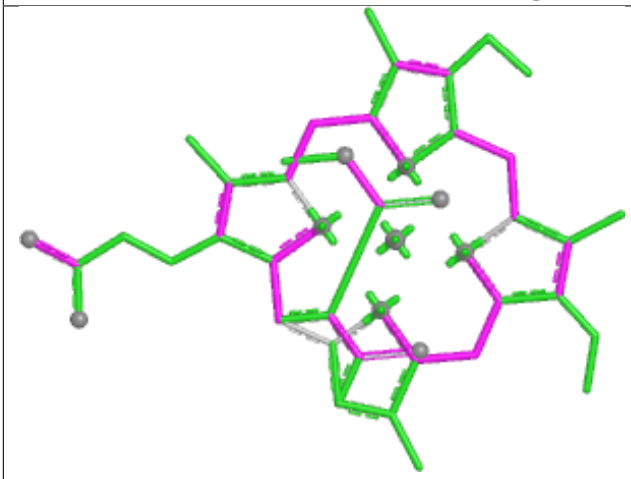


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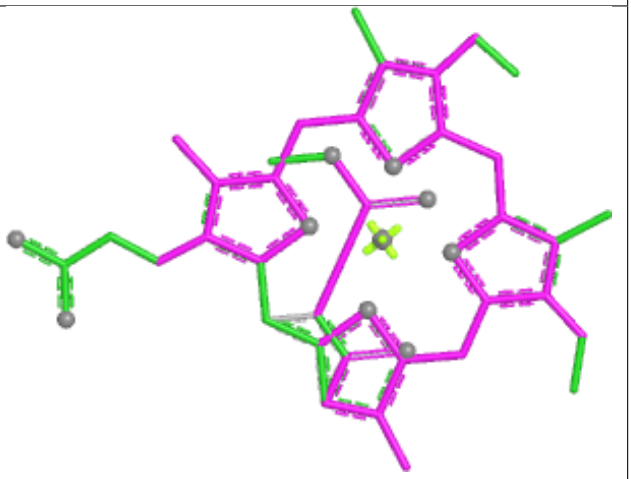


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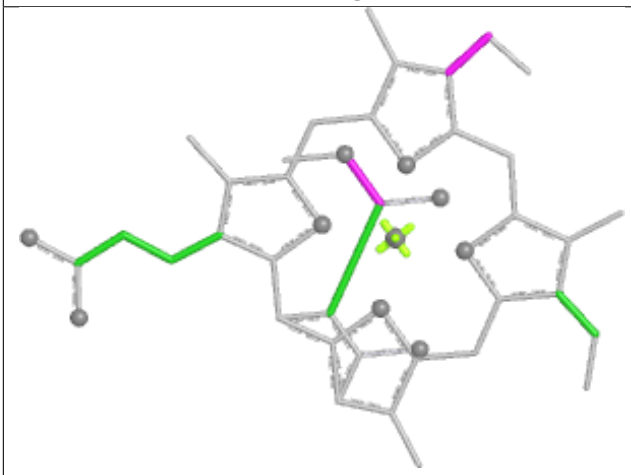
Ligand KC1 F 315



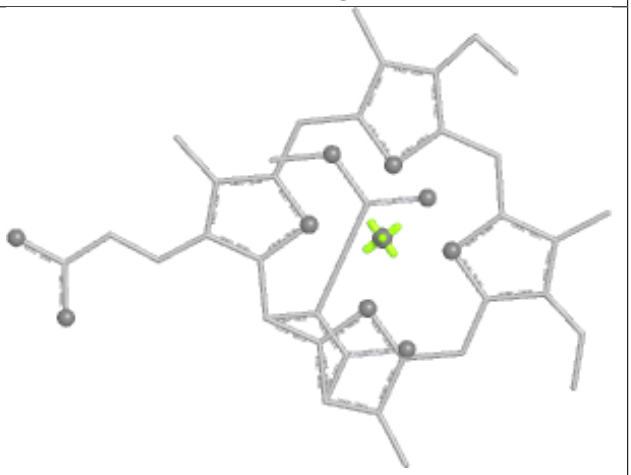
Bond lengths



Bond angles

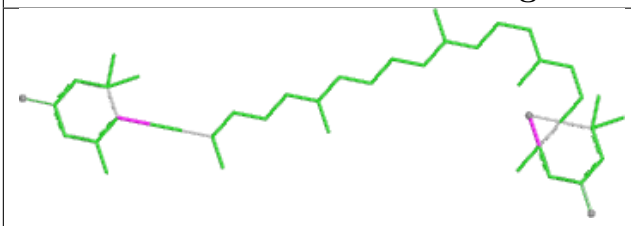


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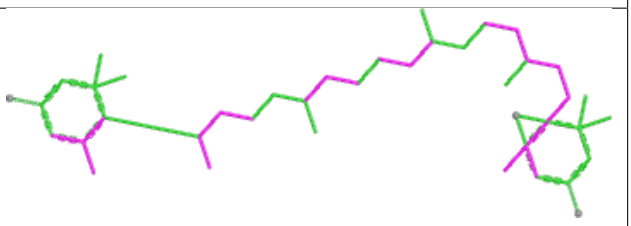


Rings

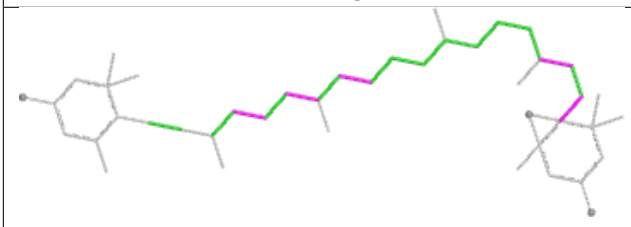
Ligand DD6 W 204



Bond lengths



Bond angles

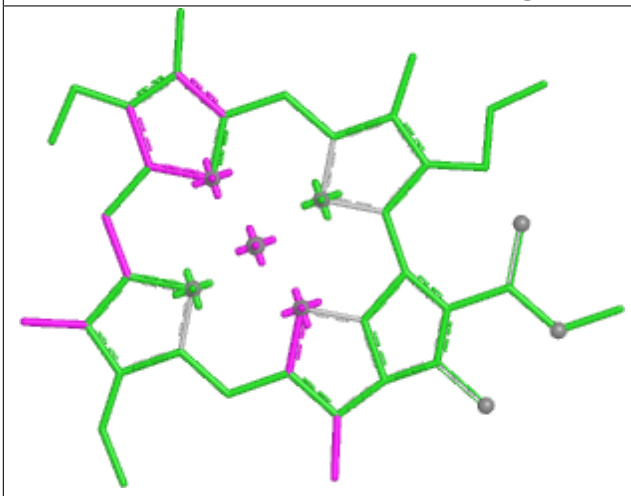


Torsions

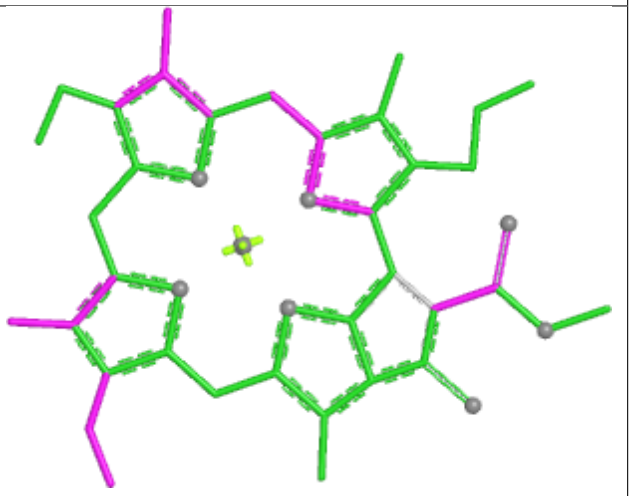


Rings

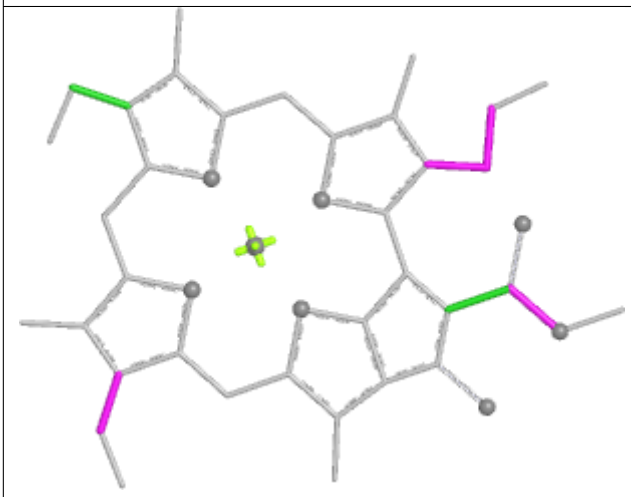
Ligand CLA W 218



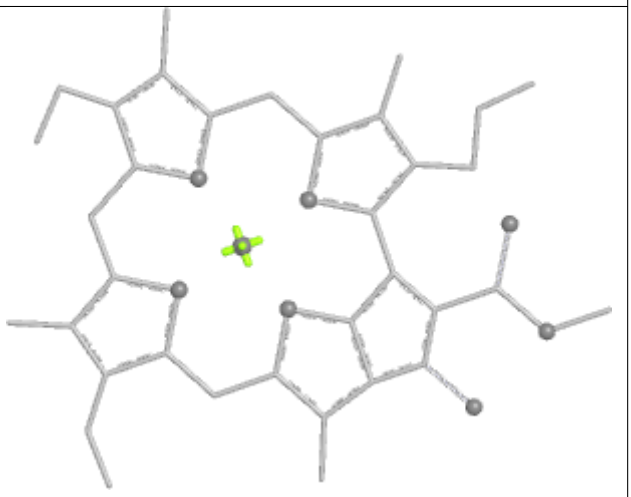
Bond lengths



Bond angles

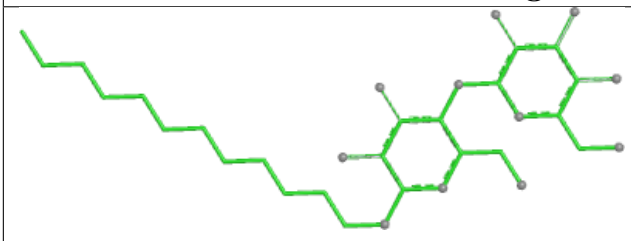


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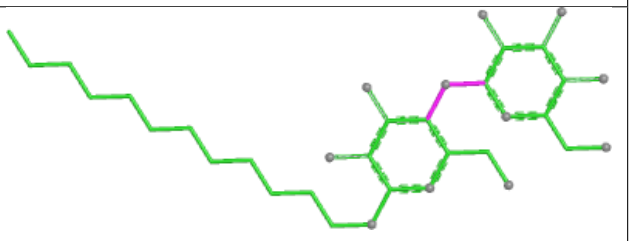


Rings

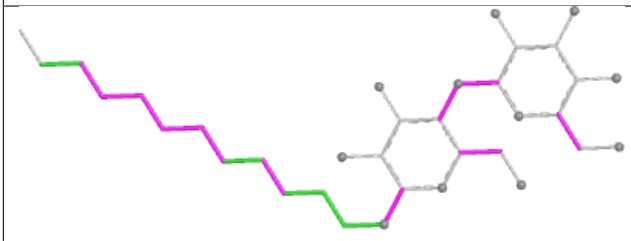
Ligand LMT a 851



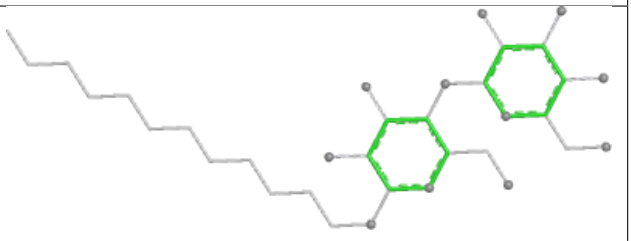
Bond lengths



Bond angles

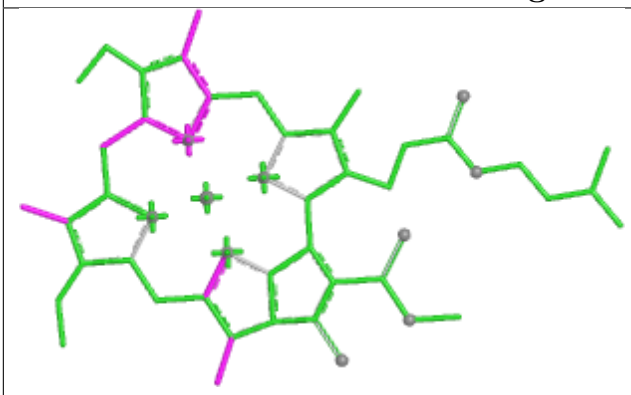


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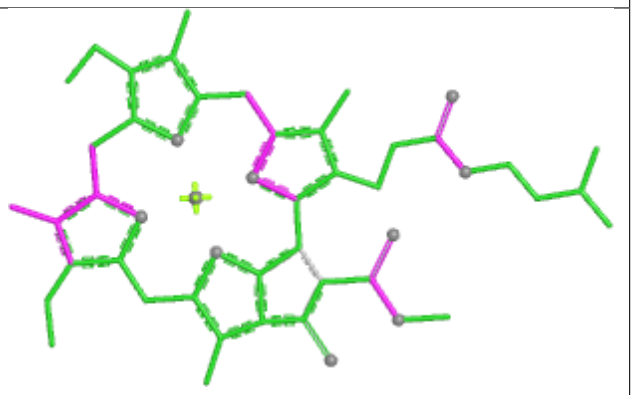


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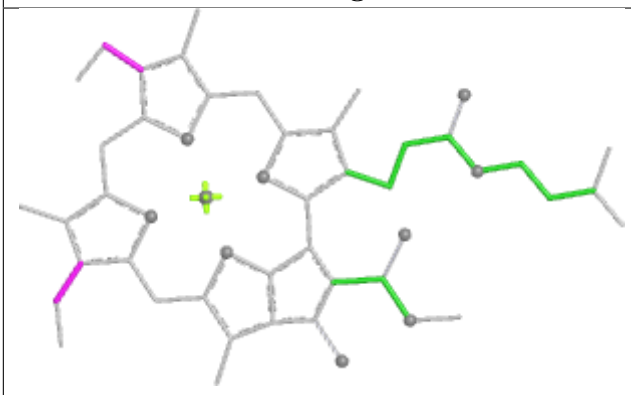
Ligand CLA a 814



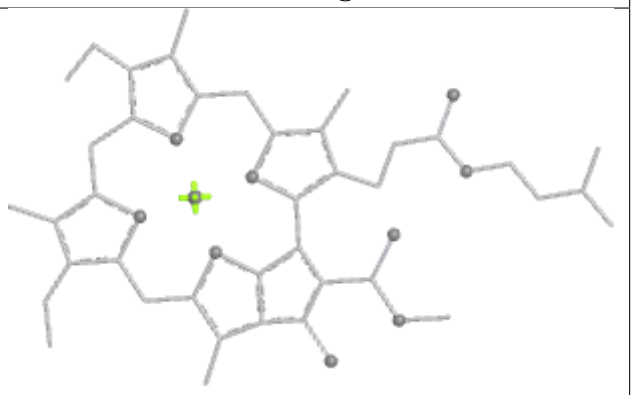
Bond lengths



Bond angles



Torsions

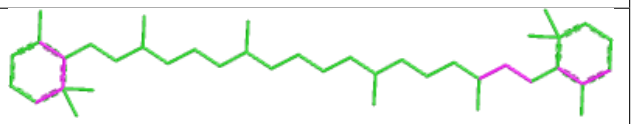


Rings

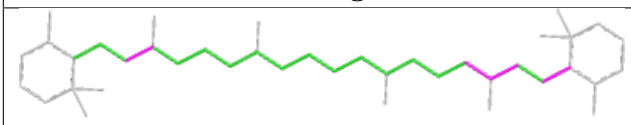
Ligand BCR a 845



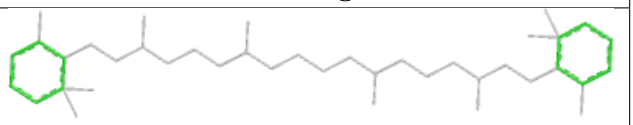
Bond lengths



Bond angles

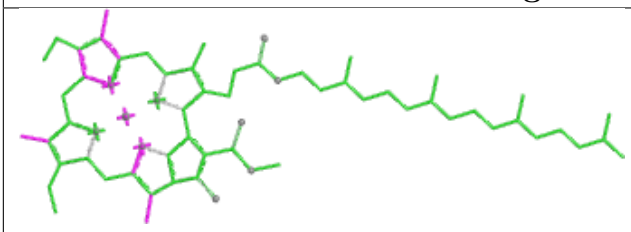


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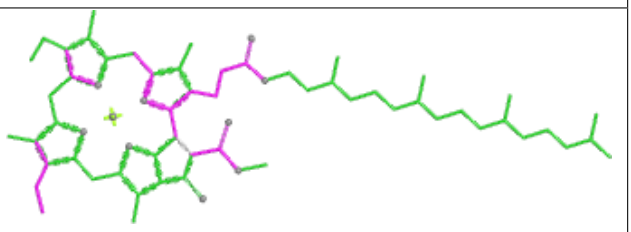


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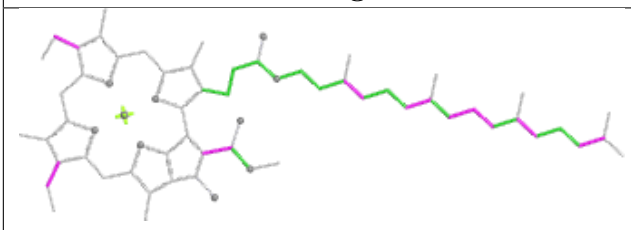
Ligand CLA H 315



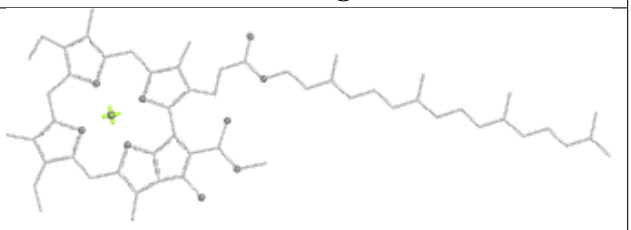
Bond lengths



Bond angles



Torsions

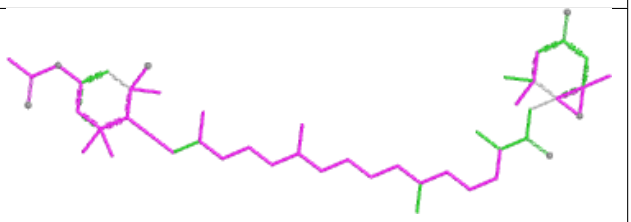


Rings

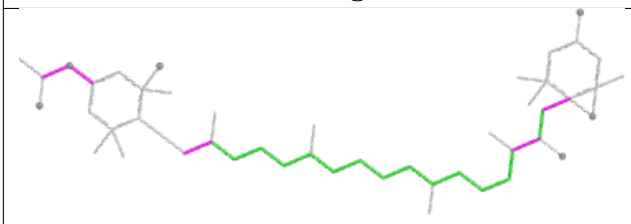
Ligand A86 N 320



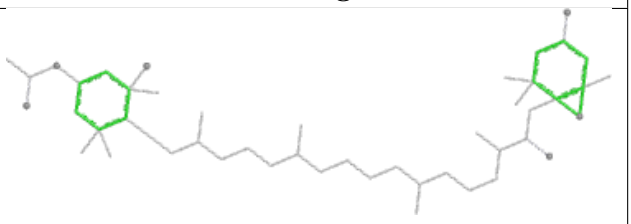
Bond lengths



Bond angles

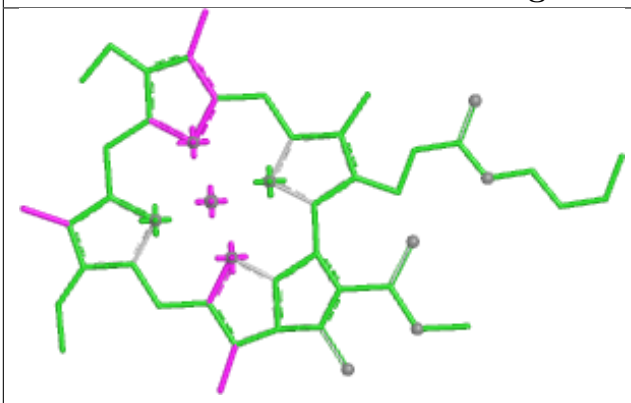


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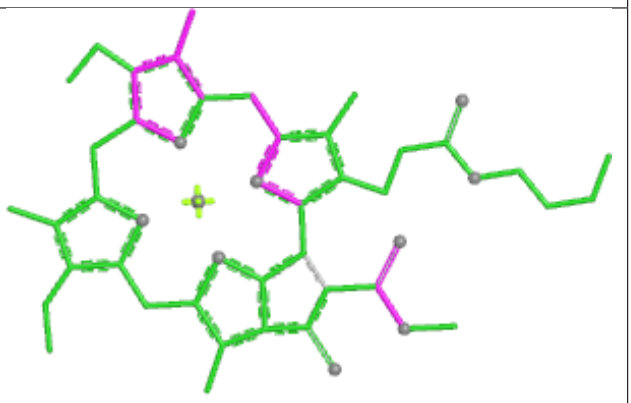


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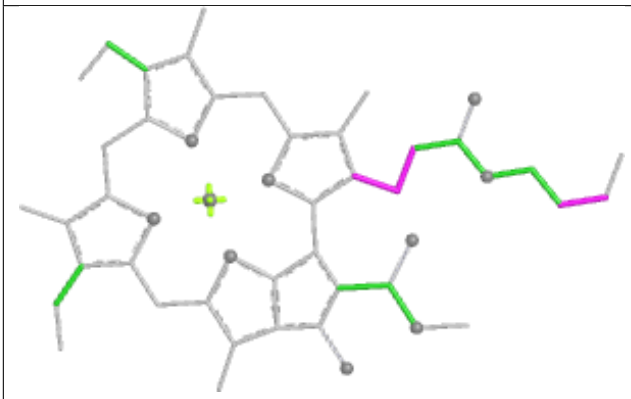
Ligand CLA a 821



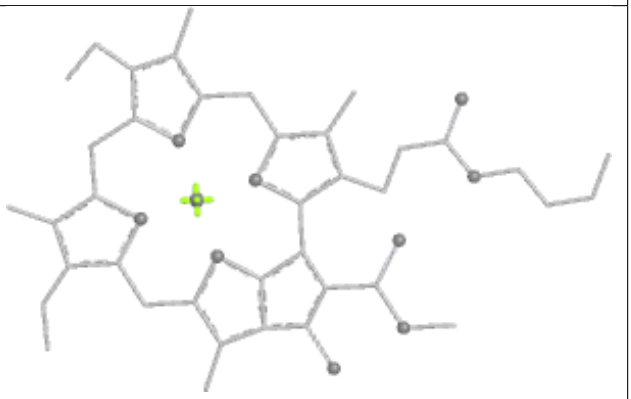
Bond lengths



Bond angles



Torsions

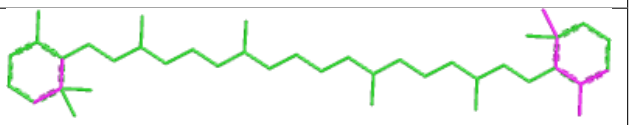


Rings

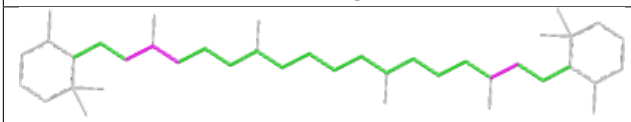
Ligand BCR f 801



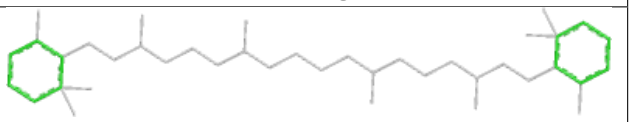
Bond lengths



Bond angles

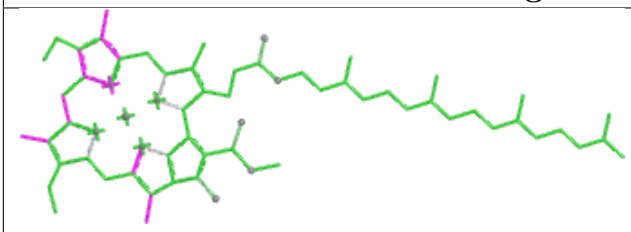


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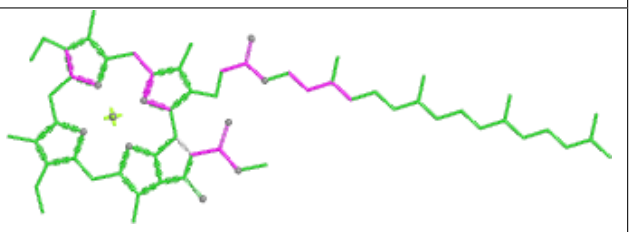


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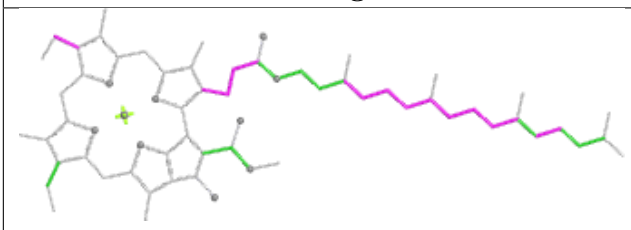
Ligand CLA P 301



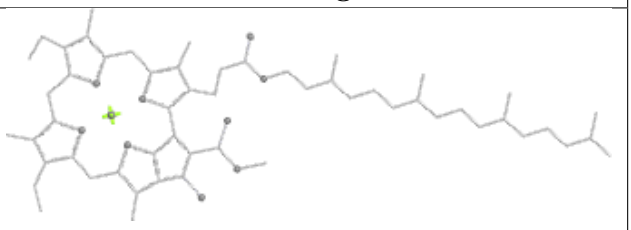
Bond lengths



Bond angles

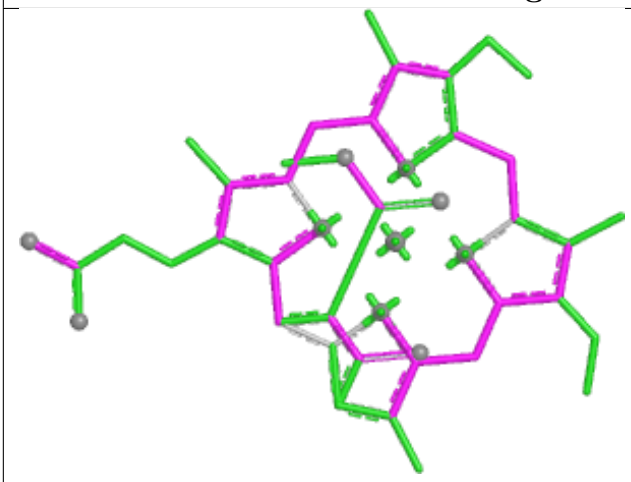


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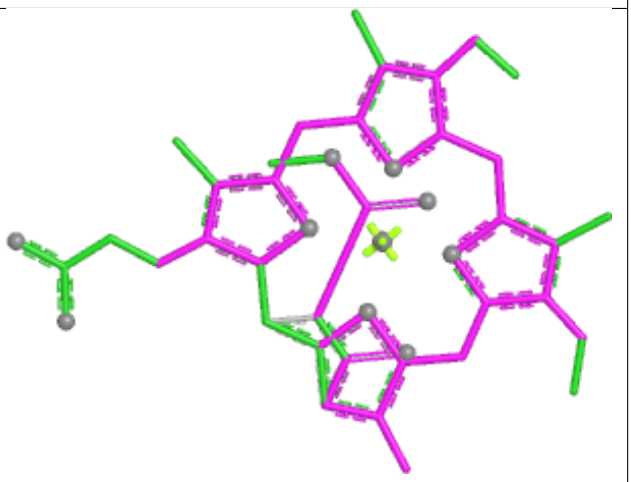


Rings

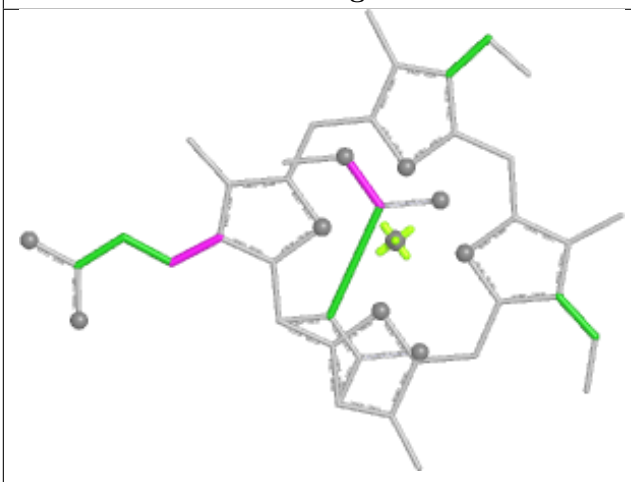
Ligand KC1 U 312



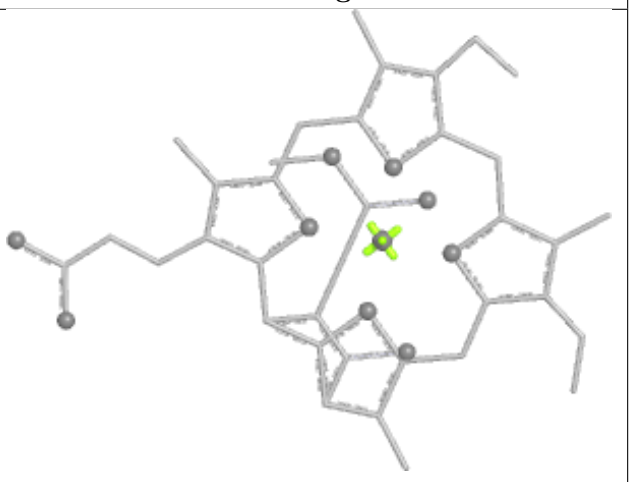
Bond lengths



Bond angles

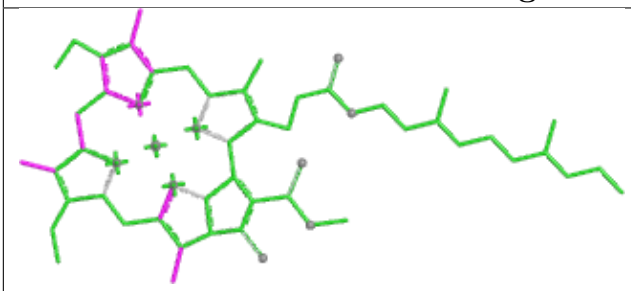


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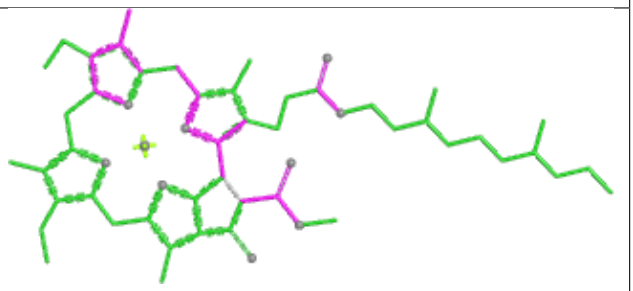


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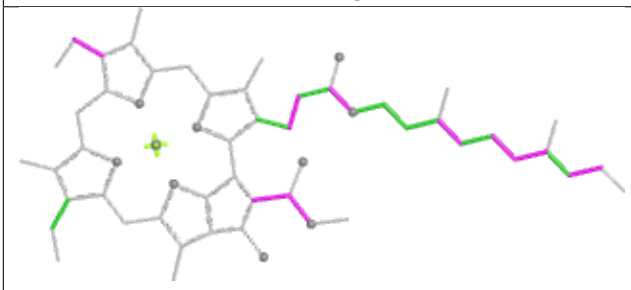
Ligand CLA W 209



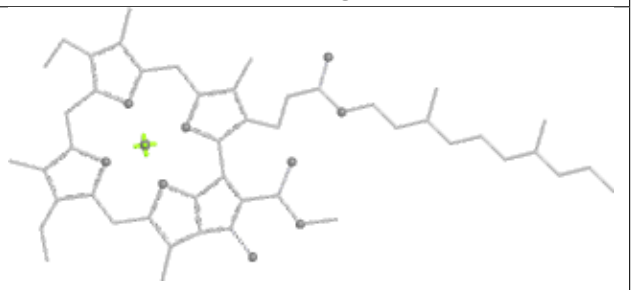
Bond lengths



Bond angles

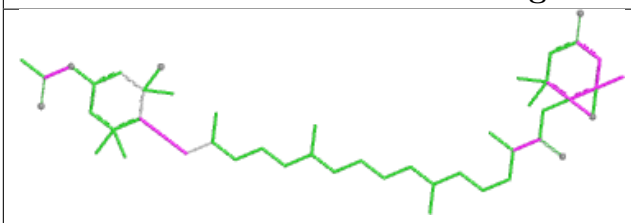


Torsions

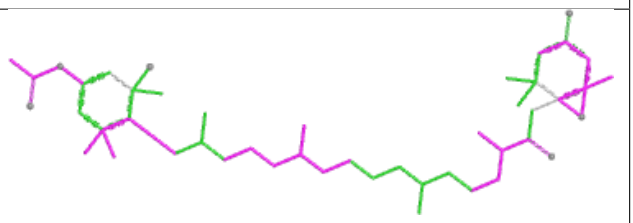


Rings

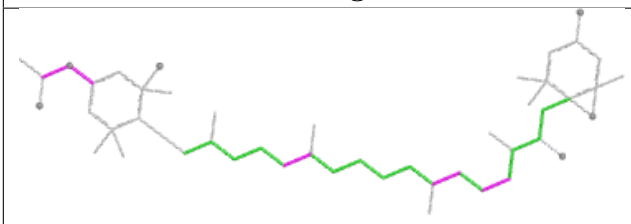
Ligand A86 N 304



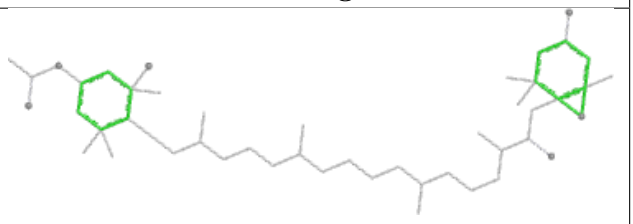
Bond lengths



Bond angles

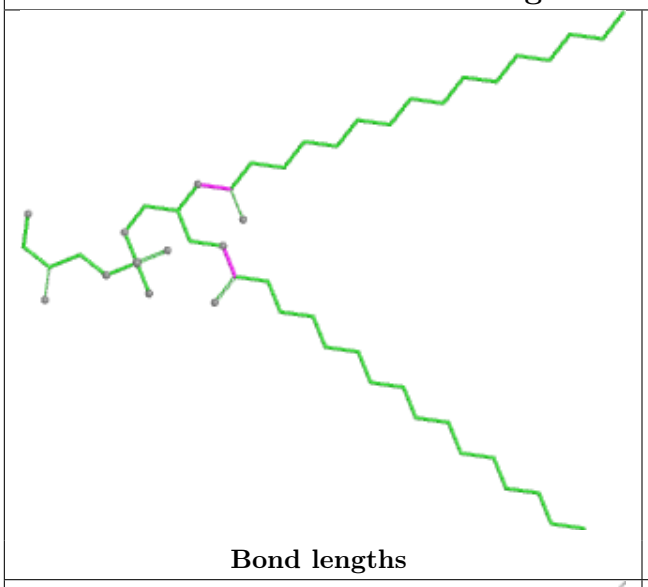


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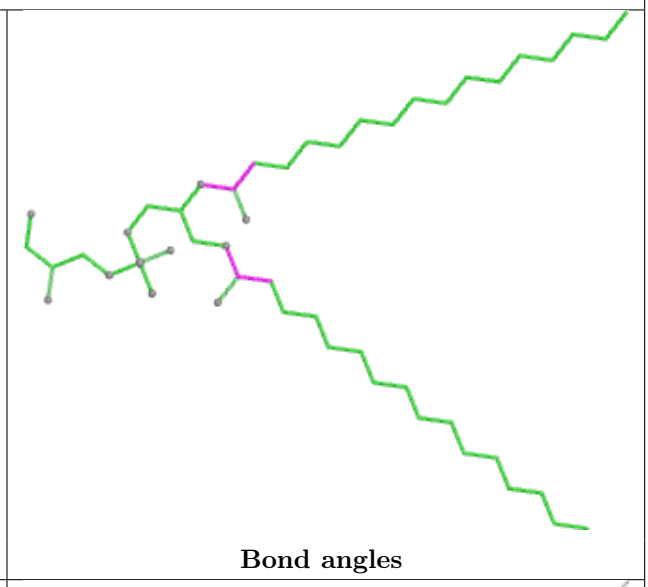


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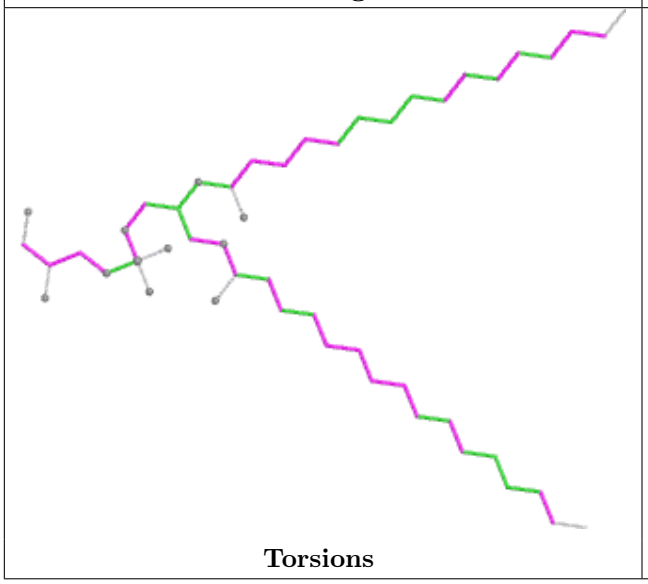
Ligand LHG E 322



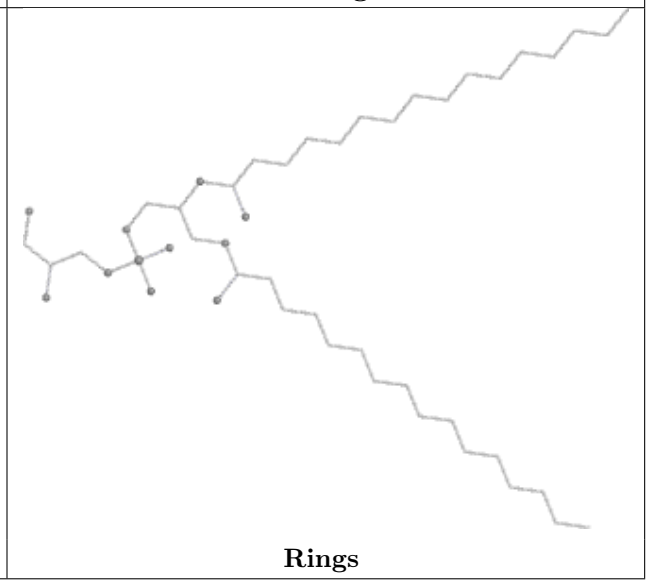
Bond lengths



Bond angles

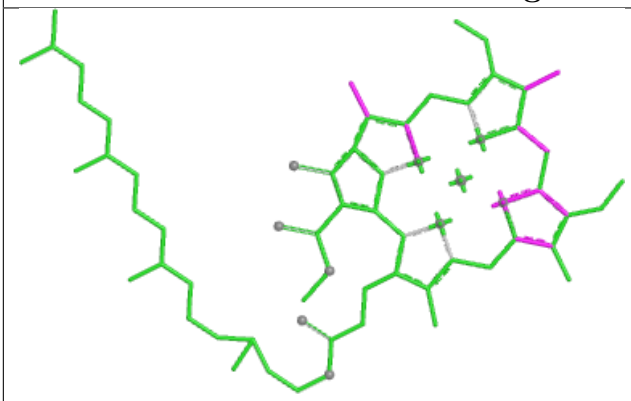


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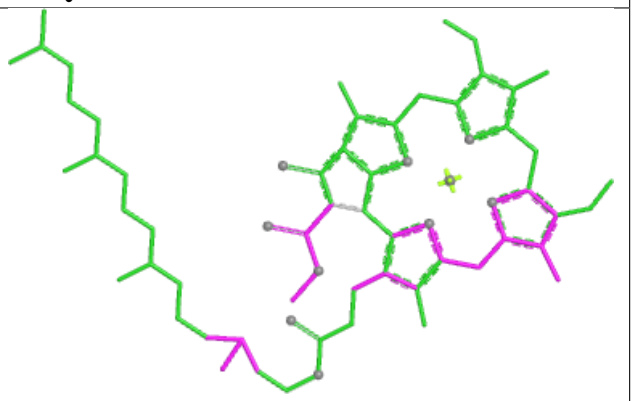


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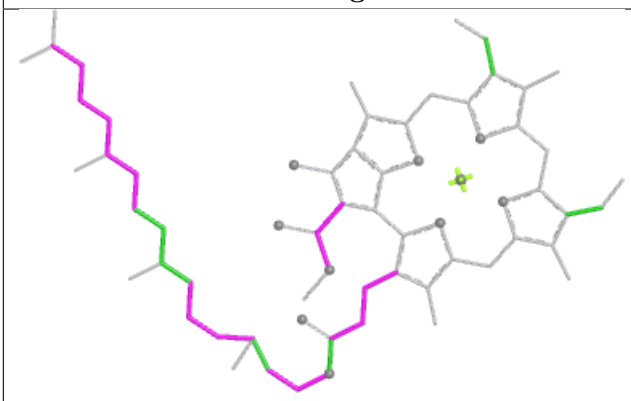
Ligand CLA Q 314



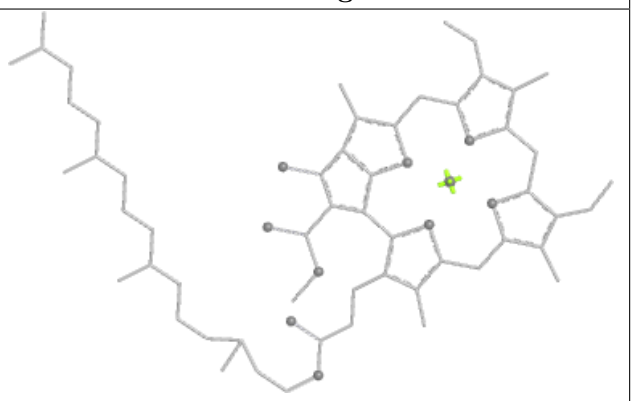
Bond lengths



Bond angles

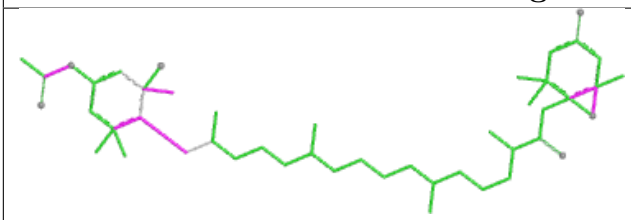


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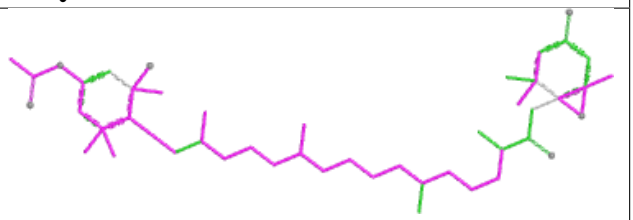


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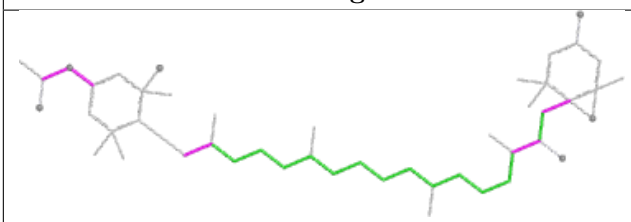
Ligand A86 Q 304



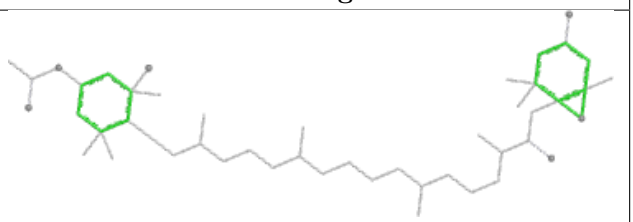
Bond lengths



Bond angles

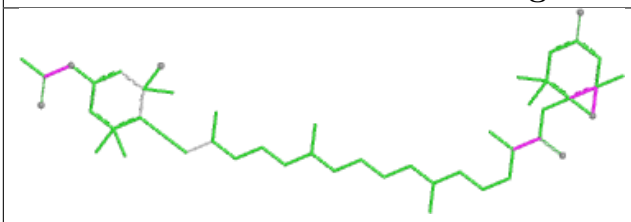


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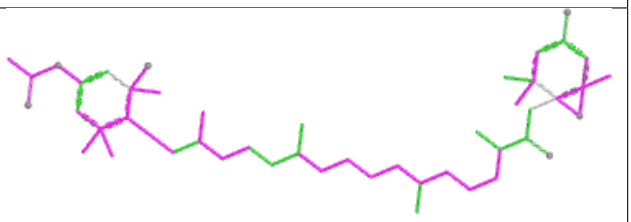


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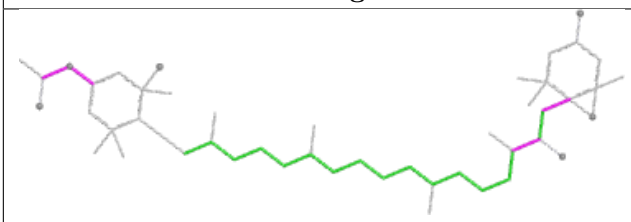
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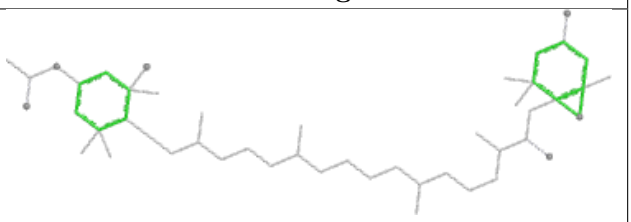
Bond lengths



Bond angles

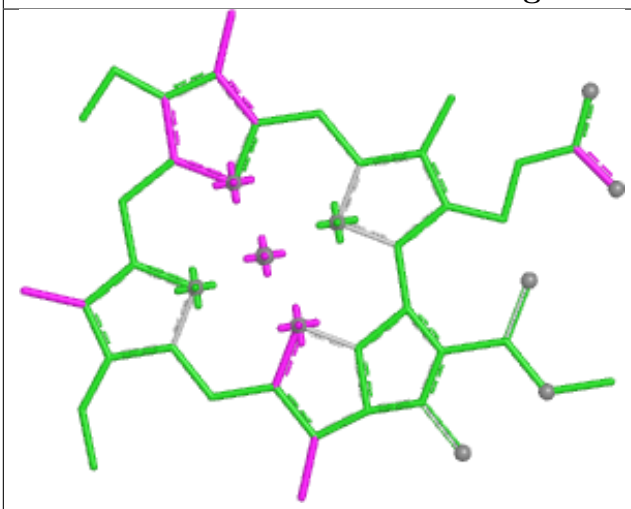


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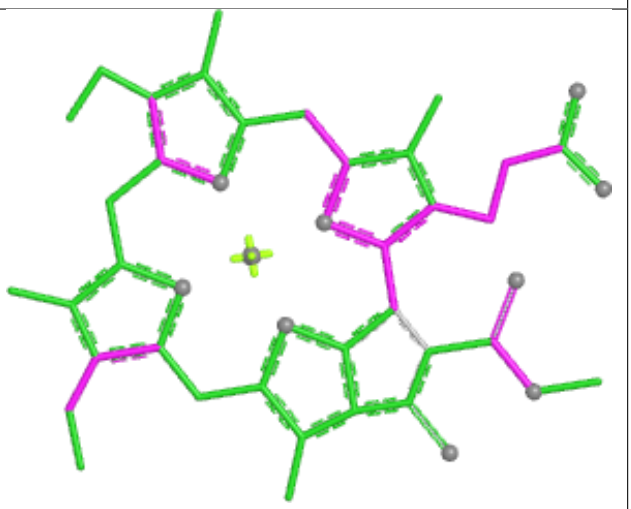


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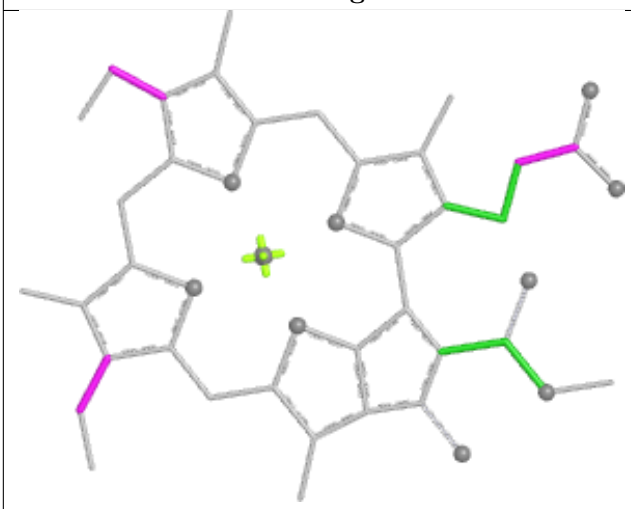
Ligand CLA D 306



Bond lengths



Bond angles

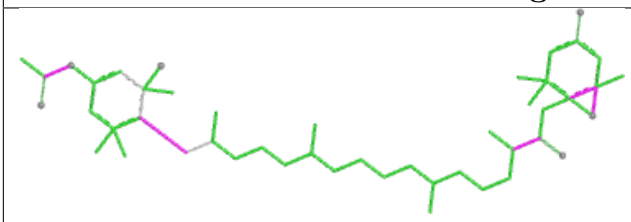


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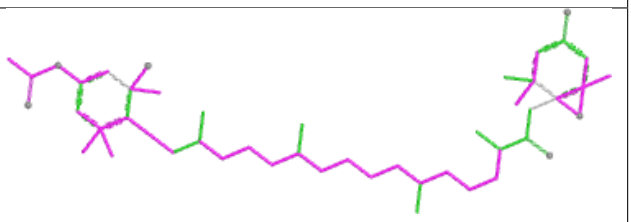


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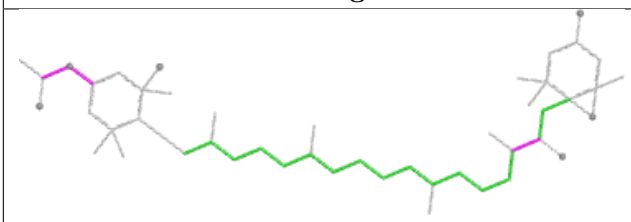
Ligand A86 R 303



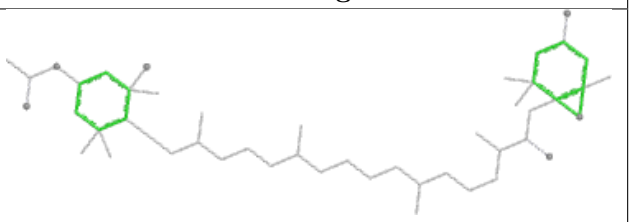
Bond lengths



Bond angles

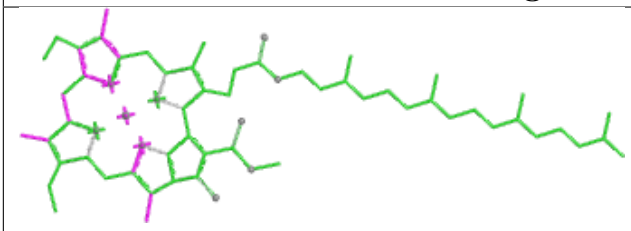


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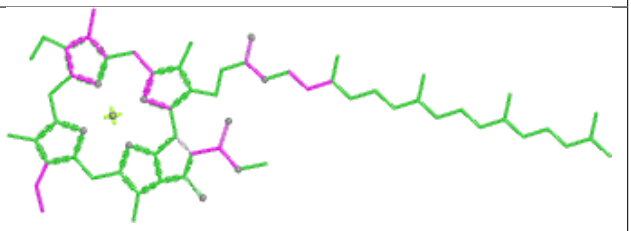


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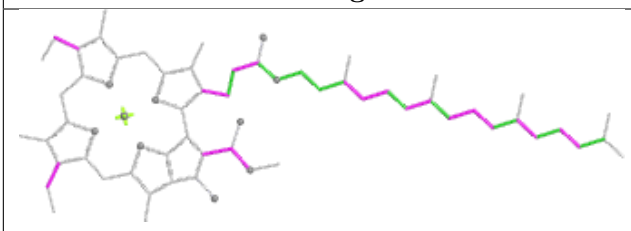
Ligand CLA O 309



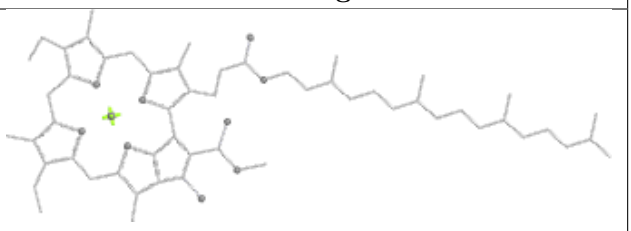
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Bond angles

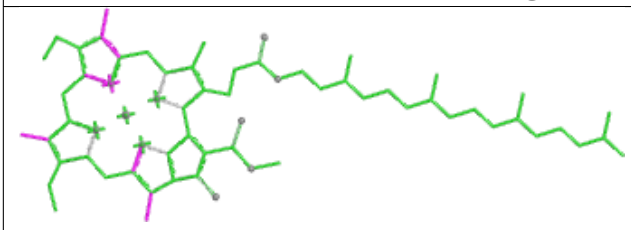


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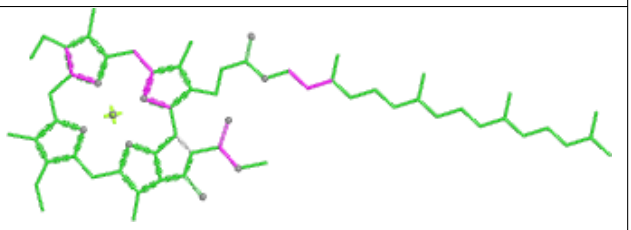


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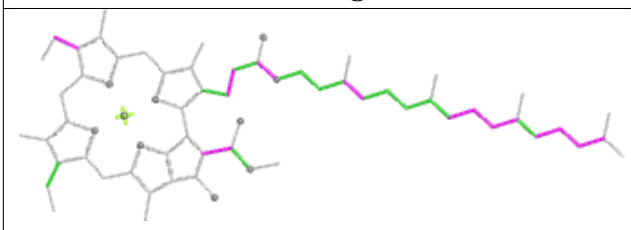
Ligand CLA H 309



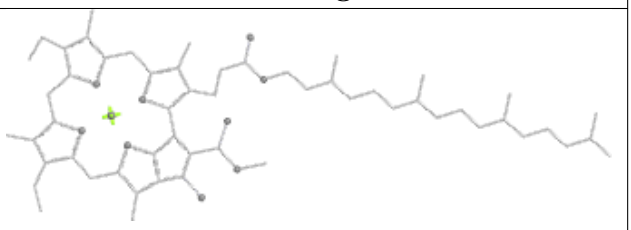
Bond lengths



Bond angles

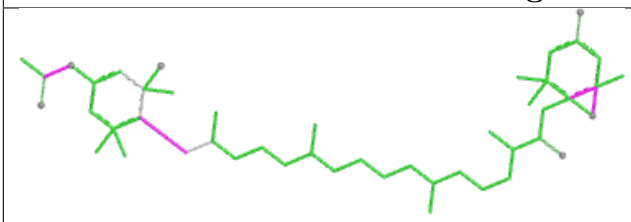


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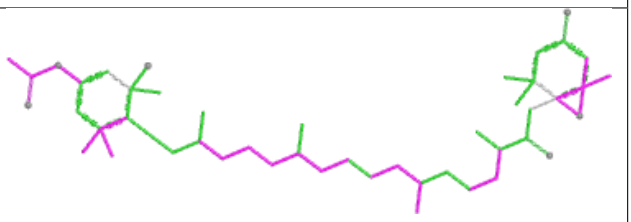


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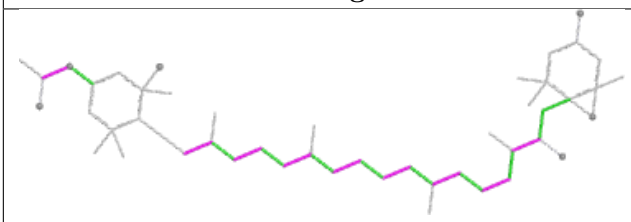
Ligand A86 M 304



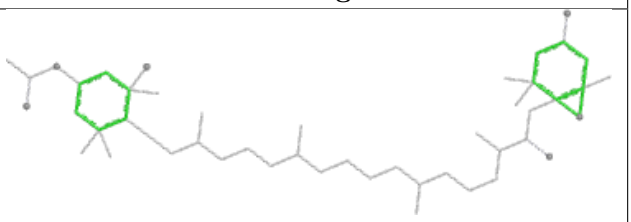
Bond lengths



Bond angles

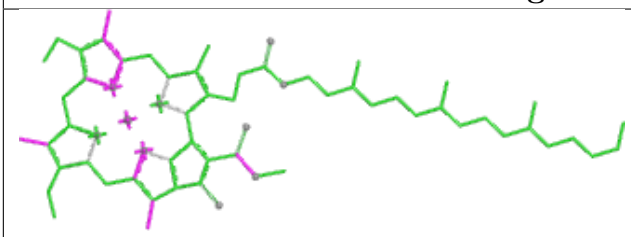


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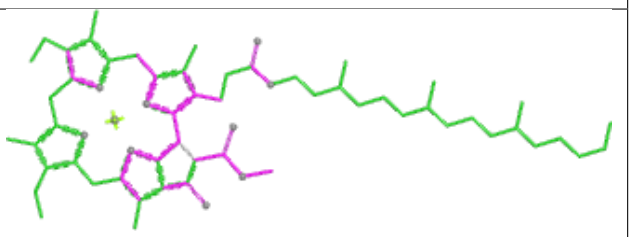


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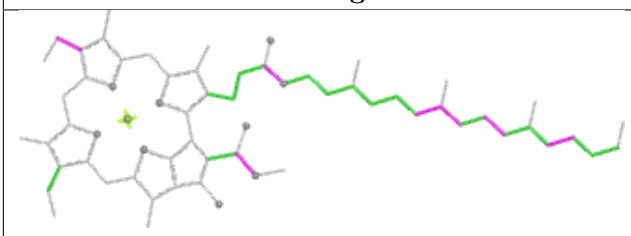
Ligand CLA b 826



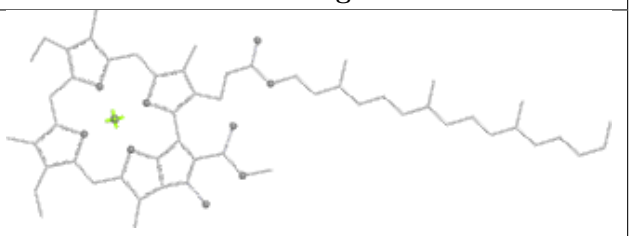
Bond lengths



Bond angles

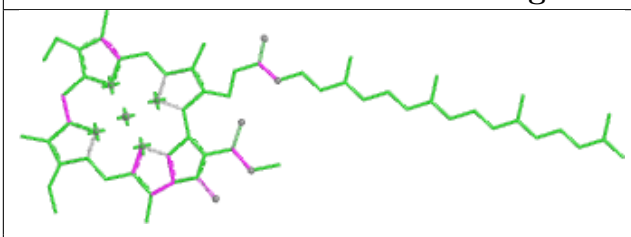


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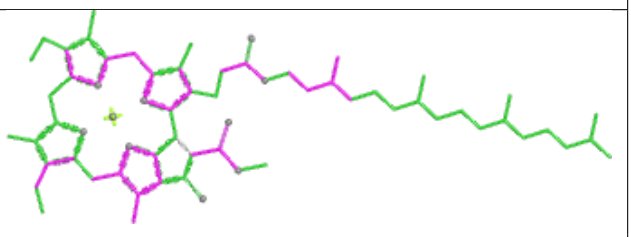


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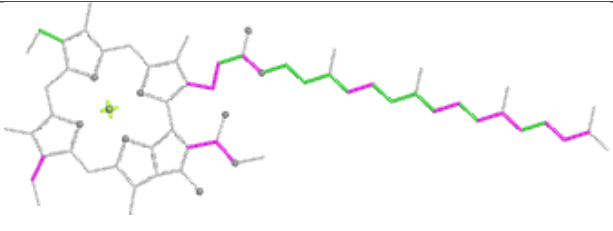
Ligand CLA a 816



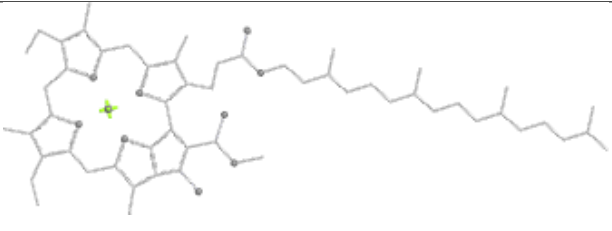
Bond lengths



Bond angles

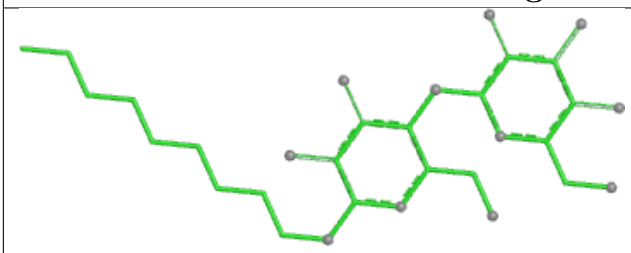


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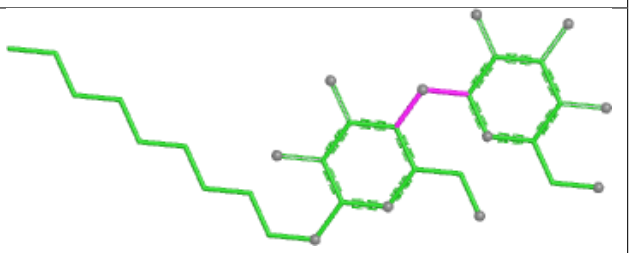


Rings

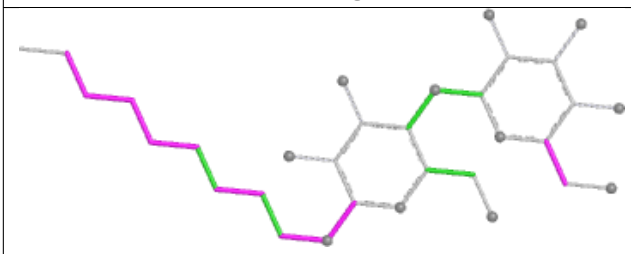
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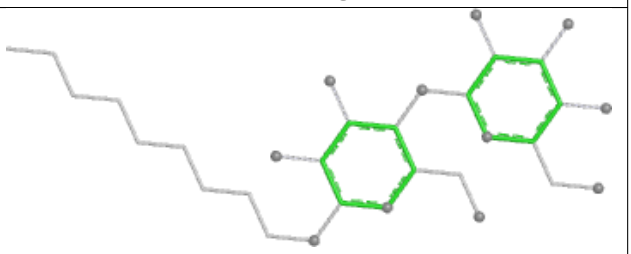
Bond lengths



Bond angles

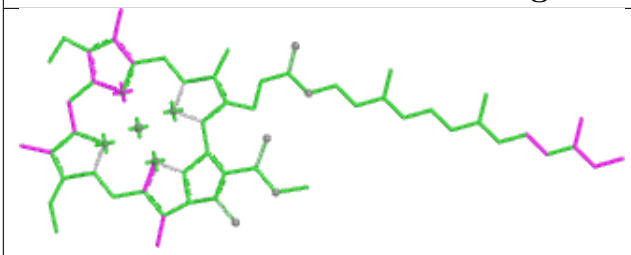


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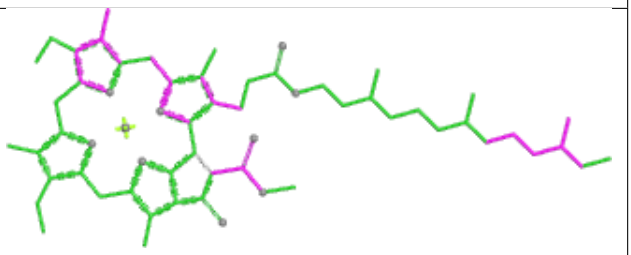


Rings

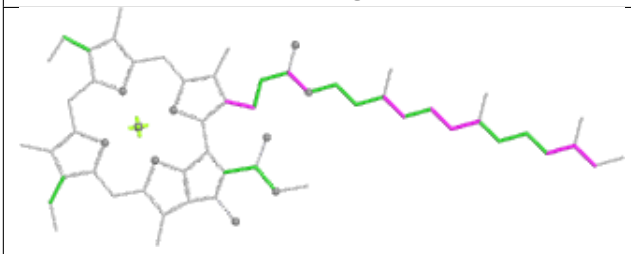
Ligand CLA I 305



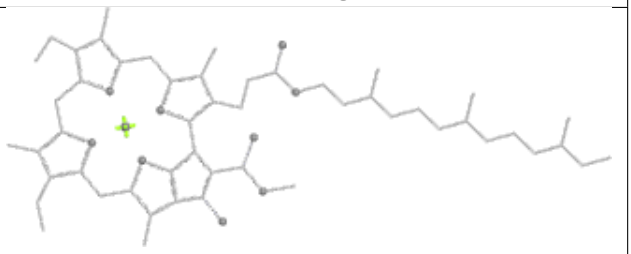
Bond lengths



Bond angles

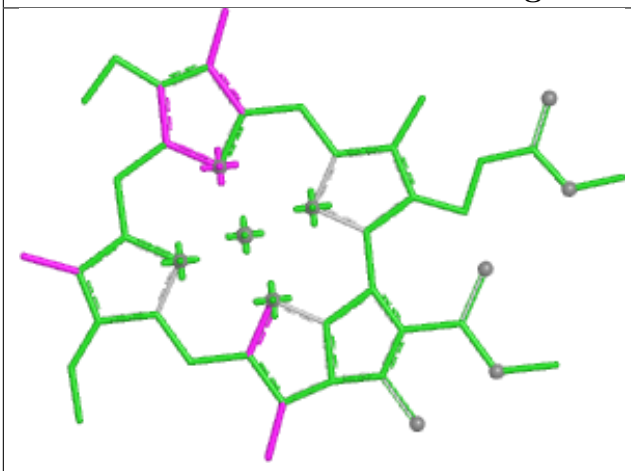


Torsions

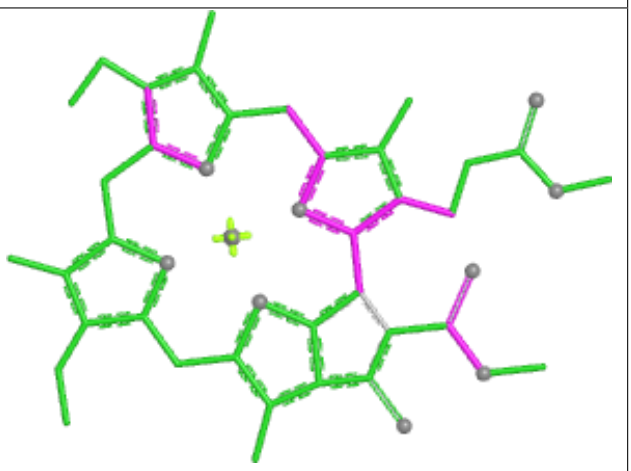


Rings

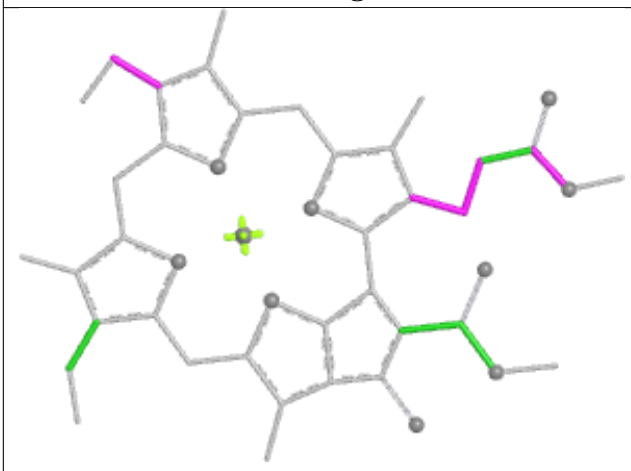
Ligand CLA B 307



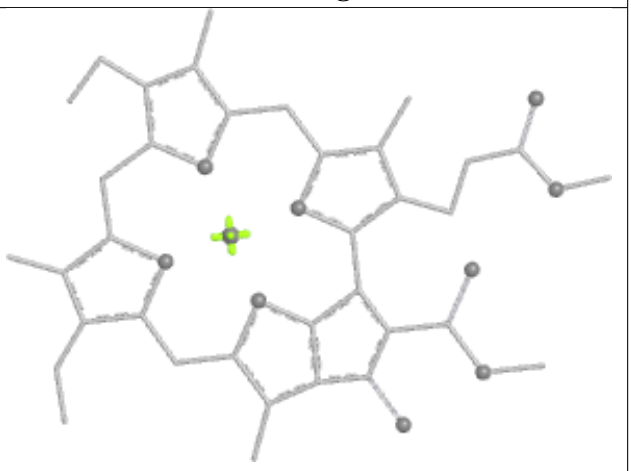
Bond lengths



Bond angles

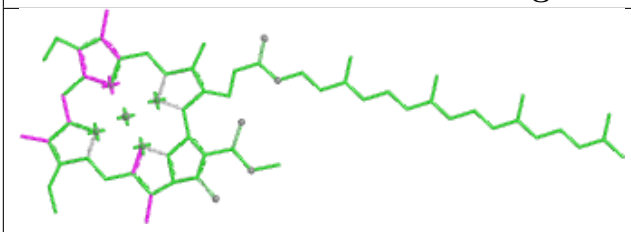


Torsions

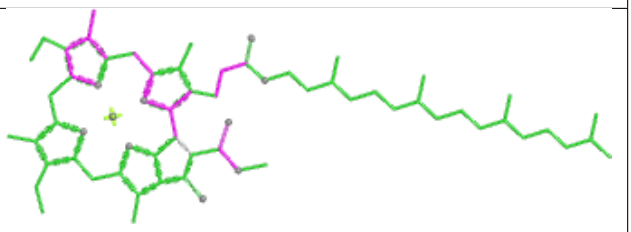


Rings

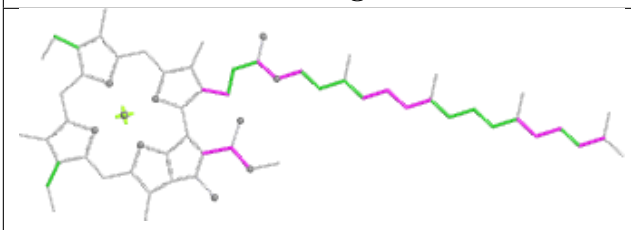
Ligand CLA i 102



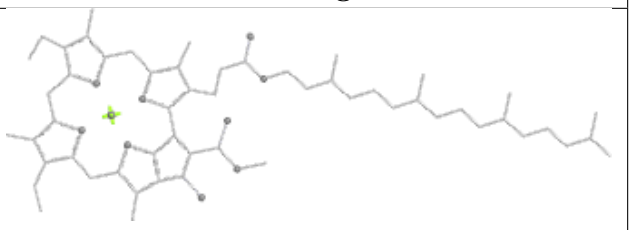
Bond lengths



Bond angles

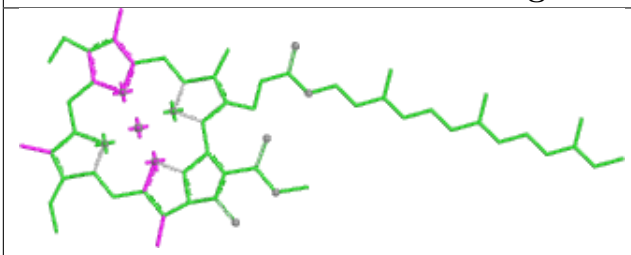


Torsions

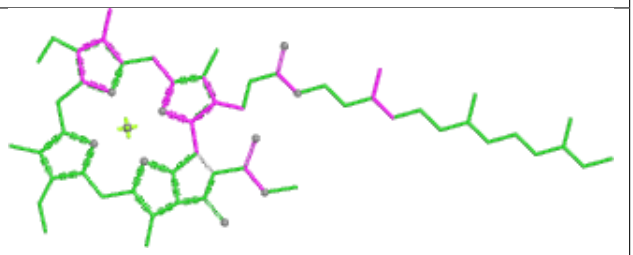


Rings

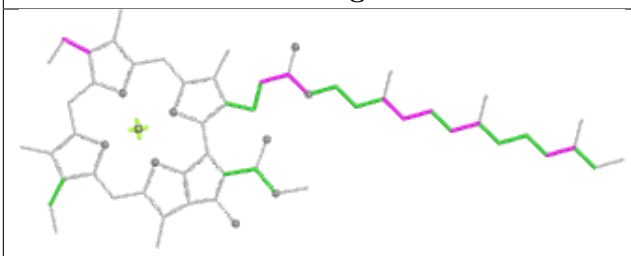
Ligand CLA J 307



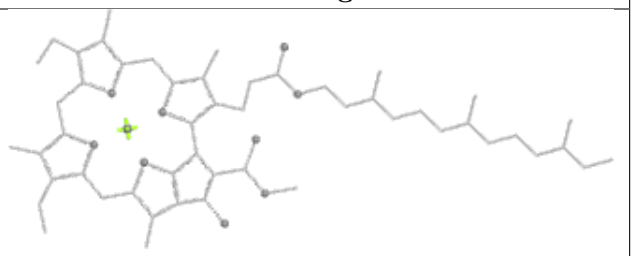
Bond lengths



Bond angles

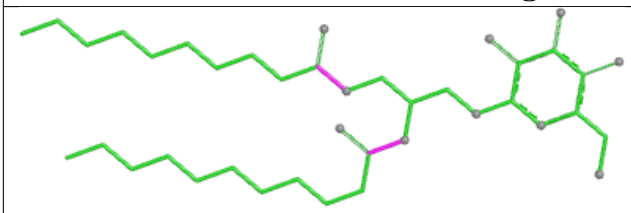


Torsions

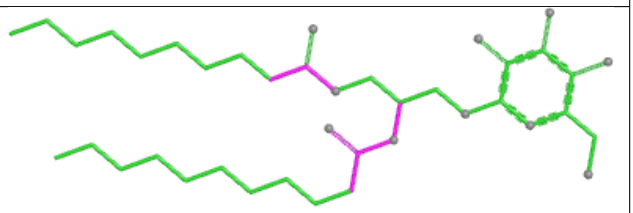


Rings

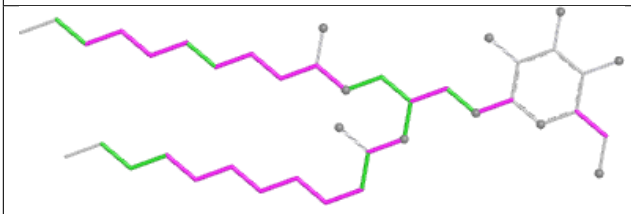
Ligand LMG E 319



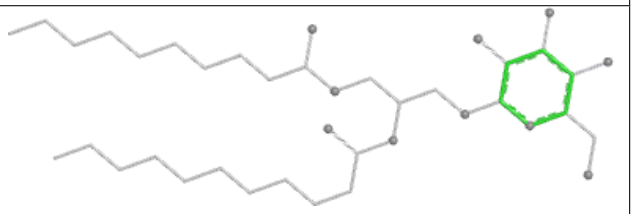
Bond lengths



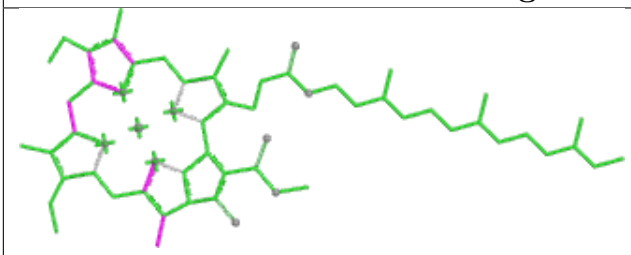
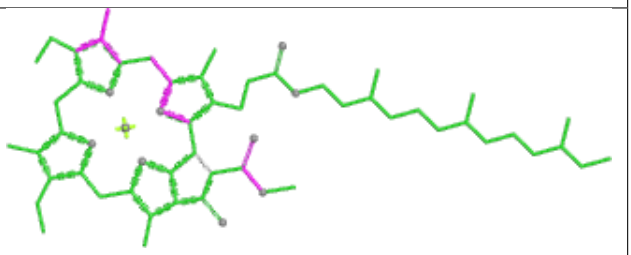
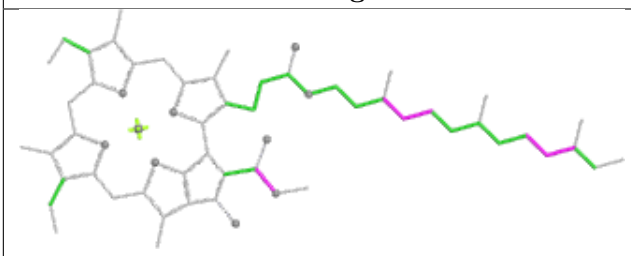
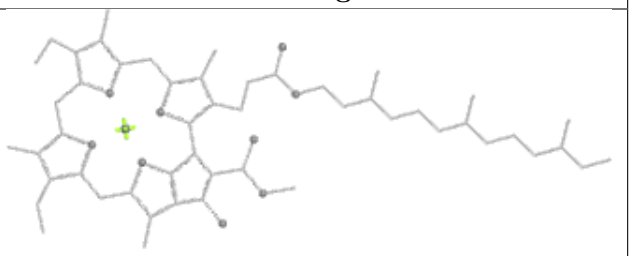
Bond angles

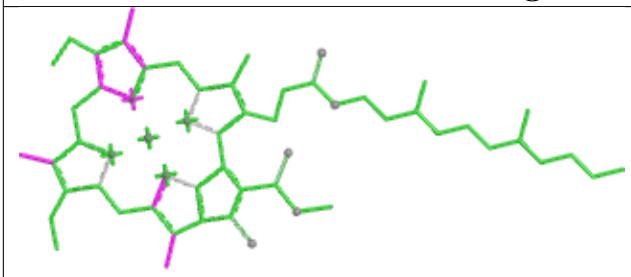
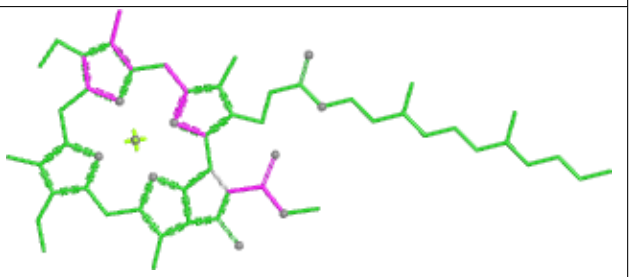
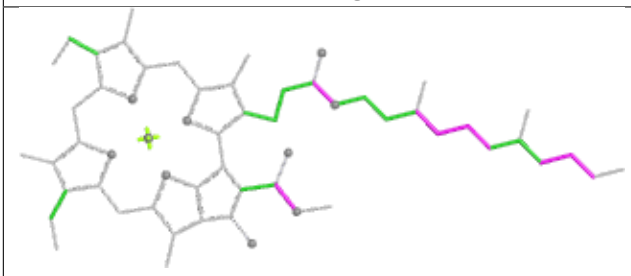
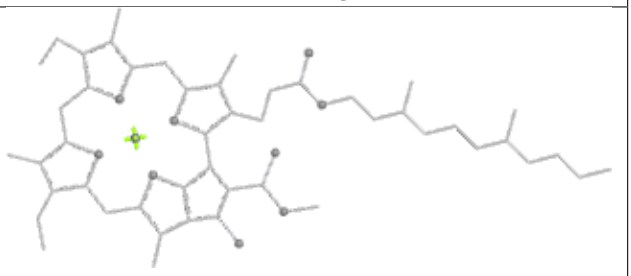


Torsions

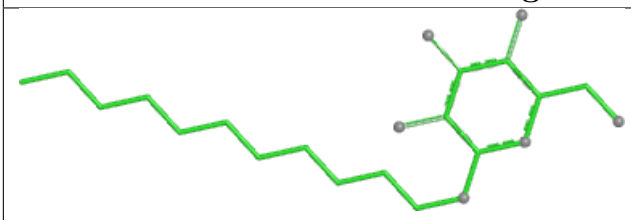


Rings

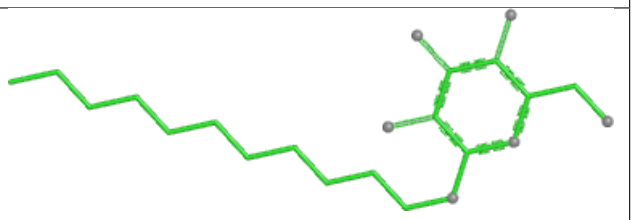
Ligand CLA W 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

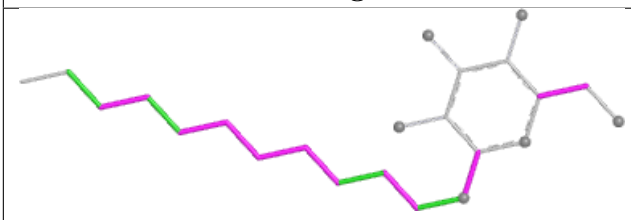
Ligand LMT P 321



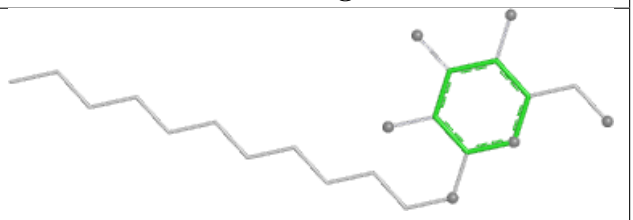
Bond lengths



Bond angles

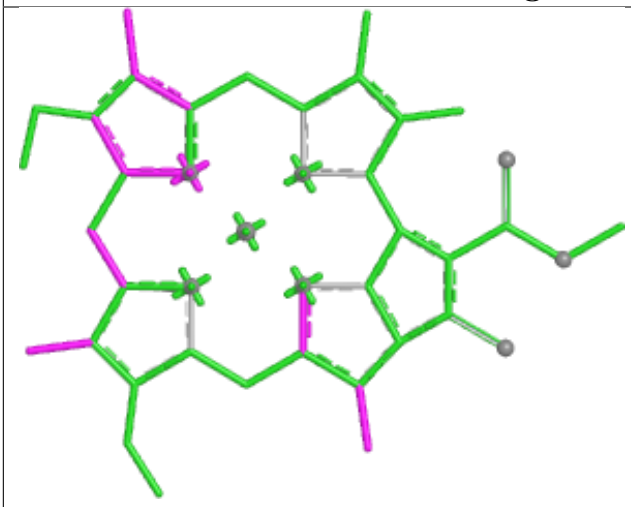


Torsions

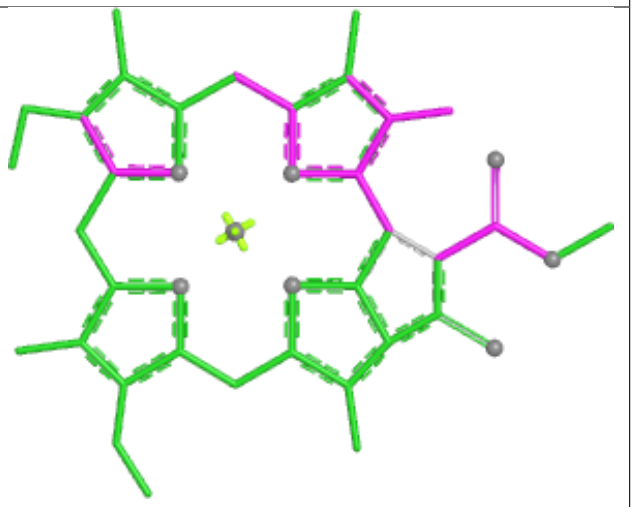


Rings

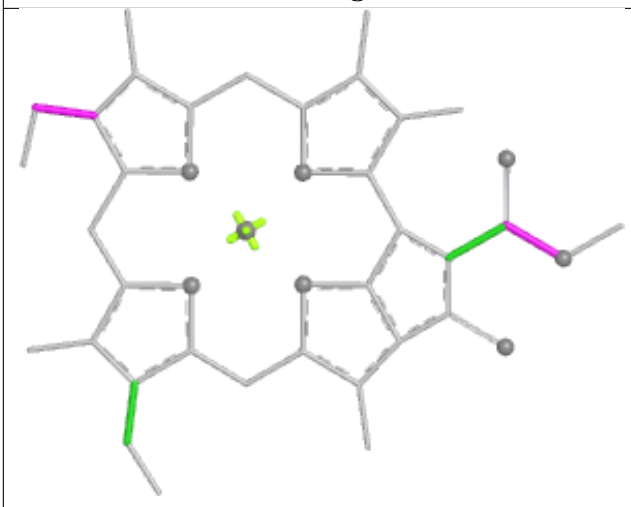
Ligand CLA A 313



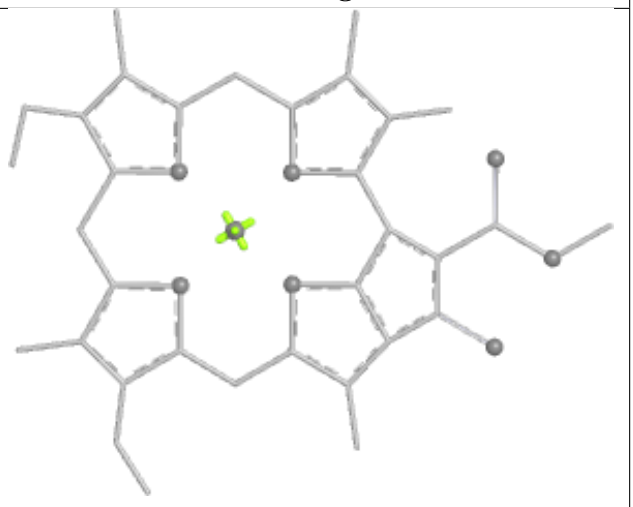
Bond lengths



Bond angles

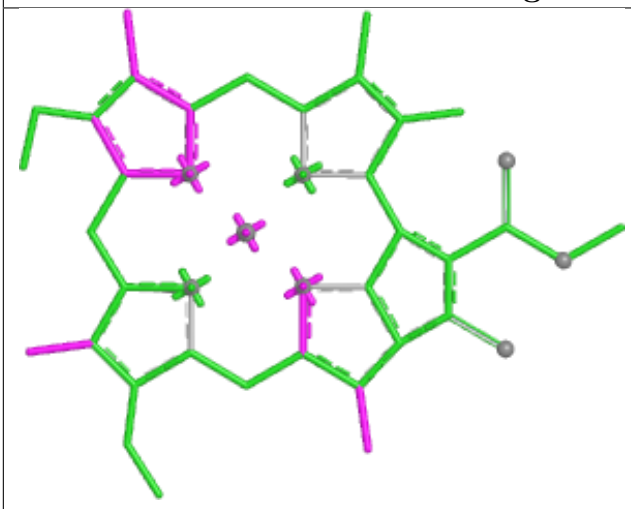


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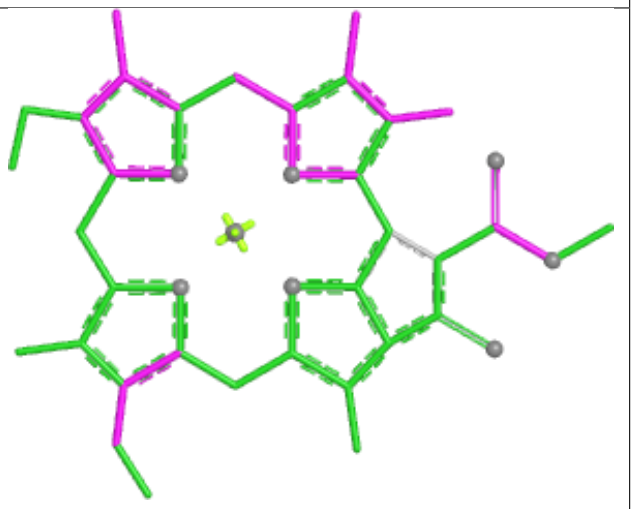


Rings

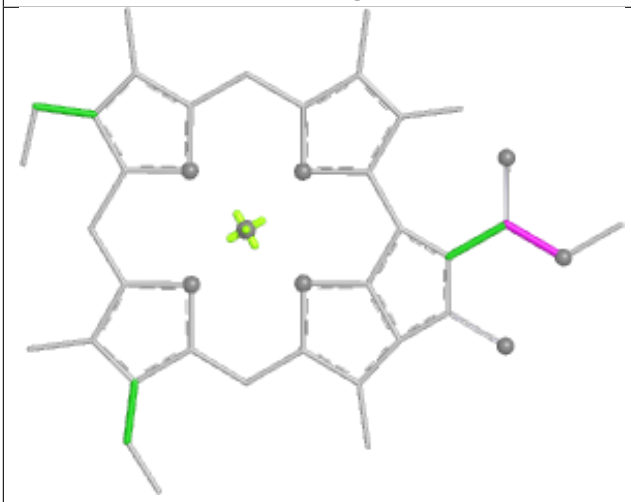
Ligand CLA H 314



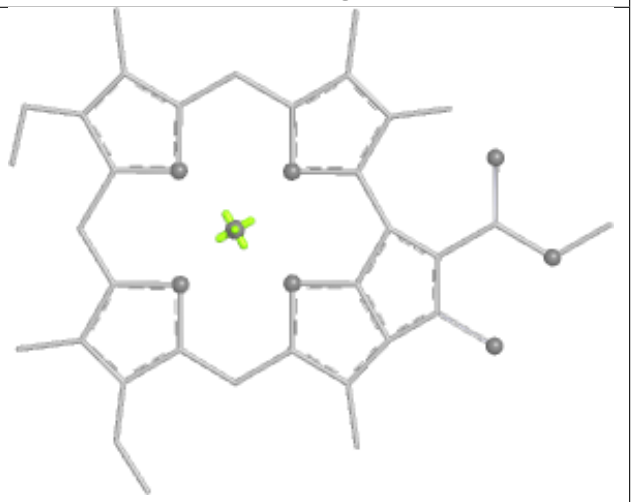
Bond lengths



Bond angles

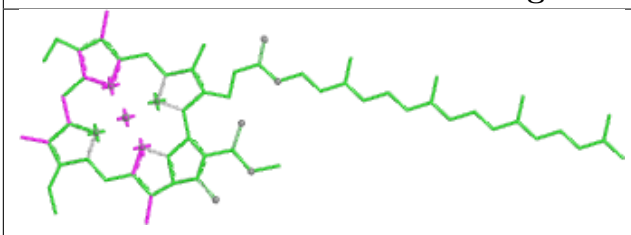


Torsions

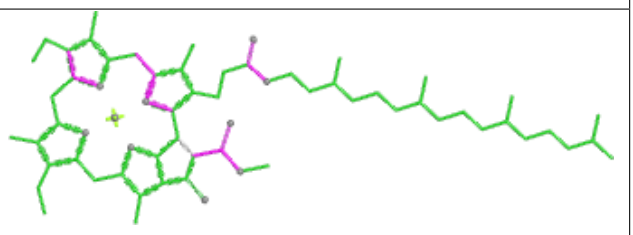


Rings

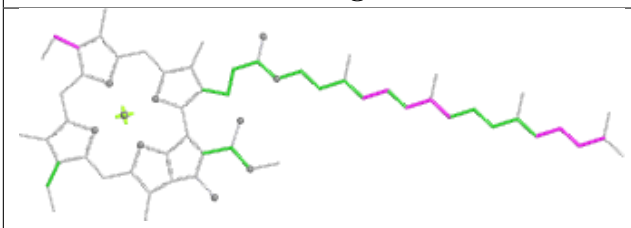
Ligand CLA b 821



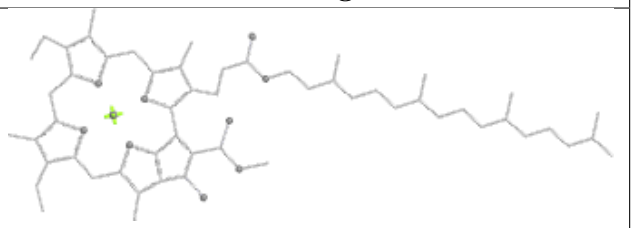
Bond lengths



Bond angles

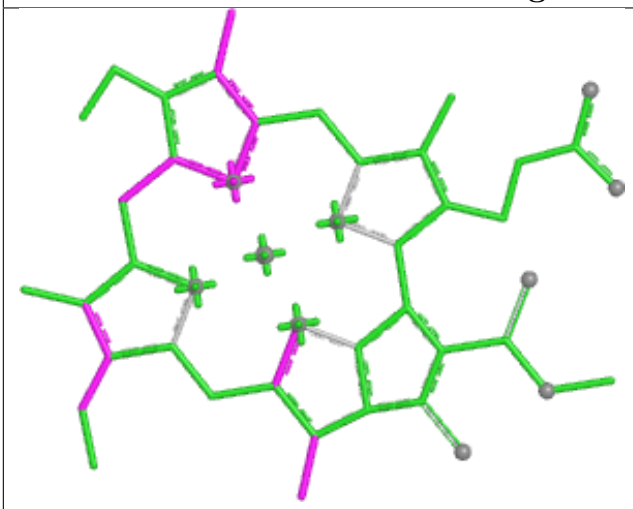


Torsions

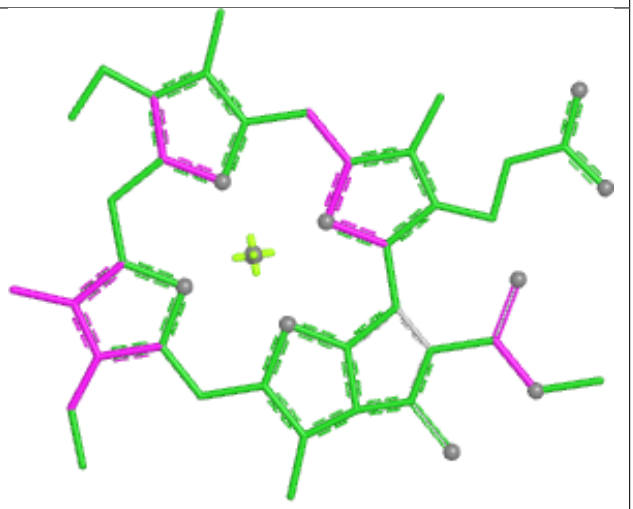


Rings

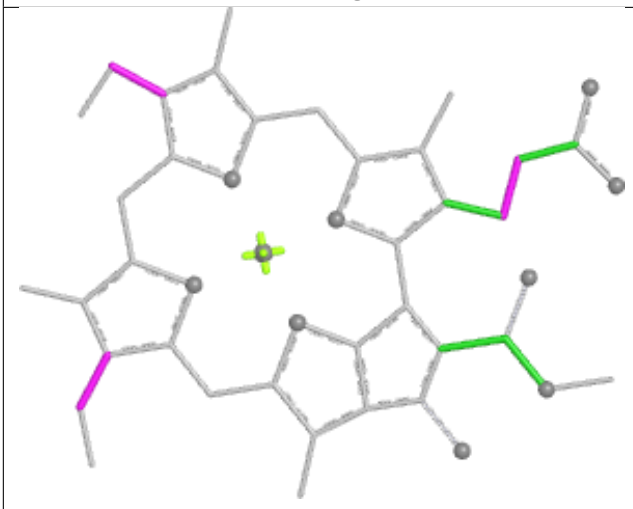
Ligand CLA a 819



Bond lengths



Bond angles

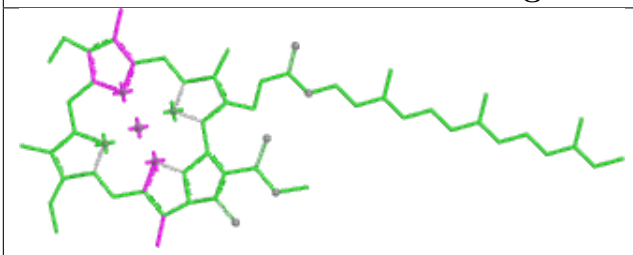


Torsions

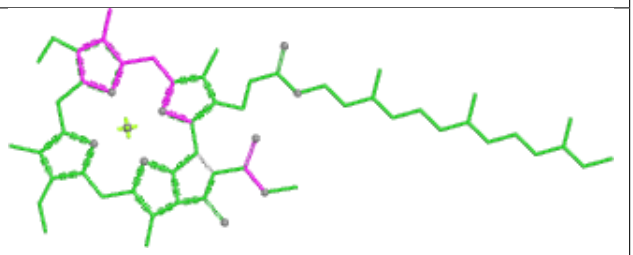


Rings

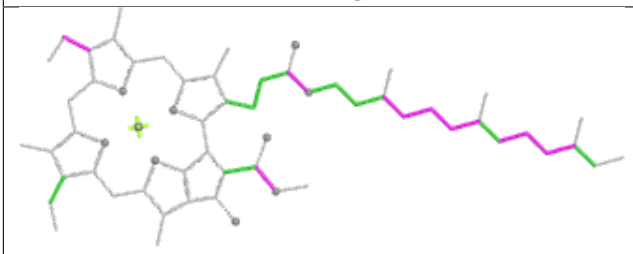
Ligand CLA R 310



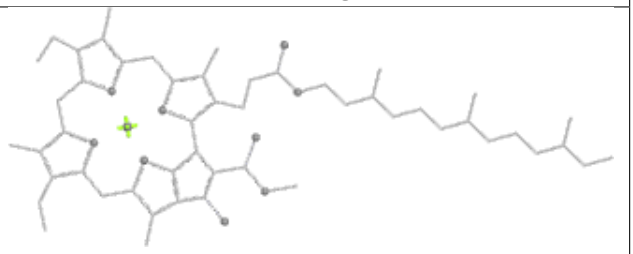
Bond lengths



Bond angles

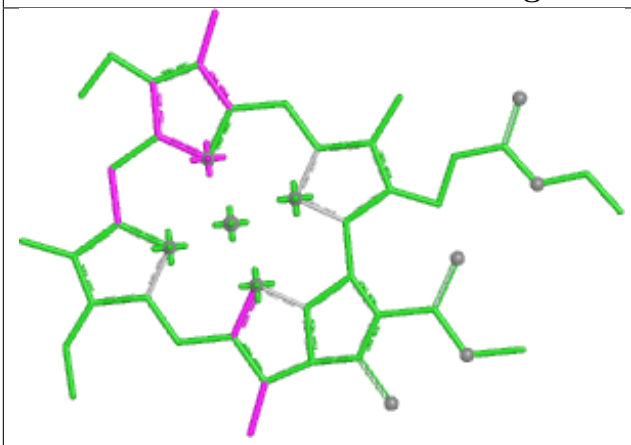


Torsions

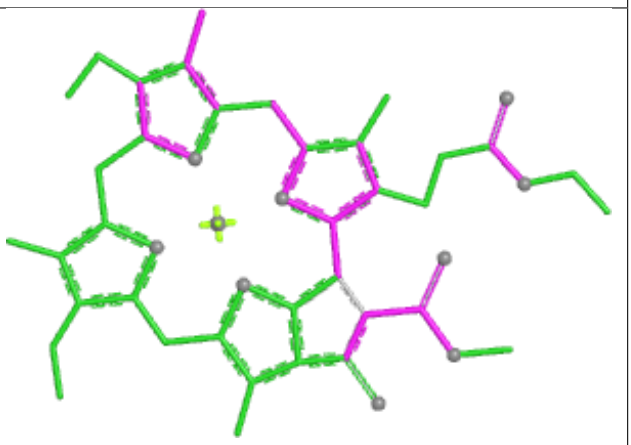


Rings

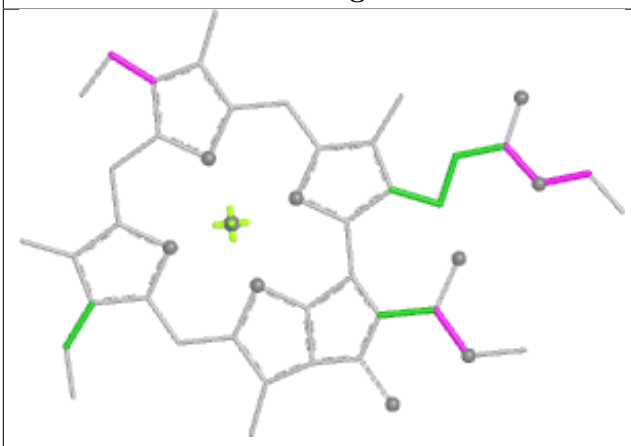
Ligand CLA N 318



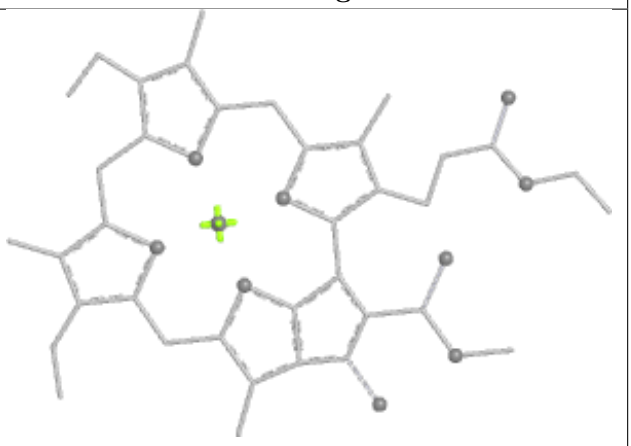
Bond lengths



Bond angles

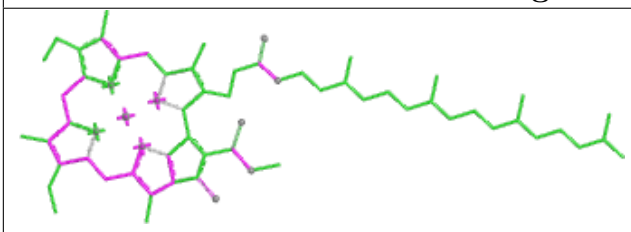


Torsions

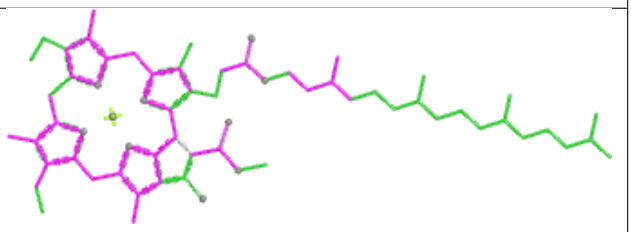


Rings

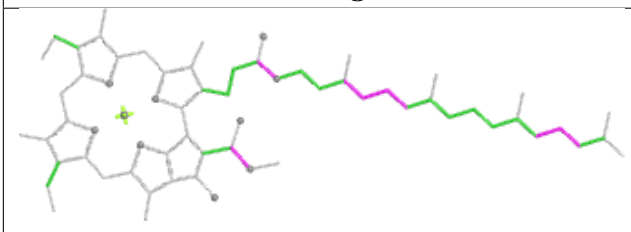
Ligand CLA f 804



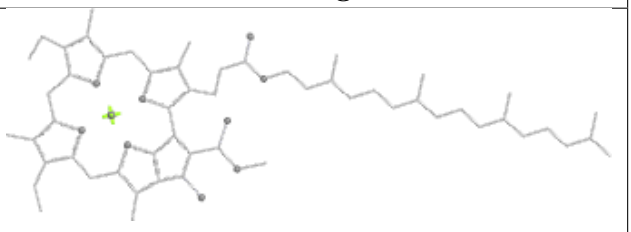
Bond lengths



Bond angles

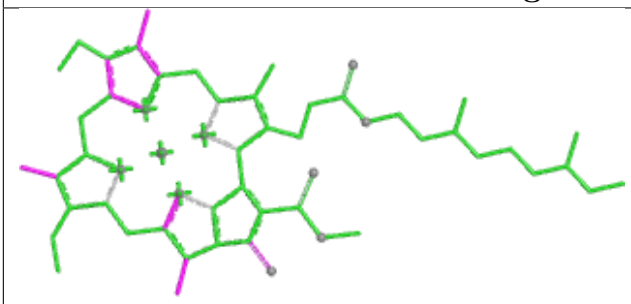


Torsions

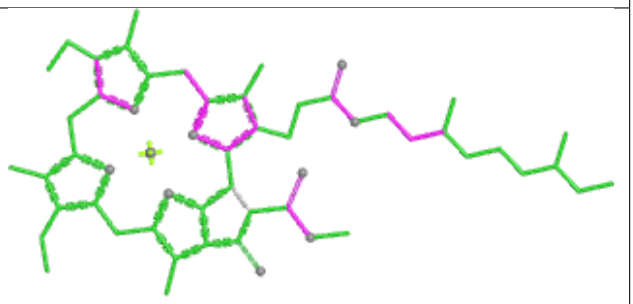


Rings

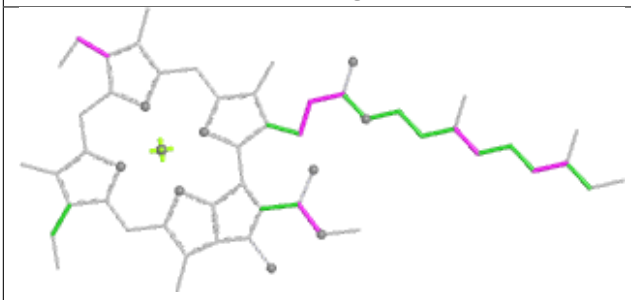
Ligand CLA U 308



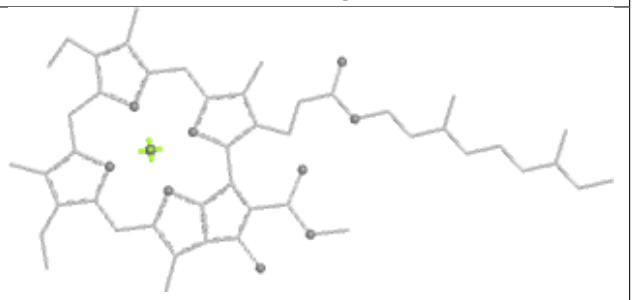
Bond lengths



Bond angles

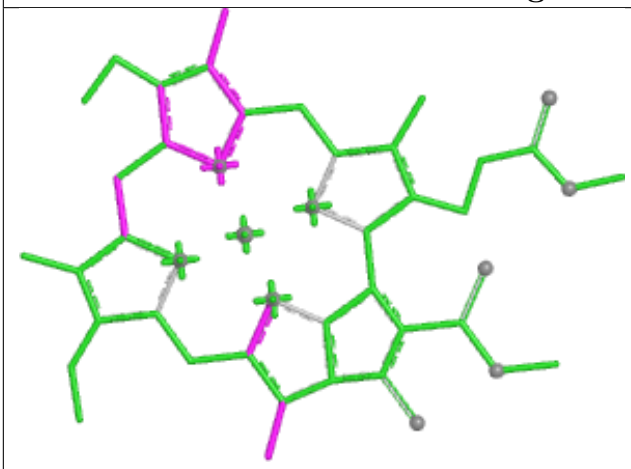


Torsions

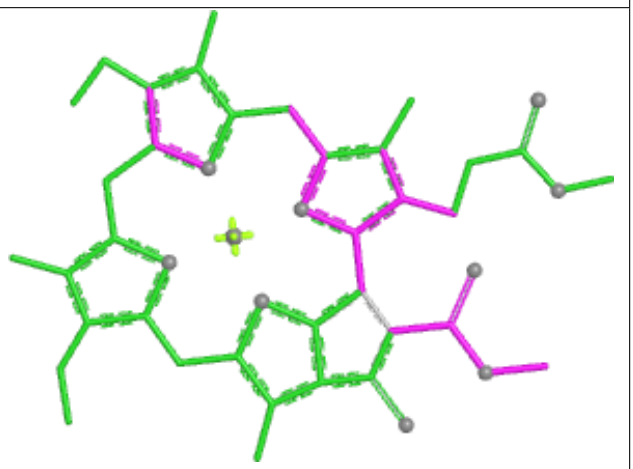


Rings

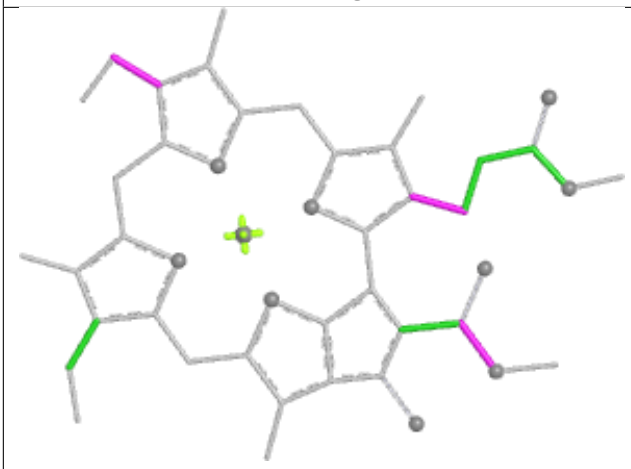
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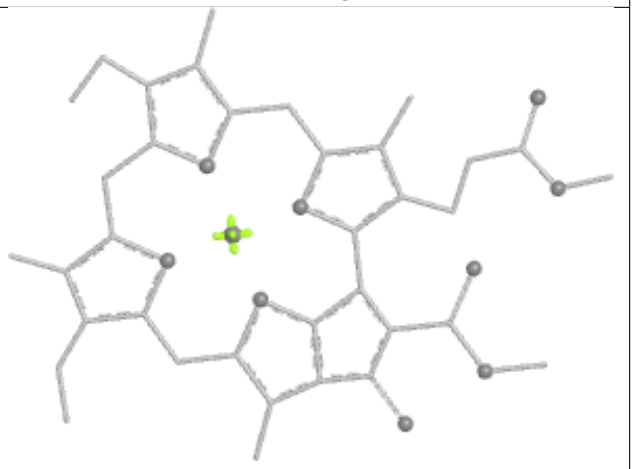
Bond lengths



Bond angles

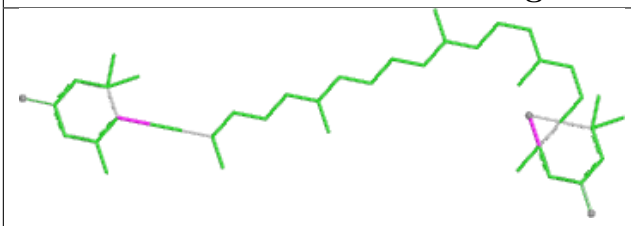


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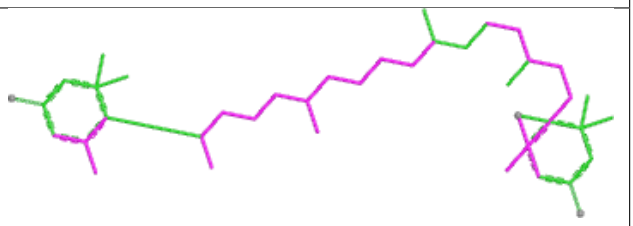


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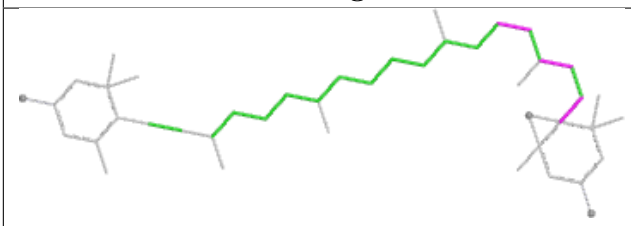
Ligand DD6 B 302



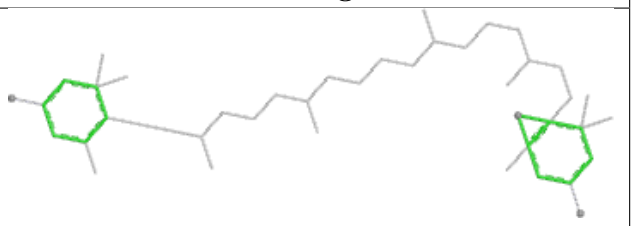
Bond lengths



Bond angles

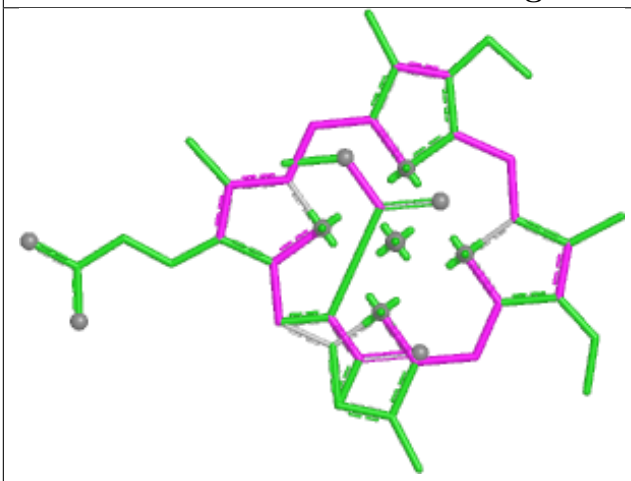


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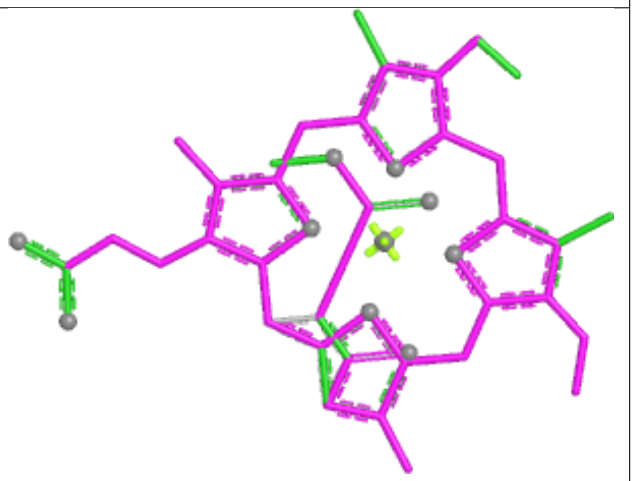


Rings

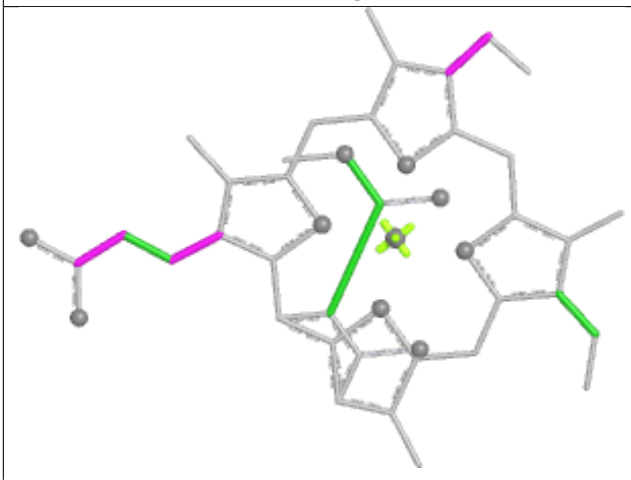
Ligand KC1 K 314



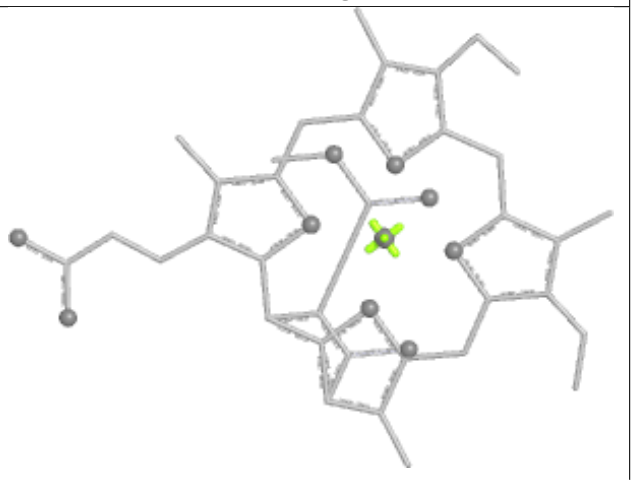
Bond lengths



Bond angles

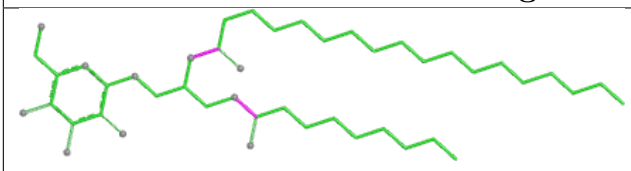


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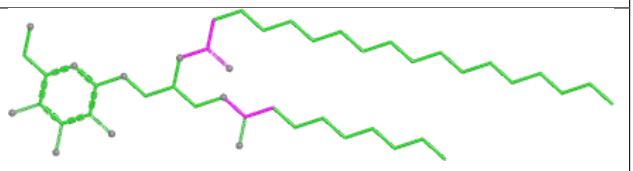


Rings

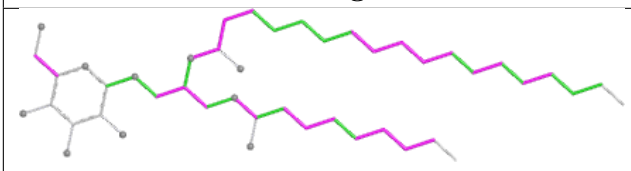
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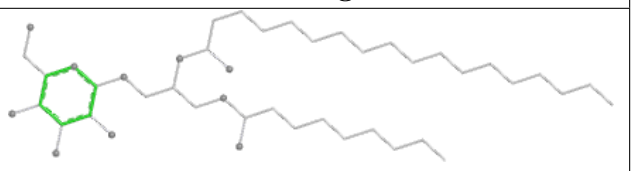
Bond lengths



Bond angles

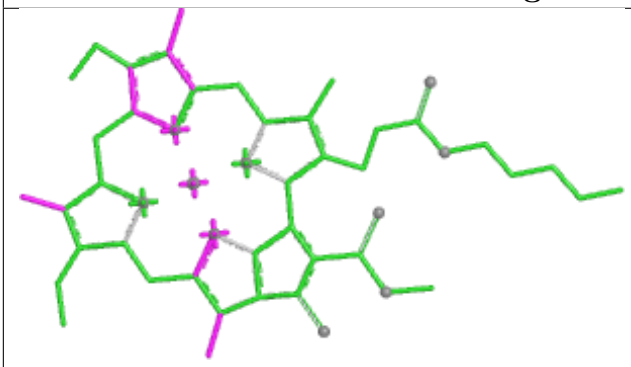


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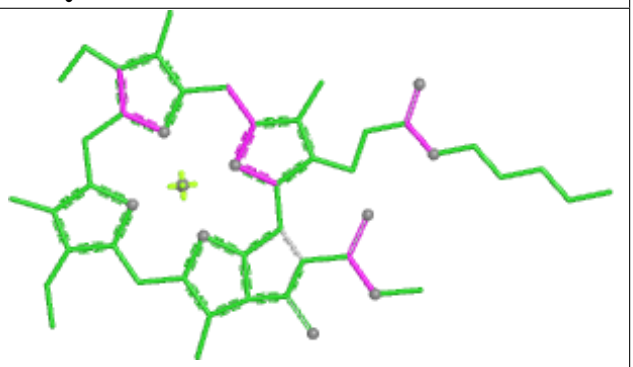


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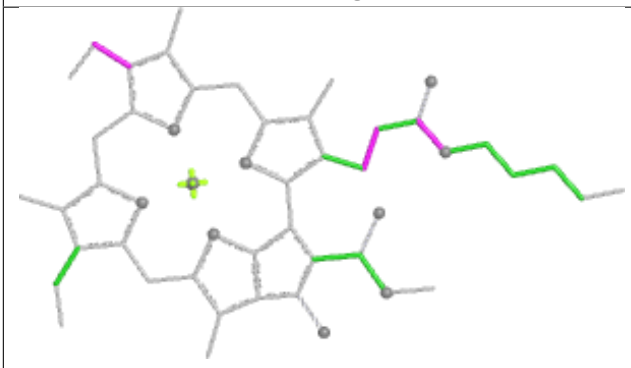
Ligand CLA Q 307



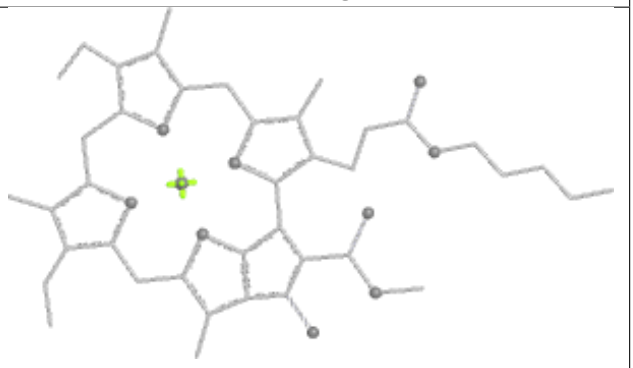
Bond lengths



Bond angles

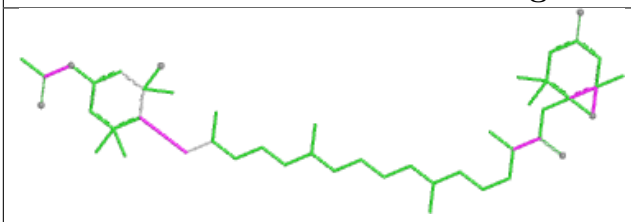


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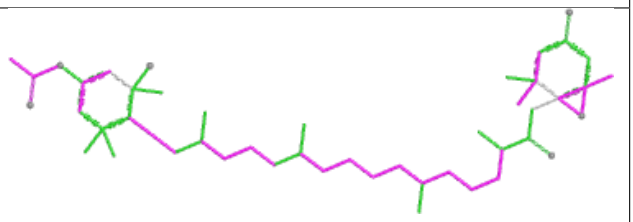


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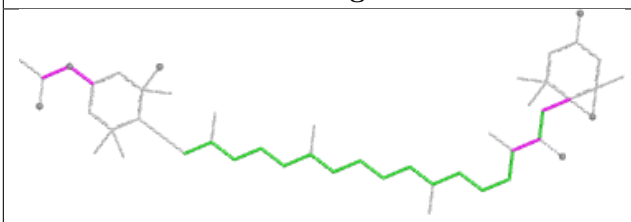
Ligand A86 R 309



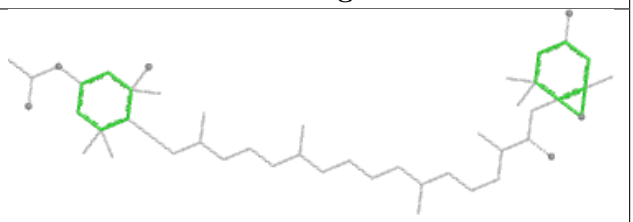
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Bond angles

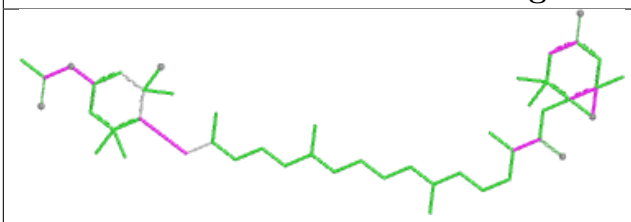


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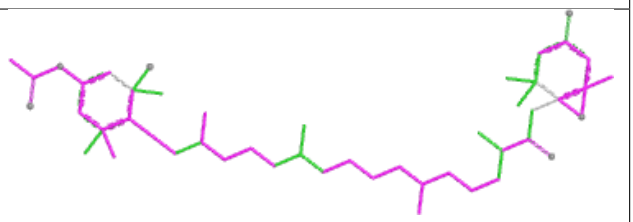


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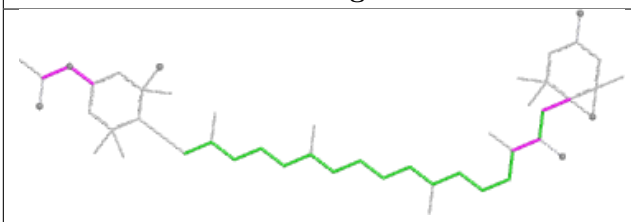
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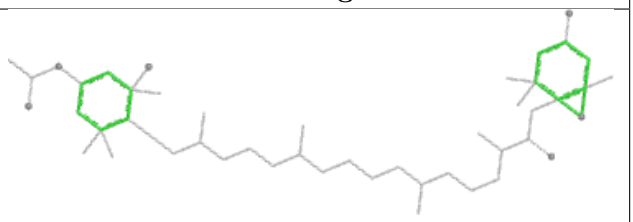
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Bond angles

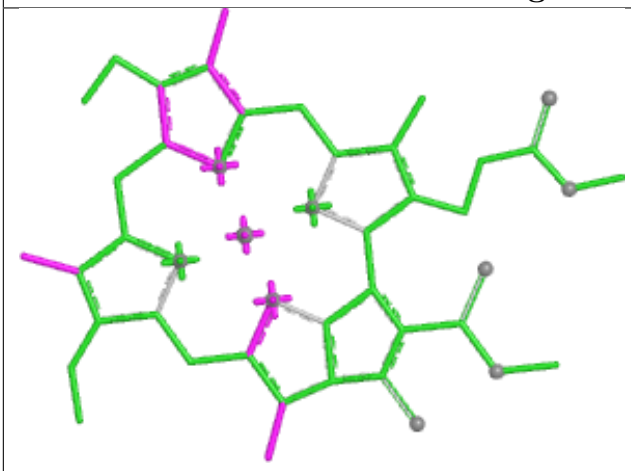


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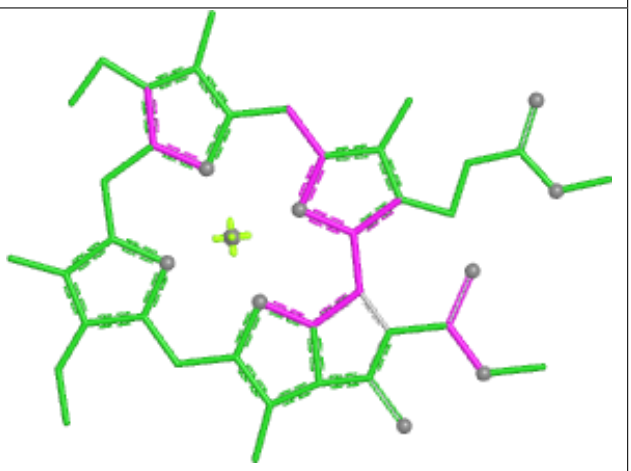


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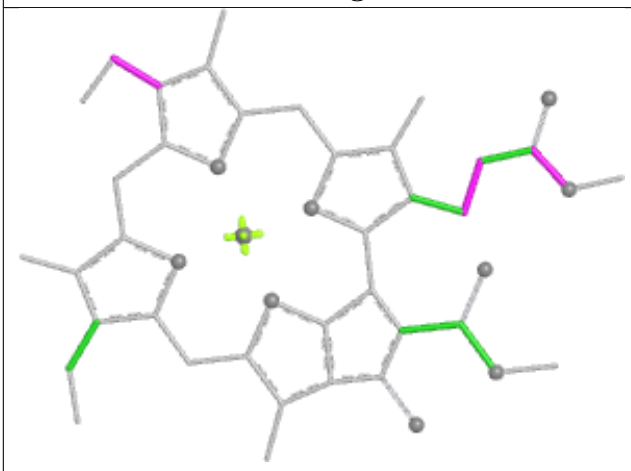
Ligand CLA J 311



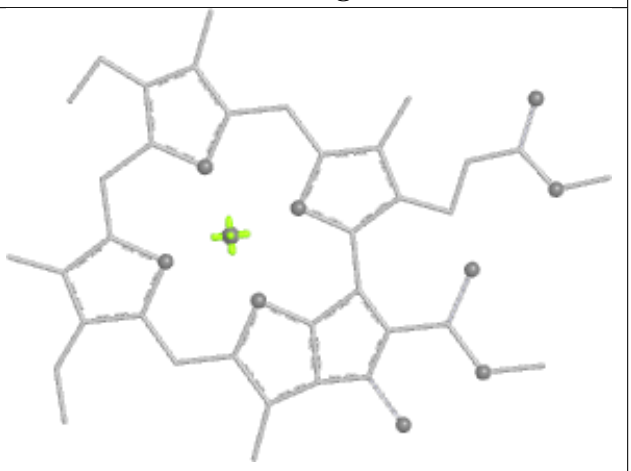
Bond lengths



Bond angles

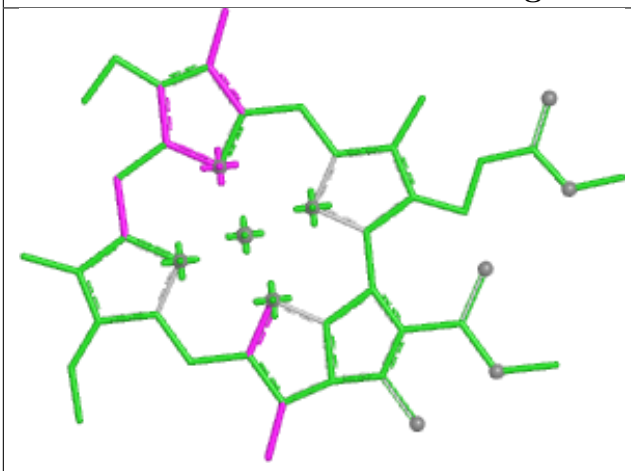


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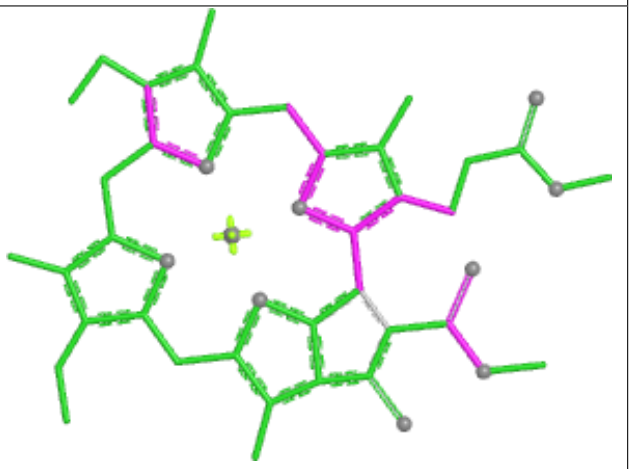


Rings

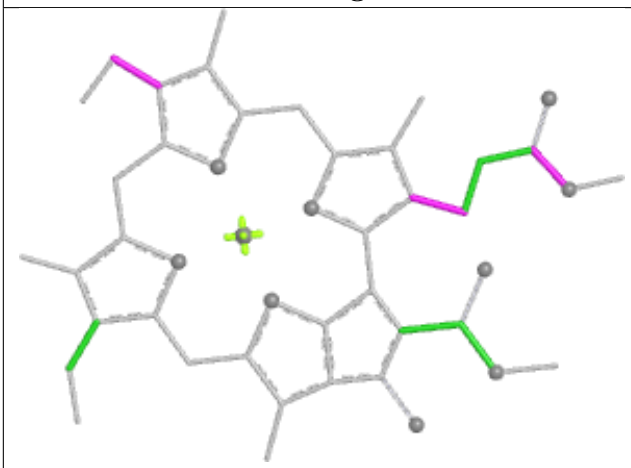
Ligand CLA C 210



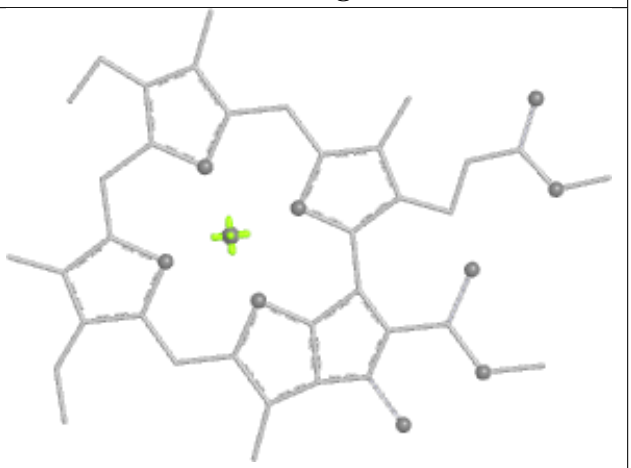
Bond lengths



Bond angles

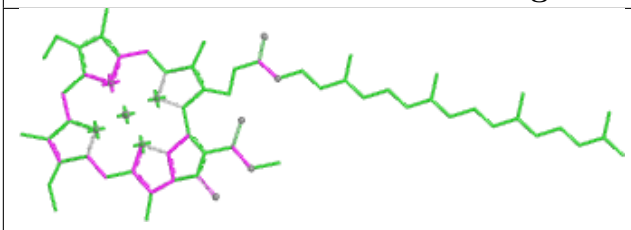


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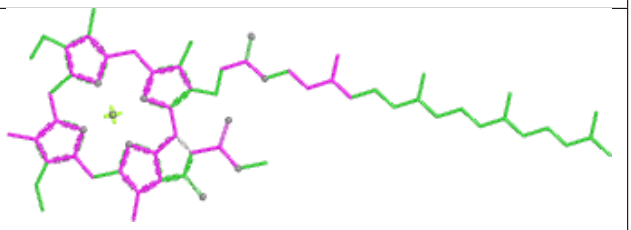


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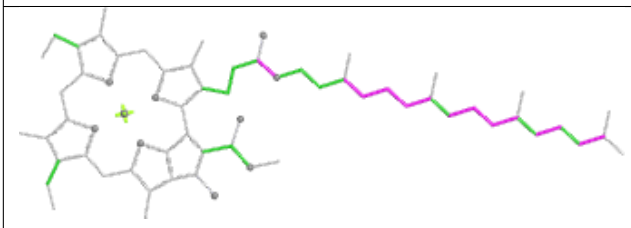
Ligand CLA I 306



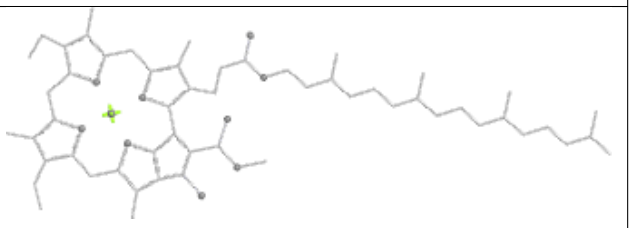
Bond lengths



Bond angles

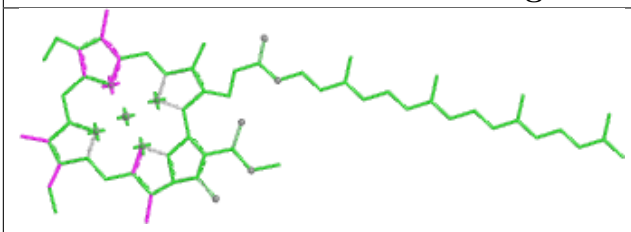


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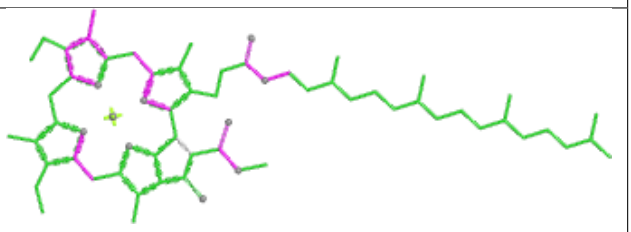


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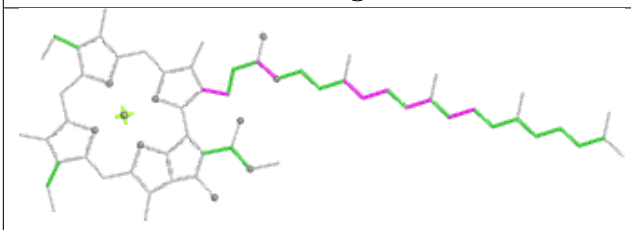
Ligand CLA E 314



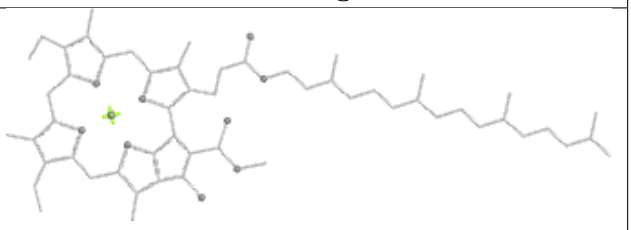
Bond lengths



Bond angles



Torsions

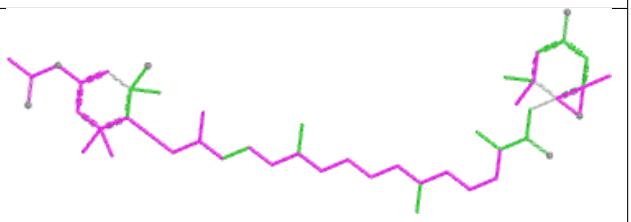


Rings

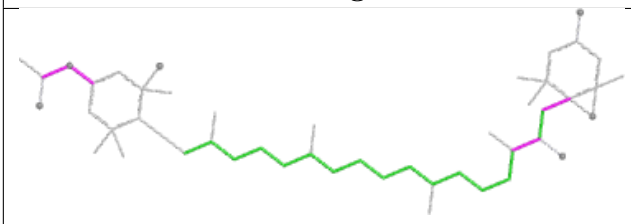
Ligand A86 P 303



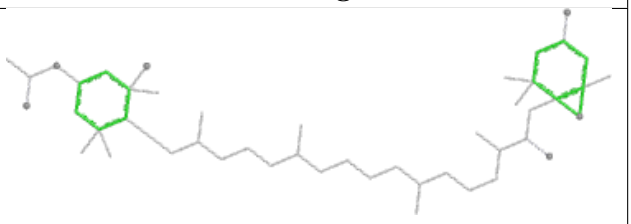
Bond lengths



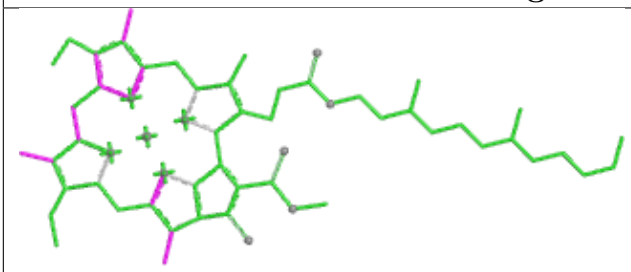
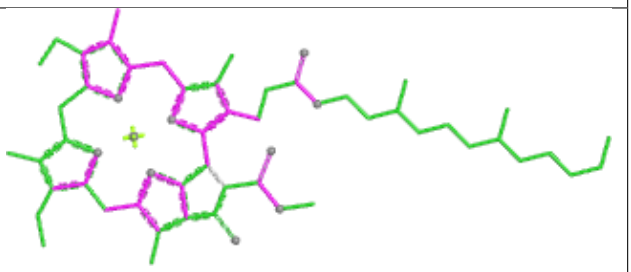
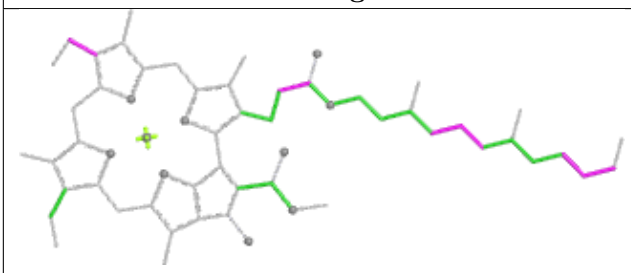
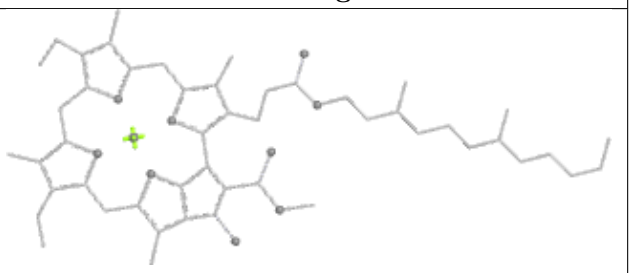
Bond angles

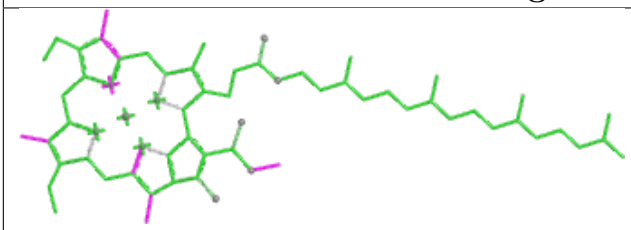
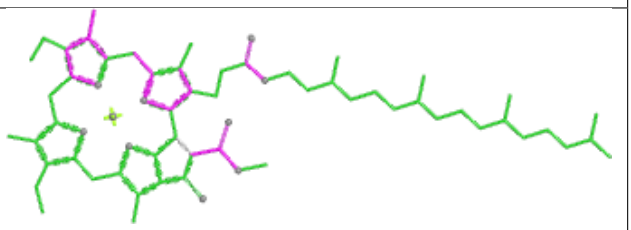
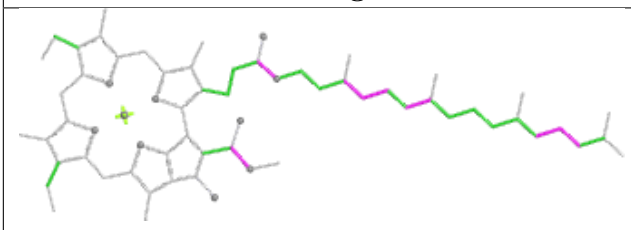
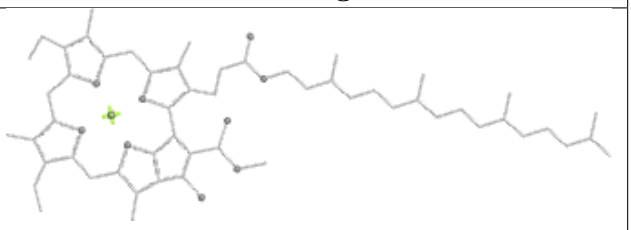


Torsions

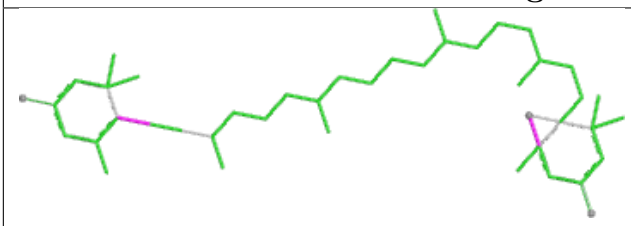


Rings

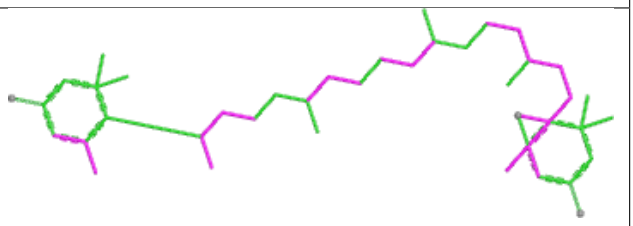
Ligand CLA b 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

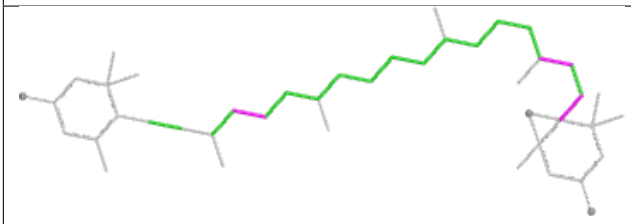
Ligand DD6 E 306



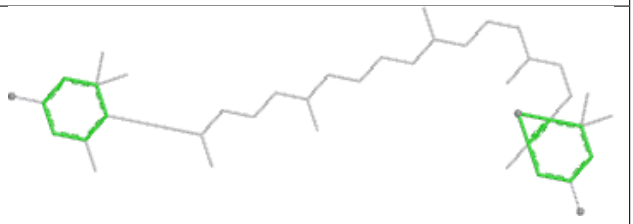
Bond lengths



Bond angles

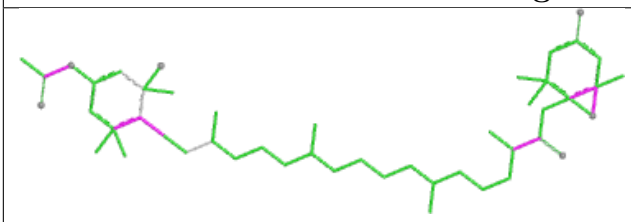


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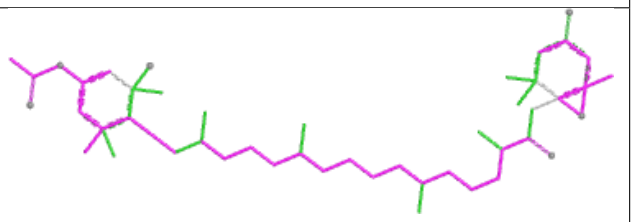


Rings

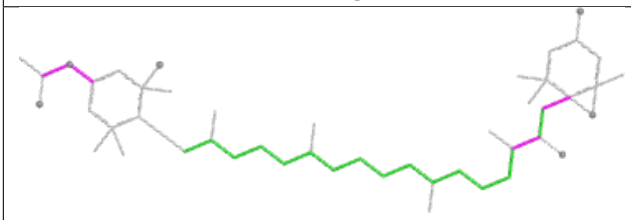
Ligand A86 S 301



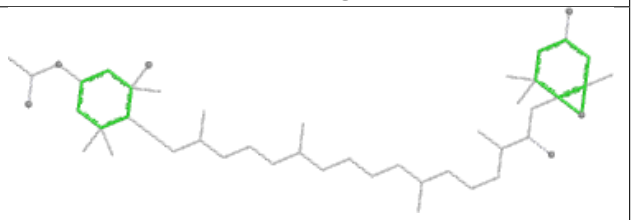
Bond lengths



Bond angles

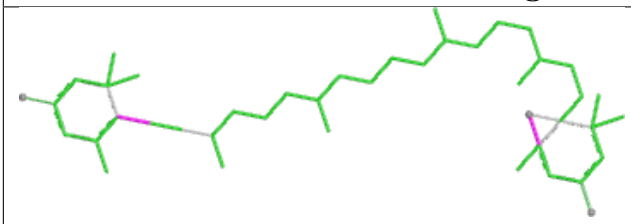


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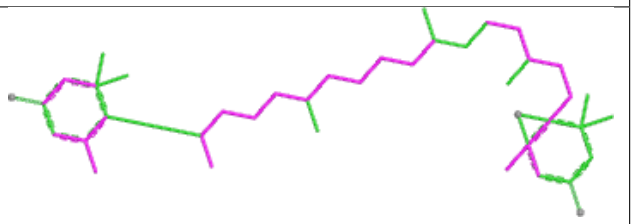


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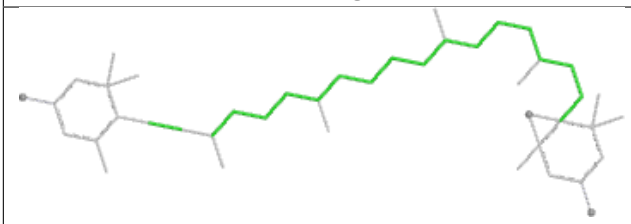
Ligand DD6 K 305



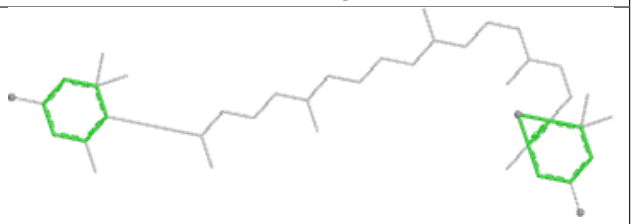
Bond lengths



Bond angles

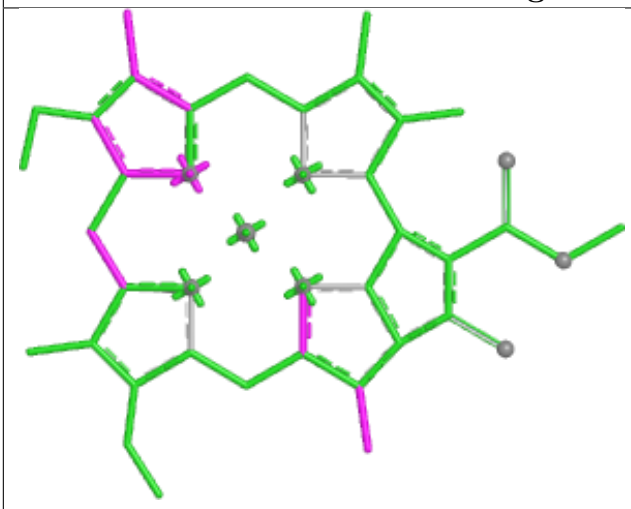


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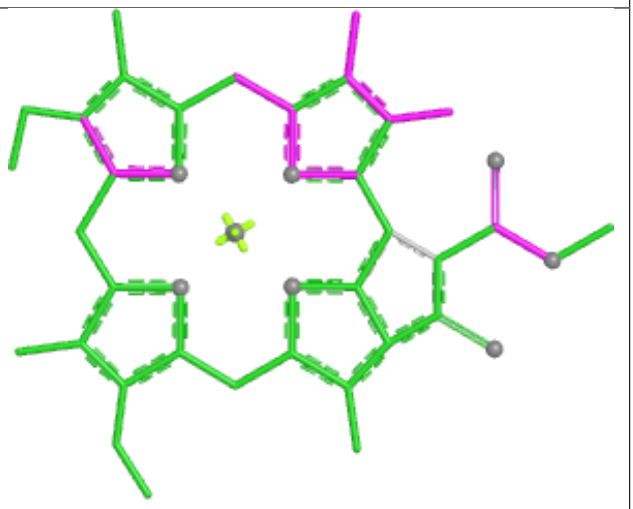


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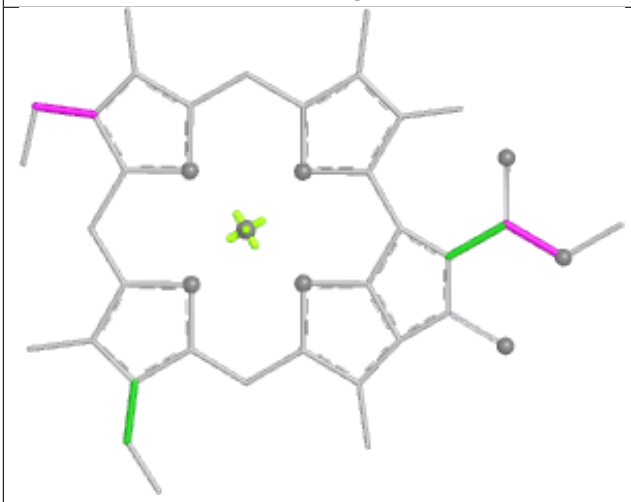
Ligand CLA S 317



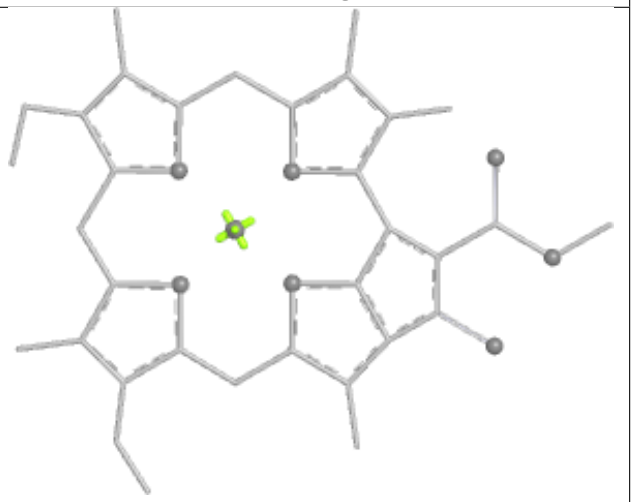
Bond lengths



Bond angles

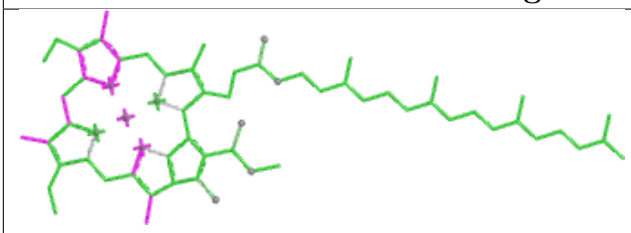


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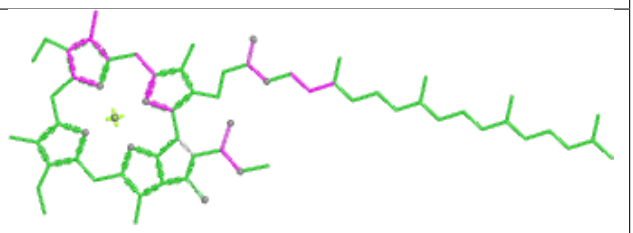


Rings

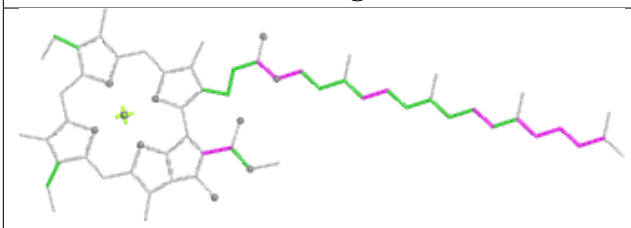
Ligand CLA A 310



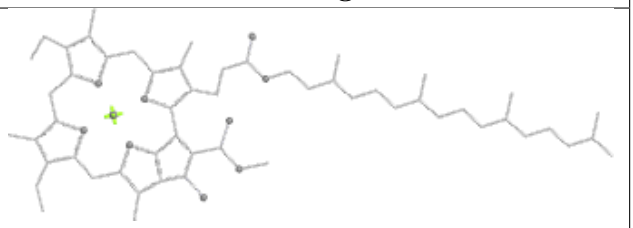
Bond lengths



Bond angles

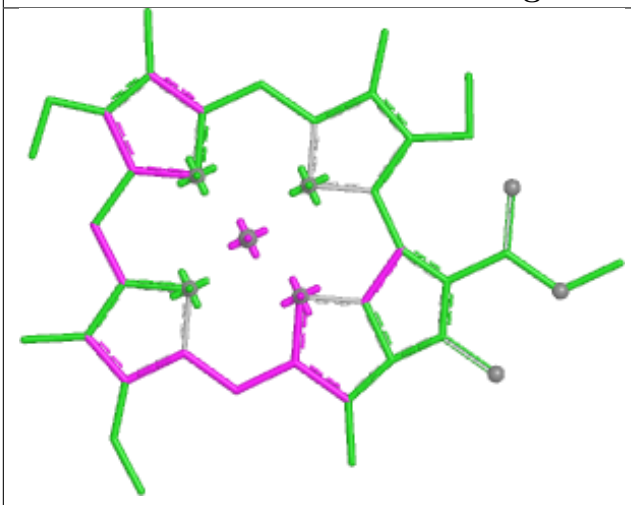


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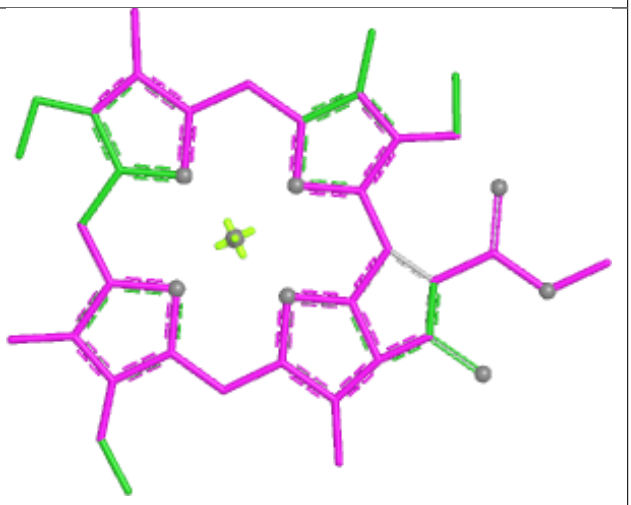


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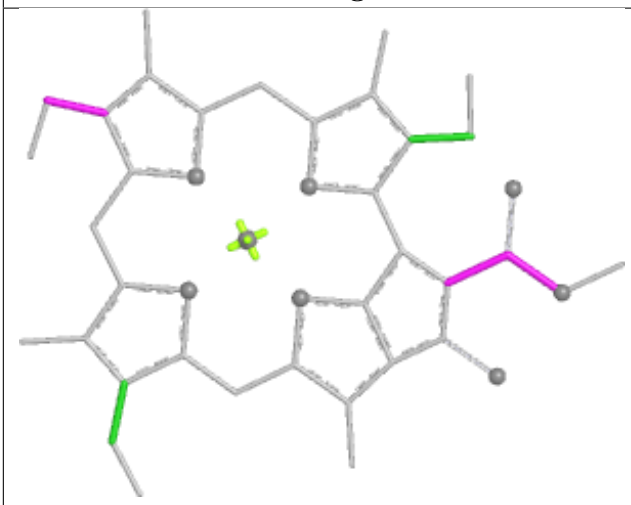
Ligand CLA N 319



Bond lengths



Bond angles

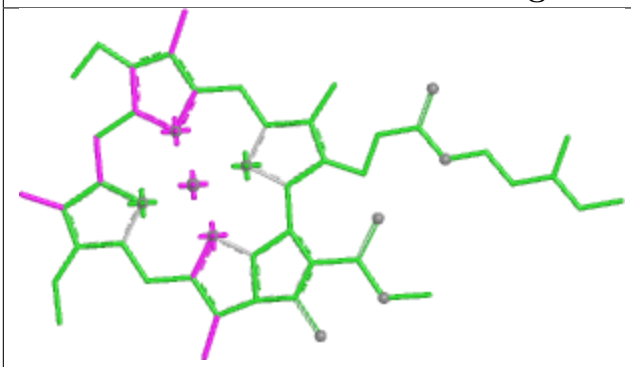


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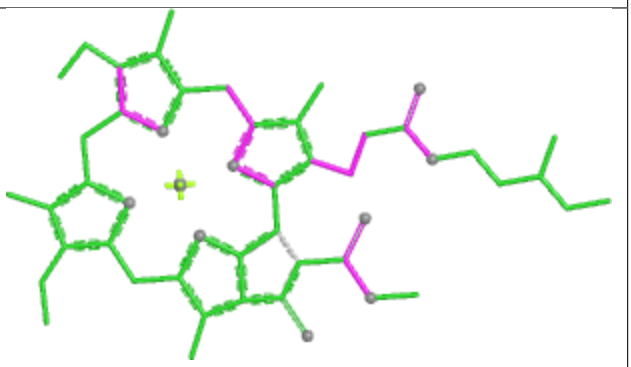


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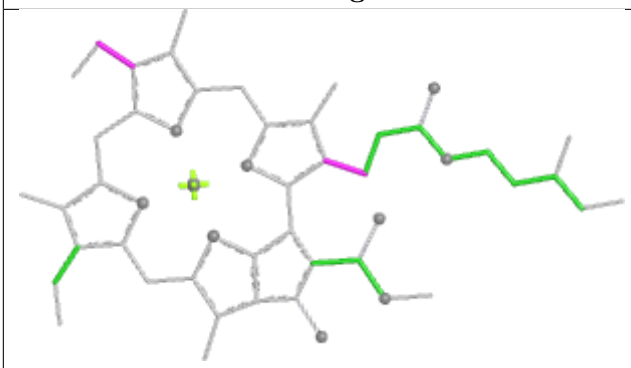
Ligand CLA a 835



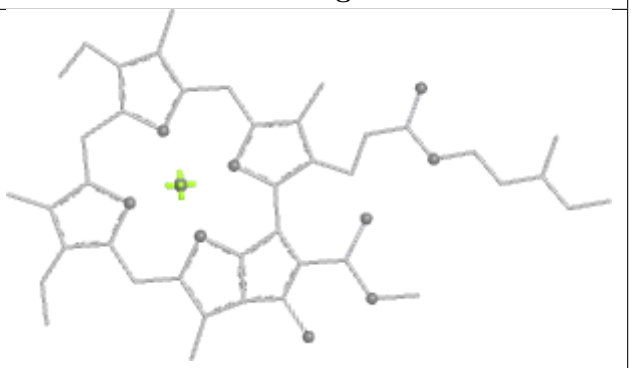
Bond lengths



Bond angles

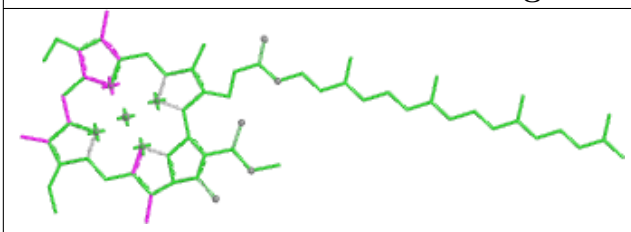


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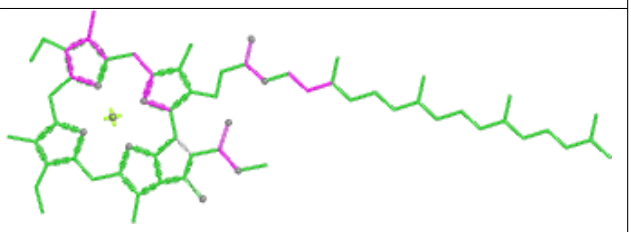


Rings

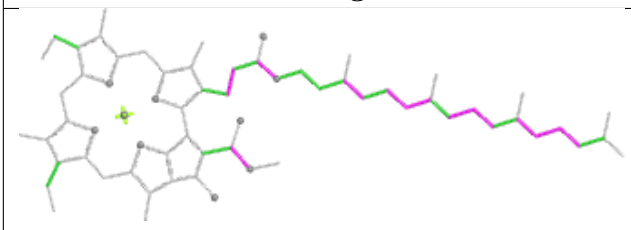
Ligand CLA V 308



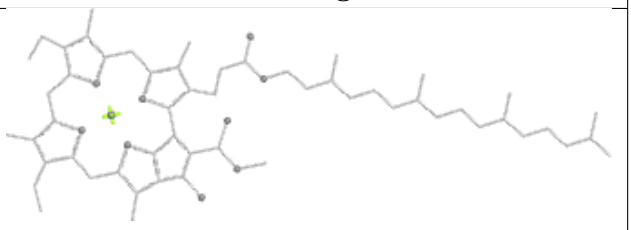
Bond lengths



Bond angles

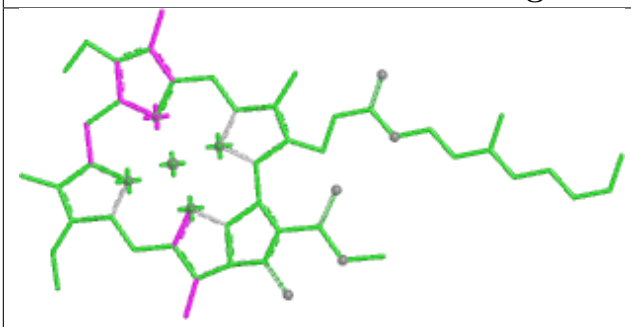


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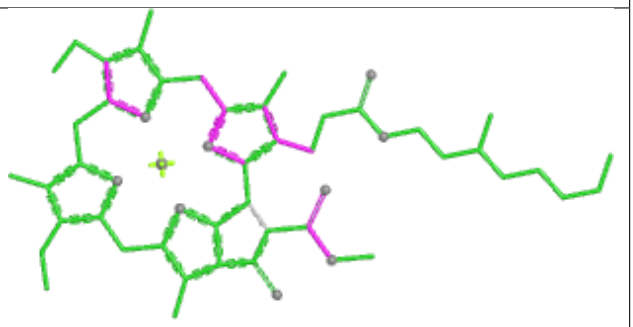


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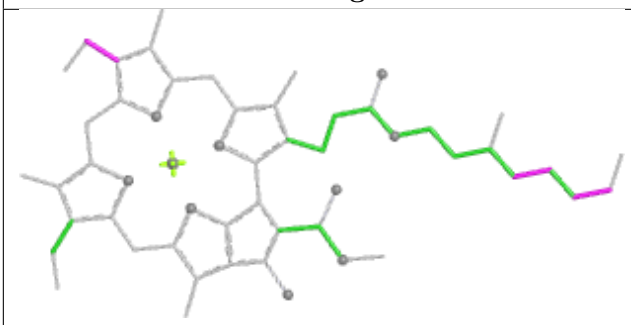
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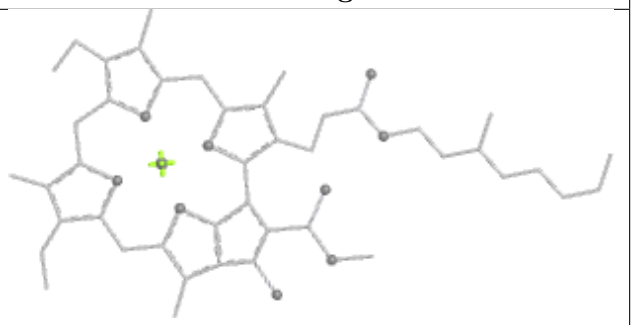
Bond lengths



Bond angles

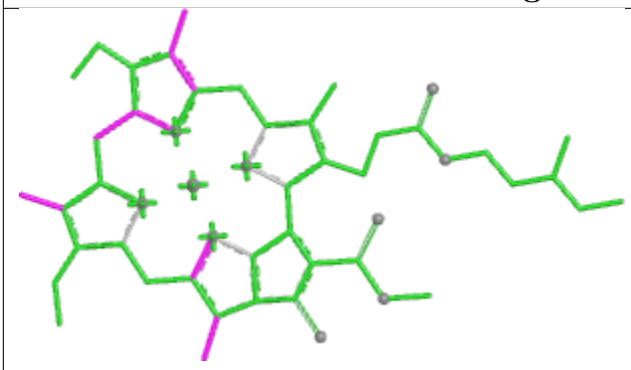


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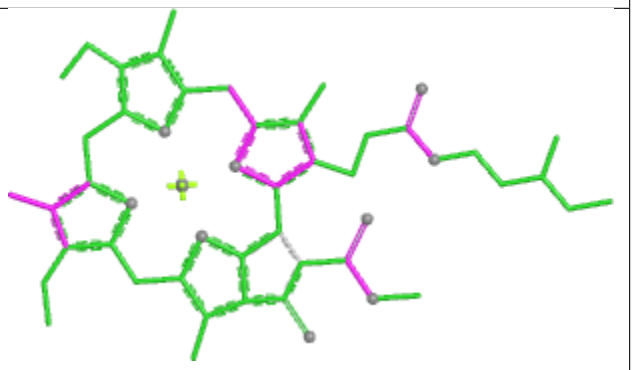


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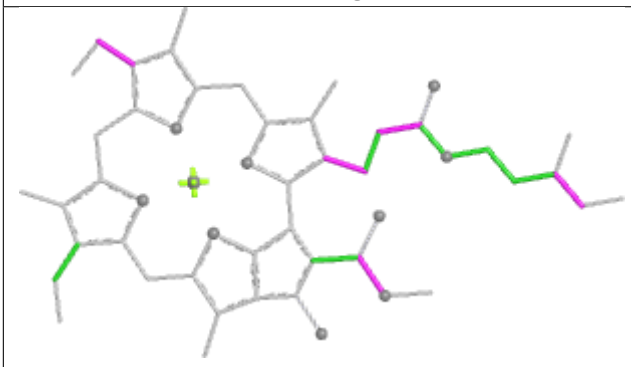
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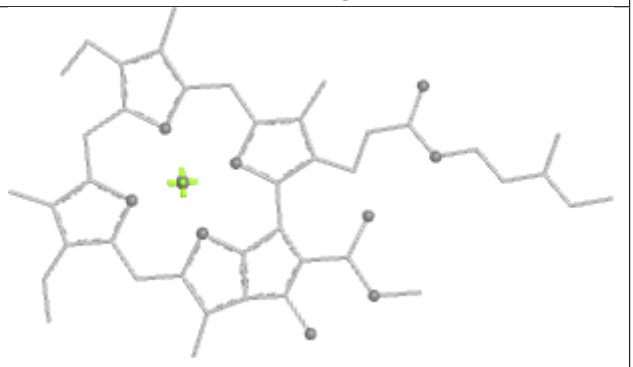
Bond lengths



Bond angles

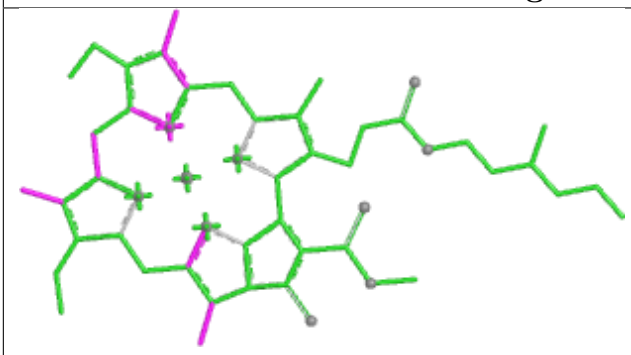


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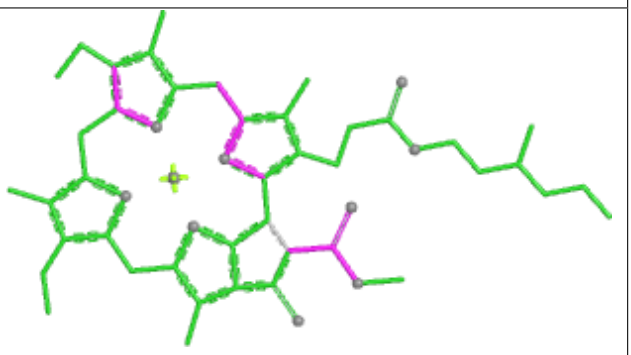


Rings

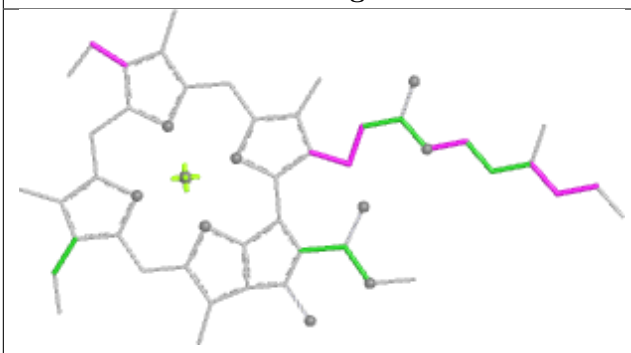
Ligand CLA F 313



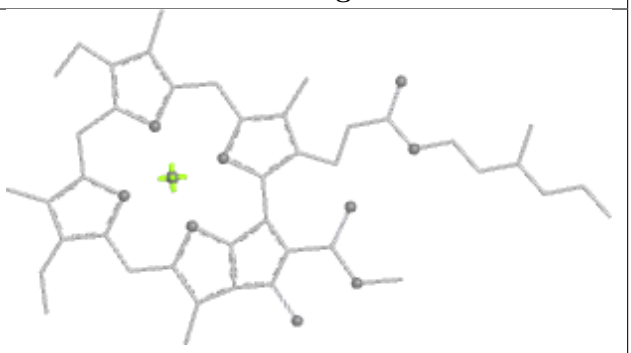
Bond lengths



Bond angles

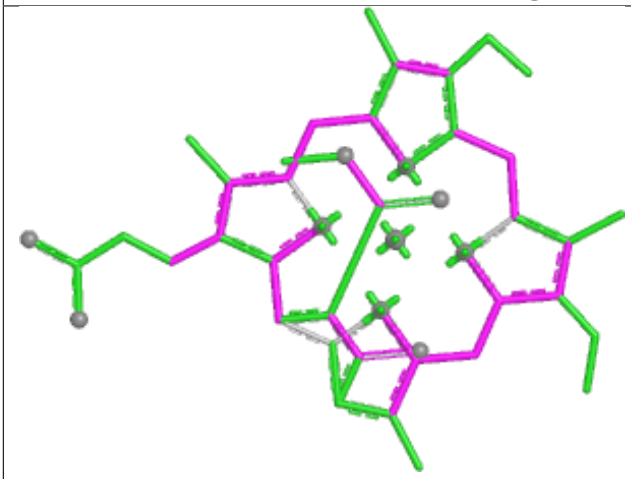


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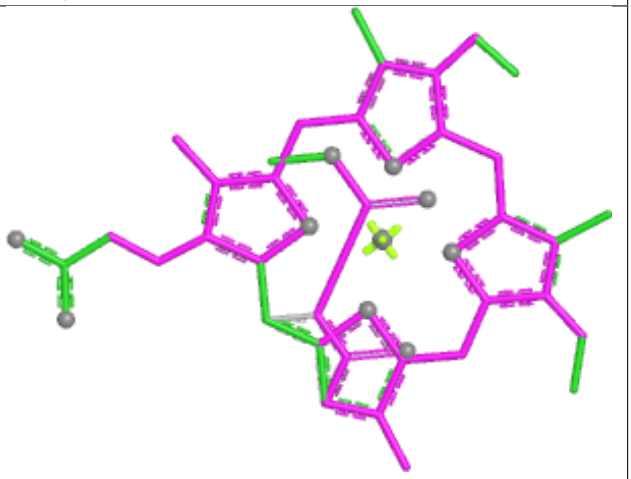


Rings

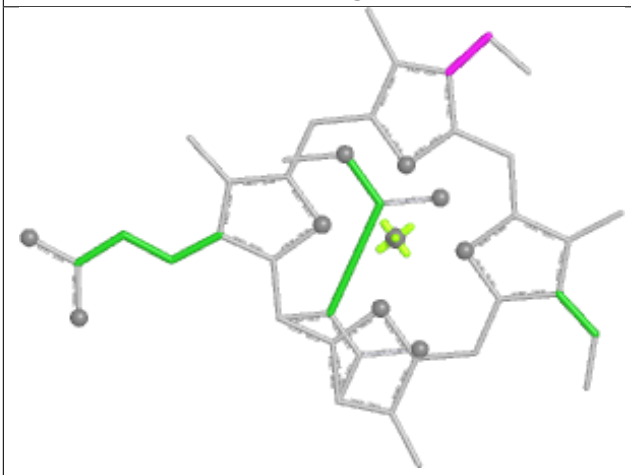
Ligand KC1 Q 313



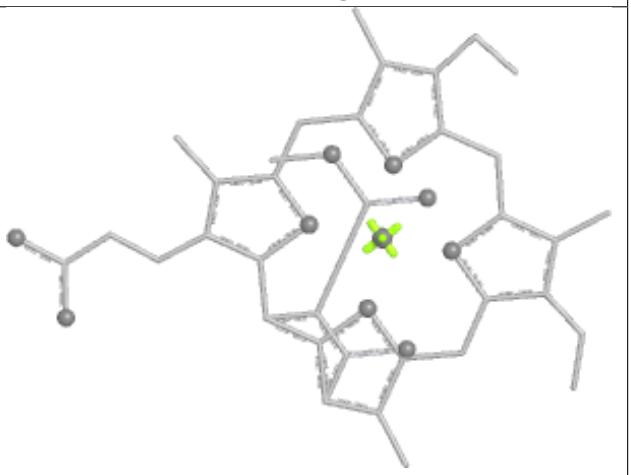
Bond lengths



Bond angles

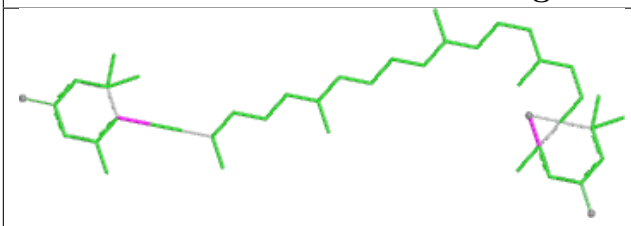


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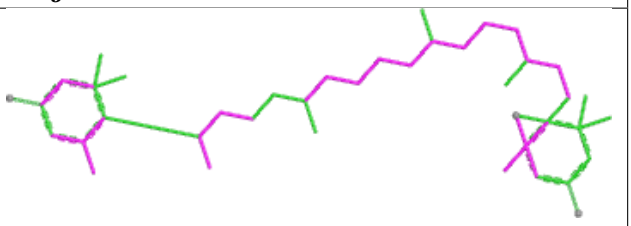


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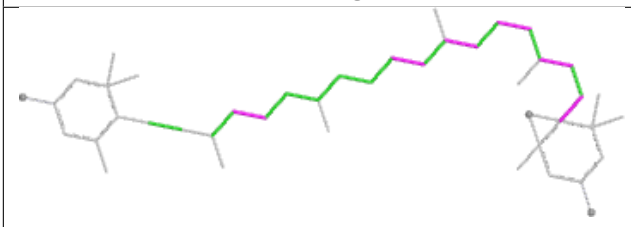
Ligand DD6 j 103



Bond lengths



Bond angles

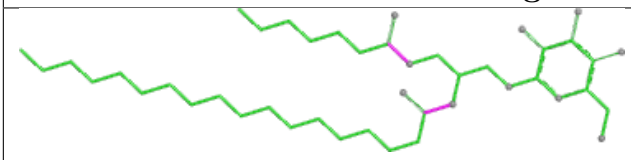


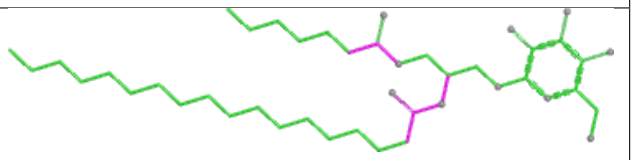
Torsions

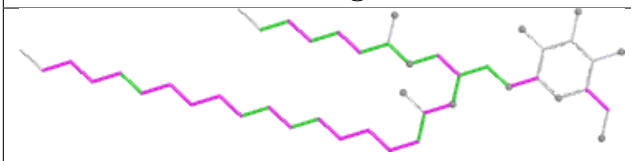


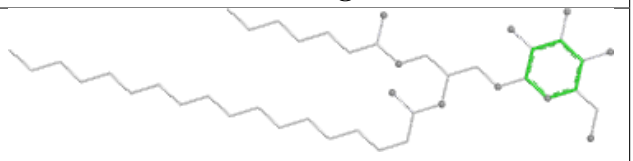
Rings

Ligand LMG J 319

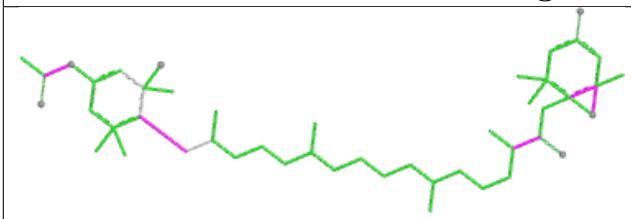

Bond lengths

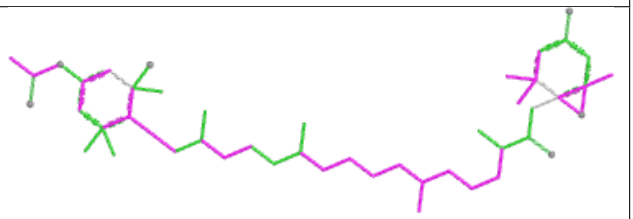

Bond angles

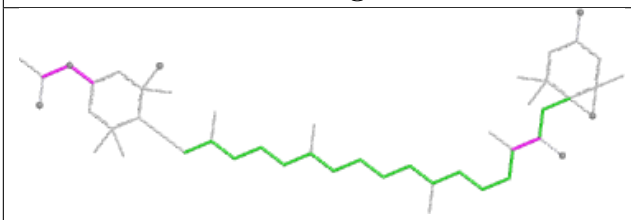

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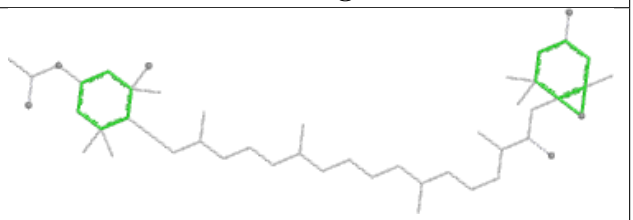

Rings

Ligand A86 I 302

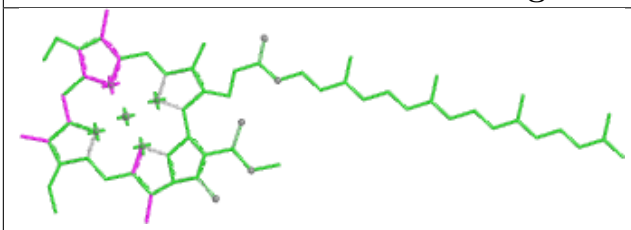

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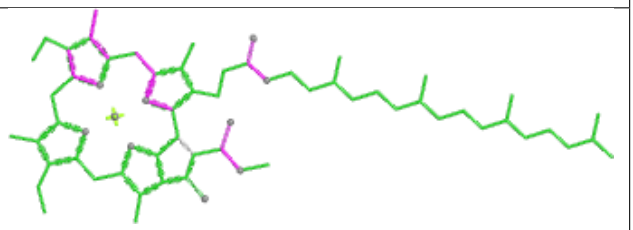

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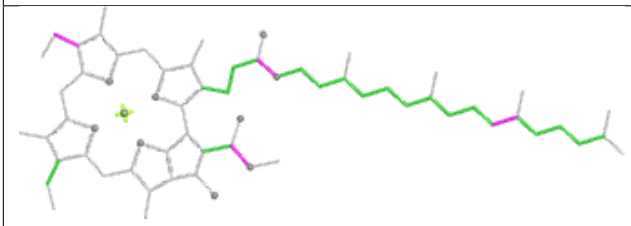

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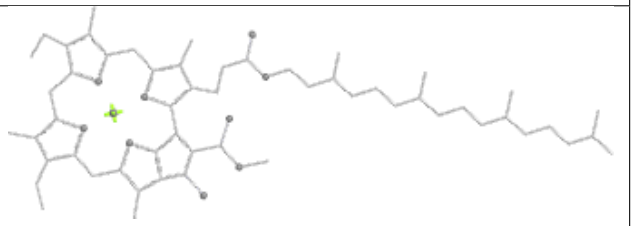

Rings

Ligand CLA J 309

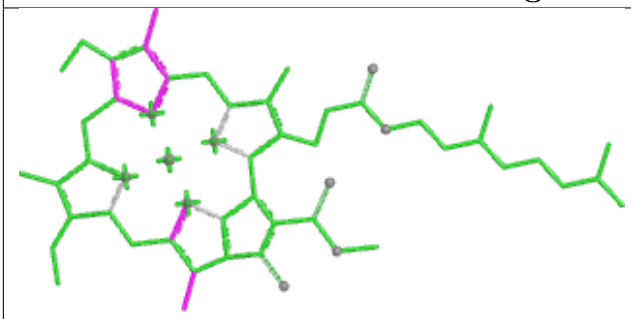

Bond lengths


Bond angles

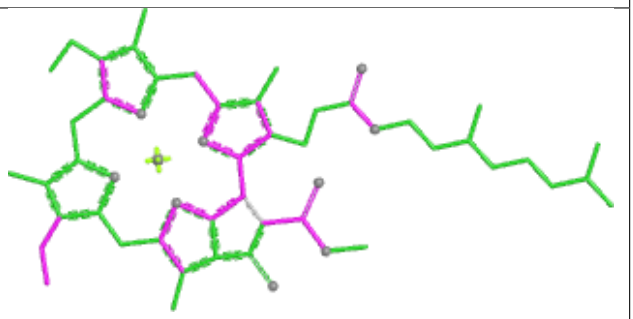

Torsions


Rings

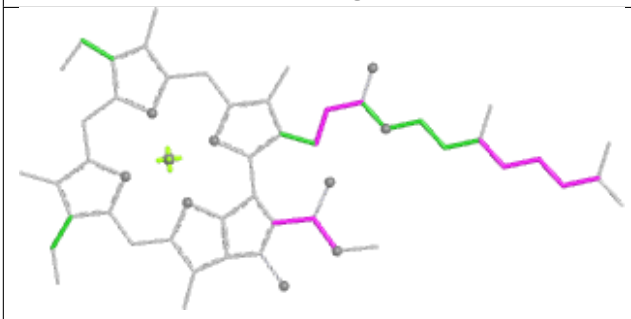
Ligand CLA B 311



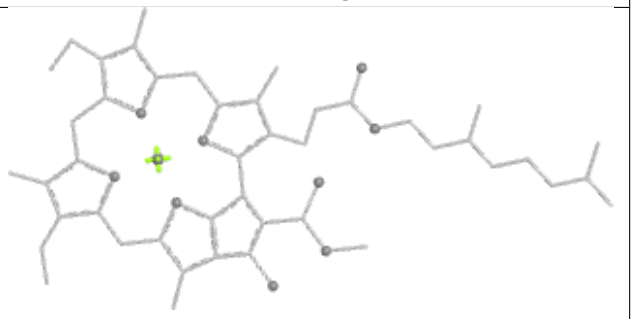
Bond lengths



Bond angles

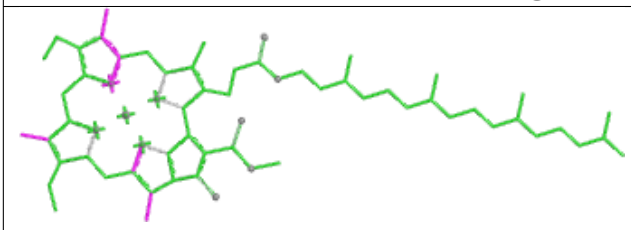


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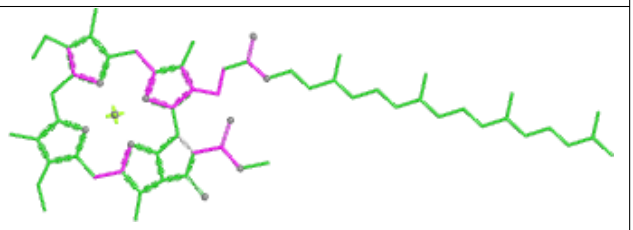


Rings

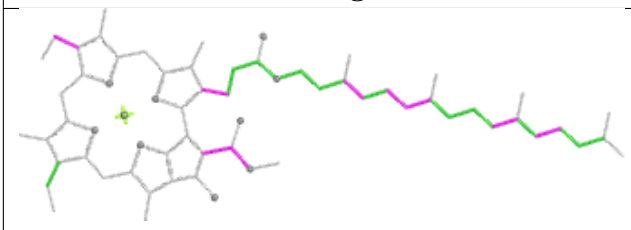
Ligand CLA a 832



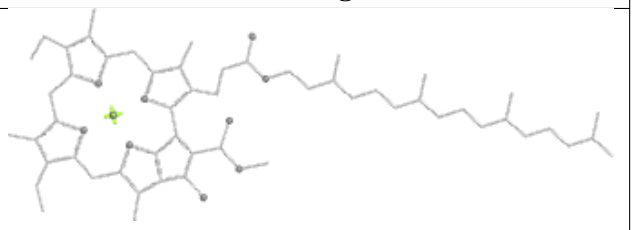
Bond lengths



Bond angles

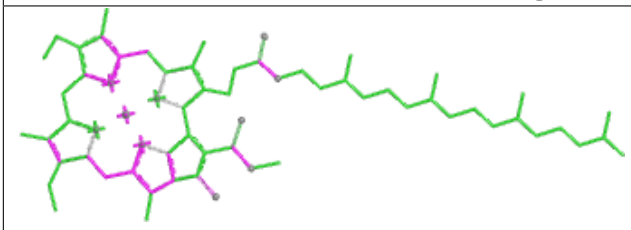


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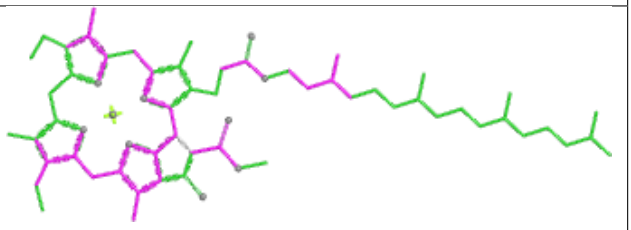


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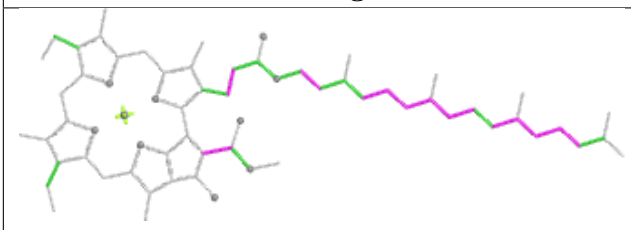
Ligand CLA I 308



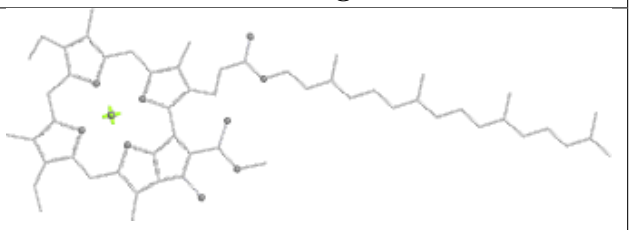
Bond lengths



Bond angles

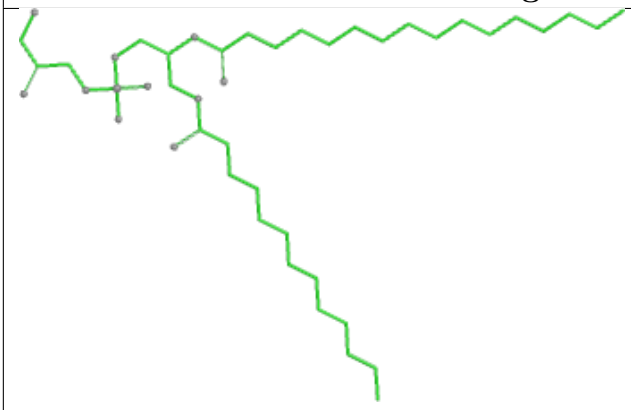


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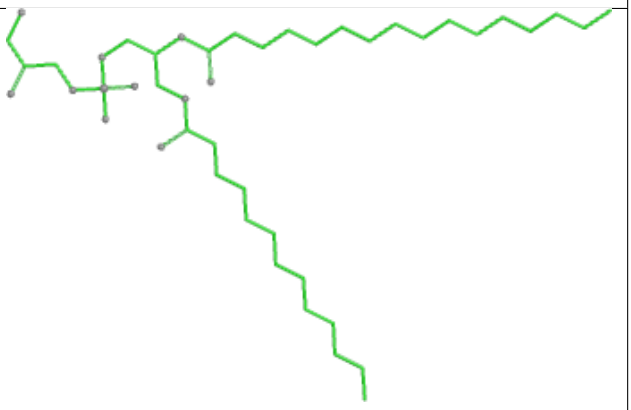


Rings

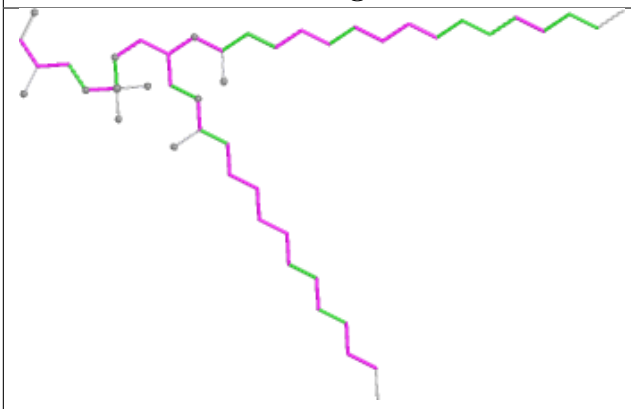
Ligand LHG D 318



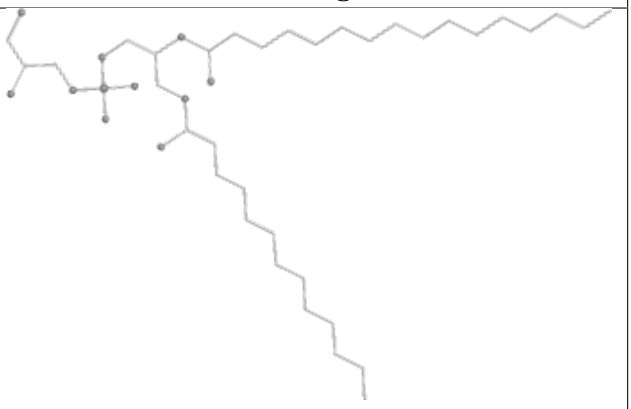
Bond lengths



Bond angles

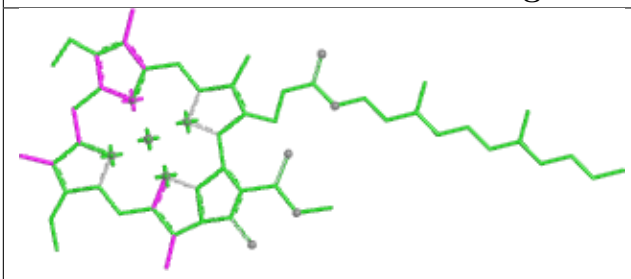


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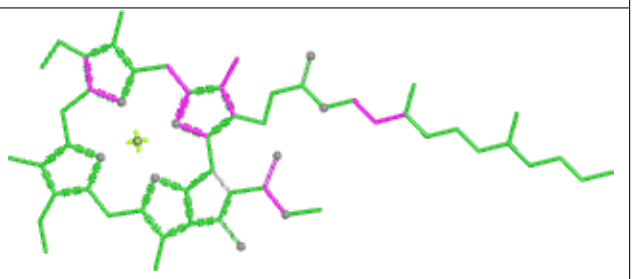


Rings

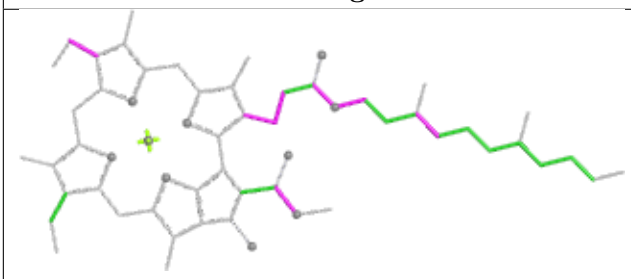
Ligand CLA D 317



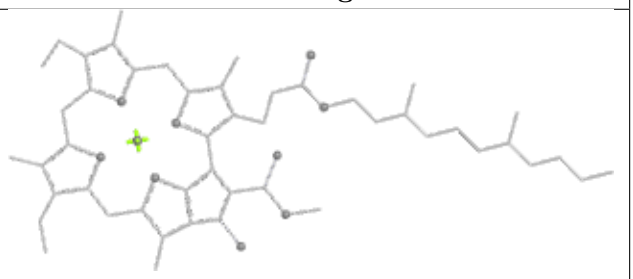
Bond lengths



Bond angles

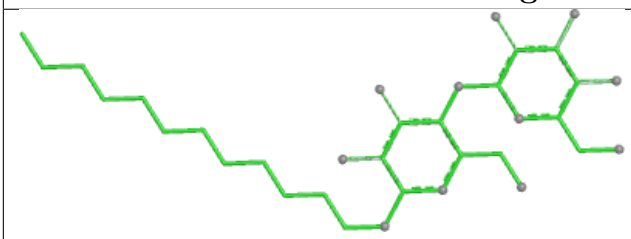


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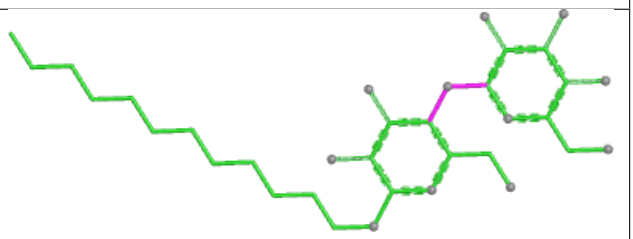


Rings

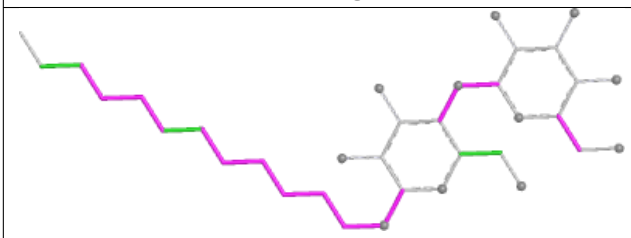
Ligand LMT G 322



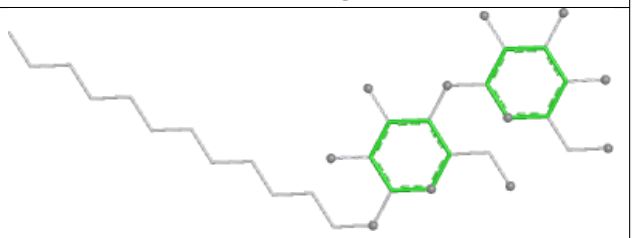
Bond lengths



Bond angles

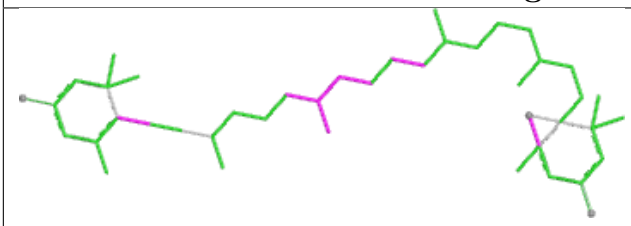


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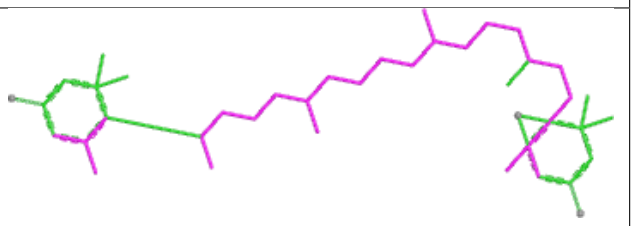


Rings

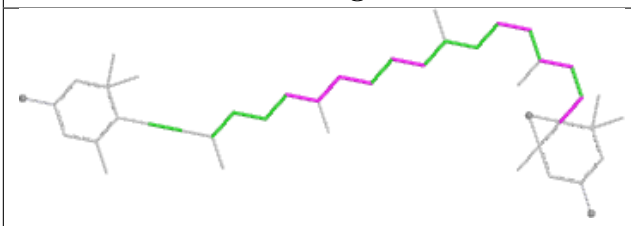
Ligand DD6 D 303



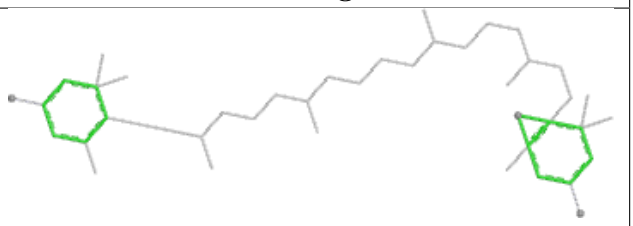
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Bond angles

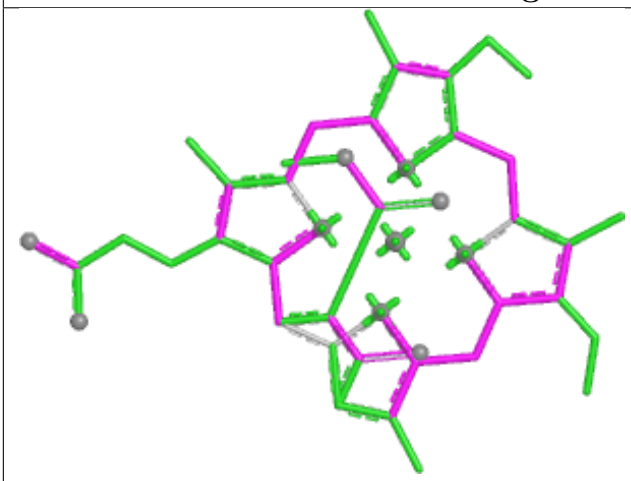


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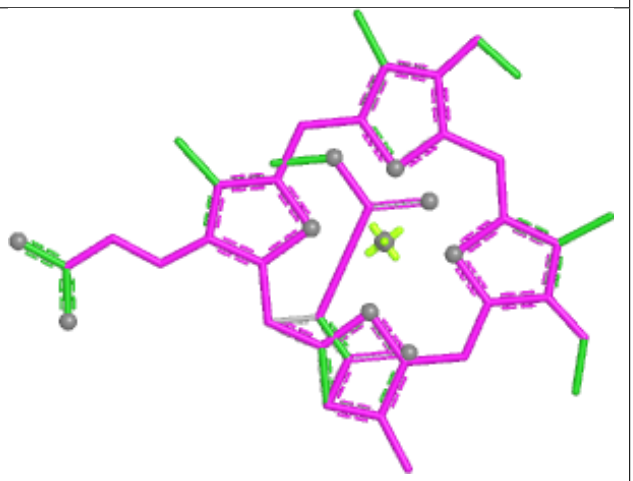


Rings

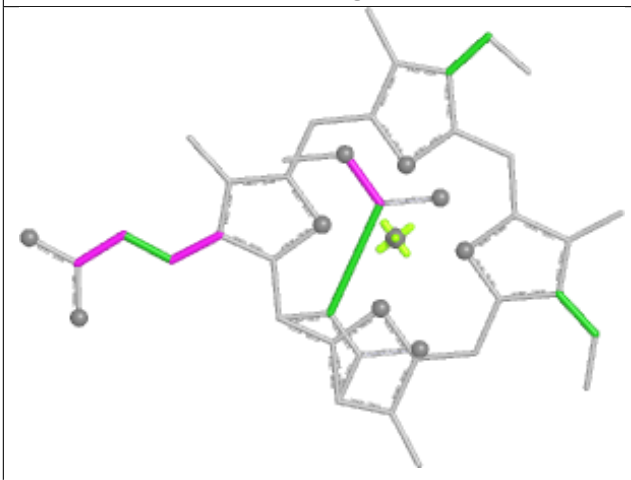
Ligand KC1 M 313



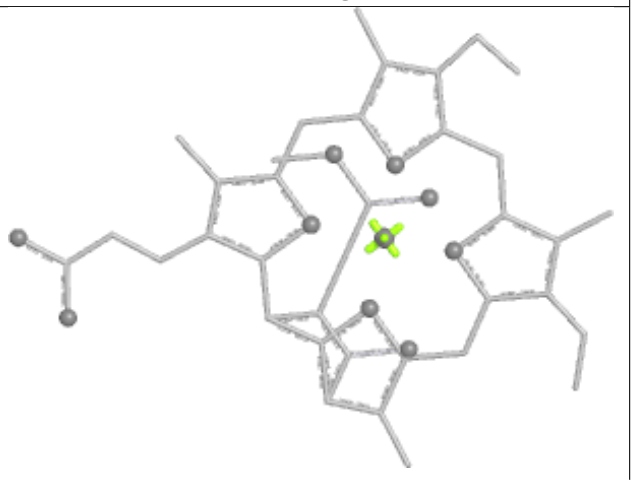
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Bond angles

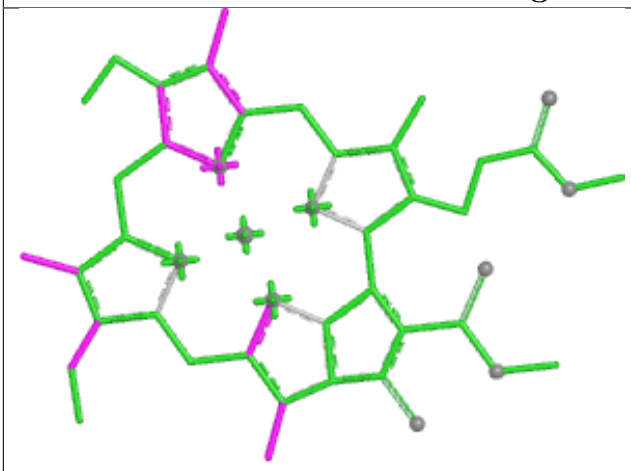


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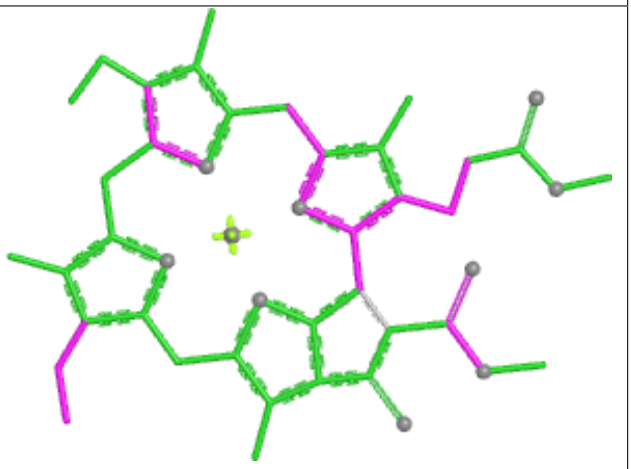


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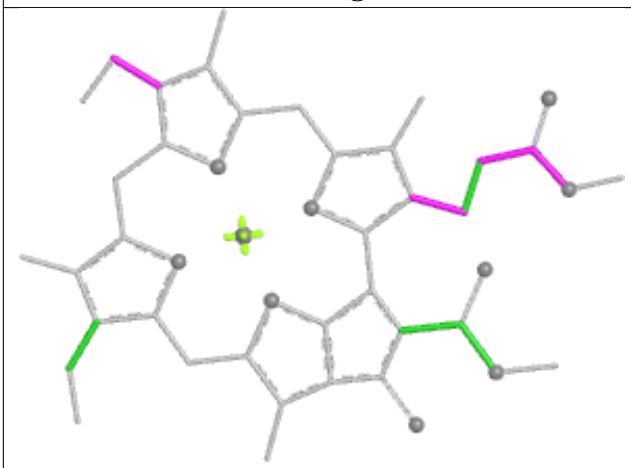
Ligand CLA I 309



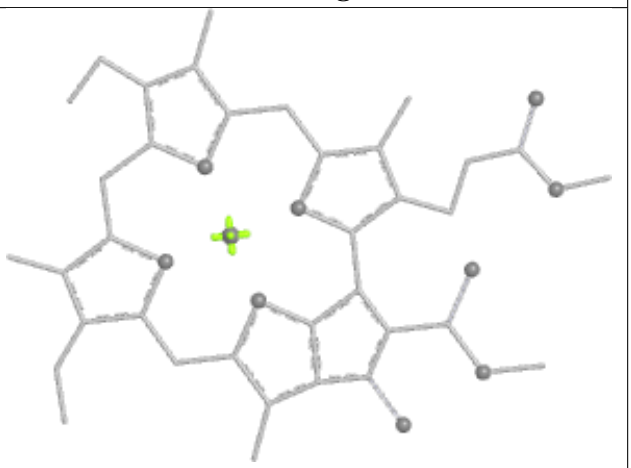
Bond lengths



Bond angles

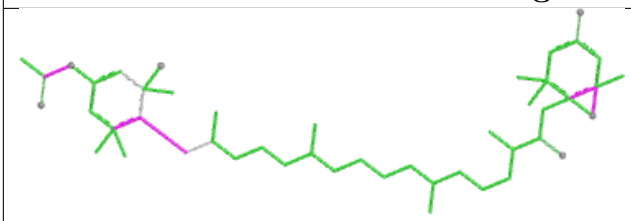


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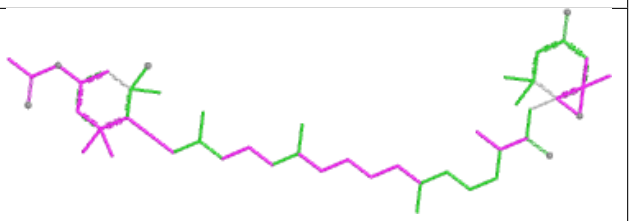


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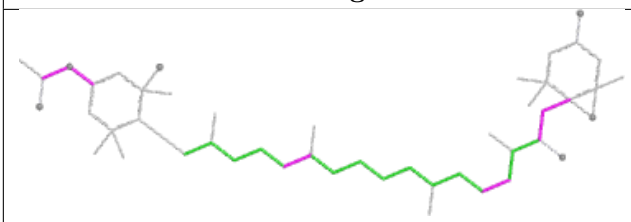
Ligand A86 S 304



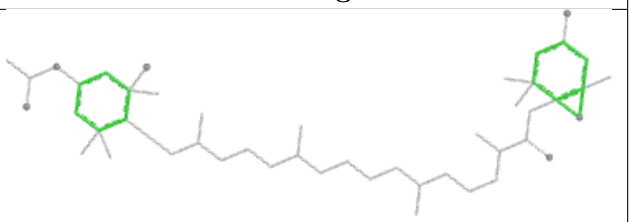
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Bond angles

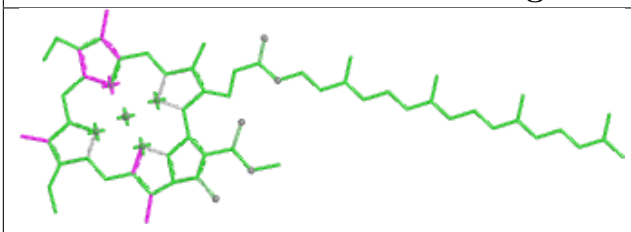


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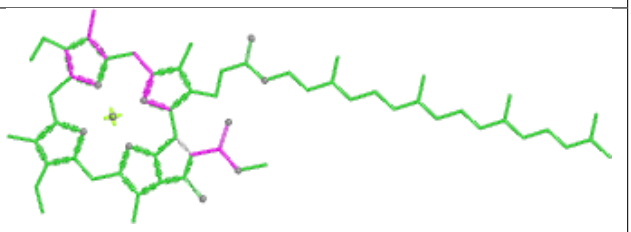


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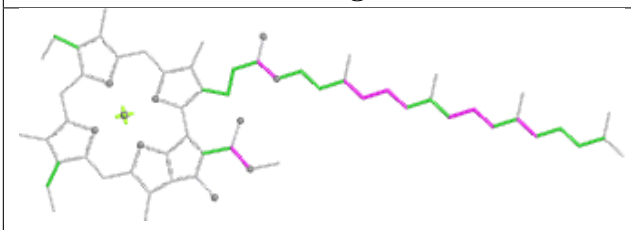
Ligand CLA L 320



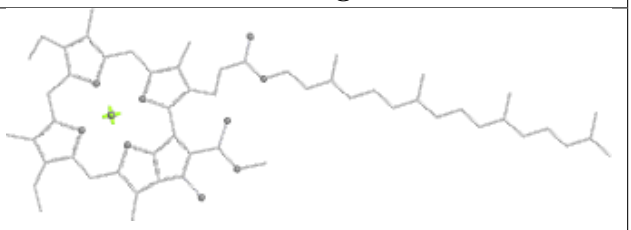
Bond lengths



Bond angles

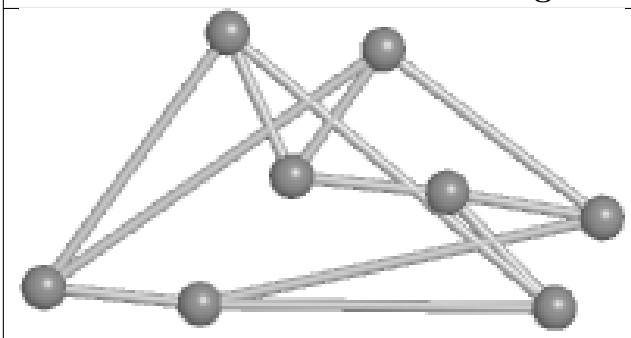


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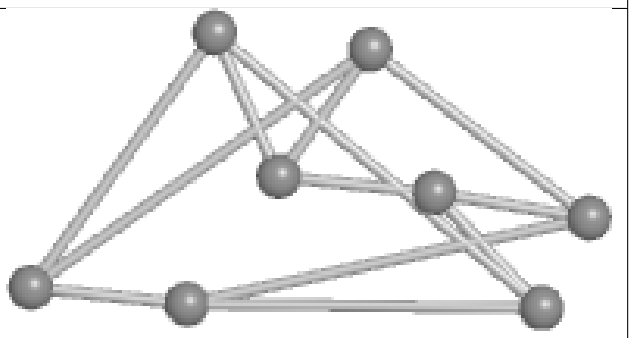


Rings

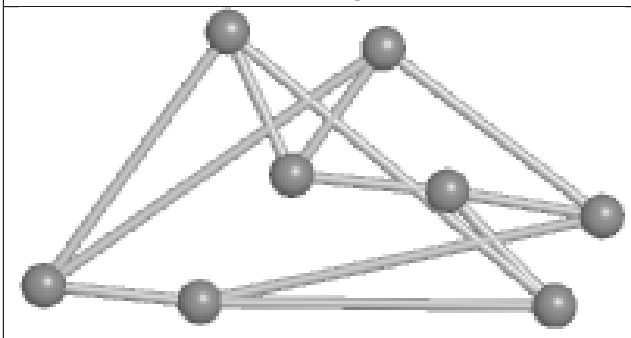
Ligand SF4 b 803



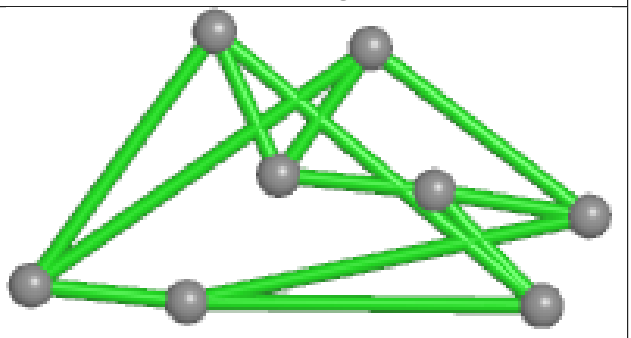
Bond lengths



Bond angles

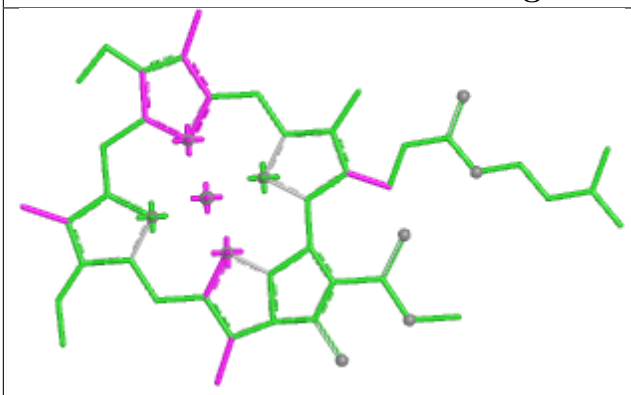


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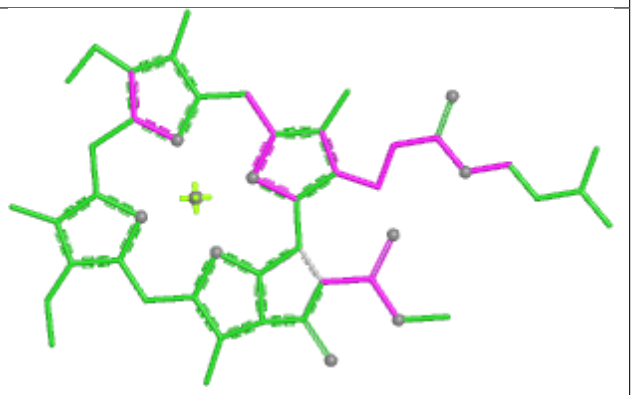


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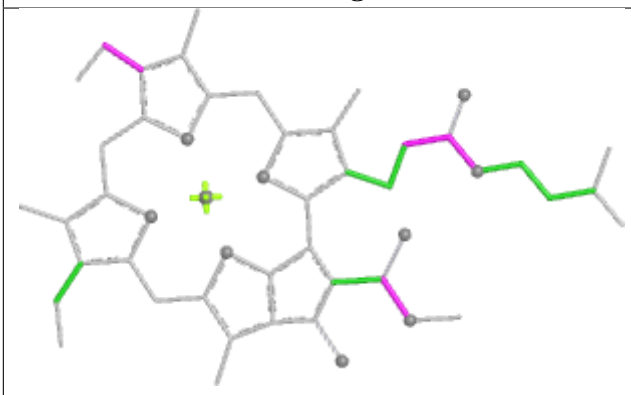
Ligand CLA H 318



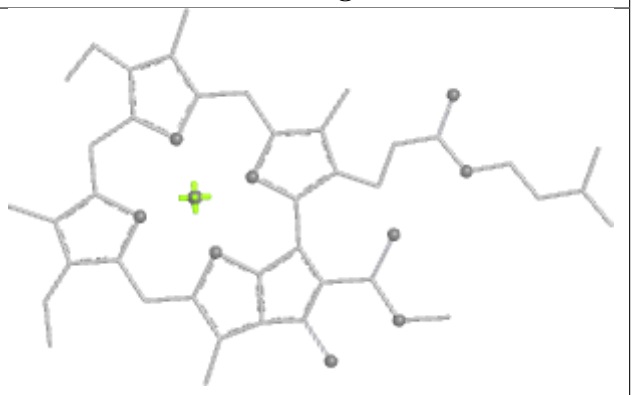
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Bond angles

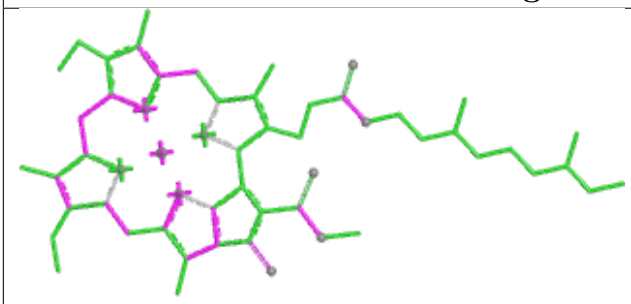


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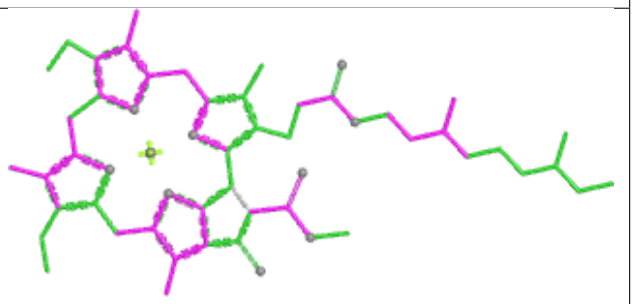


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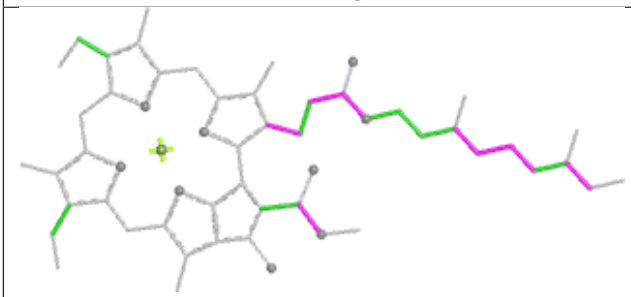
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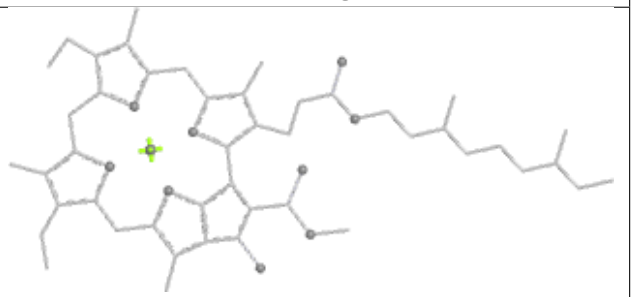
Bond lengths



Bond angles

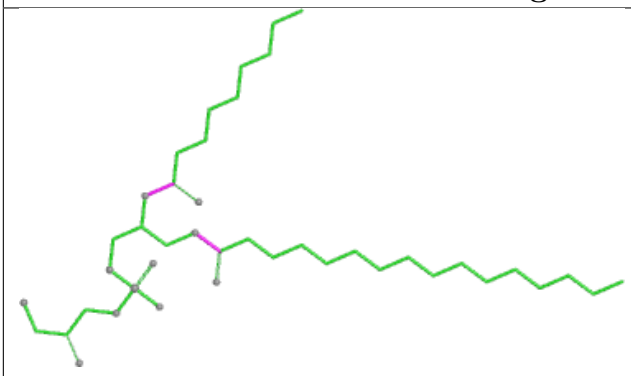


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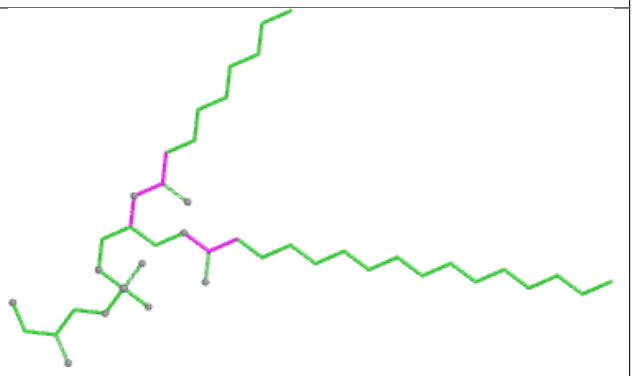


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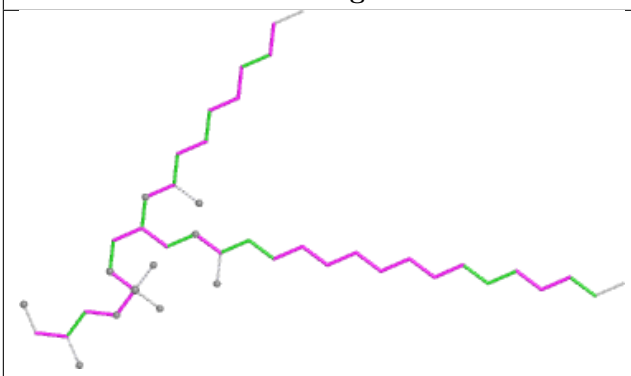
Ligand LHG f 809



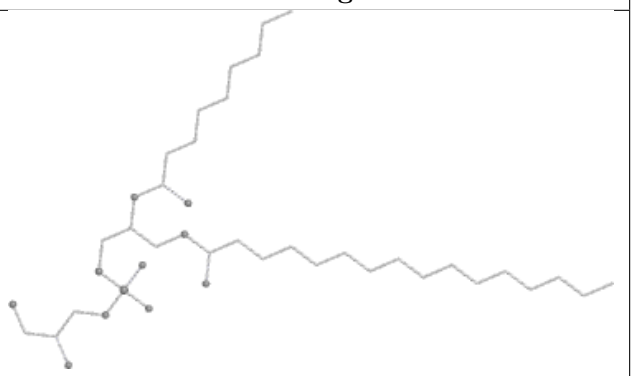
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Bond angles

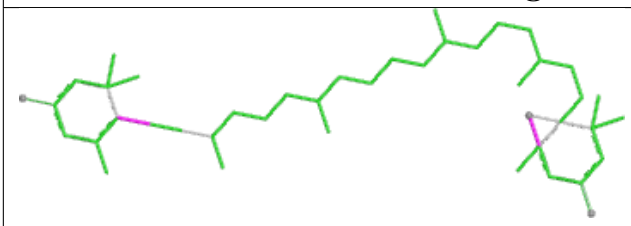


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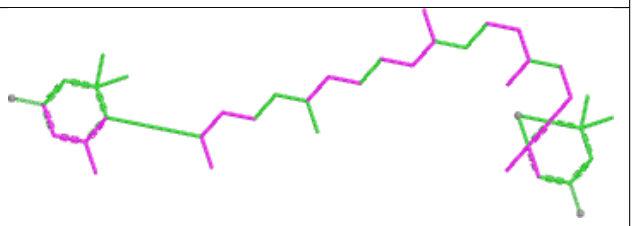


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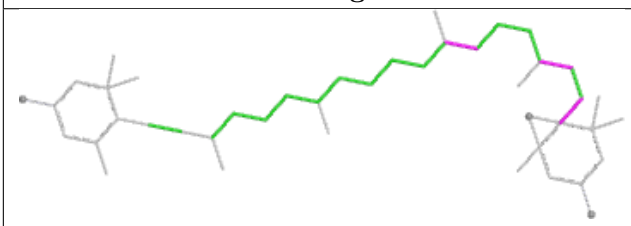
Ligand DD6 O 304



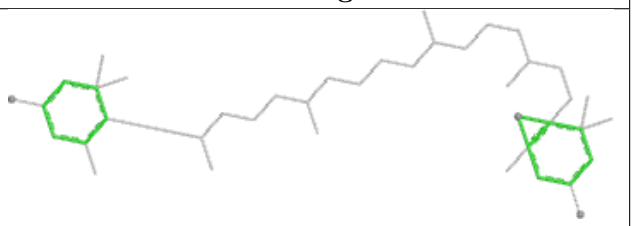
Bond lengths



Bond angles

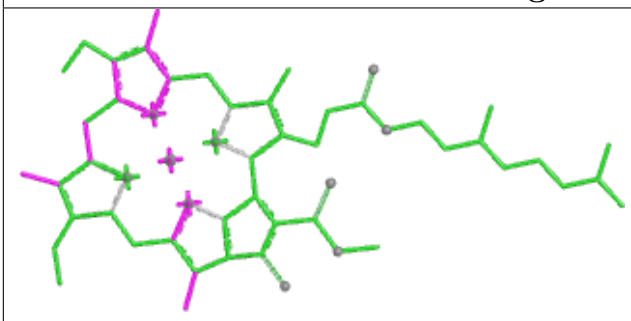


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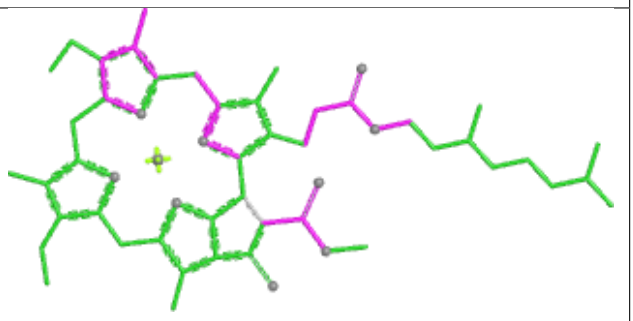


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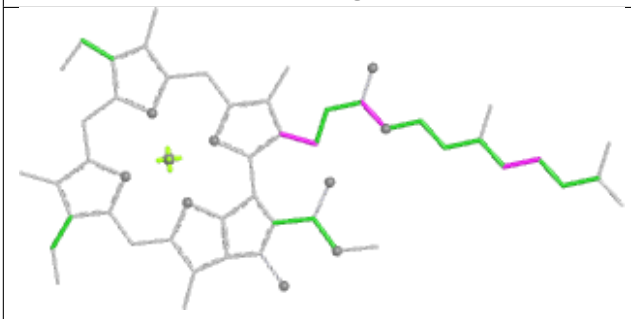
Ligand CLA a 803



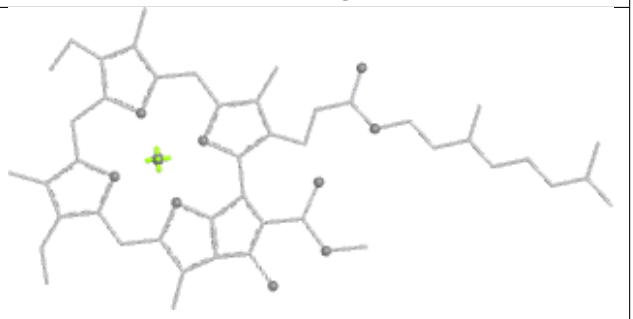
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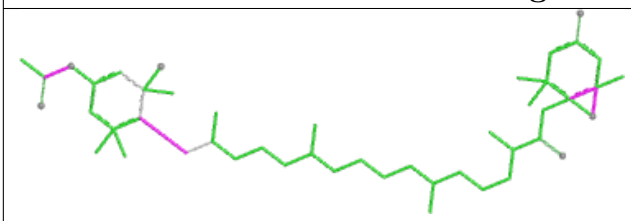


Torsions



Rings

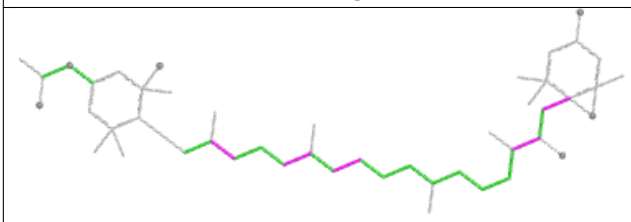
Ligand A86 U 304



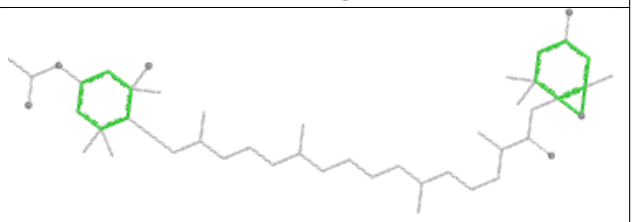
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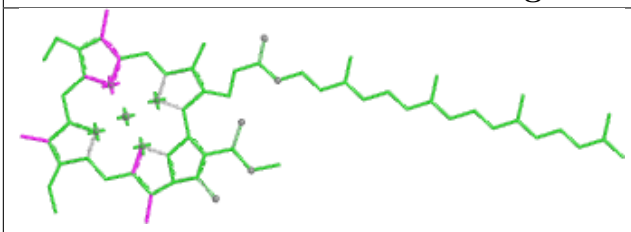


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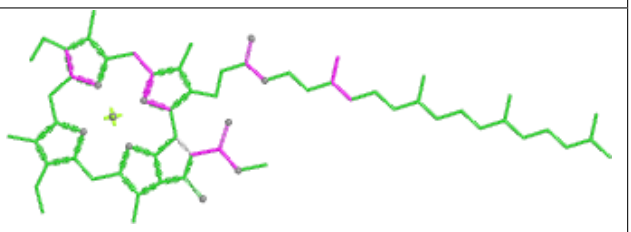


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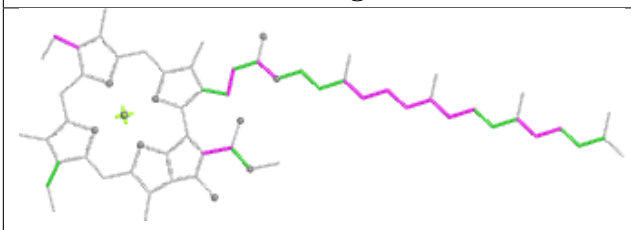
Ligand CLA C 208



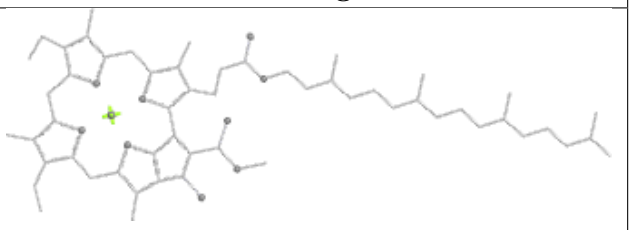
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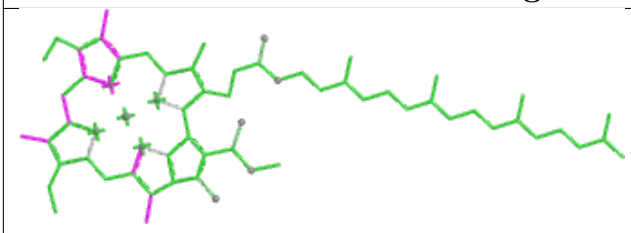


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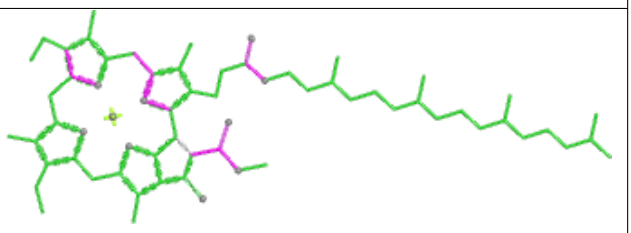


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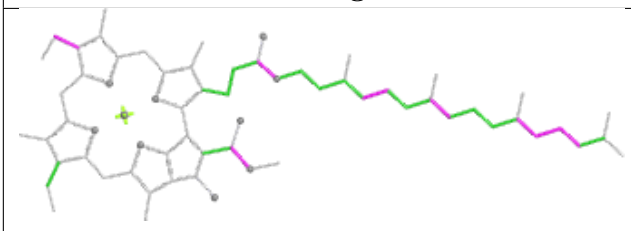
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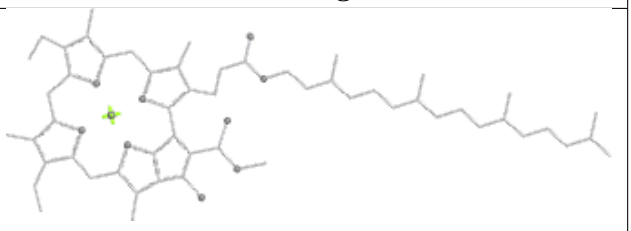
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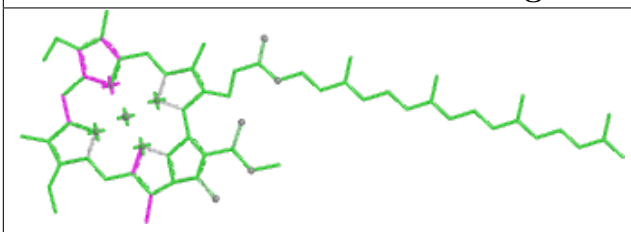


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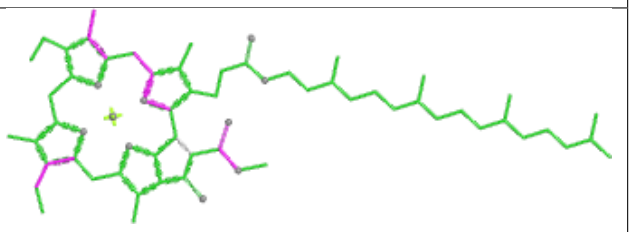


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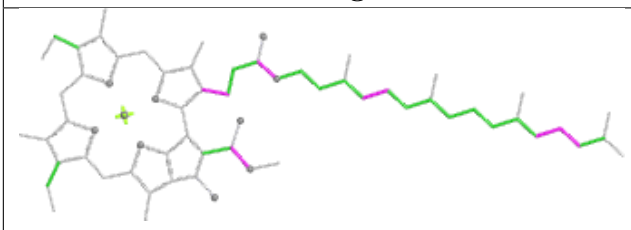
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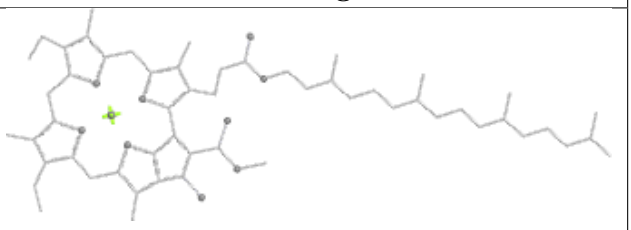
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Bond angles

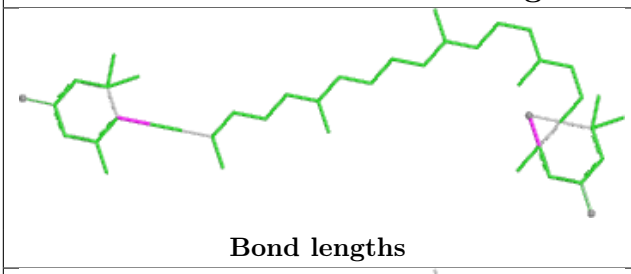


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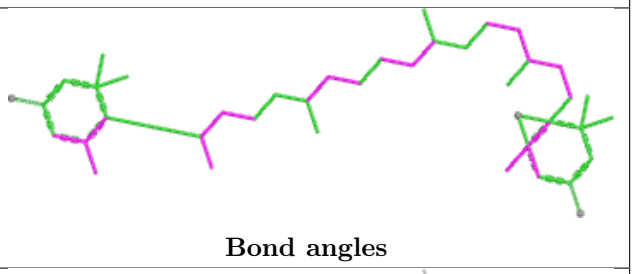


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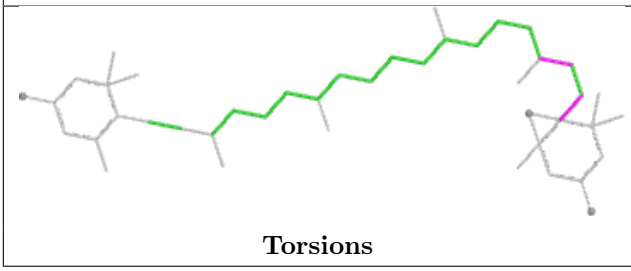
Ligand DD6 A 303



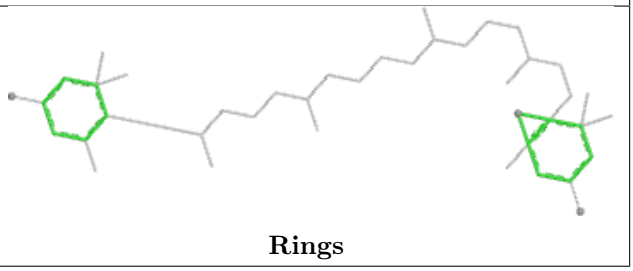
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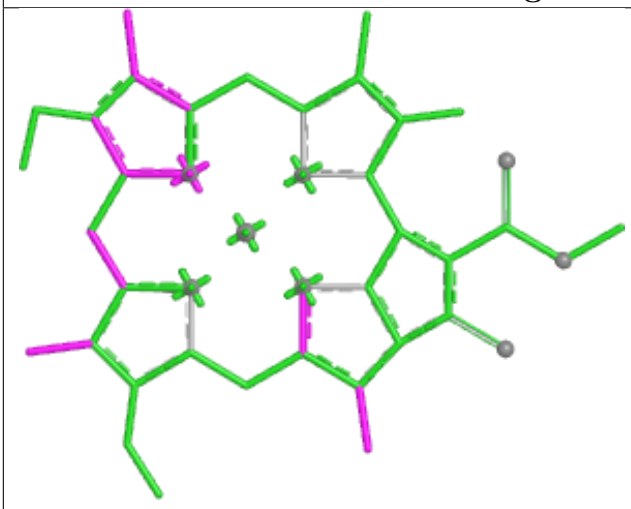


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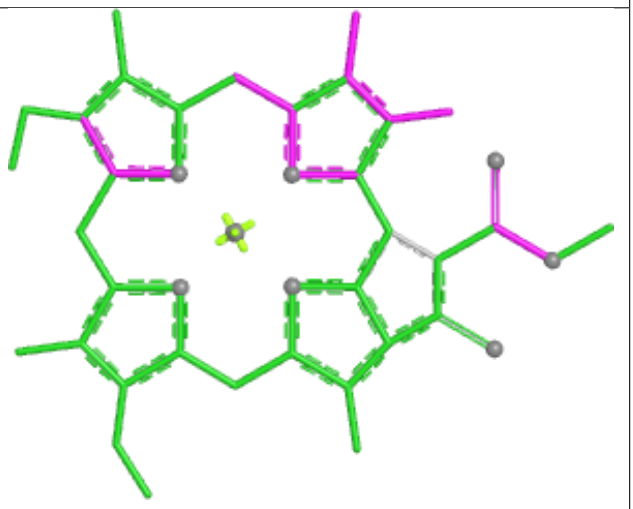


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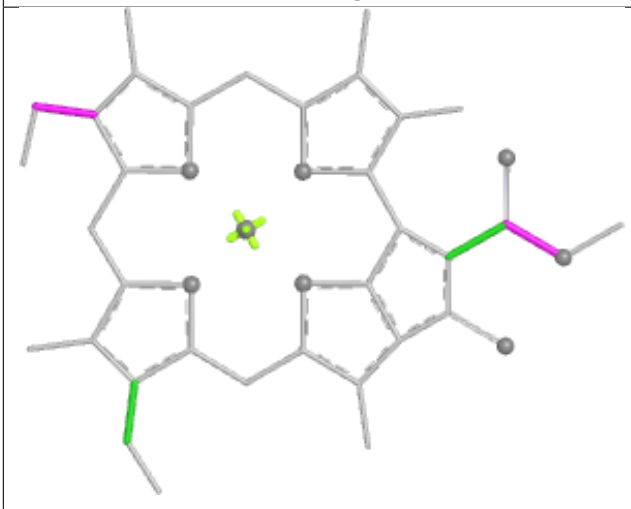
Ligand CLA C 214



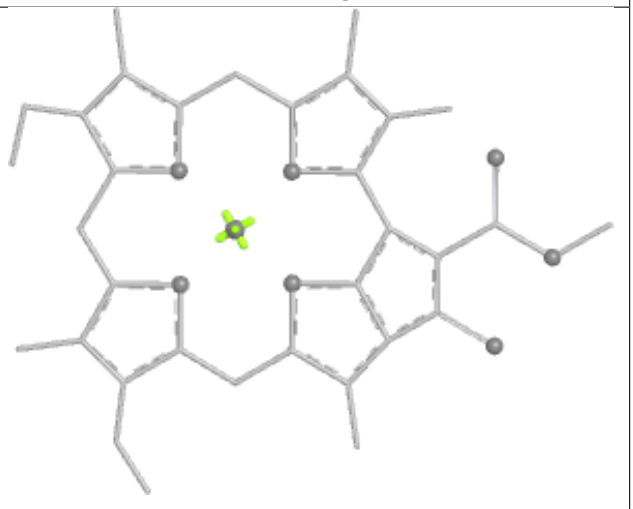
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Bond angles

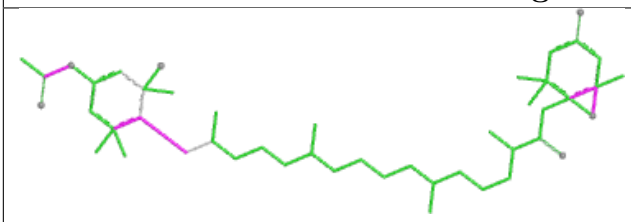


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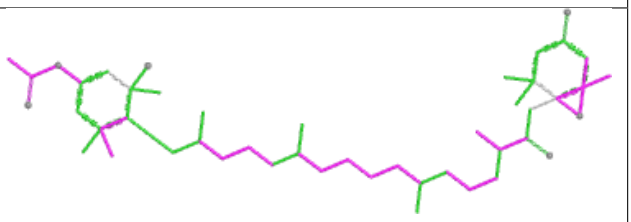


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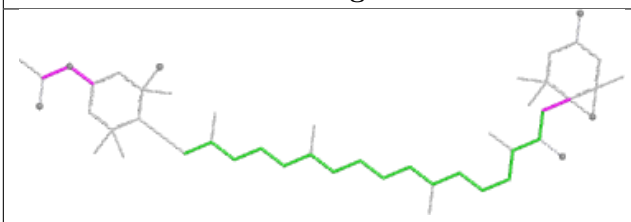
Ligand A86 F 304



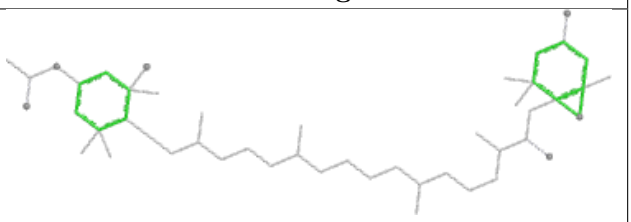
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Bond angles

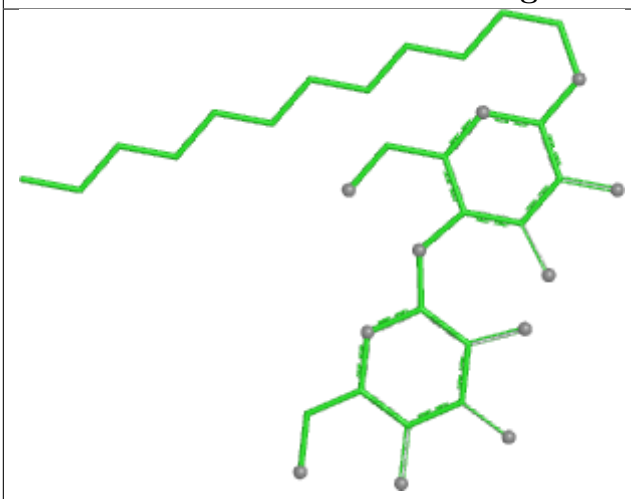


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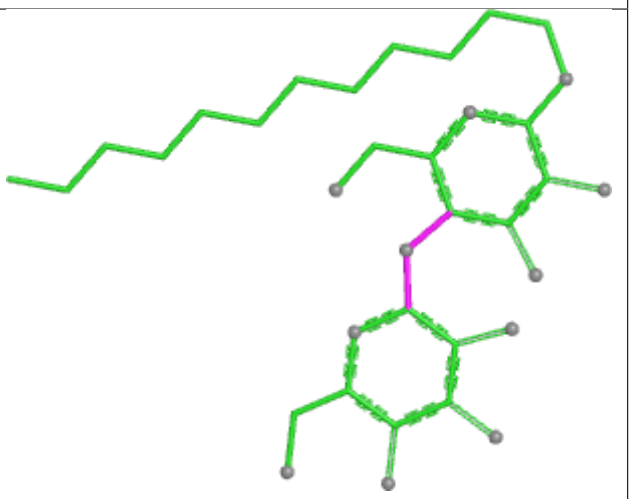


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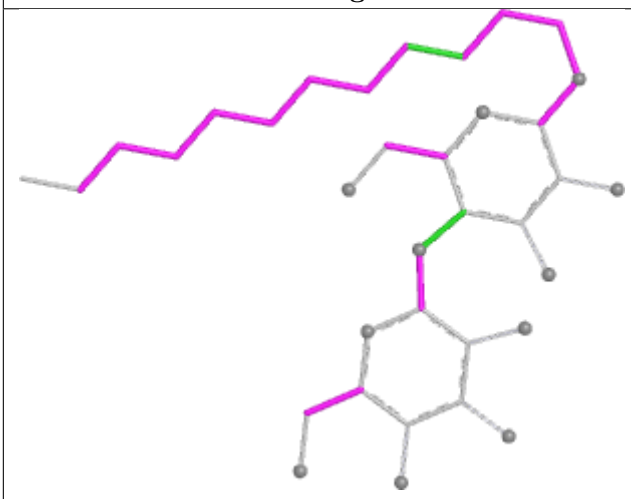
Ligand LMT U 315



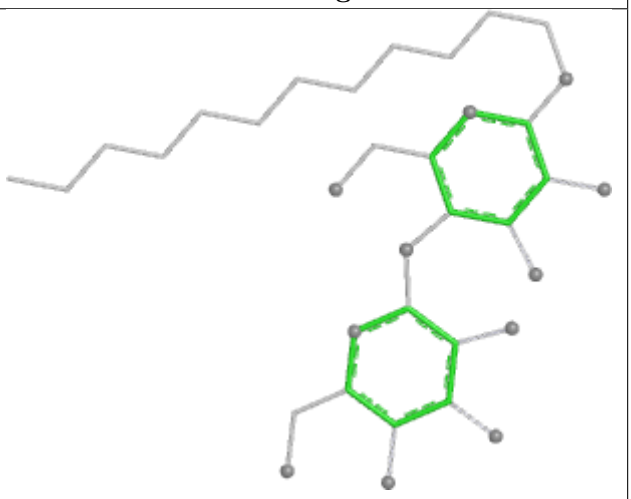
Bond lengths



Bond angles

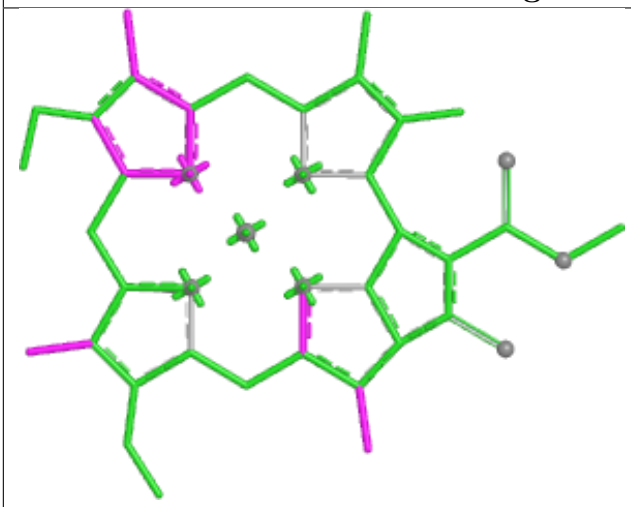


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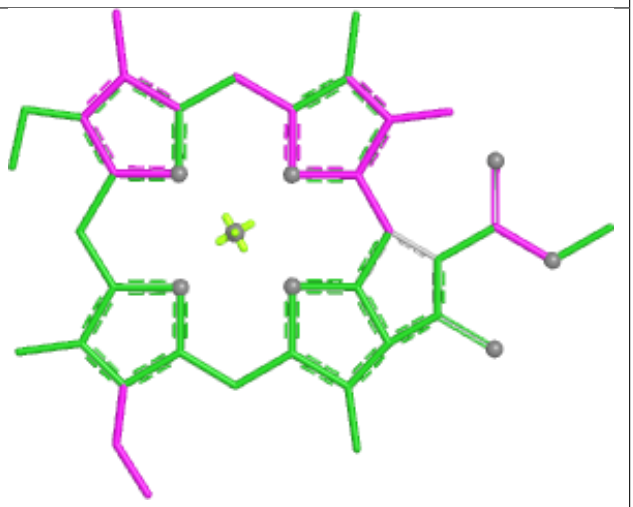


Rings

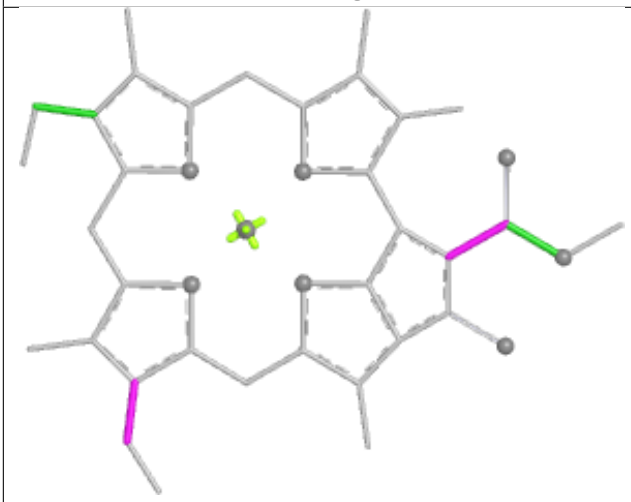
Ligand CLA D 315



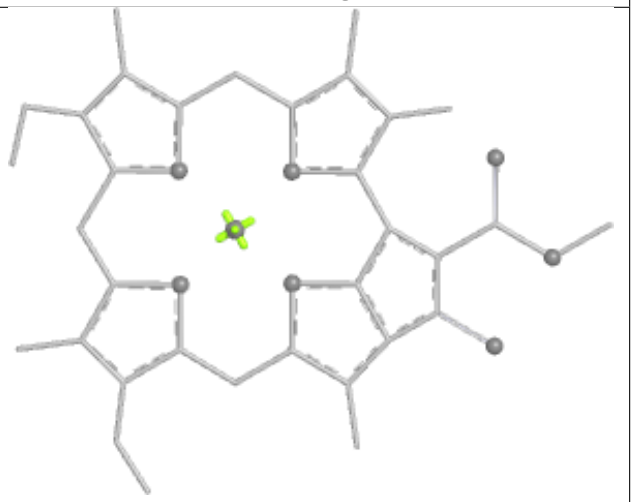
Bond lengths



Bond angles

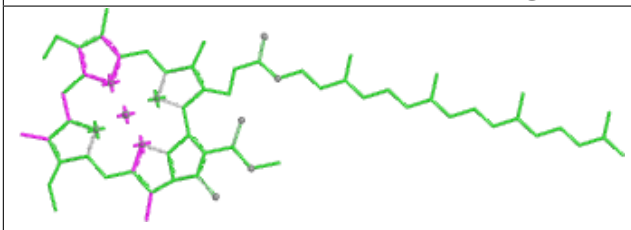


Torsions

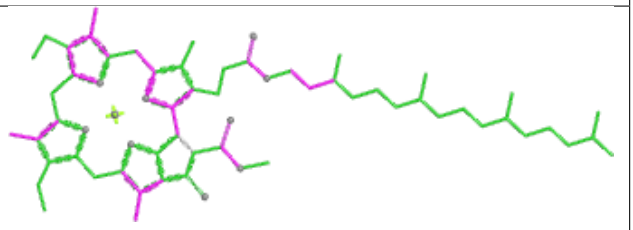


Rings

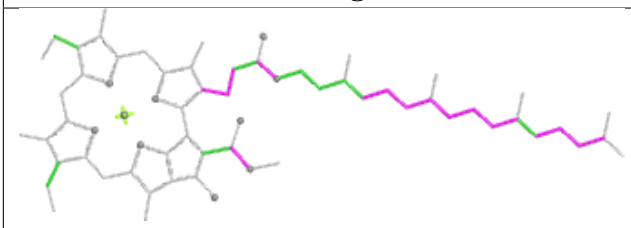
Ligand CLA U 311



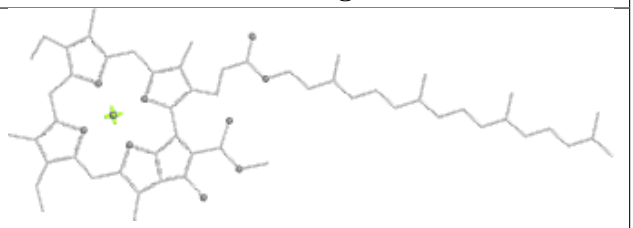
Bond lengths



Bond angles

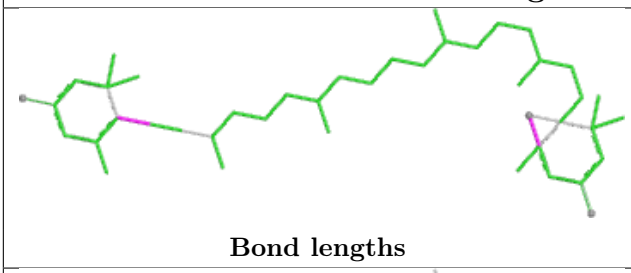


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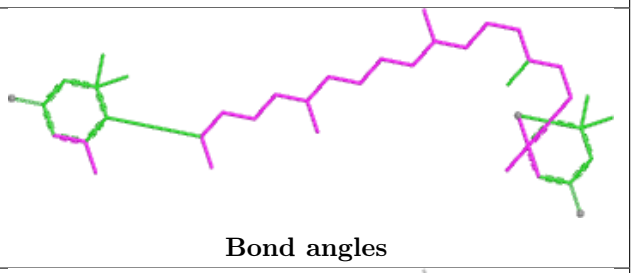


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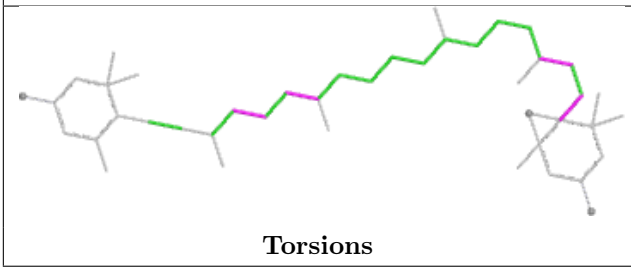
Ligand DD6 L 305



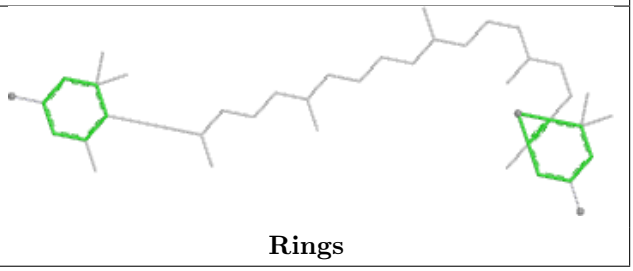
Bond lengths



Bond angles

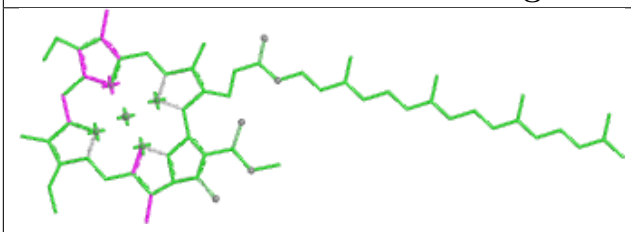


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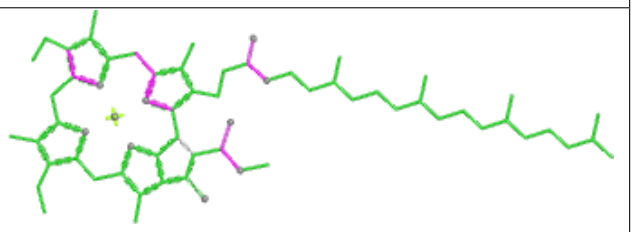


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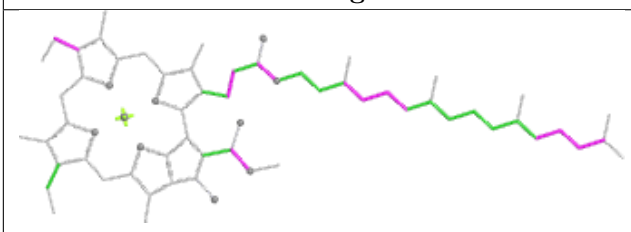
Ligand CLA R 315



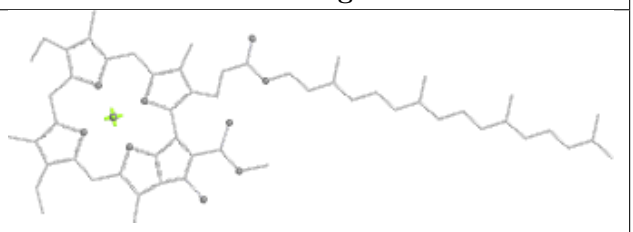
Bond lengths



Bond angles

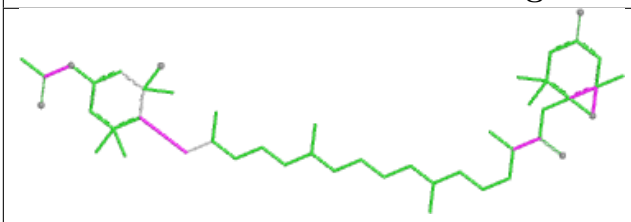


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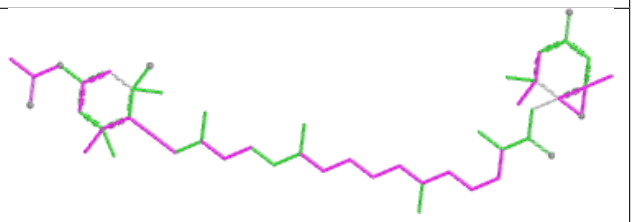


Rings

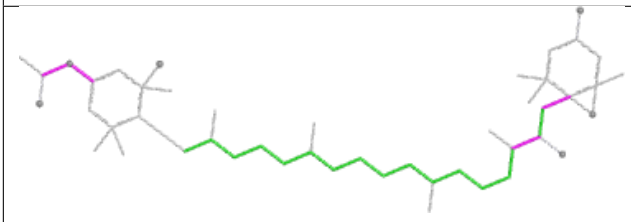
Ligand A86 M 305



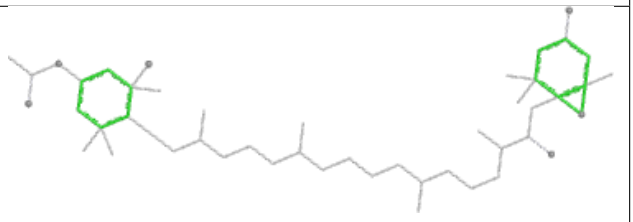
Bond lengths



Bond angles

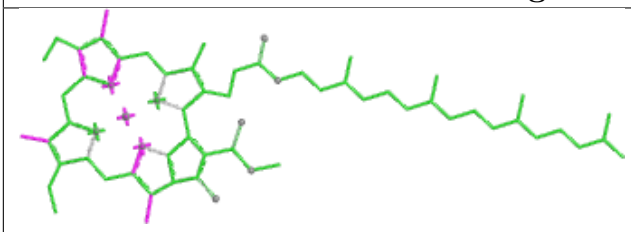


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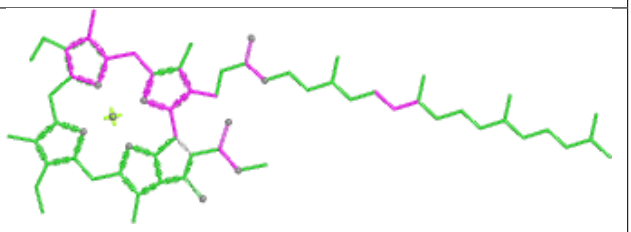


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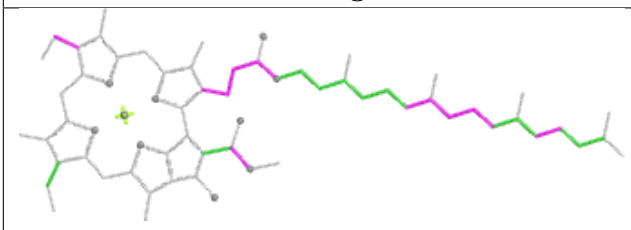
Ligand CLA a 817



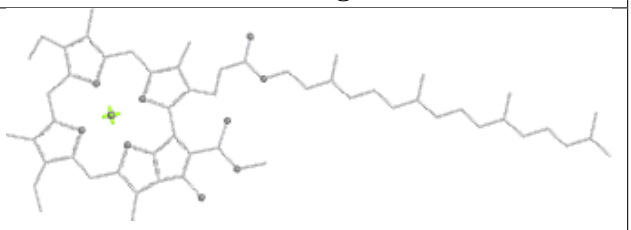
Bond lengths



Bond angles

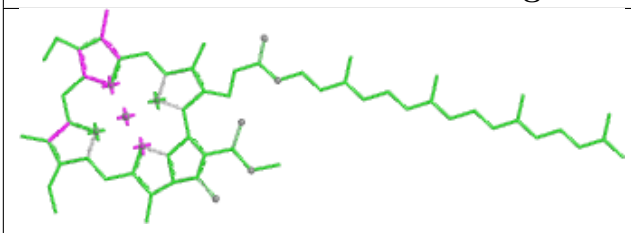


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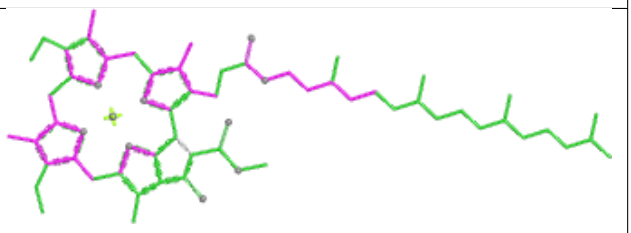


Rings

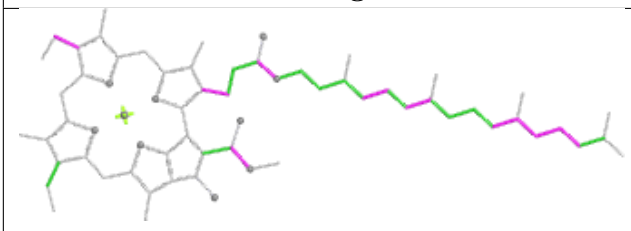
Ligand CLA N 308



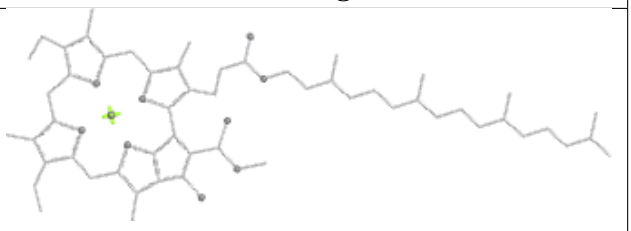
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Bond angles

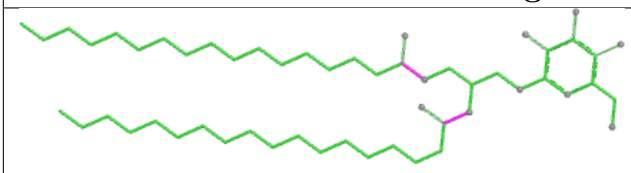


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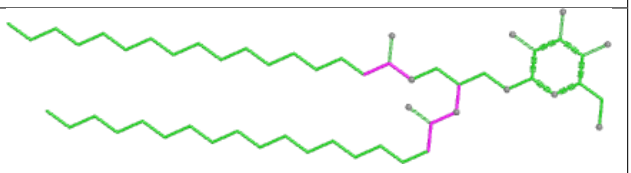


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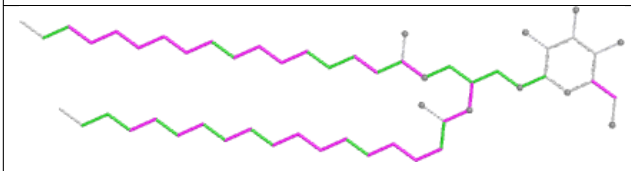
Ligand LMG a 852



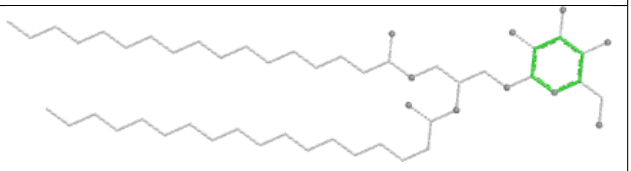
Bond lengths



Bond angles

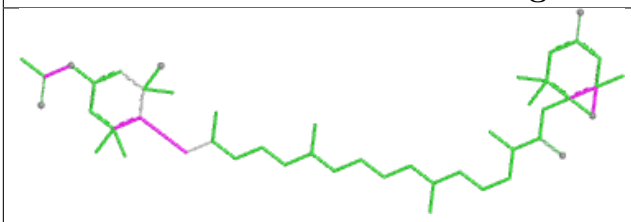


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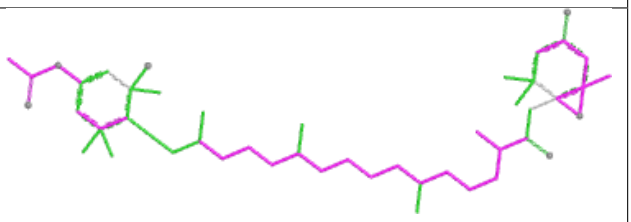


Rings

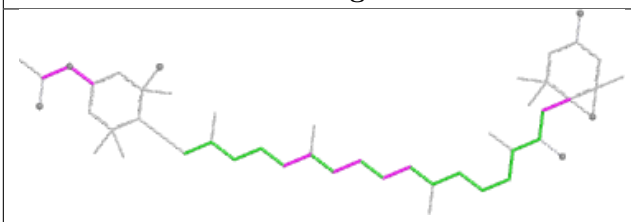
Ligand A86 V 301



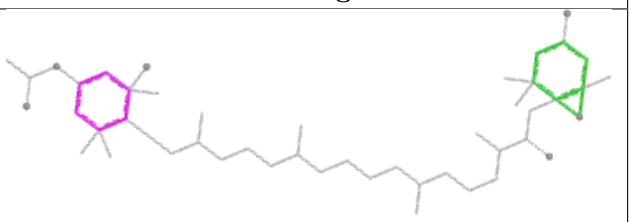
Bond lengths



Bond angles

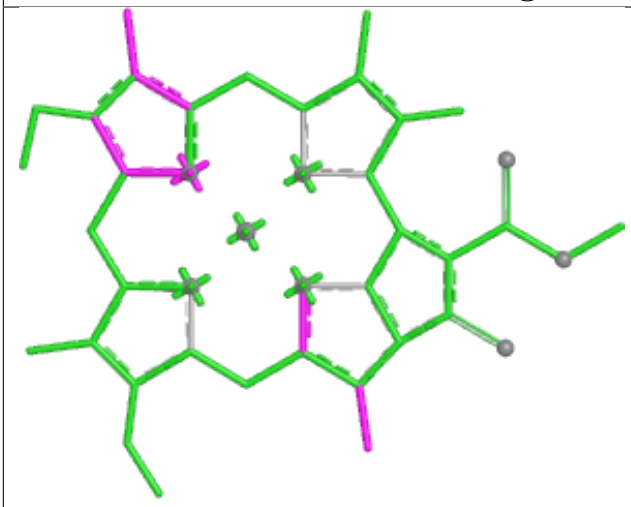


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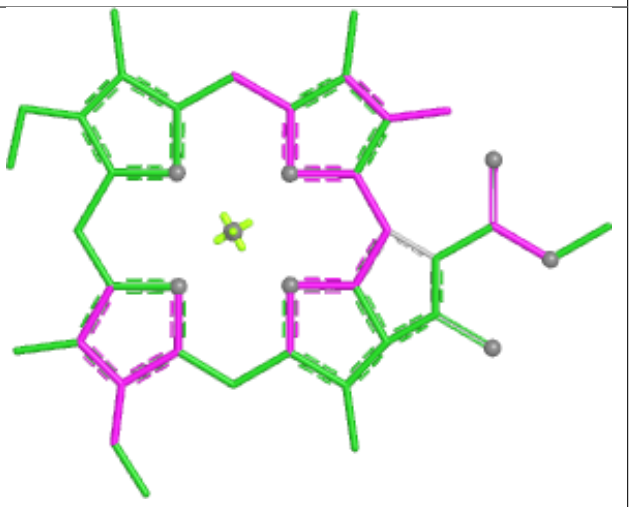


Rings

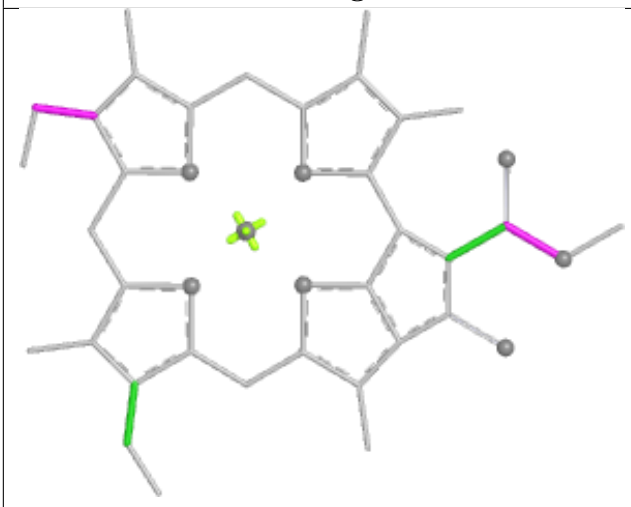
Ligand CLA W 214



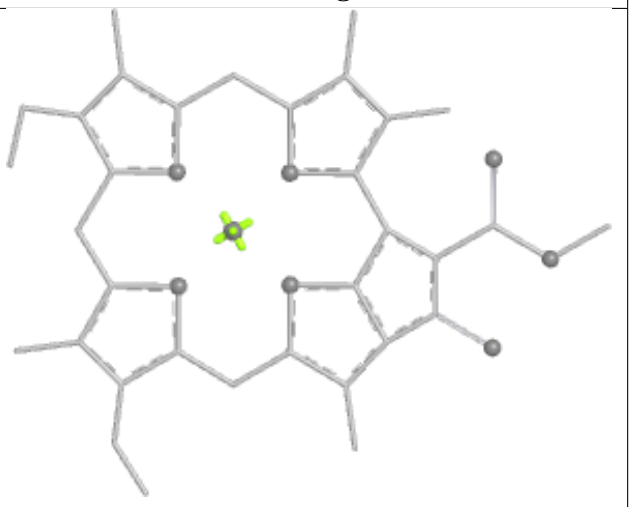
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Bond angles

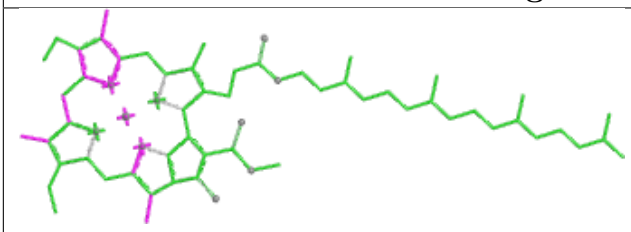


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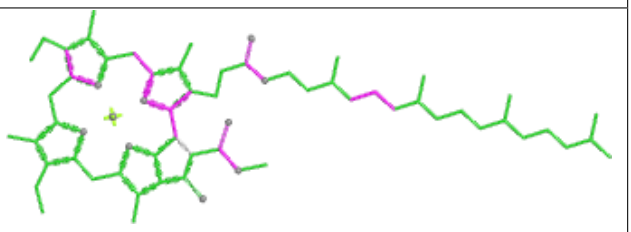


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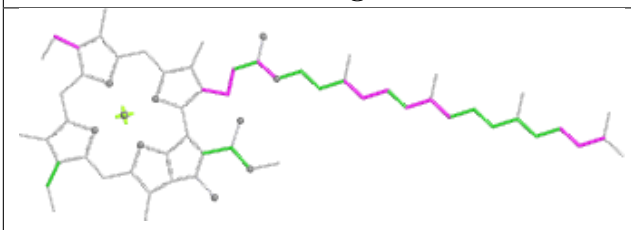
Ligand CLA F 314



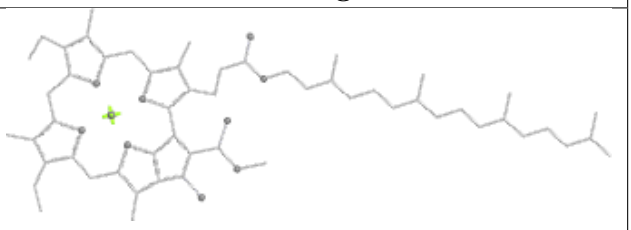
Bond lengths



Bond angles

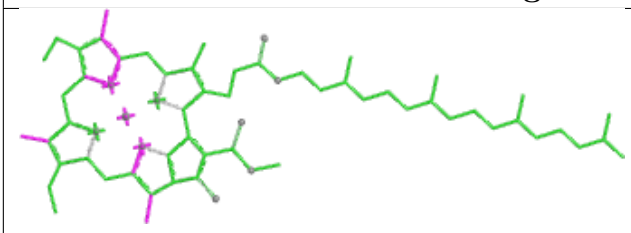


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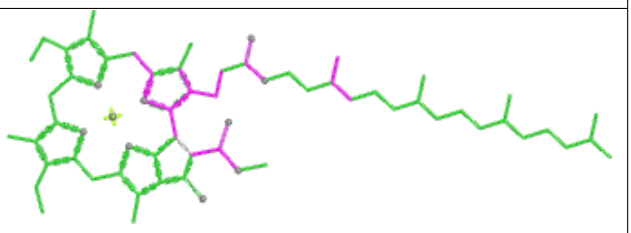


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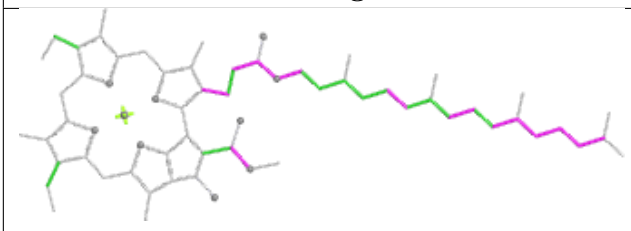
Ligand CLA H 312



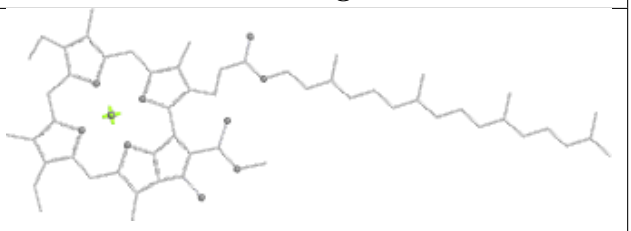
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Bond angles

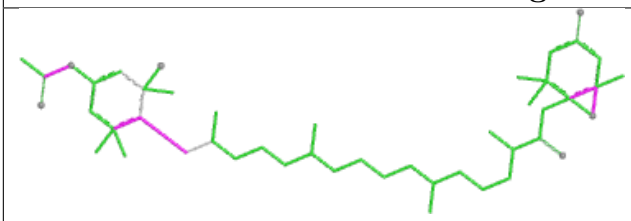


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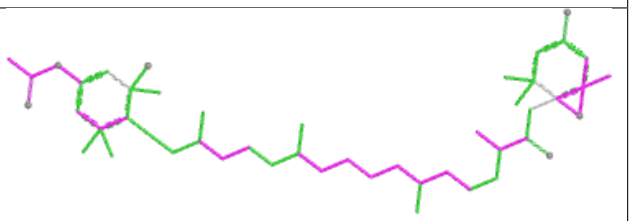


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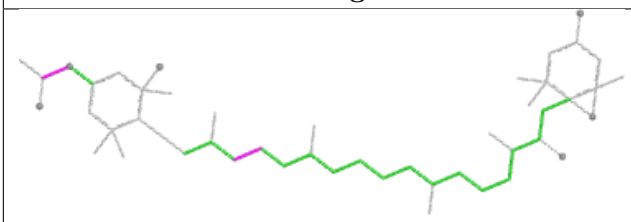
Ligand A86 X 314



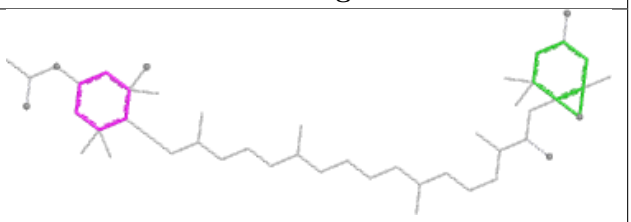
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Bond angles

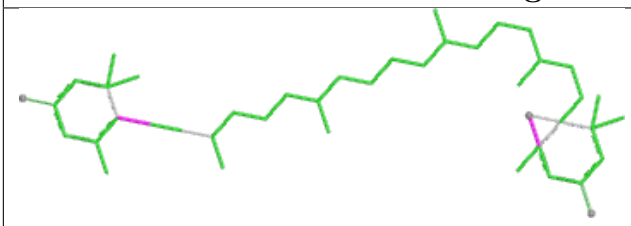


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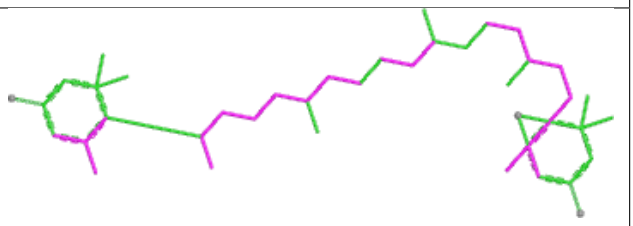


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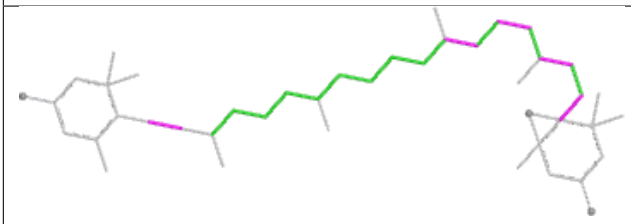
Ligand DD6 D 304



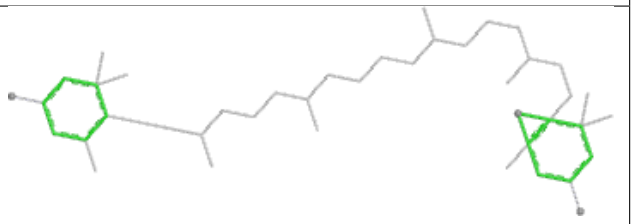
Bond lengths



Bond angles

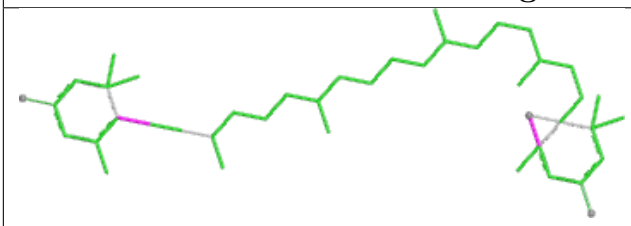


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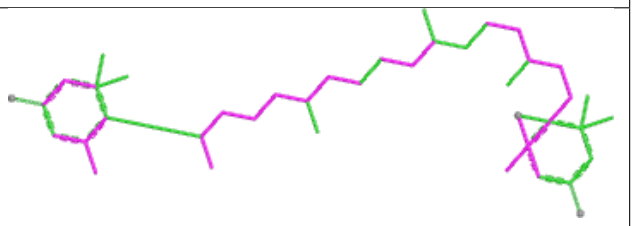


Rings

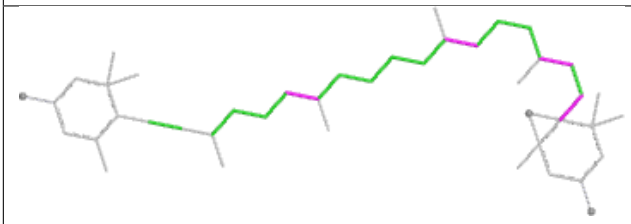
Ligand DD6 W 205



Bond lengths



Bond angles

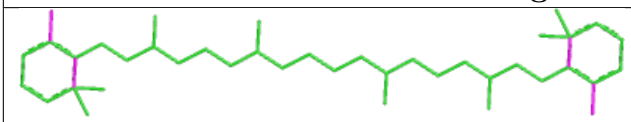


Torsions

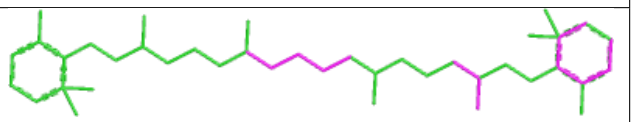


Rings

Ligand BCR i 103



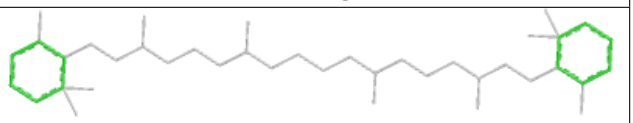
Bond lengths



Bond angles

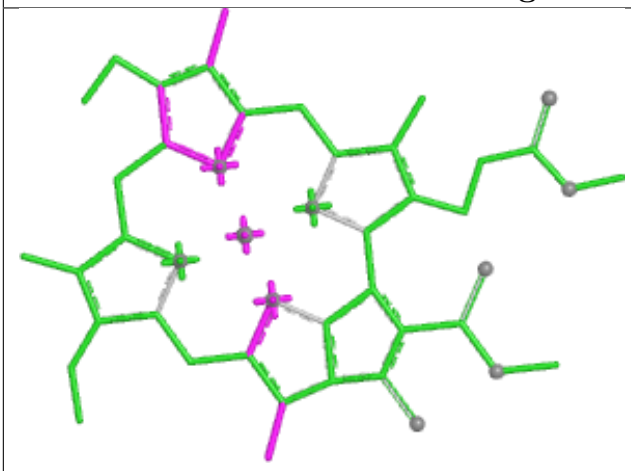


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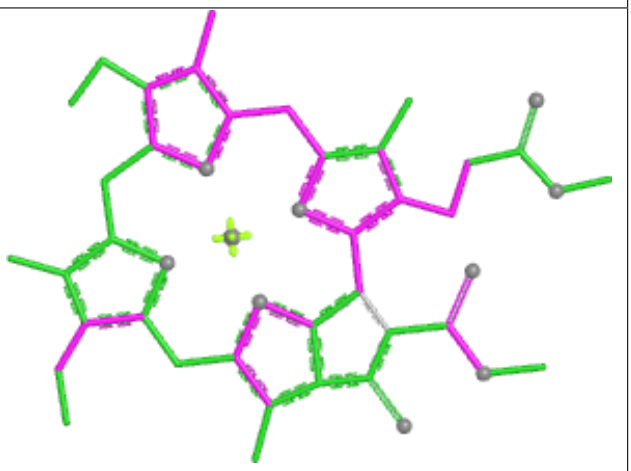


Rings

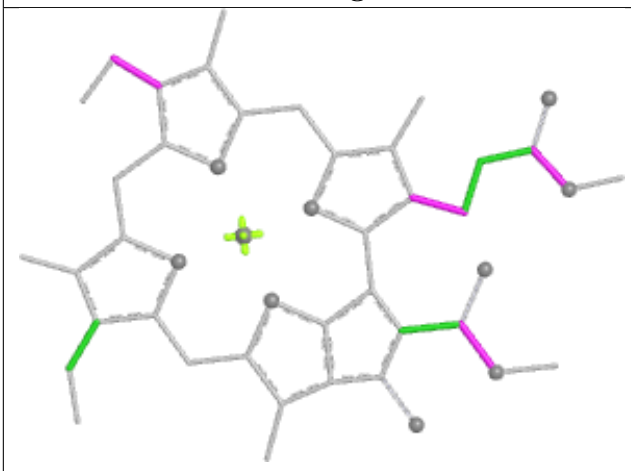
Ligand CLA W 210



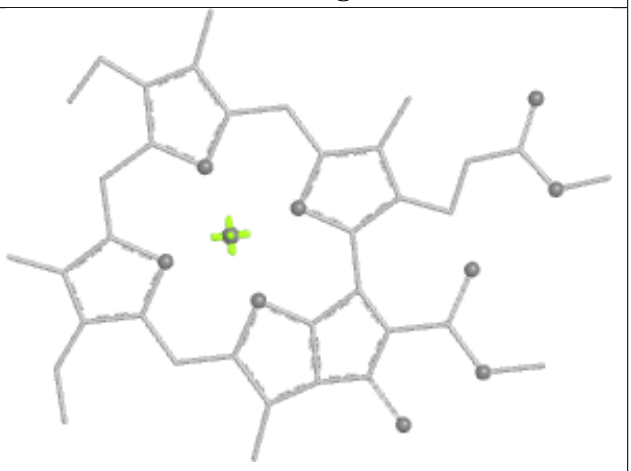
Bond lengths



Bond angles

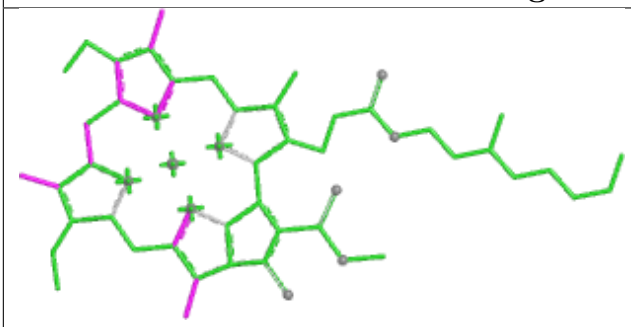


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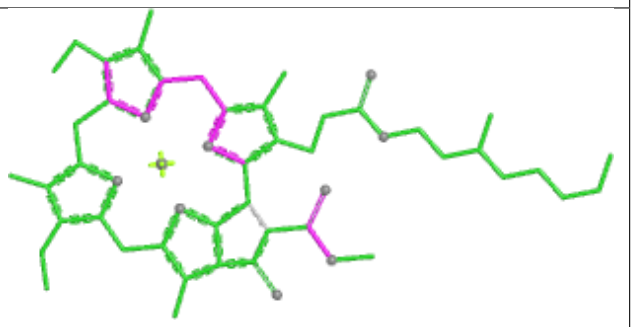


Rings

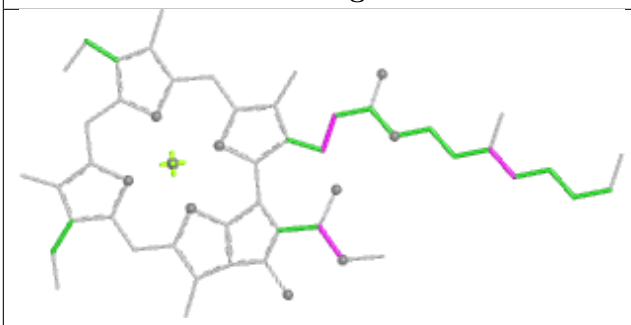
Ligand CLA a 811



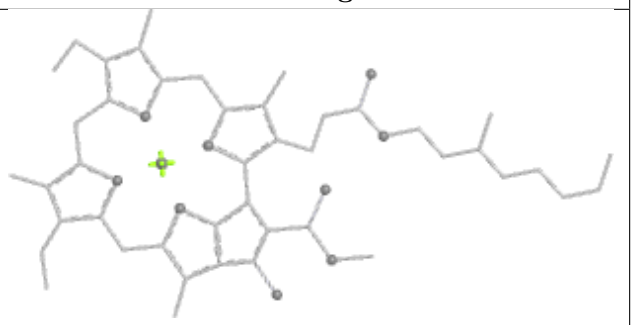
Bond lengths



Bond angles

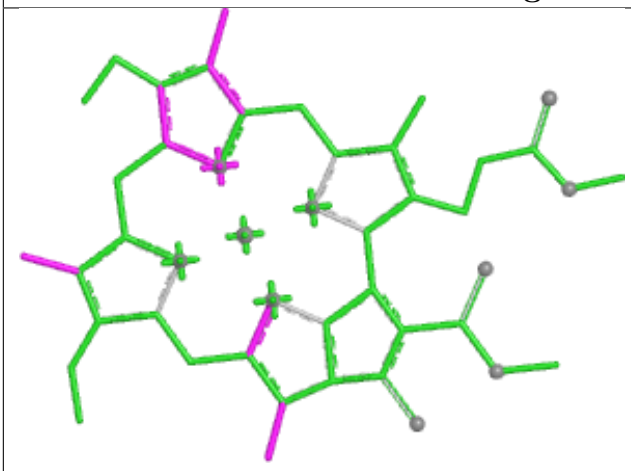


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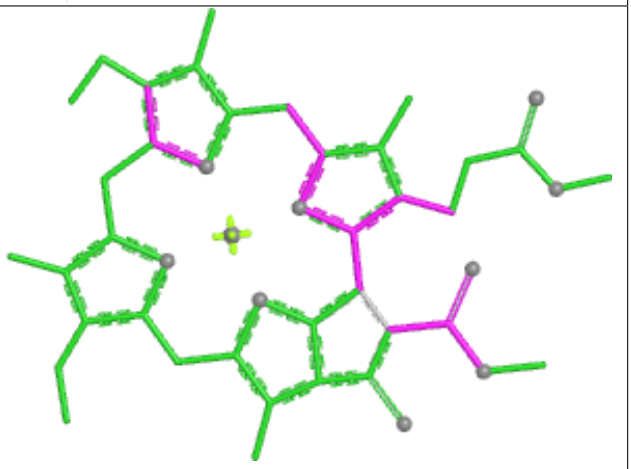


Rings

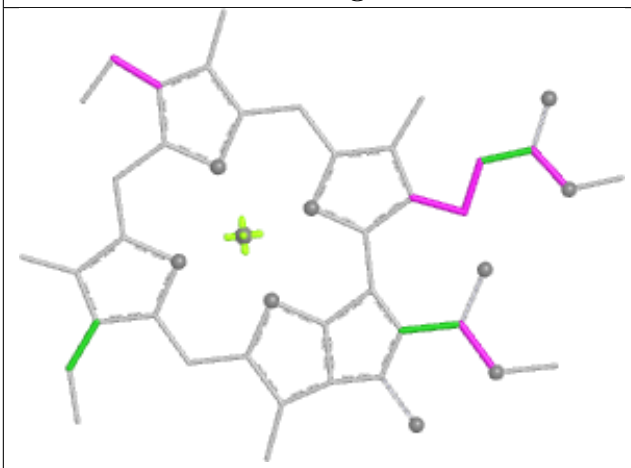
Ligand CLA Q 309



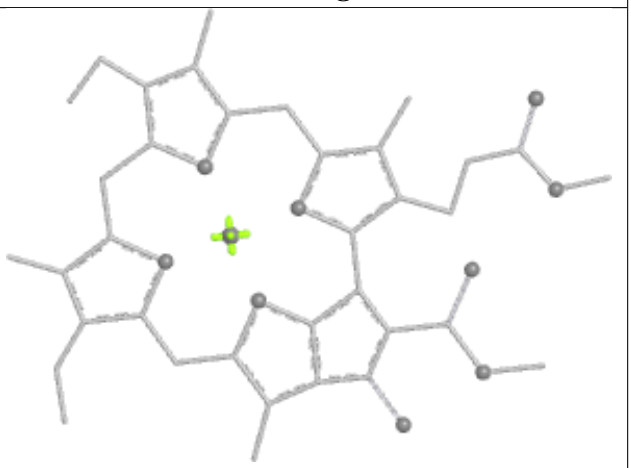
Bond lengths



Bond angles

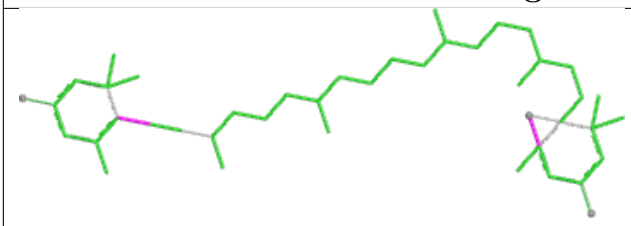


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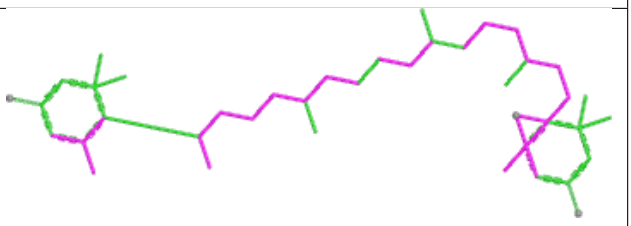


Rings

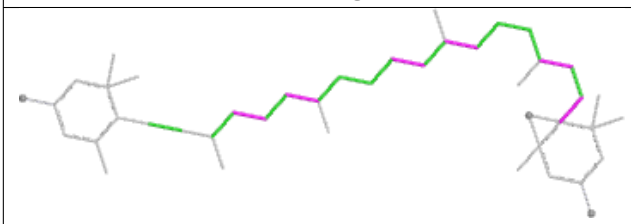
Ligand DD6 D 301



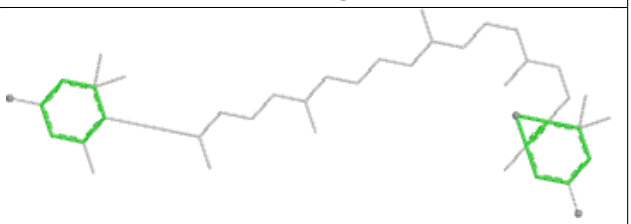
Bond lengths



Bond angles

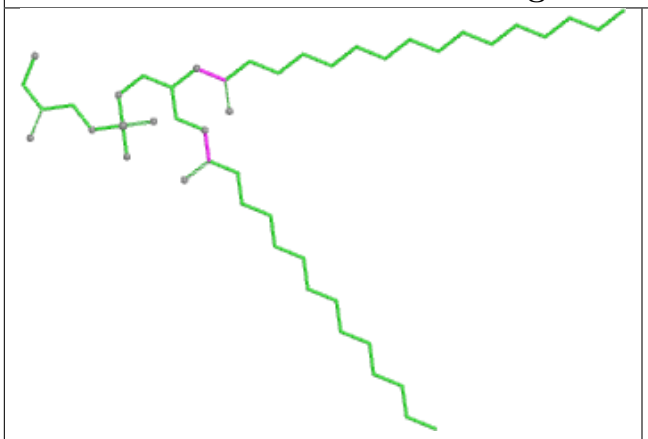


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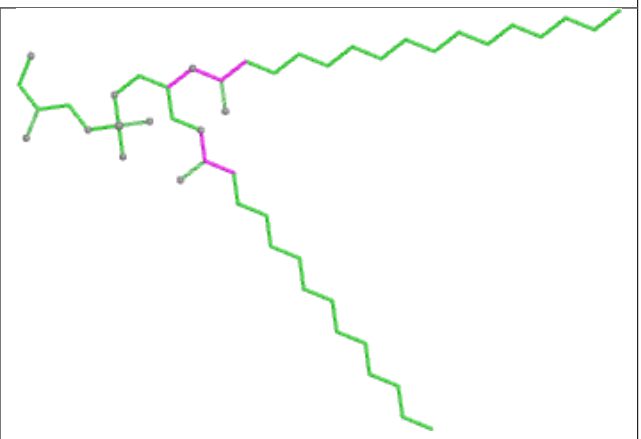


Rings

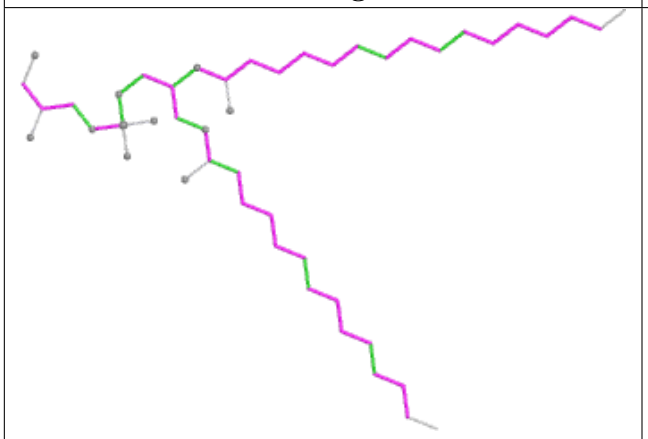
Ligand LHG a 850



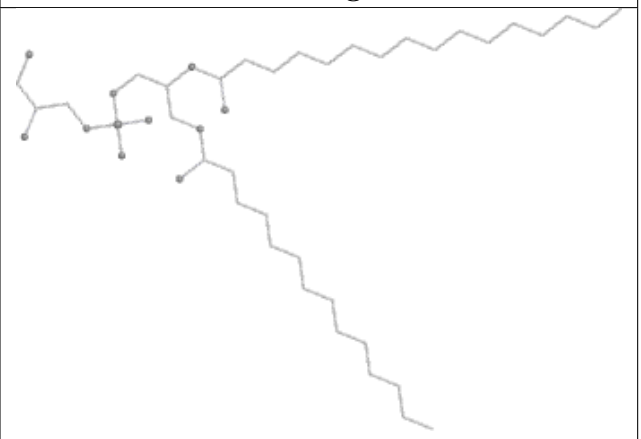
Bond lengths



Bond angles

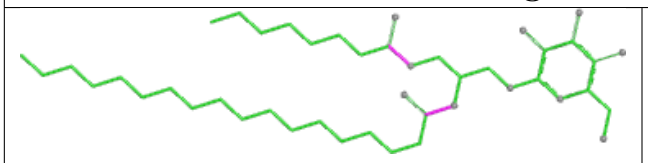


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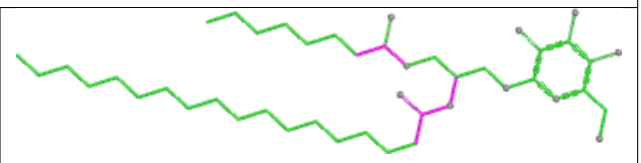


Rings

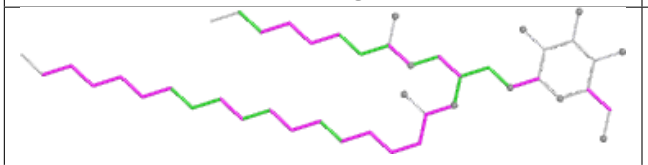
Ligand LMG h 206



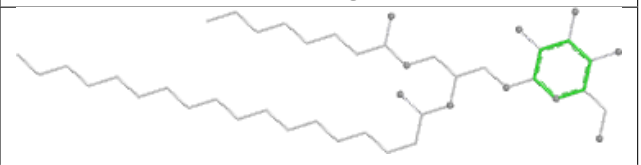
Bond lengths



Bond angles

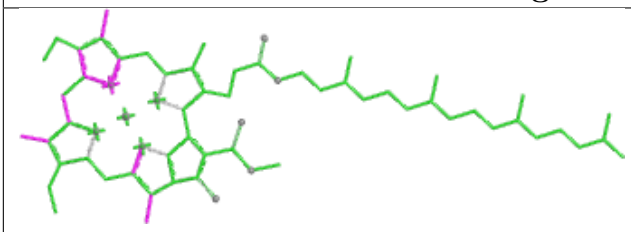


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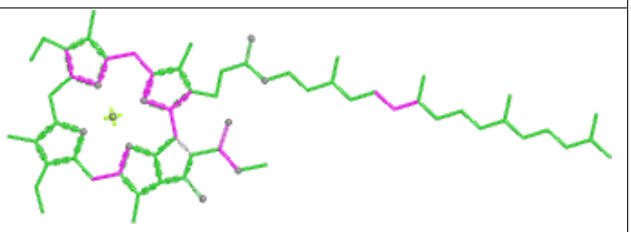


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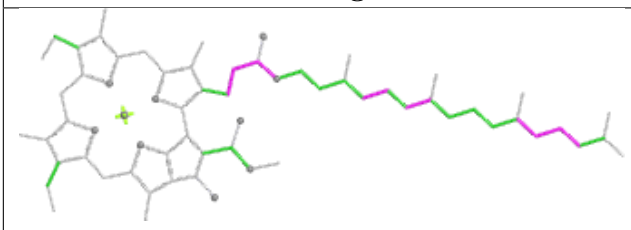
Ligand CLA f 802



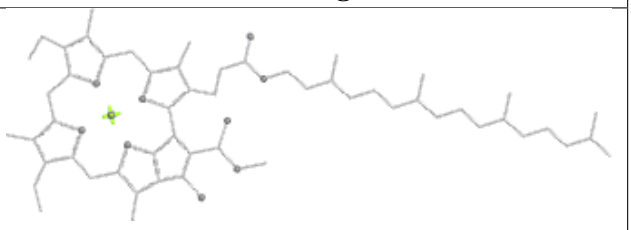
Bond lengths



Bond angles



Torsions

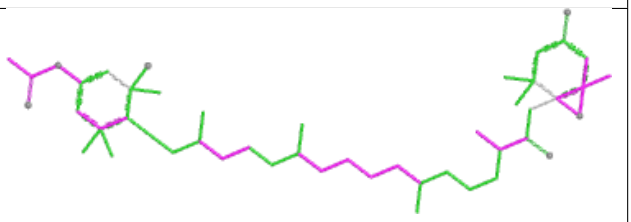


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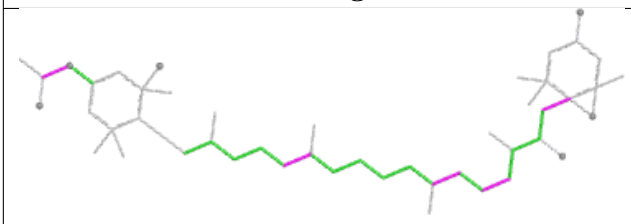
Ligand A86 L 307



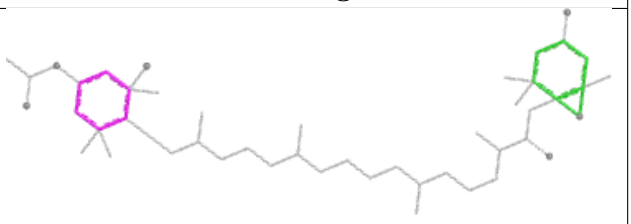
Bond lengths



Bond angles

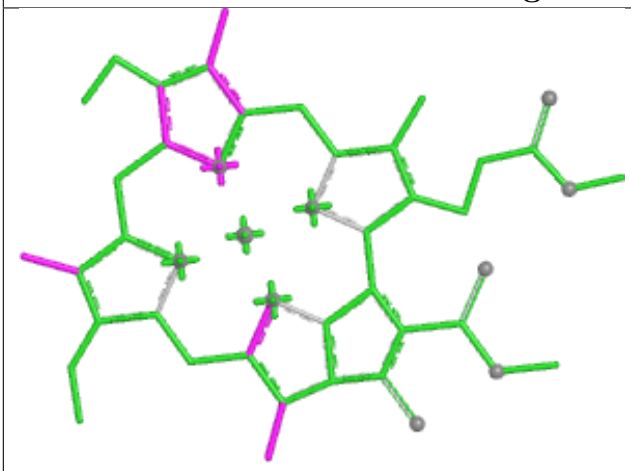


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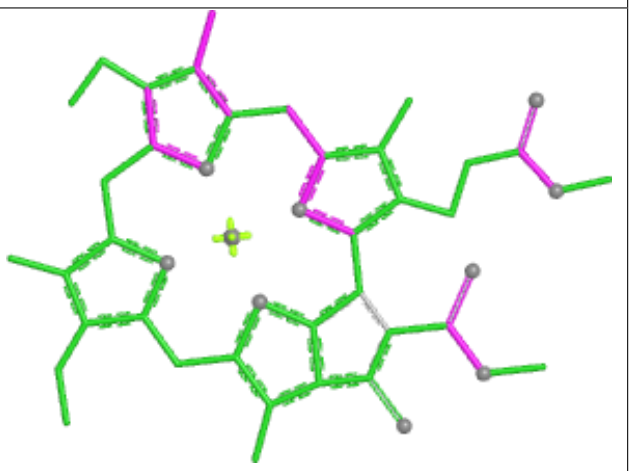


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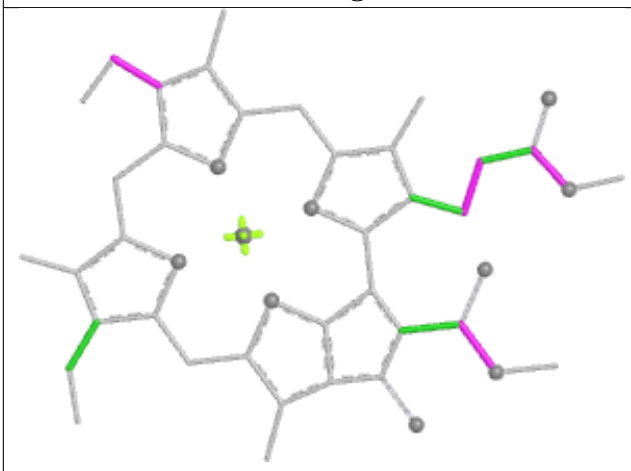
Ligand CLA D 311



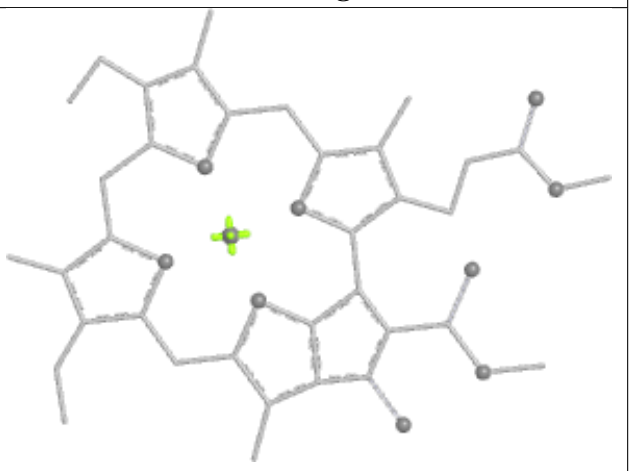
Bond lengths



Bond angles

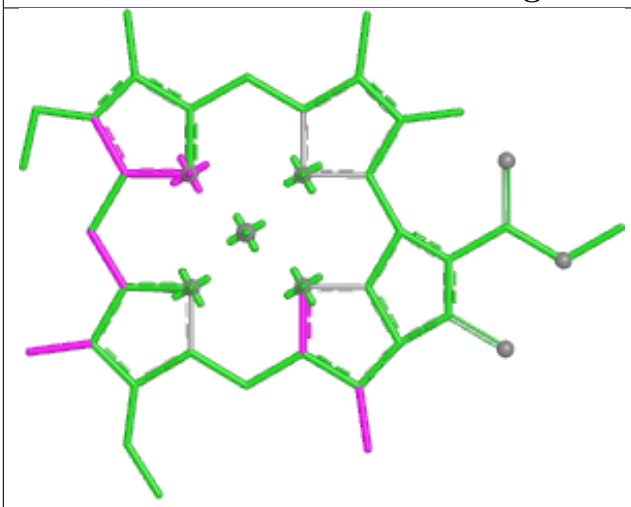


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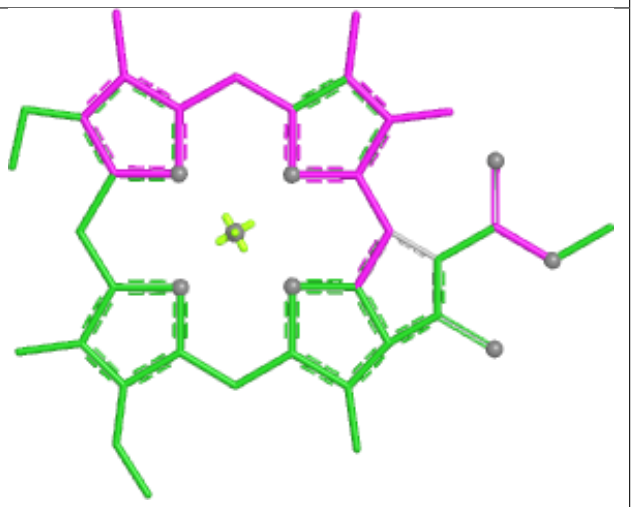


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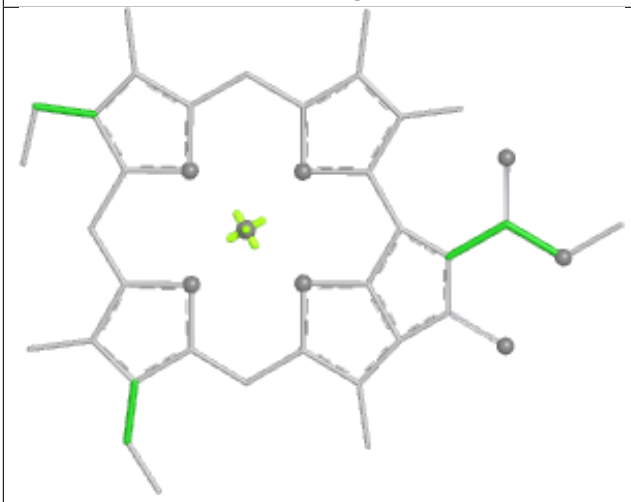
Ligand CLA N 313



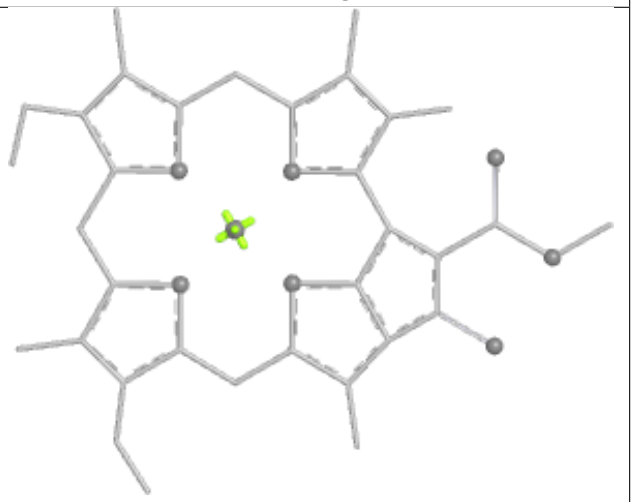
Bond lengths



Bond angles

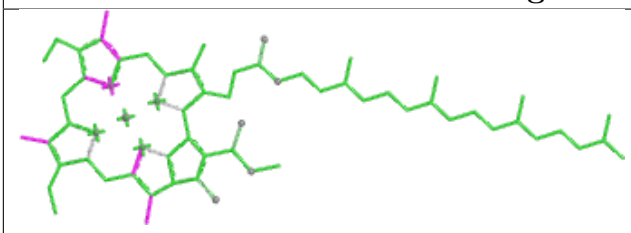


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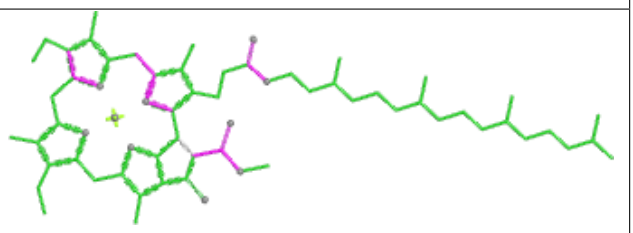


Rings

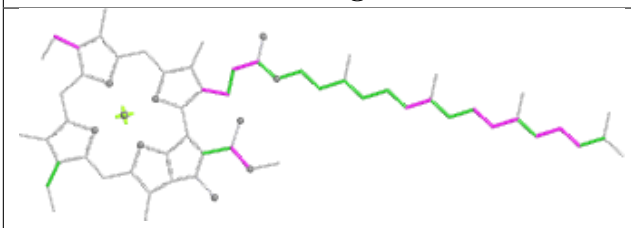
Ligand CLA b 808



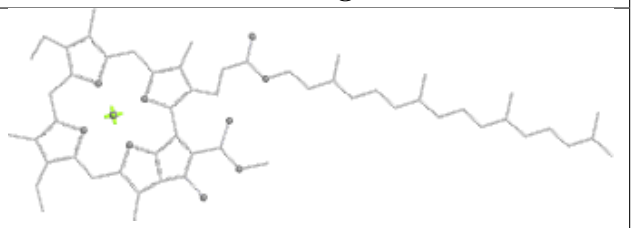
Bond lengths



Bond angles

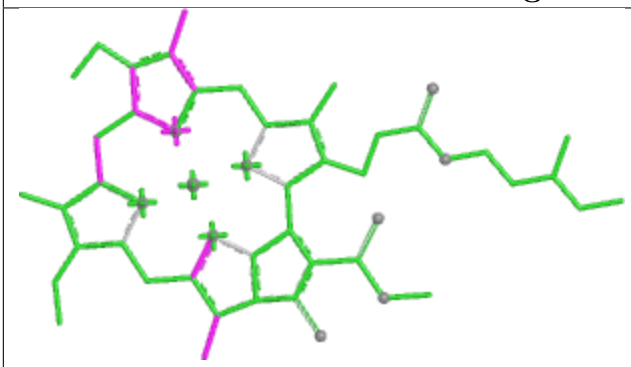


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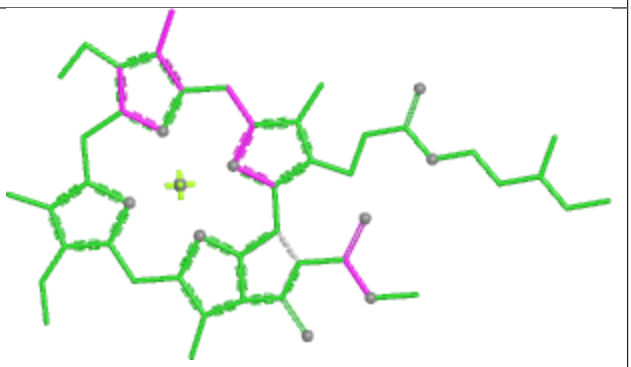


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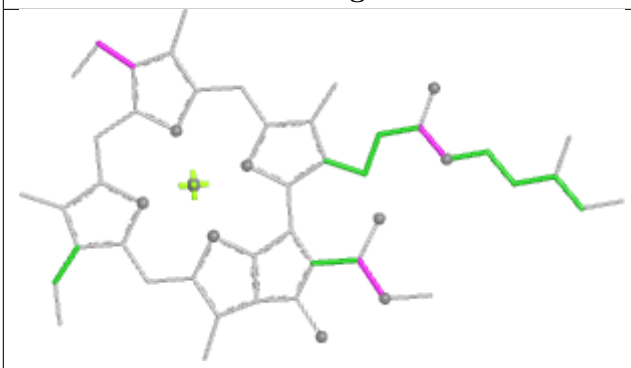
Ligand CLA V 307



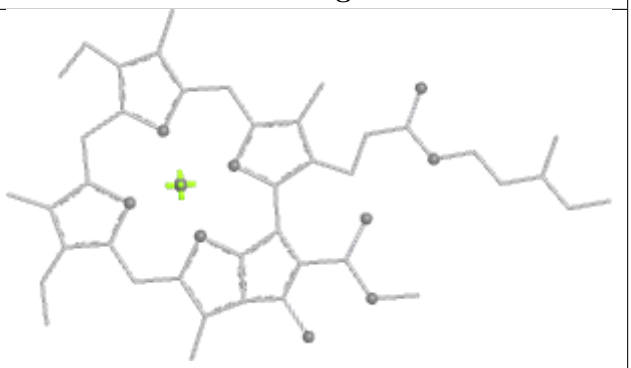
Bond lengths



Bond angles

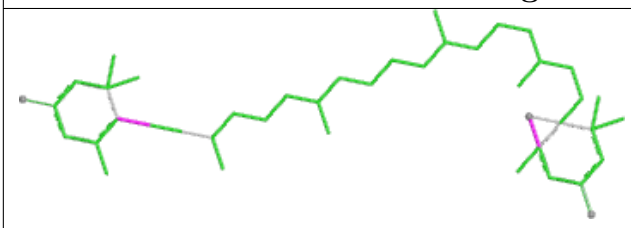


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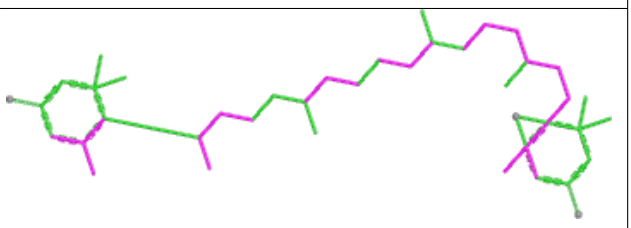


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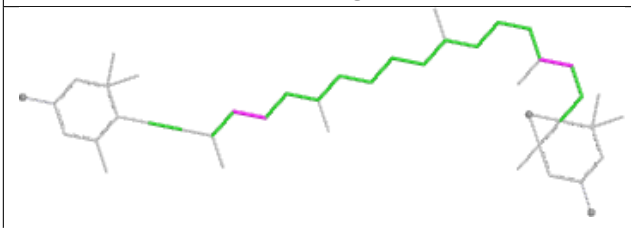
Ligand DD6 M 303



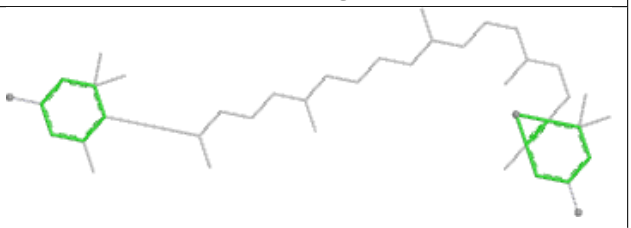
Bond lengths



Bond angles



Torsions



Rings

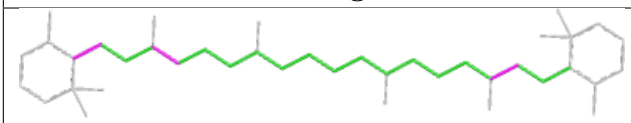
Ligand BCR b 844



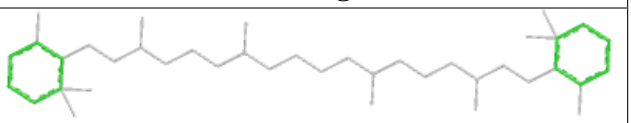
Bond lengths



Bond angles

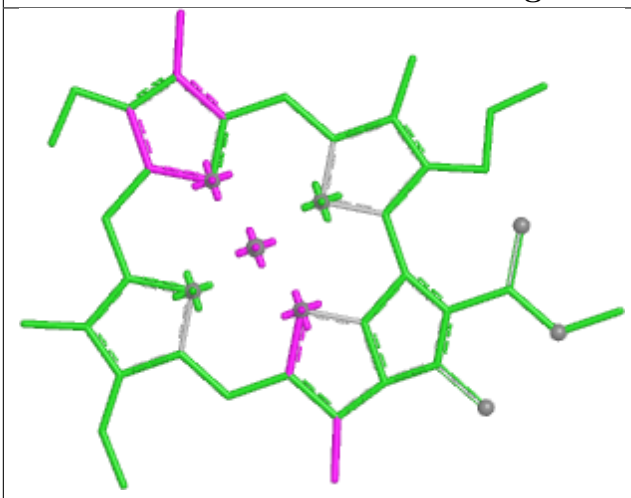


Torsions

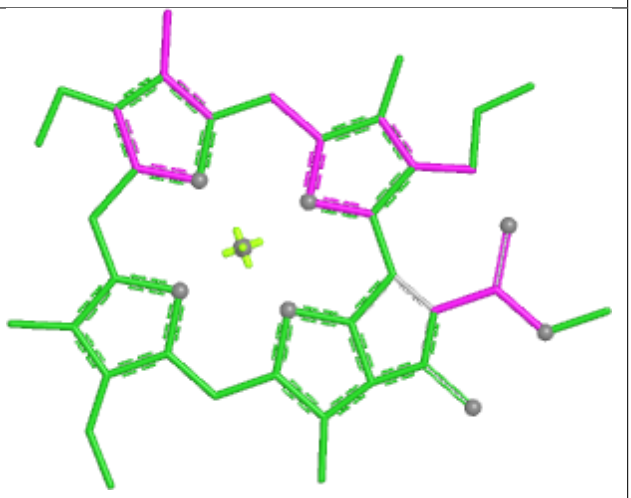


Rings

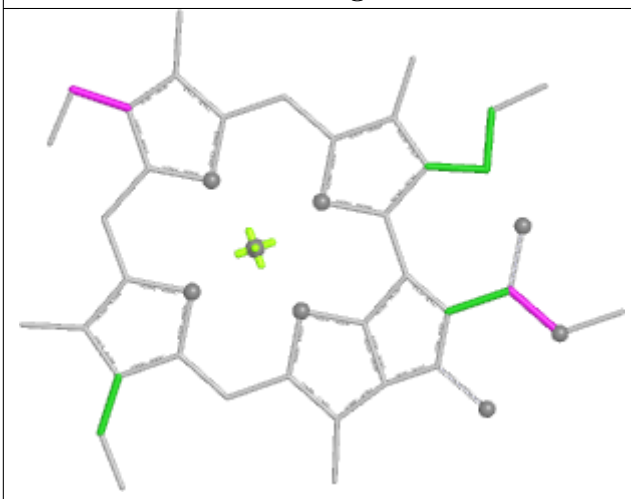
Ligand CLA C 205



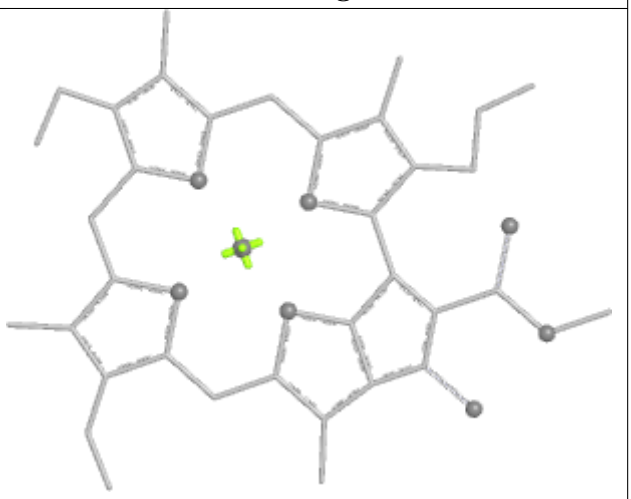
Bond lengths



Bond angles

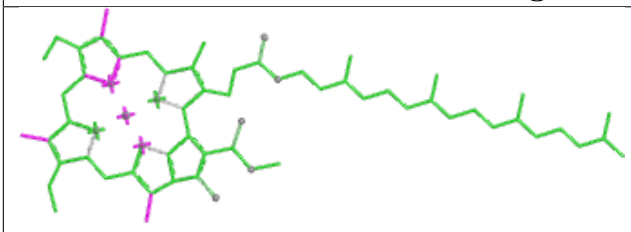


Torsions

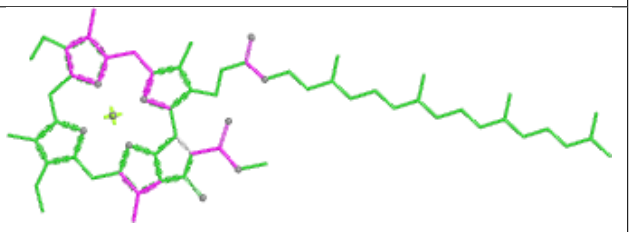


Rings

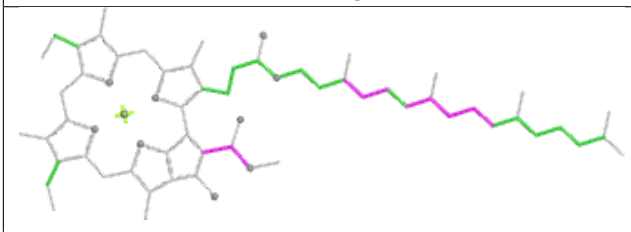
Ligand CLA a 829



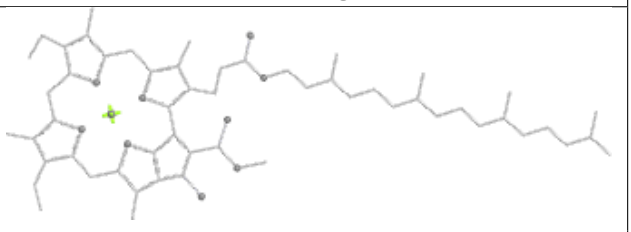
Bond lengths



Bond angles

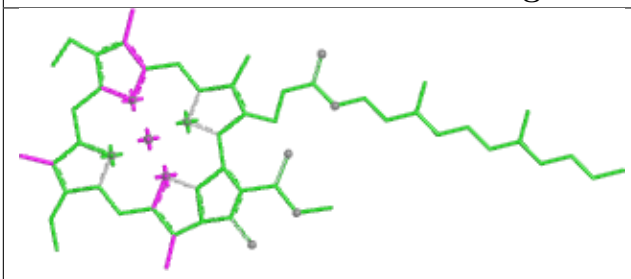


Torsions

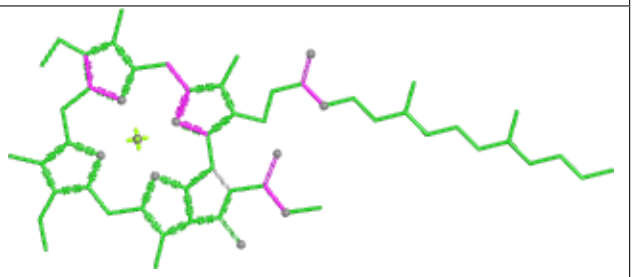


Rings

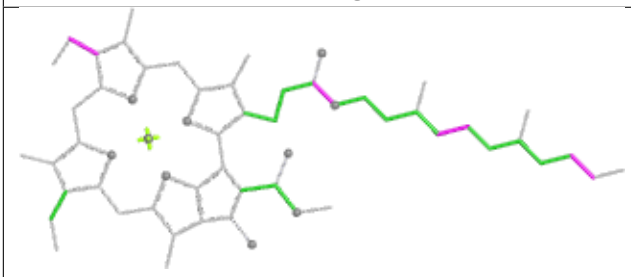
Ligand CLA G 312



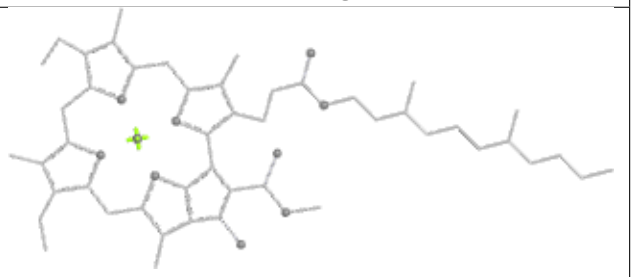
Bond lengths



Bond angles

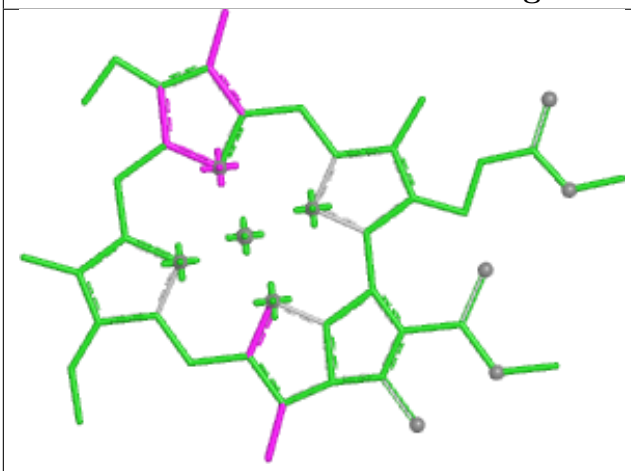


Torsions

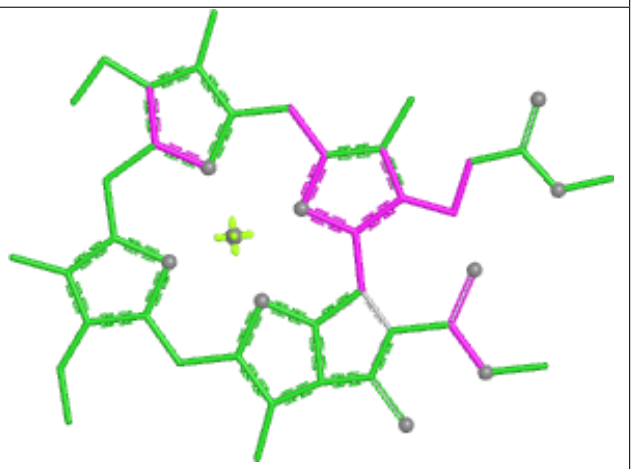


Rings

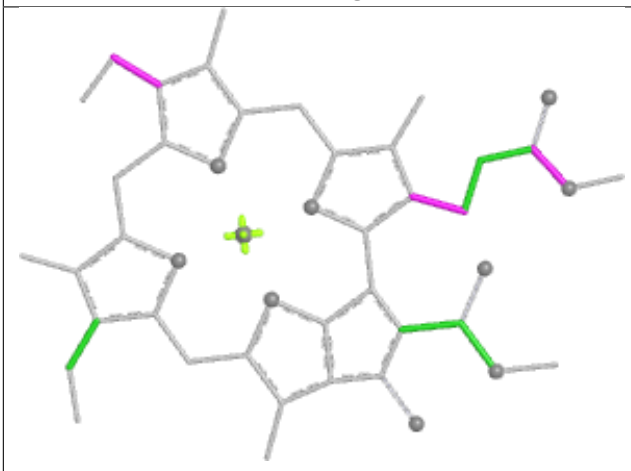
Ligand CLA U 309



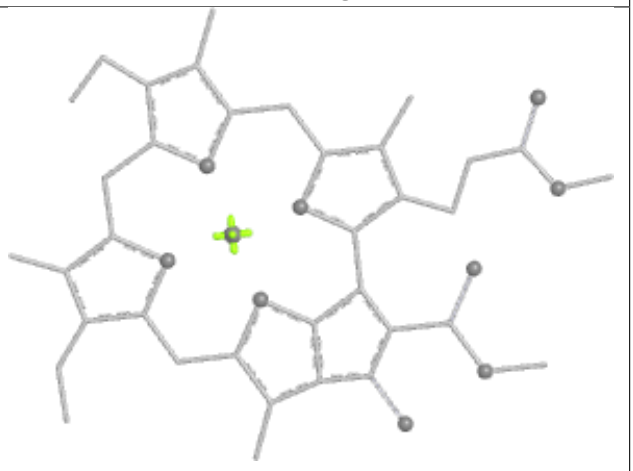
Bond lengths



Bond angles

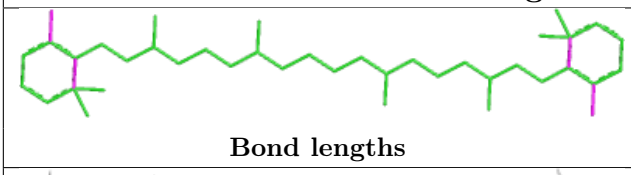


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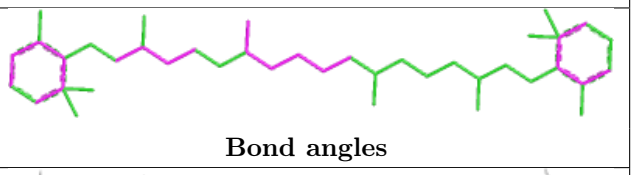


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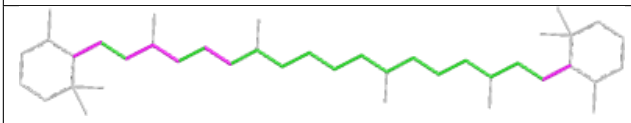
Ligand BCR b 846



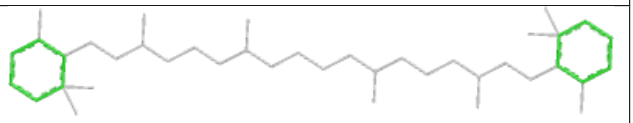
Bond lengths



Bond angles



Torsions

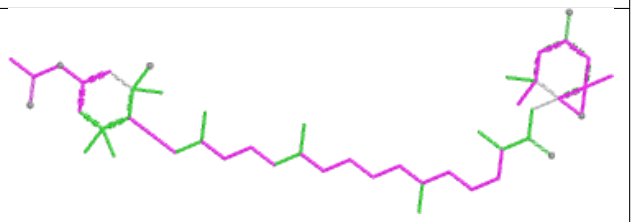


Rings

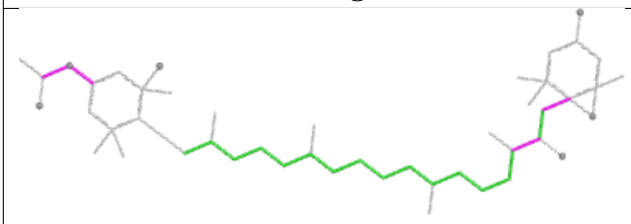
Ligand A86 K 302



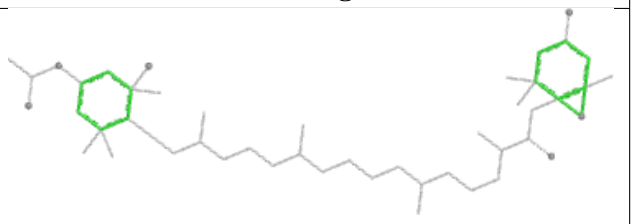
Bond lengths



Bond angles

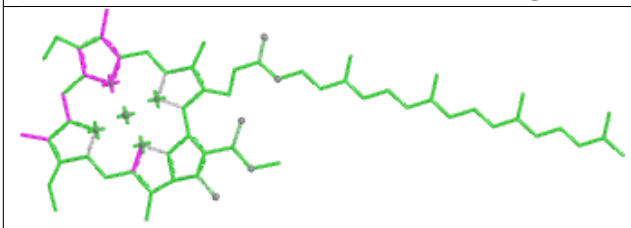


Torsions

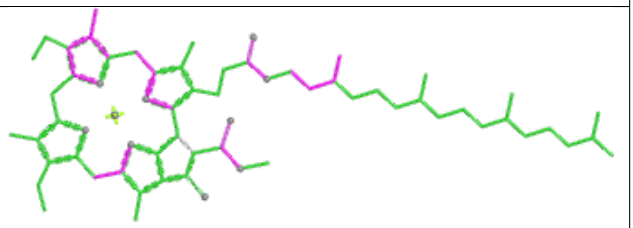


Rings

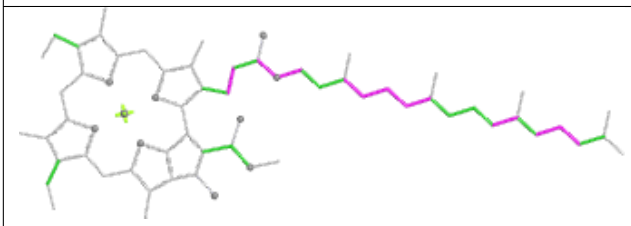
Ligand CLA F 309



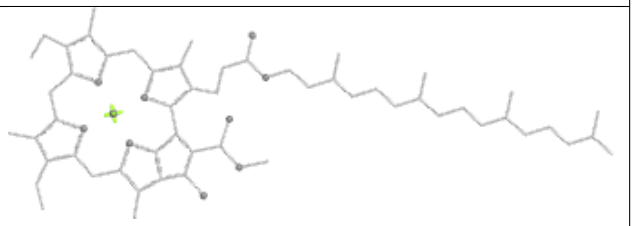
Bond lengths



Bond angles

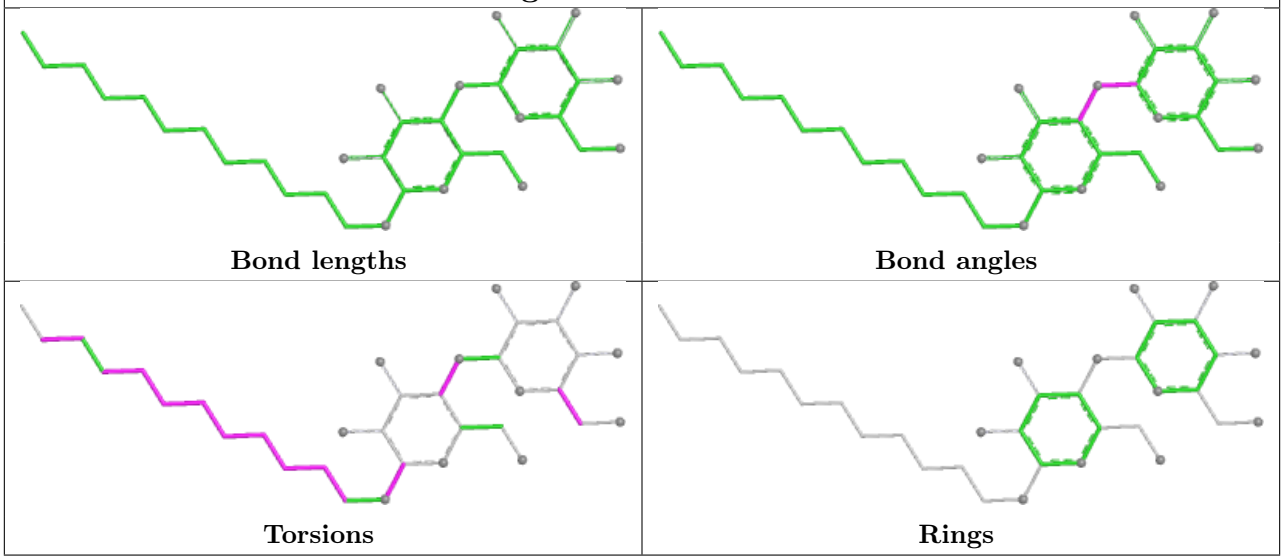


Torsions

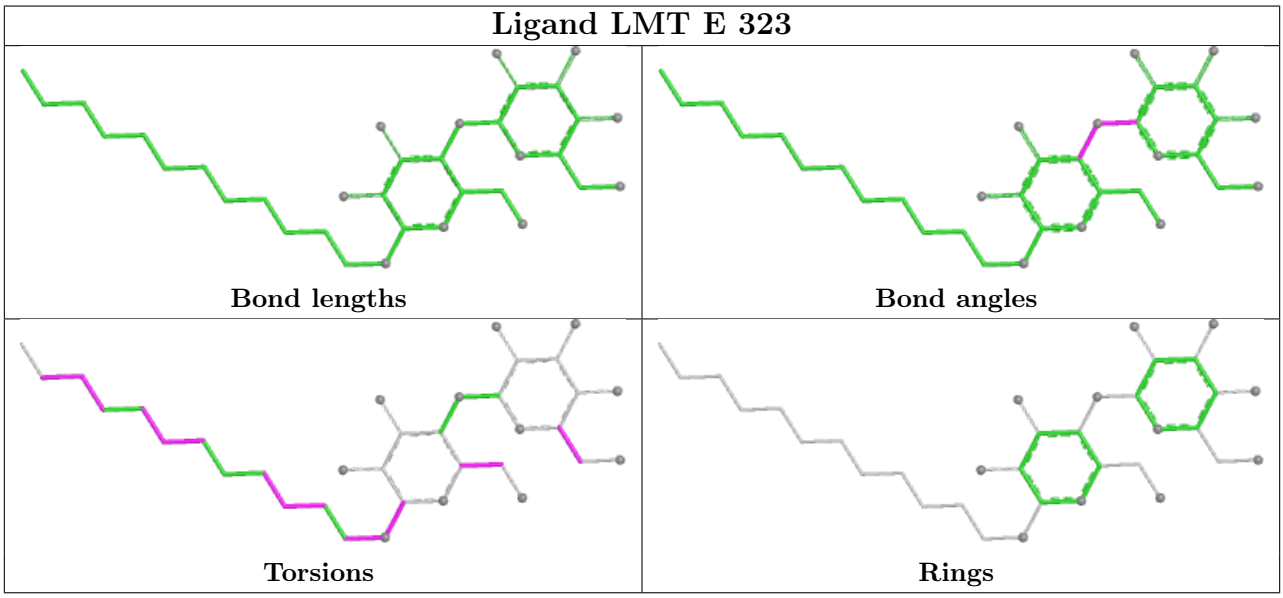


Rings

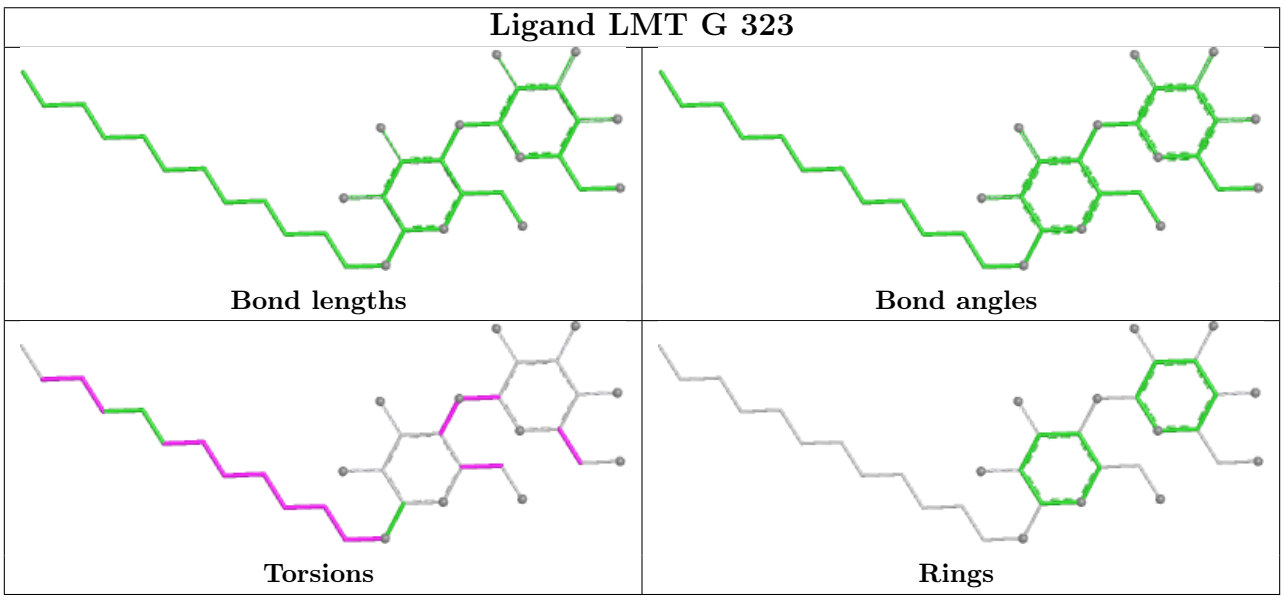
Ligand LMT U 314



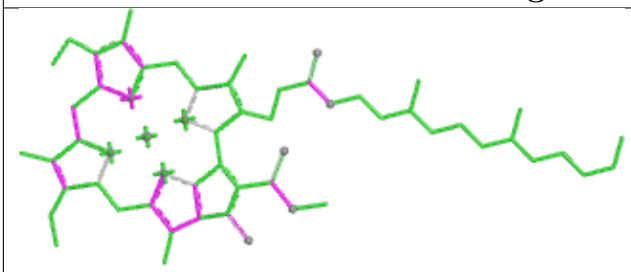
Ligand LMT E 323



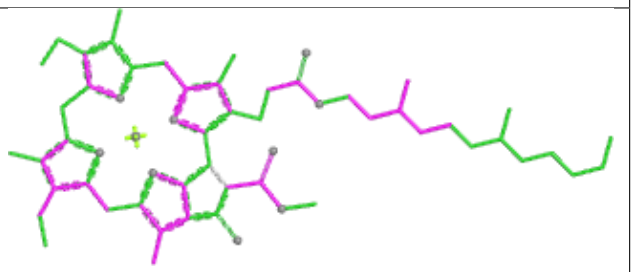
Ligand LMT G 323



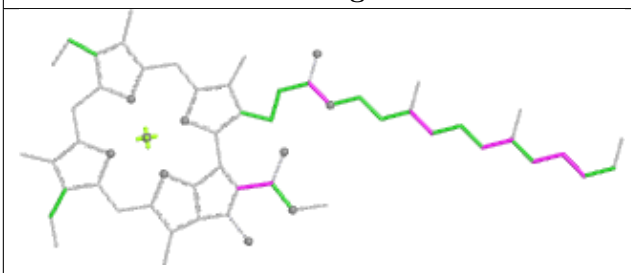
Ligand CLA b 817



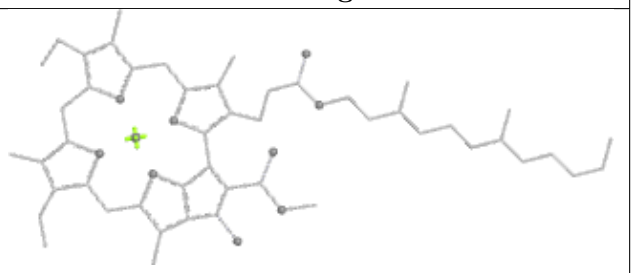
Bond lengths



Bond angles

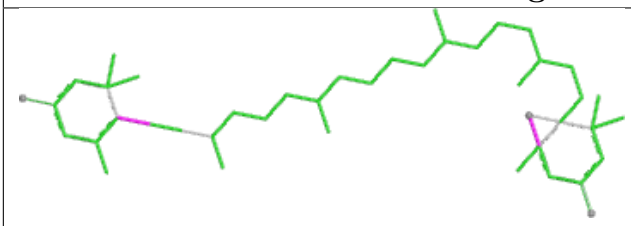


Torsions

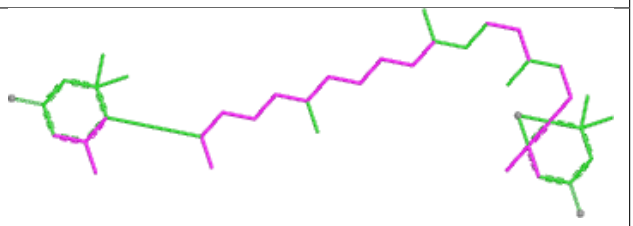


Rings

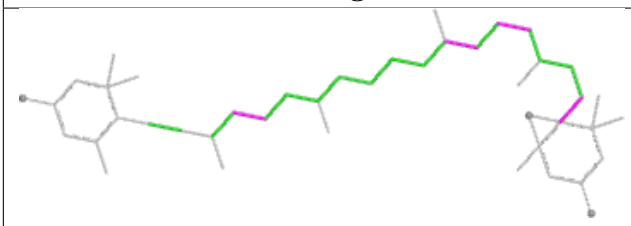
Ligand DD6 S 306



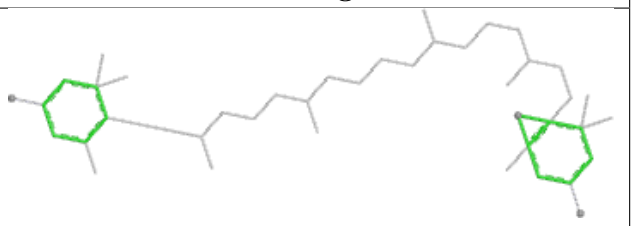
Bond lengths



Bond angles

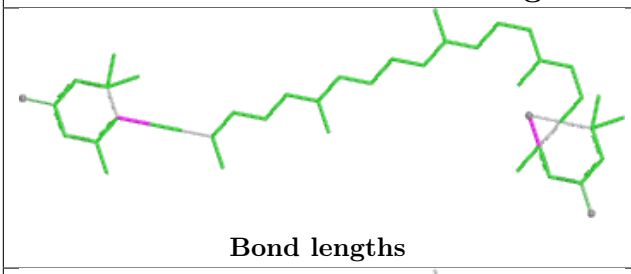


Torsions

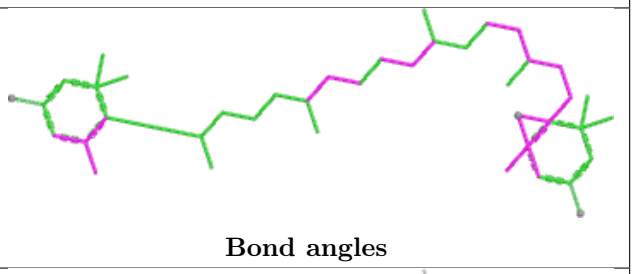


Rings

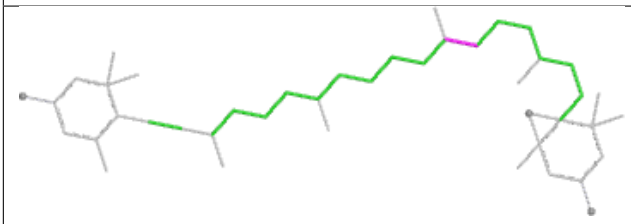
Ligand DD6 K 304



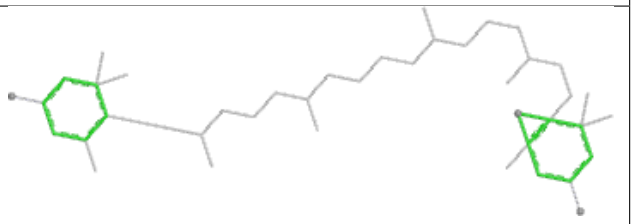
Bond lengths



Bond angles

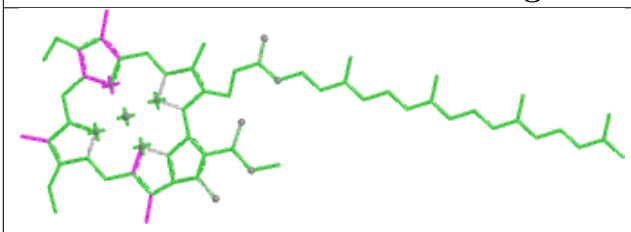


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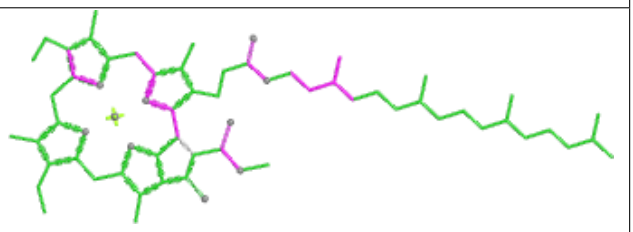


Rings

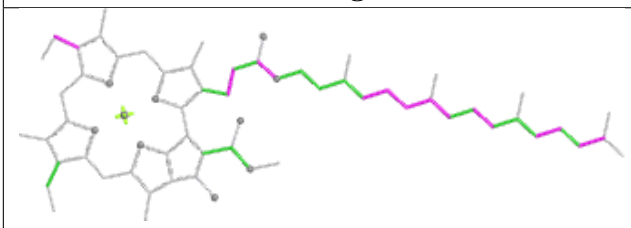
Ligand CLA O 308



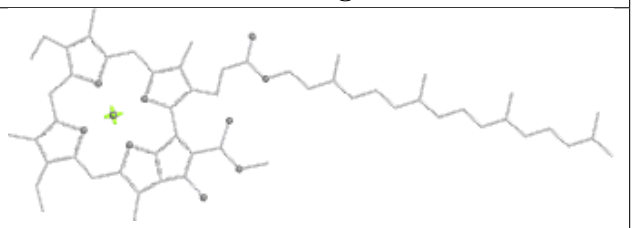
Bond lengths



Bond angles

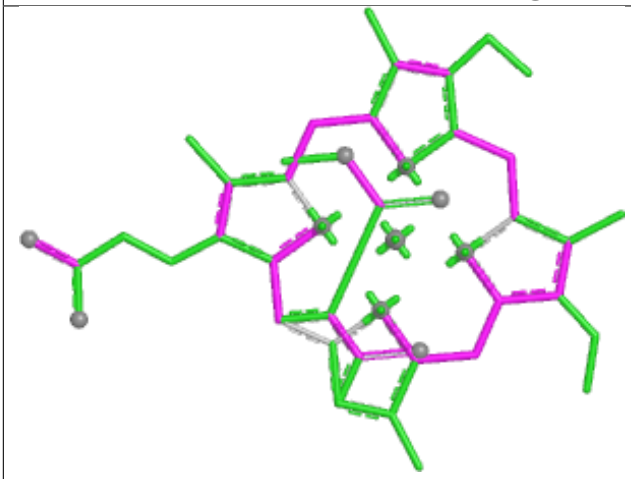


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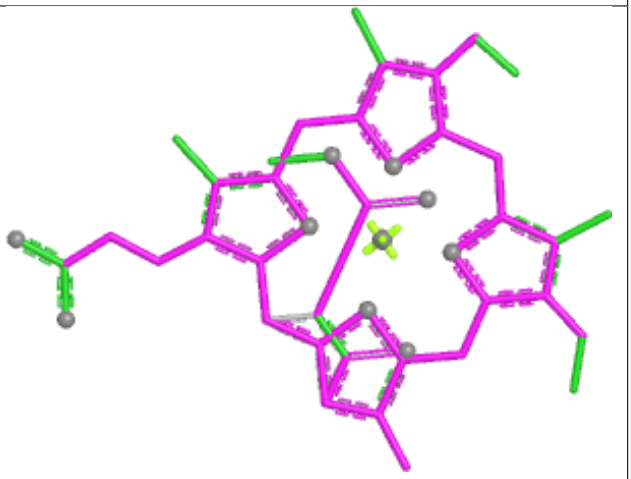


Rings

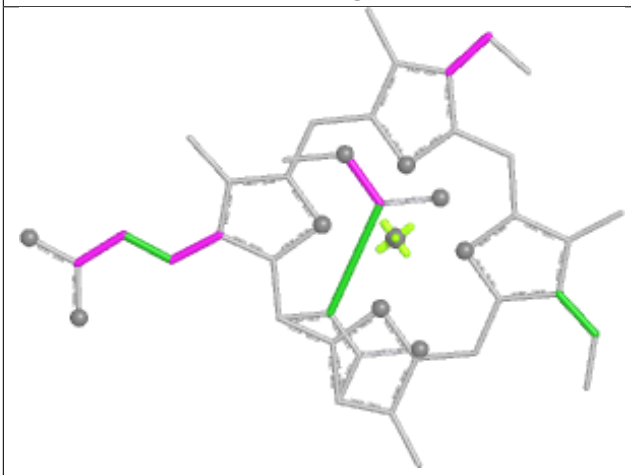
Ligand KC1 T 315



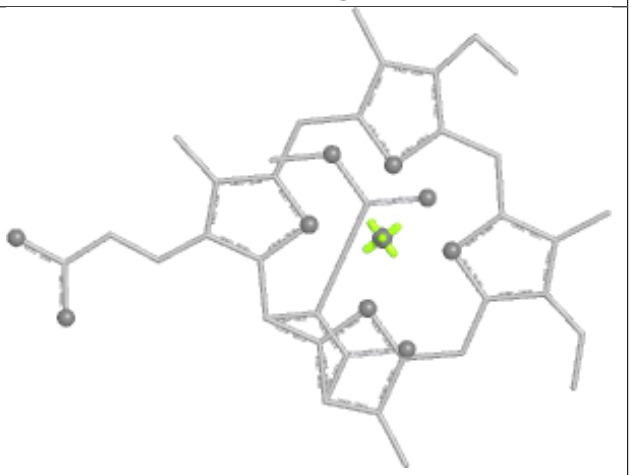
Bond lengths



Bond angles

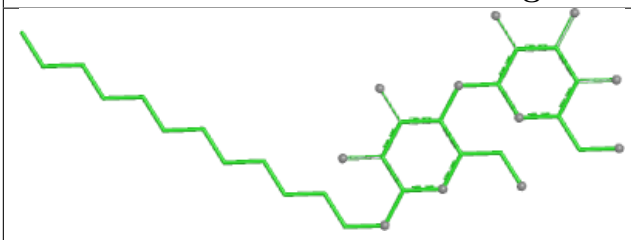


Torsions

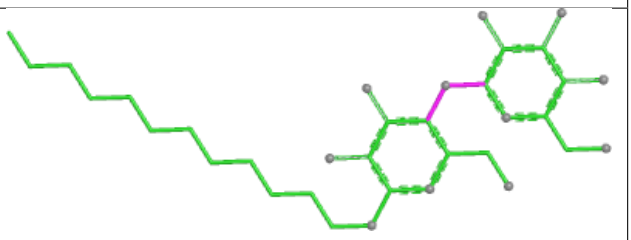


Rings

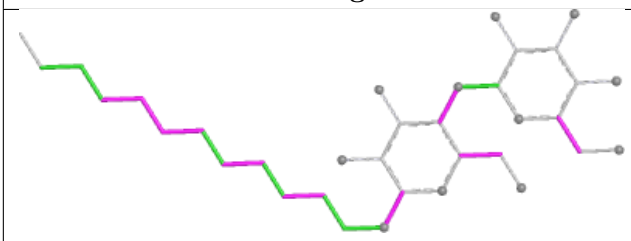
Ligand LMT F 320



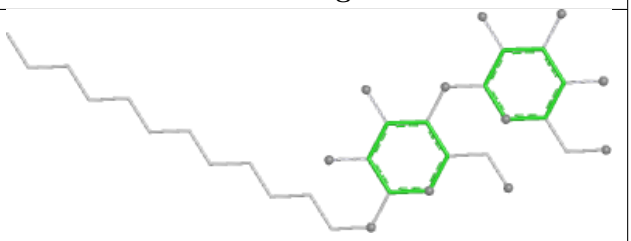
Bond lengths



Bond angles

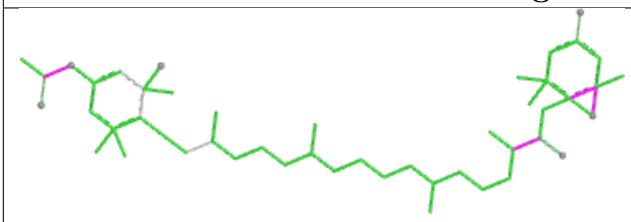


Torsions

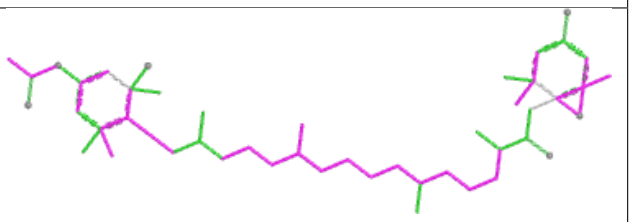


Rings

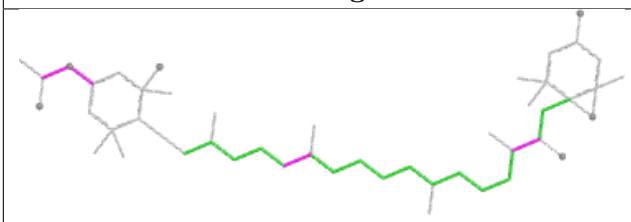
Ligand A86 L 306



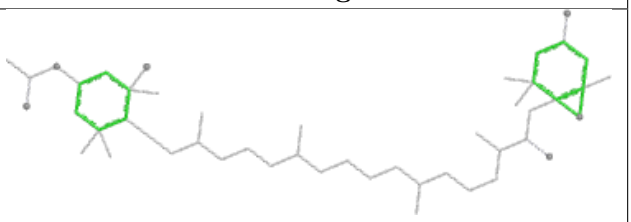
Bond lengths



Bond angles

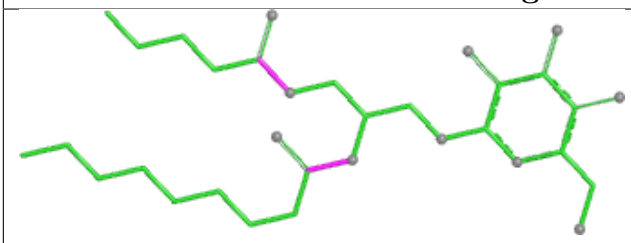


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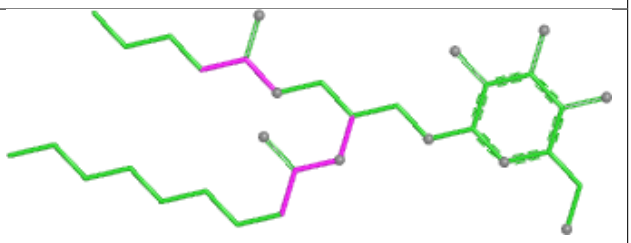


Rings

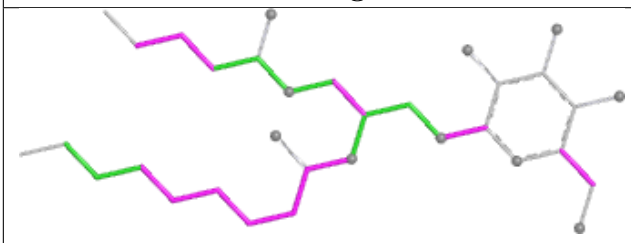
Ligand LMG L 321



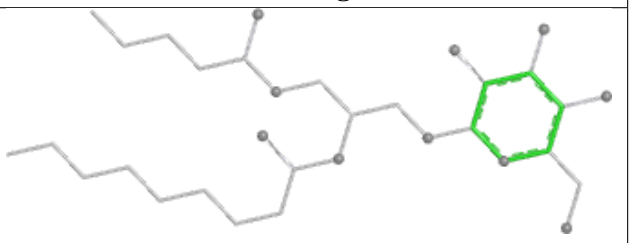
Bond lengths



Bond angles

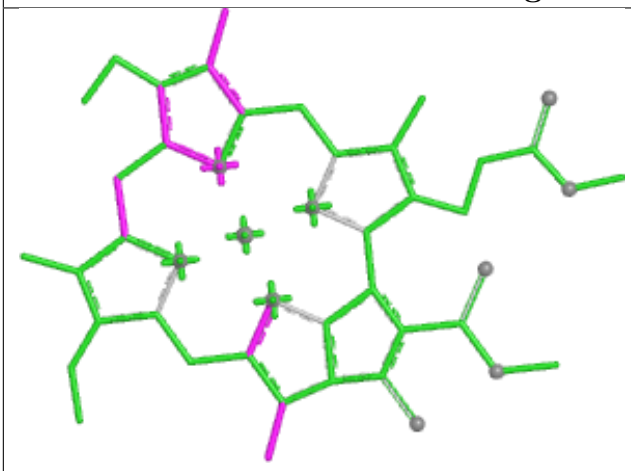


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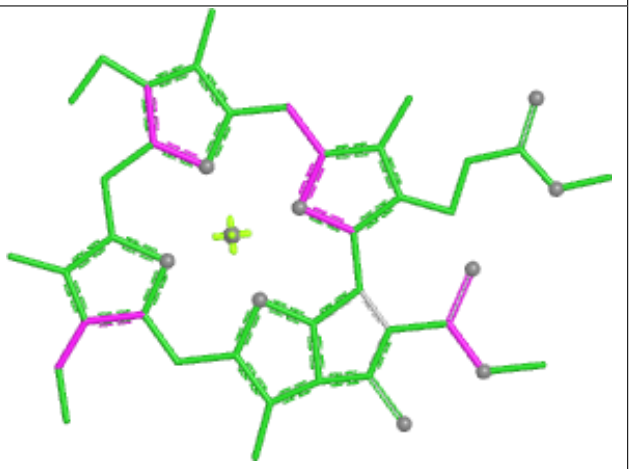


Rings

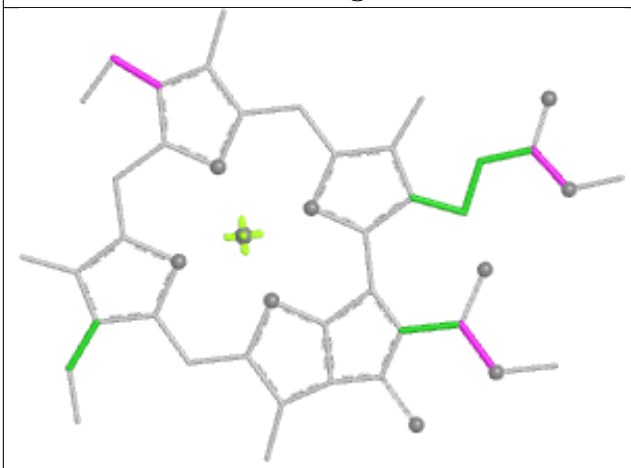
Ligand CLA B 306



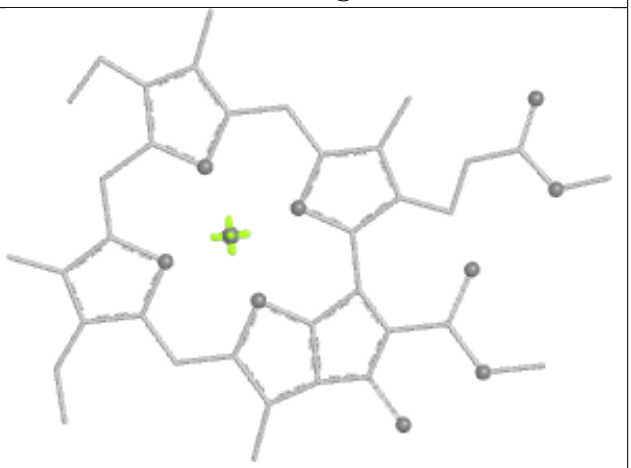
Bond lengths



Bond angles

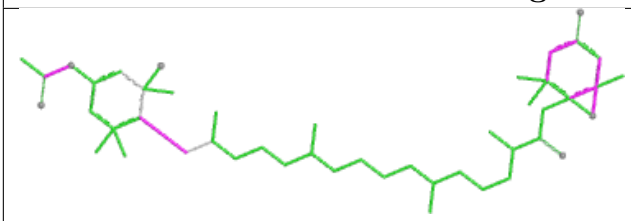


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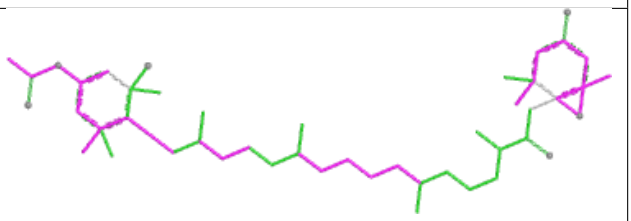


Rings

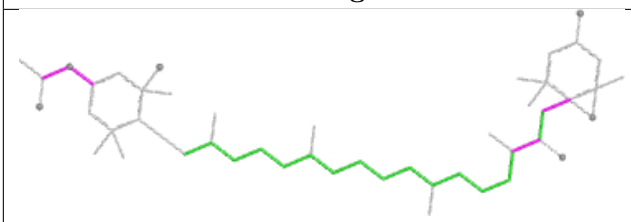
Ligand A86 V 304



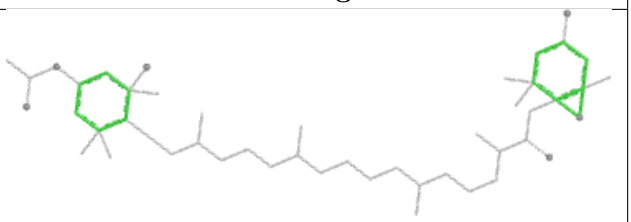
Bond lengths



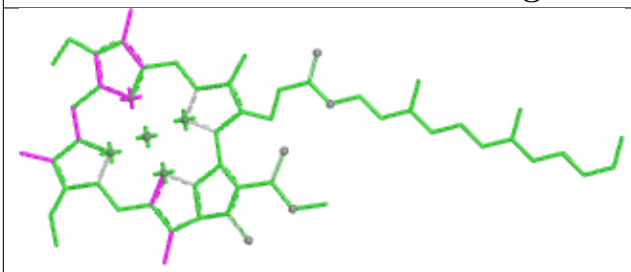
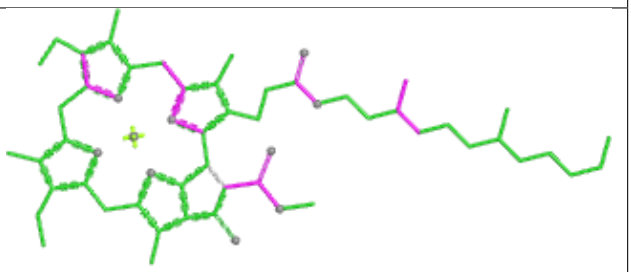
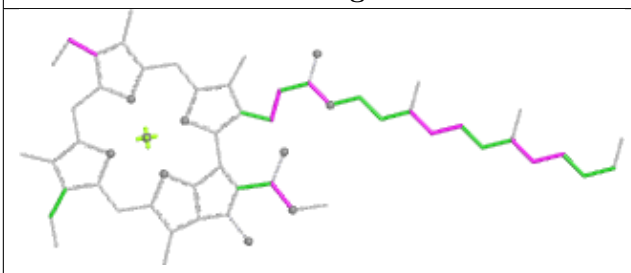
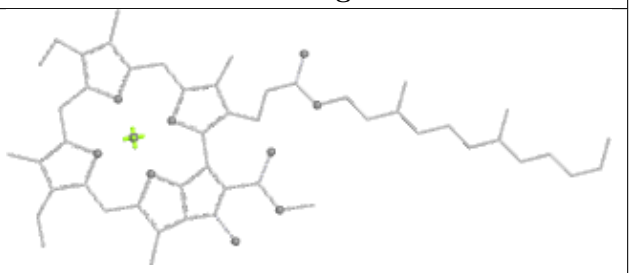
Bond angles

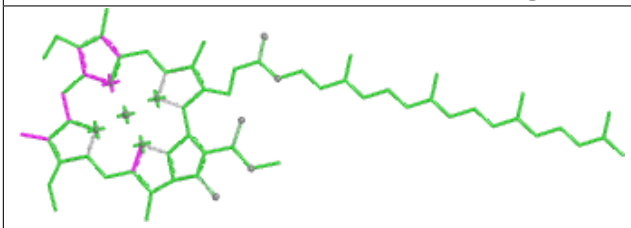
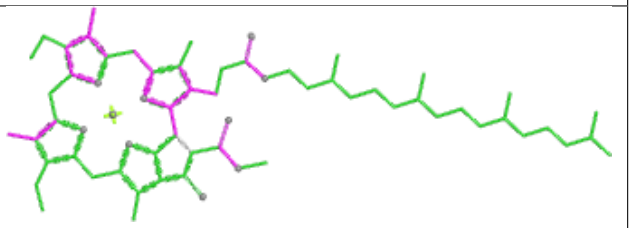
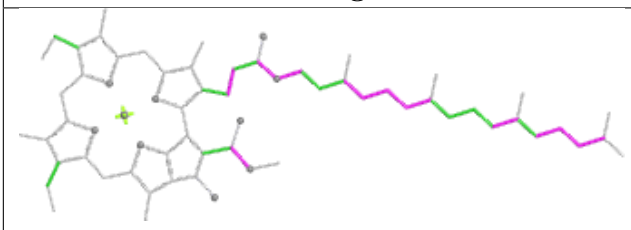
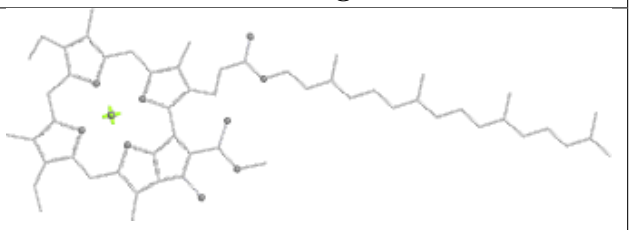


Torsions

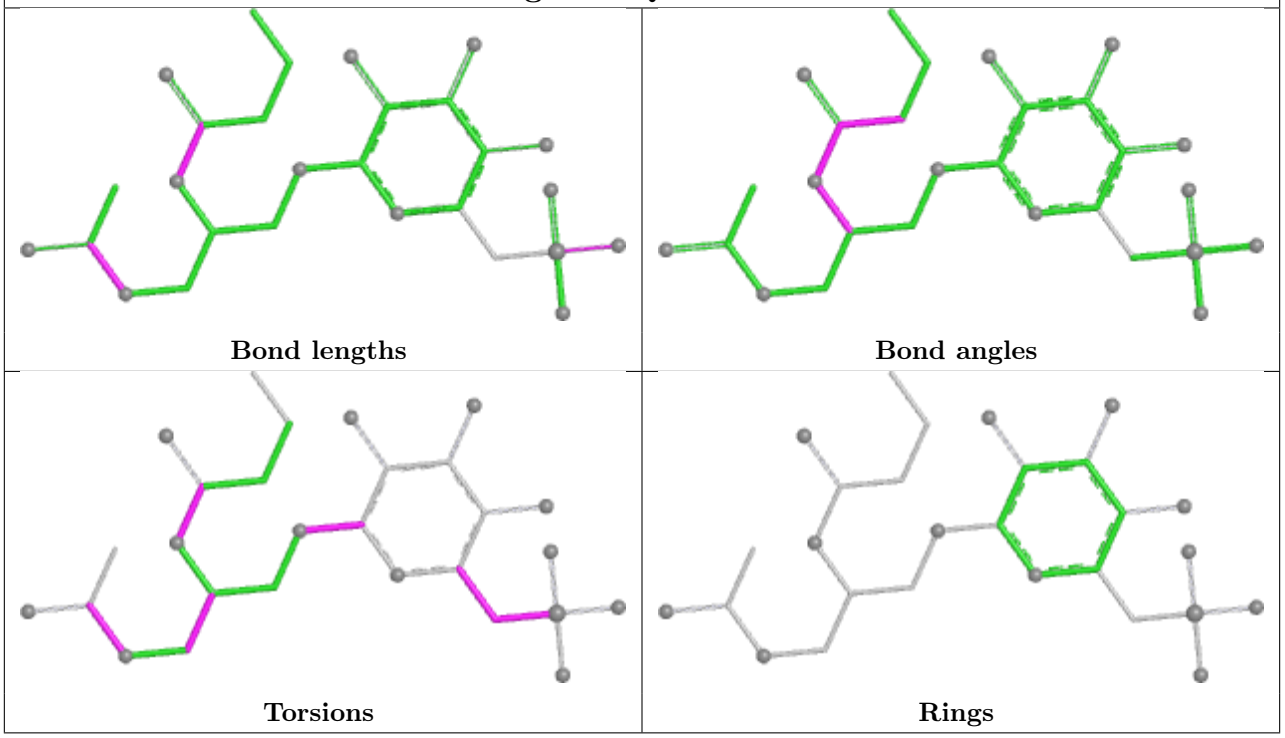


Rings

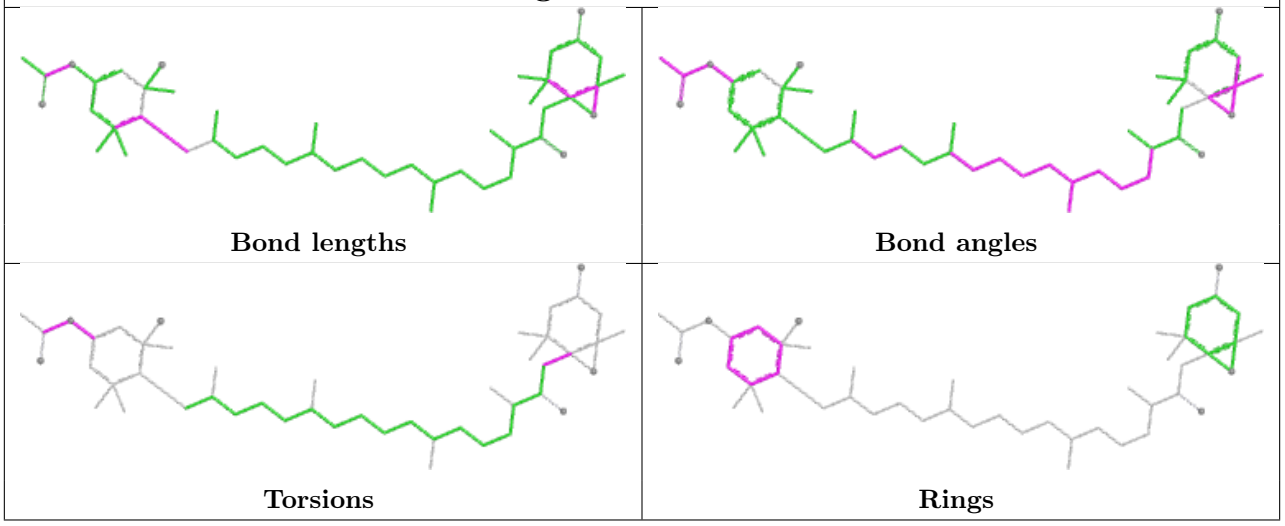
Ligand CLA K 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA V 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

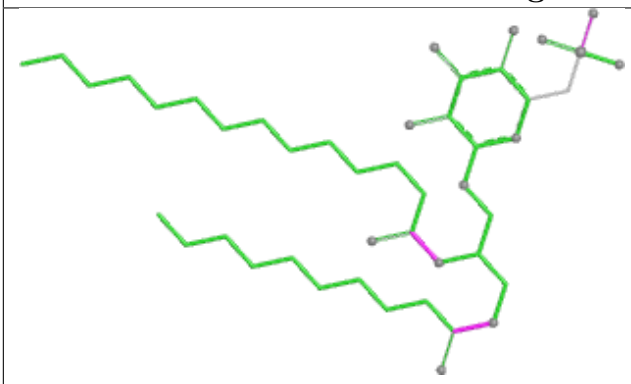
Ligand SQD A 315



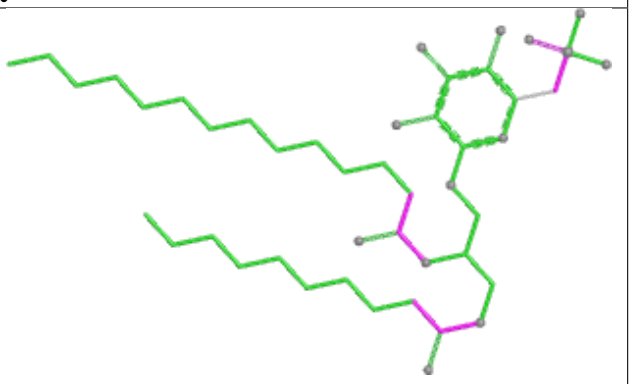
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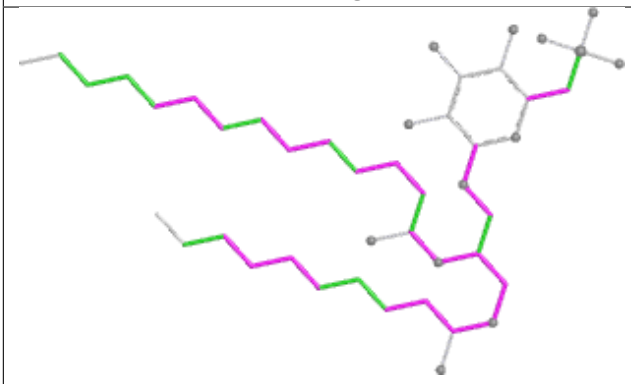
Ligand SQD b 804



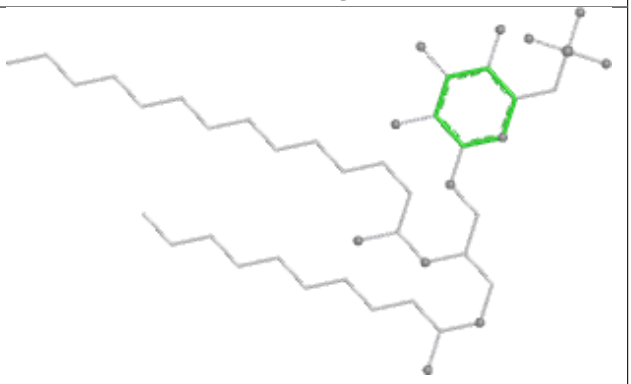
Bond lengths



Bond angles

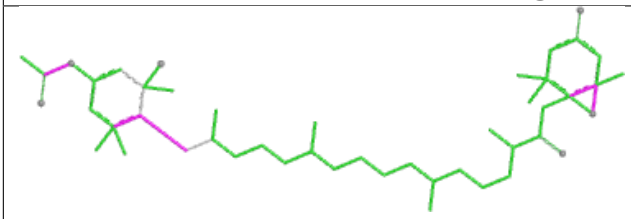


Torsions

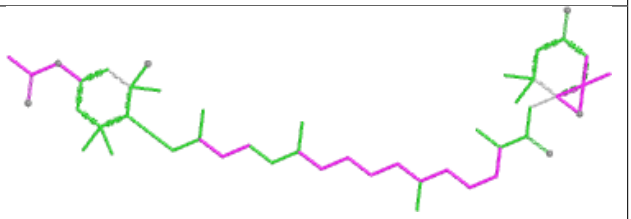


Rings

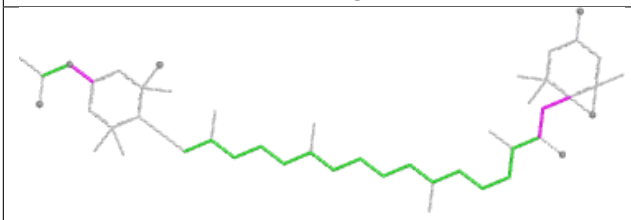
Ligand A86 E 302



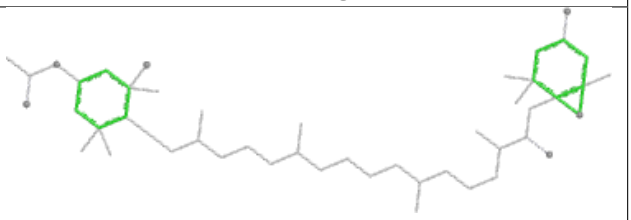
Bond lengths



Bond angles

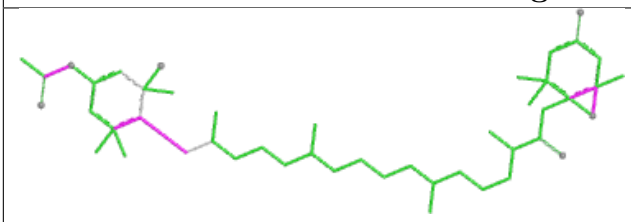


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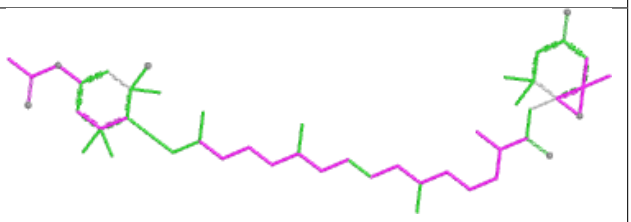


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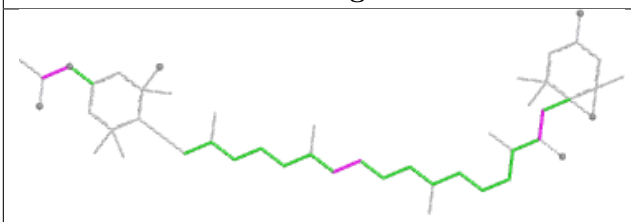
Ligand A86 T 301



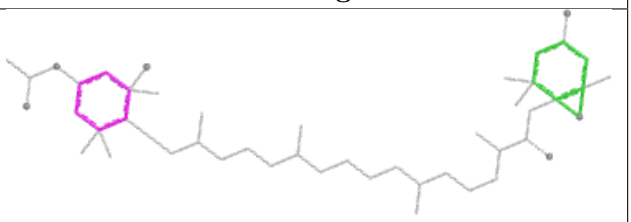
Bond lengths



Bond angles

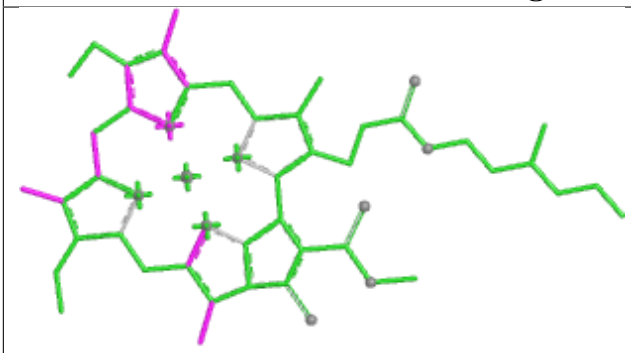


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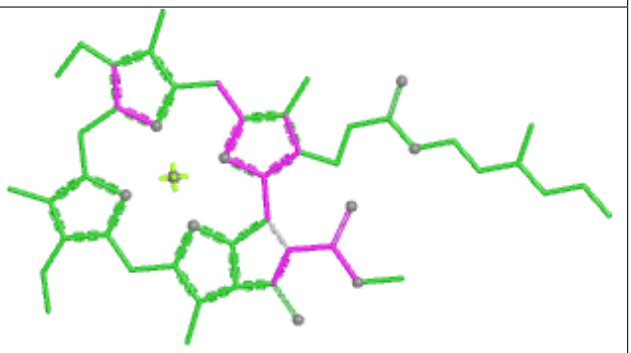


Rings

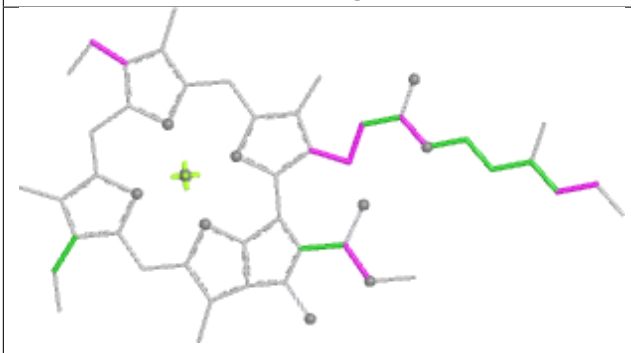
Ligand CLA S 321



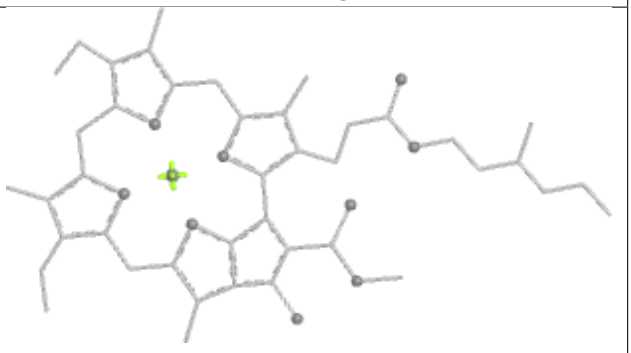
Bond lengths



Bond angles

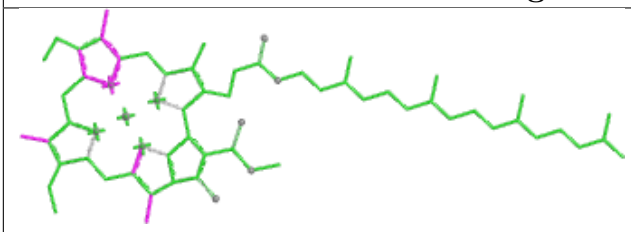


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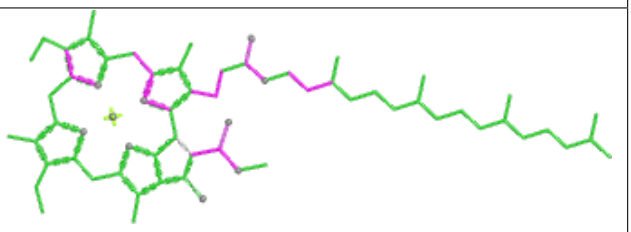


Rings

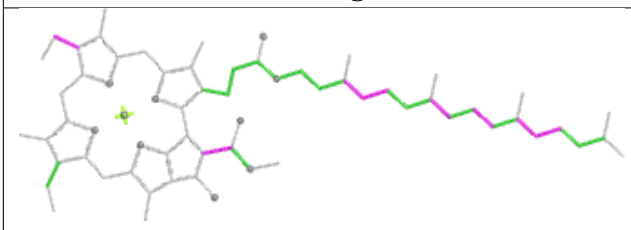
Ligand CLA b 811



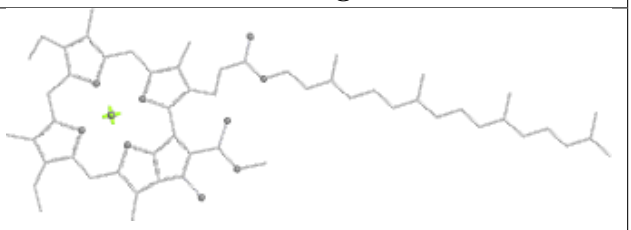
Bond lengths



Bond angles



Torsions

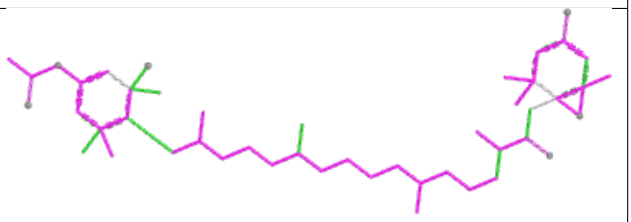


Rings

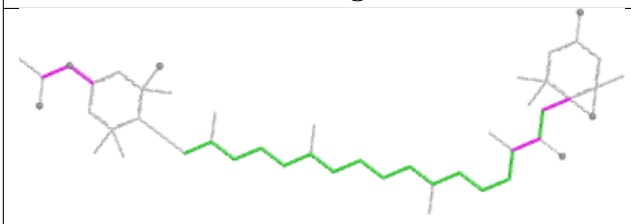
Ligand A86 W 202



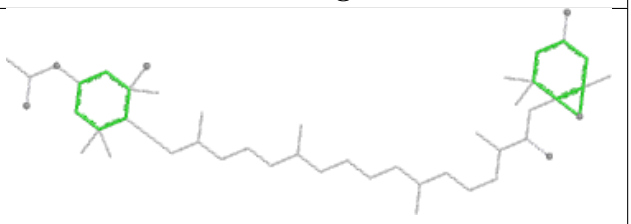
Bond lengths



Bond angles

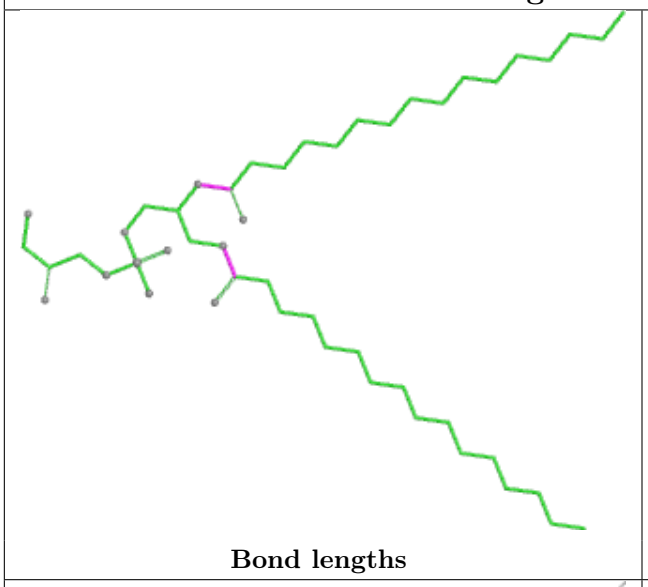


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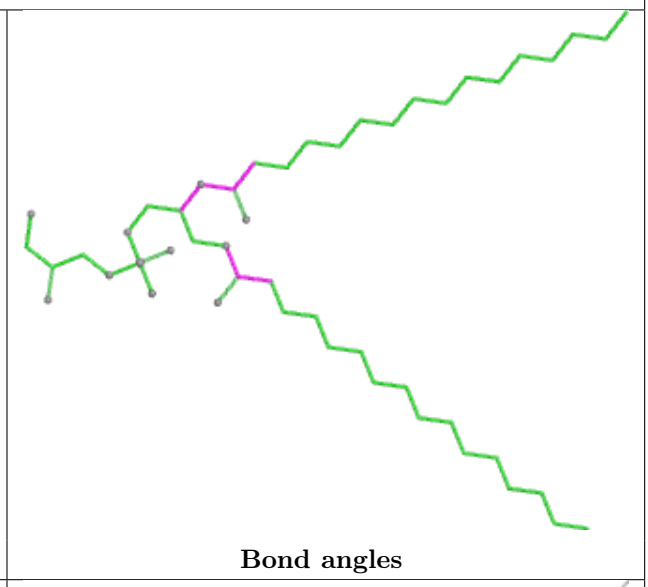


Rings

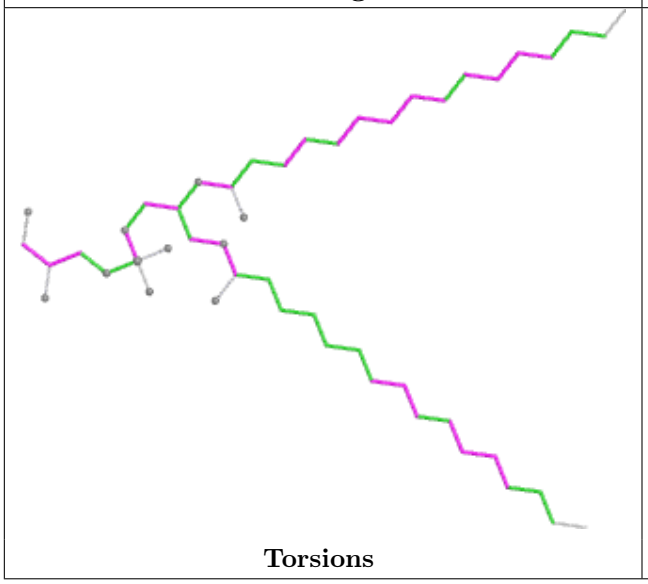
Ligand LHG b 850



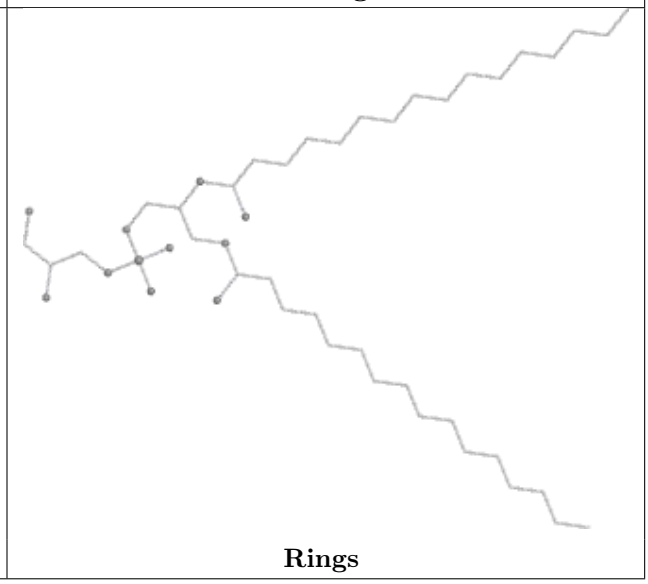
Bond lengths



Bond angles

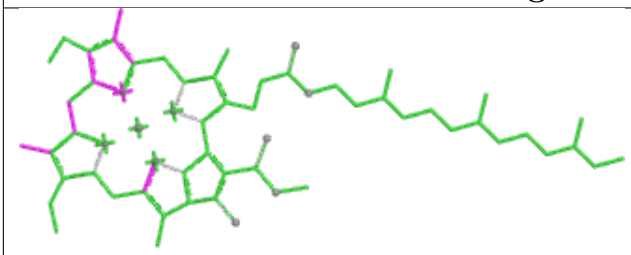


Torsions

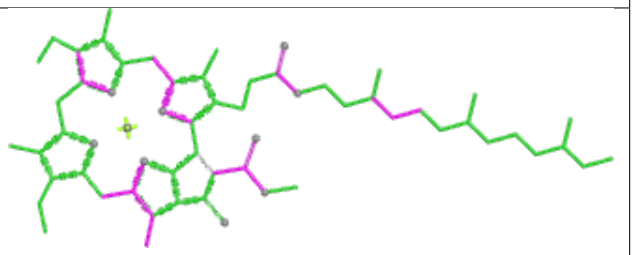


Rings

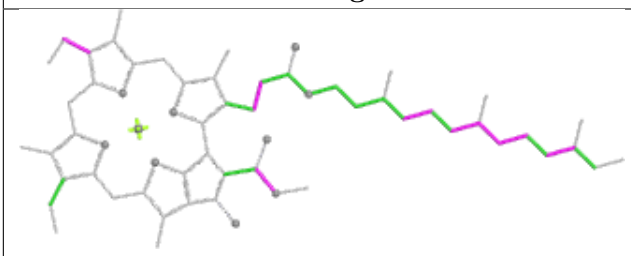
Ligand CLA J 308



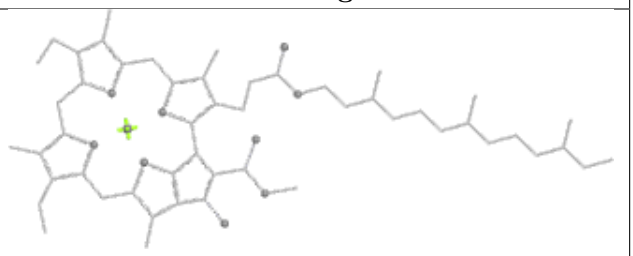
Bond lengths



Bond angles

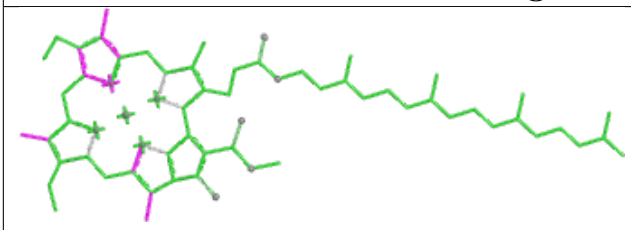


Torsions

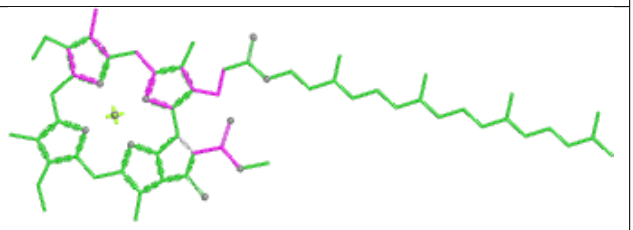


Rings

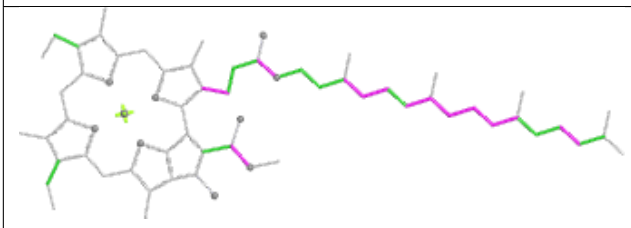
Ligand CLA h 203



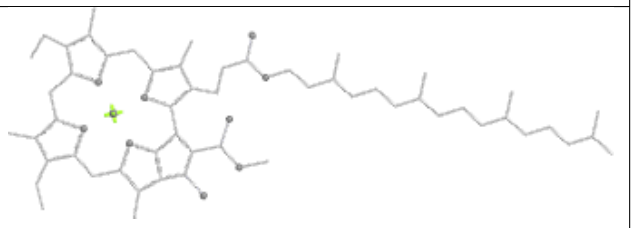
Bond lengths



Bond angles

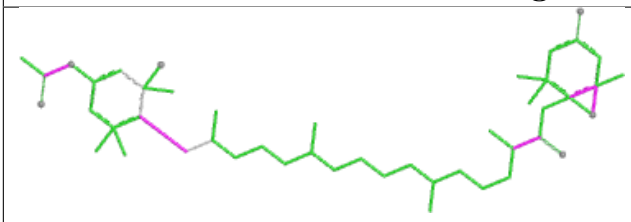


Torsions

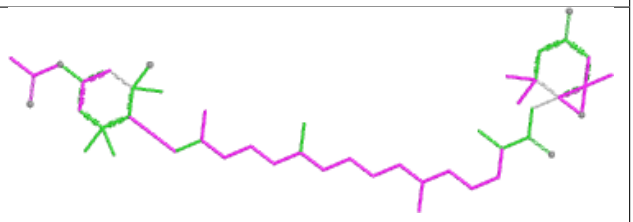


Rings

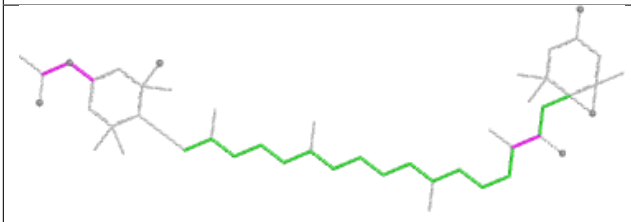
Ligand A86 T 306



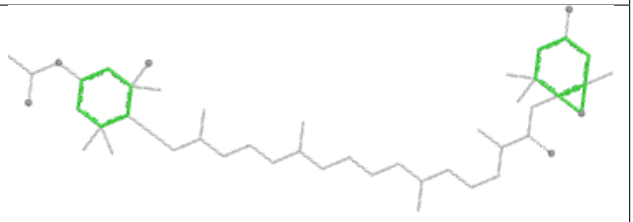
Bond lengths



Bond angles

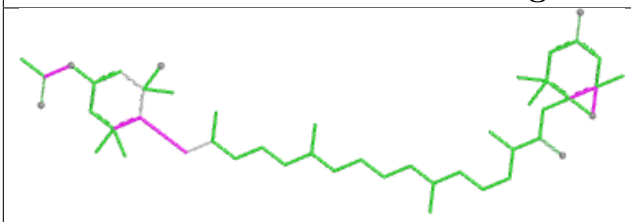


Torsions

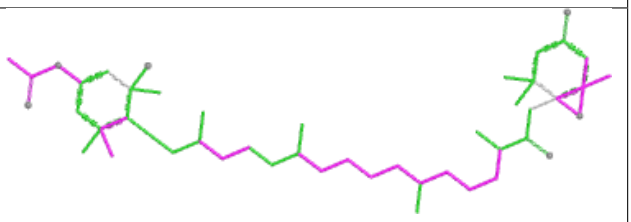


Rings

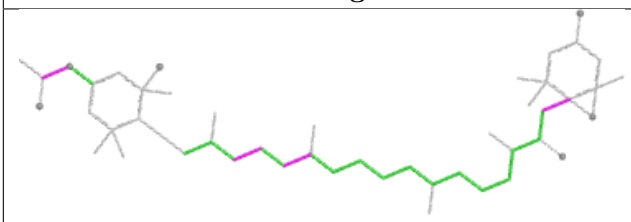
Ligand A86 K 301



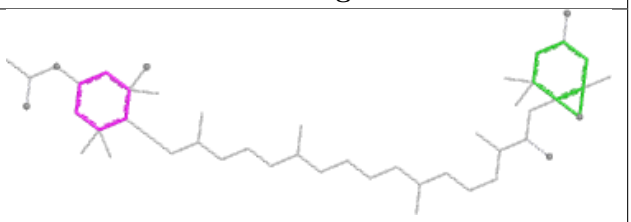
Bond lengths



Bond angles

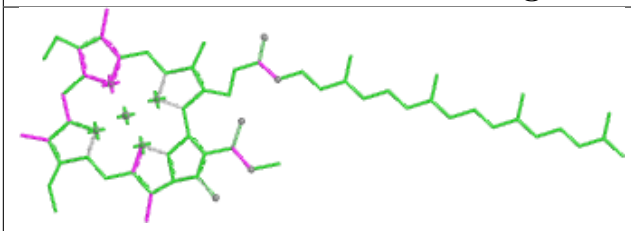


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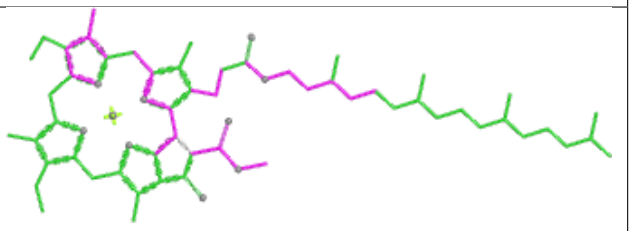


Rings

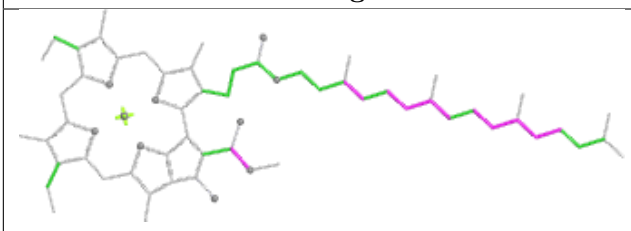
Ligand CLA G 309



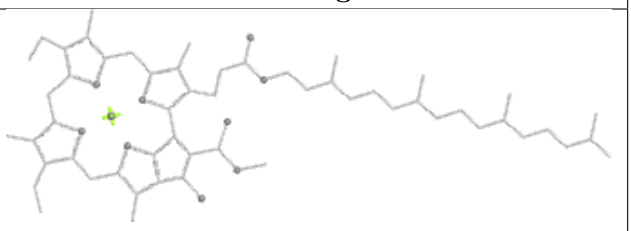
Bond lengths



Bond angles

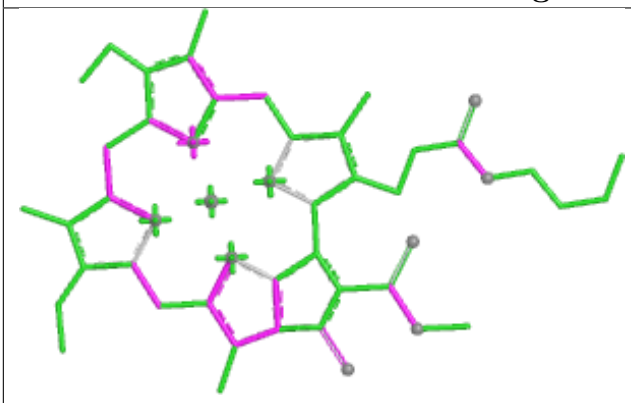


Torsions

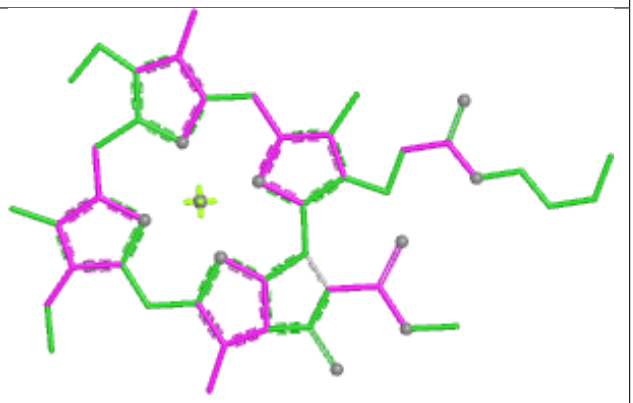


Rings

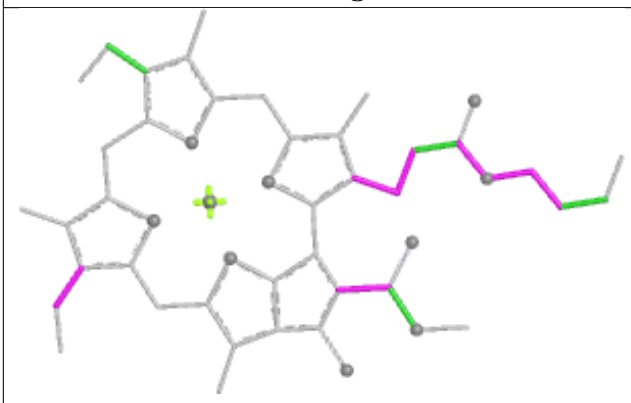
Ligand CLA l 204



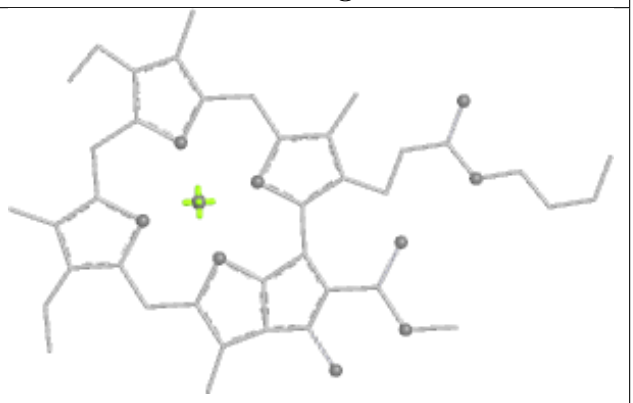
Bond lengths



Bond angles

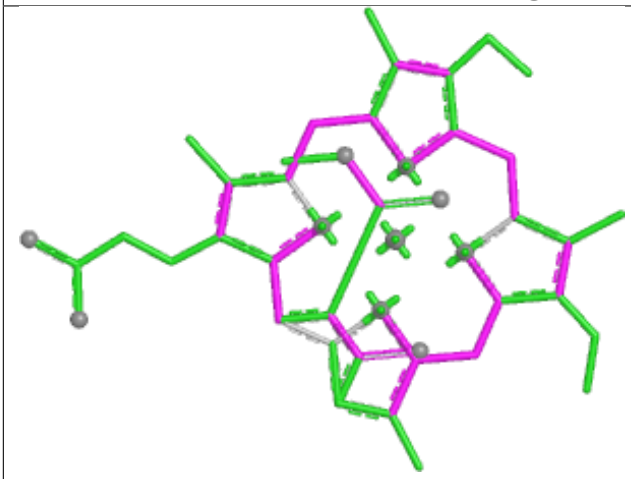


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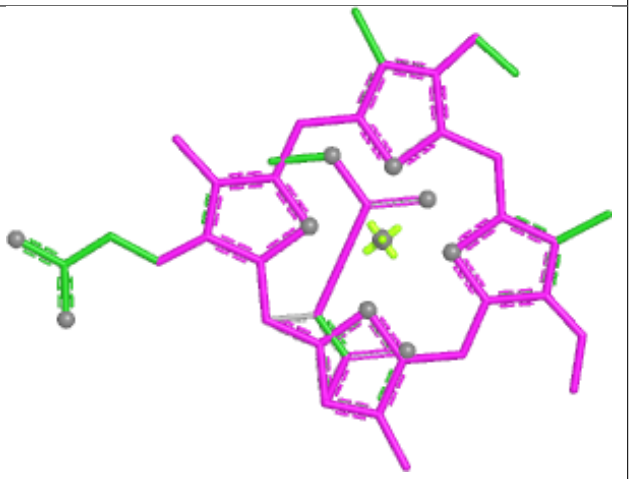


Rings

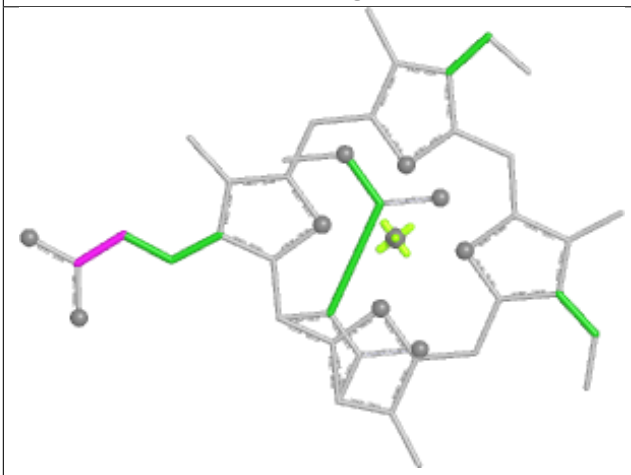
Ligand KC1 A 312



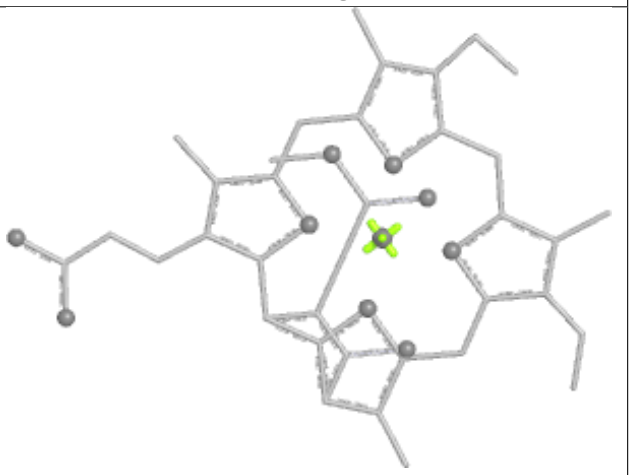
Bond lengths



Bond angles

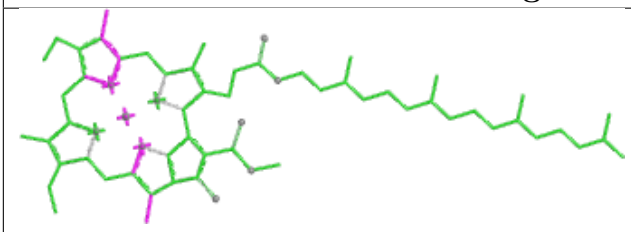


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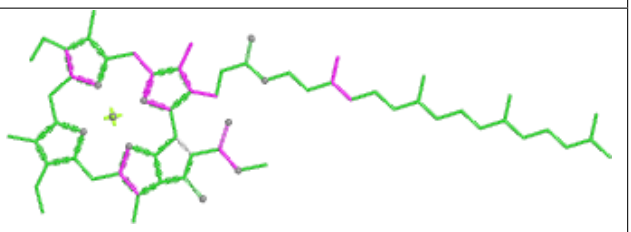


Rings

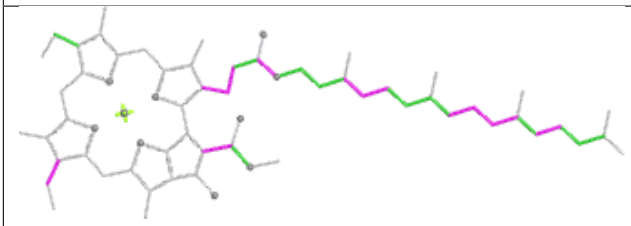
Ligand CLA G 311



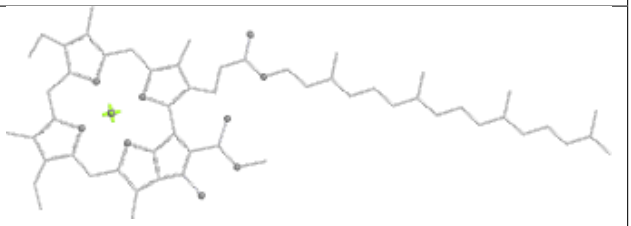
Bond lengths



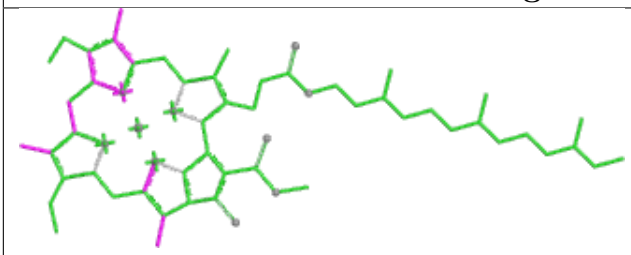
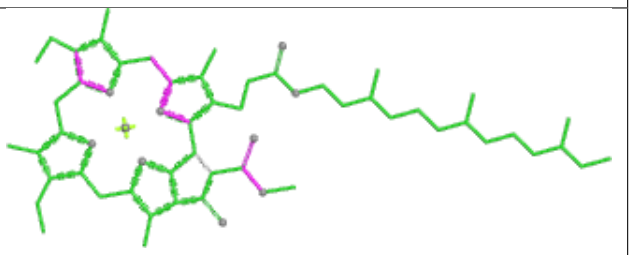
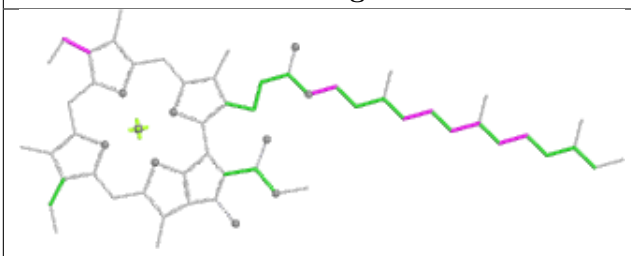
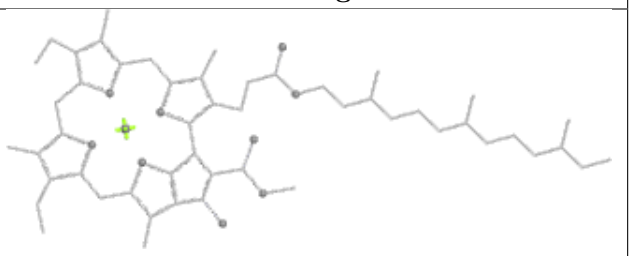
Bond angles

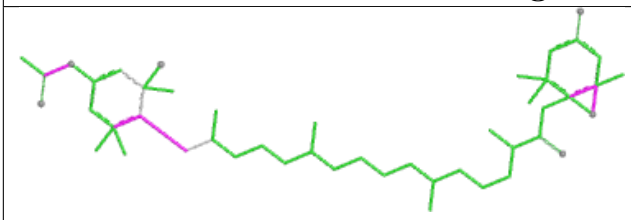
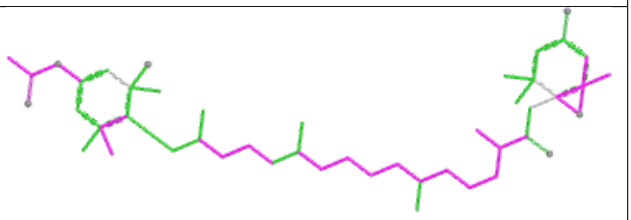
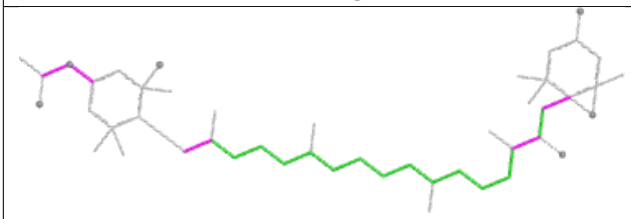
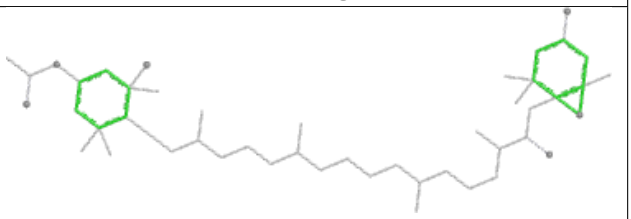


Torsions

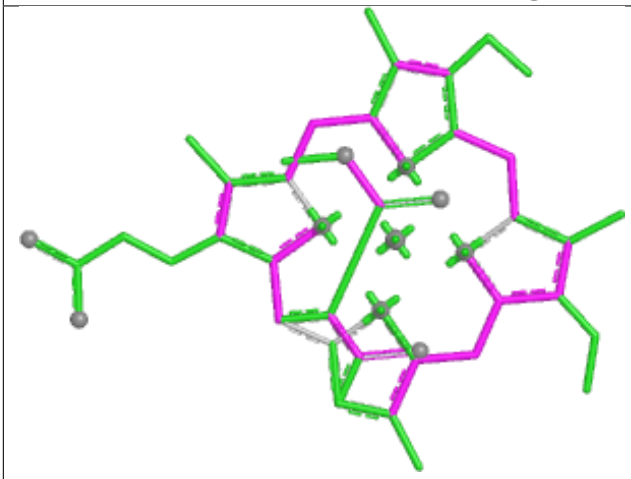


Rings

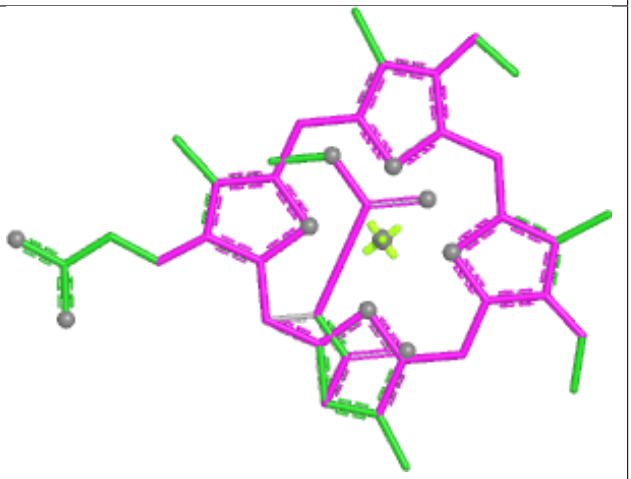
Ligand CLA H 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 A 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

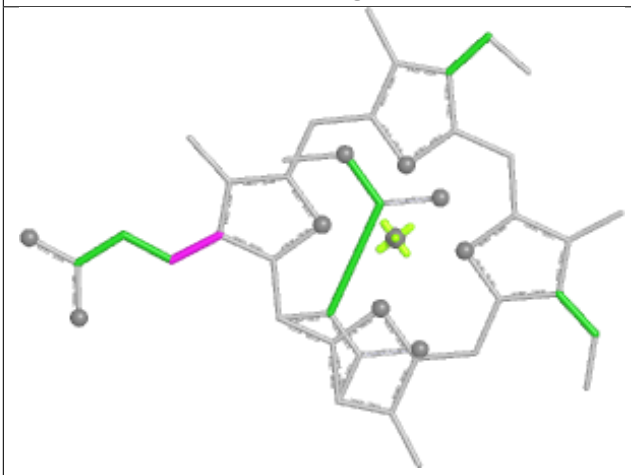
Ligand KC1 X 311



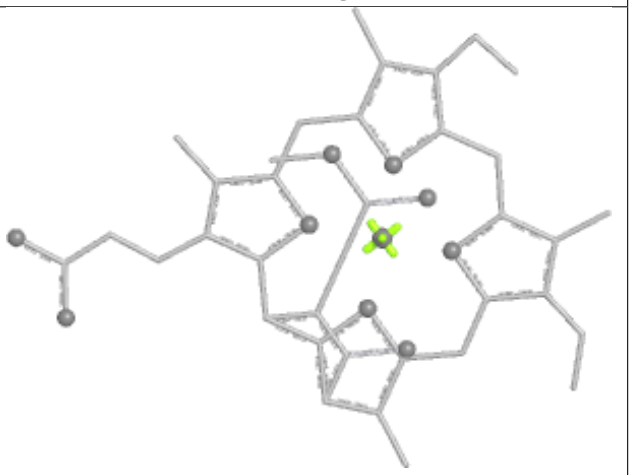
Bond lengths



Bond angles

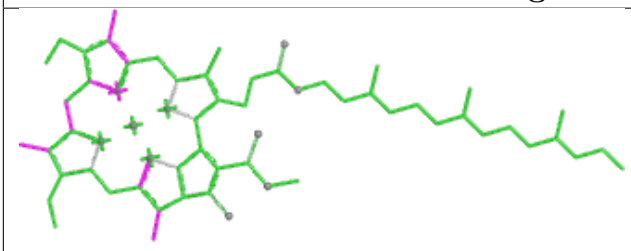


Torsions

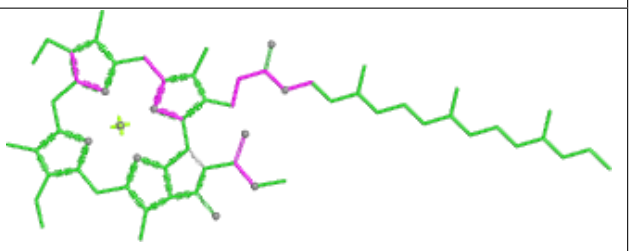


Rings

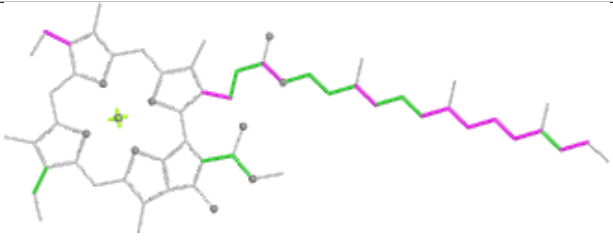
Ligand CLA a 810



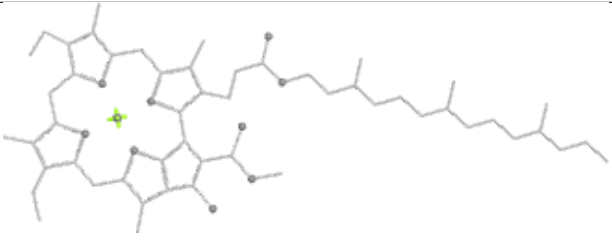
Bond lengths



Bond angles

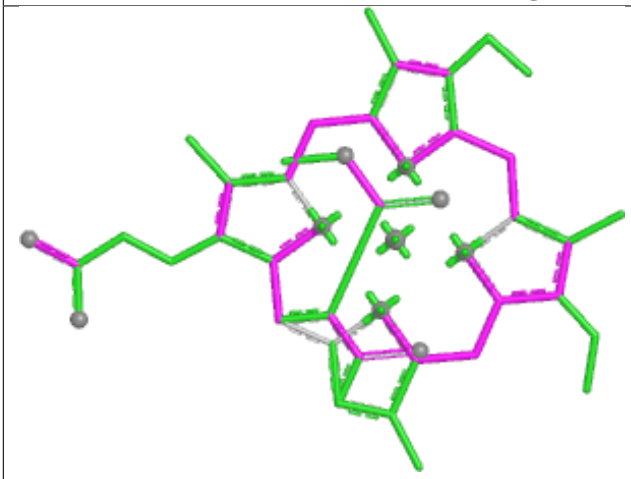


Torsions

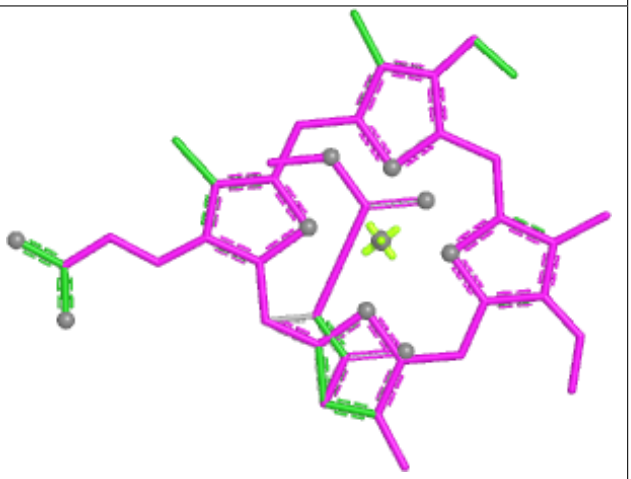


Rings

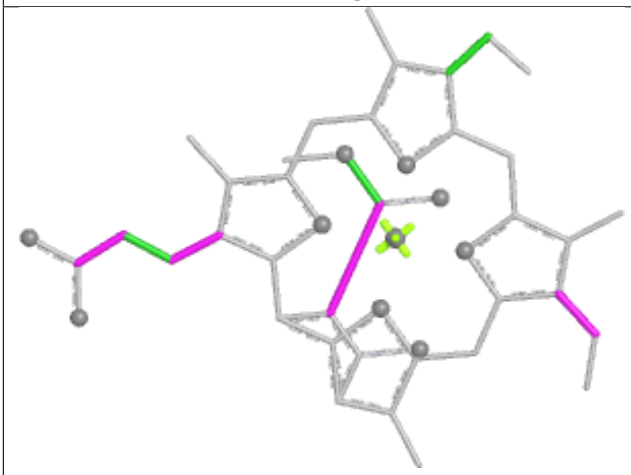
Ligand KC1 G 318



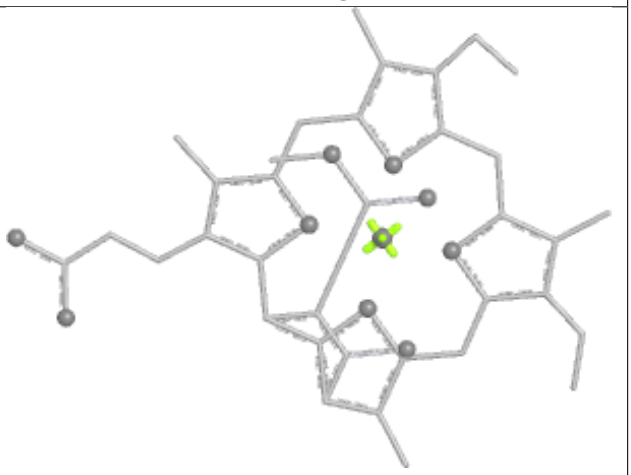
Bond lengths



Bond angles

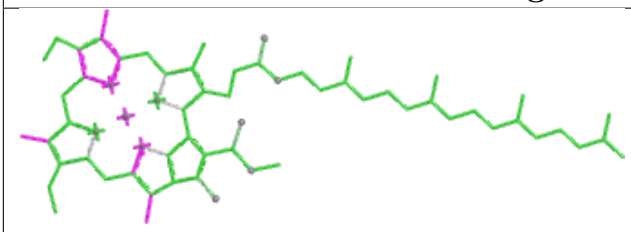


Torsions

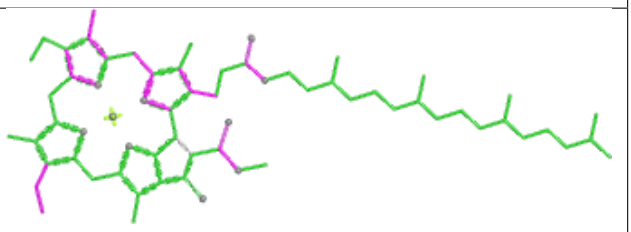


Rings

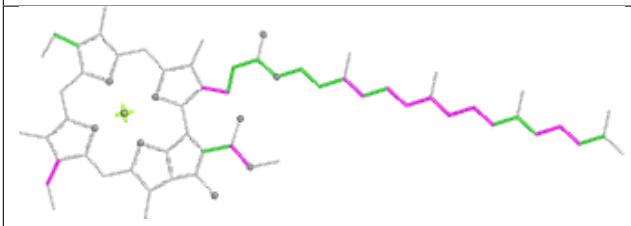
Ligand CLA b 815



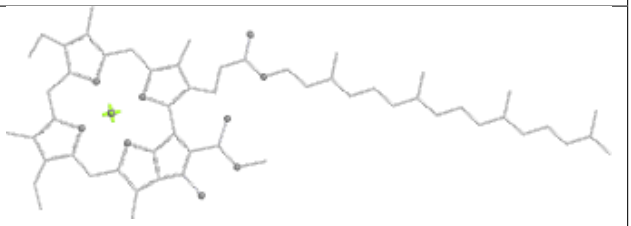
Bond lengths



Bond angles

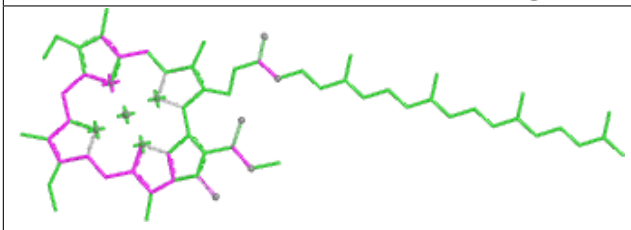


Torsions

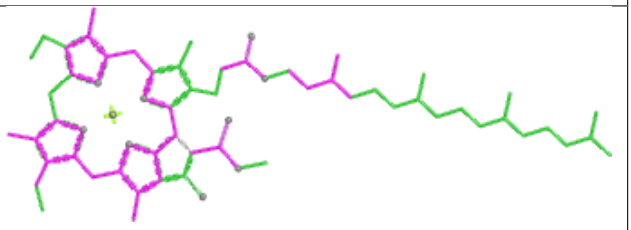


Rings

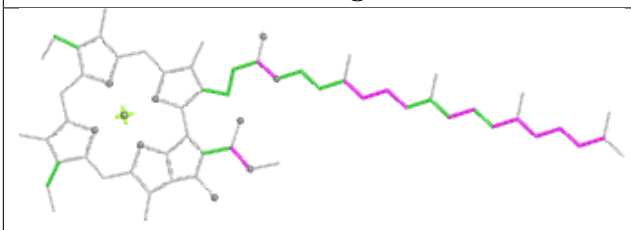
Ligand CLA E 315



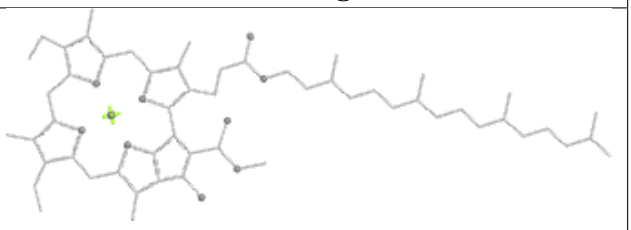
Bond lengths



Bond angles

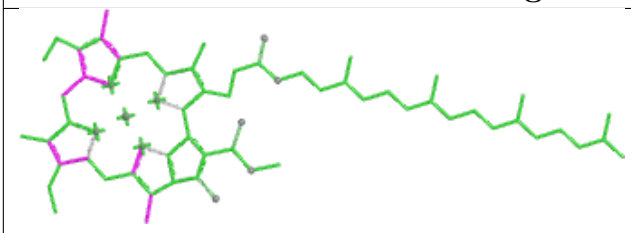


Torsions

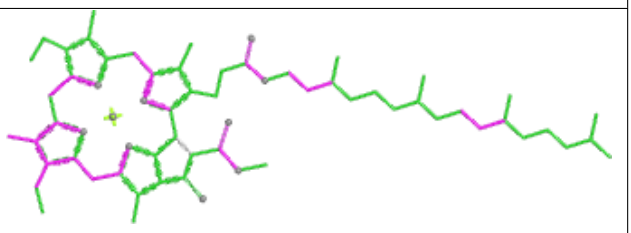


Rings

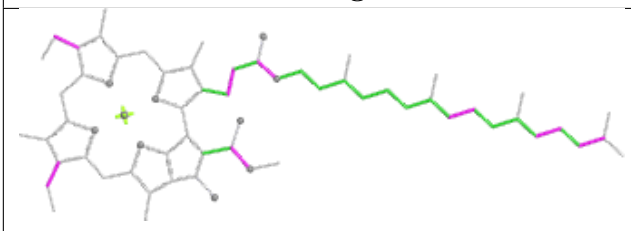
Ligand CLA T 311



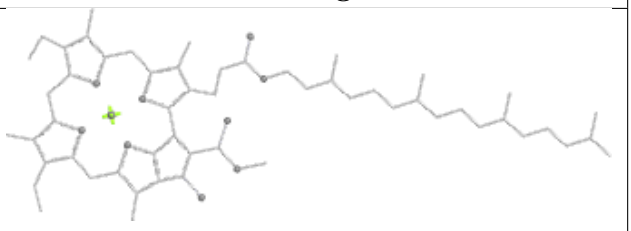
Bond lengths



Bond angles

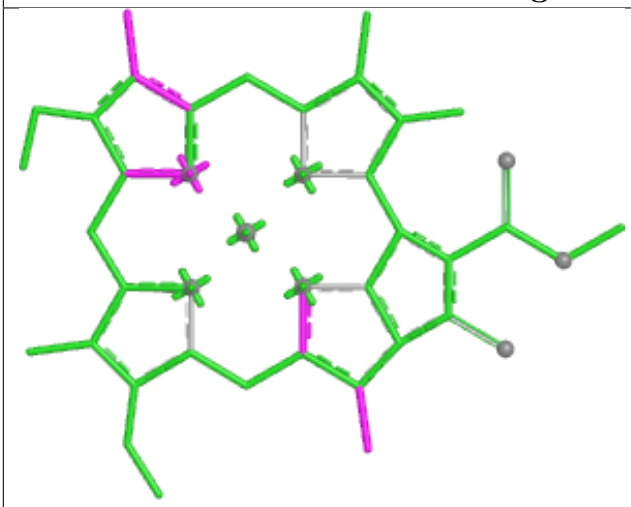


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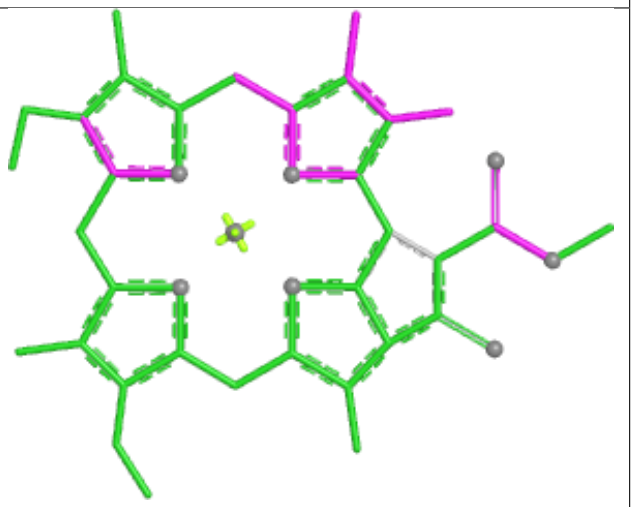


Rings

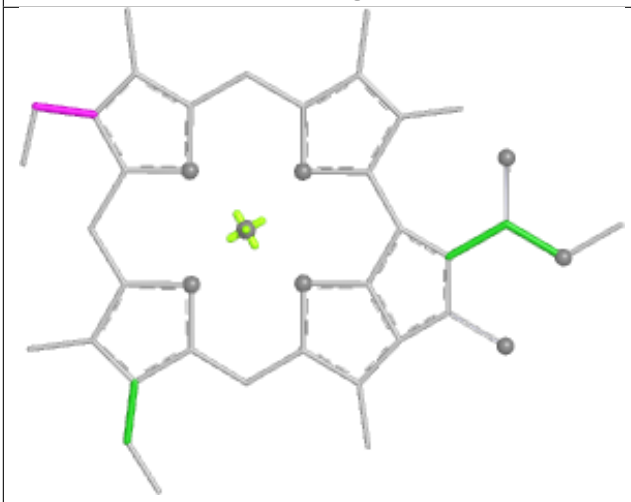
Ligand CLA I 314



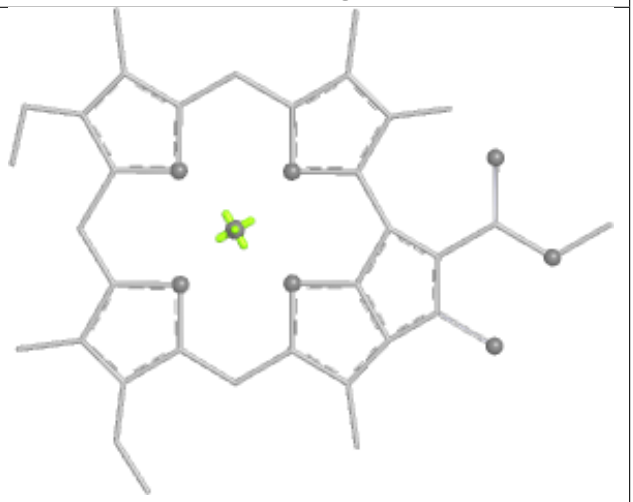
Bond lengths



Bond angles

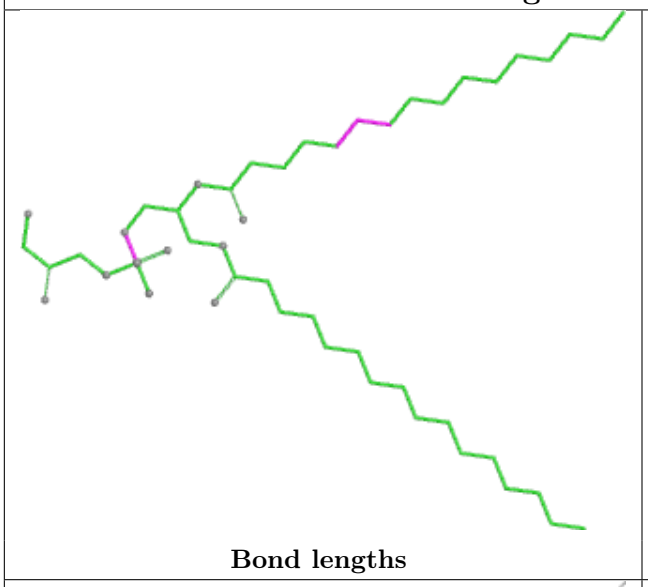


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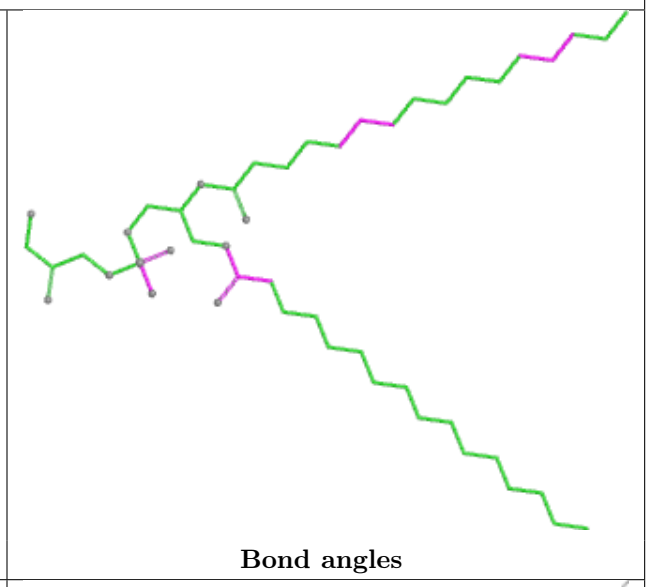


Rings

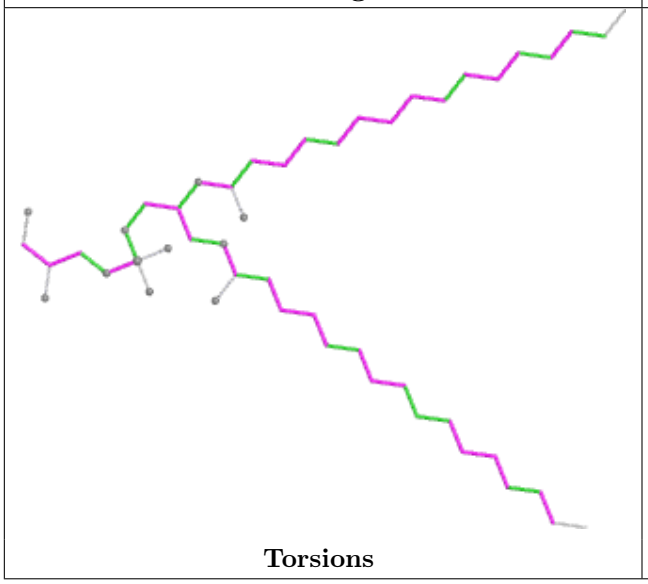
Ligand LHG O 318



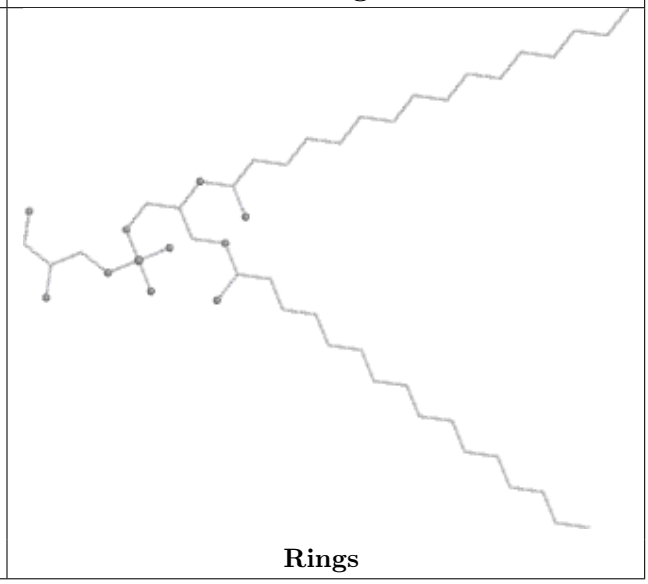
Bond lengths



Bond angles

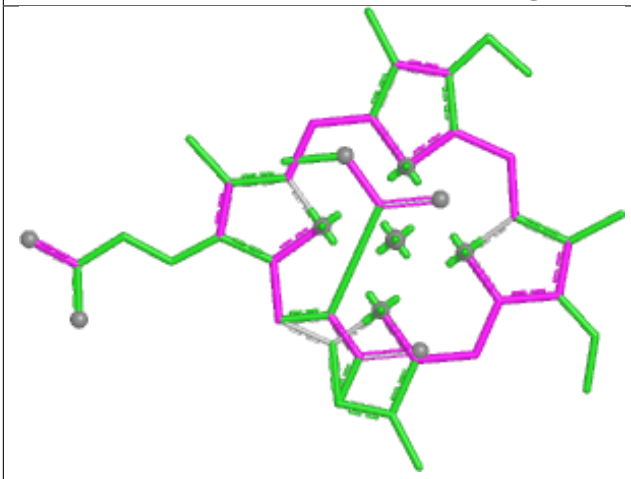


Torsions

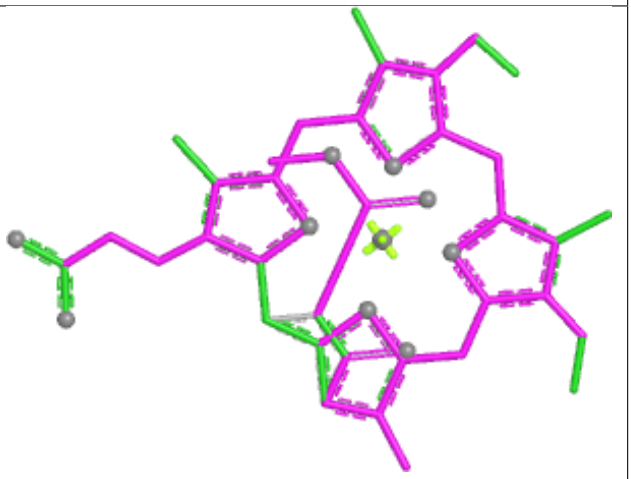


Rings

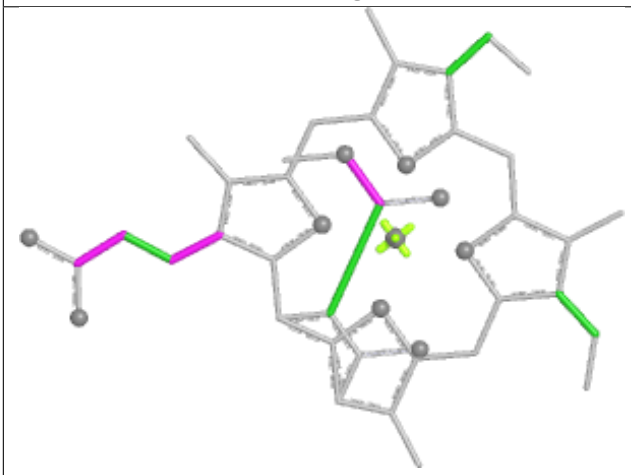
Ligand KC1 G 317



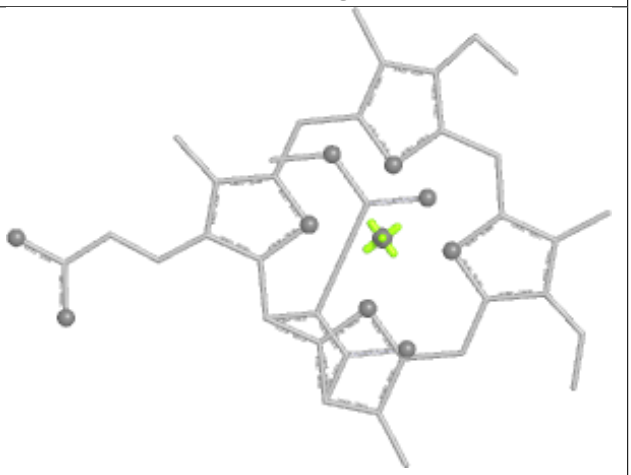
Bond lengths



Bond angles

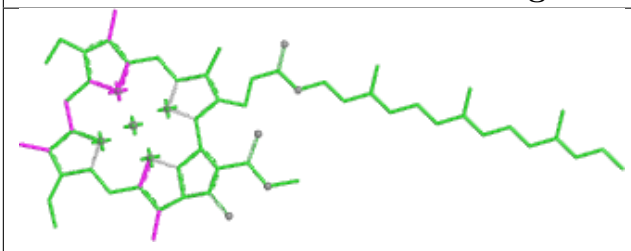


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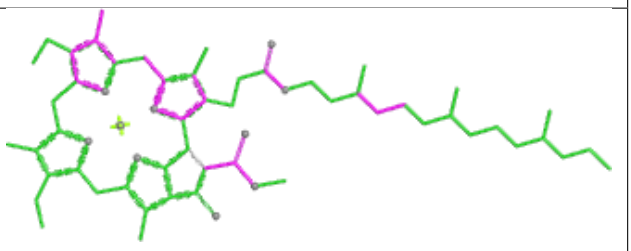


Rings

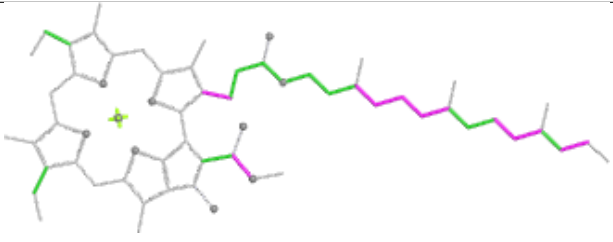
Ligand CLA a 827



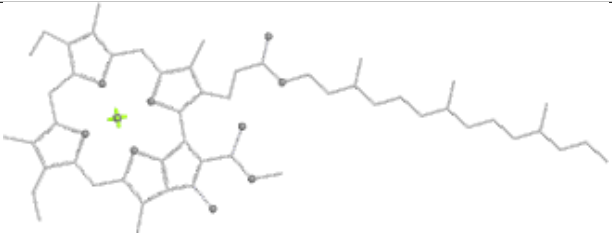
Bond lengths



Bond angles

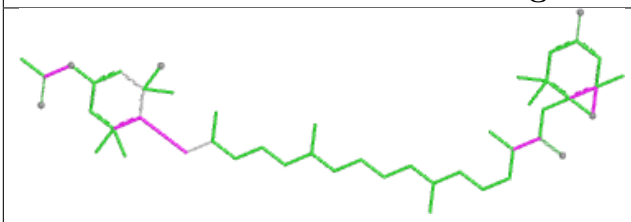


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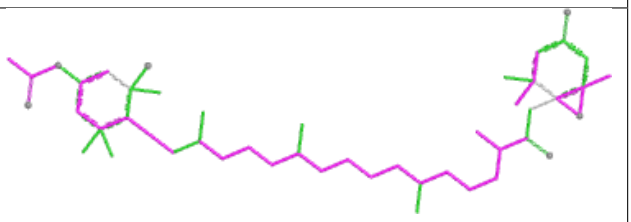


Rings

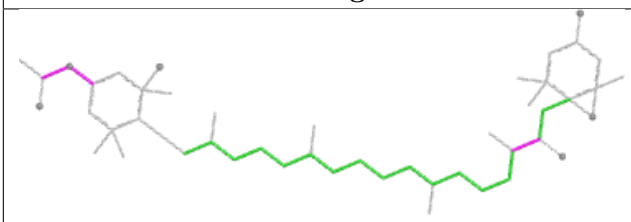
Ligand A86 O 303



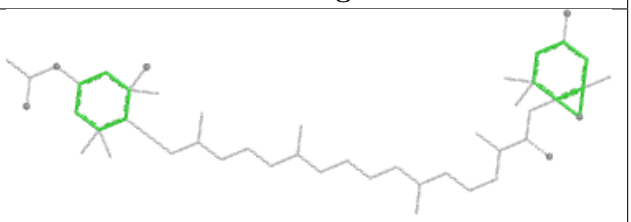
Bond lengths



Bond angles

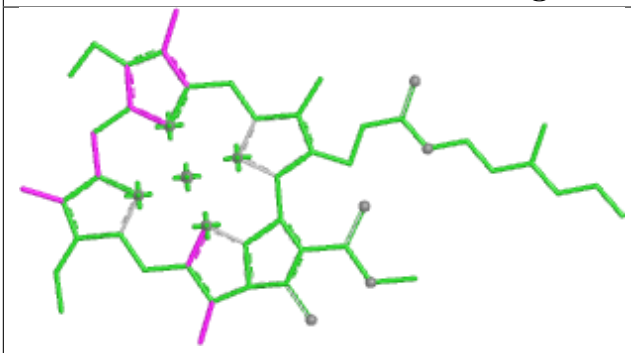


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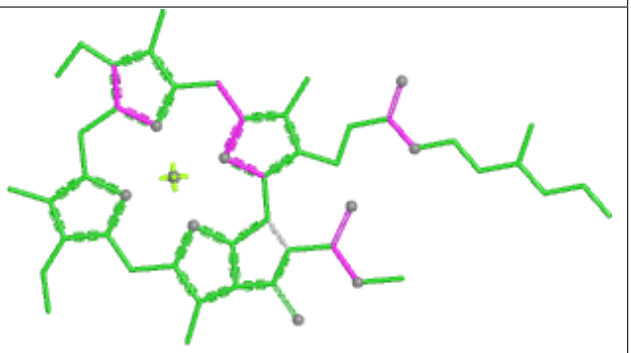


Rings

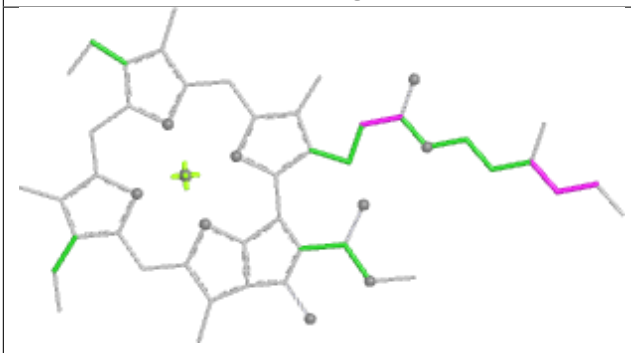
Ligand CLA I 312



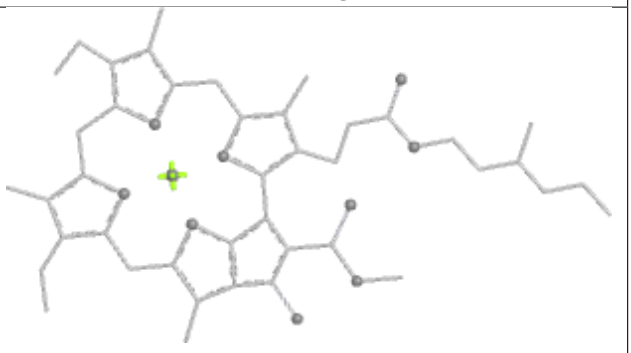
Bond lengths



Bond angles

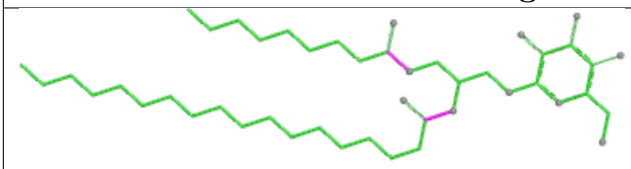


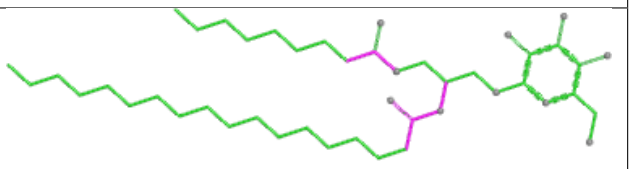
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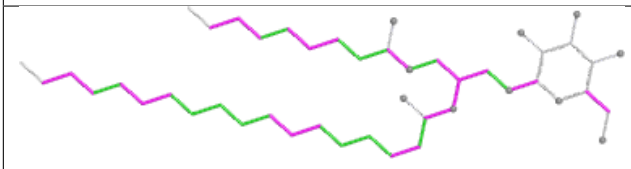


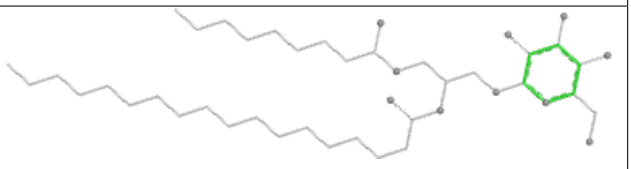
Rings

Ligand LMG D 320

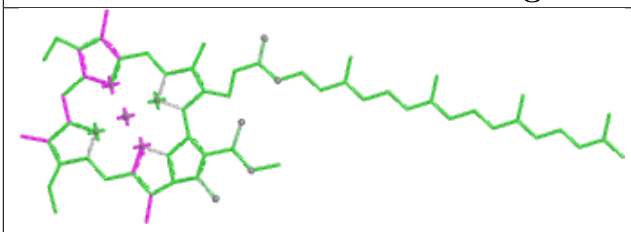

Bond lengths

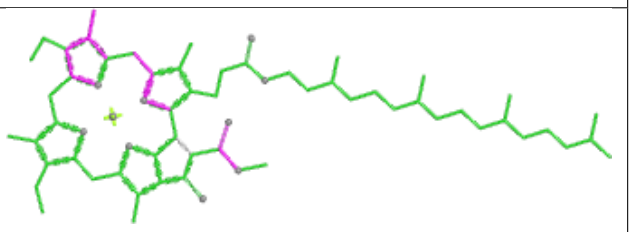

Bond angles

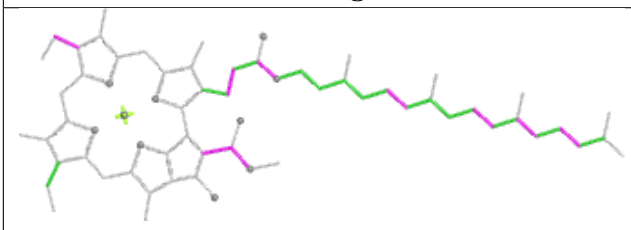

Torsions

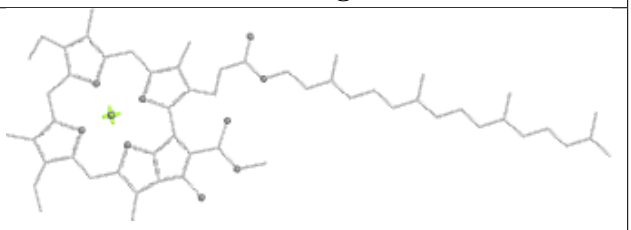

Rings

Ligand CLA R 313


Bond lengths

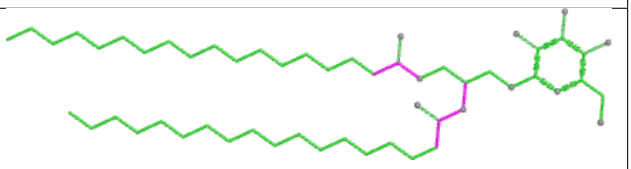

Bond angles

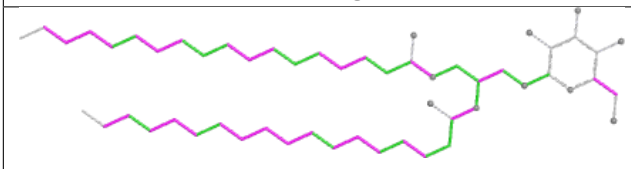

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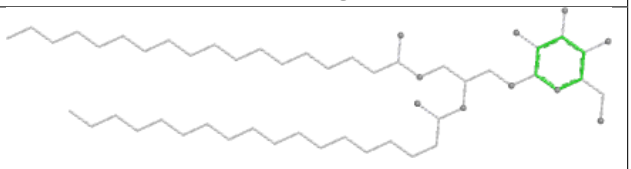

Rings

Ligand LMG G 325

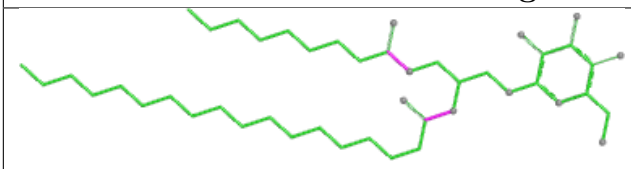

Bond lengths


Bond angles

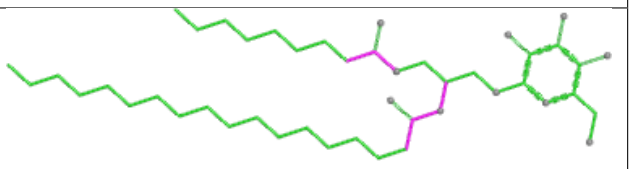

Torsions


Rings

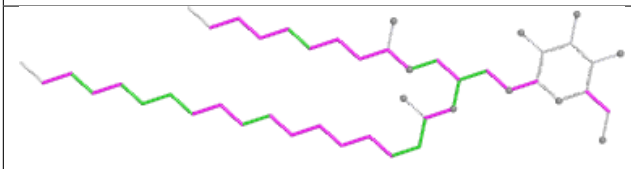
Ligand LMG V 316



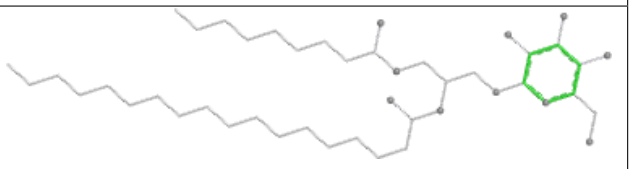
Bond lengths



Bond angles

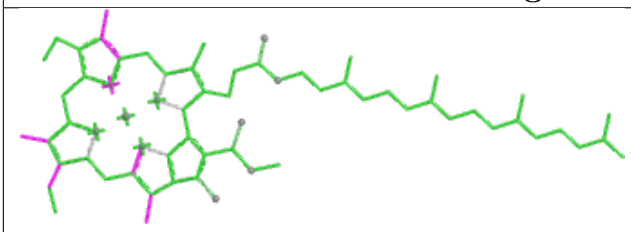


Torsions

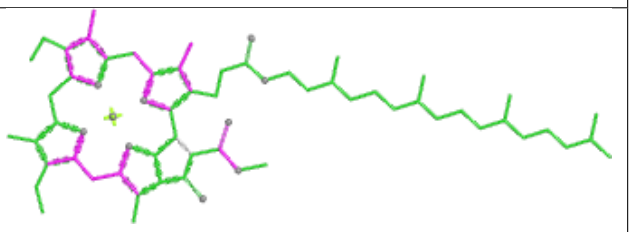


Rings

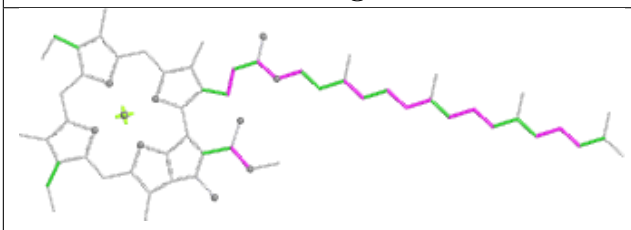
Ligand CLA B 308



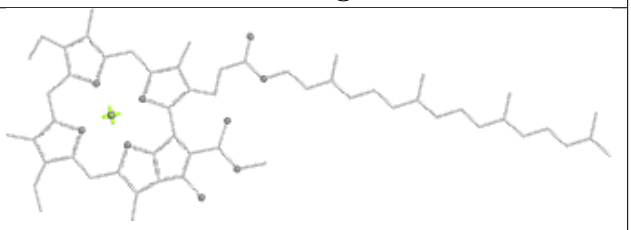
Bond lengths



Bond angles

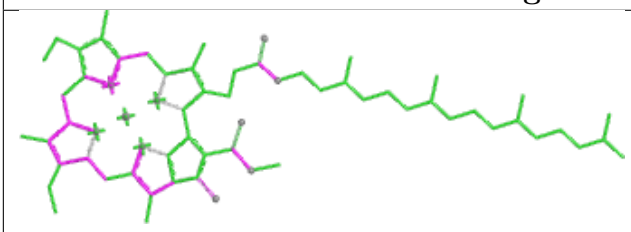


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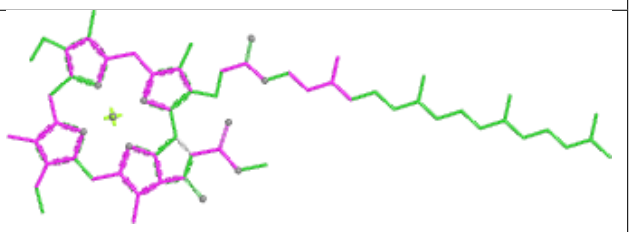


Rings

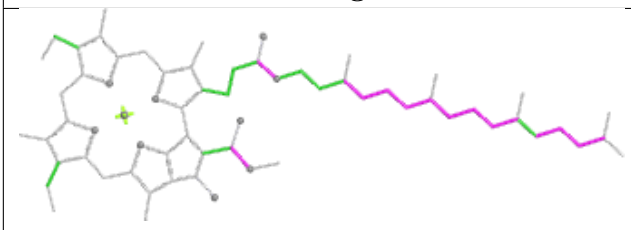
Ligand CLA U 306



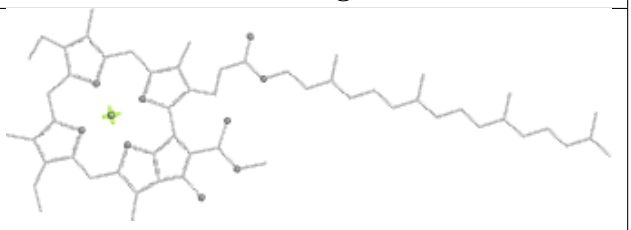
Bond lengths



Bond angles

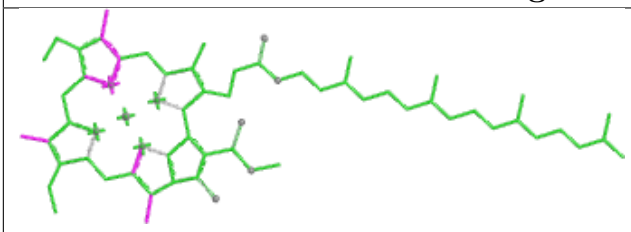


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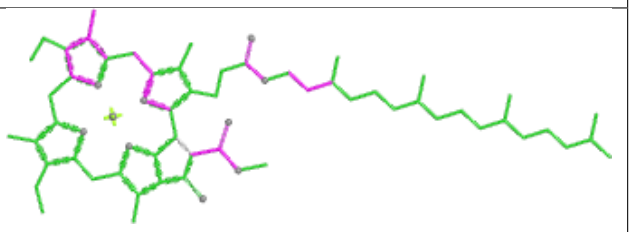


Rings

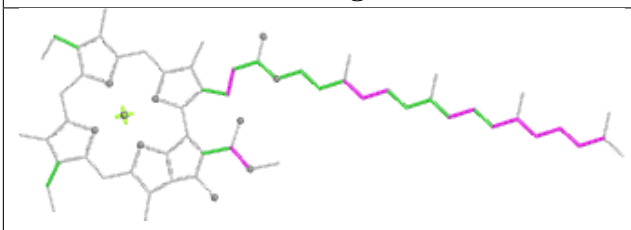
Ligand CLA a 828



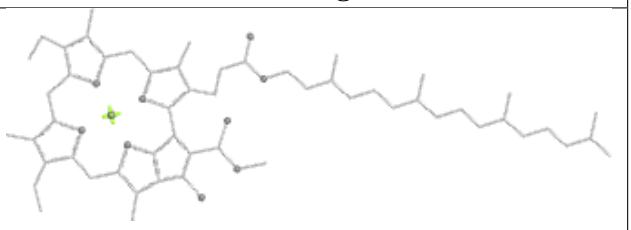
Bond lengths



Bond angles

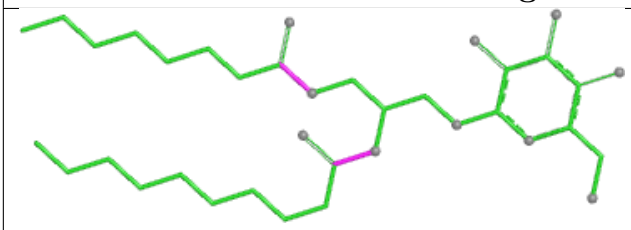


Torsions

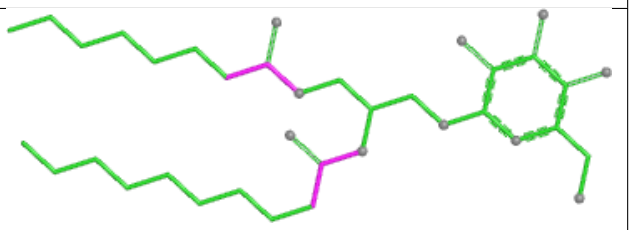


Rings

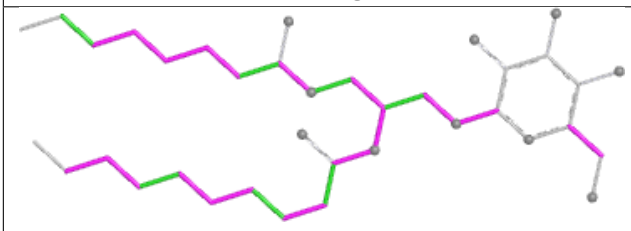
Ligand LMG D 321



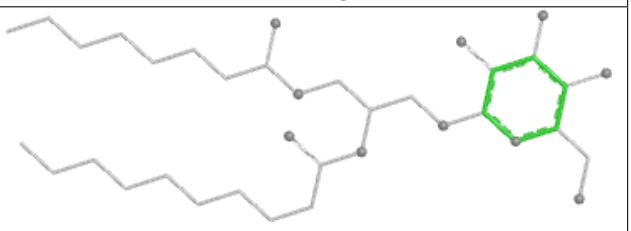
Bond lengths



Bond angles

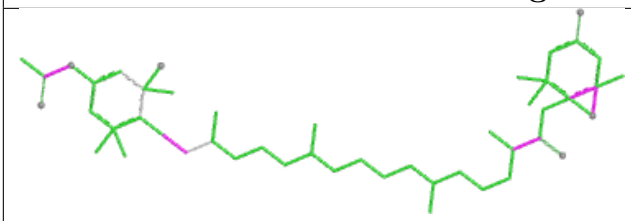


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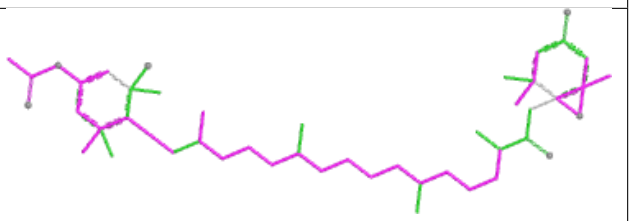


Rings

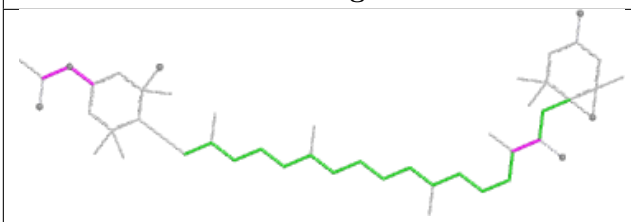
Ligand A86 V 303



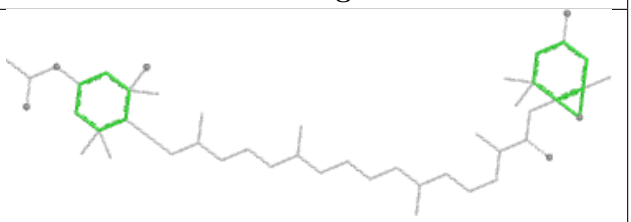
Bond lengths



Bond angles

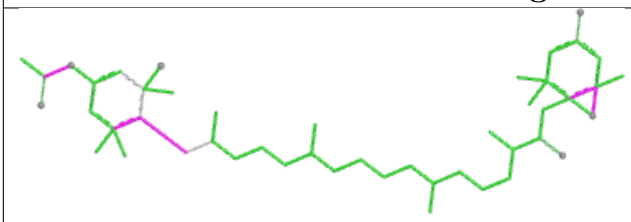


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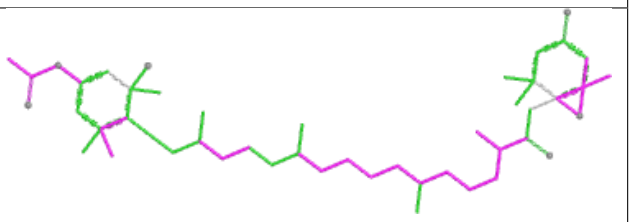


Rings

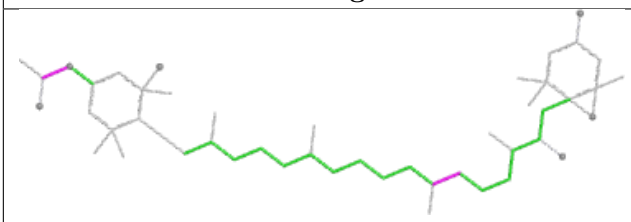
Ligand A86 O 301



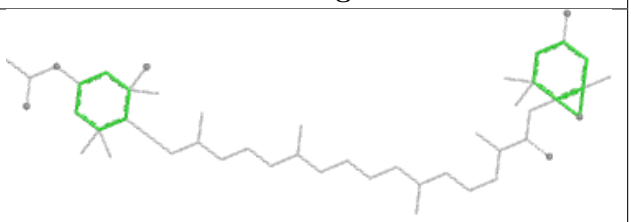
Bond lengths



Bond angles

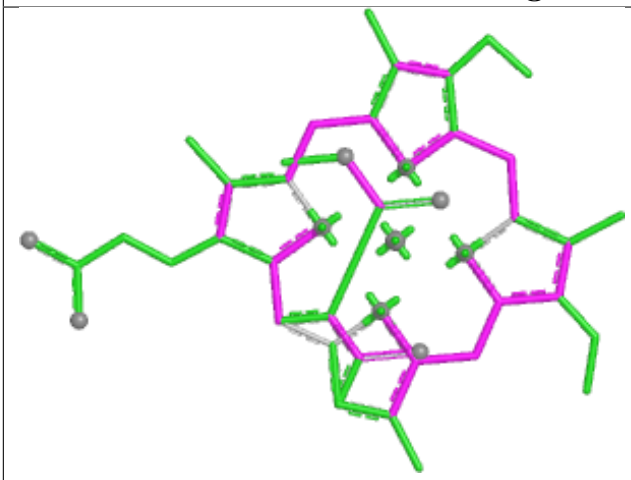


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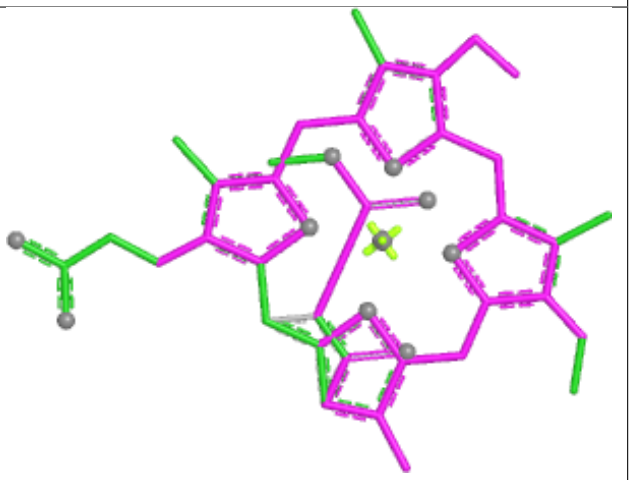


Rings

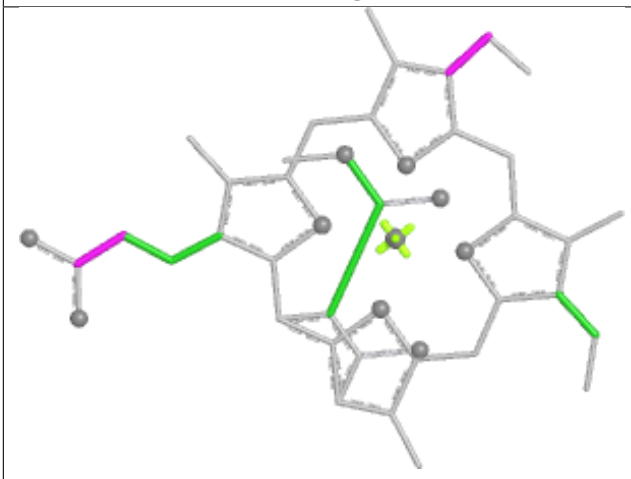
Ligand KC1 R 317



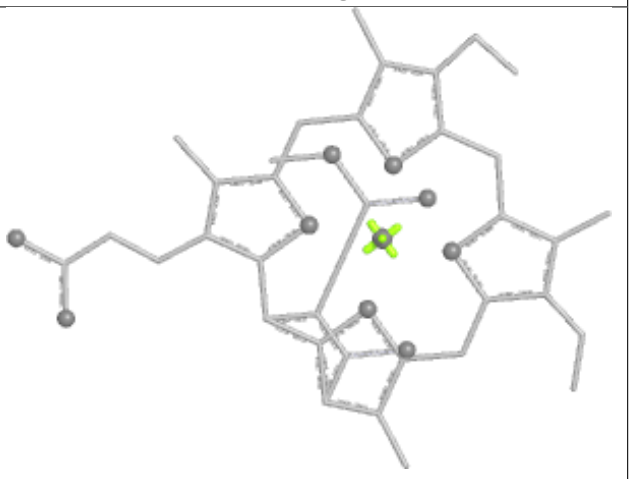
Bond lengths



Bond angles

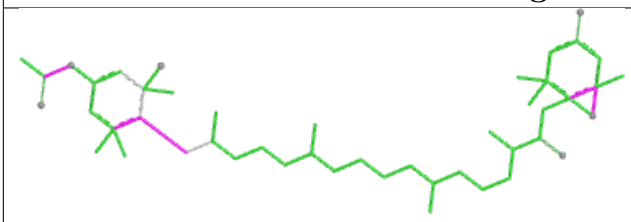


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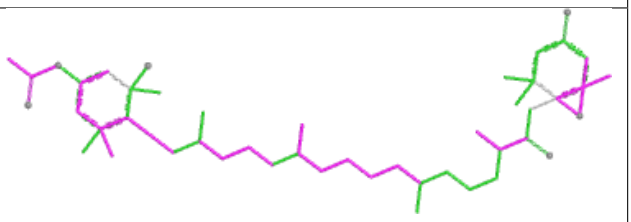


Rings

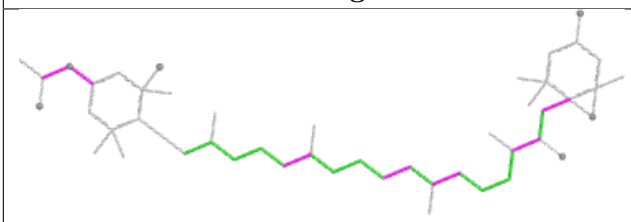
Ligand A86 O 305



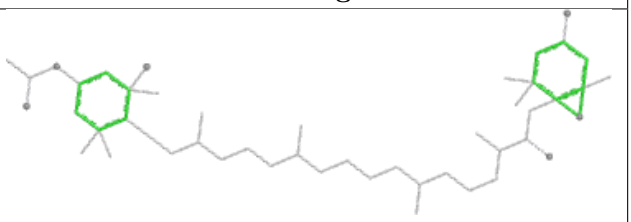
Bond lengths



Bond angles

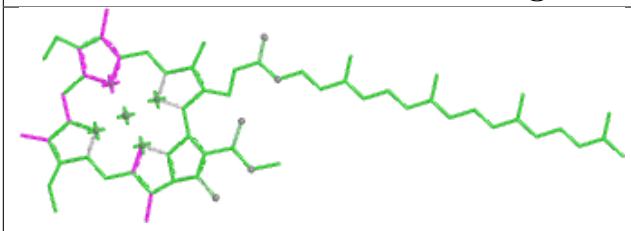


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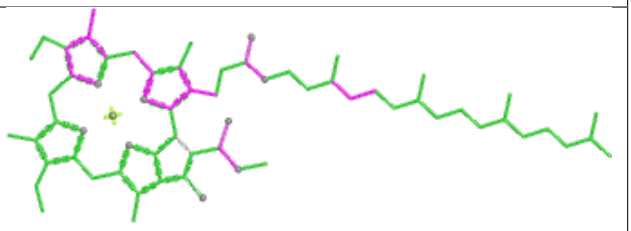


Rings

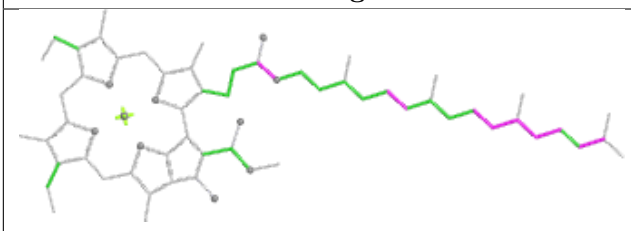
Ligand CLA a 826



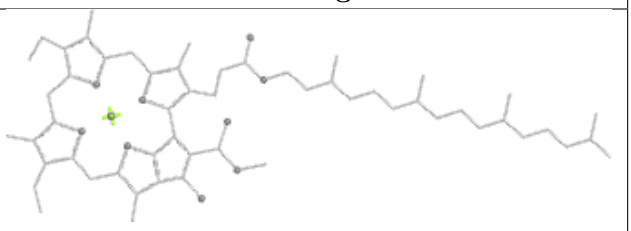
Bond lengths



Bond angles

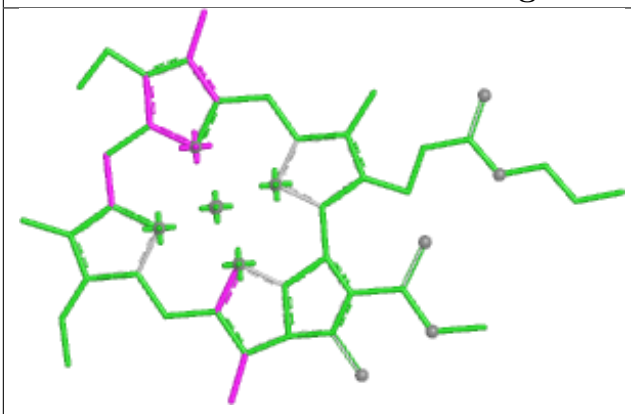


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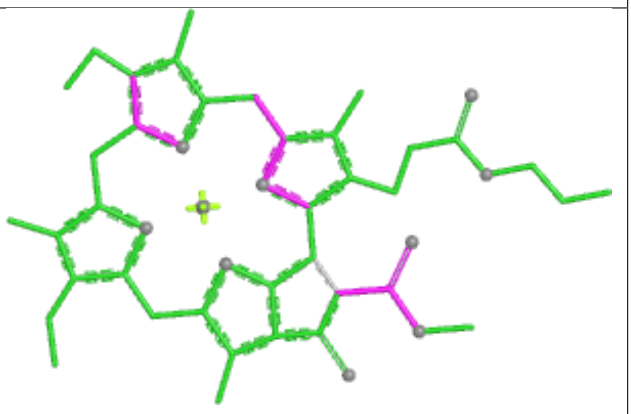


Rings

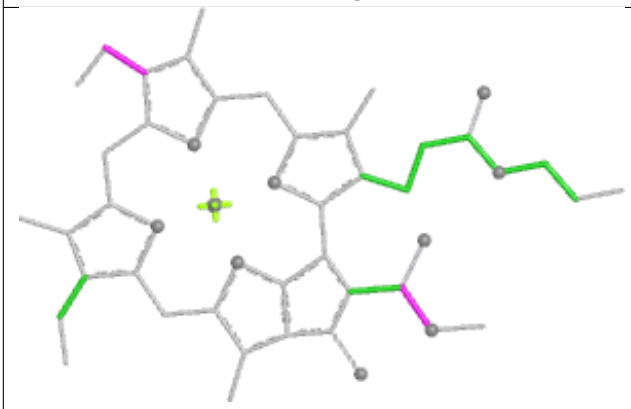
Ligand CLA W 201



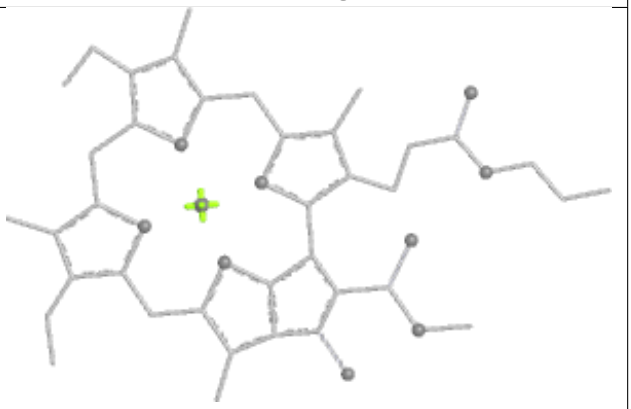
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Bond angles

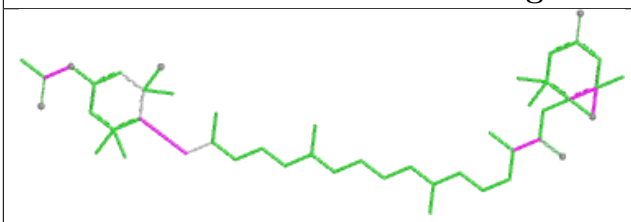


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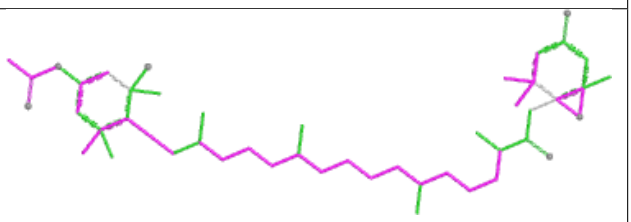


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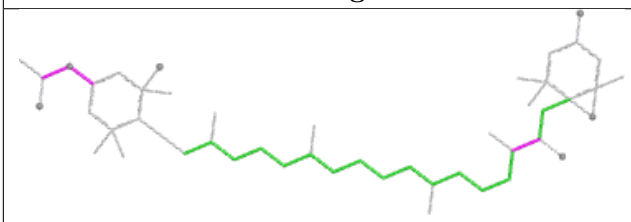
Ligand A86 M 302



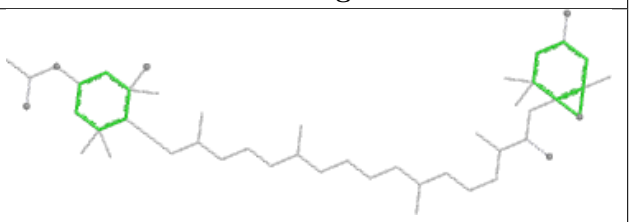
Bond lengths



Bond angles

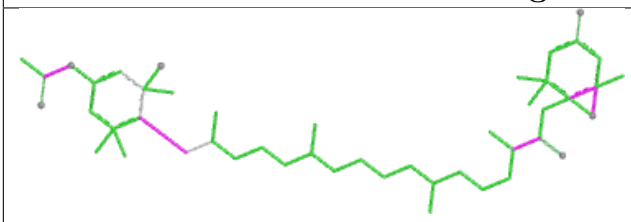


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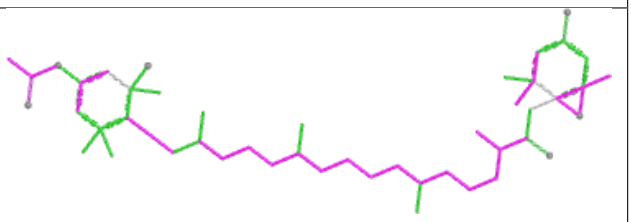


Rings

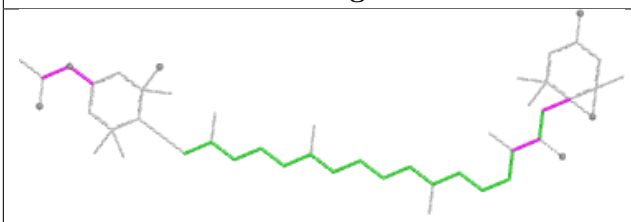
Ligand A86 X 305



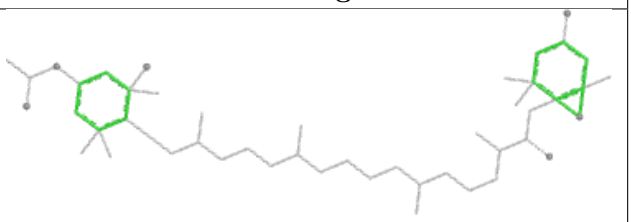
Bond lengths



Bond angles

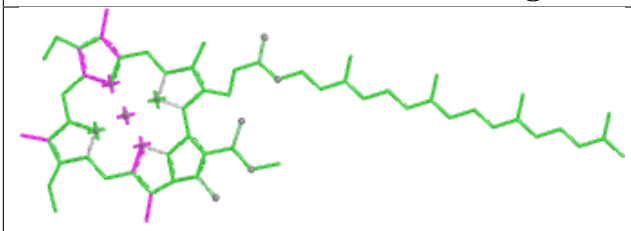


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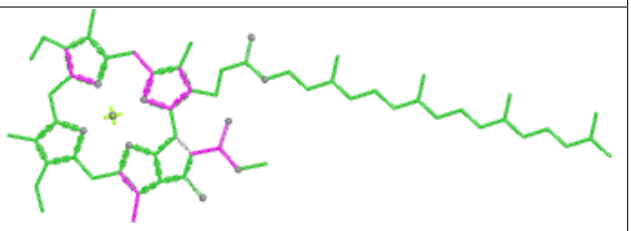


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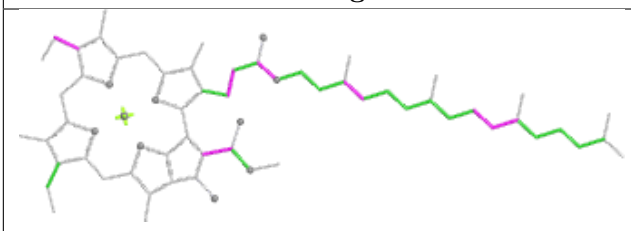
Ligand CLA C 209



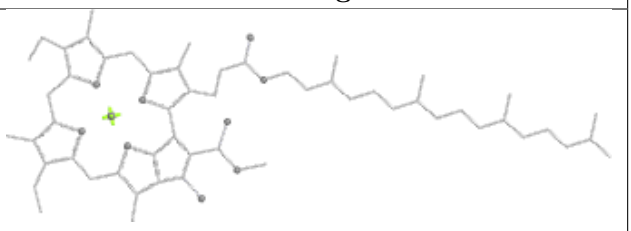
Bond lengths



Bond angles

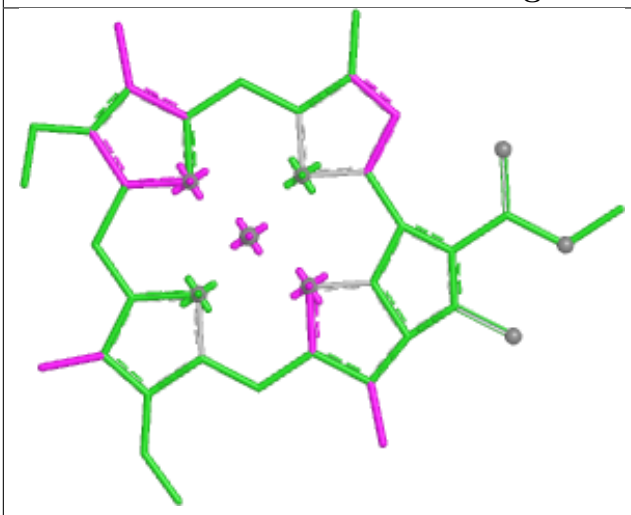


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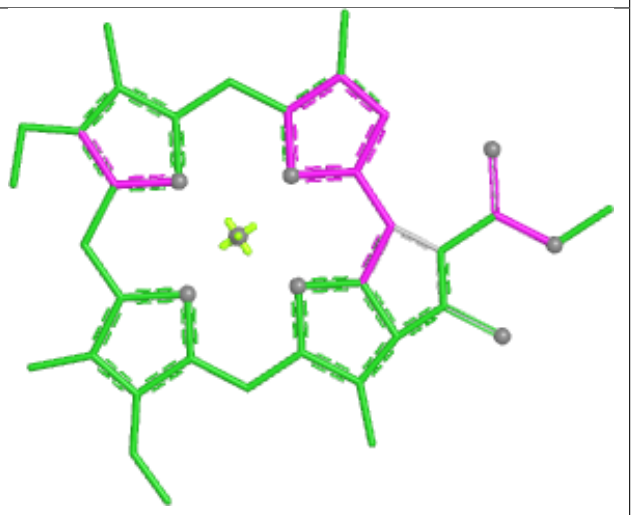


Rings

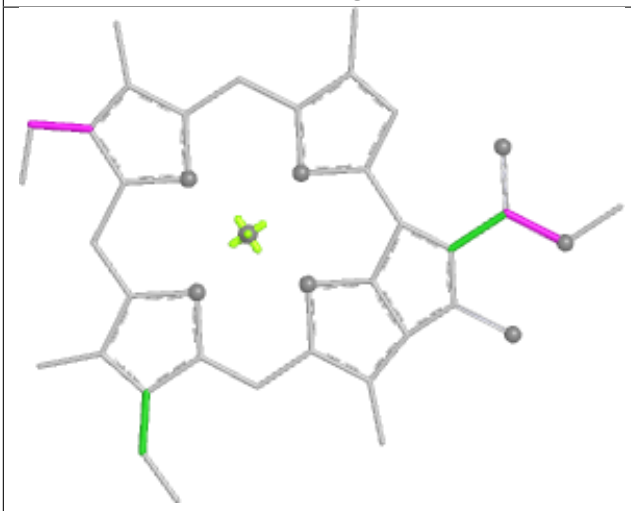
Ligand CLA O 312



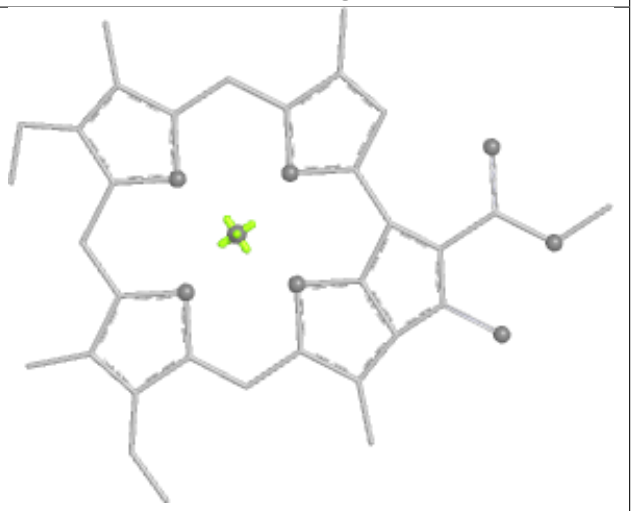
Bond lengths



Bond angles

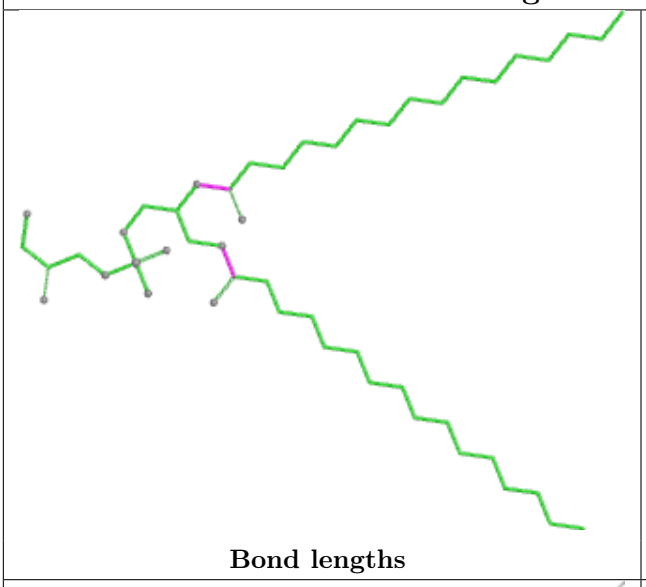


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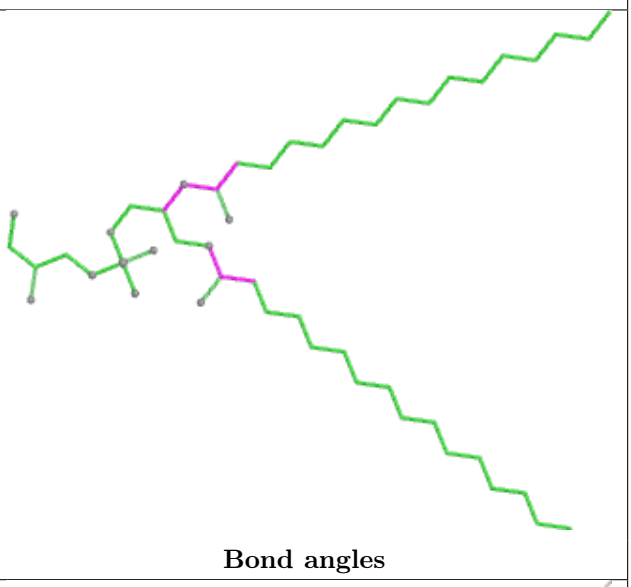


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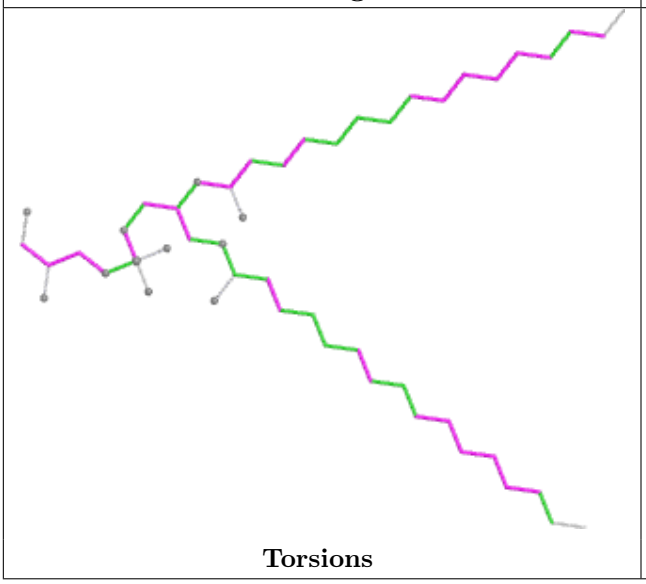
Ligand LHG R 323



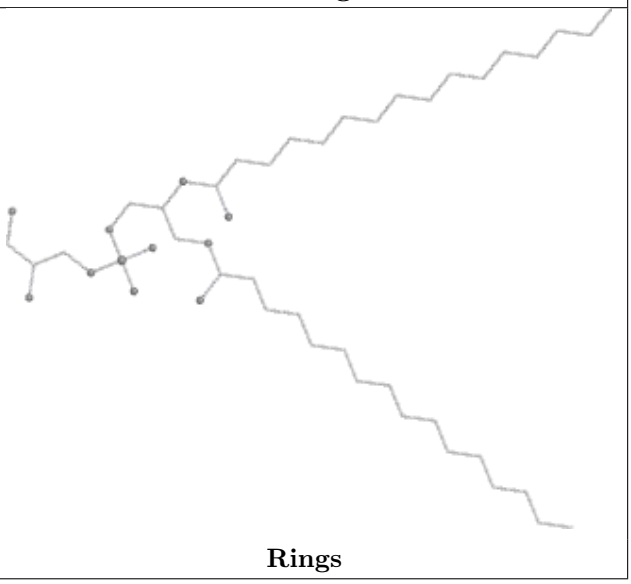
Bond lengths



Bond angles

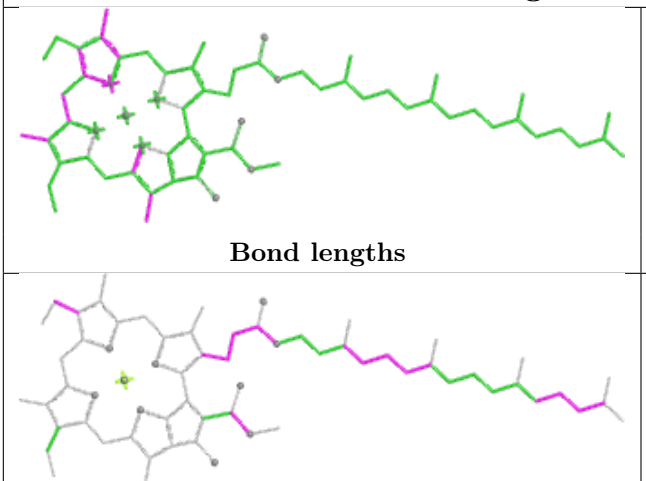


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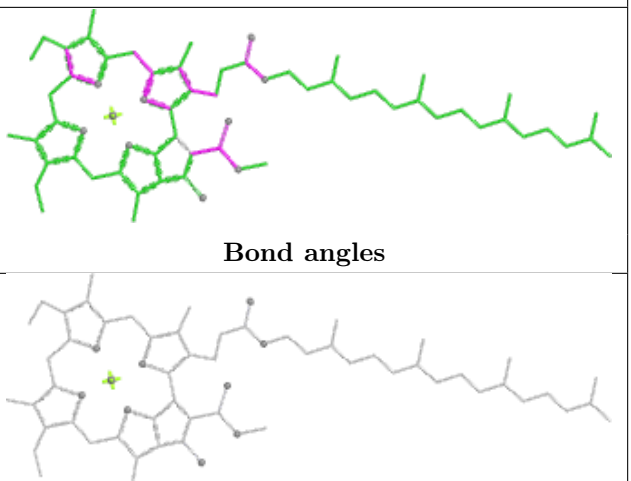


Rings

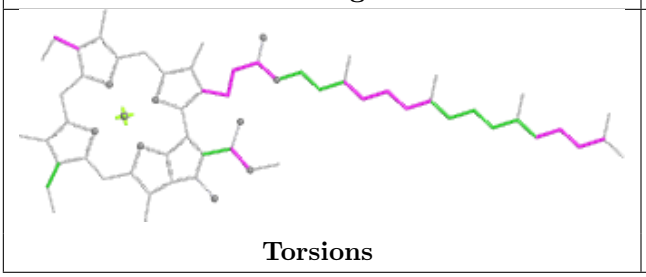
Ligand CLA T 309



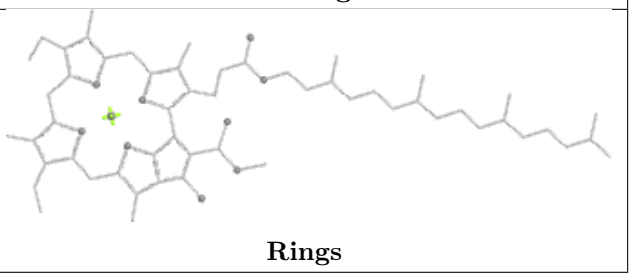
Bond lengths



Bond angles

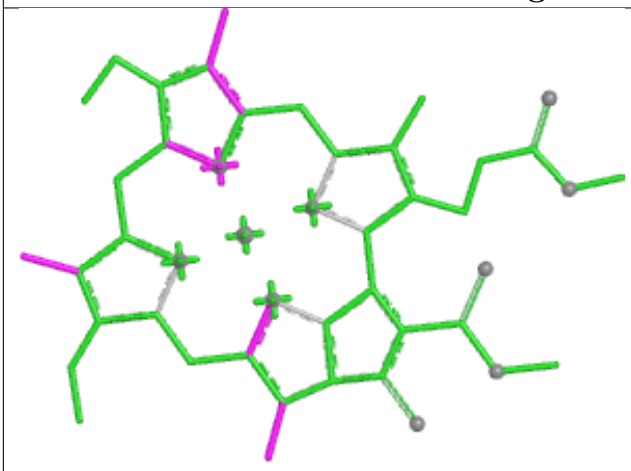


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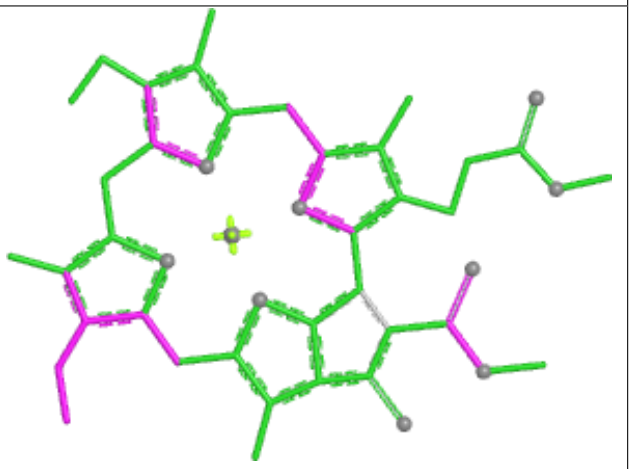


Rings

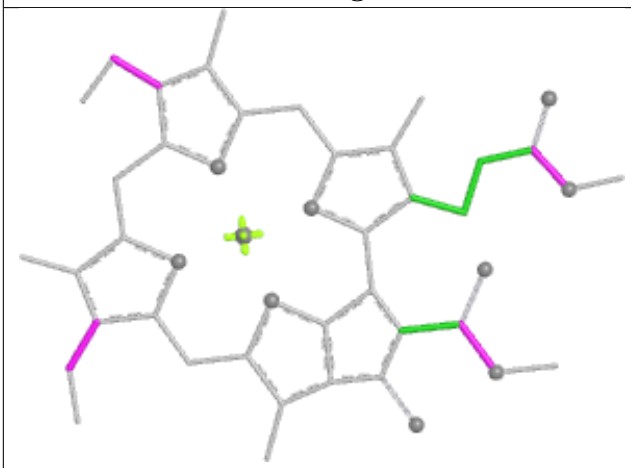
Ligand CLA J 316



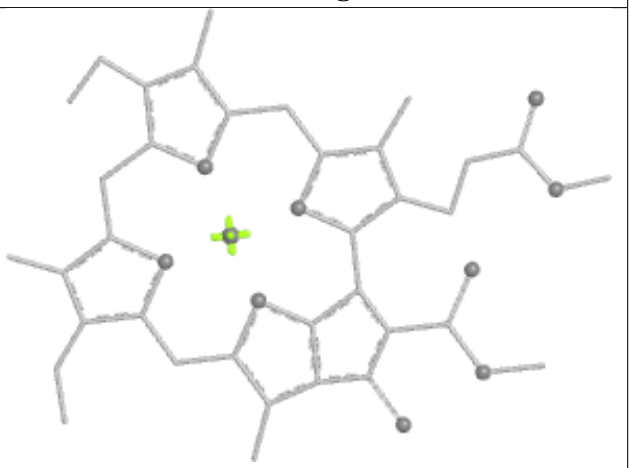
Bond lengths



Bond angles

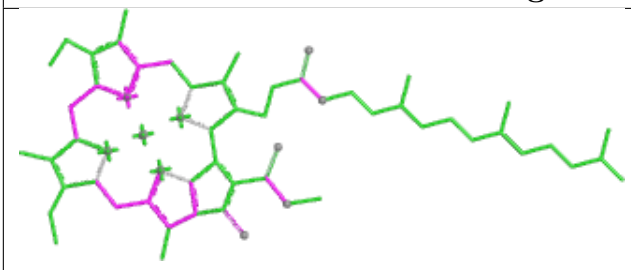


Torsions

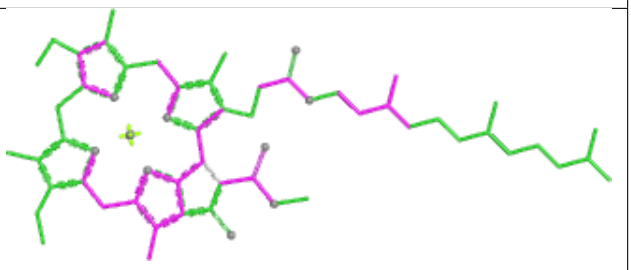


Rings

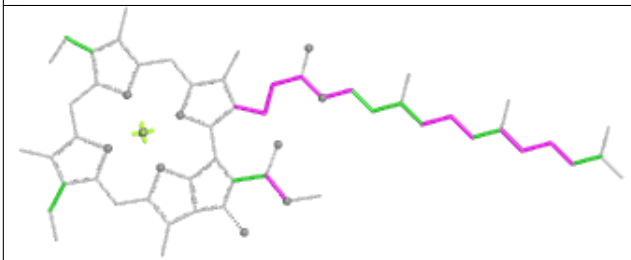
Ligand CLA b 816



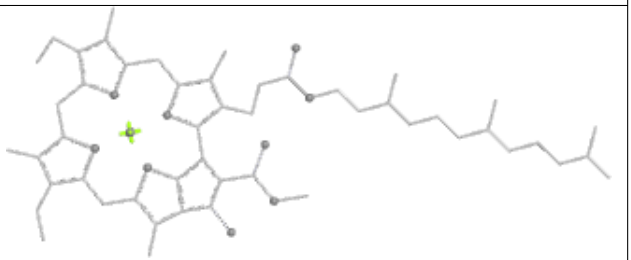
Bond lengths



Bond angles

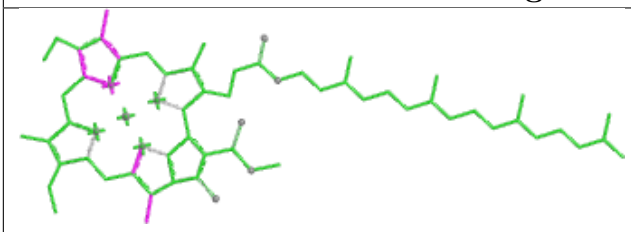


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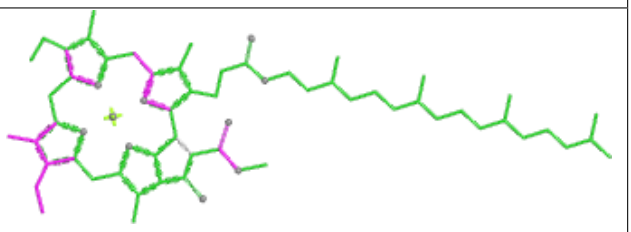


Rings

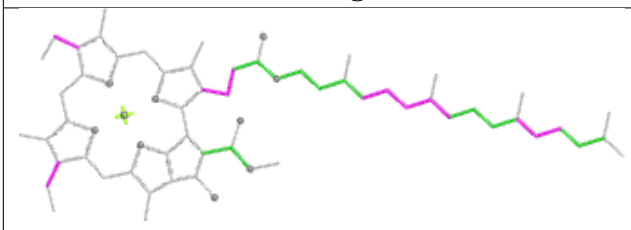
Ligand CLA E 316



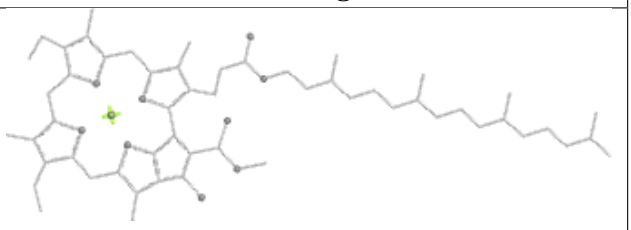
Bond lengths



Bond angles

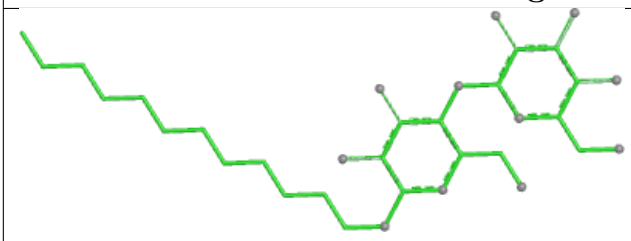


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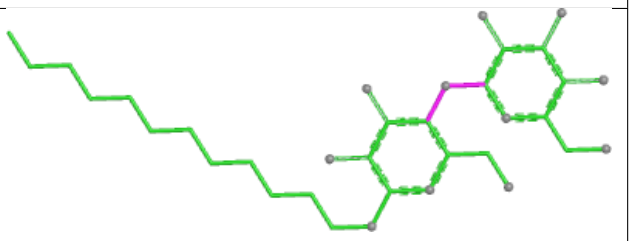


Rings

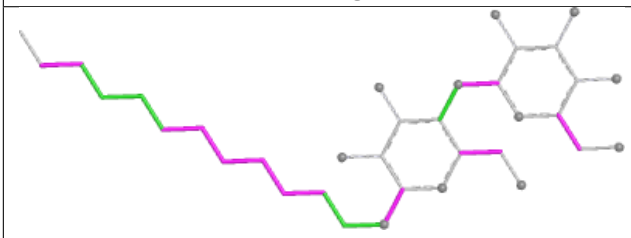
Ligand LMT I 317



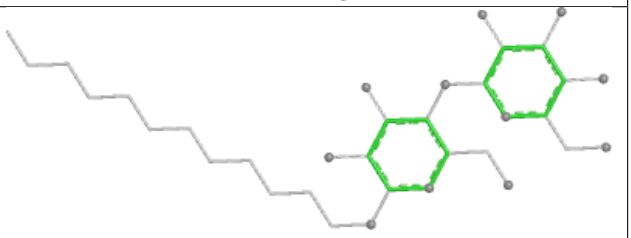
Bond lengths



Bond angles

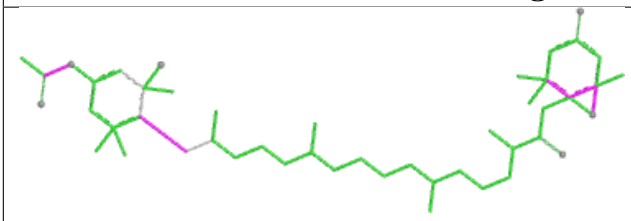


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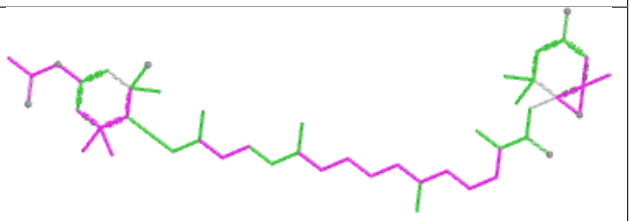


Rings

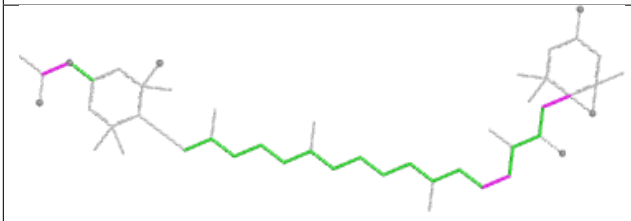
Ligand A86 G 305



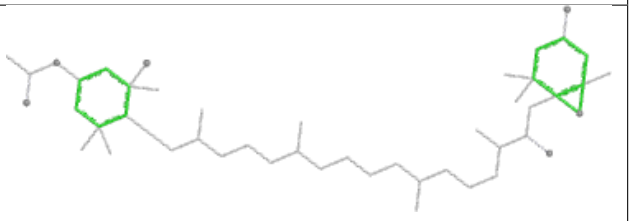
Bond lengths



Bond angles

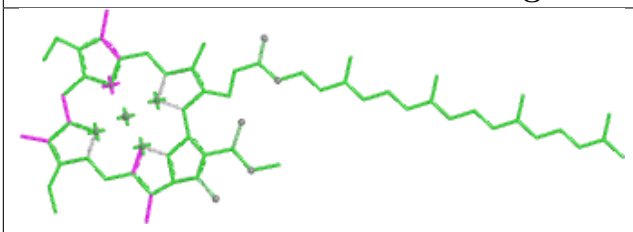


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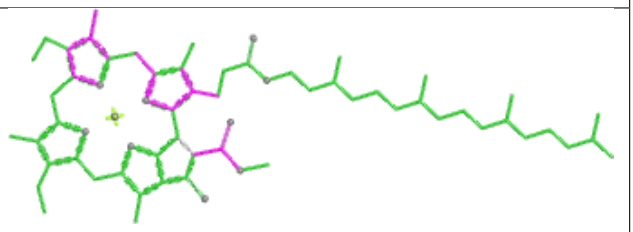


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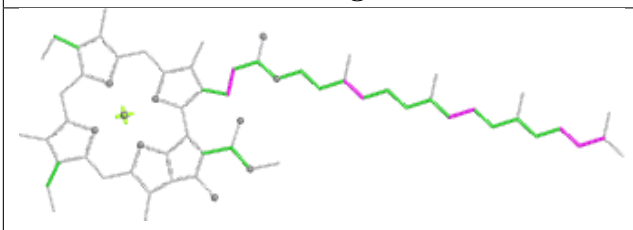
Ligand CLA D 310



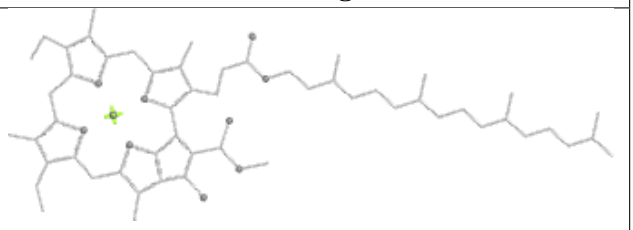
Bond lengths



Bond angles

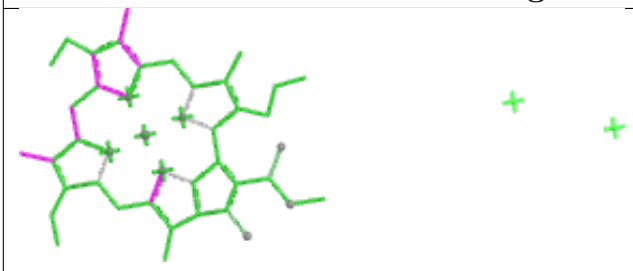


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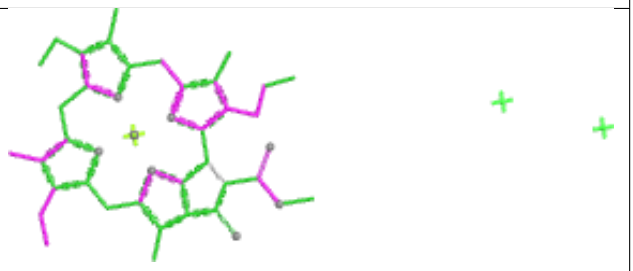


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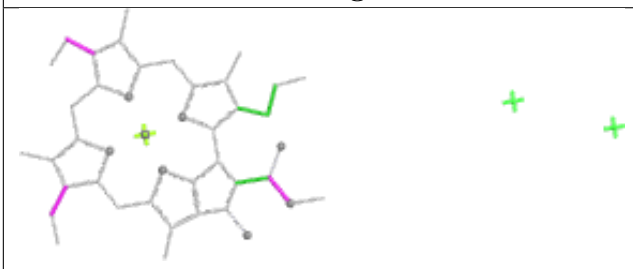
Ligand CLA S 315



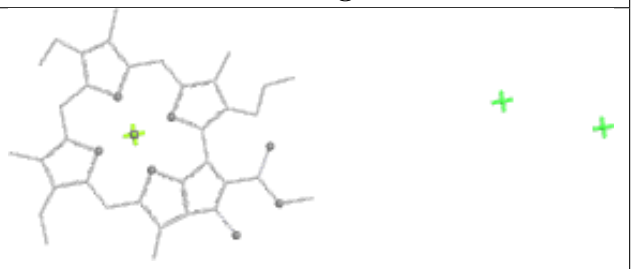
Bond lengths



Bond angles

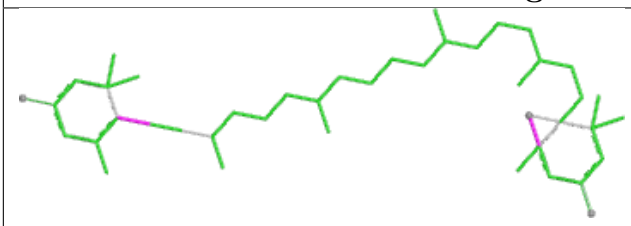


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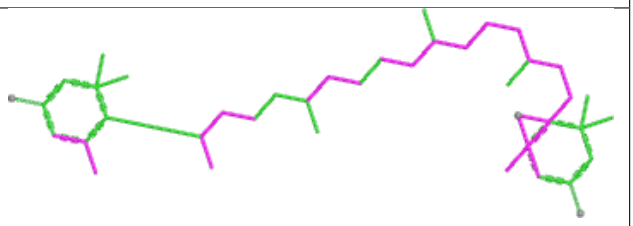


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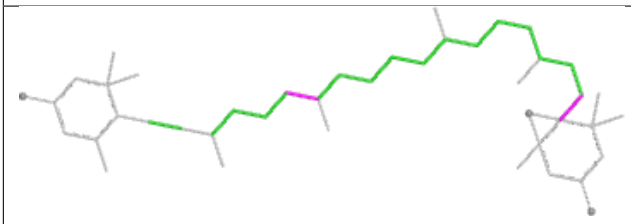
Ligand DD6 P 305



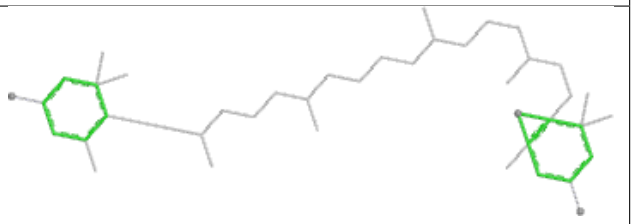
Bond lengths



Bond angles

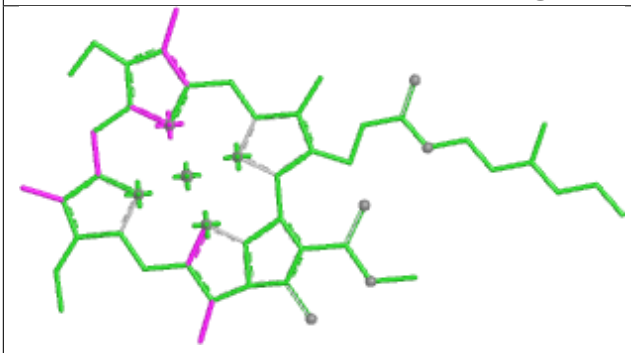


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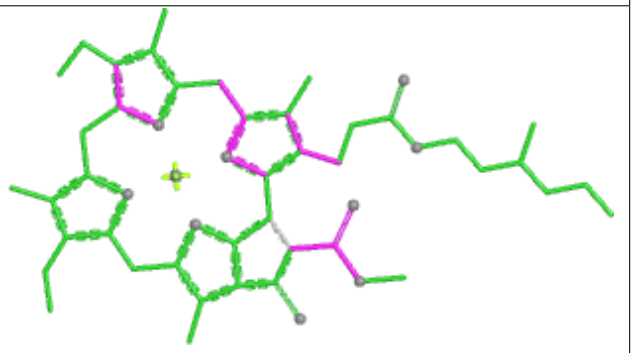


Rings

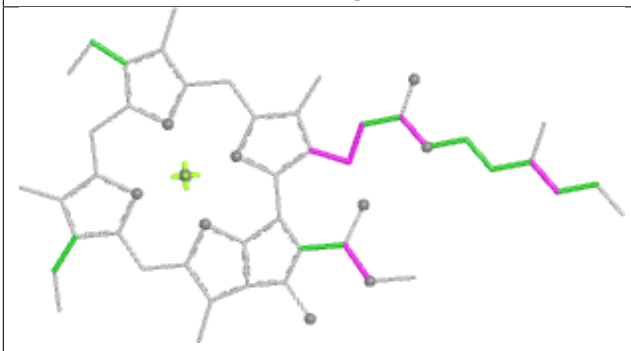
Ligand CLA f 805



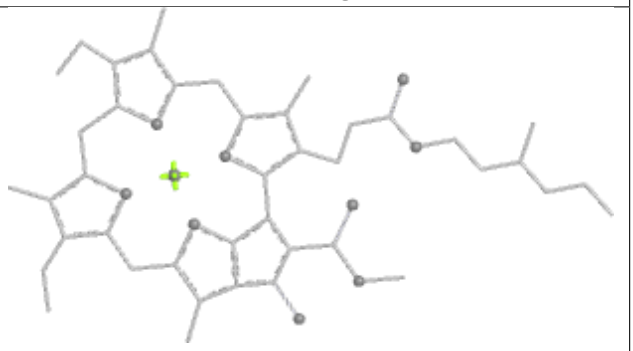
Bond lengths



Bond angles

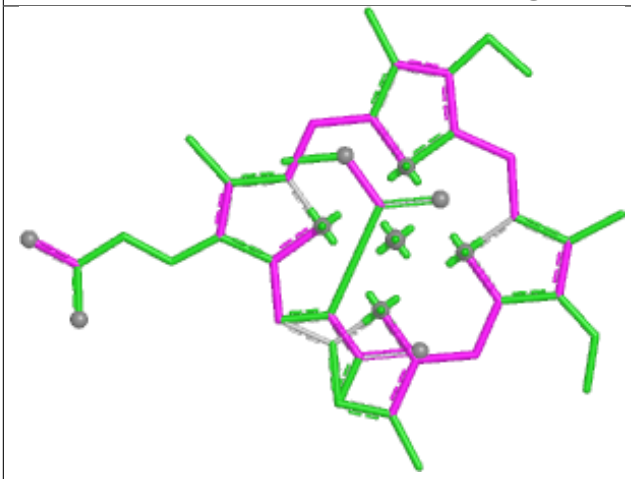


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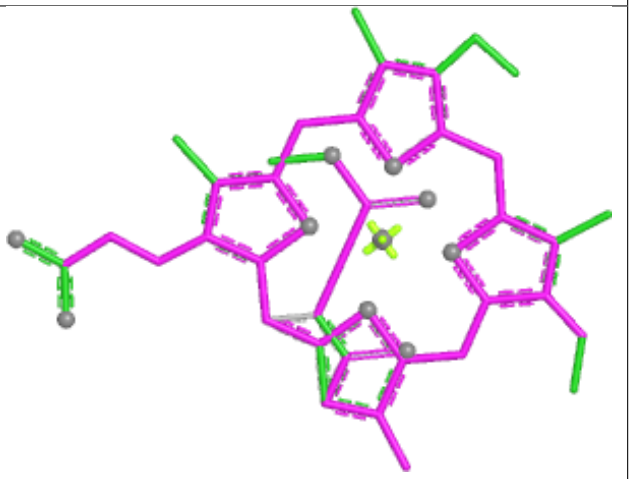


Rings

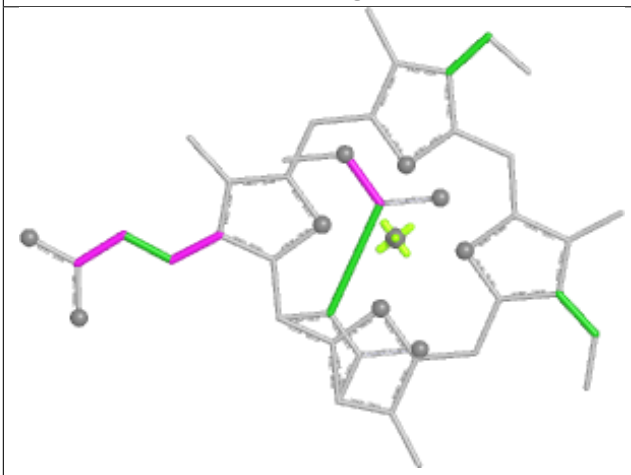
Ligand KC1 H 313



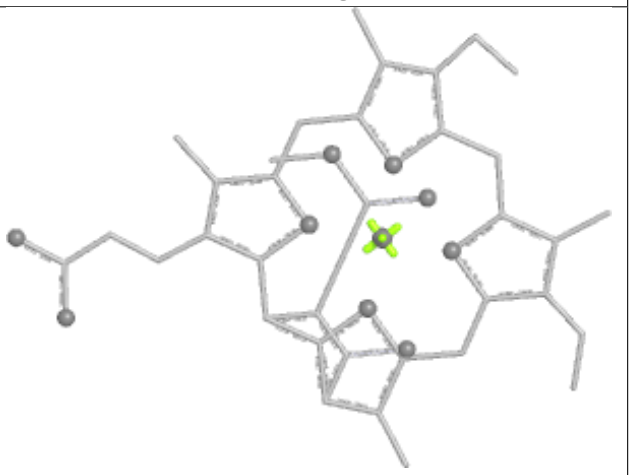
Bond lengths



Bond angles

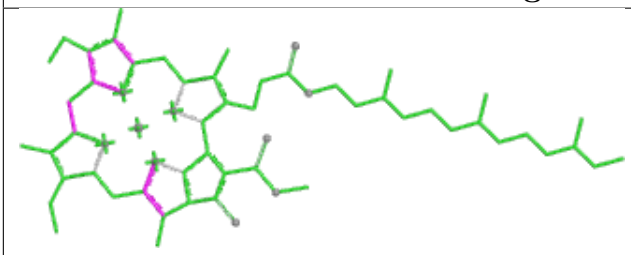


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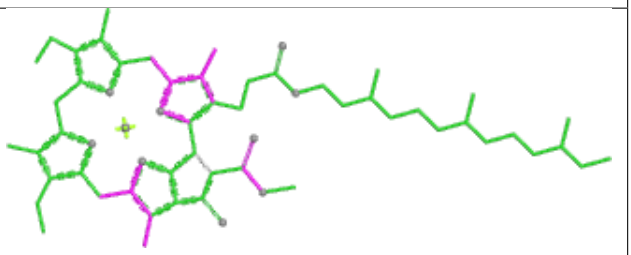


Rings

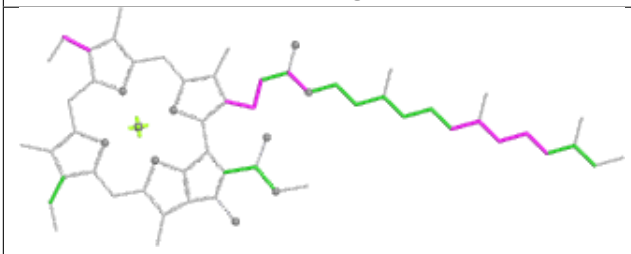
Ligand CLA V 305



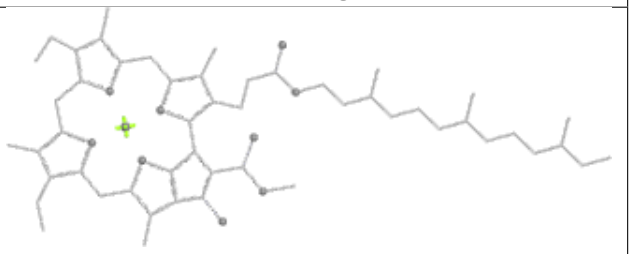
Bond lengths



Bond angles

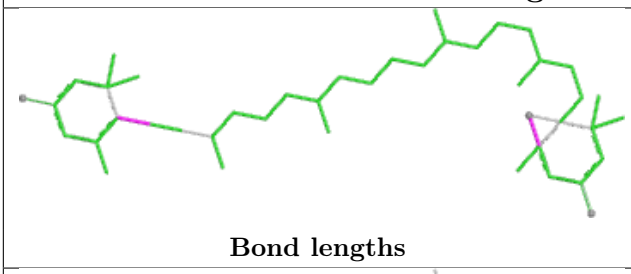


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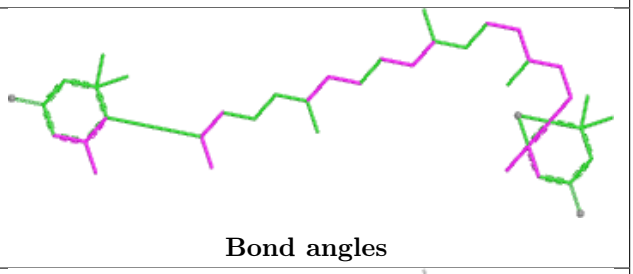


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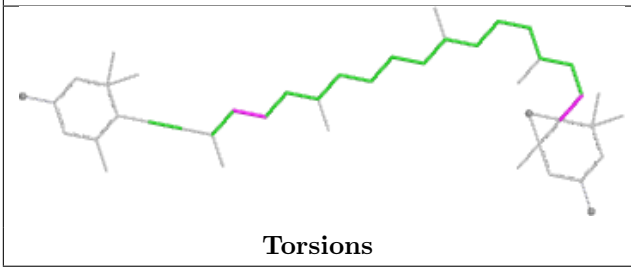
Ligand DD6 E 301



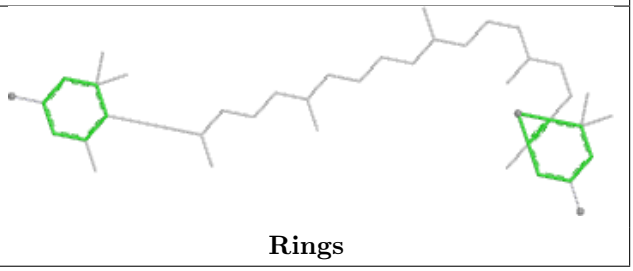
Bond lengths



Bond angles

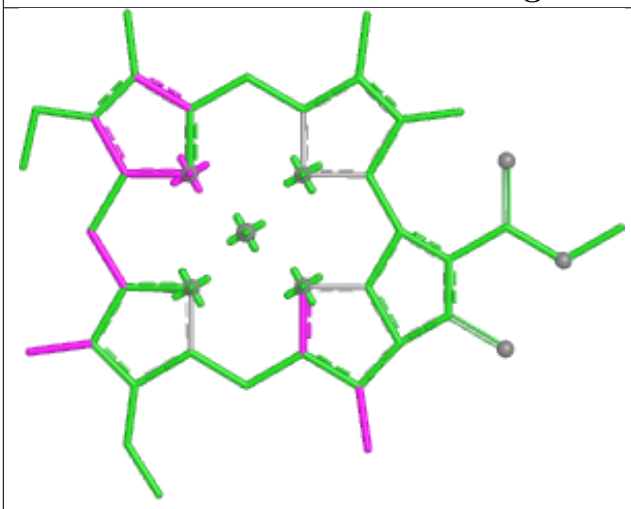


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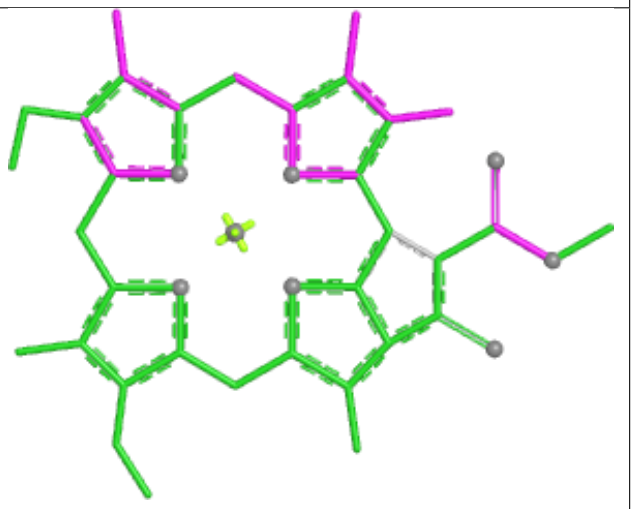


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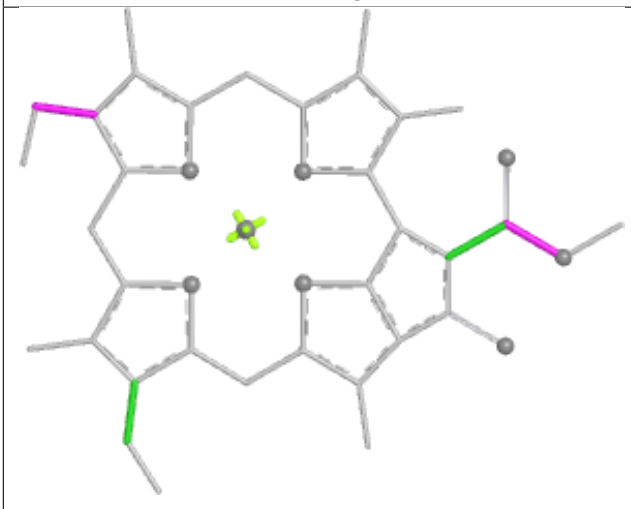
Ligand CLA R 318



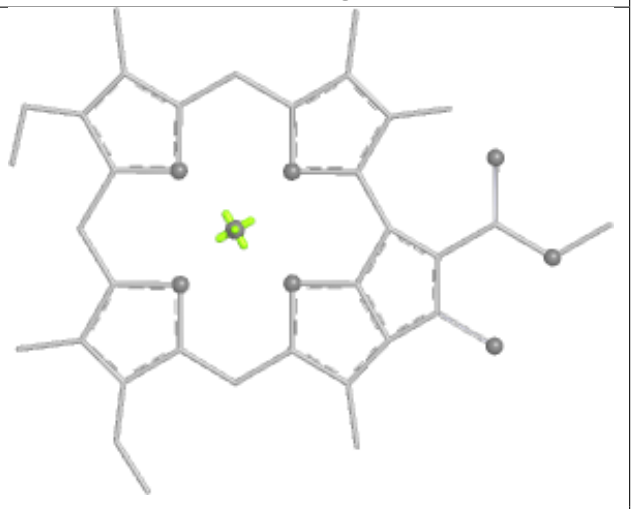
Bond lengths



Bond angles

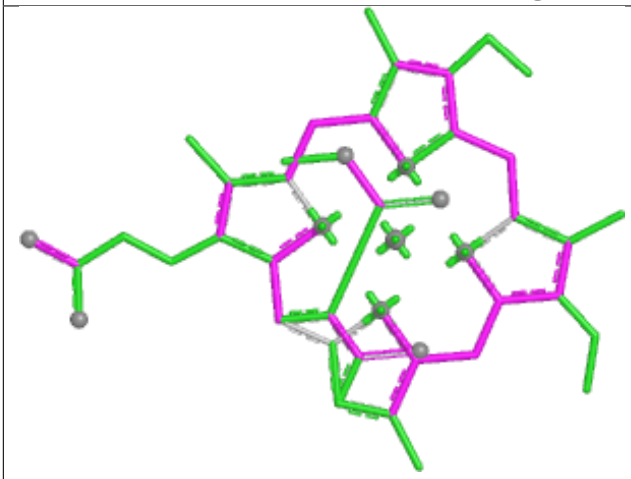


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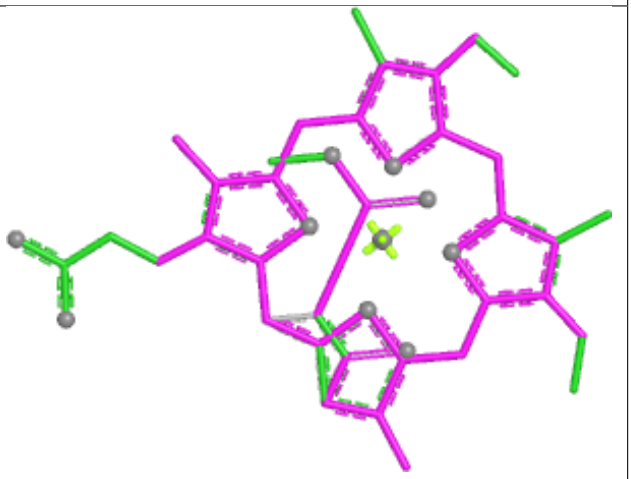


Rings

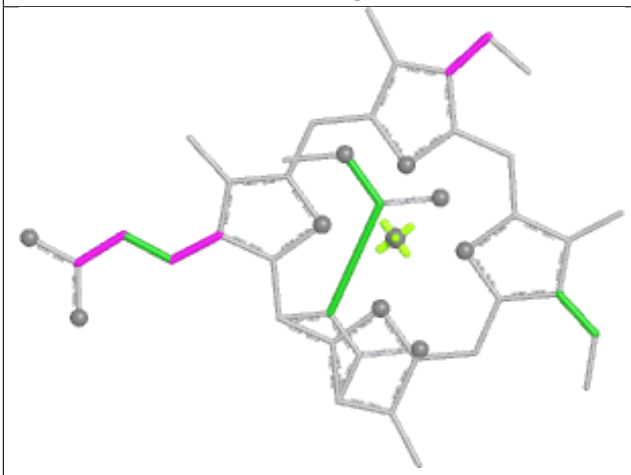
Ligand KC1 S 316



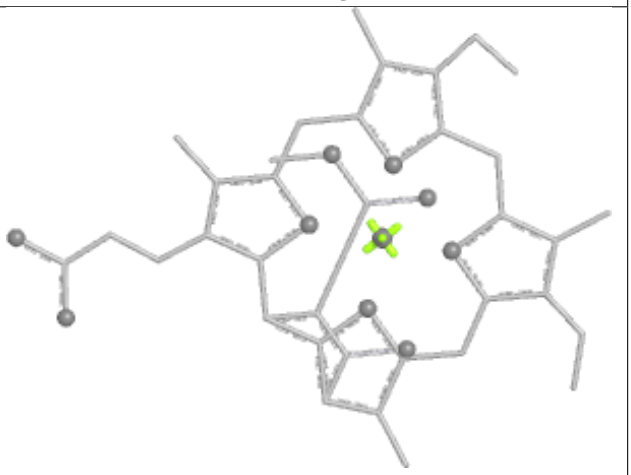
Bond lengths



Bond angles

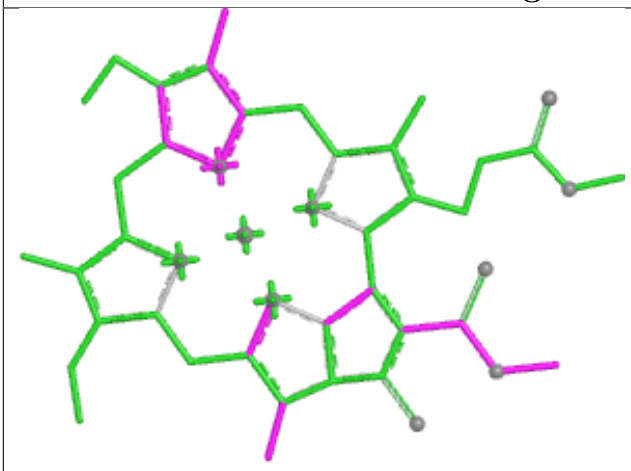


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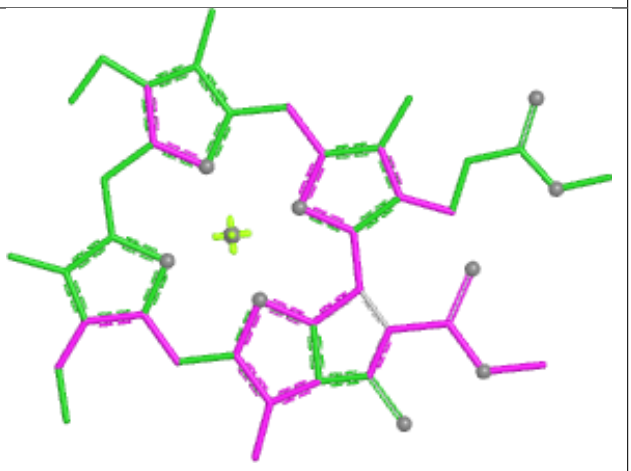


Rings

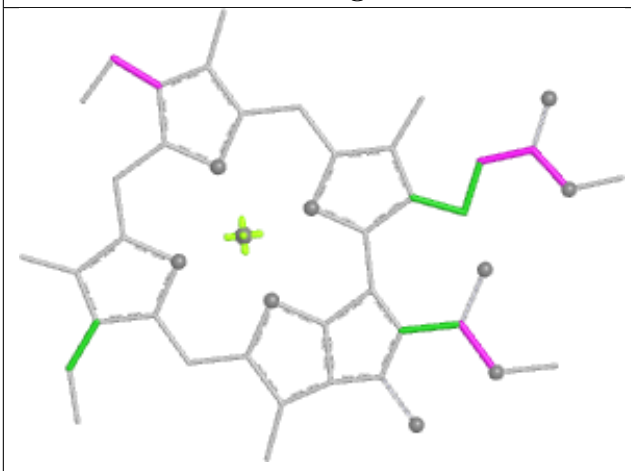
Ligand CLA H 310



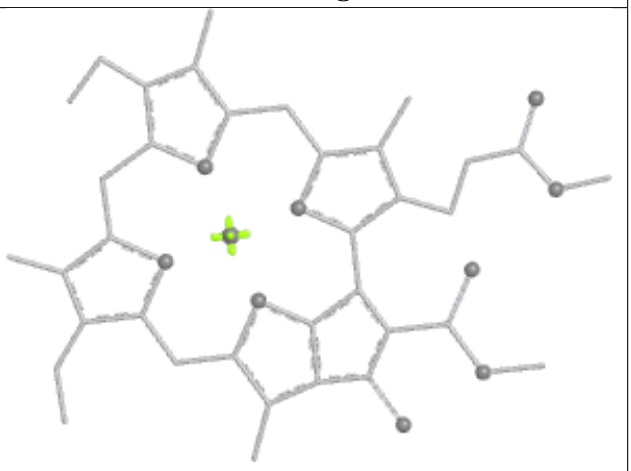
Bond lengths



Bond angles

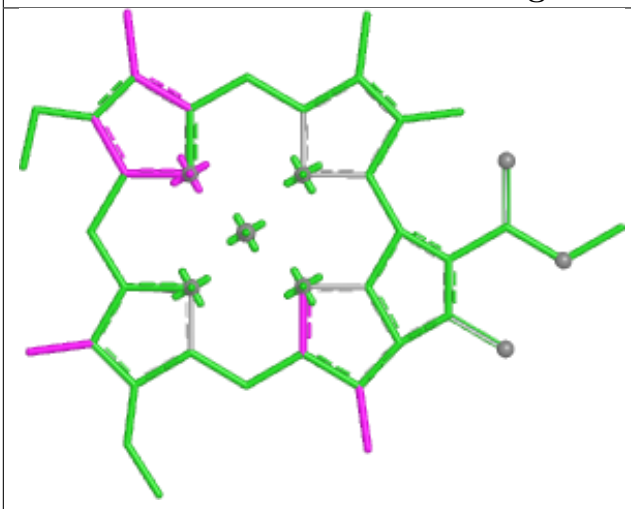


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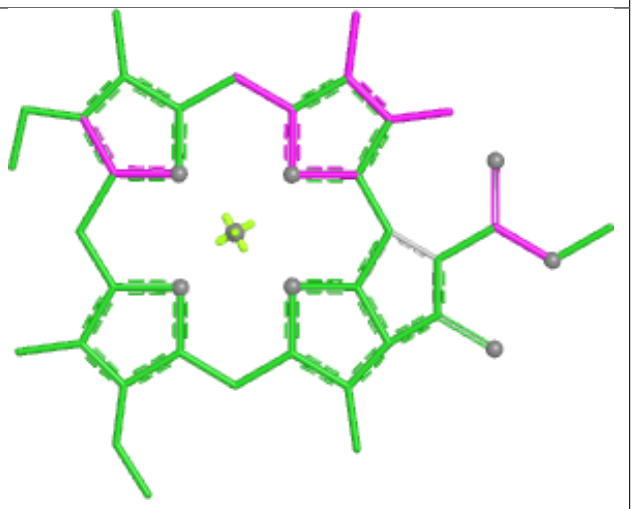


Rings

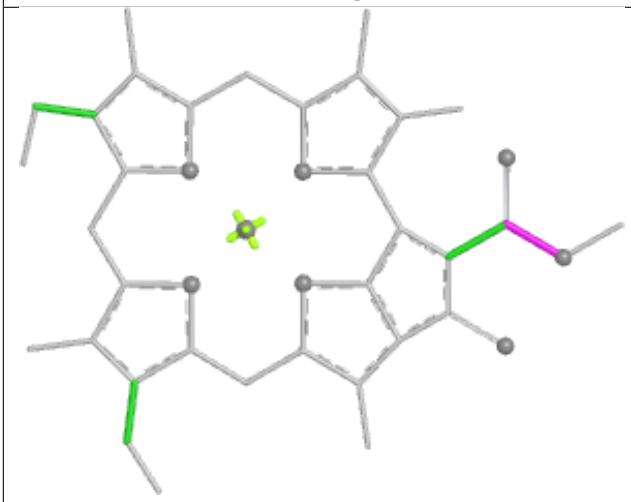
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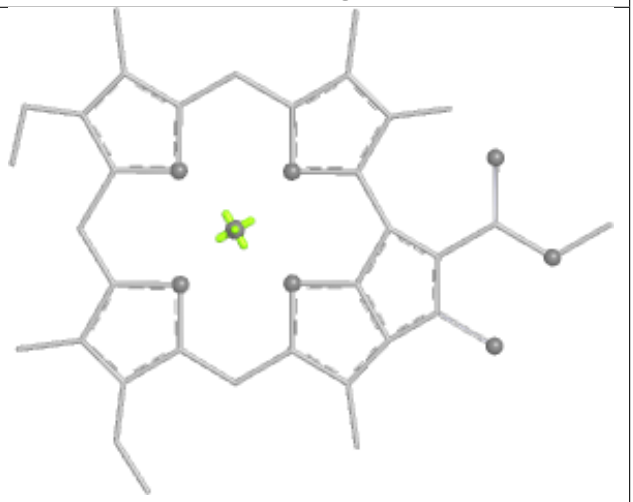
Bond lengths



Bond angles

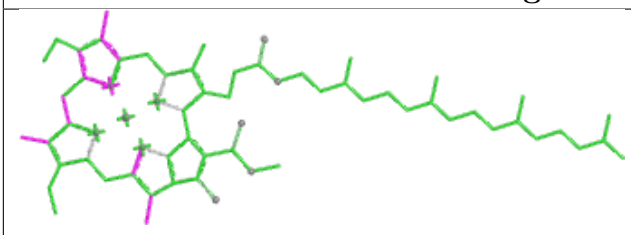


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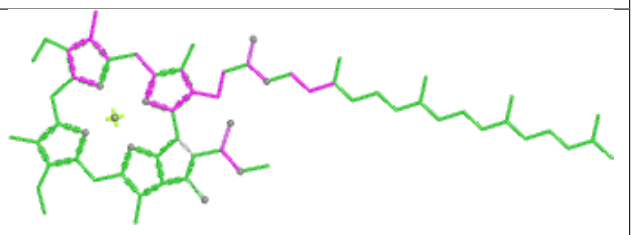


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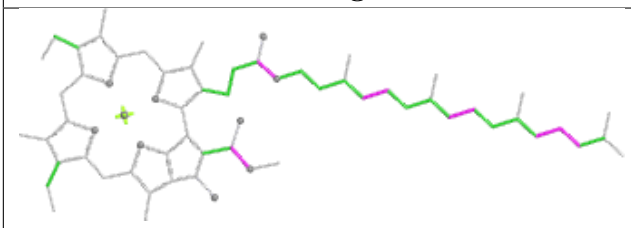
Ligand CLA D 313



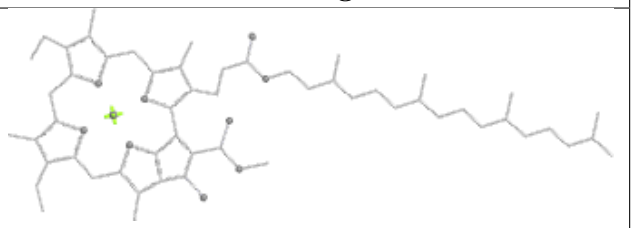
Bond lengths



Bond angles

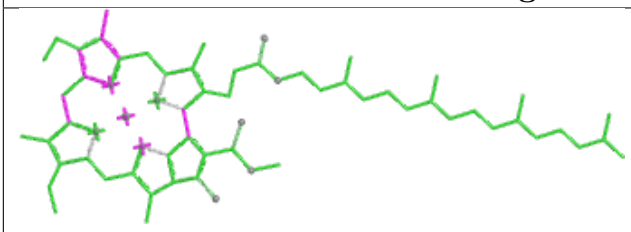


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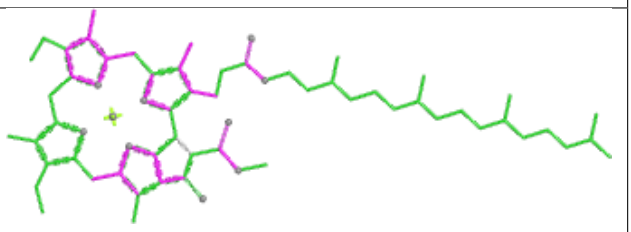


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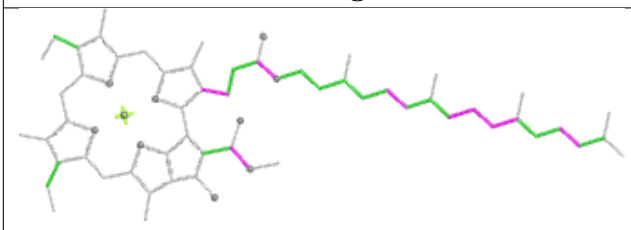
Ligand CLA W 212



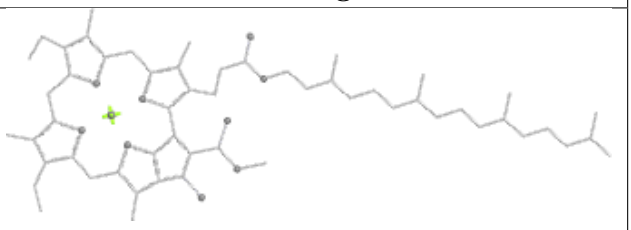
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Bond angles

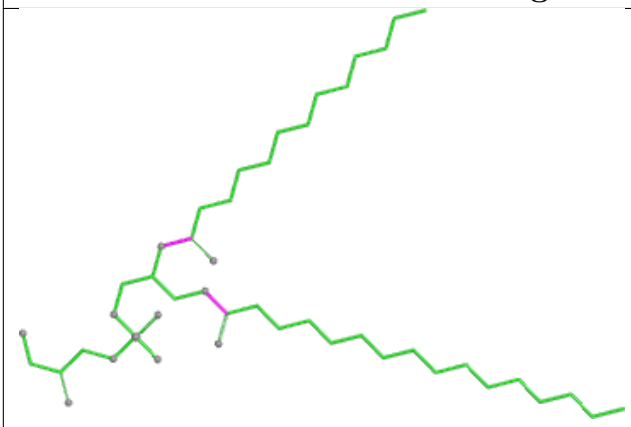


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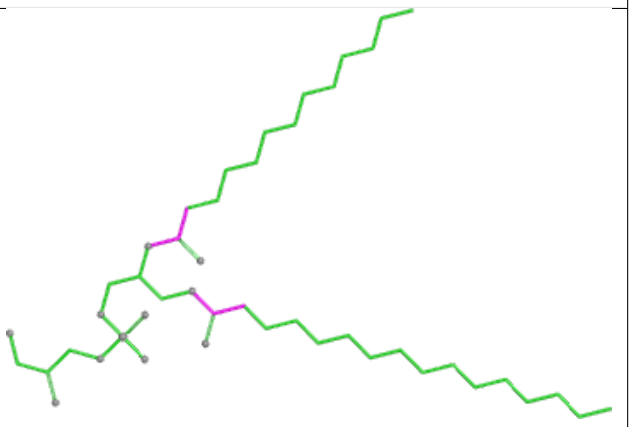


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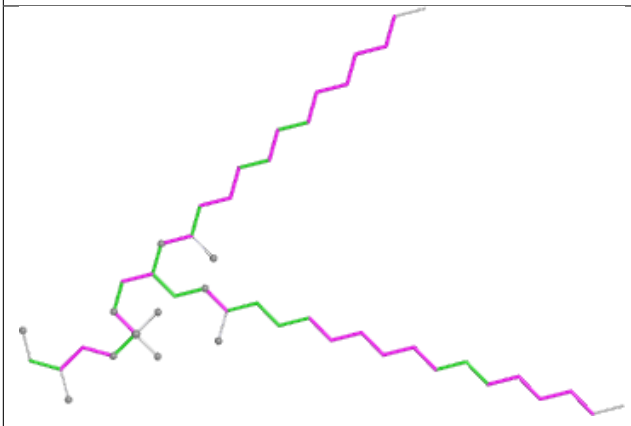
Ligand LHG i 104



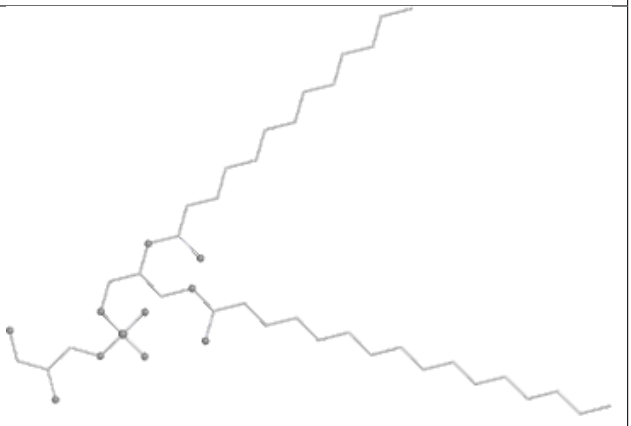
Bond lengths



Bond angles

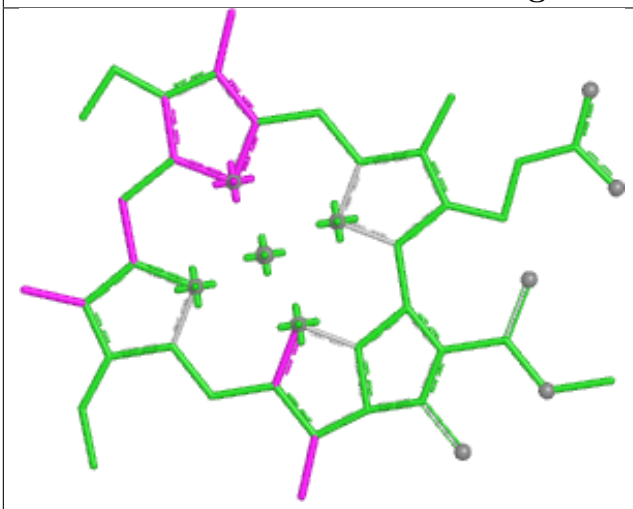


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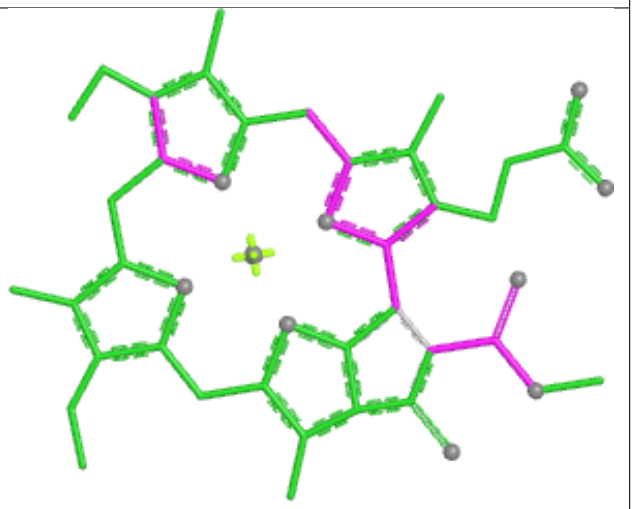


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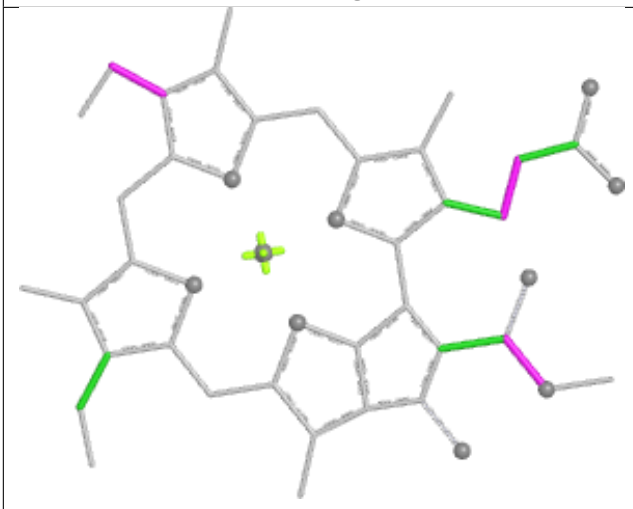
Ligand CLA a 834



Bond lengths



Bond angles

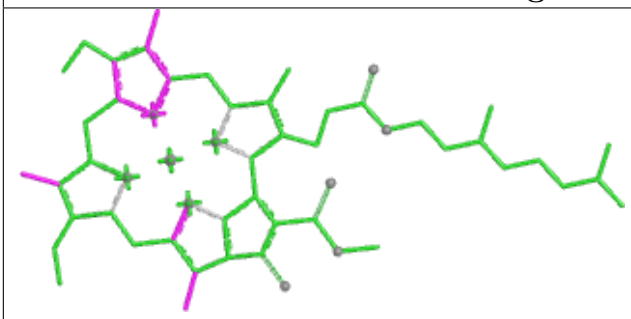


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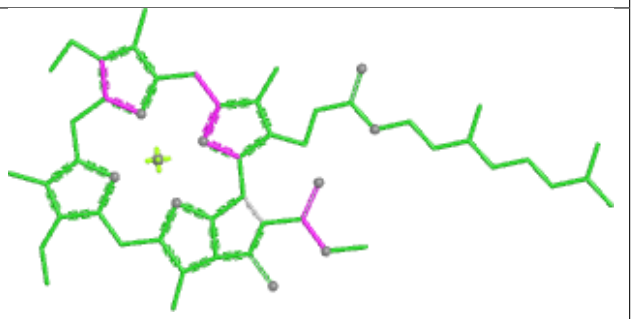


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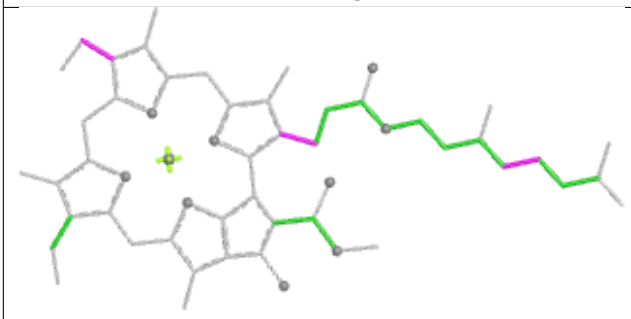
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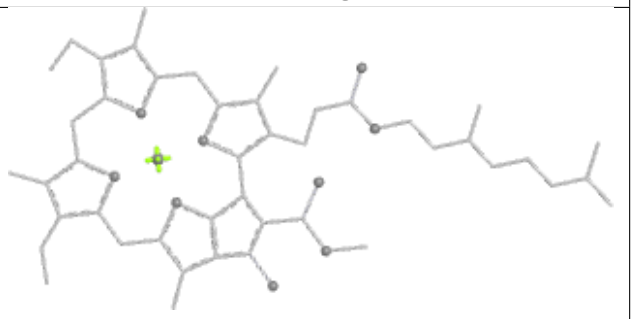
Bond lengths



Bond angles

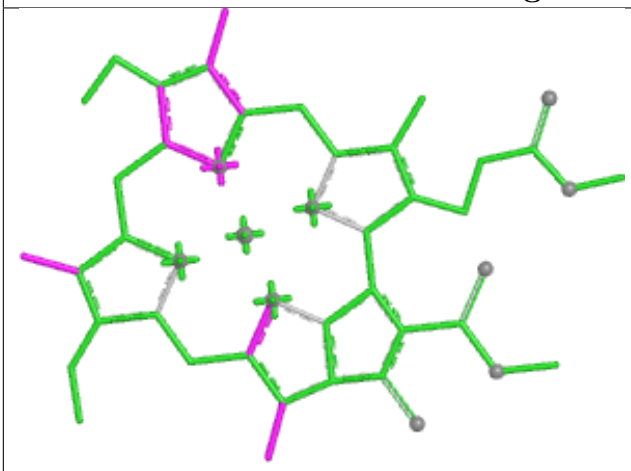


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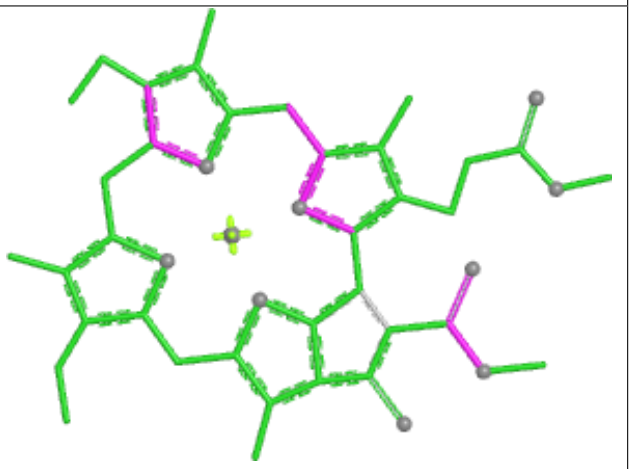


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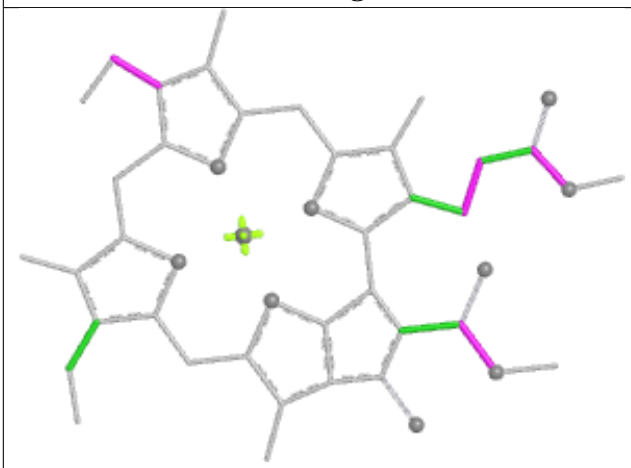
Ligand CLA A 309



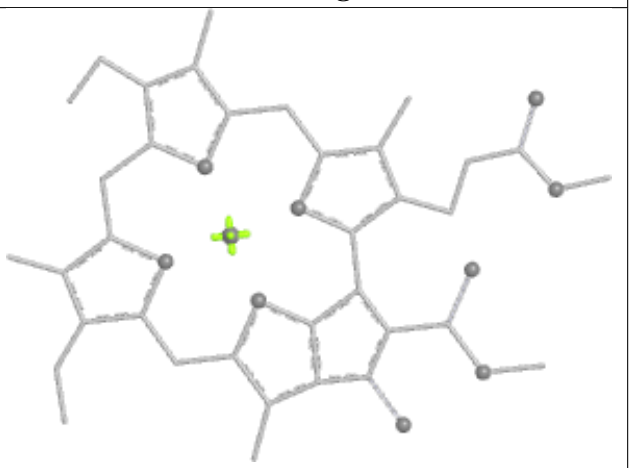
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Bond angles

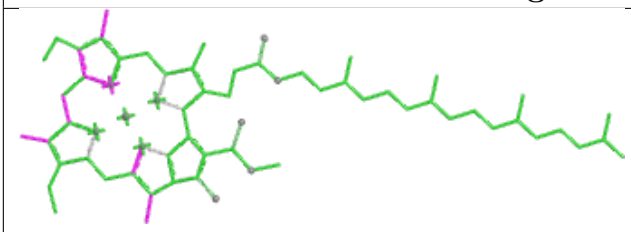


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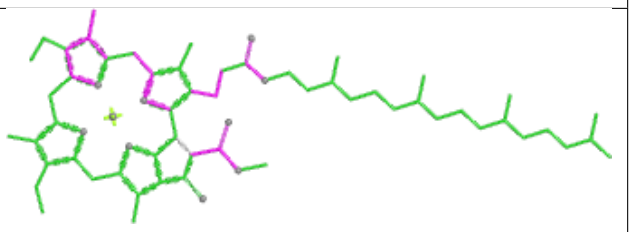


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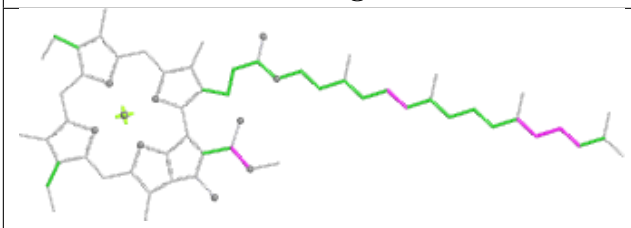
Ligand CLA b 837



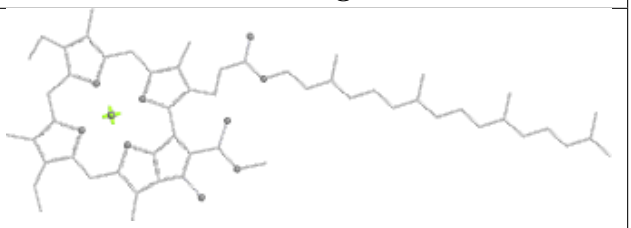
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Bond angles

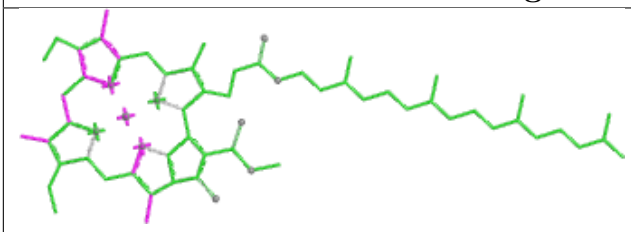


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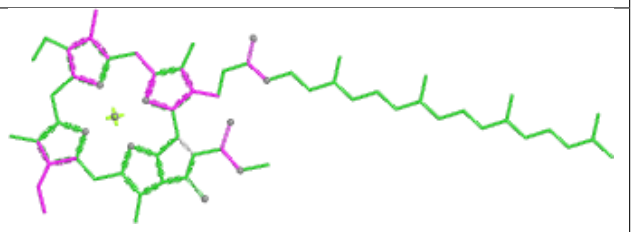


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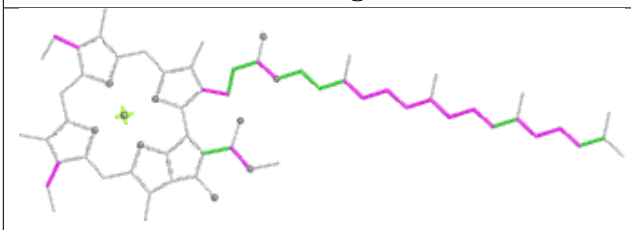
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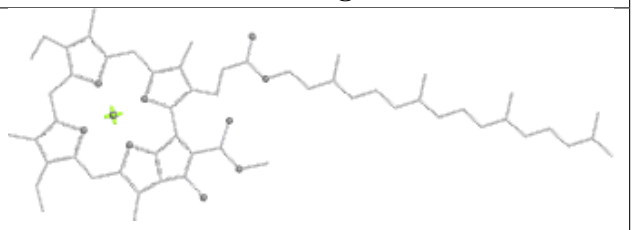
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Bond angles

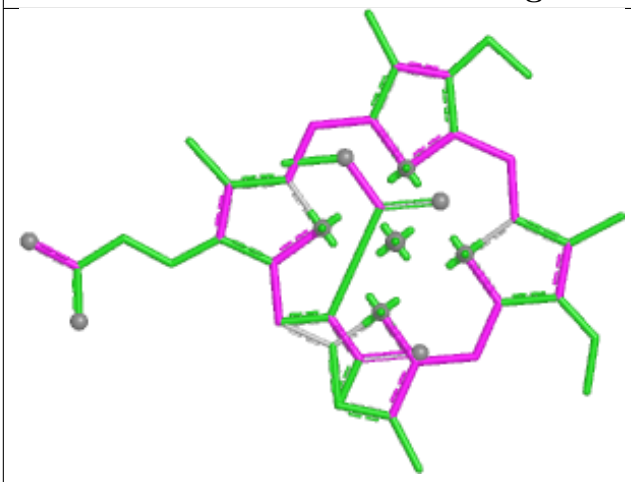


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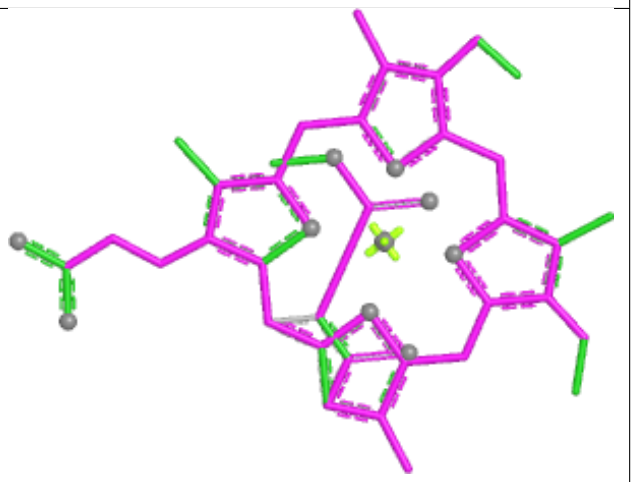


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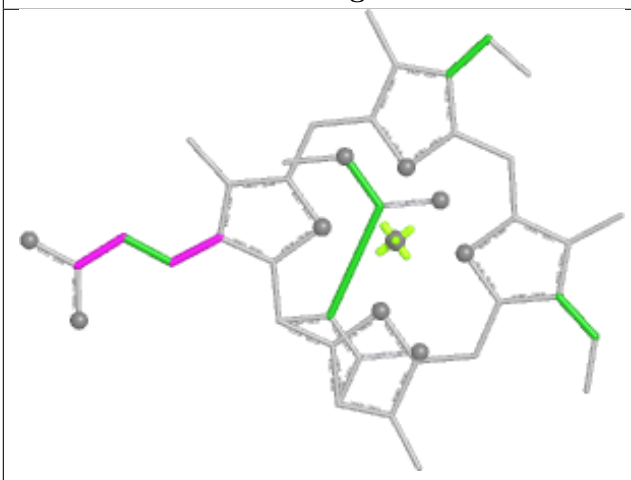
Ligand KC1 D 314



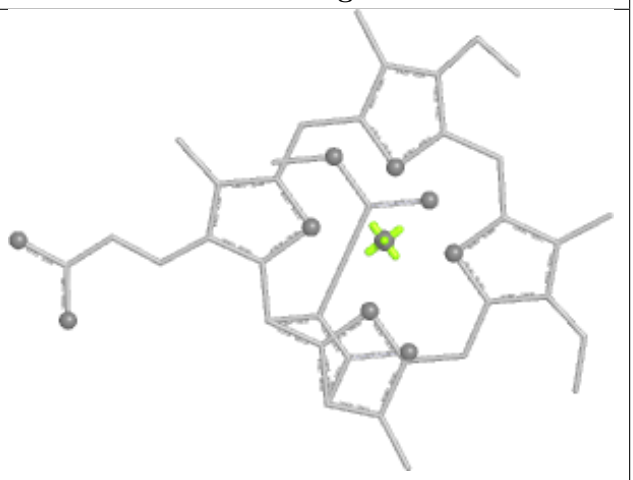
Bond lengths



Bond angles

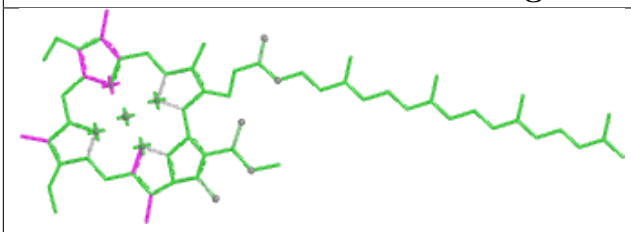


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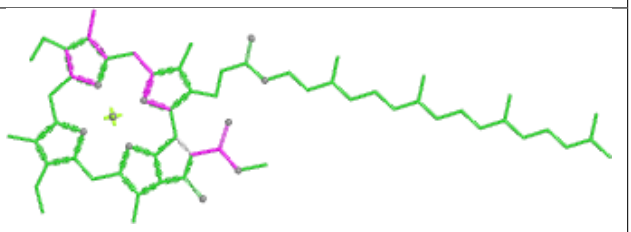


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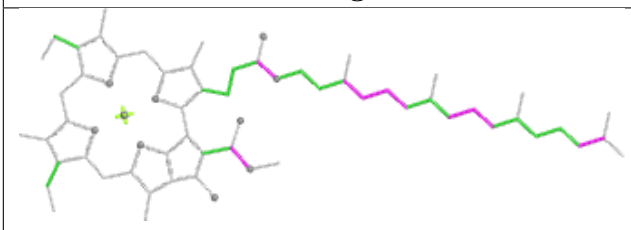
Ligand CLA P 313



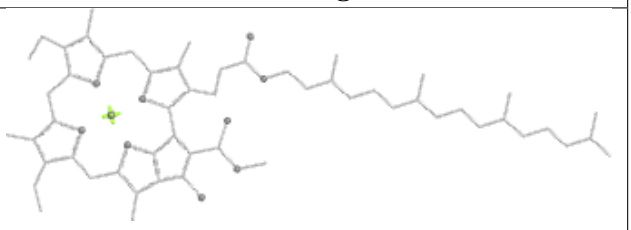
Bond lengths



Bond angles

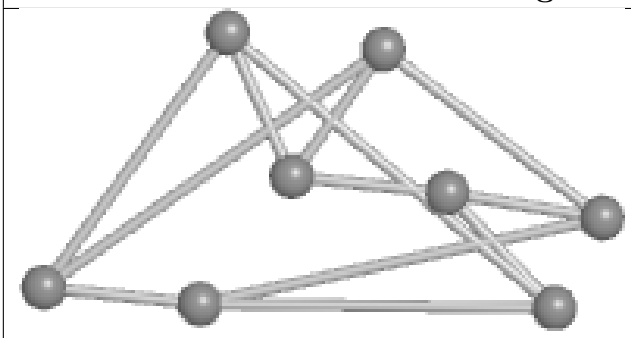


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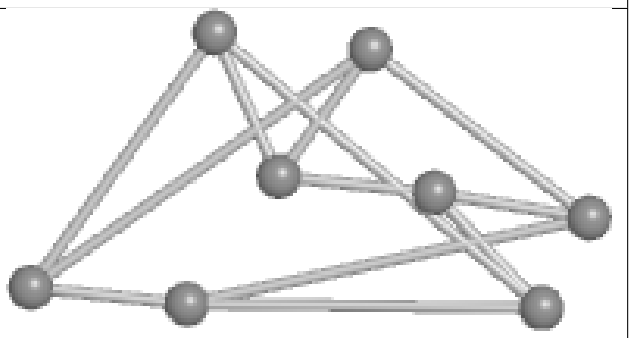


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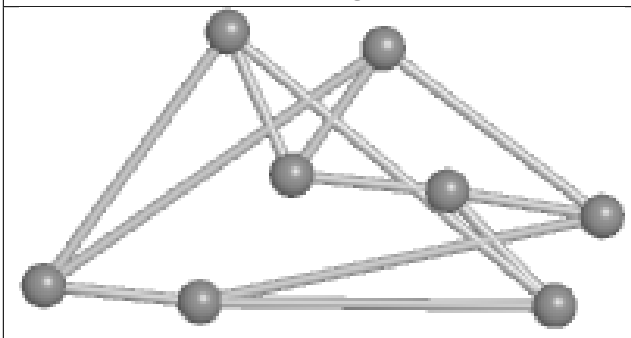
Ligand SF4 c 102



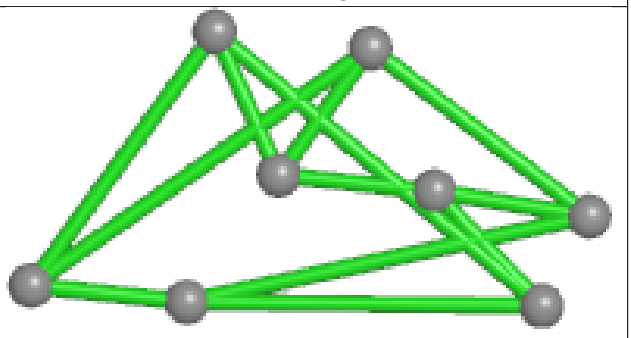
Bond lengths



Bond angles

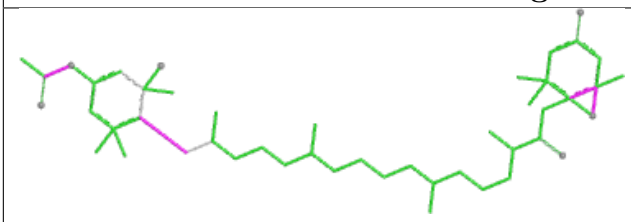


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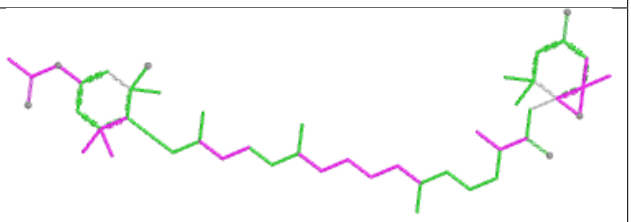


Rings

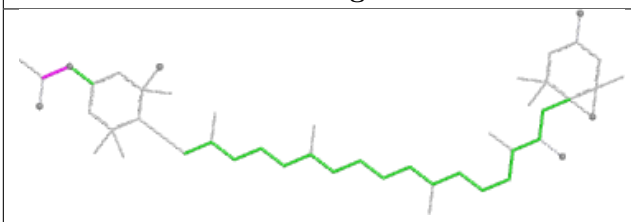
Ligand A86 P 307



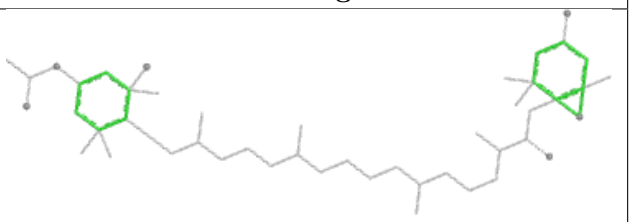
Bond lengths



Bond angles

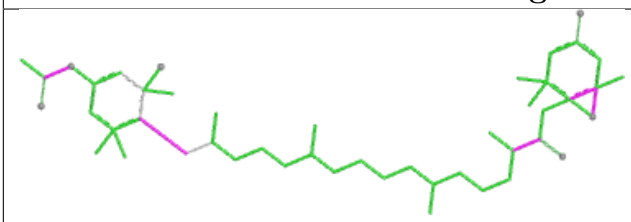


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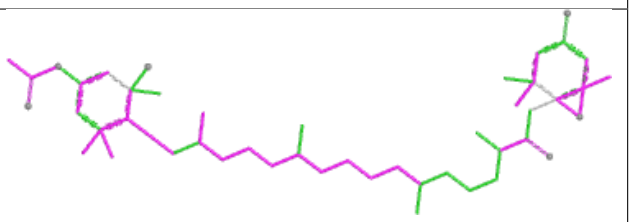


Rings

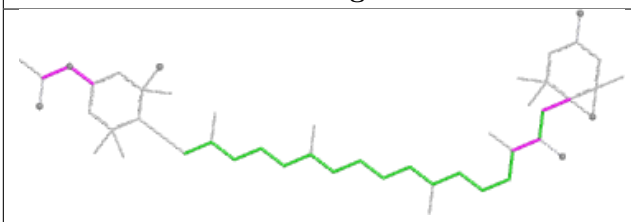
Ligand A86 X 304



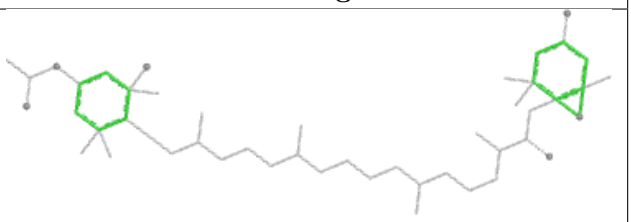
Bond lengths



Bond angles

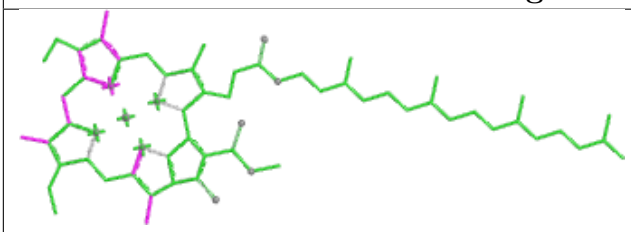


Torsions

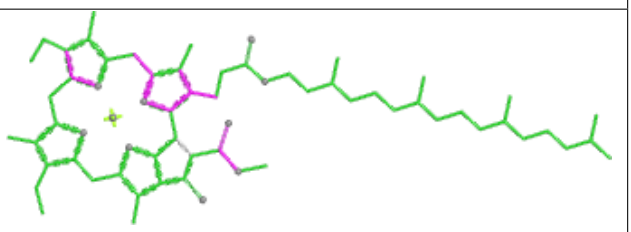


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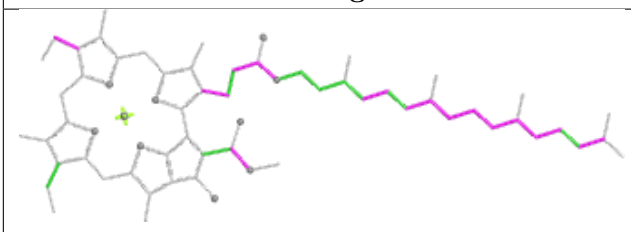
Ligand CLA F 312



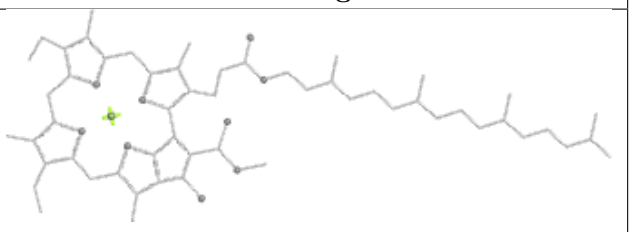
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Bond angles

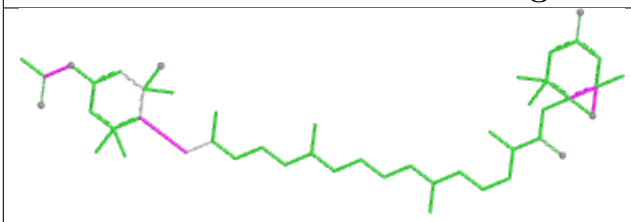


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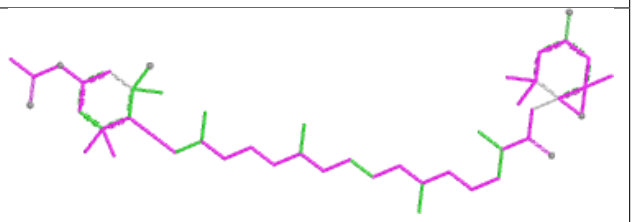


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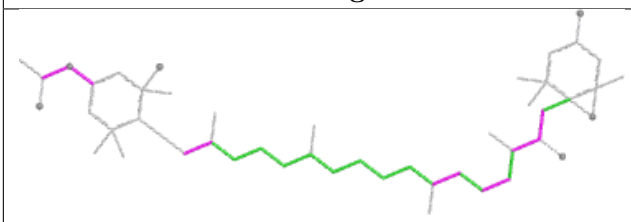
Ligand A86 B 303



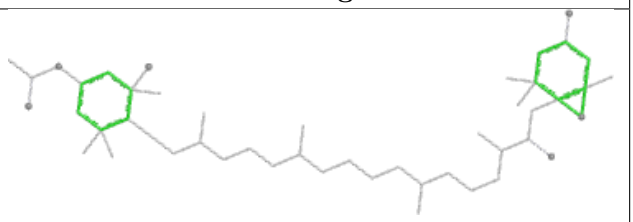
Bond lengths



Bond angles

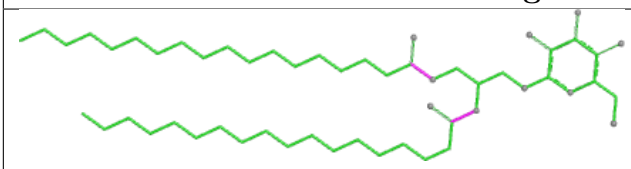


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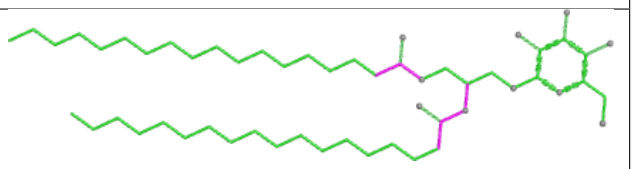


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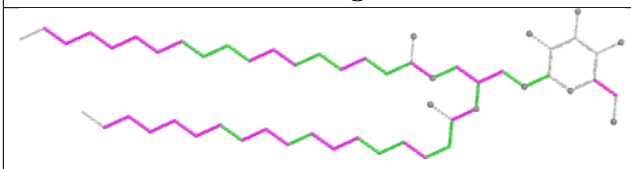
Ligand LMG J 318



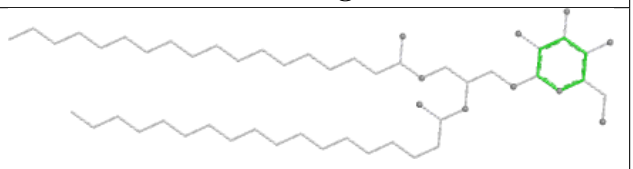
Bond lengths



Bond angles

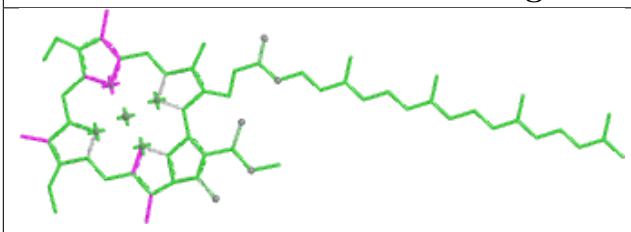


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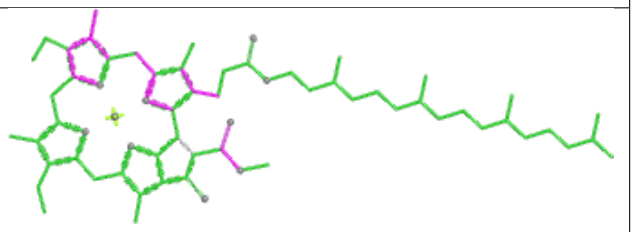


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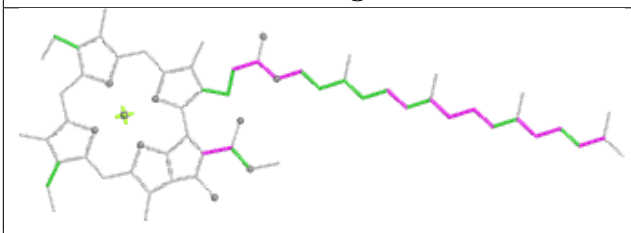
Ligand CLA E 311



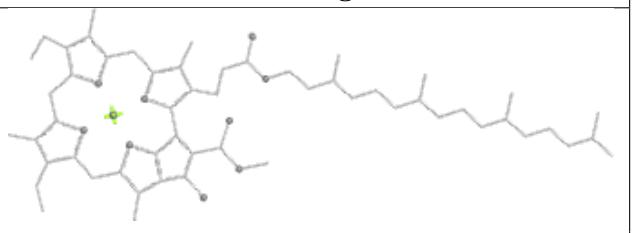
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Bond angles

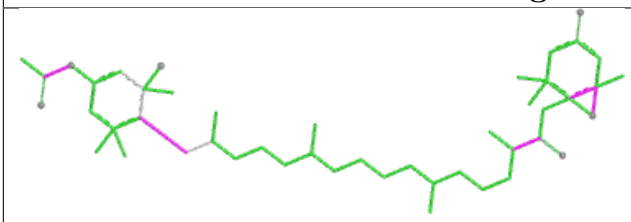


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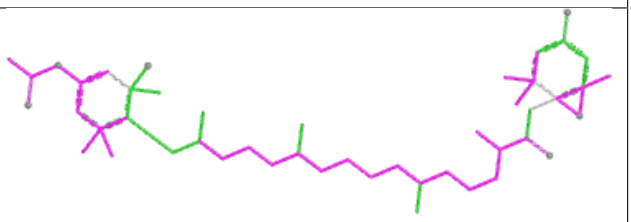


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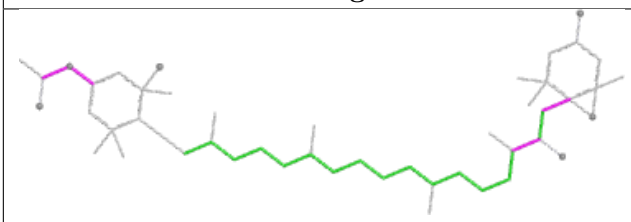
Ligand A86 R 301



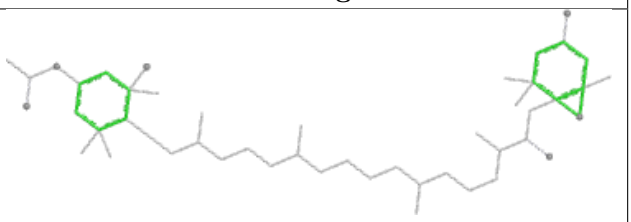
Bond lengths



Bond angles

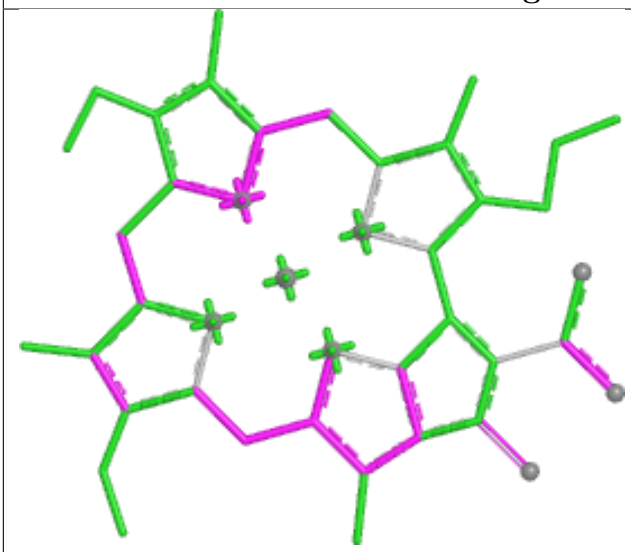


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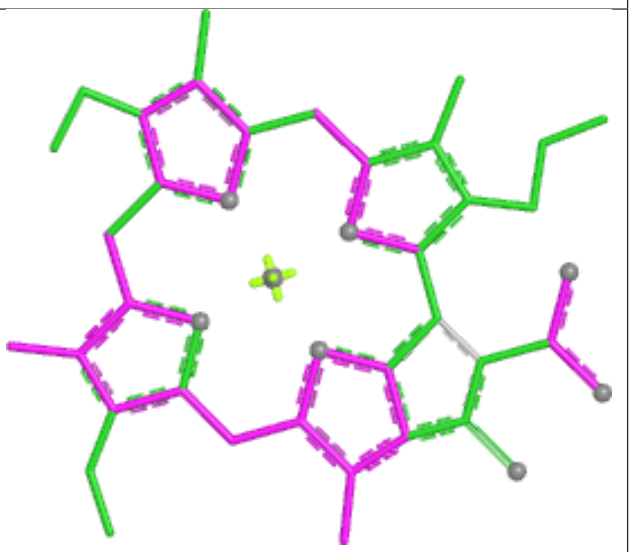


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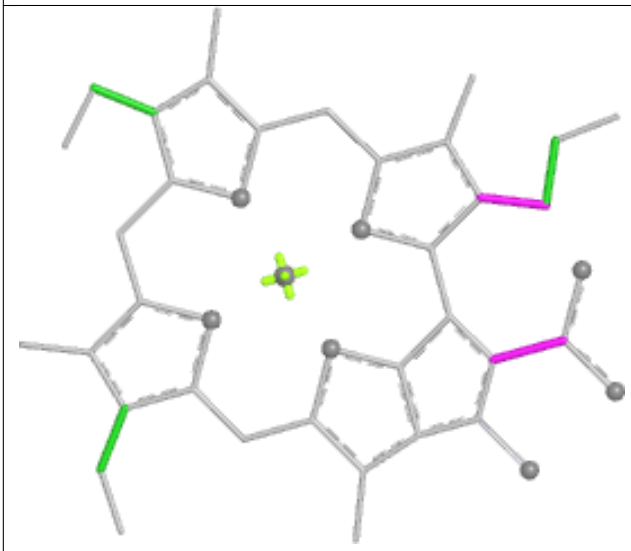
Ligand CLA G 307



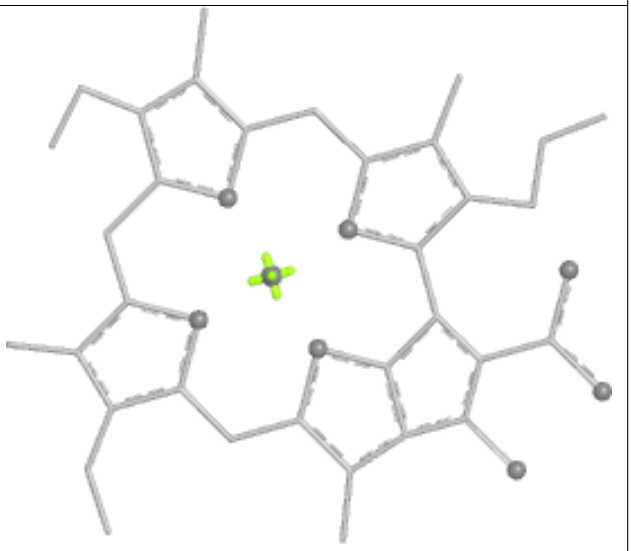
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Bond angles

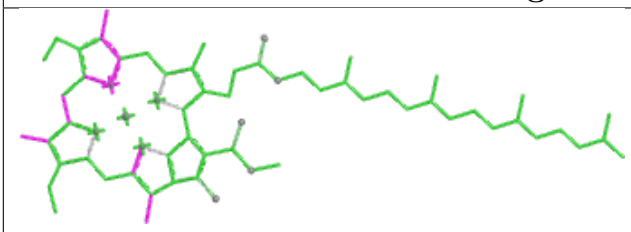


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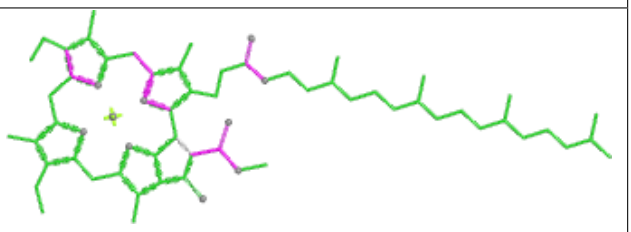


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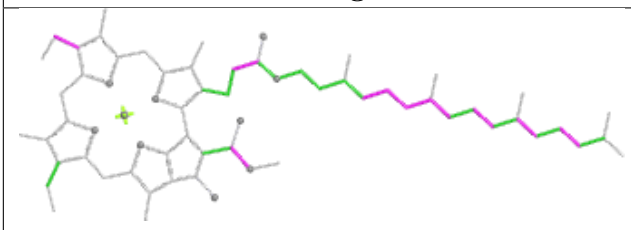
Ligand CLA b 809



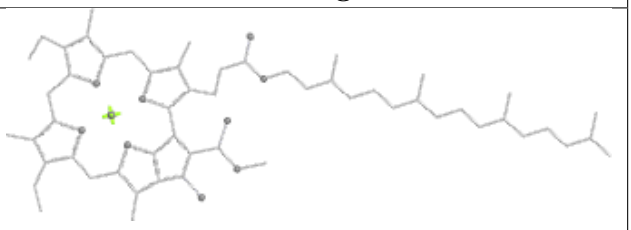
Bond lengths



Bond angles



Torsions

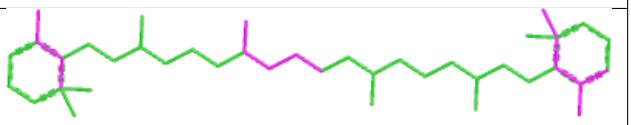


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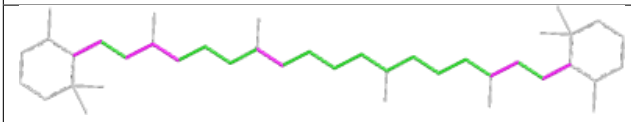
Ligand BCR f 806



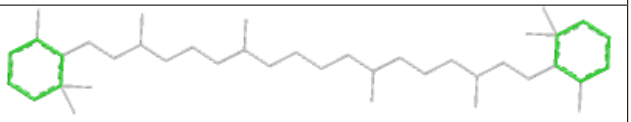
Bond lengths



Bond angles

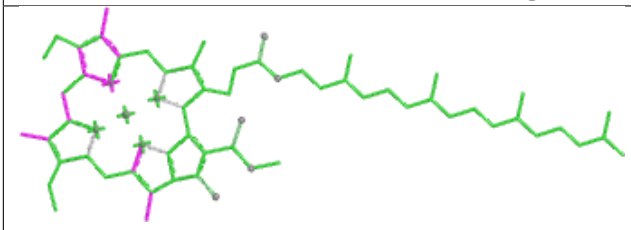


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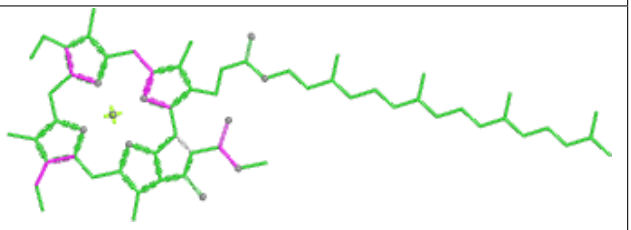


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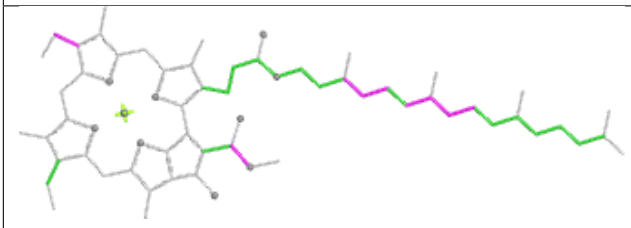
Ligand CLA H 317



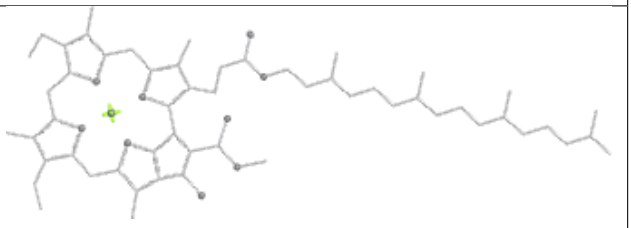
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Bond angles

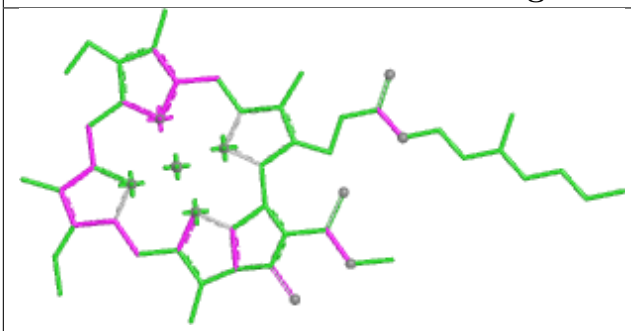


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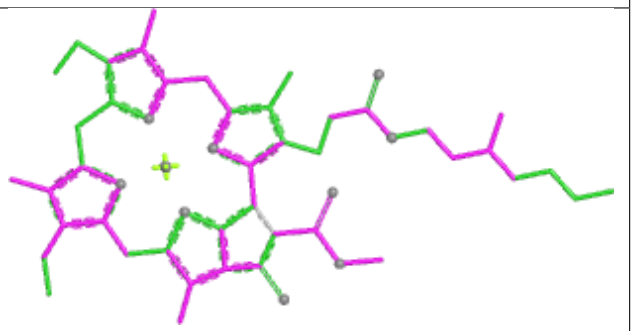


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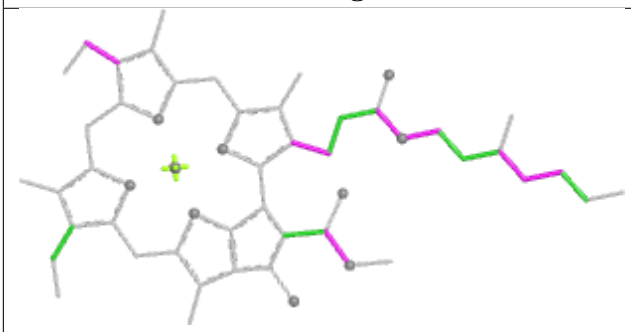
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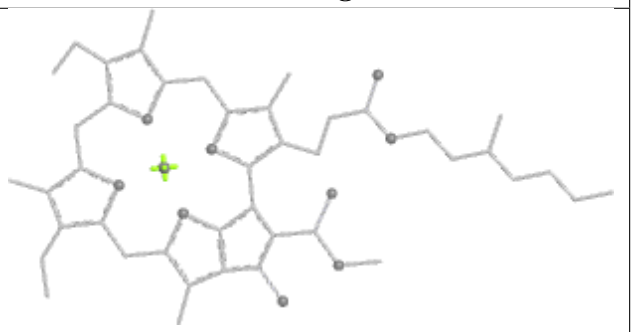
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Bond angles

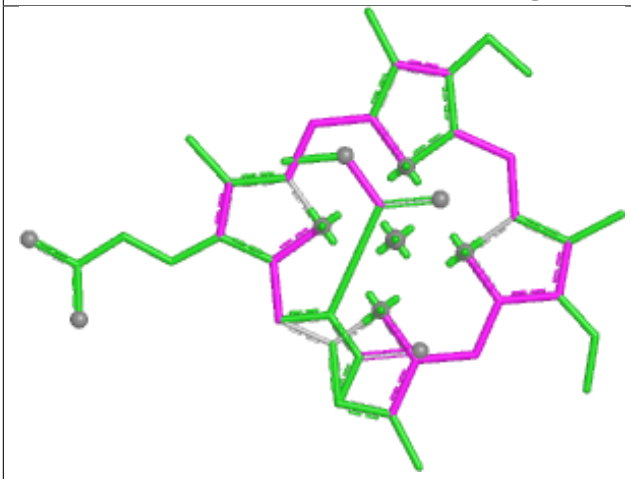


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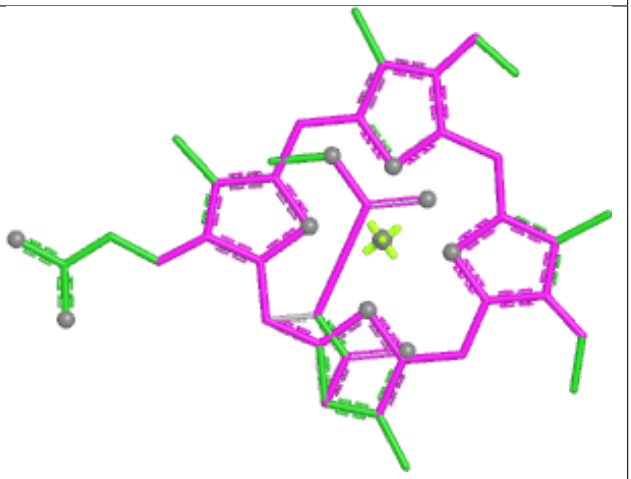


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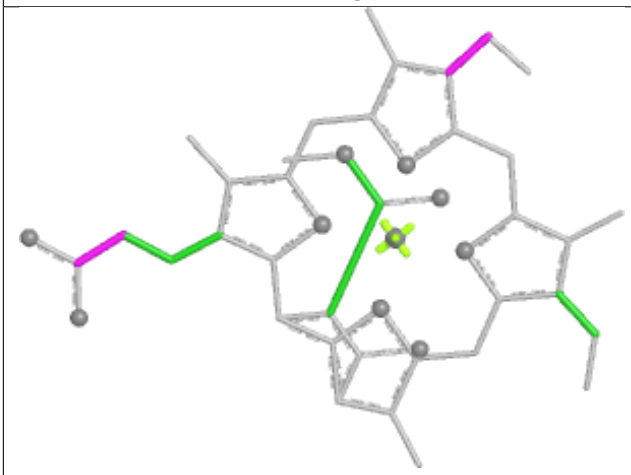
Ligand KC1 B 310



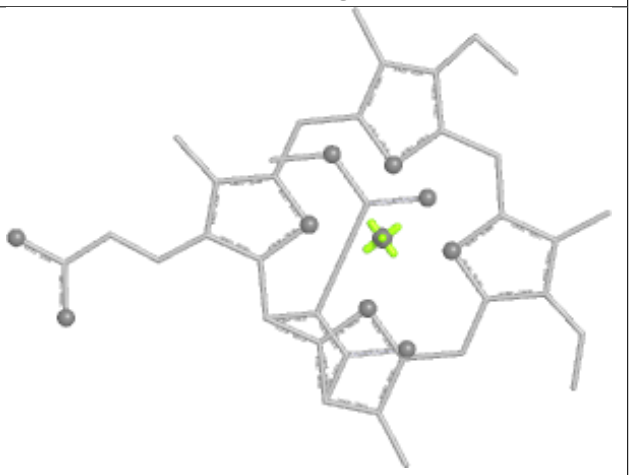
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Bond angles

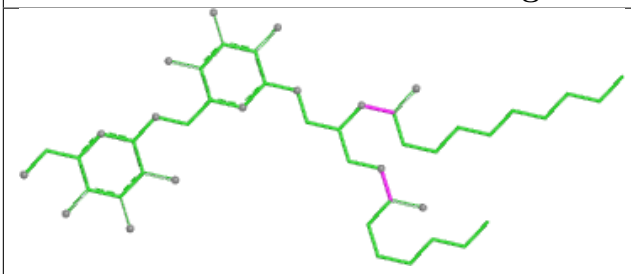


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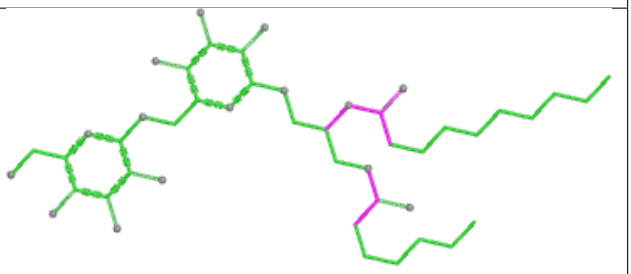


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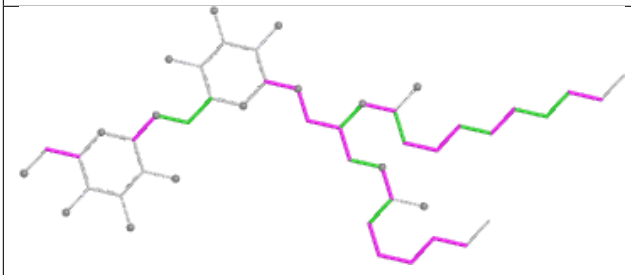
Ligand DGD L 302



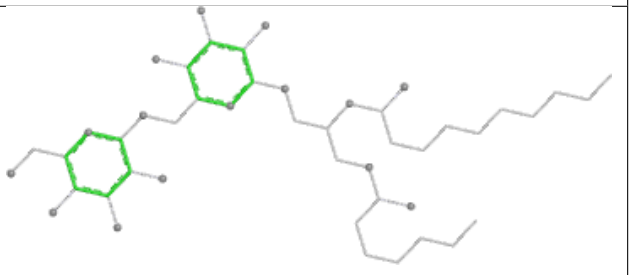
Bond lengths



Bond angles

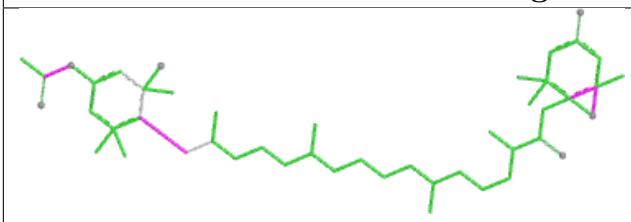


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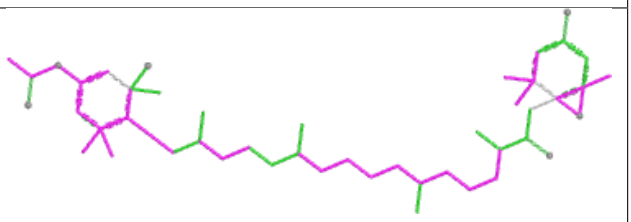


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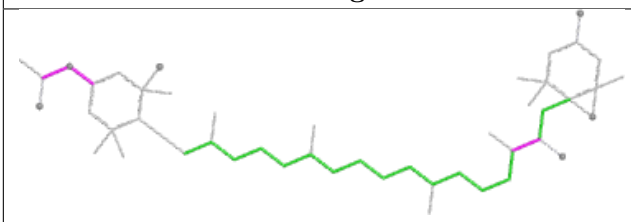
Ligand A86 T 302



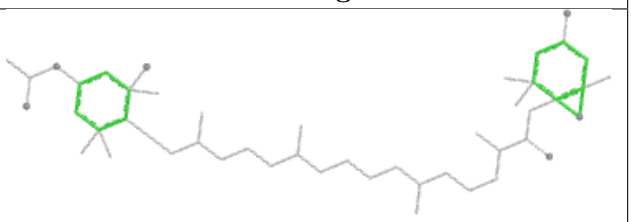
Bond lengths



Bond angles



Torsions

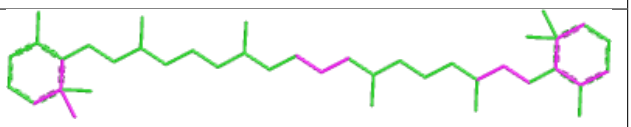


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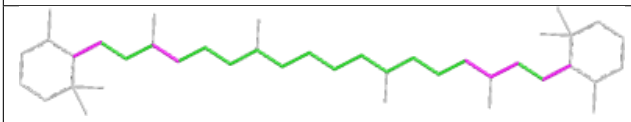
Ligand BCR l 203



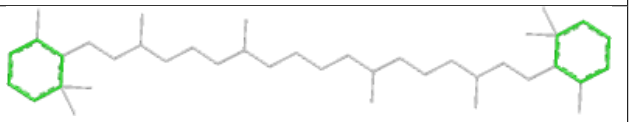
Bond lengths



Bond angles

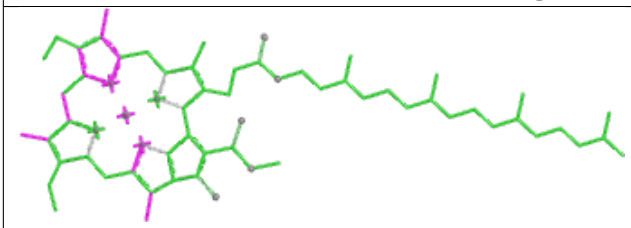


Torsions

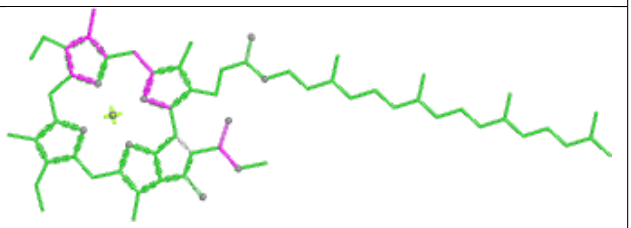


Rings

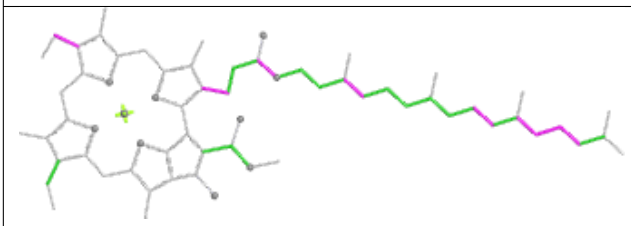
Ligand CLA I 310



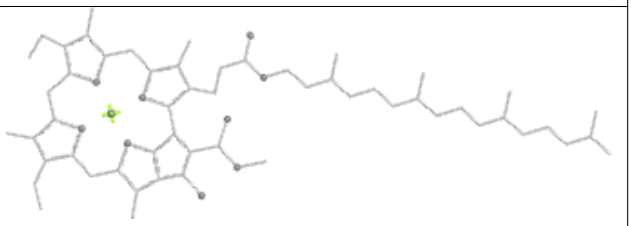
Bond lengths



Bond angles

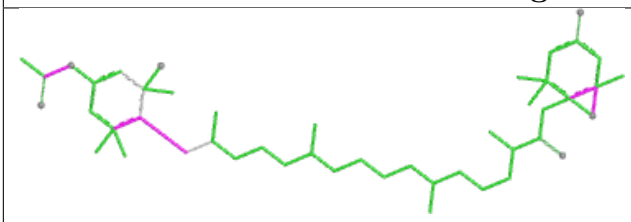


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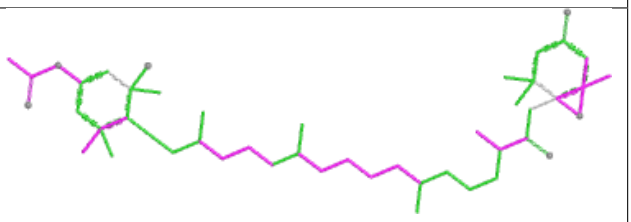


Rings

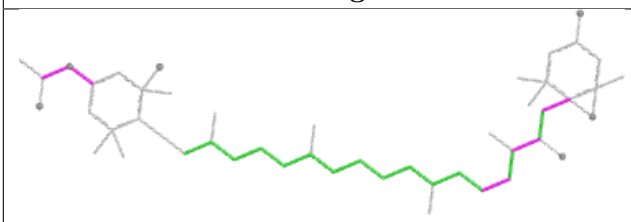
Ligand A86 B 301



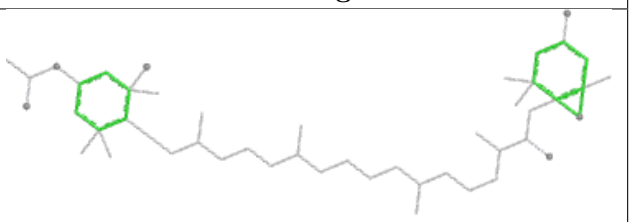
Bond lengths



Bond angles

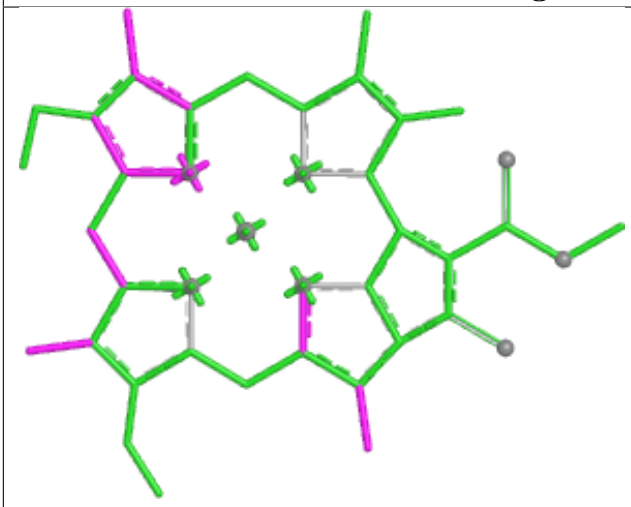


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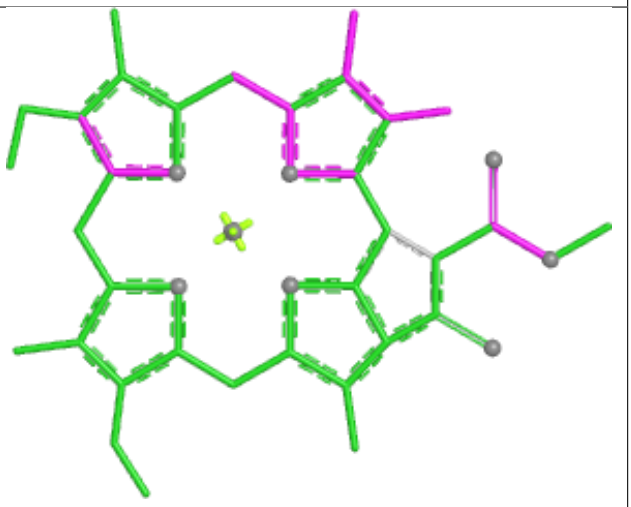


Rings

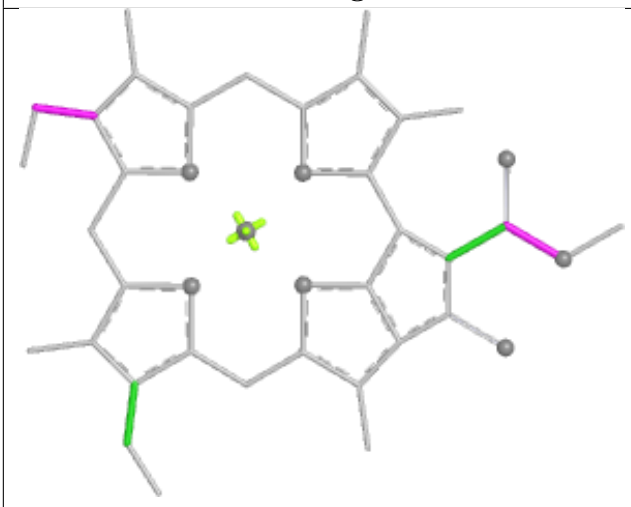
Ligand CLA I 313



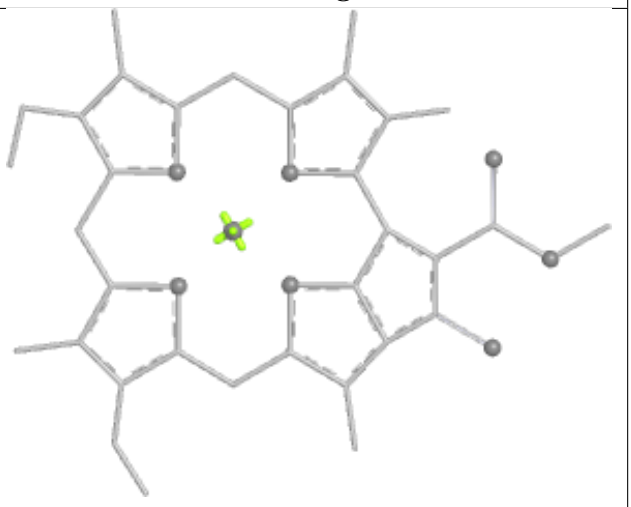
Bond lengths



Bond angles

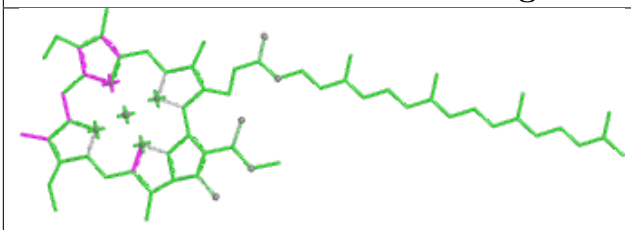


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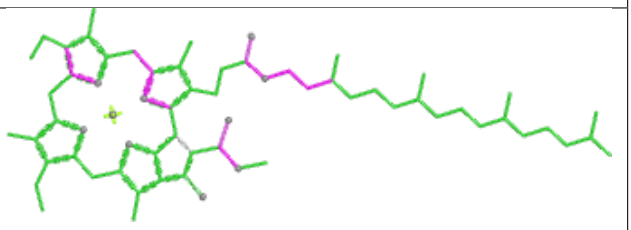


Rings

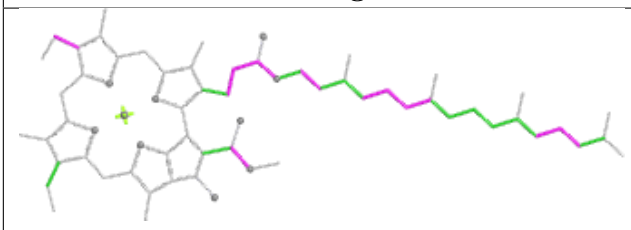
Ligand CLA W 207



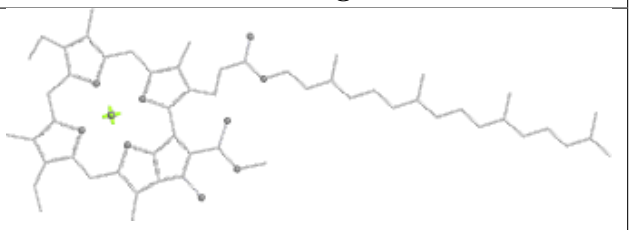
Bond lengths



Bond angles

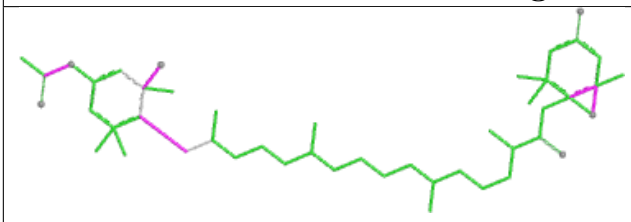


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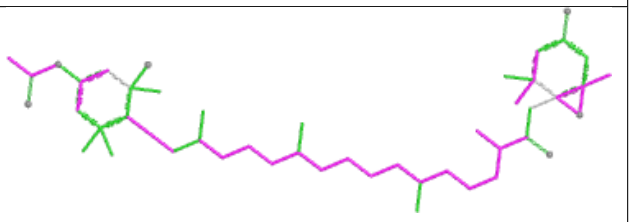


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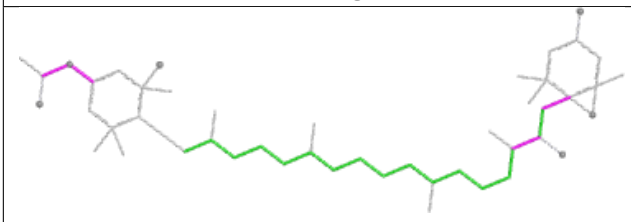
Ligand A86 R 306



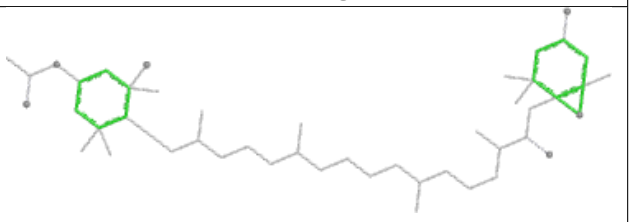
Bond lengths



Bond angles

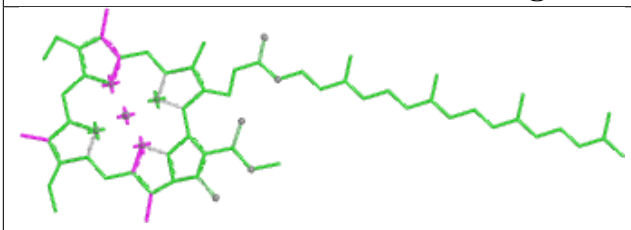


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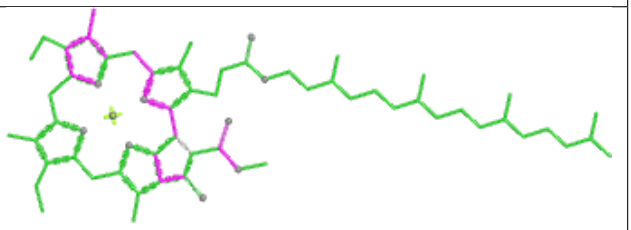


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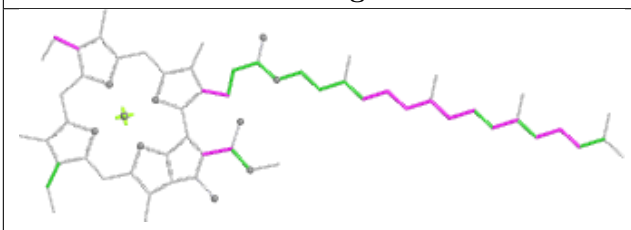
Ligand CLA a 831



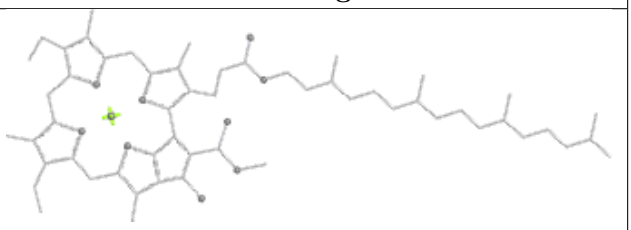
Bond lengths



Bond angles

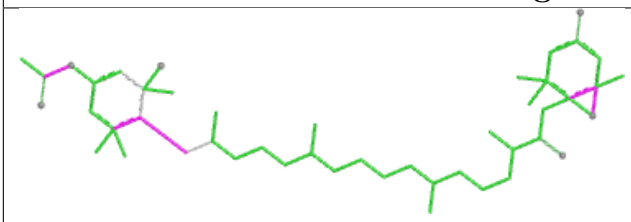


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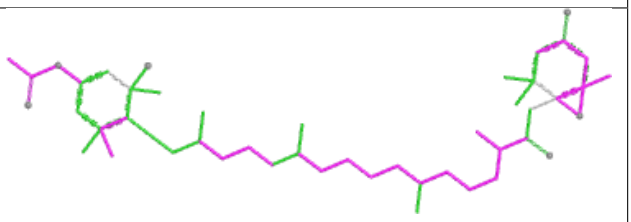


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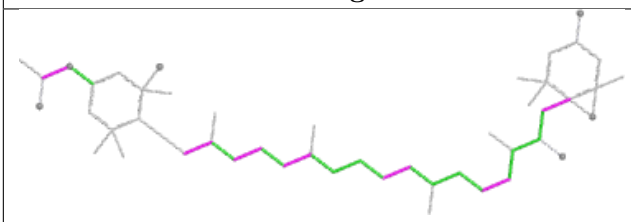
Ligand A86 J 301



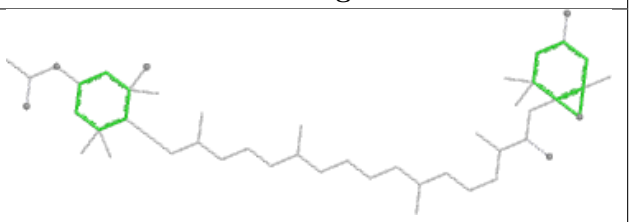
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Bond angles

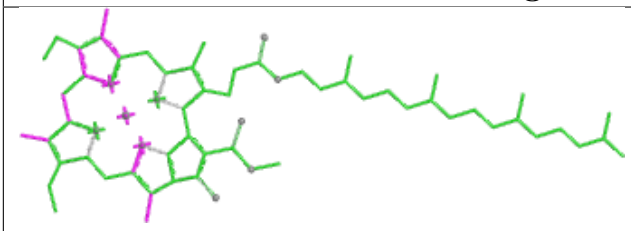


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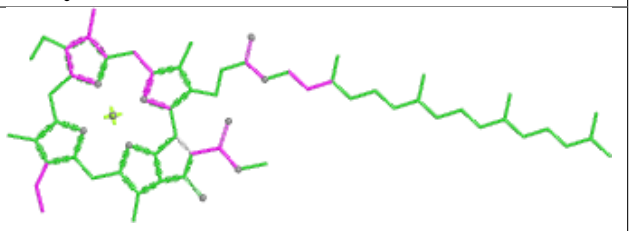


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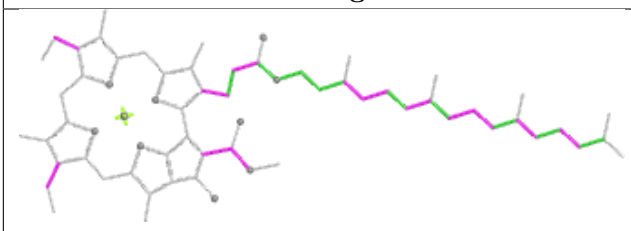
Ligand CLA Q 308



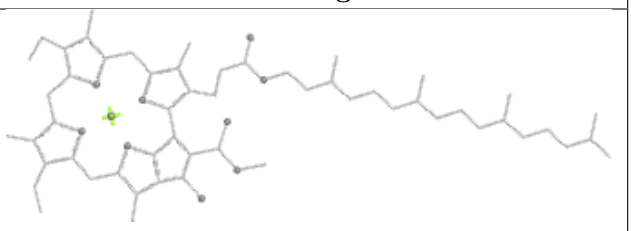
Bond lengths



Bond angles

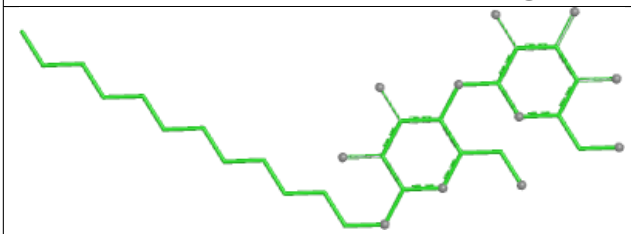


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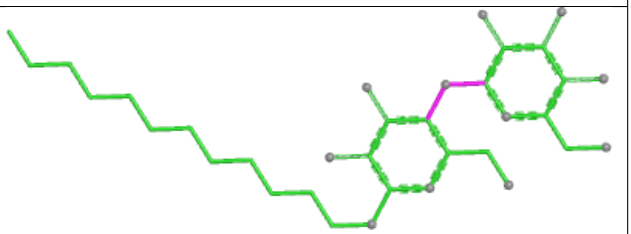


Rings

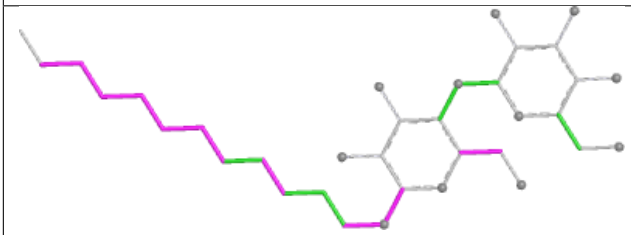
Ligand LMT K 318



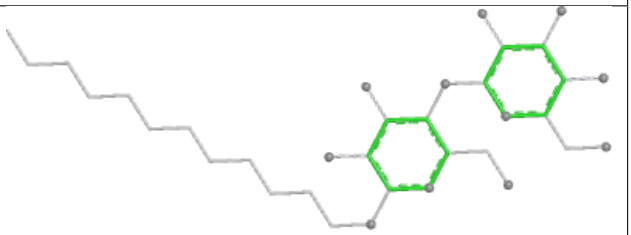
Bond lengths



Bond angles

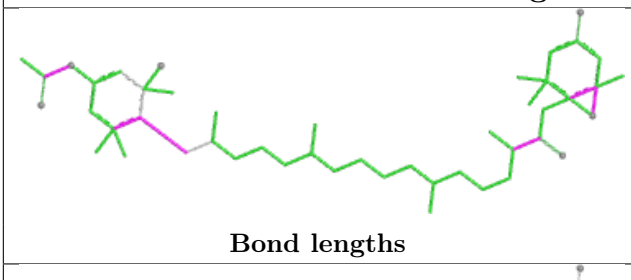


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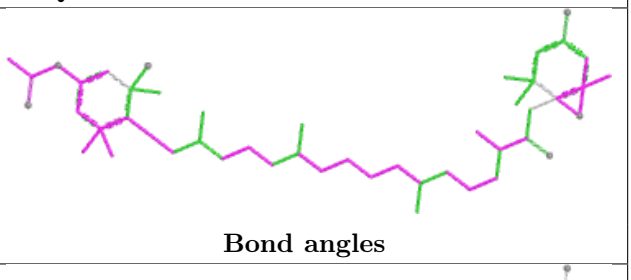


Rings

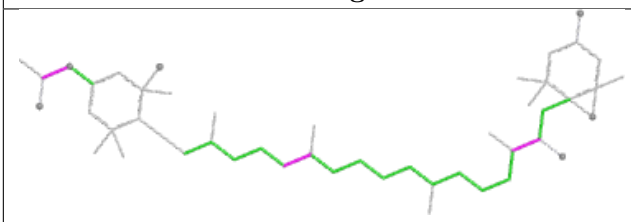
Ligand A86 Q 303



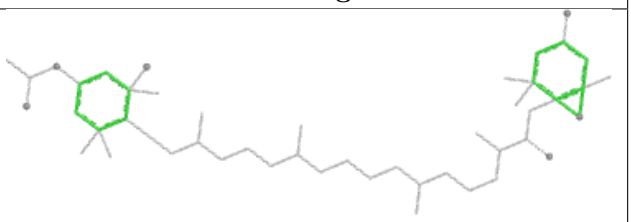
Bond lengths



Bond angles

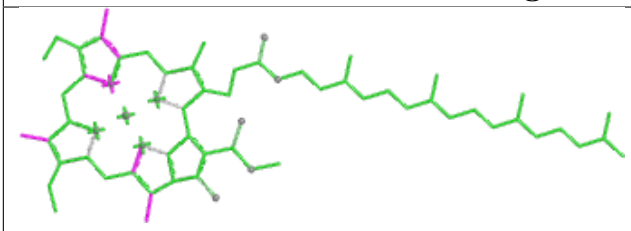


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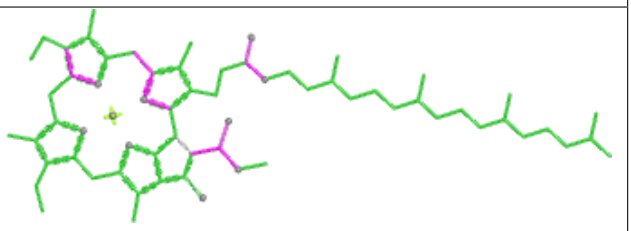


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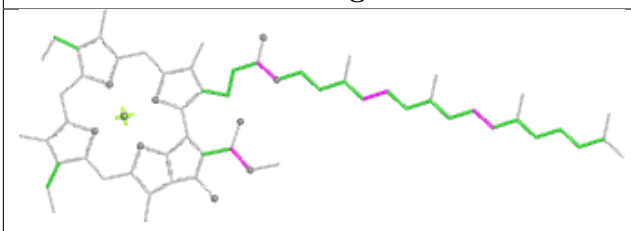
Ligand CLA V 310



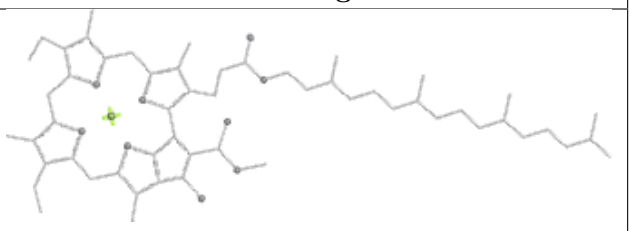
Bond lengths



Bond angles

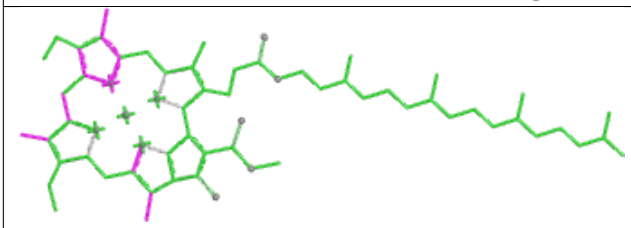


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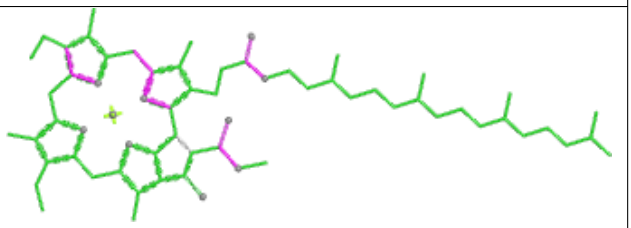


Rings

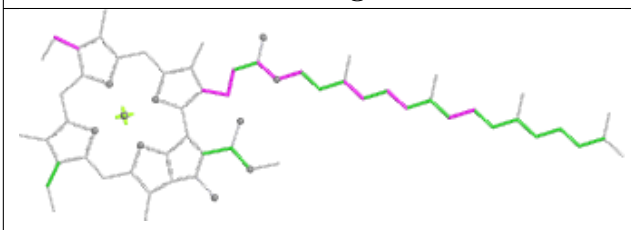
Ligand CLA b 829



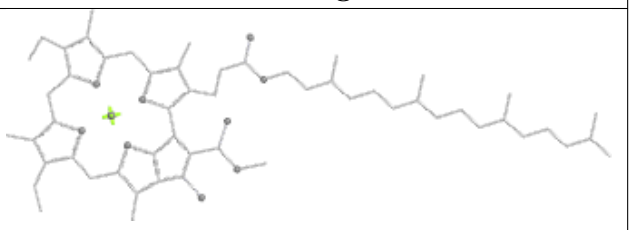
Bond lengths



Bond angles

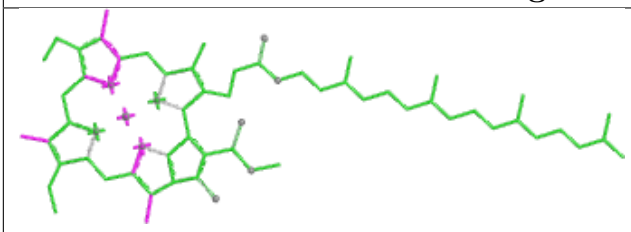


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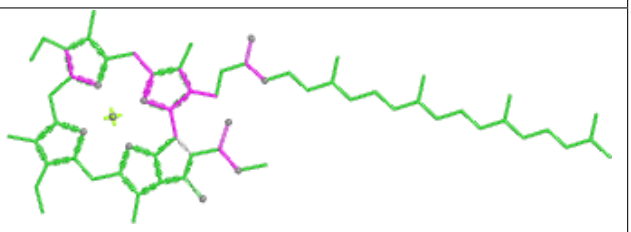


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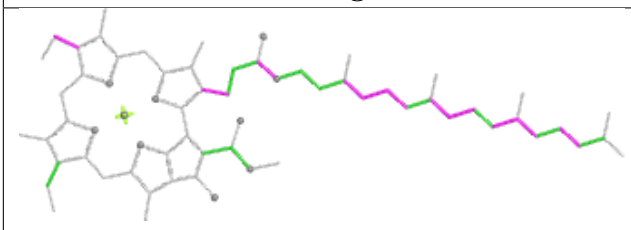
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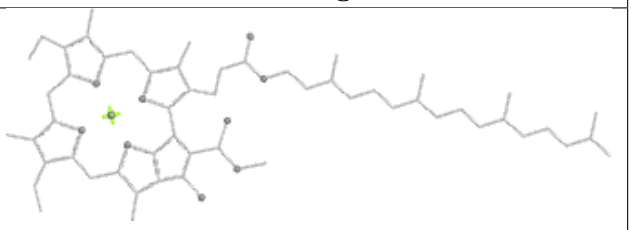
Bond lengths



Bond angles

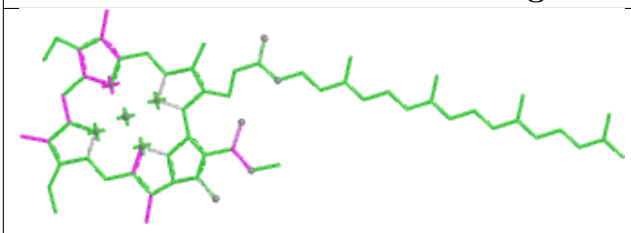


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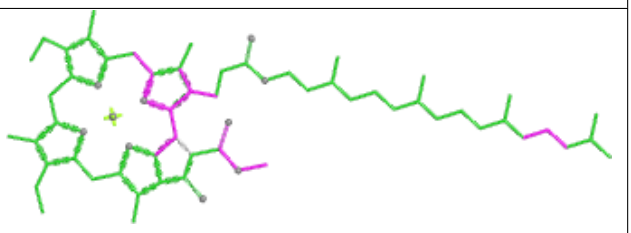


Rings

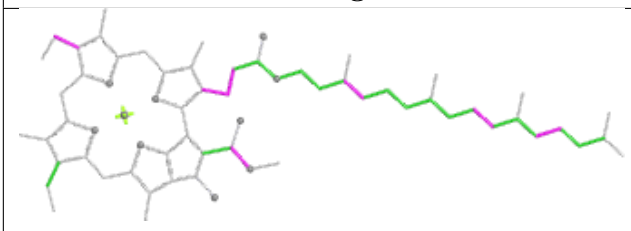
Ligand CLA S 314



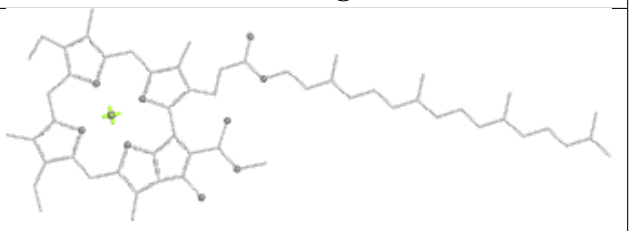
Bond lengths



Bond angles

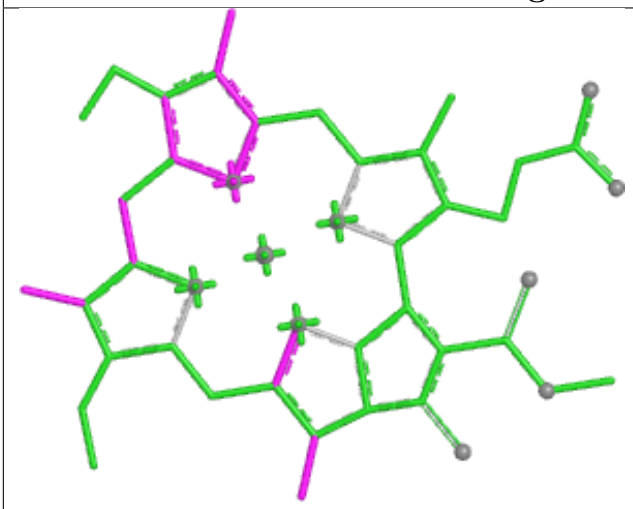


Torsions

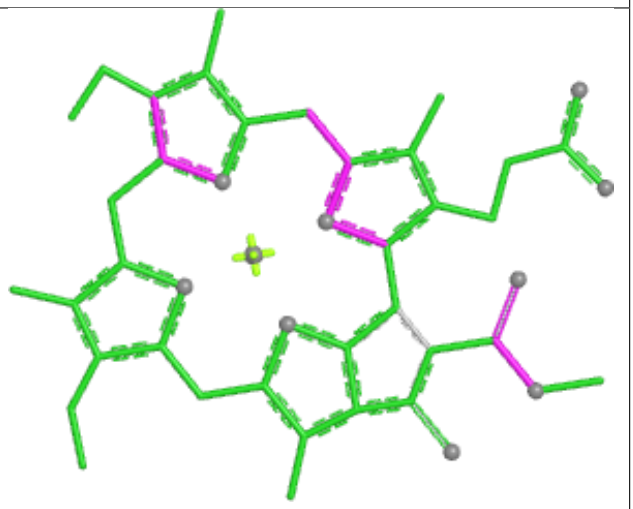


Rings

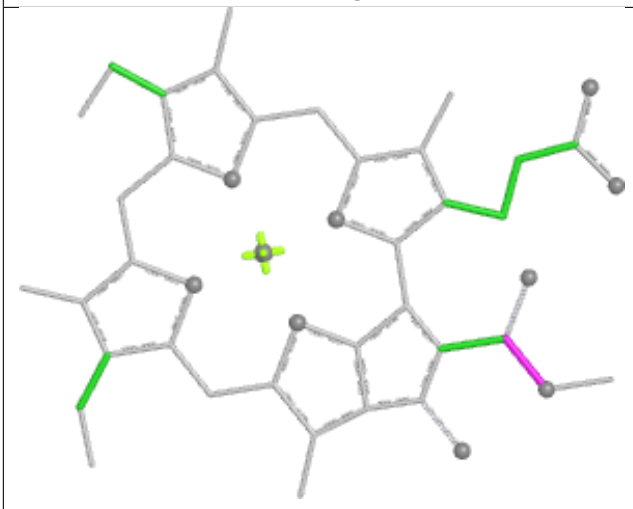
Ligand CLA a 815



Bond lengths



Bond angles

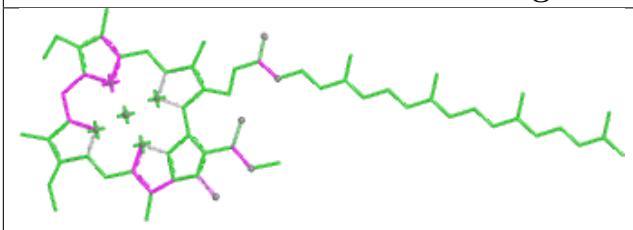


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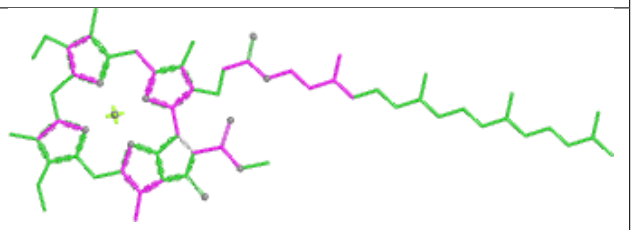


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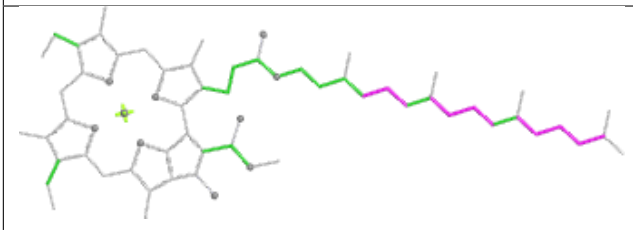
Ligand CLA l 205



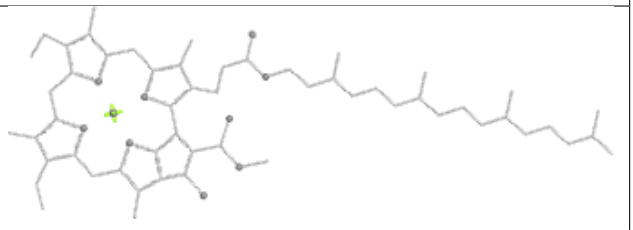
Bond lengths



Bond angles

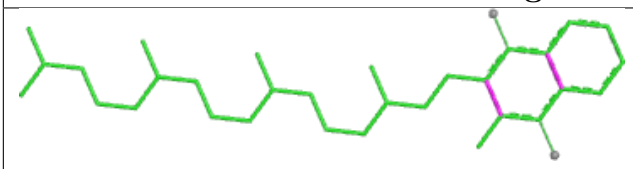


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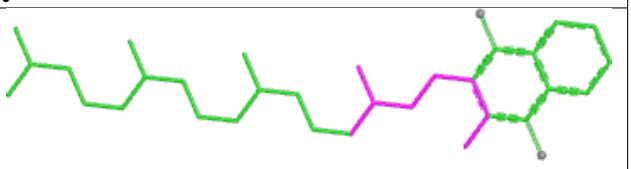


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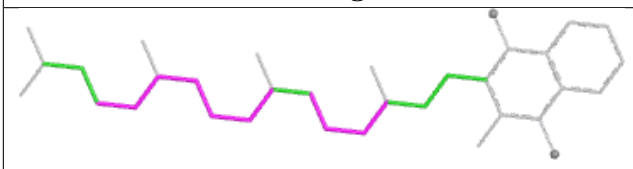
Ligand PQN b 842



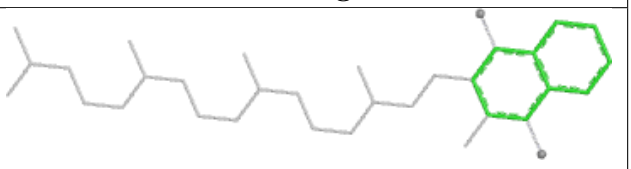
Bond lengths



Bond angles

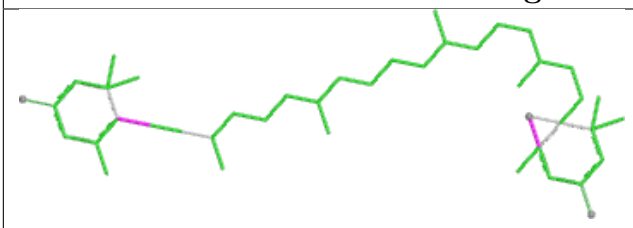


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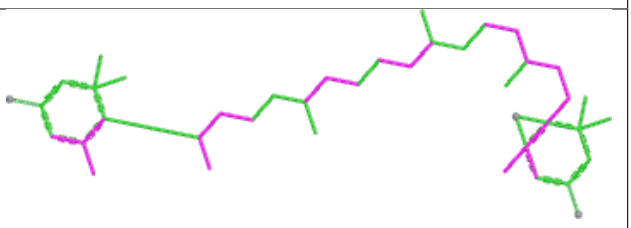


Rings

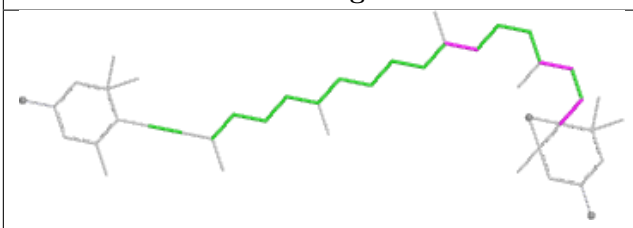
Ligand DD6 H 303



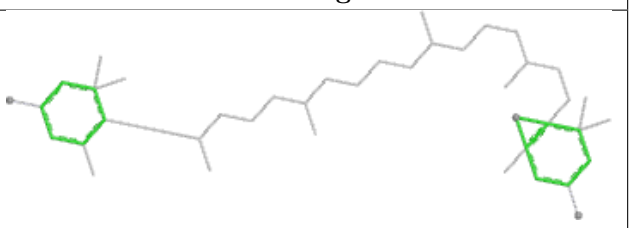
Bond lengths



Bond angles

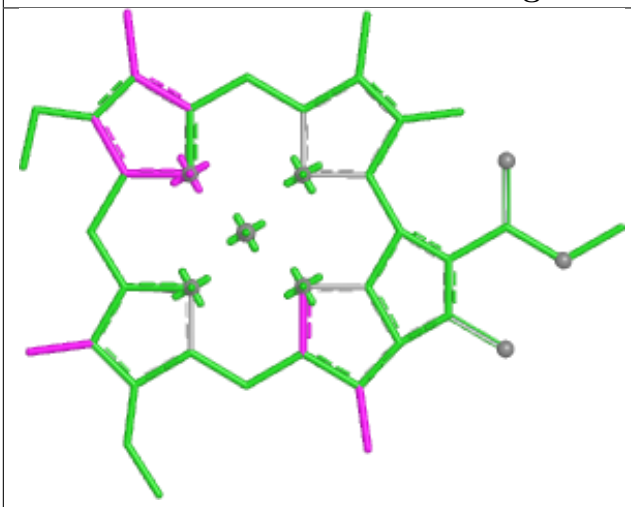


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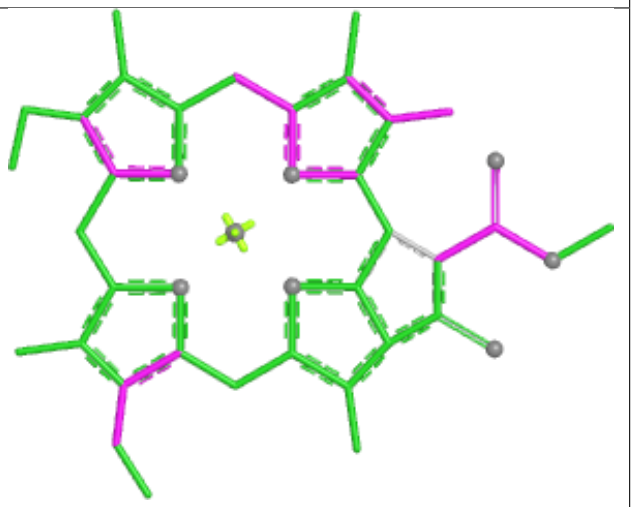


Rings

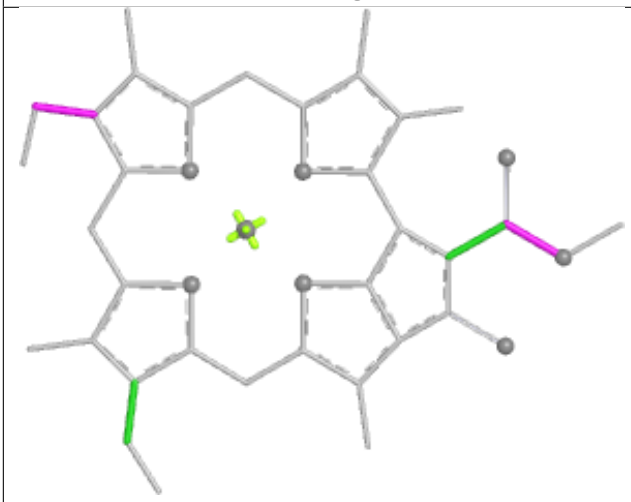
Ligand CLA G 314



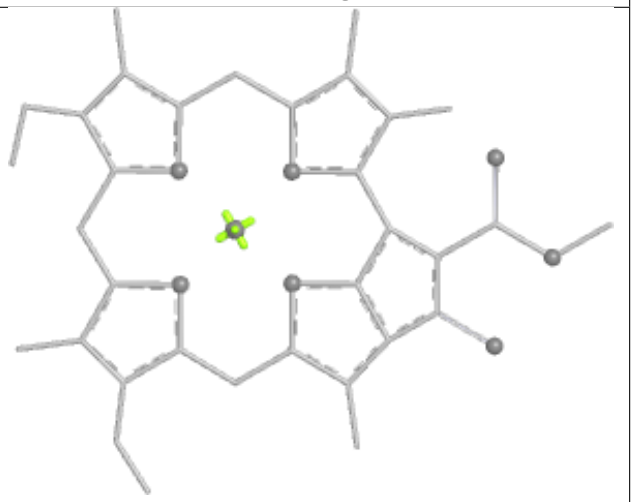
Bond lengths



Bond angles

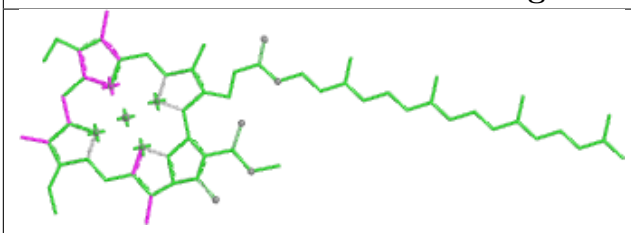


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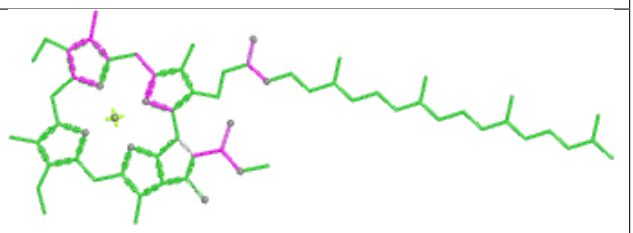


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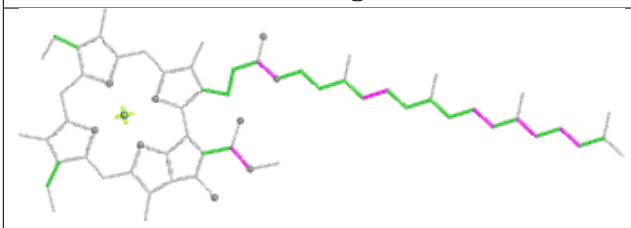
Ligand CLA J 312



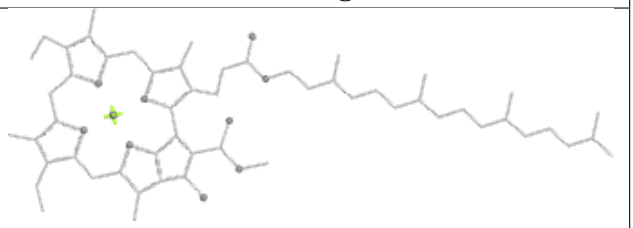
Bond lengths



Bond angles

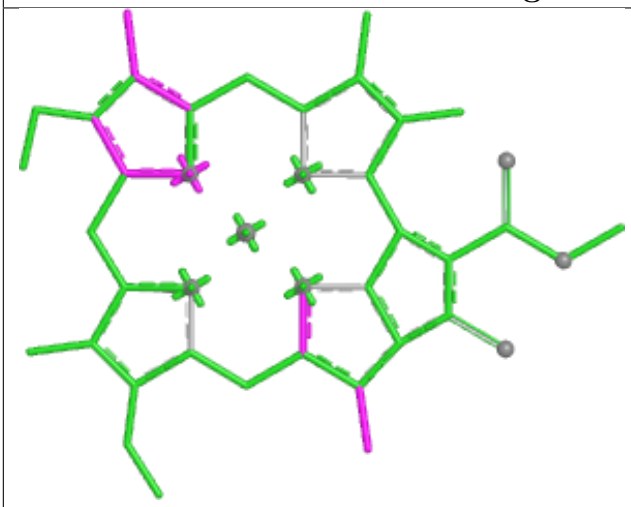


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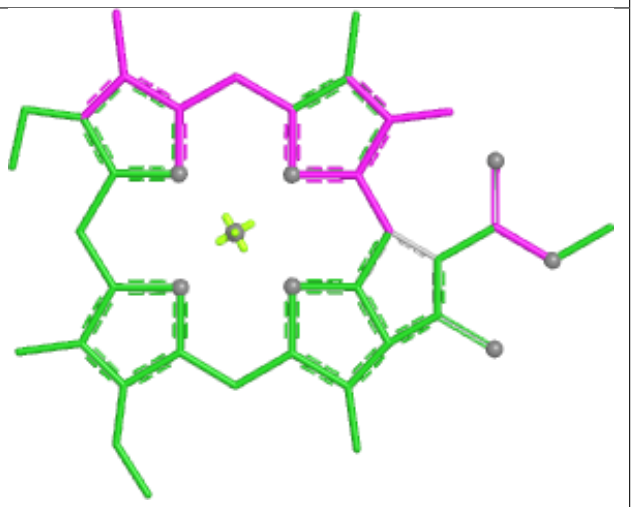


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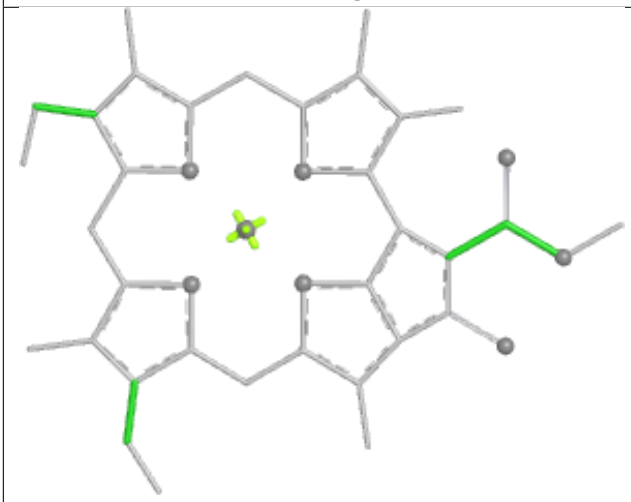
Ligand CLA N 315



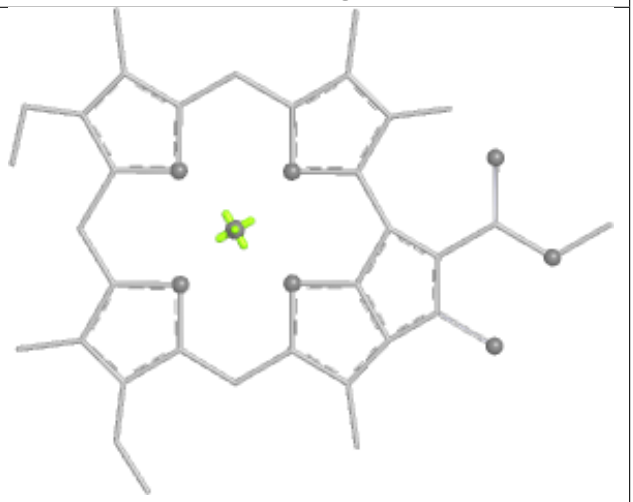
Bond lengths



Bond angles

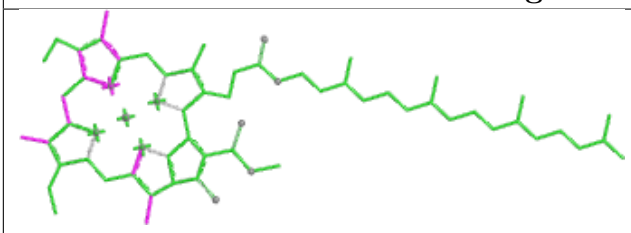


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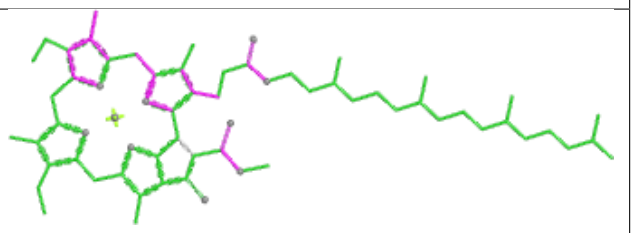


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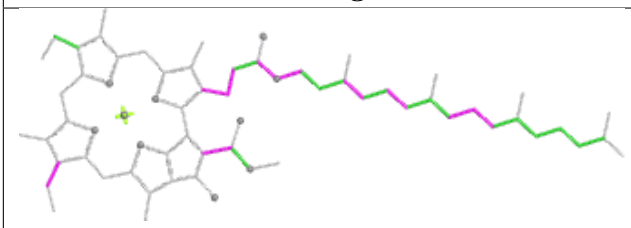
Ligand CLA E 312



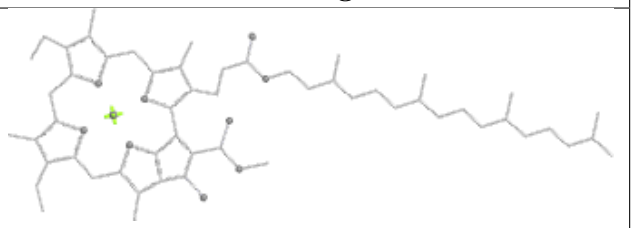
Bond lengths



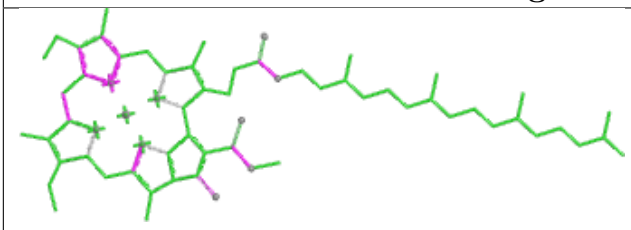
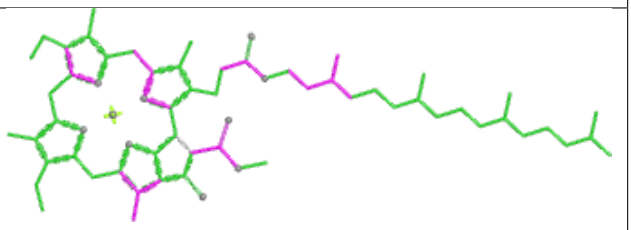
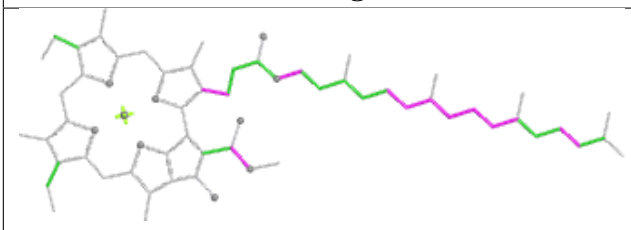
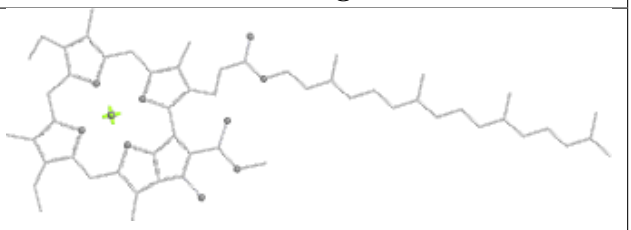
Bond angles

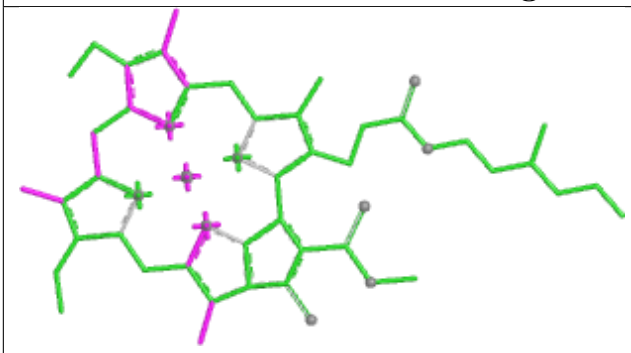
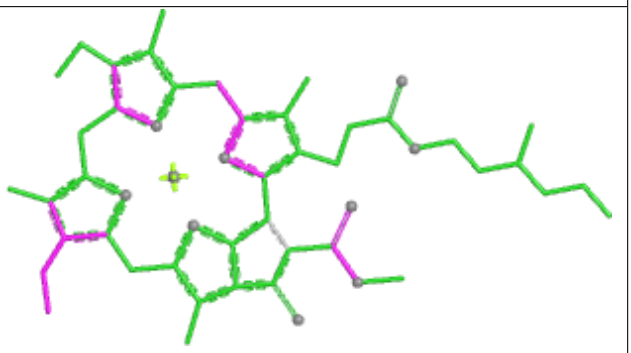
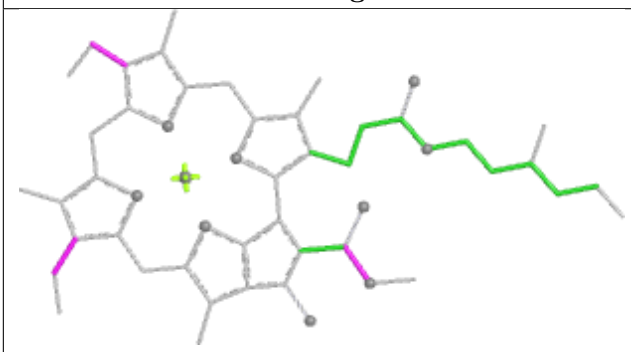
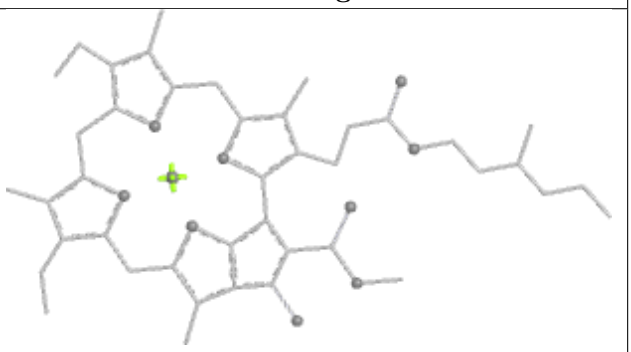


Torsions

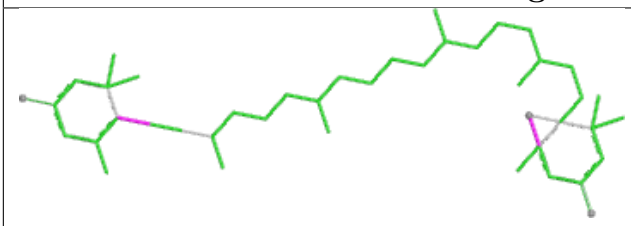


Rings

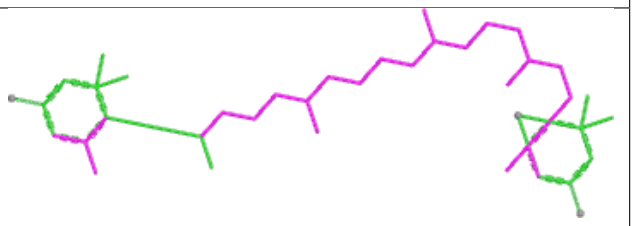
Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA M 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

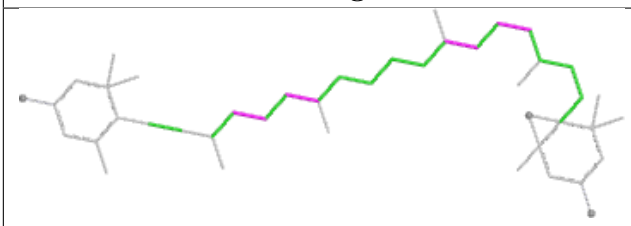
Ligand DD6 S 307



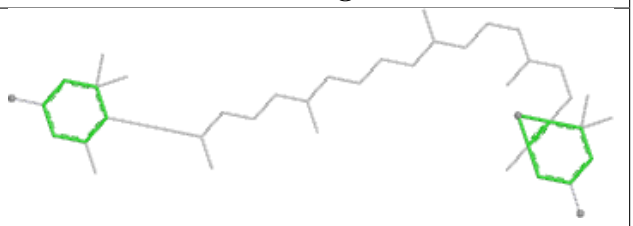
Bond lengths



Bond angles

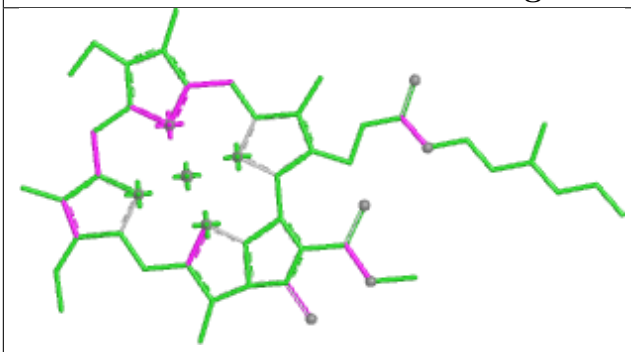


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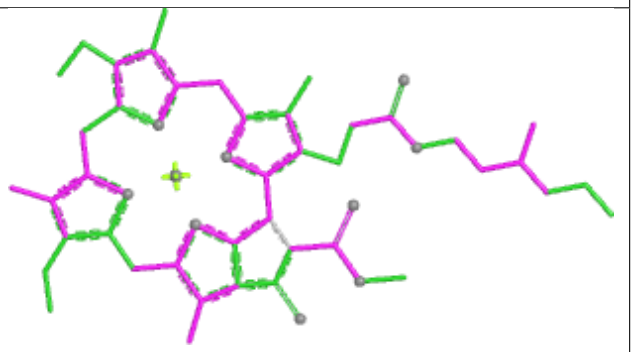


Rings

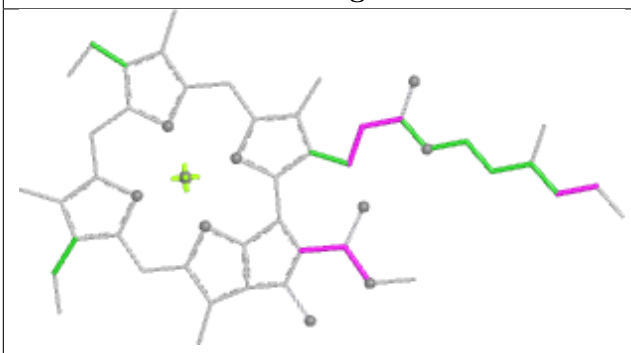
Ligand CLA B 309



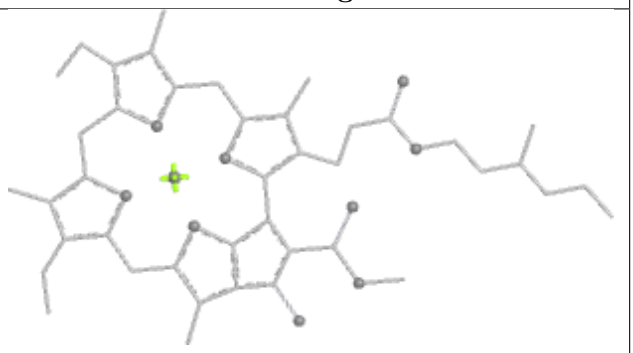
Bond lengths



Bond angles

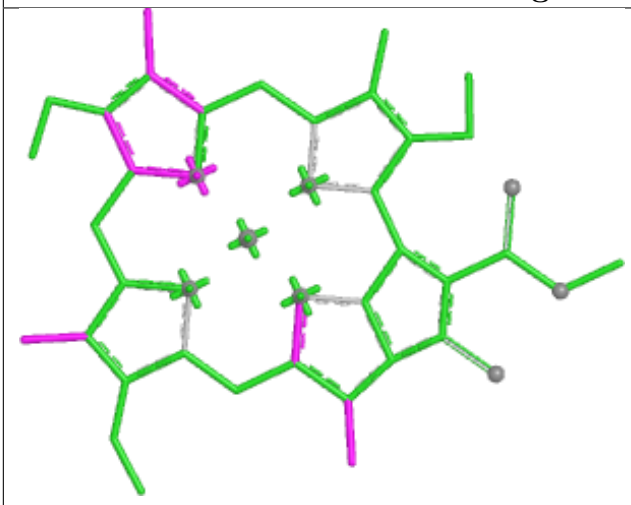


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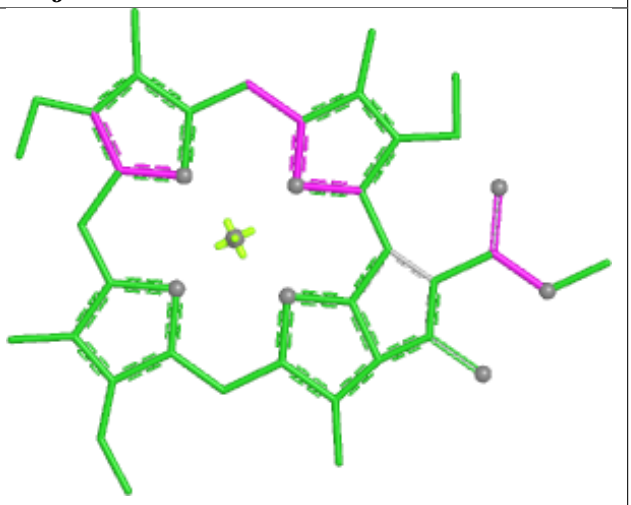


Rings

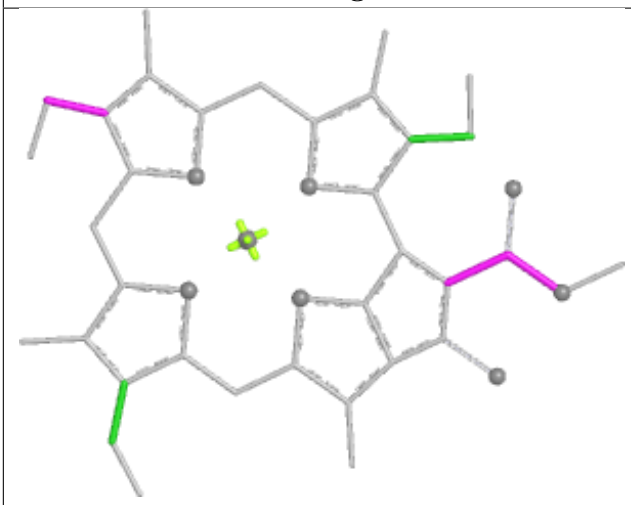
Ligand CLA j 106



Bond lengths



Bond angles

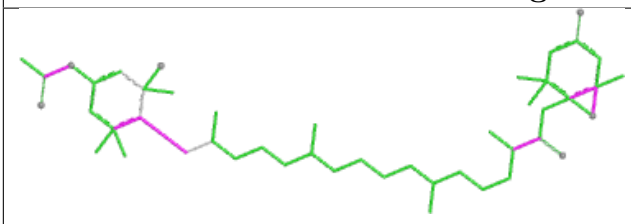


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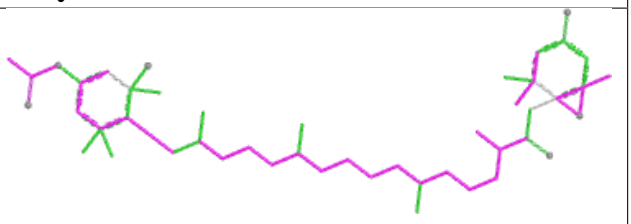


Rings

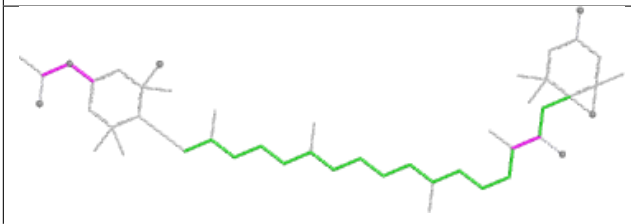
Ligand A86 Q 301



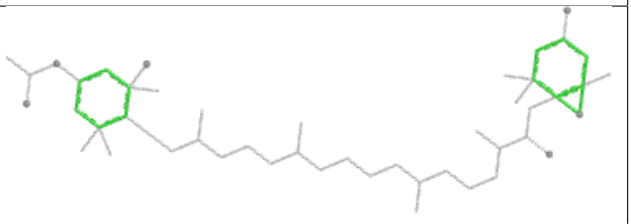
Bond lengths



Bond angles

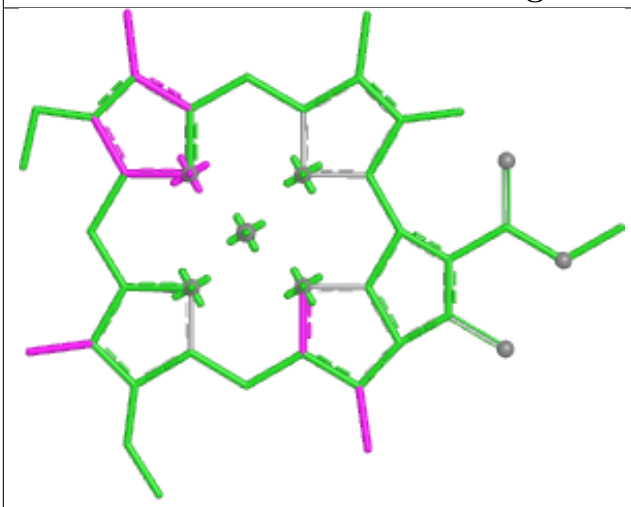


Torsions

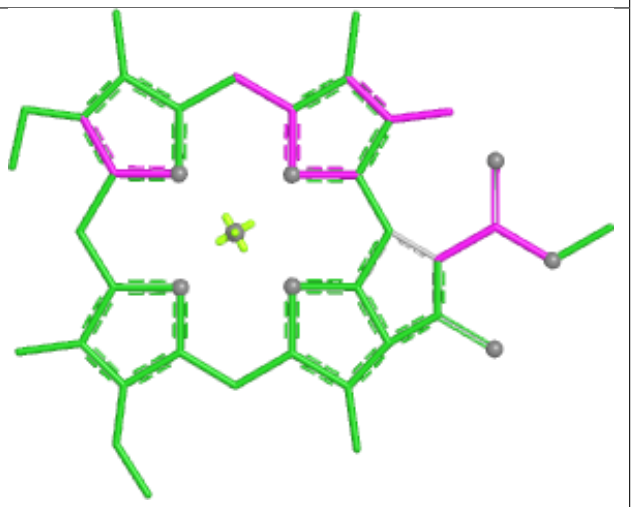


Rings

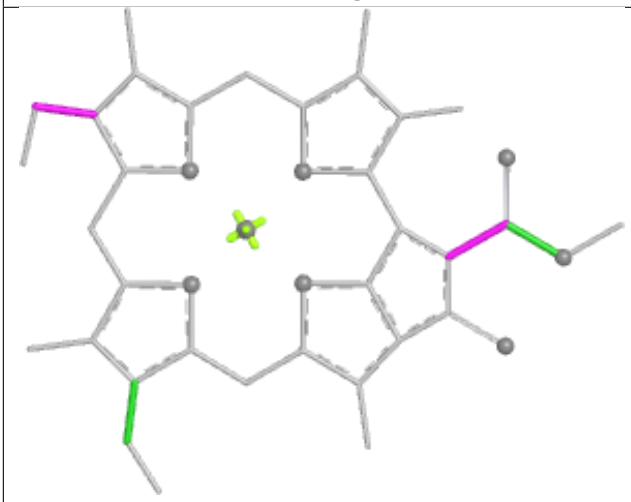
Ligand CLA L 316



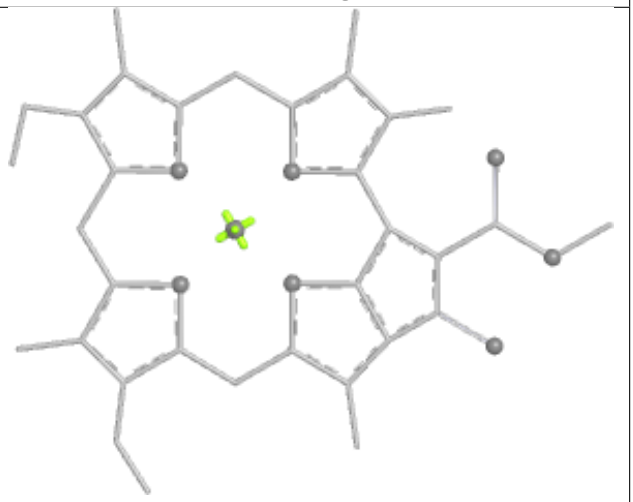
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Bond angles

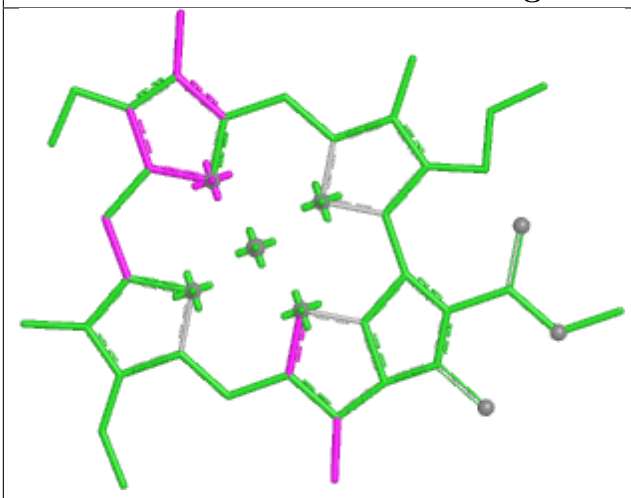


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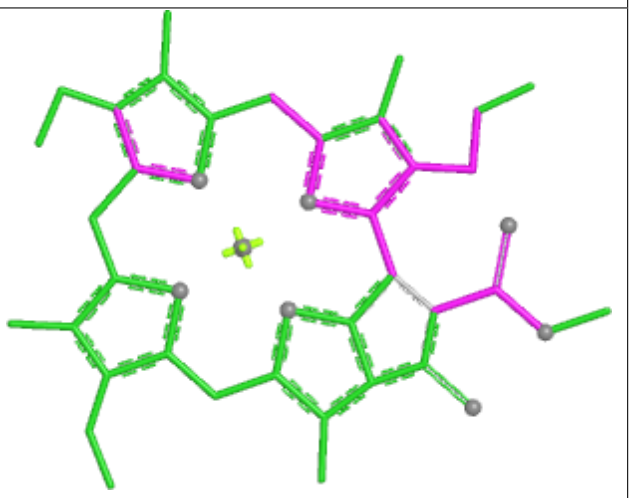


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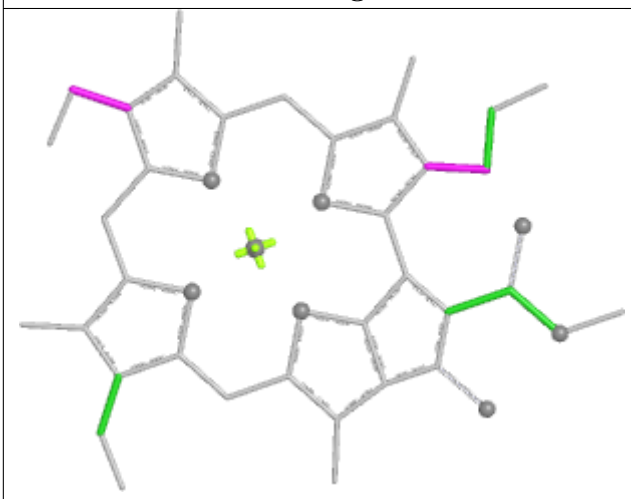
Ligand CLA V 309



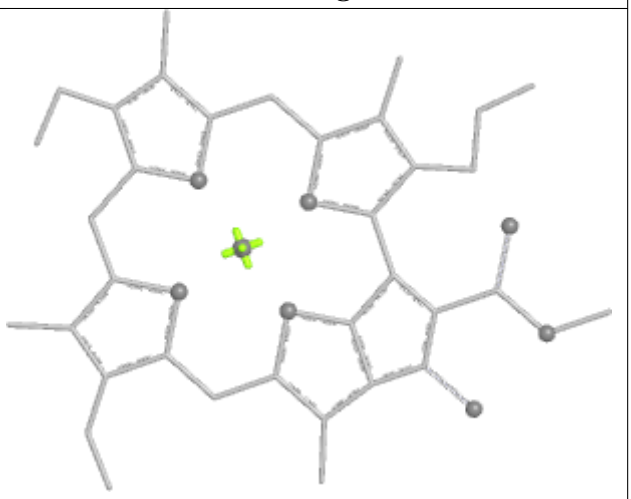
Bond lengths



Bond angles

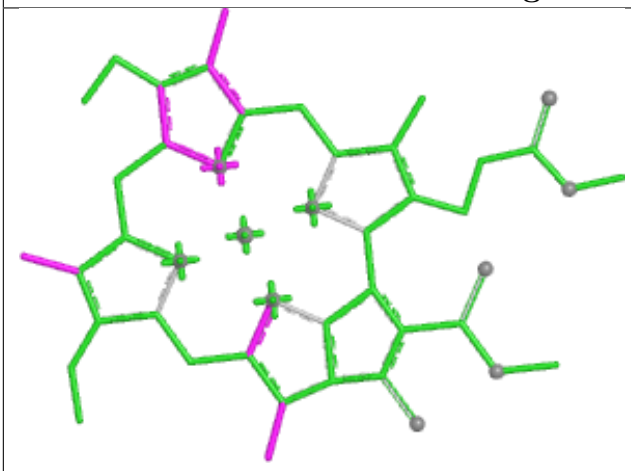


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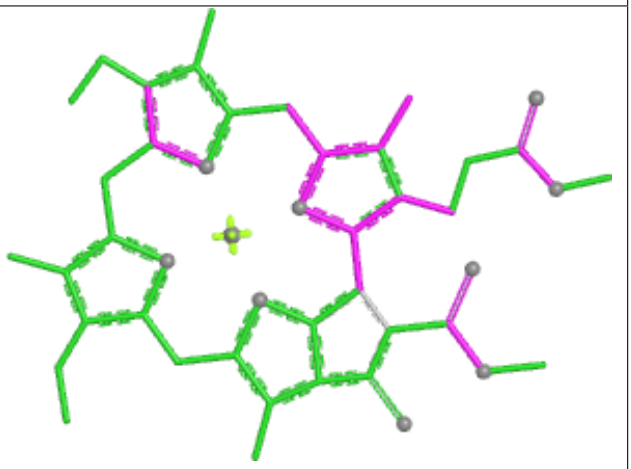


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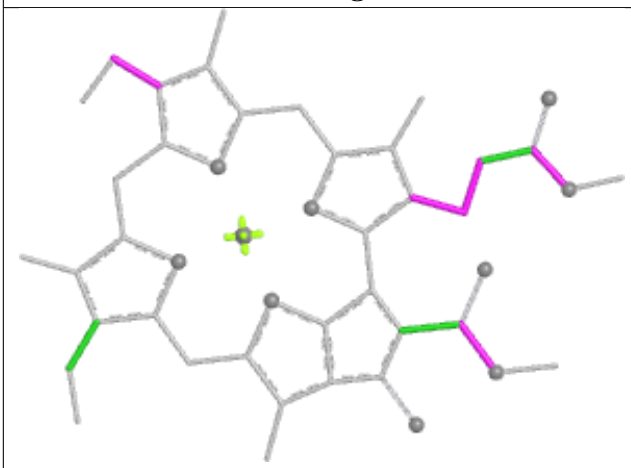
Ligand CLA K 311



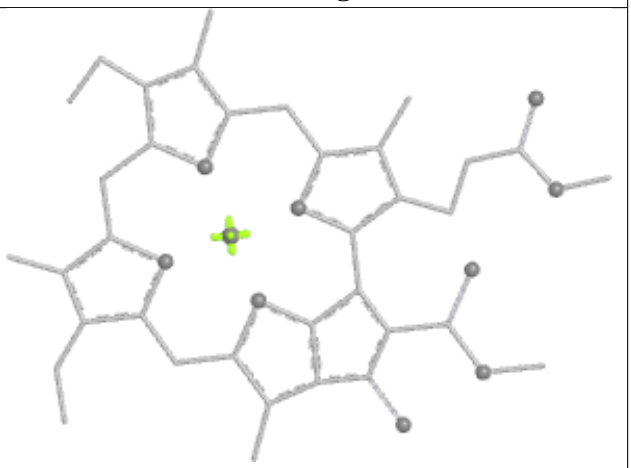
Bond lengths



Bond angles

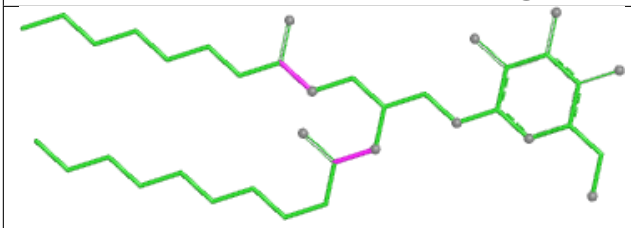


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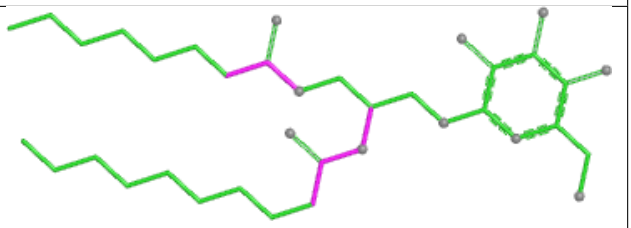


Rings

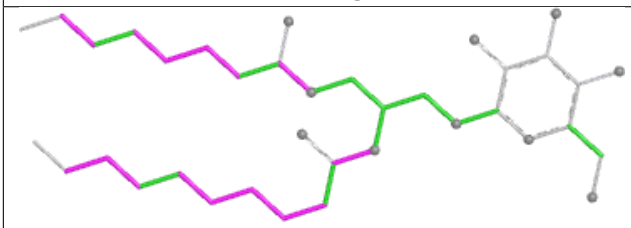
Ligand LMG m 102



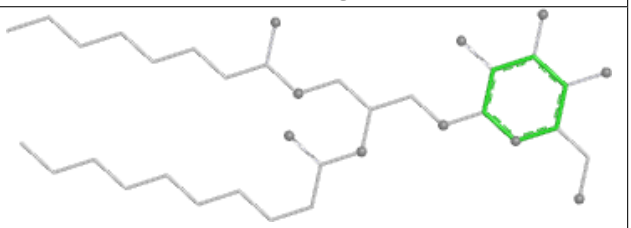
Bond lengths



Bond angles

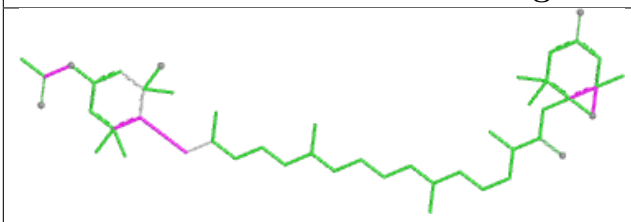


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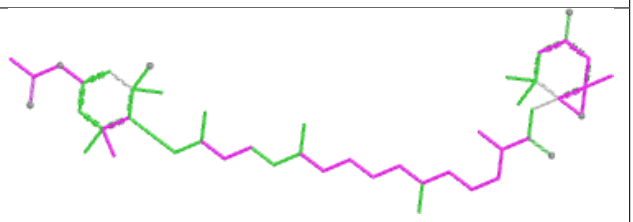


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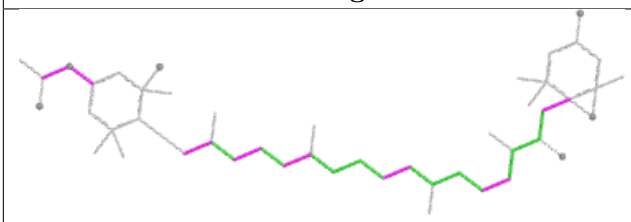
Ligand A86 S 308



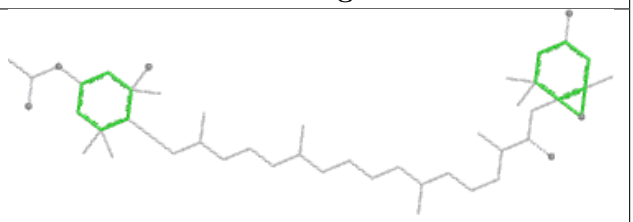
Bond lengths



Bond angles

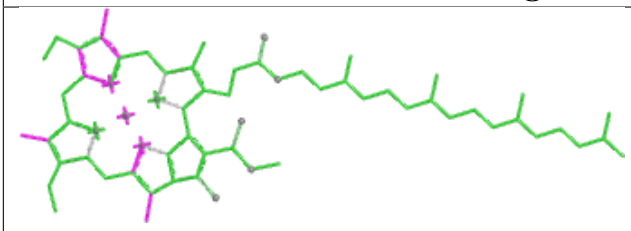


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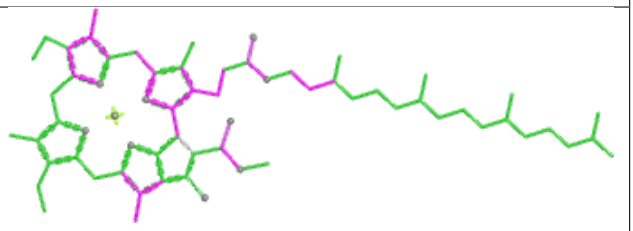


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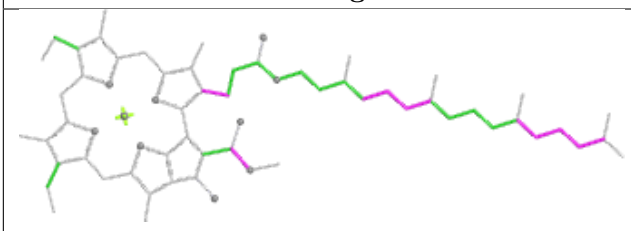
Ligand CLA V 311



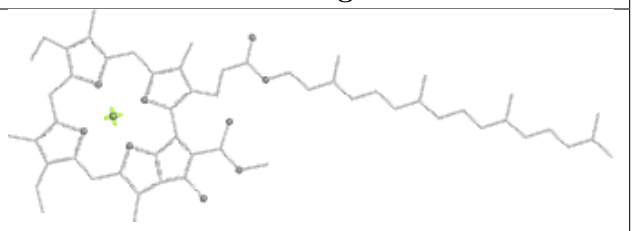
Bond lengths



Bond angles

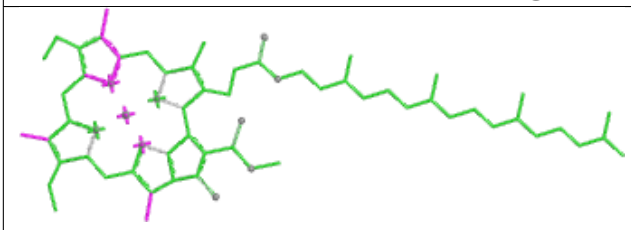


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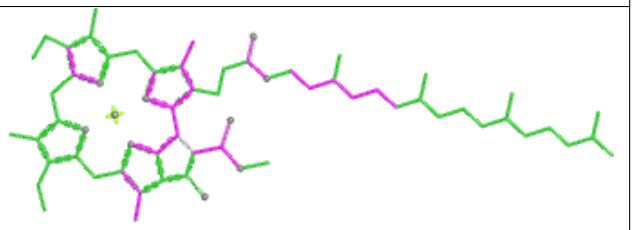


Rings

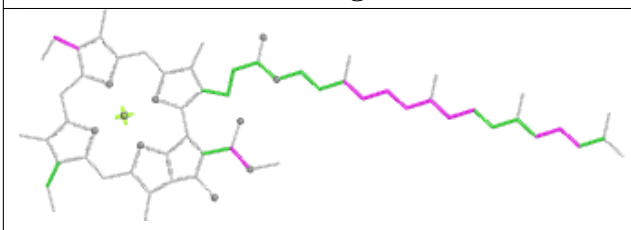
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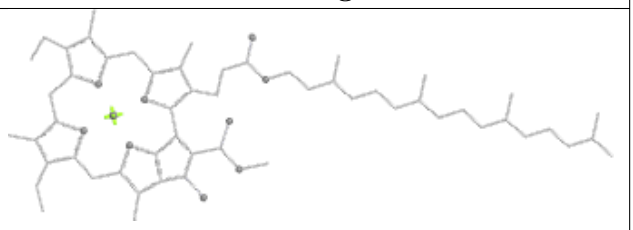
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Bond angles

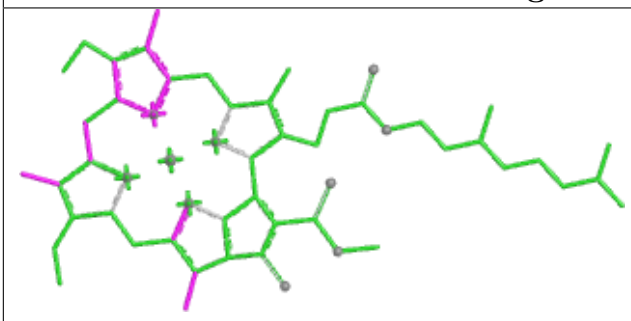


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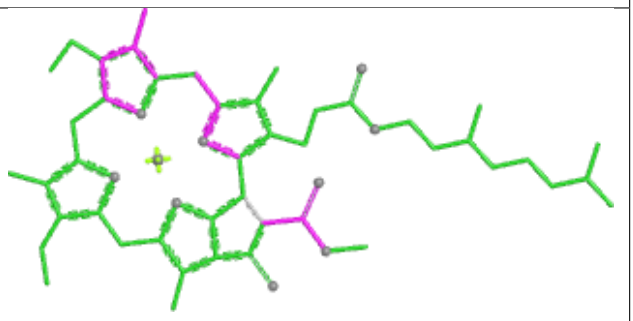


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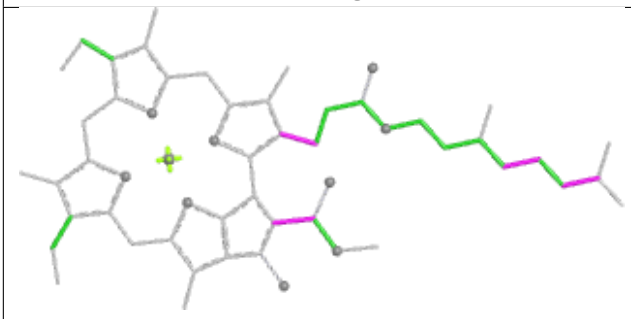
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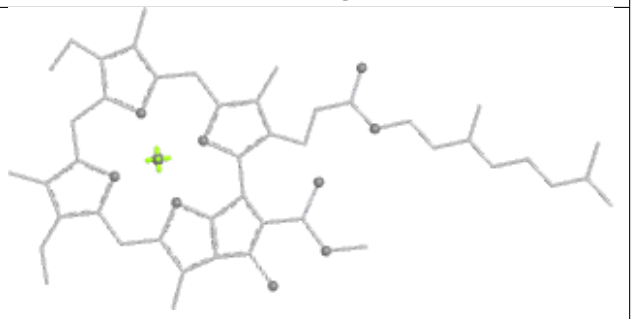
Bond lengths



Bond angles

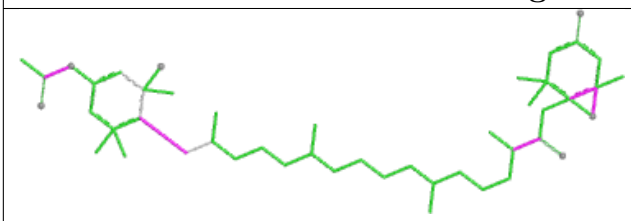


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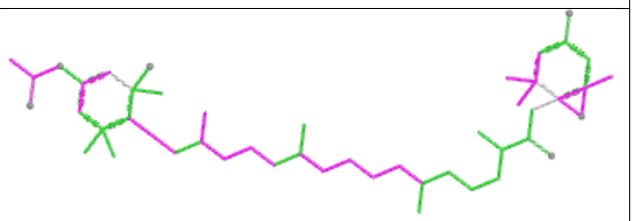


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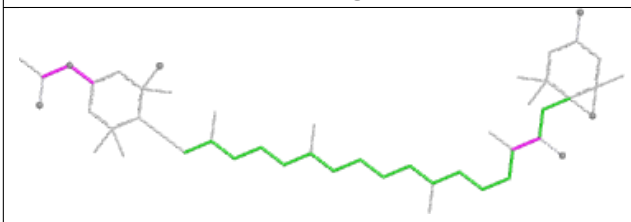
Ligand A86 N 302



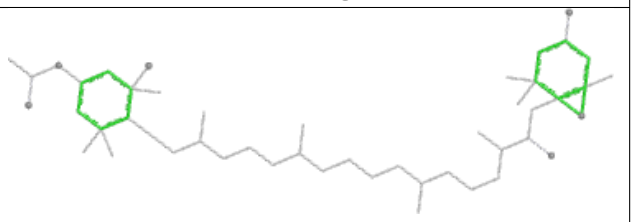
Bond lengths



Bond angles

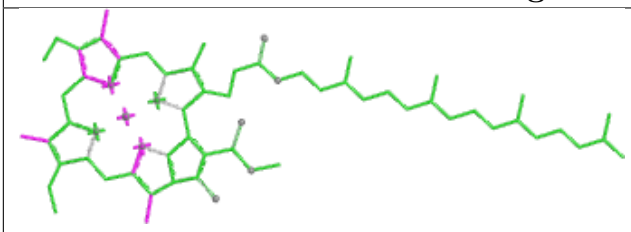


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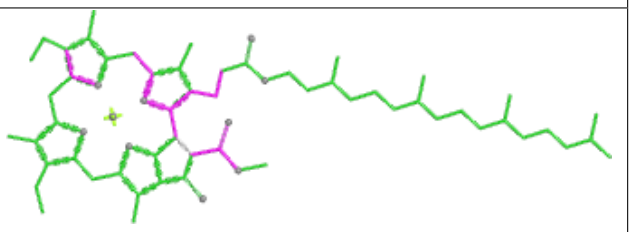


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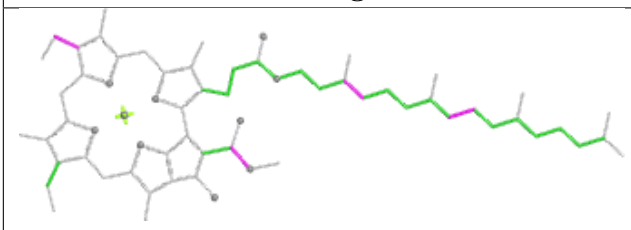
Ligand CLA S 319



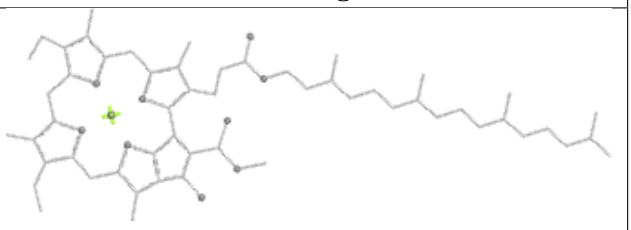
Bond lengths



Bond angles



Torsions

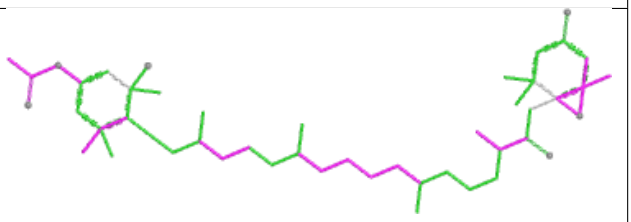


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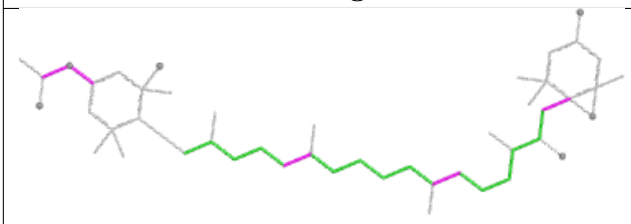
Ligand A86 F 302



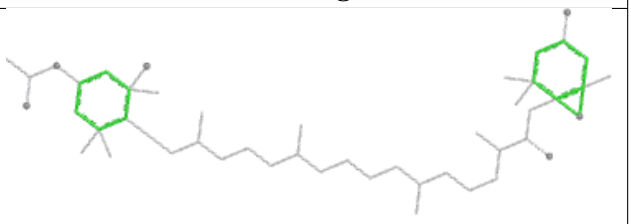
Bond lengths



Bond angles

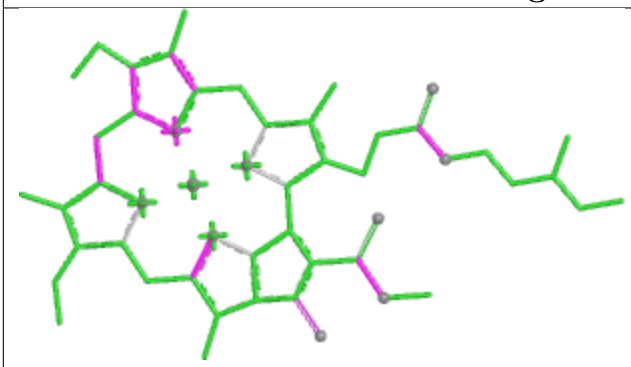


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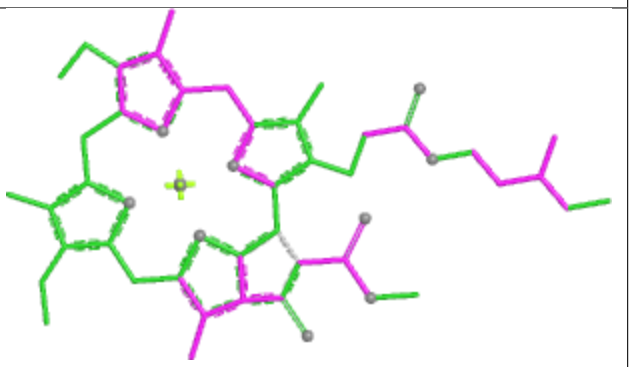


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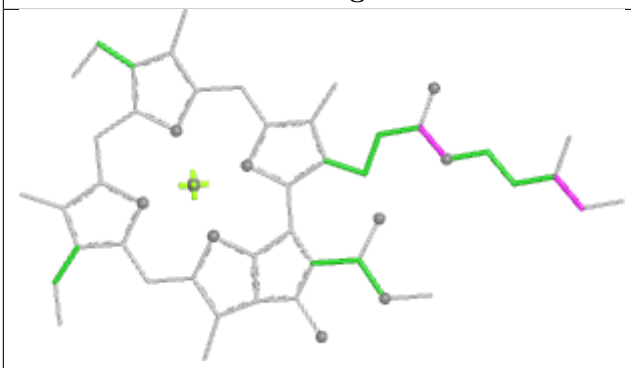
Ligand CLA a 822



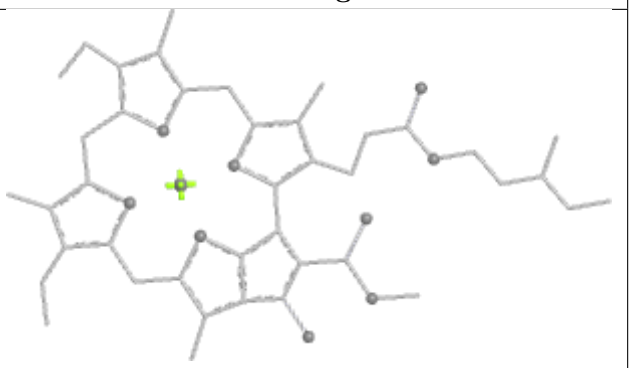
Bond lengths



Bond angles

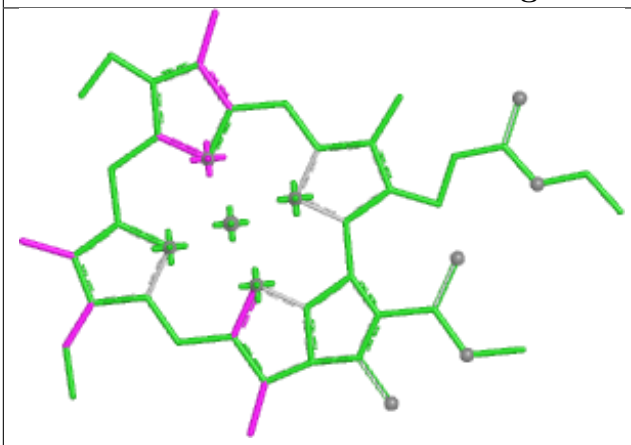


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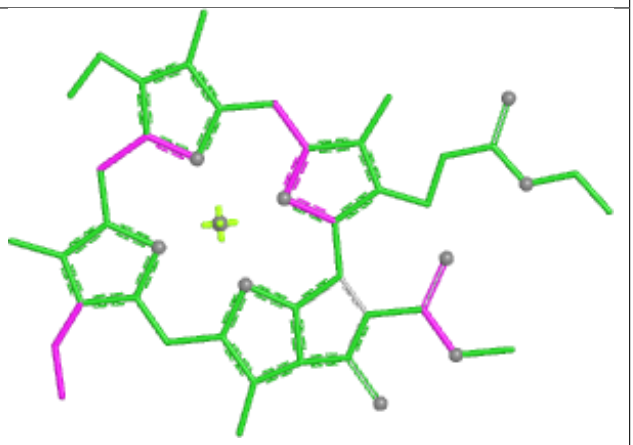


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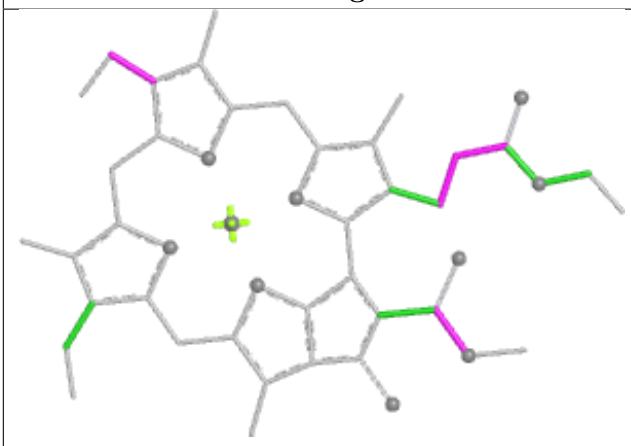
Ligand CLA M 315



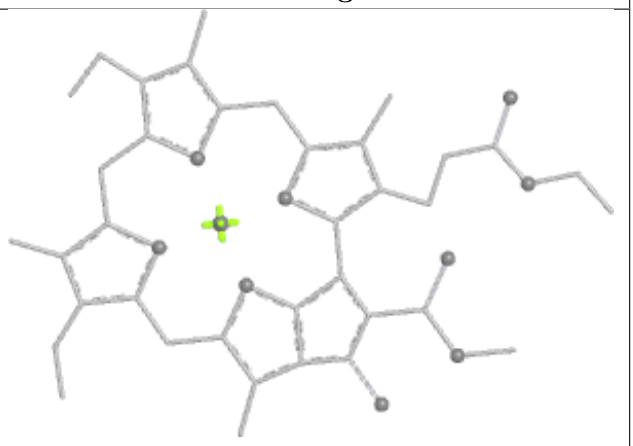
Bond lengths



Bond angles

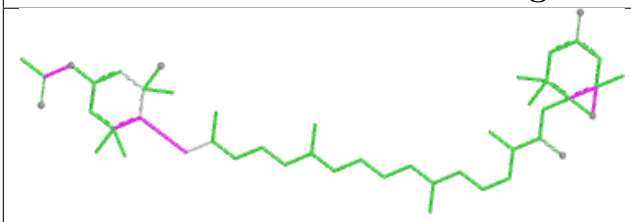


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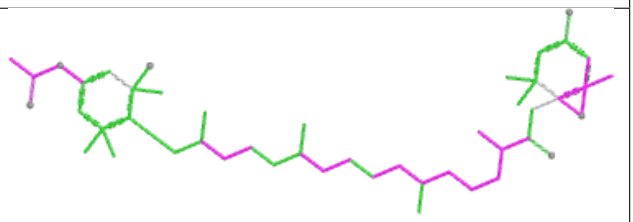


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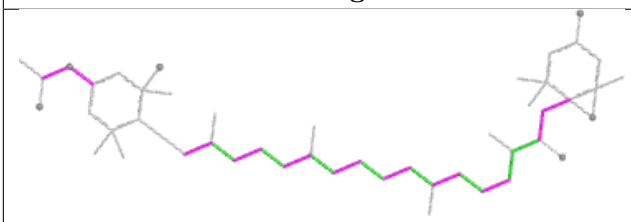
Ligand A86 U 303



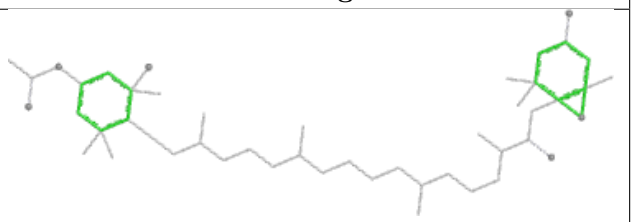
Bond lengths



Bond angles

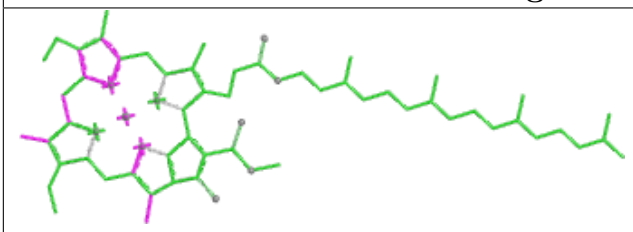


Torsions

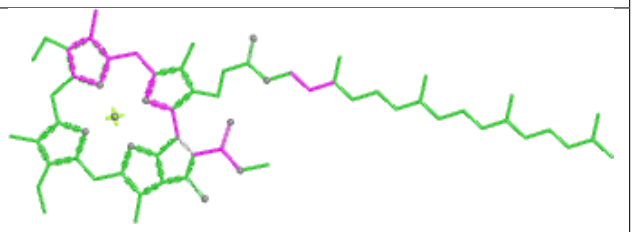


Rings

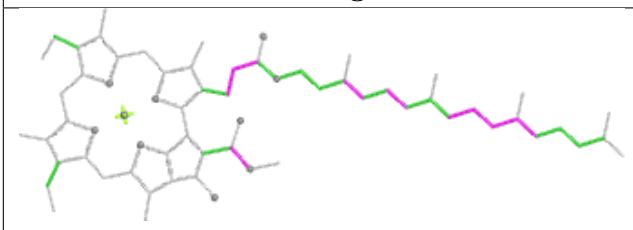
Ligand CLA L 311



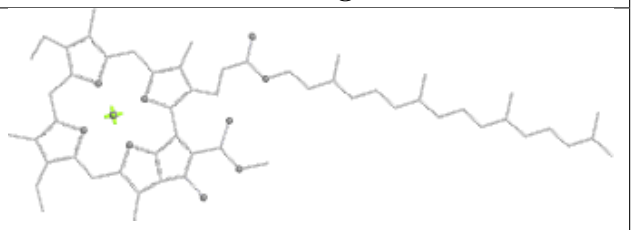
Bond lengths



Bond angles

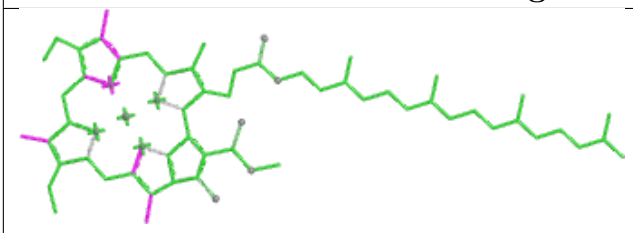


Torsions

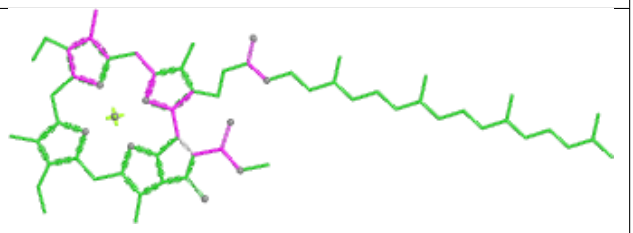


Rings

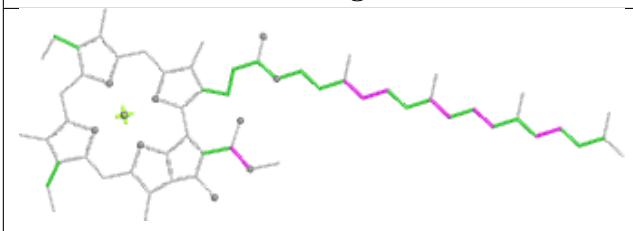
Ligand CLA a 837



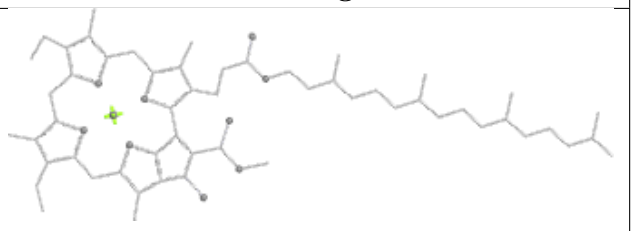
Bond lengths



Bond angles

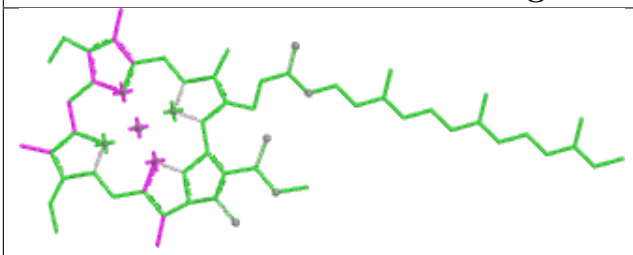


Torsions

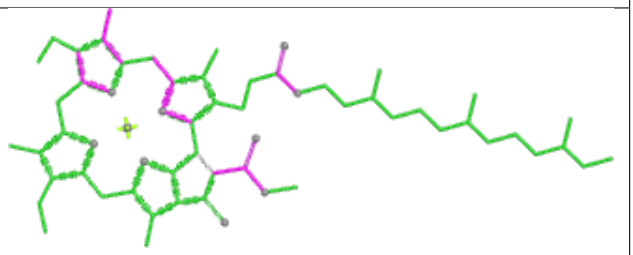


Rings

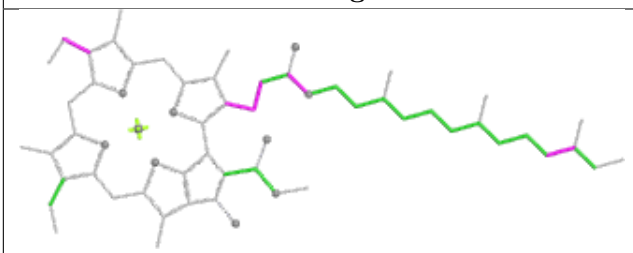
Ligand CLA S 309



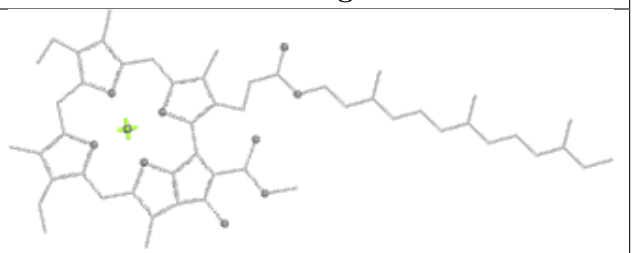
Bond lengths



Bond angles

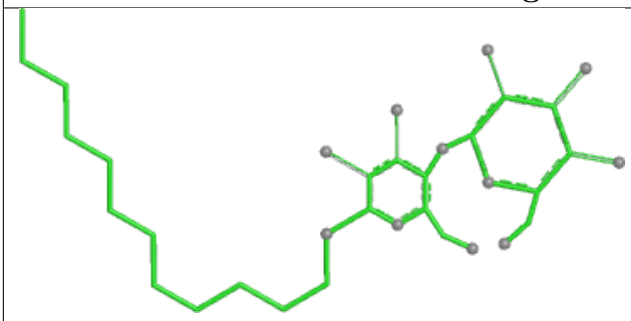


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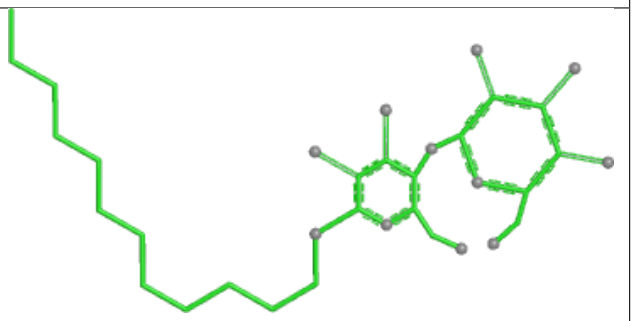


Rings

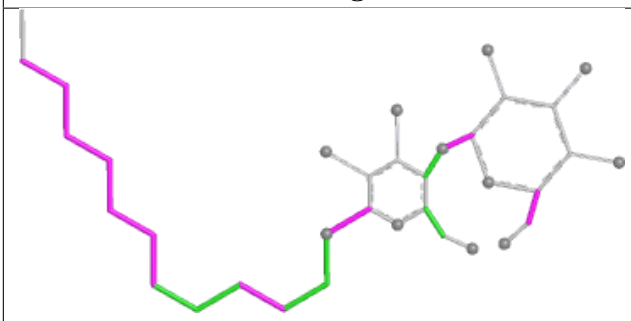
Ligand LMT E 320



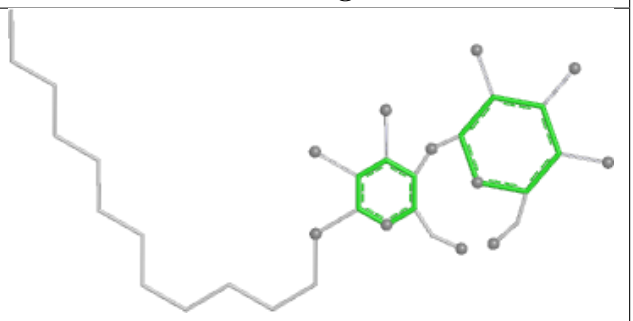
Bond lengths



Bond angles

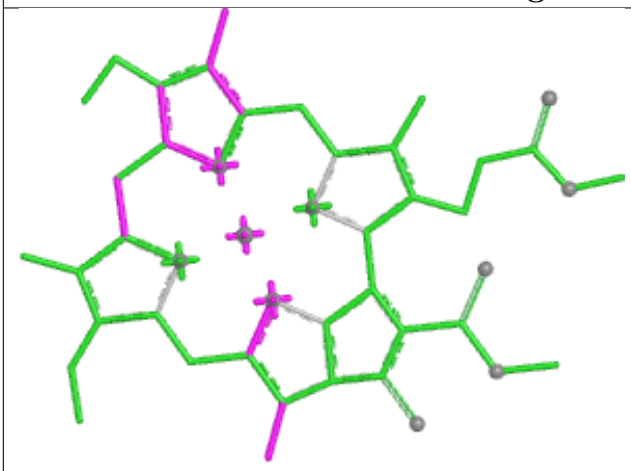


Torsions

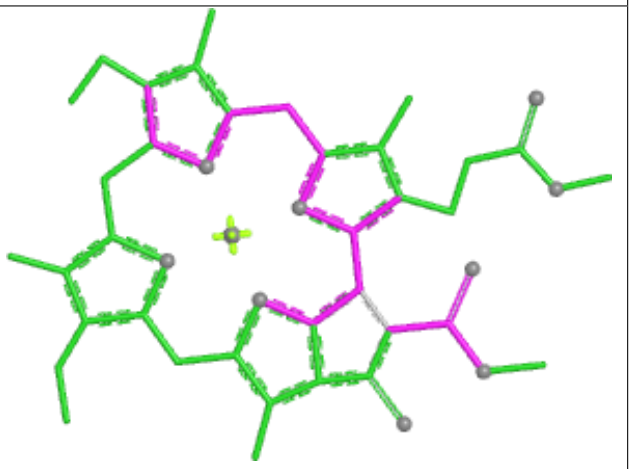


Rings

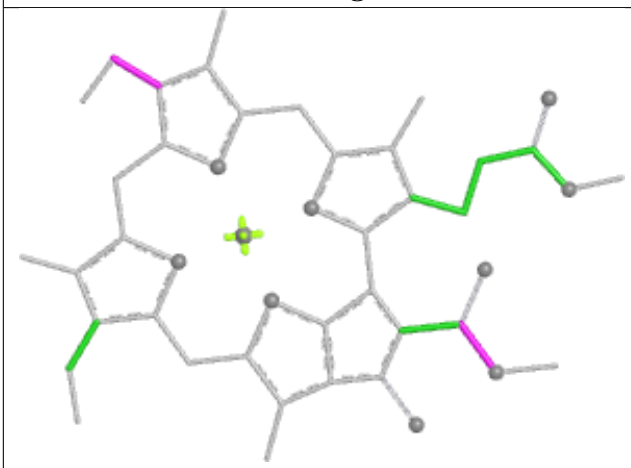
Ligand CLA S 311



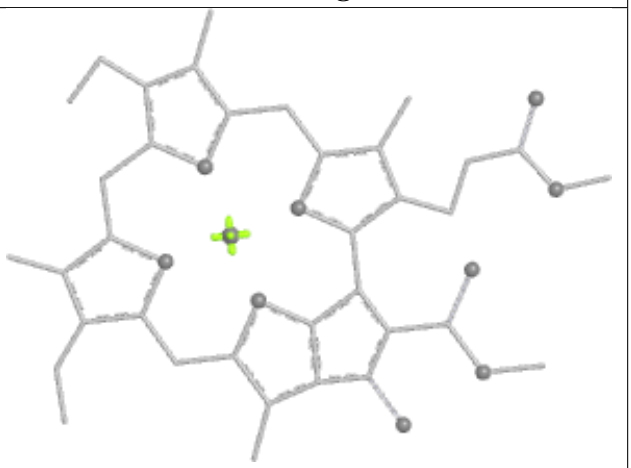
Bond lengths



Bond angles

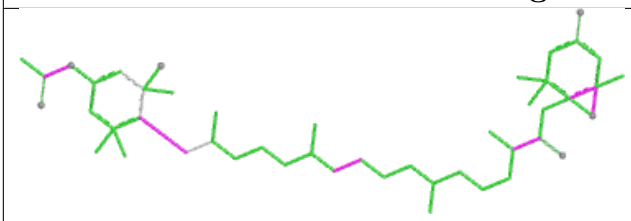


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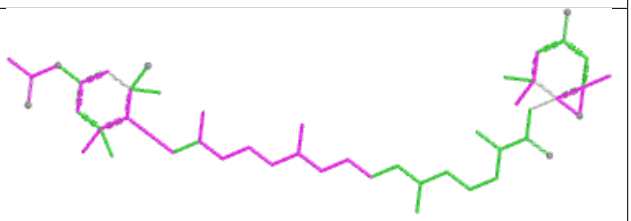


Rings

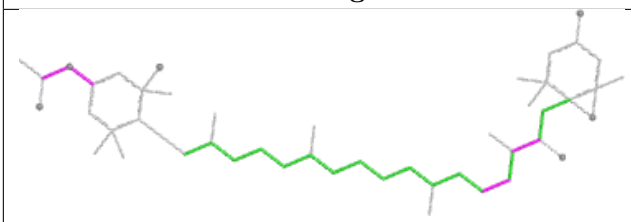
Ligand A86 O 319



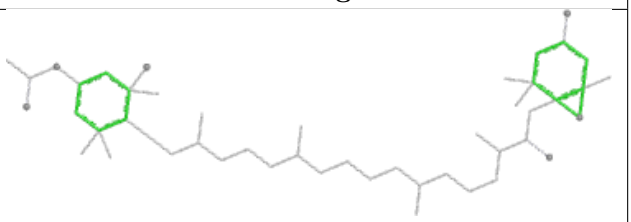
Bond lengths



Bond angles

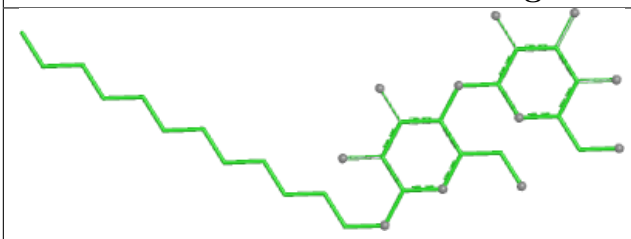


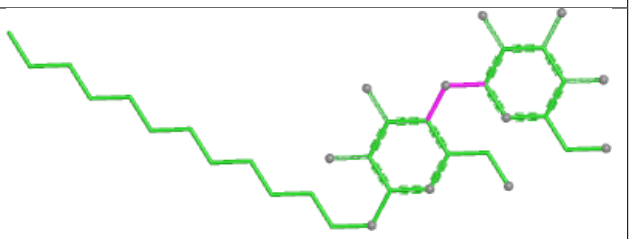
Torsions

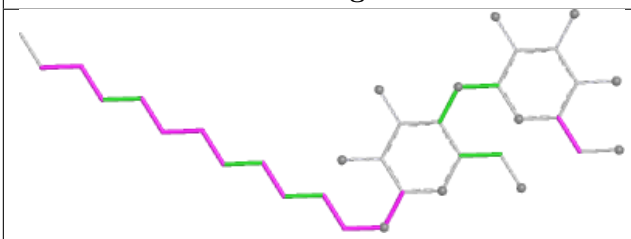


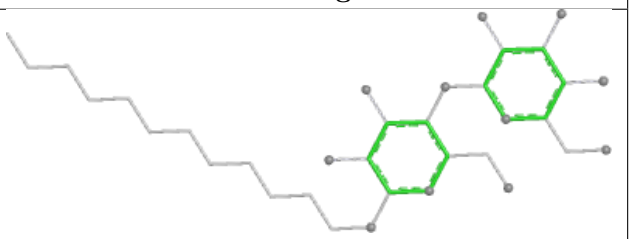
Rings

Ligand LMT b 848

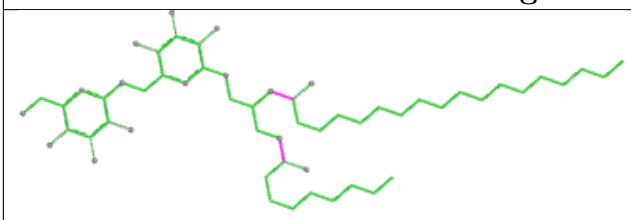

Bond lengths

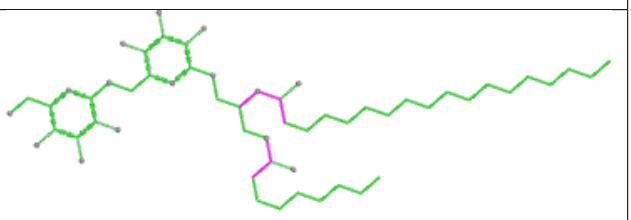

Bond angles

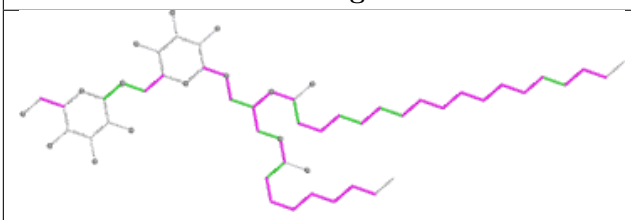

Torsions

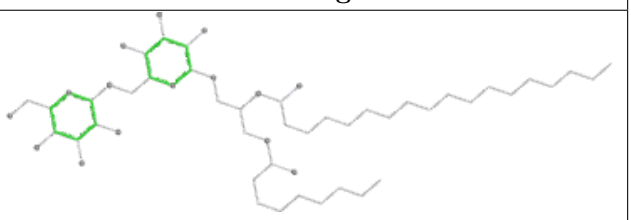

Rings

Ligand DGD C 215

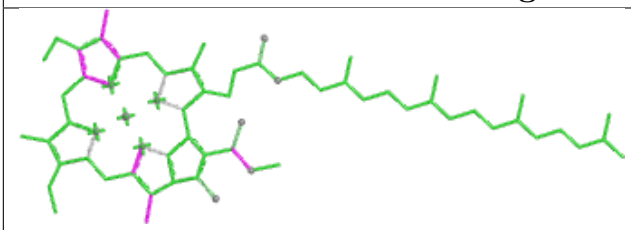

Bond lengths

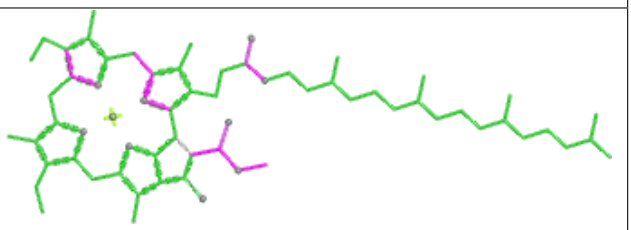

Bond angles

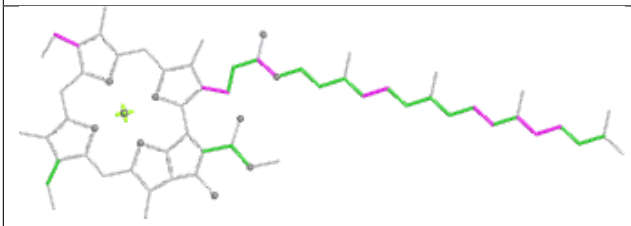

Torsions

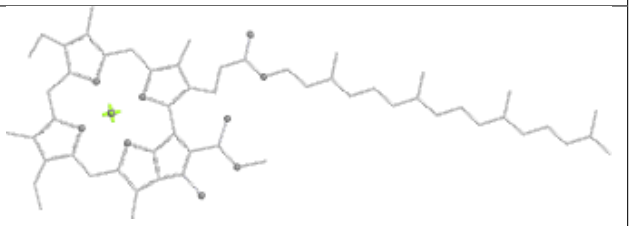

Rings

Ligand CLA W 211

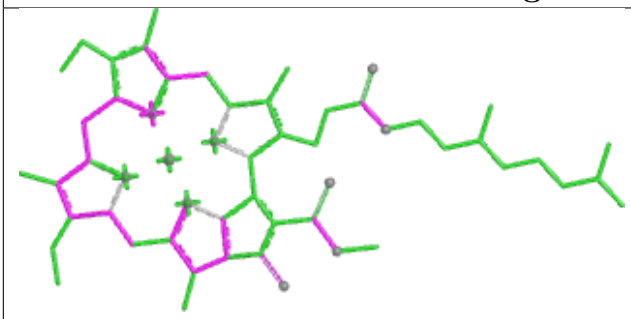

Bond lengths


Bond angles

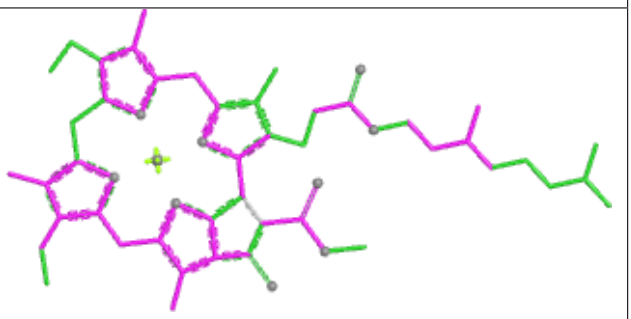

Torsions


Rings

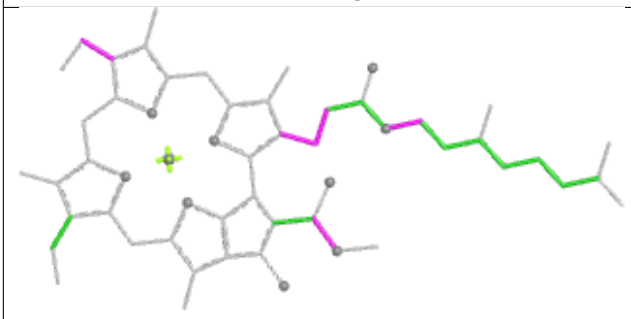
Ligand CLA D 309



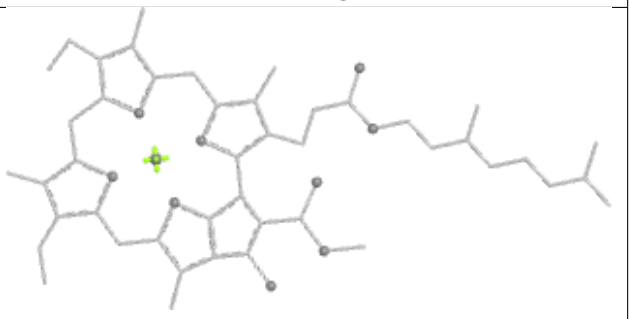
Bond lengths



Bond angles

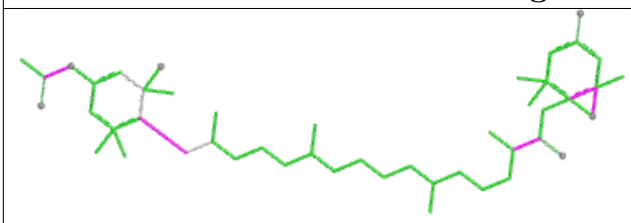


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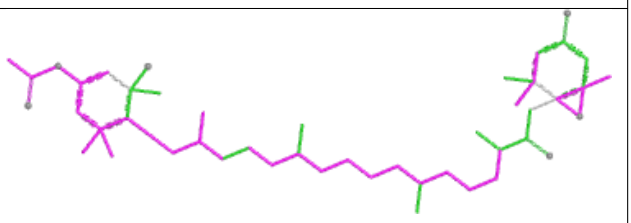


Rings

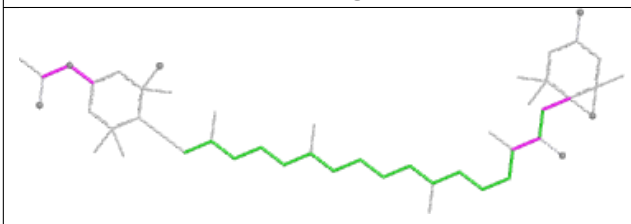
Ligand A86 O 302



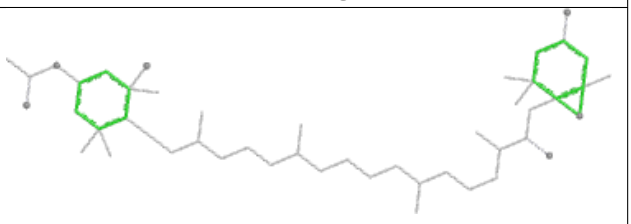
Bond lengths



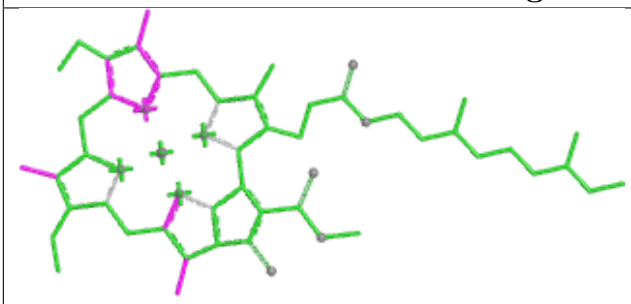
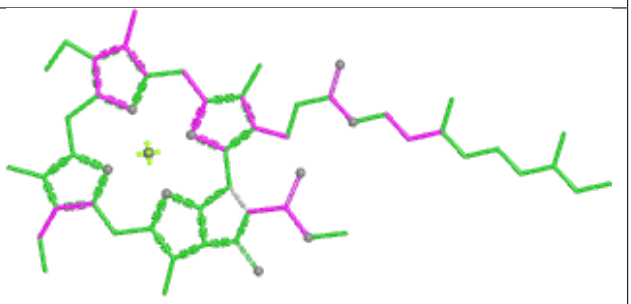
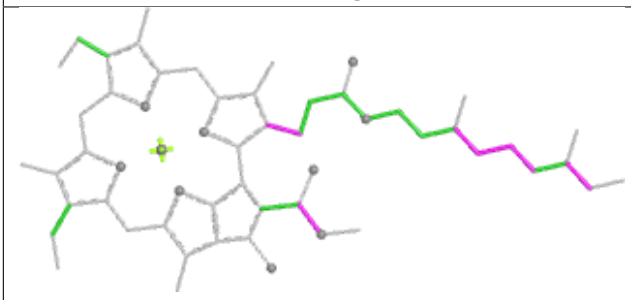
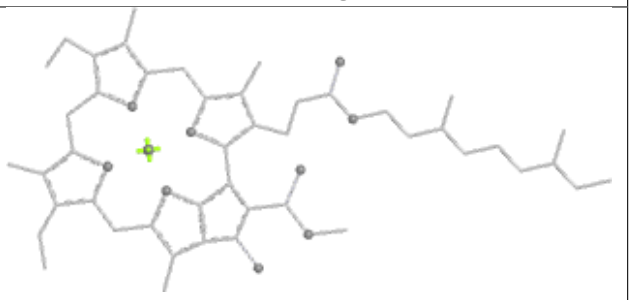
Bond angles

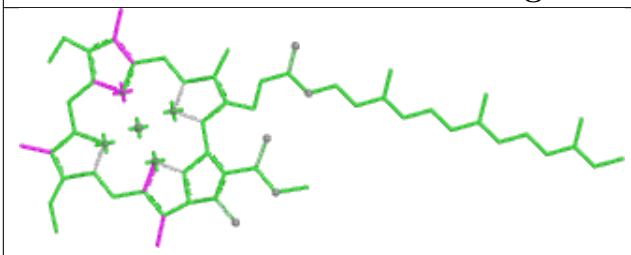
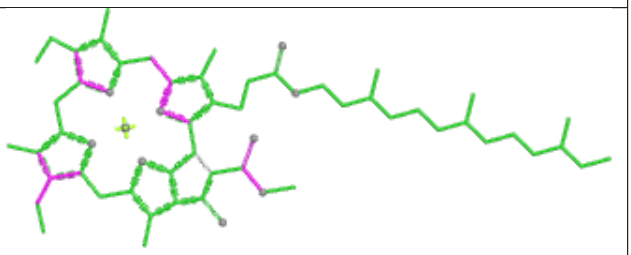
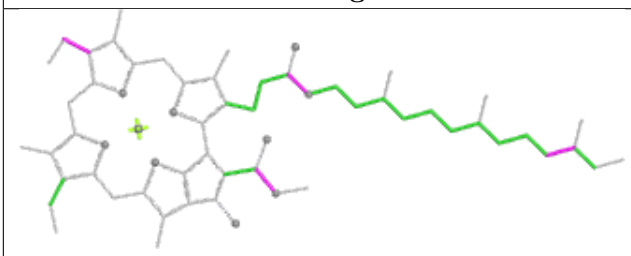
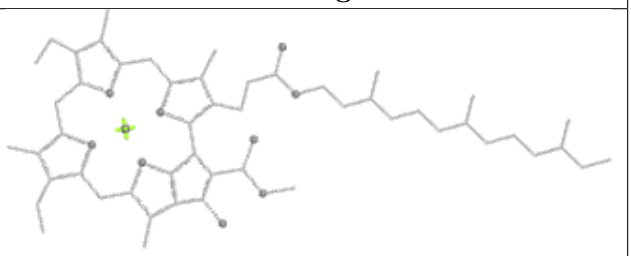


Torsions

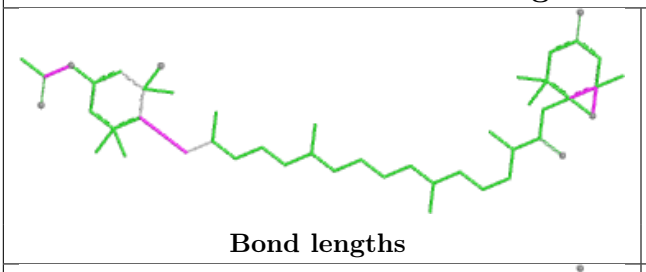


Rings

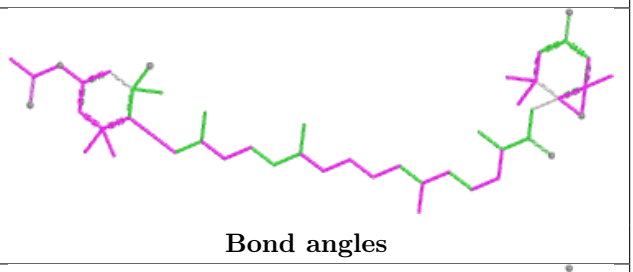
Ligand CLA F 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA T 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

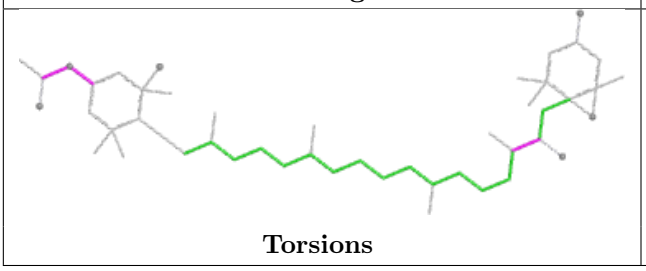
Ligand A86 F 307



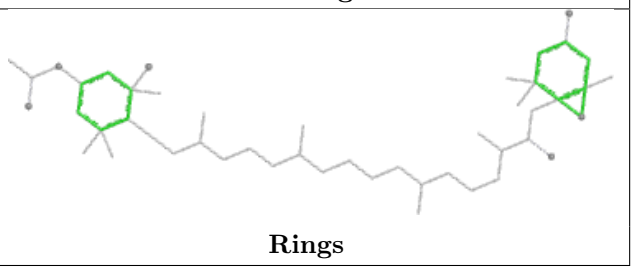
Bond lengths



Bond angles

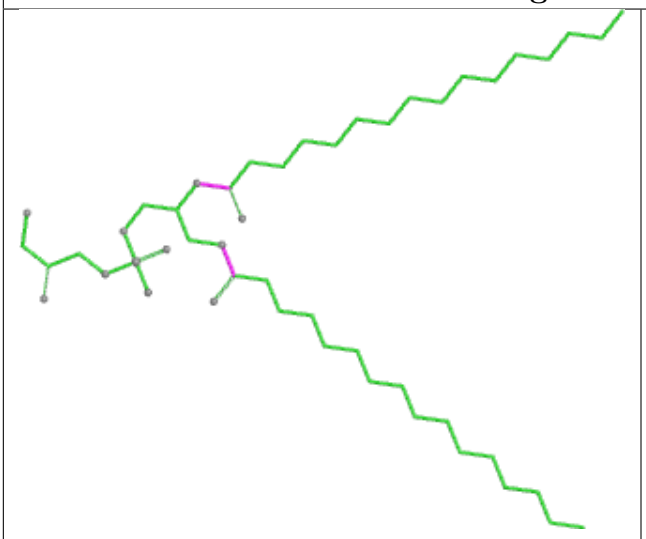


Torsions

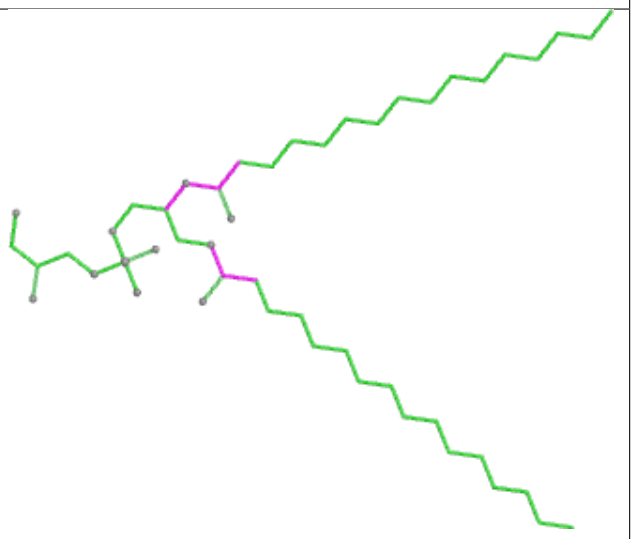


Rings

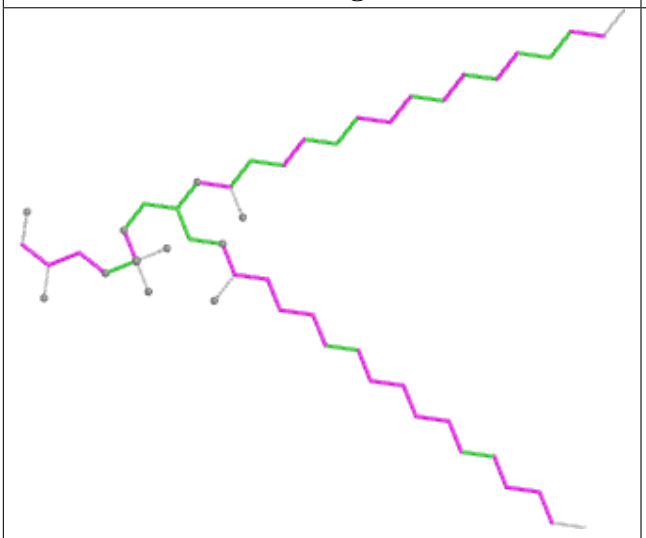
Ligand LHG f 808



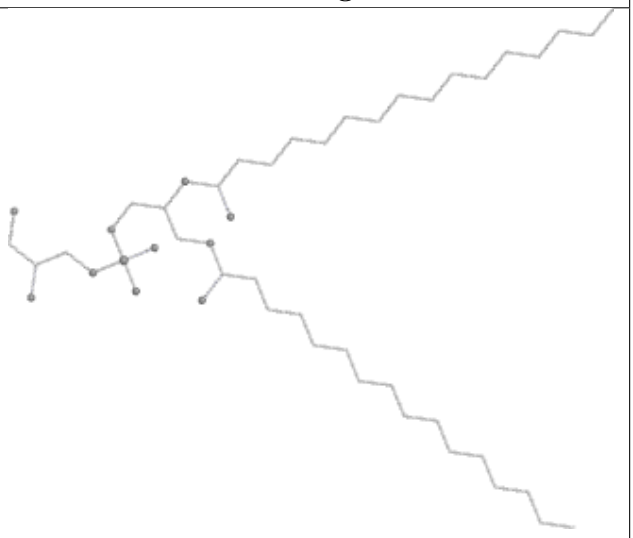
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Bond angles

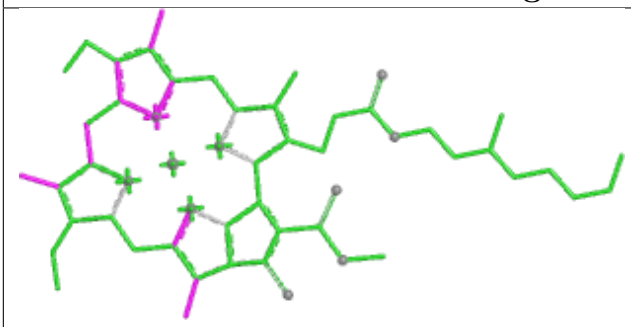


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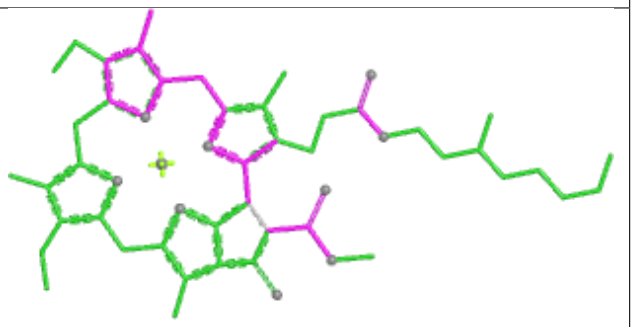


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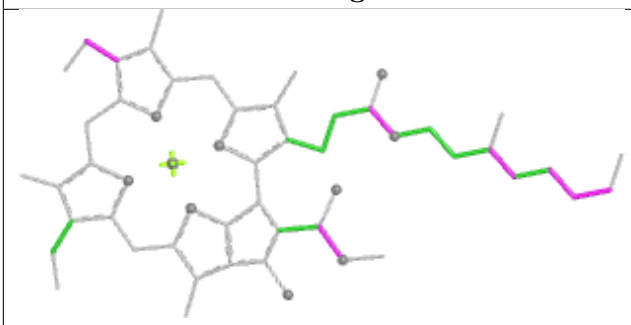
Ligand CLA N 317



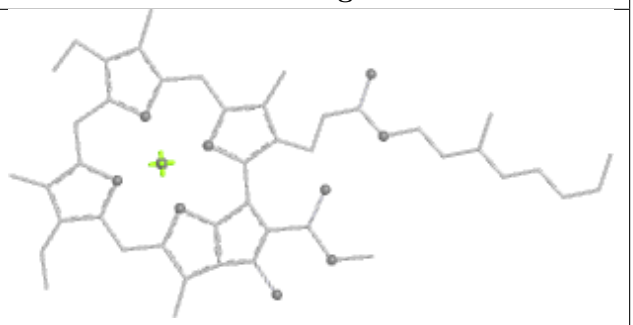
Bond lengths



Bond angles

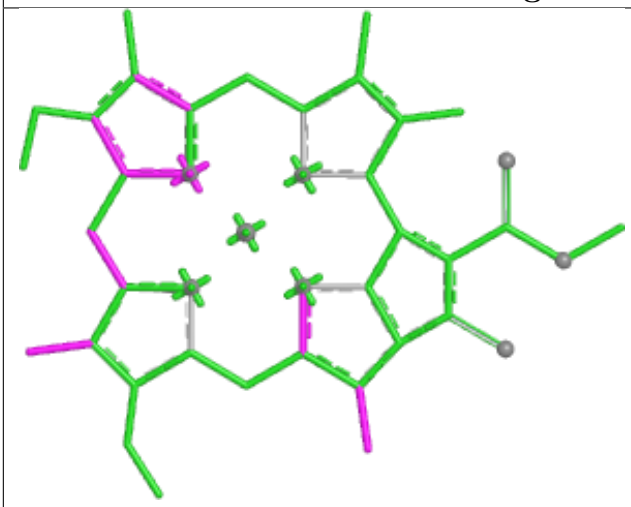


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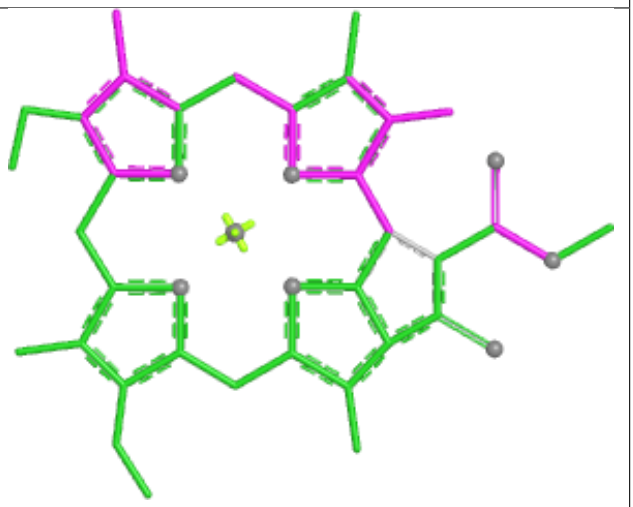


Rings

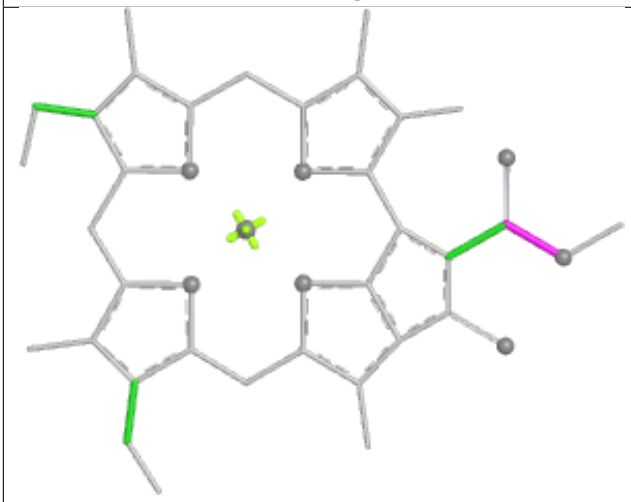
Ligand CLA X 312



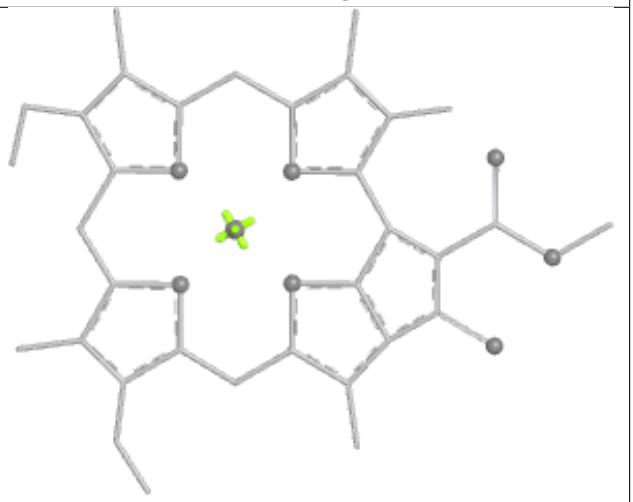
Bond lengths



Bond angles

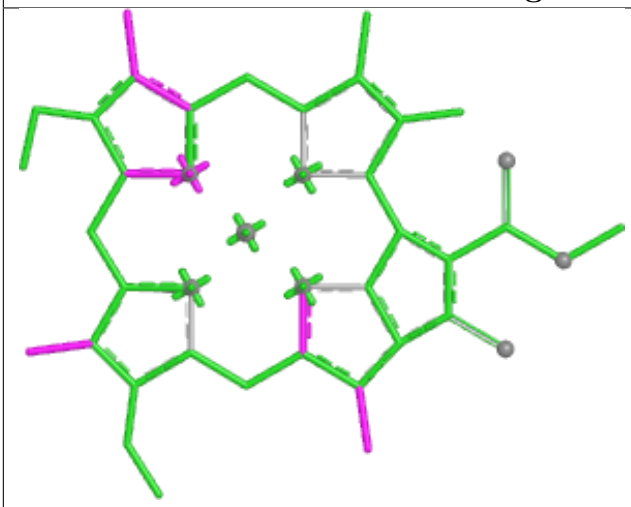


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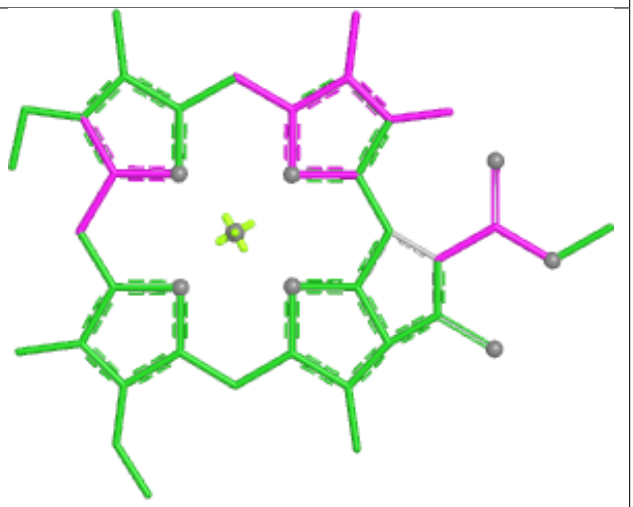


Rings

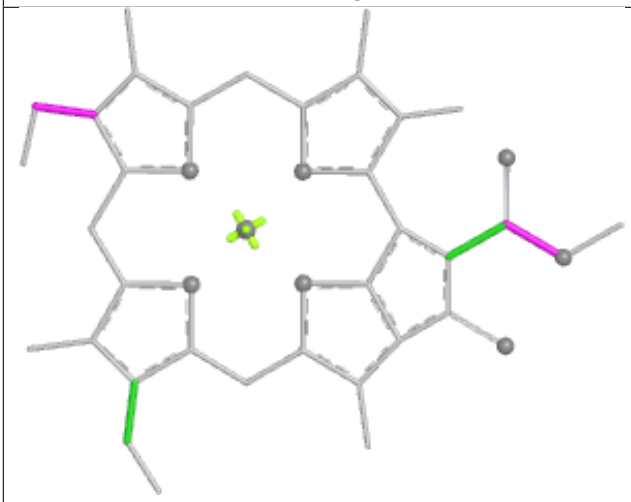
Ligand CLA P 316



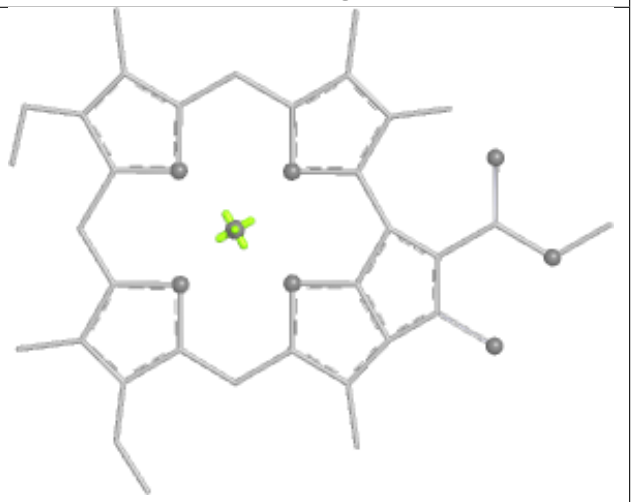
Bond lengths



Bond angles

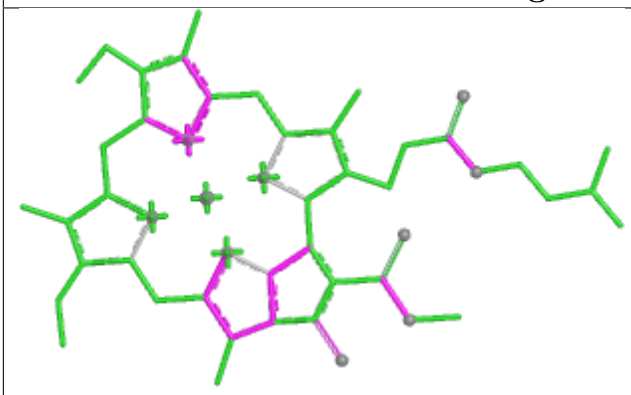


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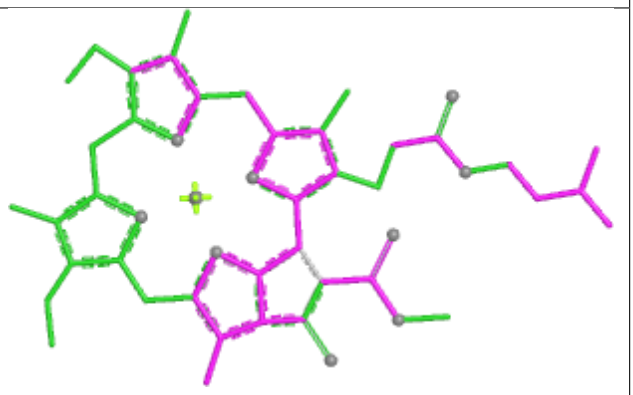


Rings

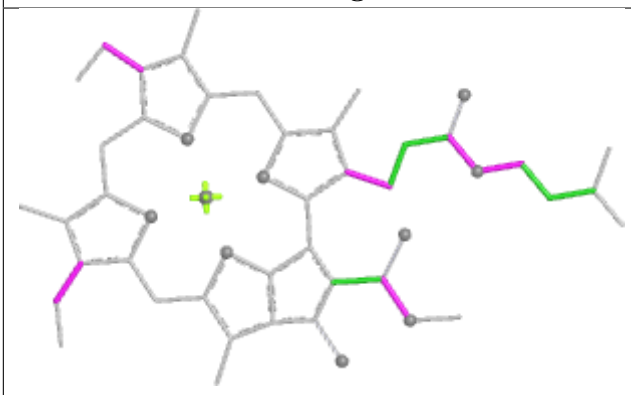
Ligand CLA a 830



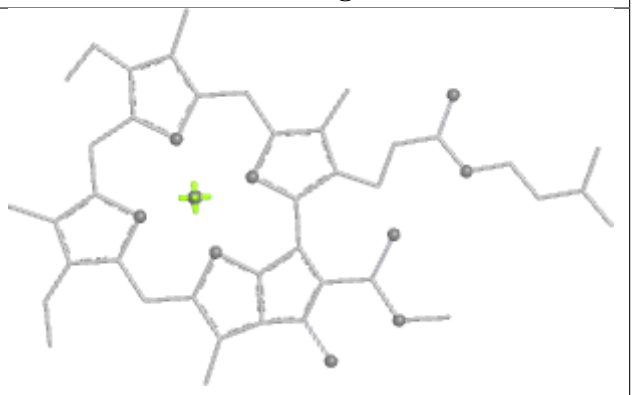
Bond lengths



Bond angles

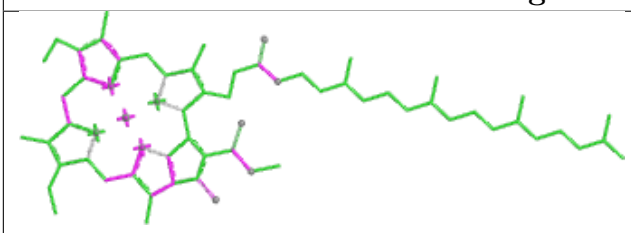


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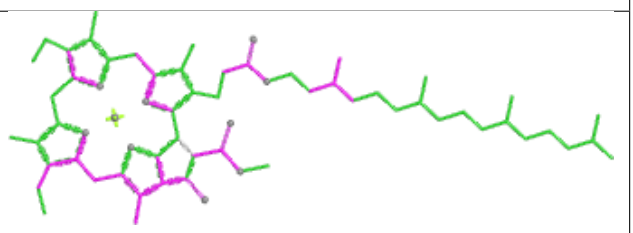


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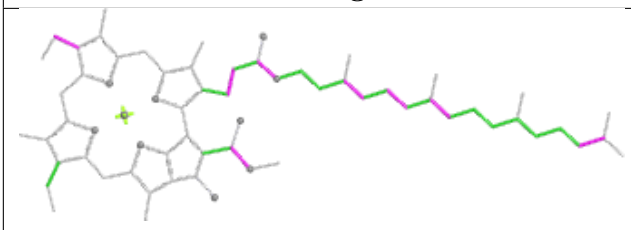
Ligand CLA a 848



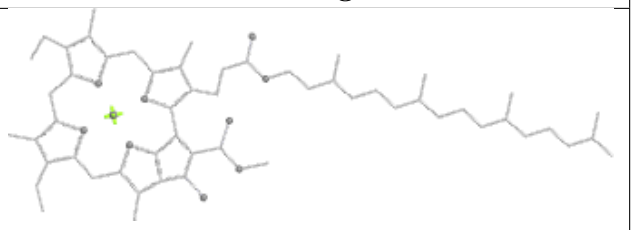
Bond lengths



Bond angles

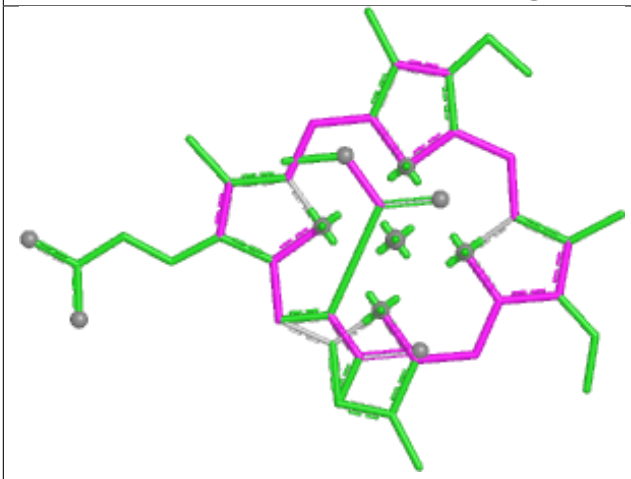


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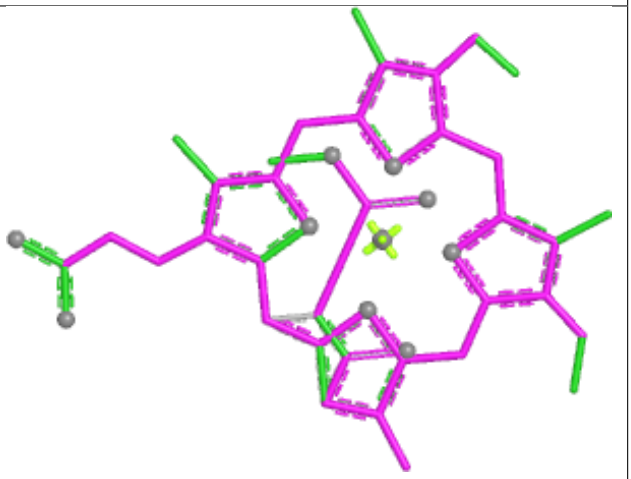


Rings

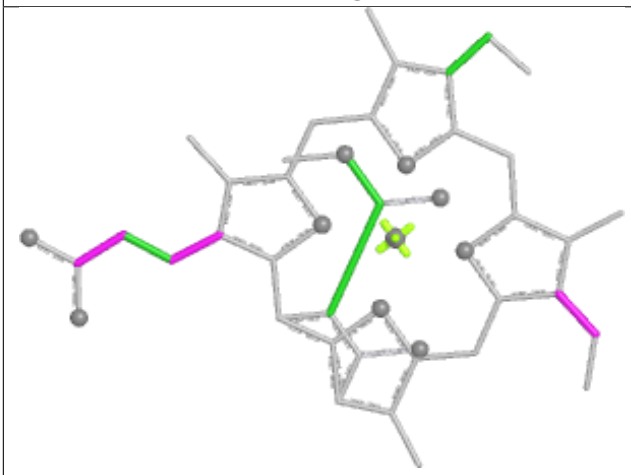
Ligand KC1 V 312



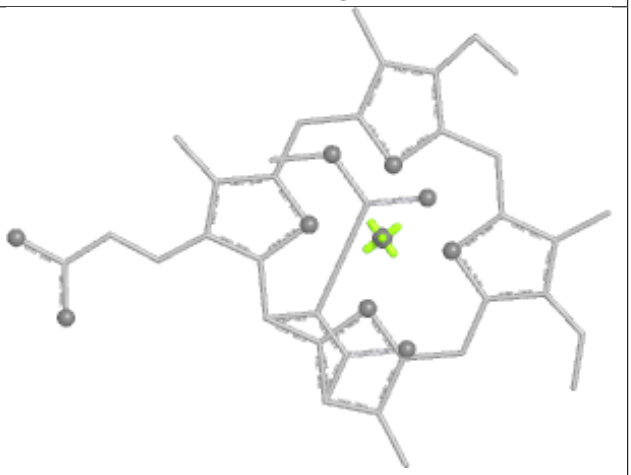
Bond lengths



Bond angles

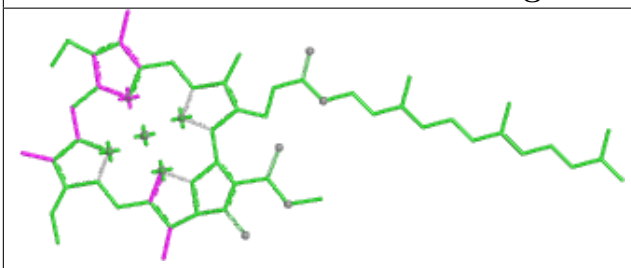


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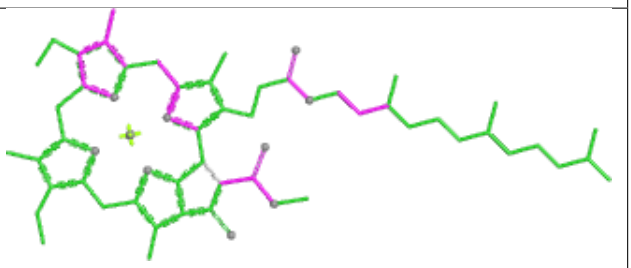


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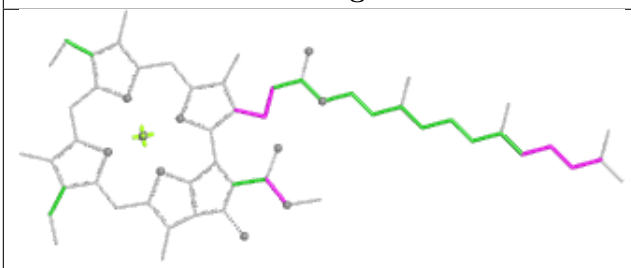
Ligand CLA A 307



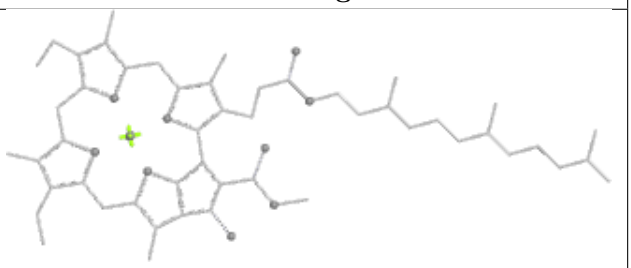
Bond lengths



Bond angles

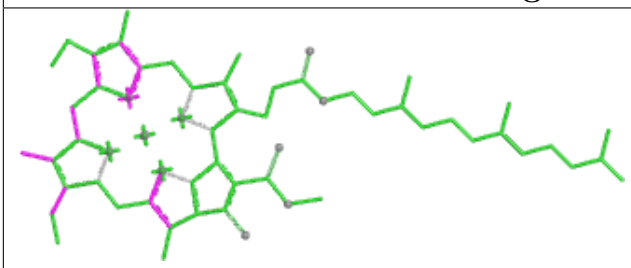


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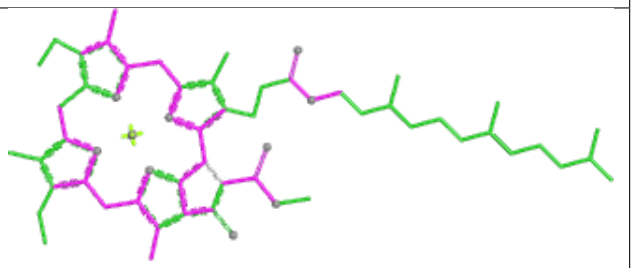


Rings

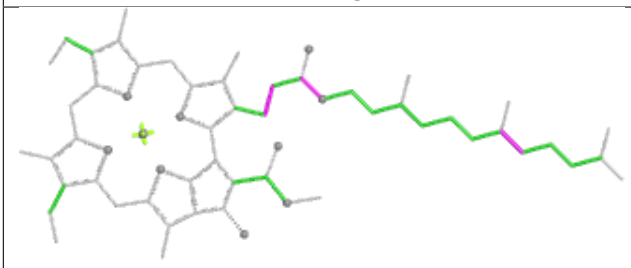
Ligand CLA H 307



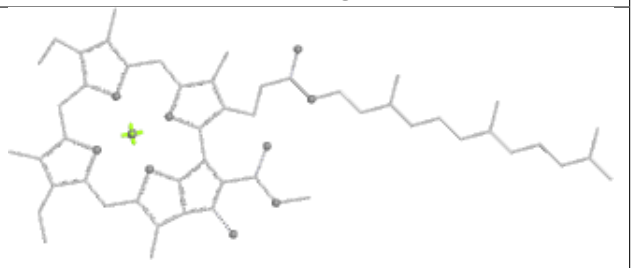
Bond lengths



Bond angles

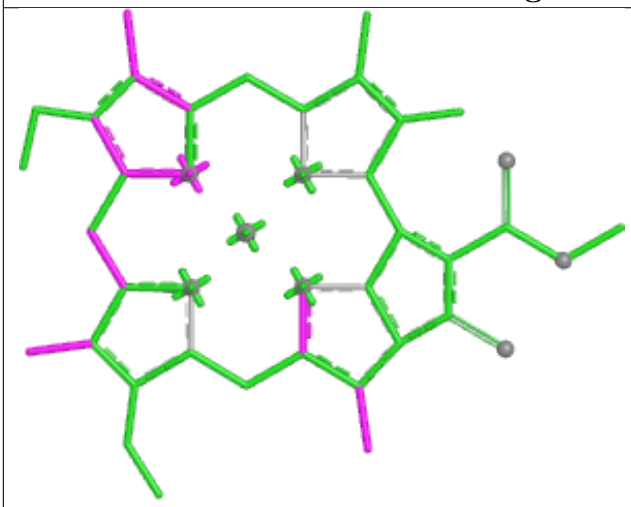


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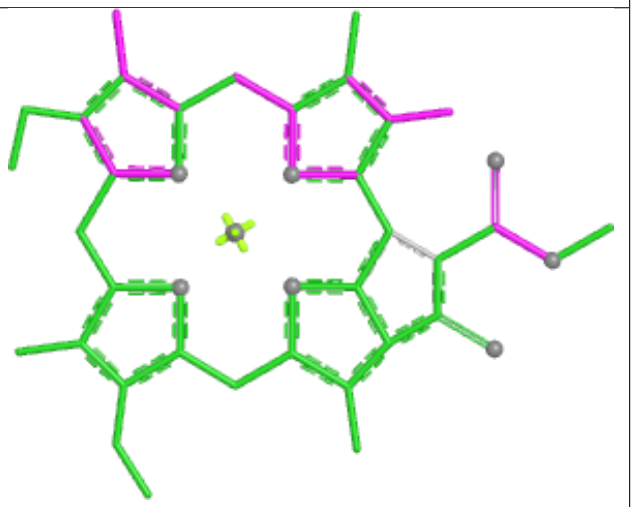


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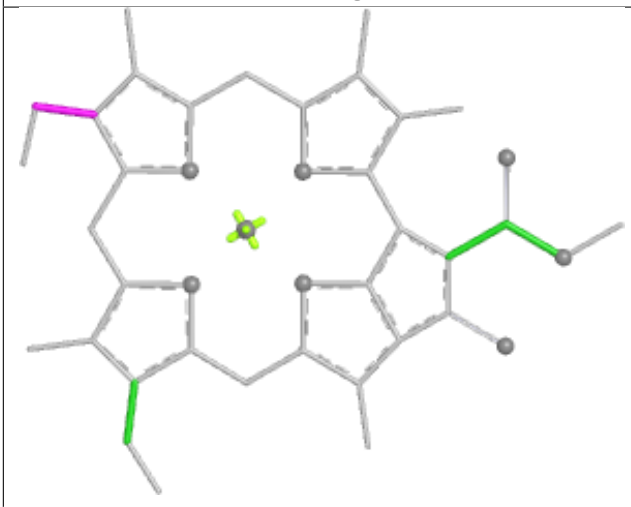
Ligand CLA T 316



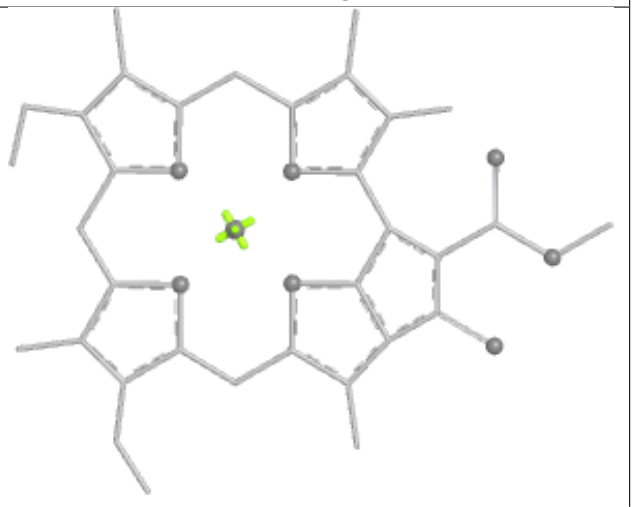
Bond lengths



Bond angles

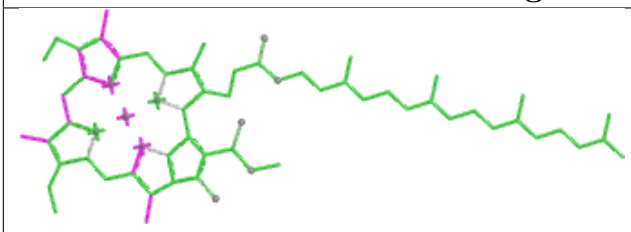


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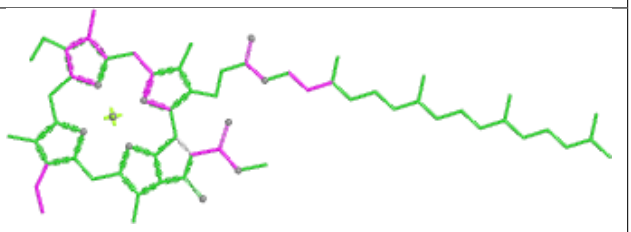


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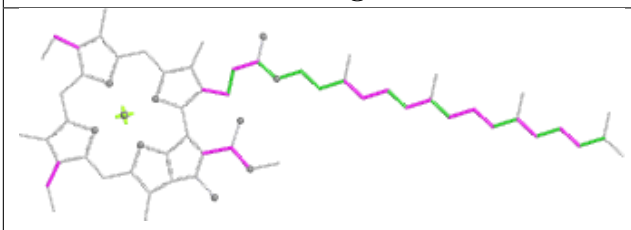
Ligand CLA P 311



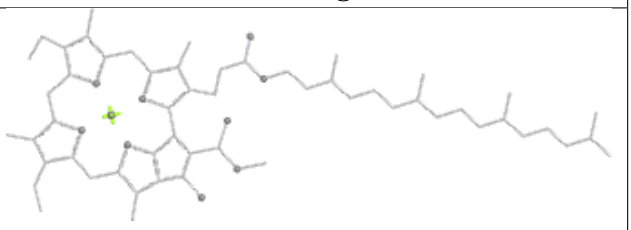
Bond lengths



Bond angles

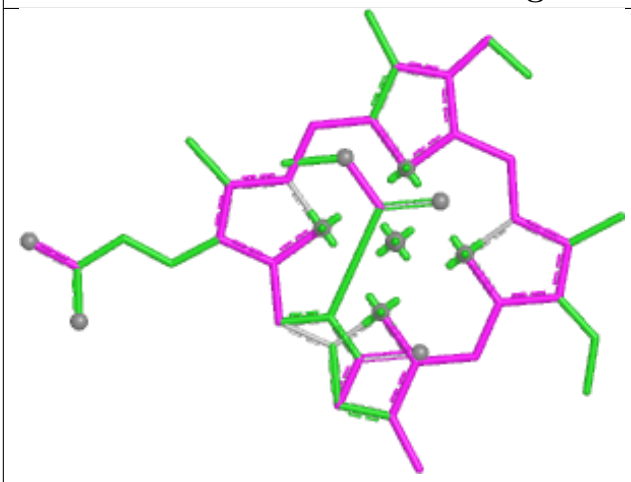


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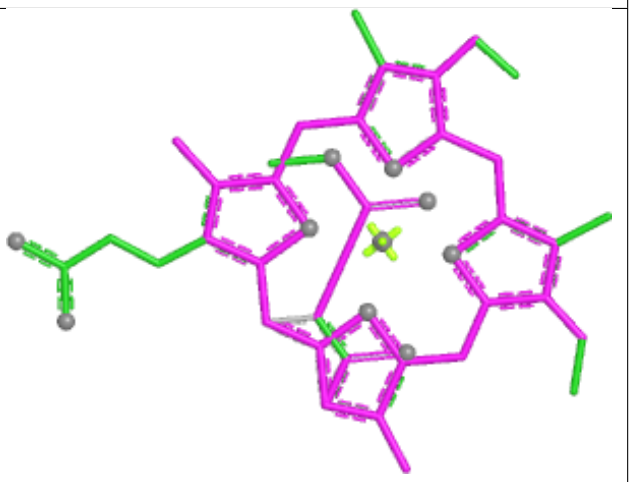


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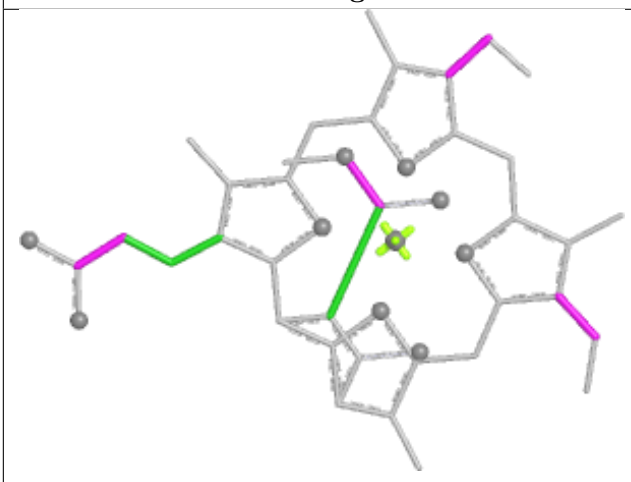
Ligand KC1 T 310



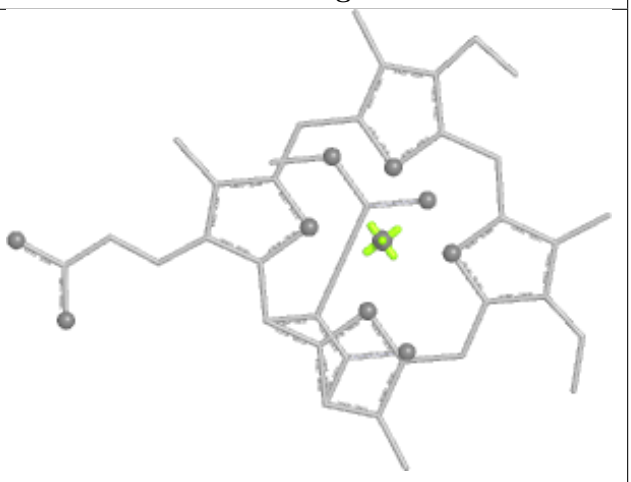
Bond lengths



Bond angles

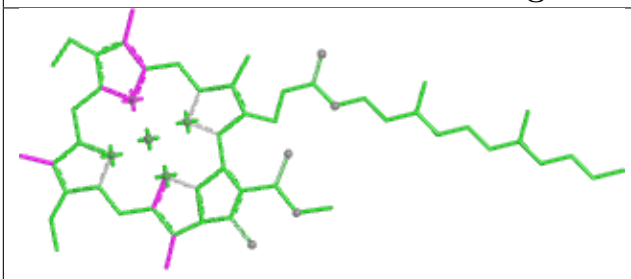


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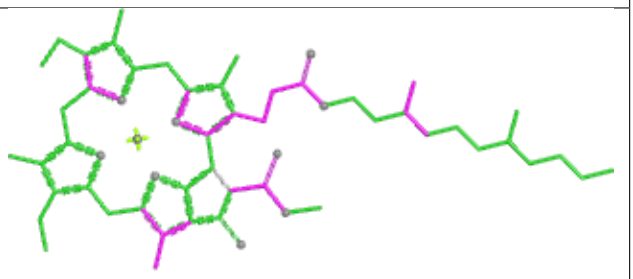


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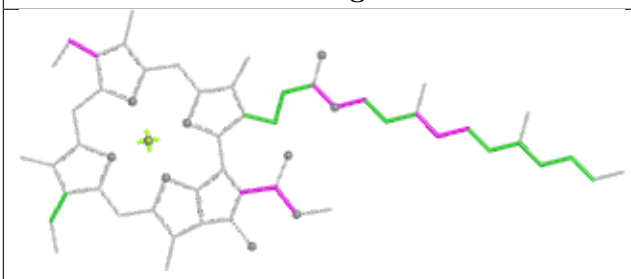
Ligand CLA b 833



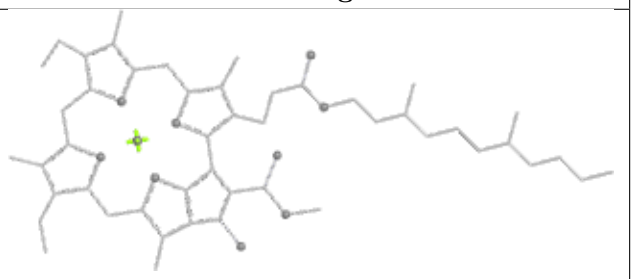
Bond lengths



Bond angles

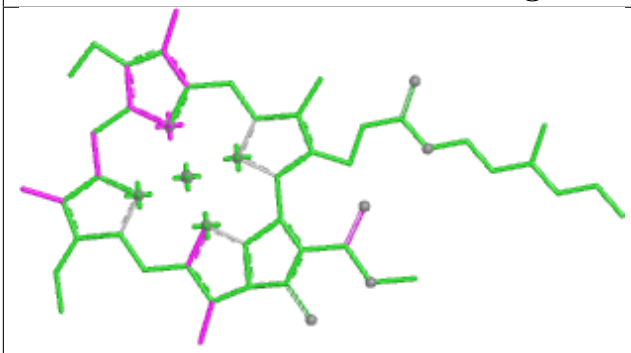


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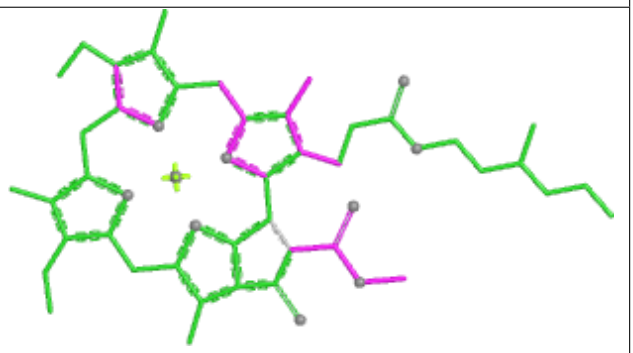


Rings

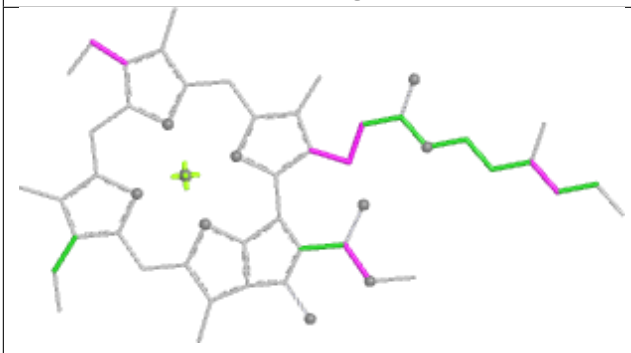
Ligand CLA R 322



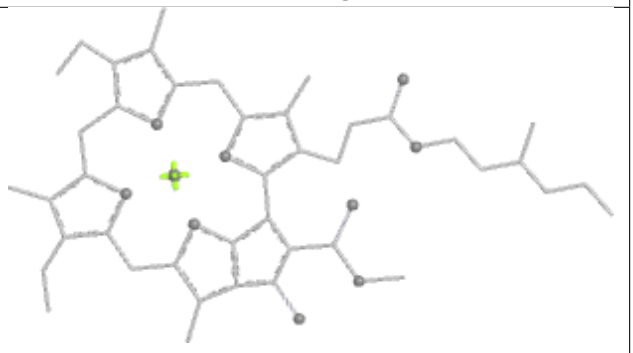
Bond lengths



Bond angles

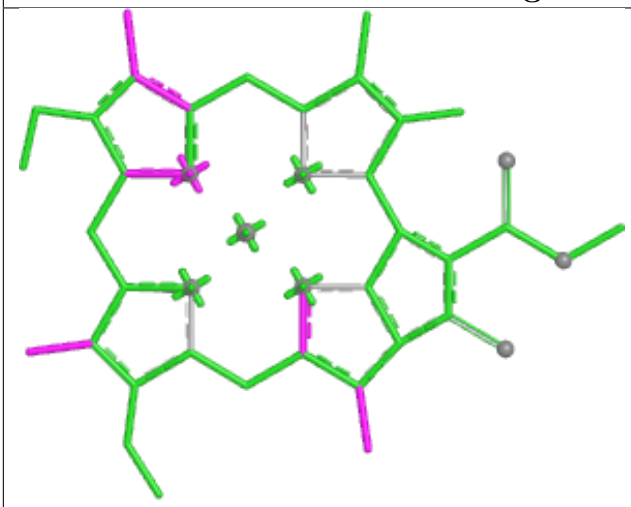


Torsions

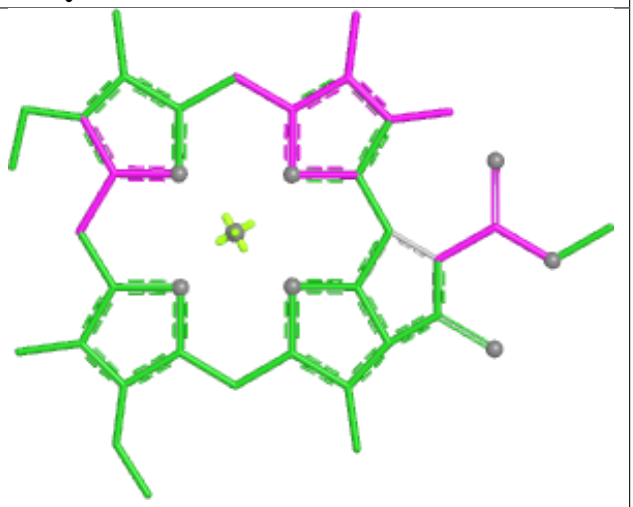


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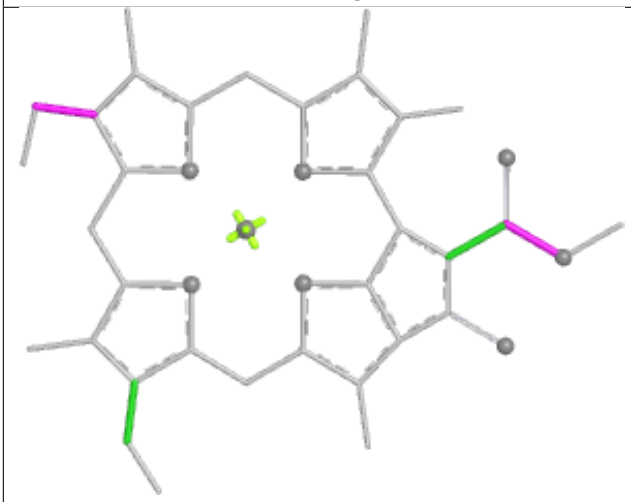
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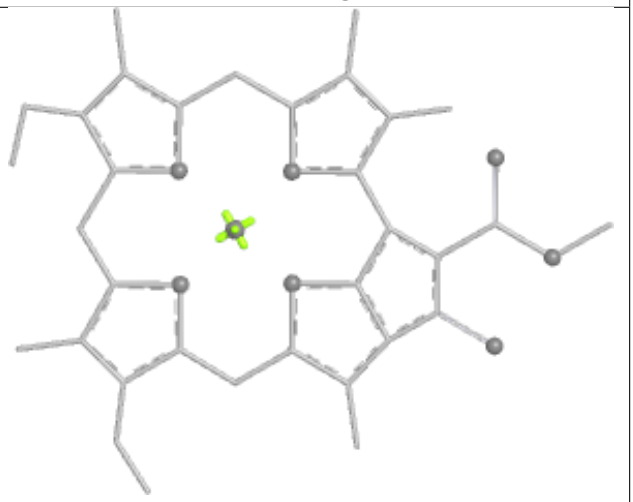
Bond lengths



Bond angles

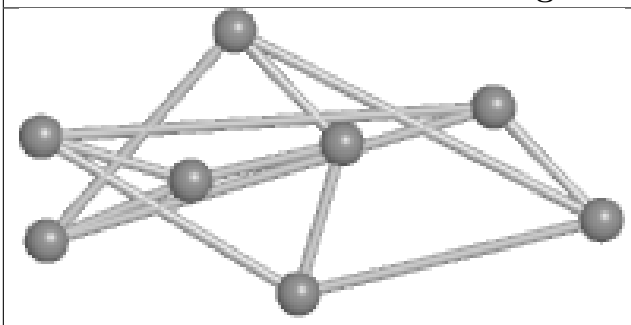


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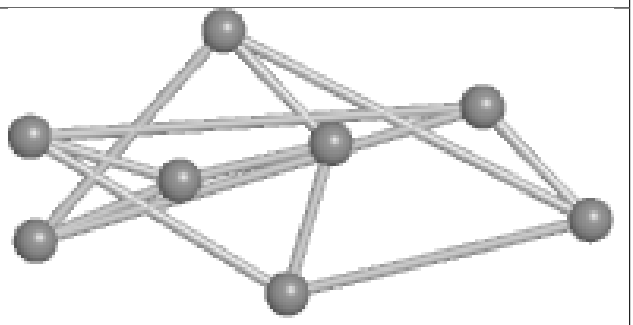


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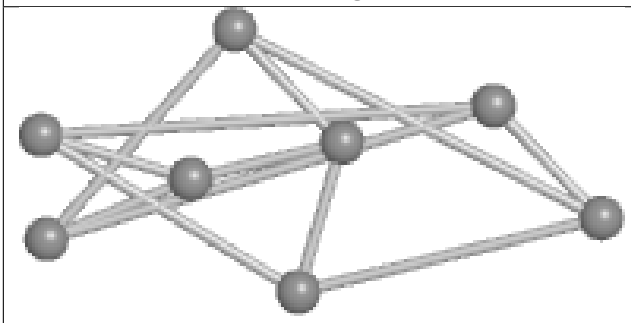
Ligand SF4 c 101



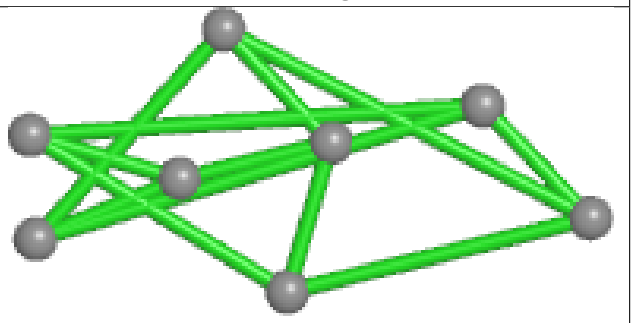
Bond lengths



Bond angles

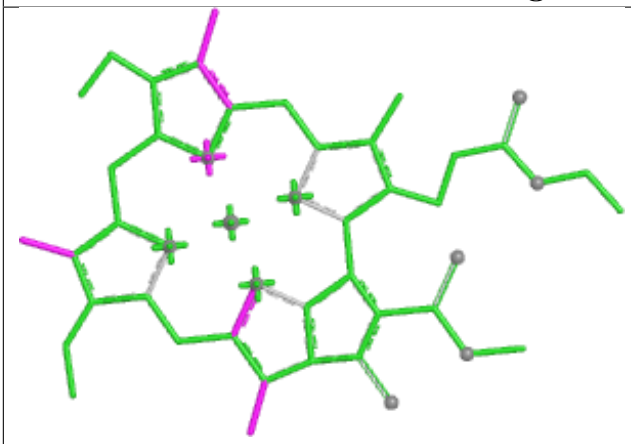


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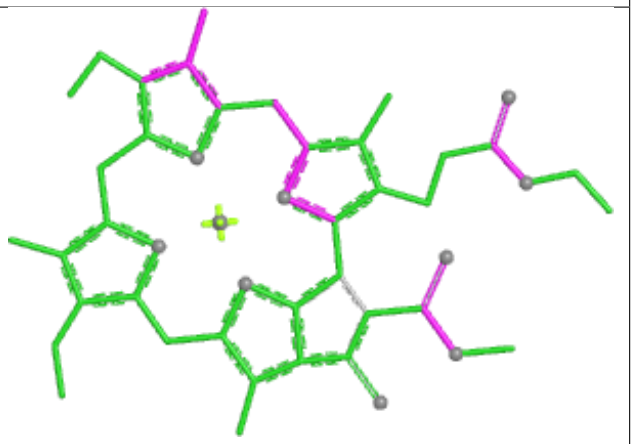


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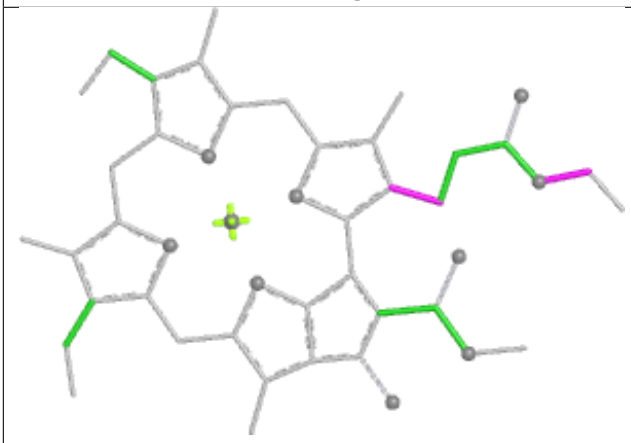
Ligand CLA b 838



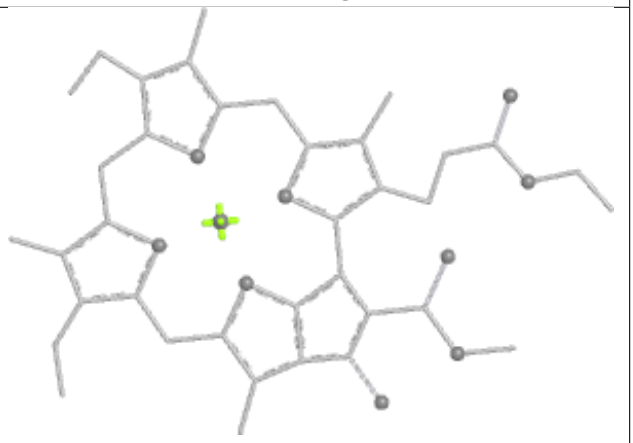
Bond lengths



Bond angles

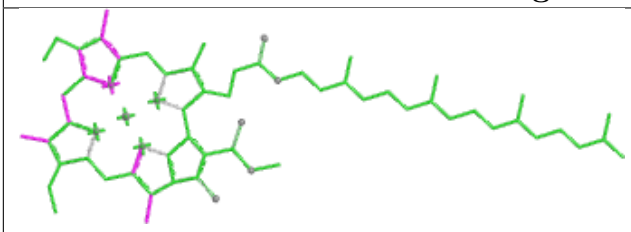


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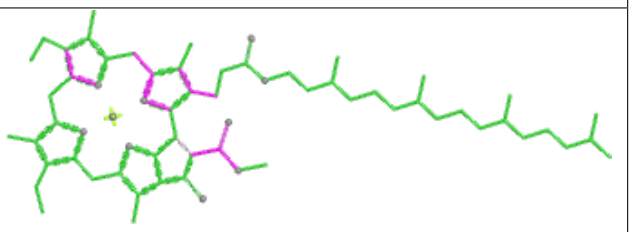


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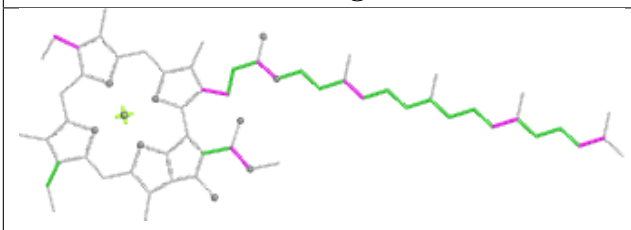
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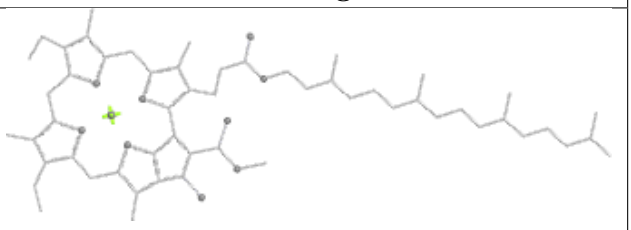
Bond lengths



Bond angles



Torsions

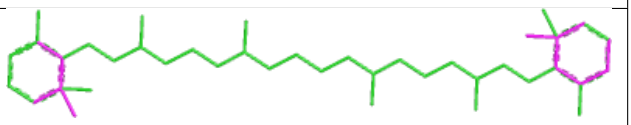


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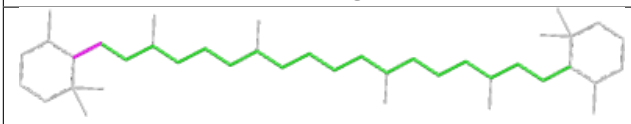
Ligand BCR i 101



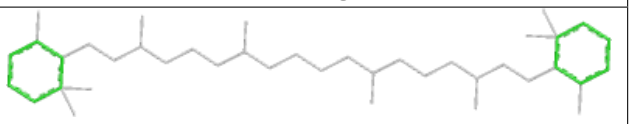
Bond lengths



Bond angles

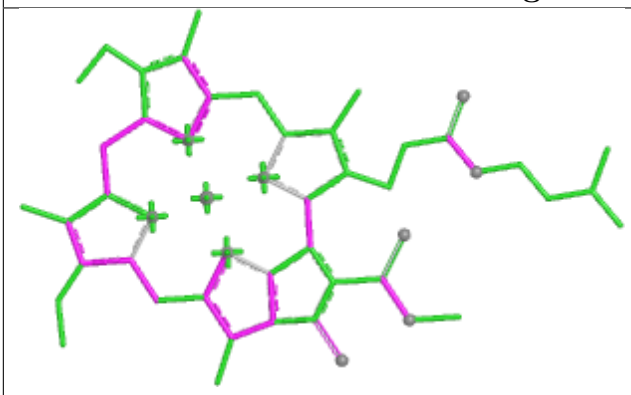


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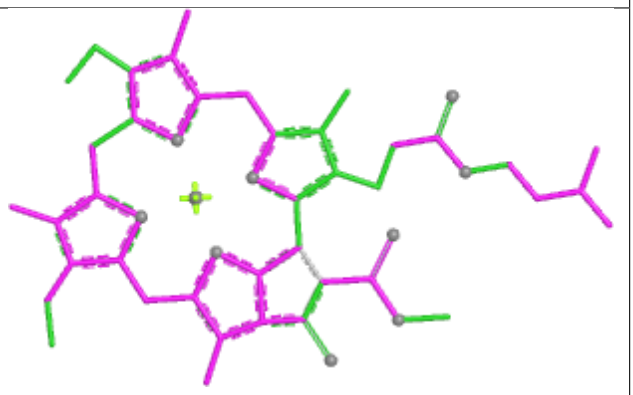


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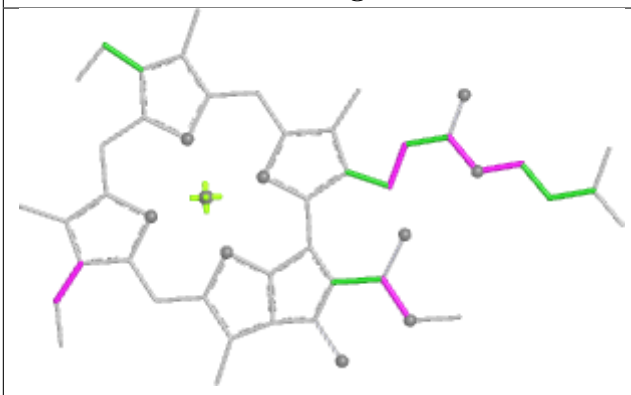
Ligand CLA G 319



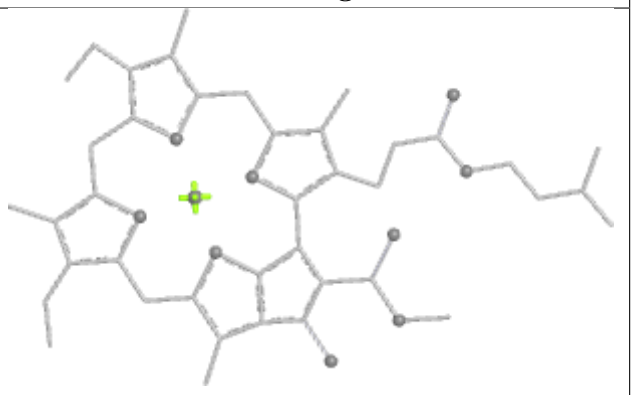
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Bond angles

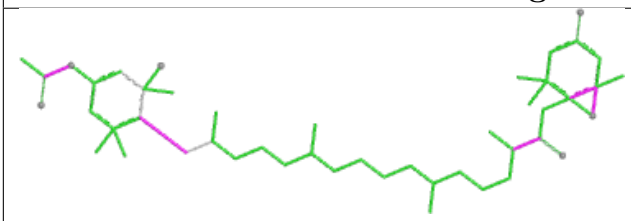


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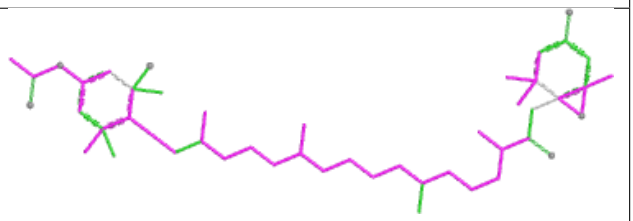


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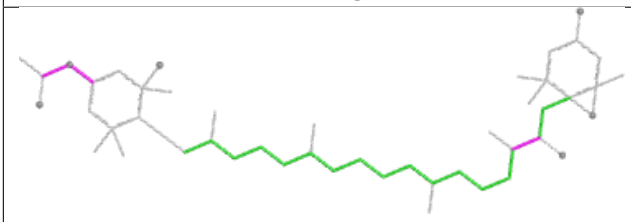
Ligand A86 K 303



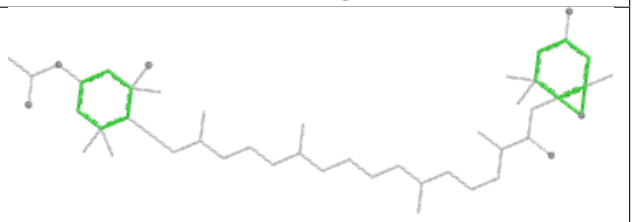
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Bond angles

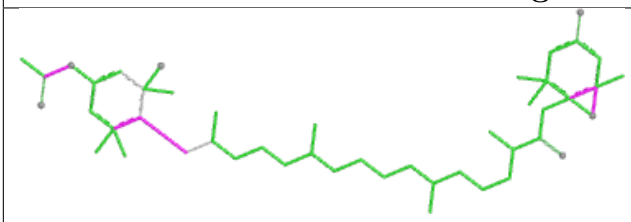


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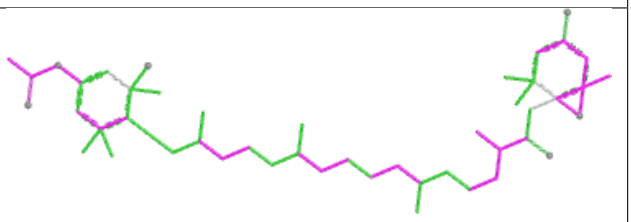


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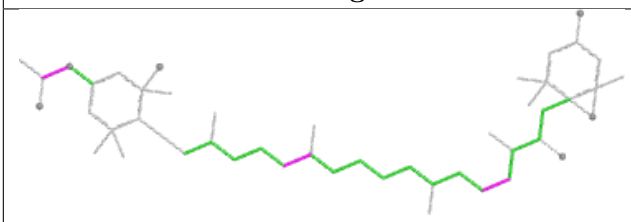
Ligand A86 F 301



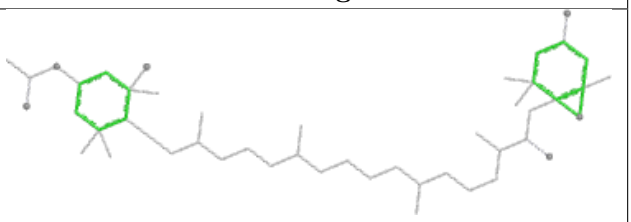
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Bond angles

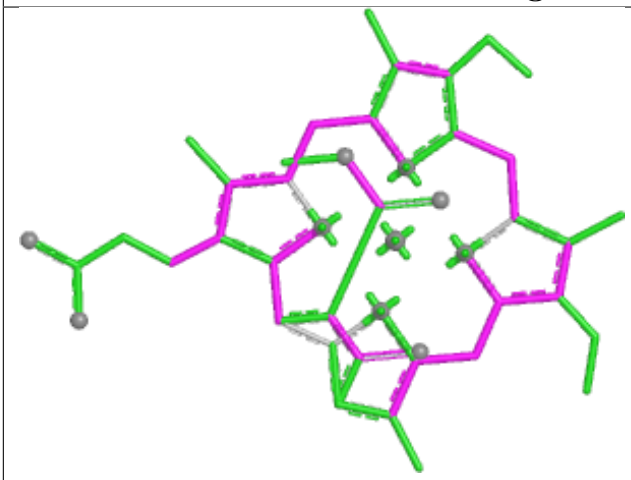


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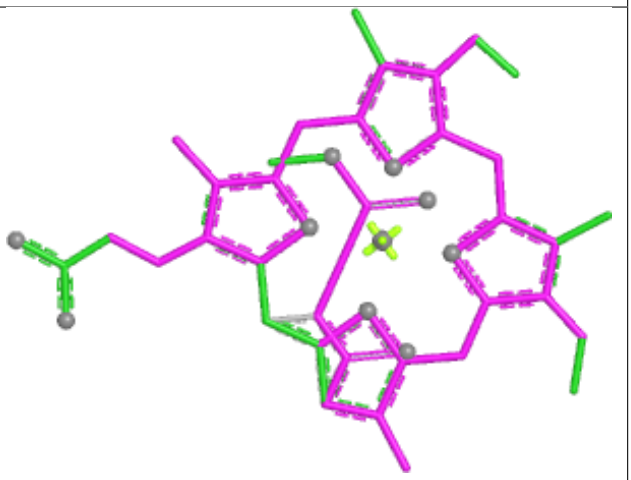


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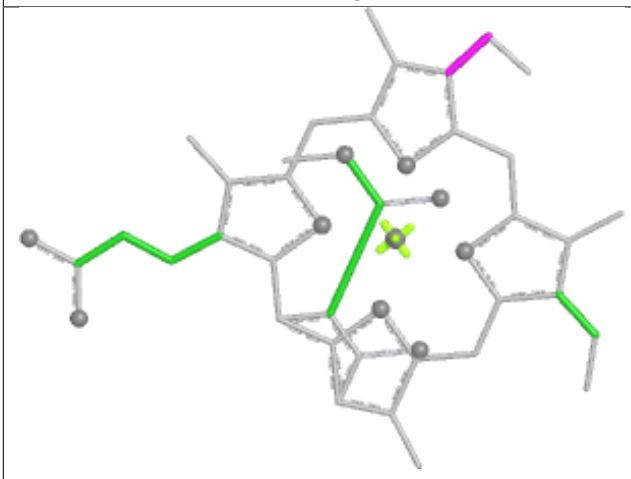
Ligand KC1 P 315



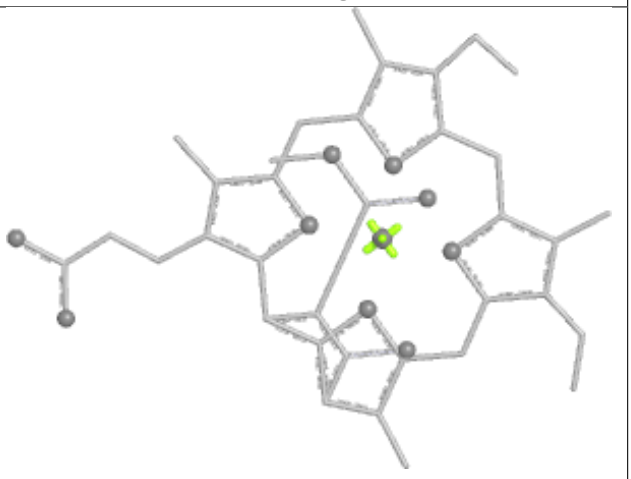
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Bond angles

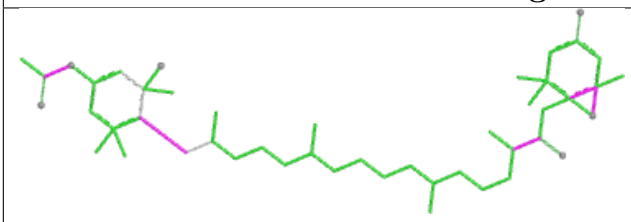


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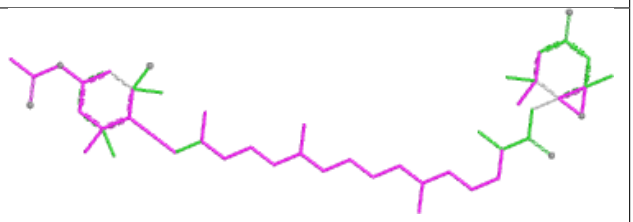


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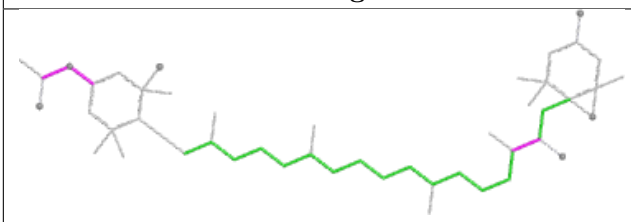
Ligand A86 N 303



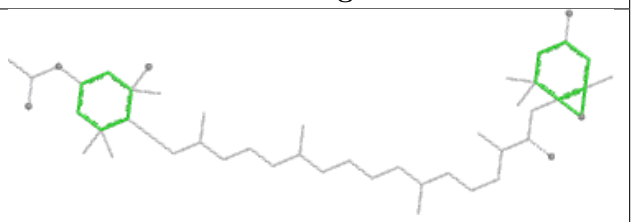
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Bond angles

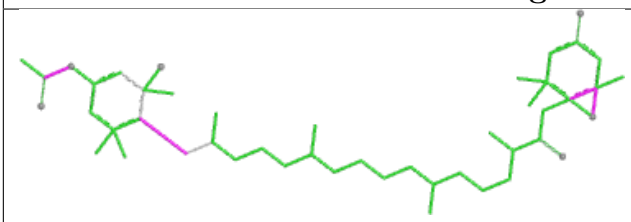


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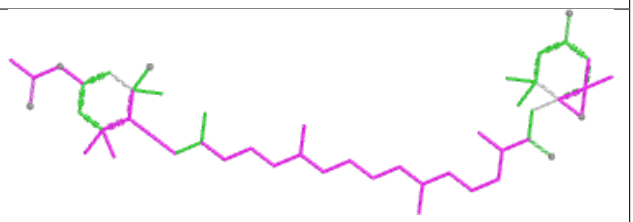


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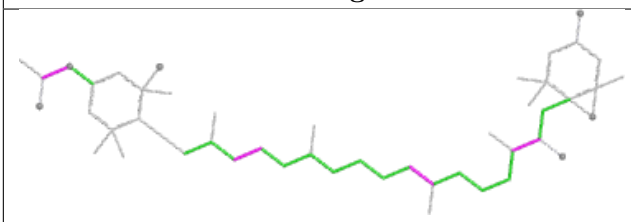
Ligand A86 U 301



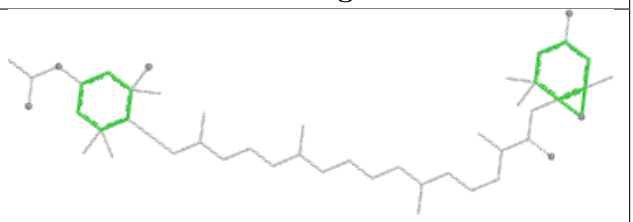
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Bond angles

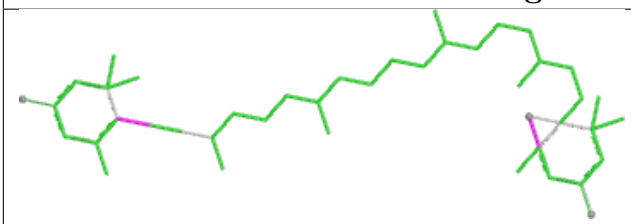


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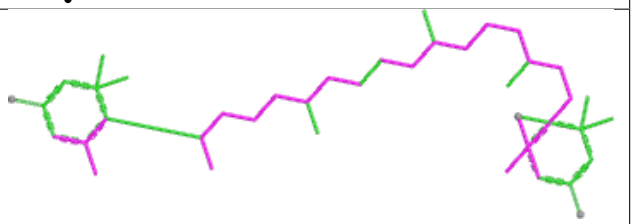


Rings

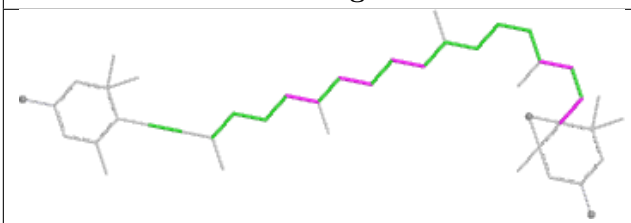
Ligand DD6 Q 302



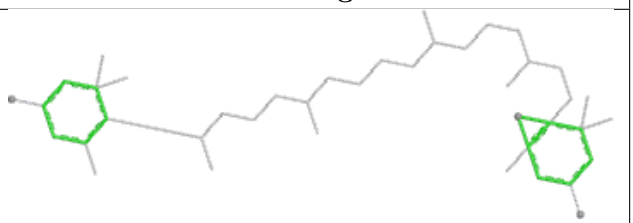
Bond lengths



Bond angles

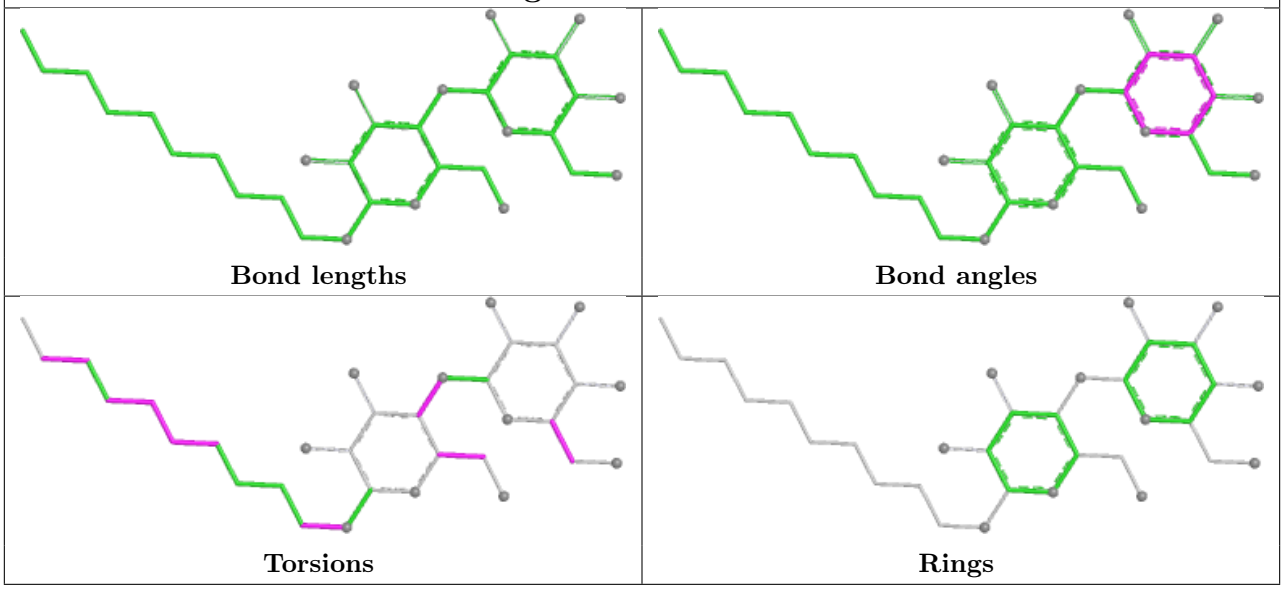


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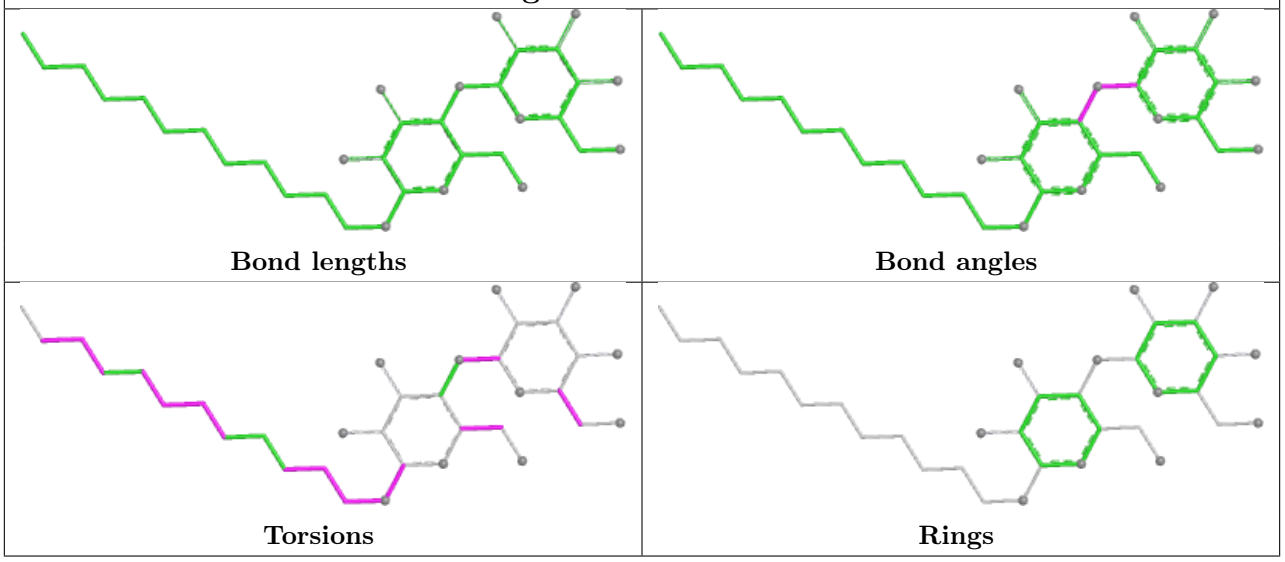


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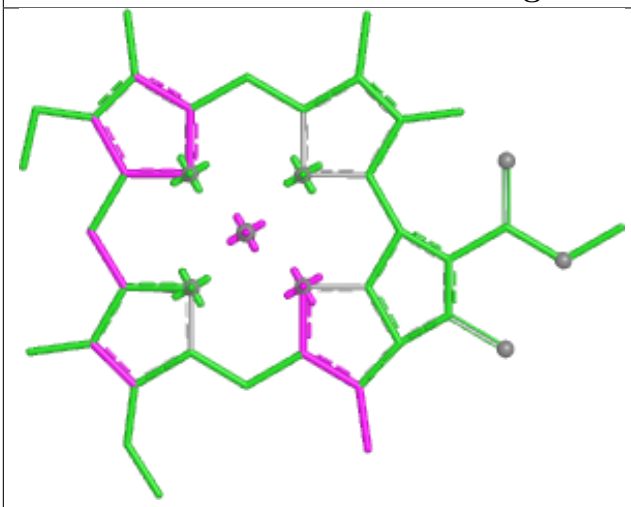
Ligand LMT F 321



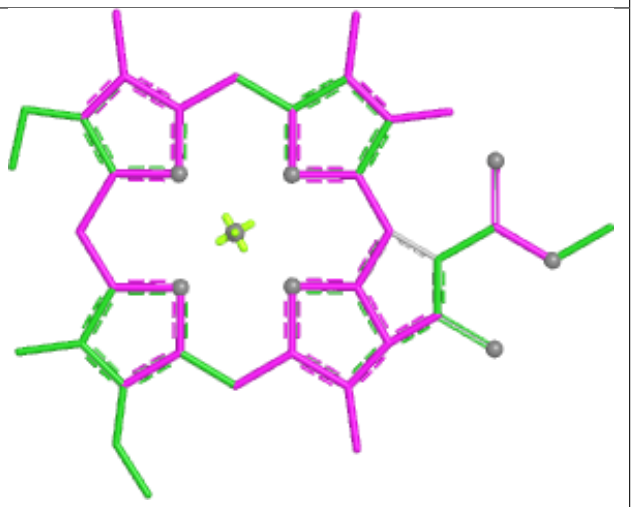
Ligand LMT B 312



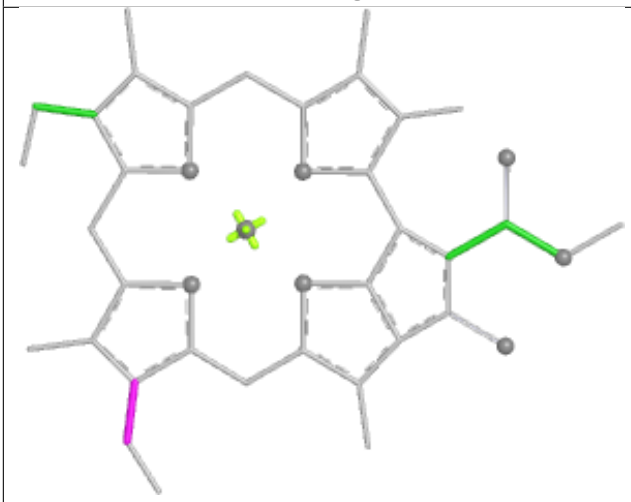
Ligand CLA N 310



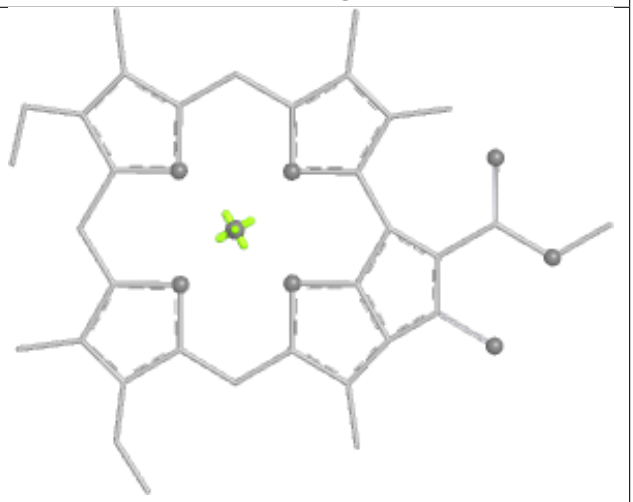
Bond lengths



Bond angles

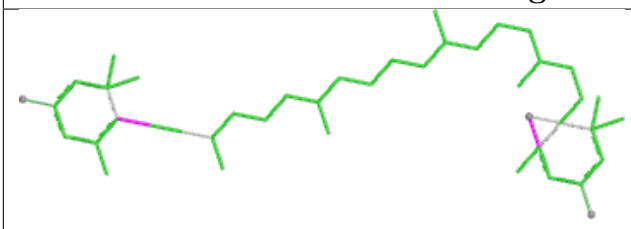


Torsions

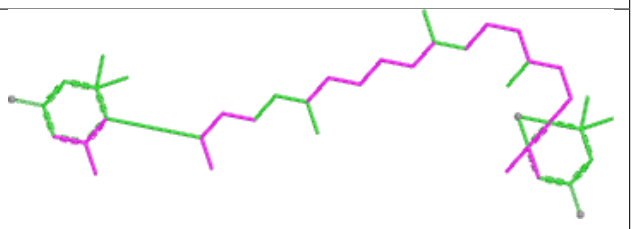


Rings

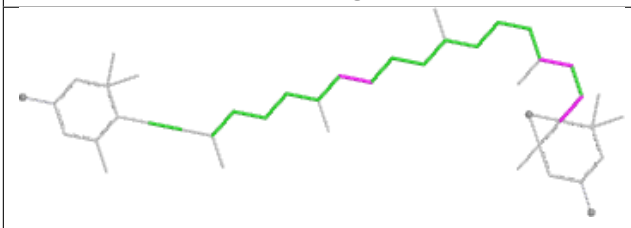
Ligand DD6 J 304



Bond lengths



Bond angles

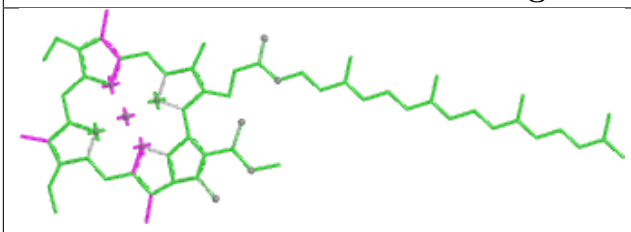


Torsions

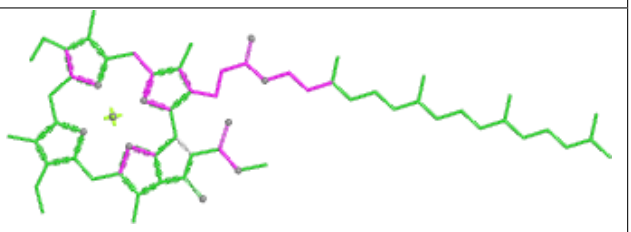


Rings

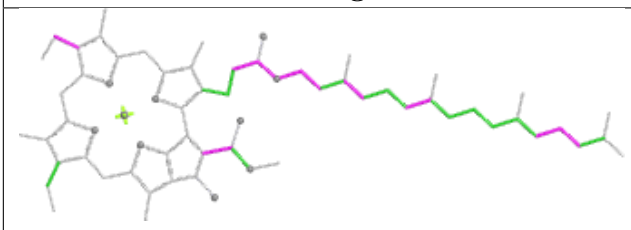
Ligand CLA a 804



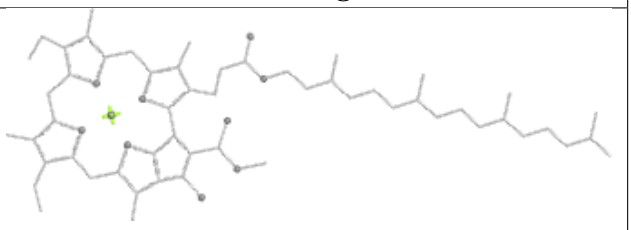
Bond lengths



Bond angles



Torsions



Rings

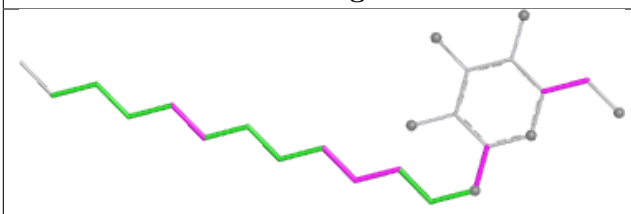
Ligand LMT f 807



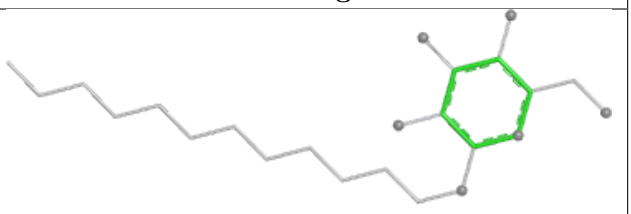
Bond lengths



Bond angles

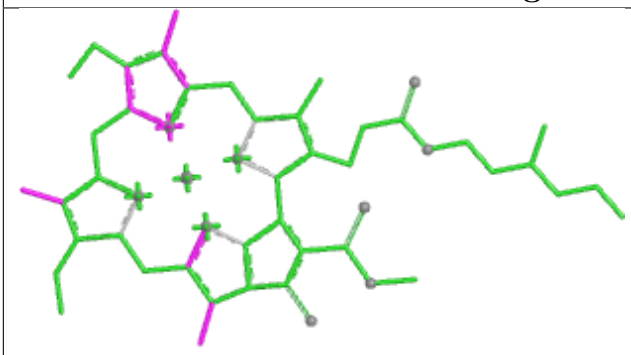


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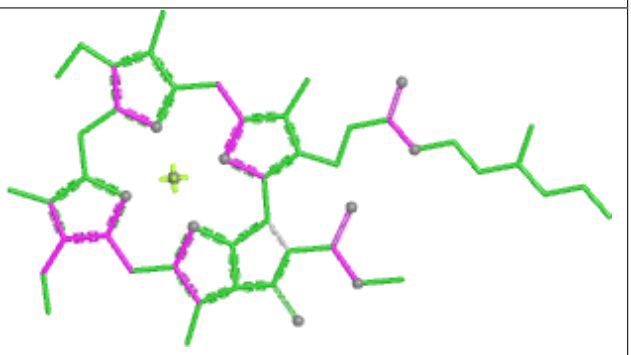


Rings

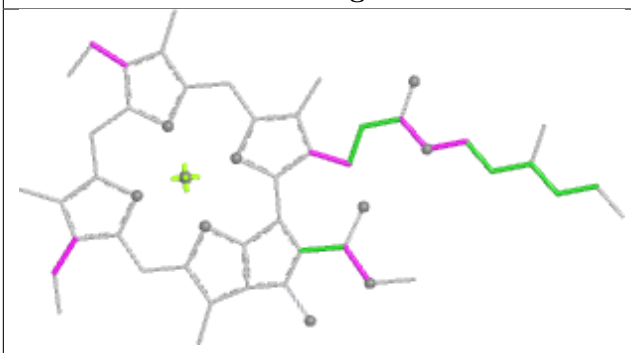
Ligand CLA D 316



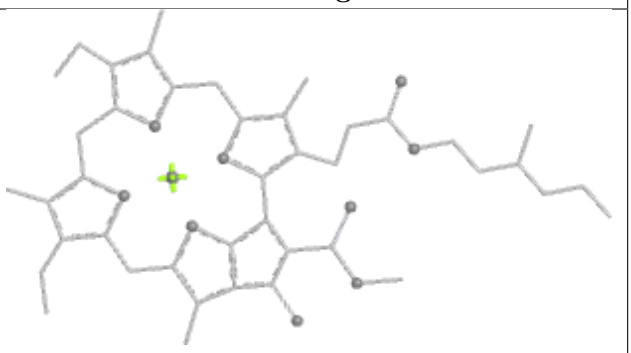
Bond lengths



Bond angles

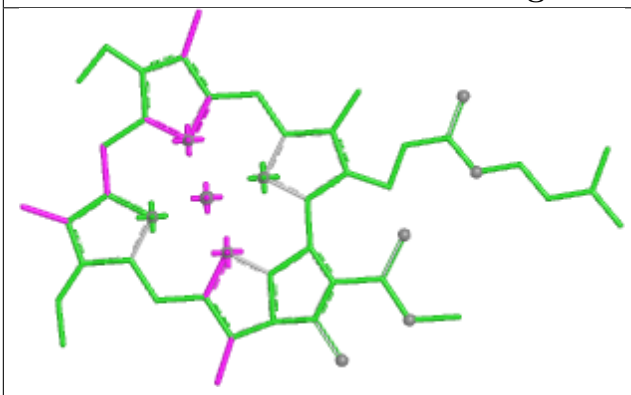


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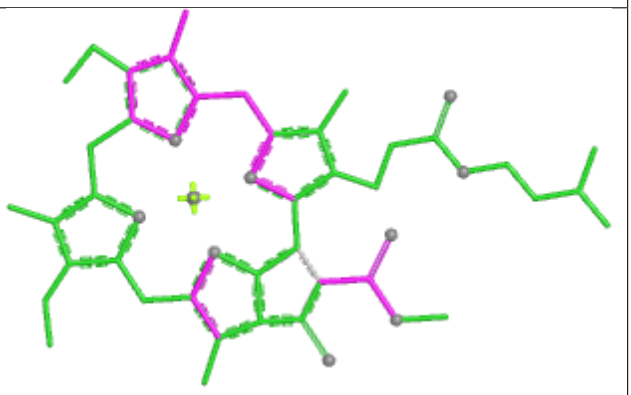


Rings

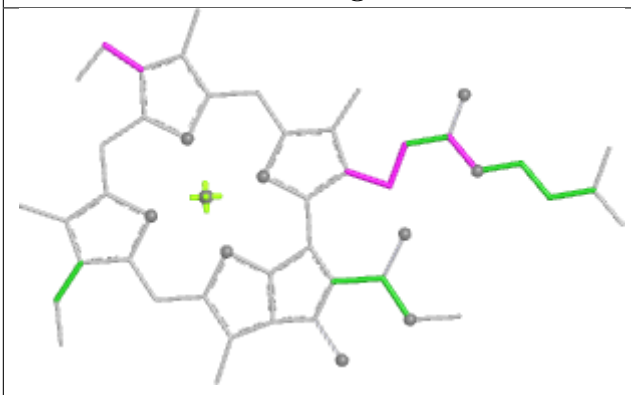
Ligand CLA b 831



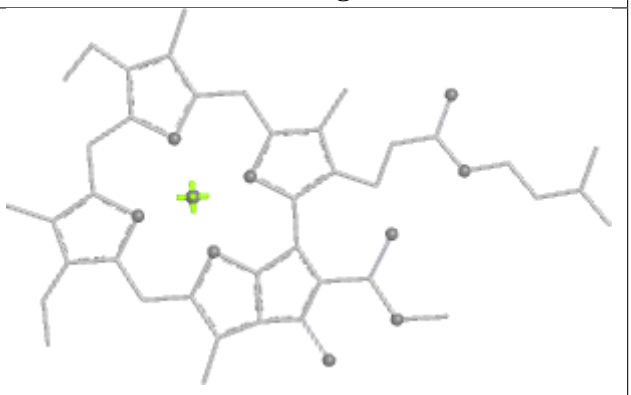
Bond lengths



Bond angles

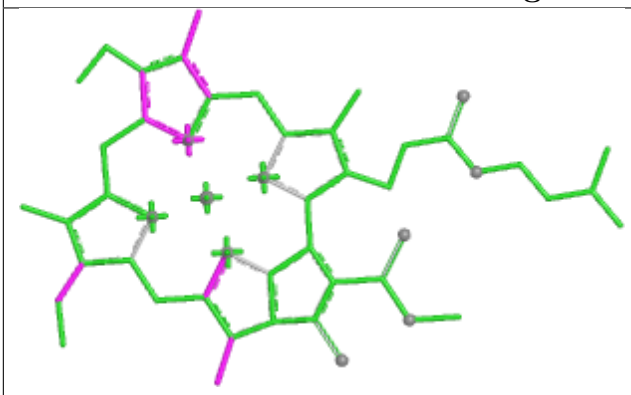


Torsions

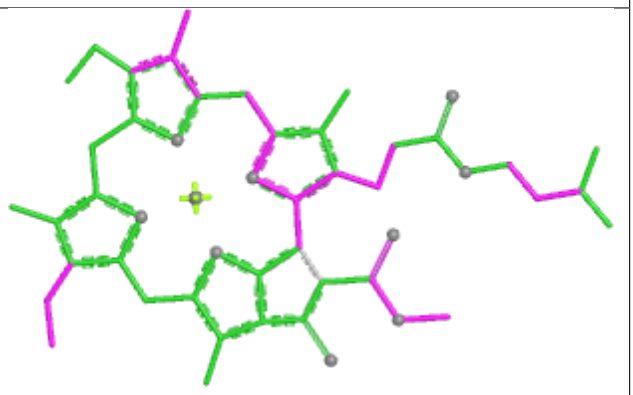


Rings

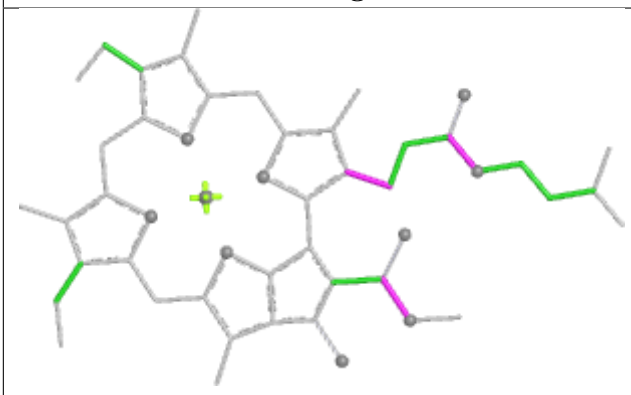
Ligand CLA X 307



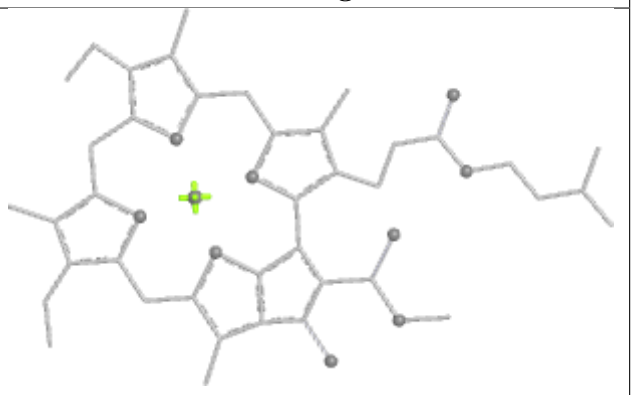
Bond lengths



Bond angles

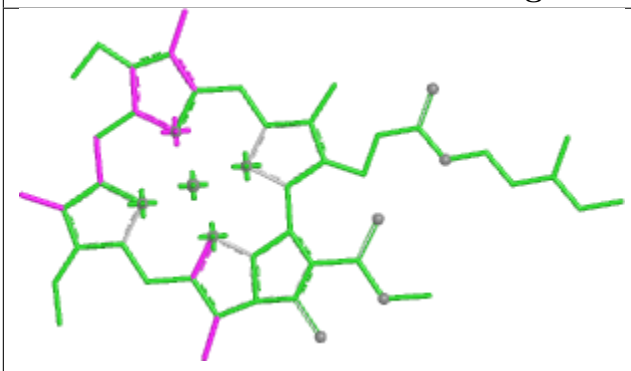


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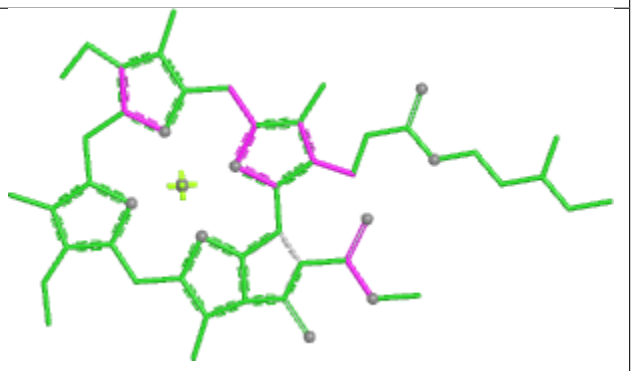


Rings

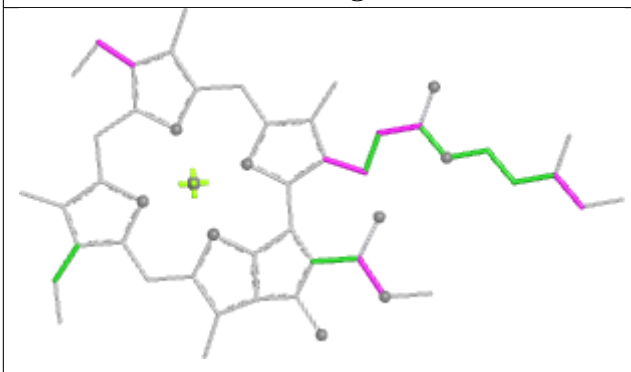
Ligand CLA P 318



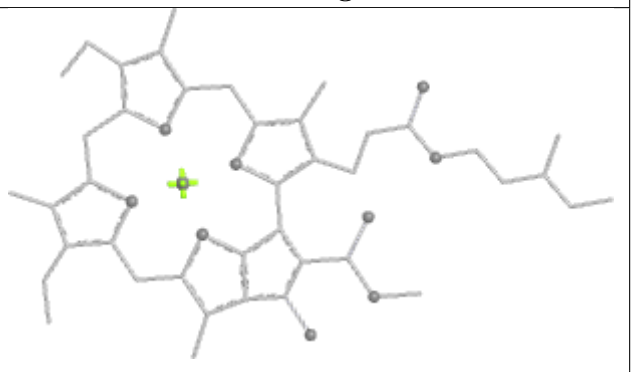
Bond lengths



Bond angles

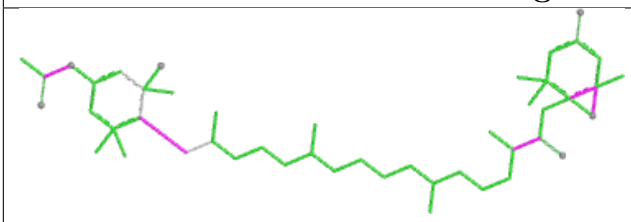


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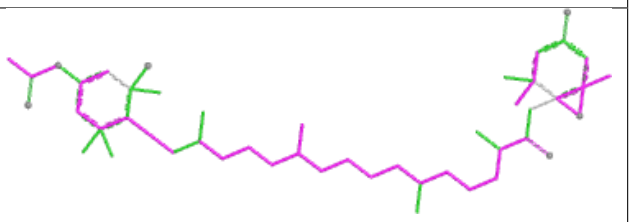


Rings

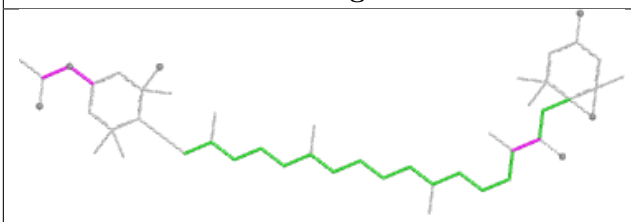
Ligand A86 J 303



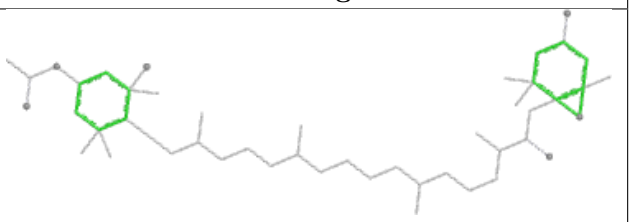
Bond lengths



Bond angles

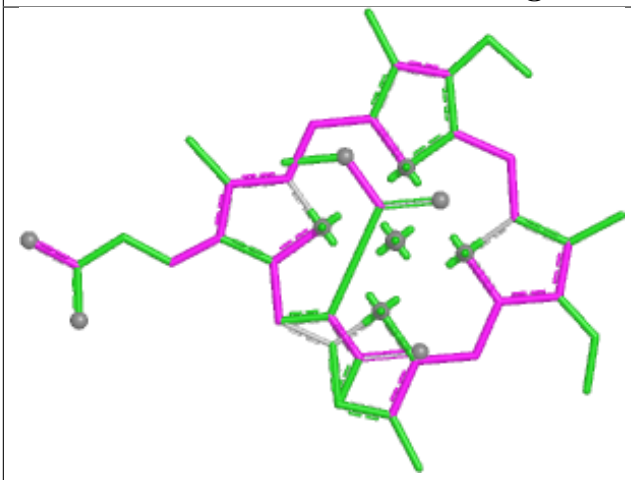


Torsions

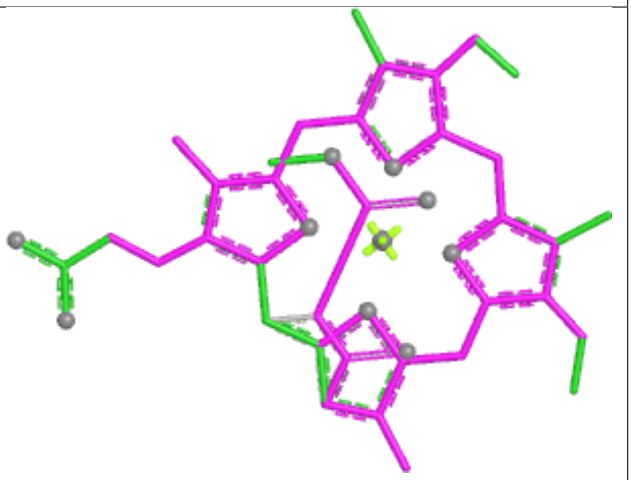


Rings

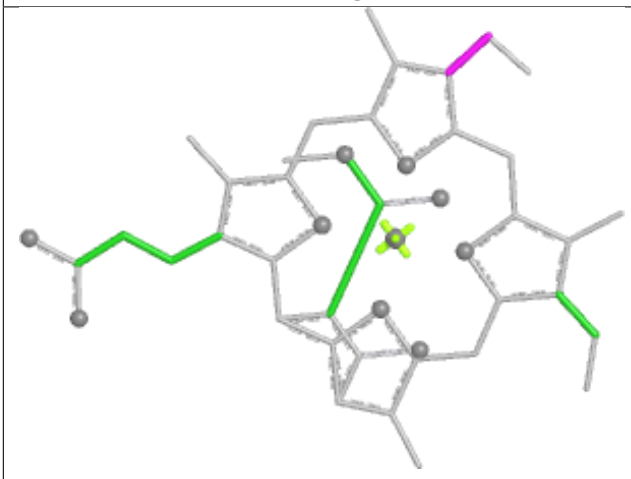
Ligand KC1 O 313



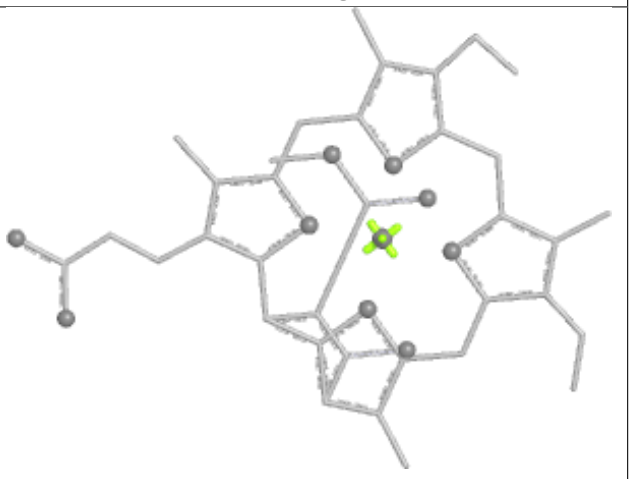
Bond lengths



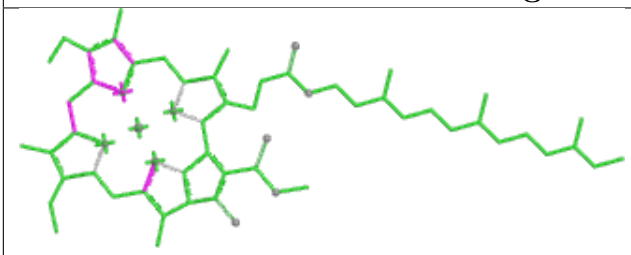
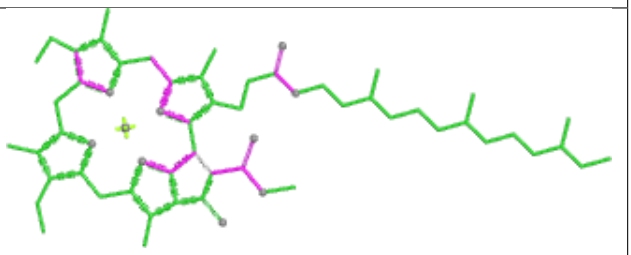
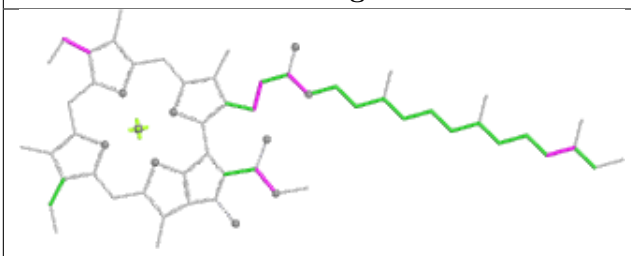
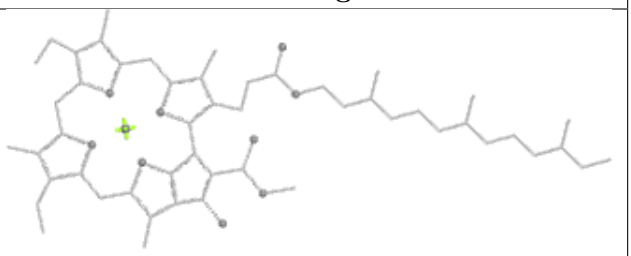
Bond angles

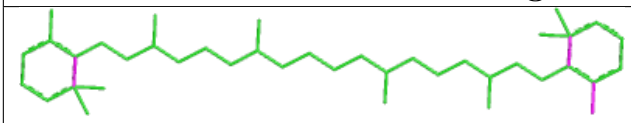
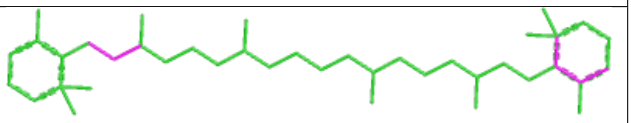
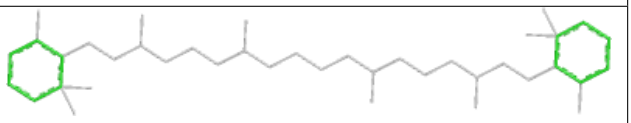


Torsions

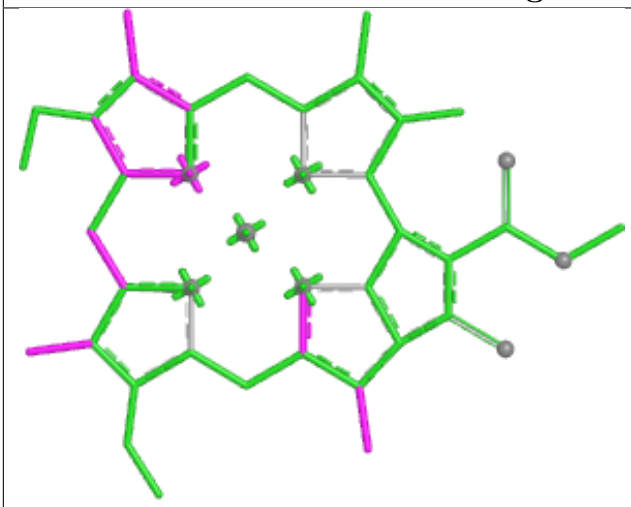


Rings

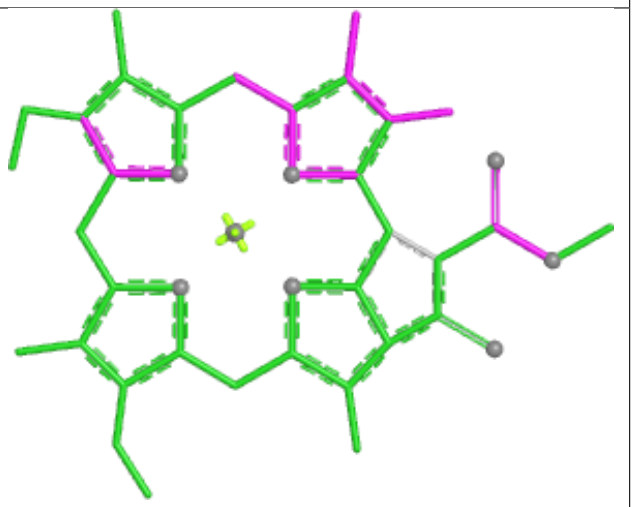
Ligand CLA X 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR a 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

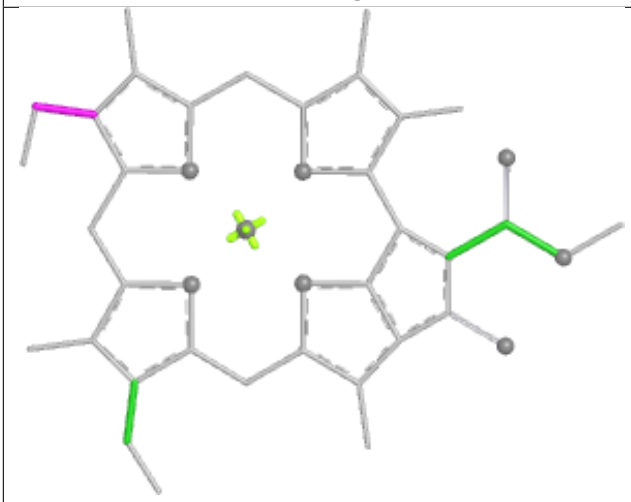
Ligand CLA F 316



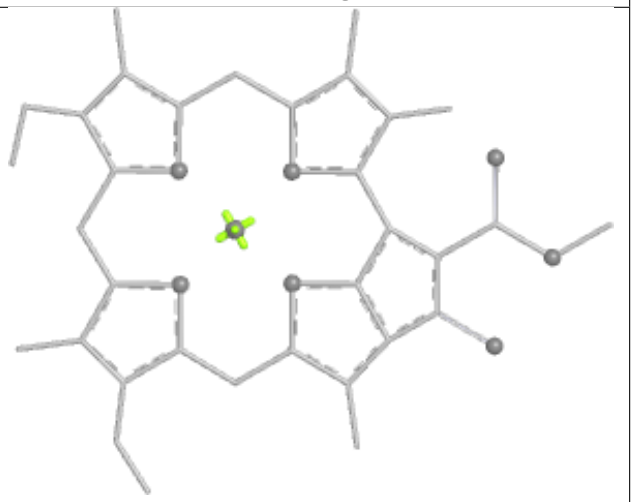
Bond lengths



Bond angles

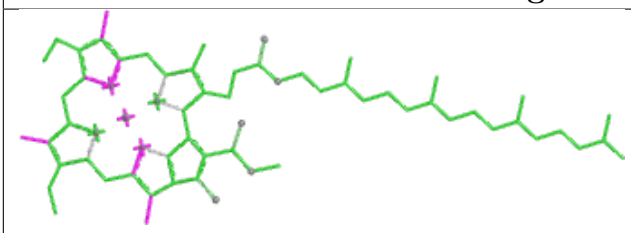


Torsions

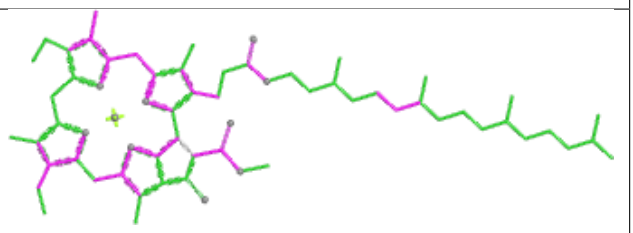


Rings

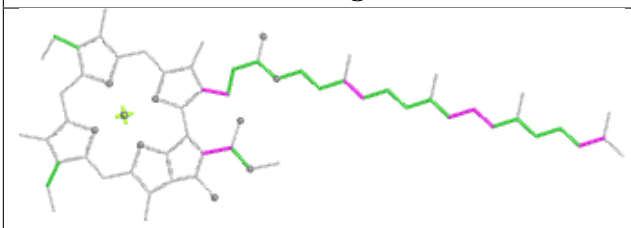
Ligand CLA b 830



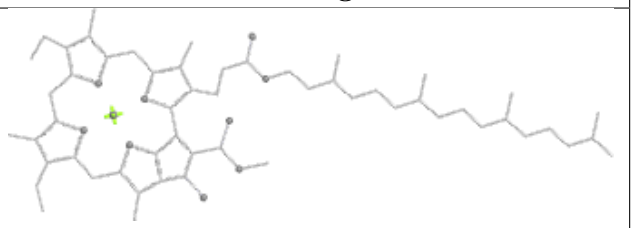
Bond lengths



Bond angles

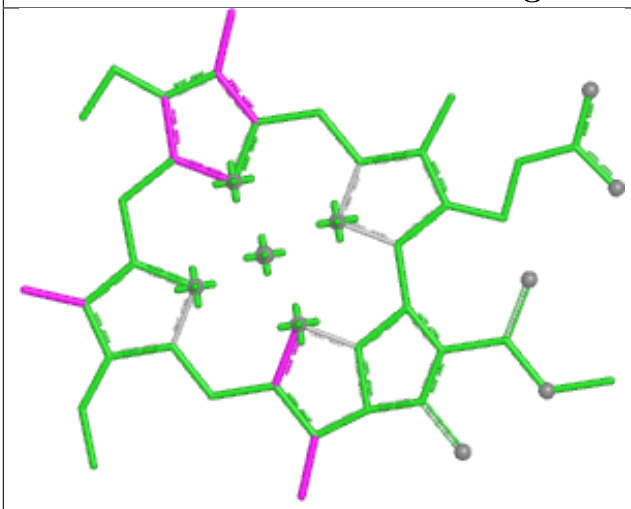


Torsions

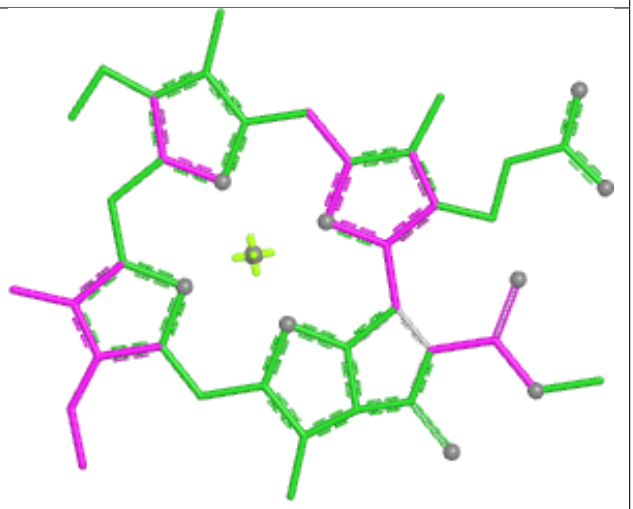


Rings

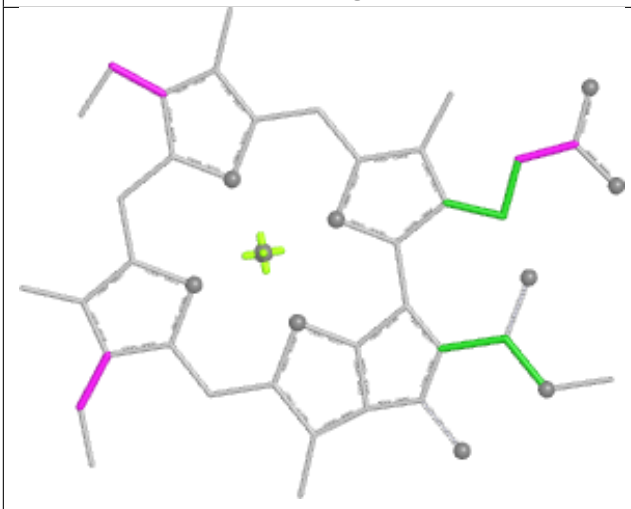
Ligand CLA R 319



Bond lengths



Bond angles

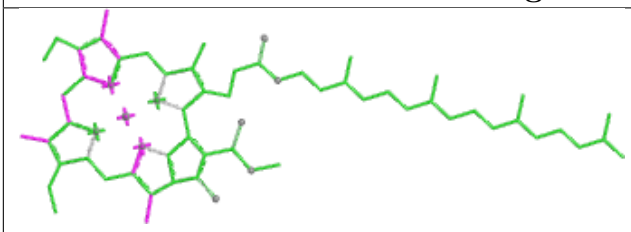


Torsions

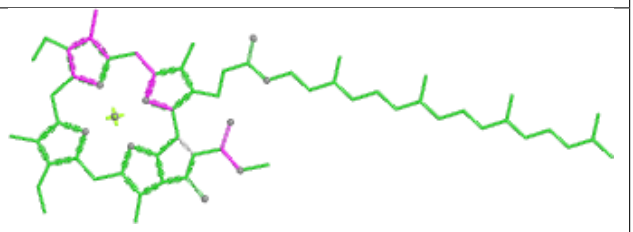


Rings

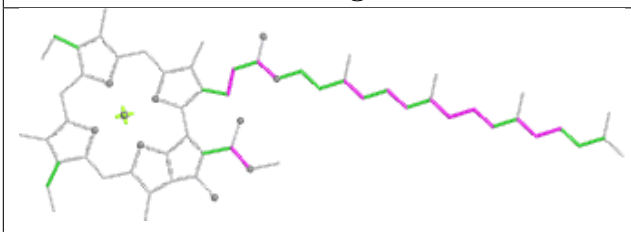
Ligand CLA P 309



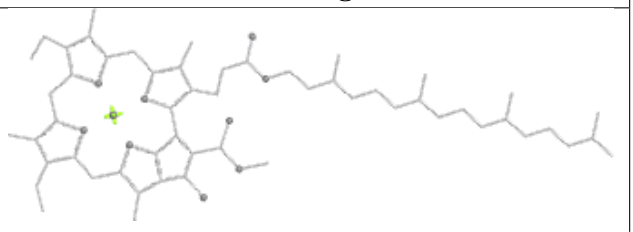
Bond lengths



Bond angles

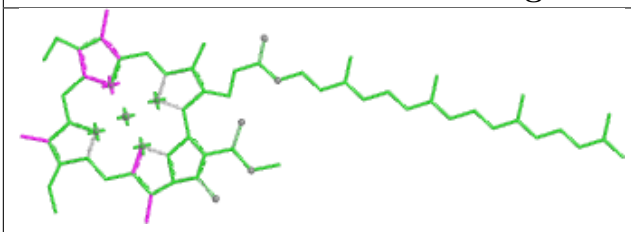


Torsions

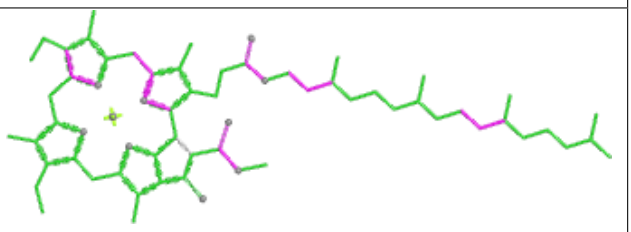


Rings

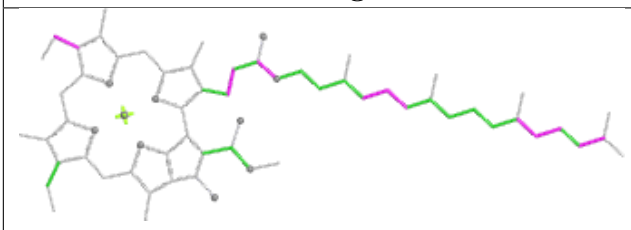
Ligand CLA P 310



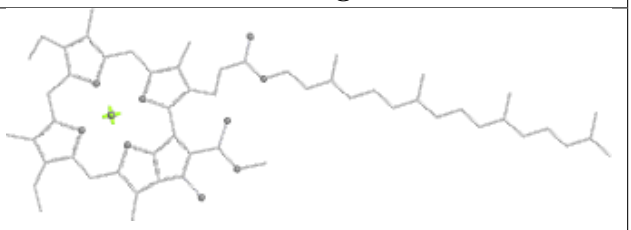
Bond lengths



Bond angles

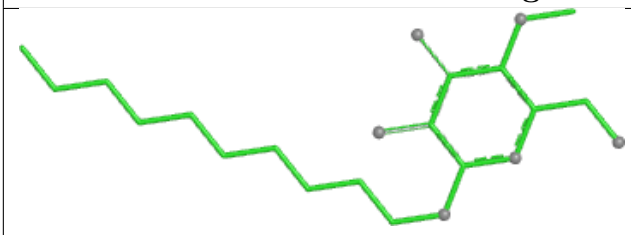


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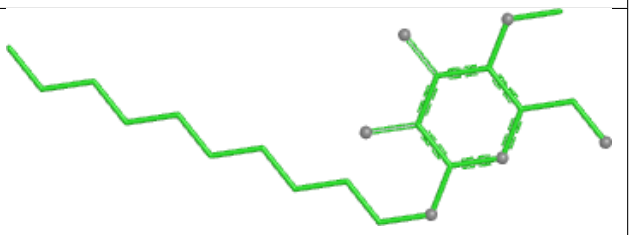


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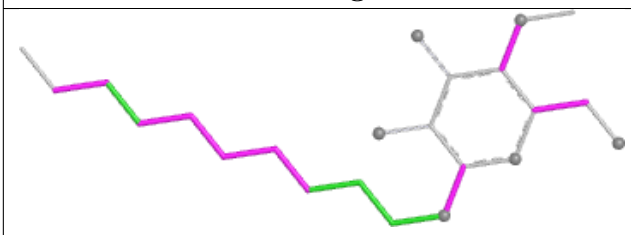
Ligand LMT E 321



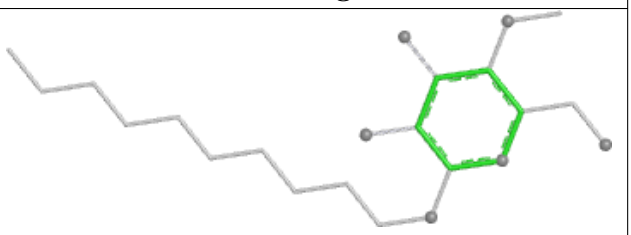
Bond lengths



Bond angles

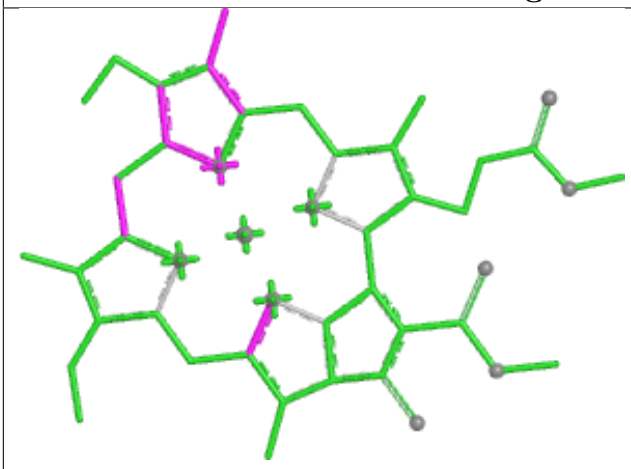


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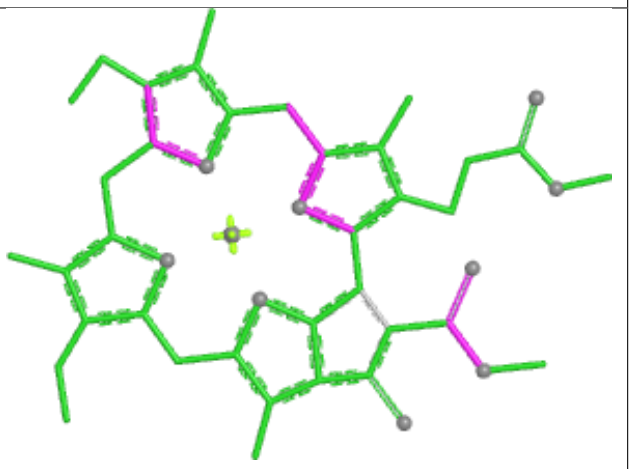


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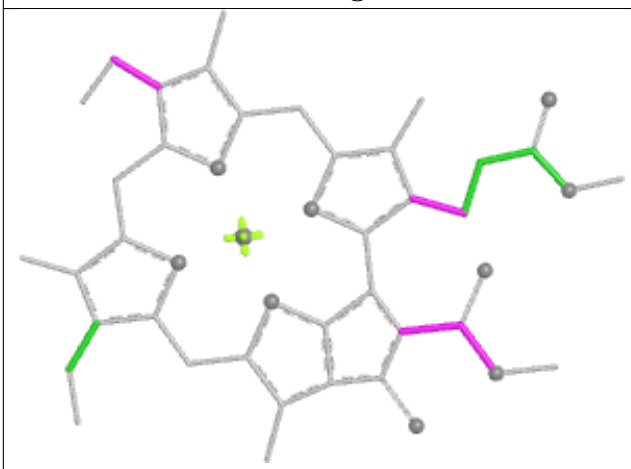
Ligand CLA E 317



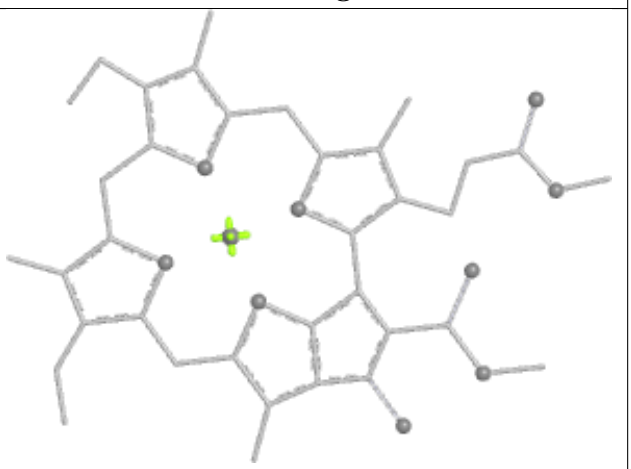
Bond lengths



Bond angles



Torsions



Rings

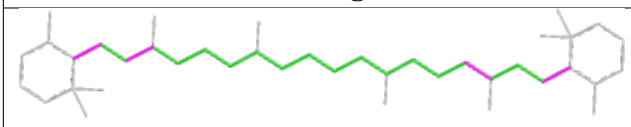
Ligand BCR a 844



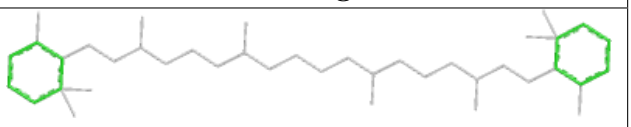
Bond lengths



Bond angles

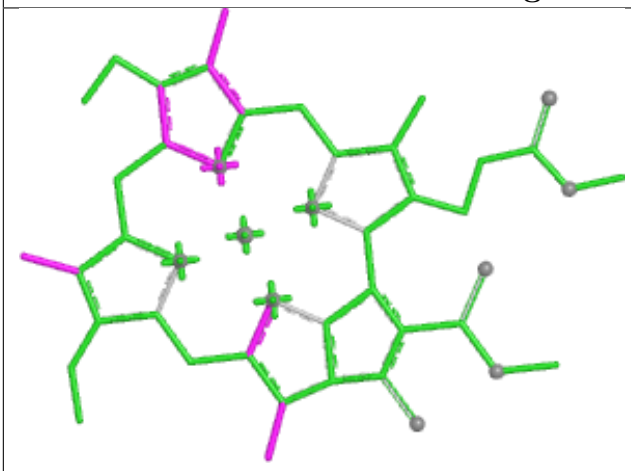


Torsions

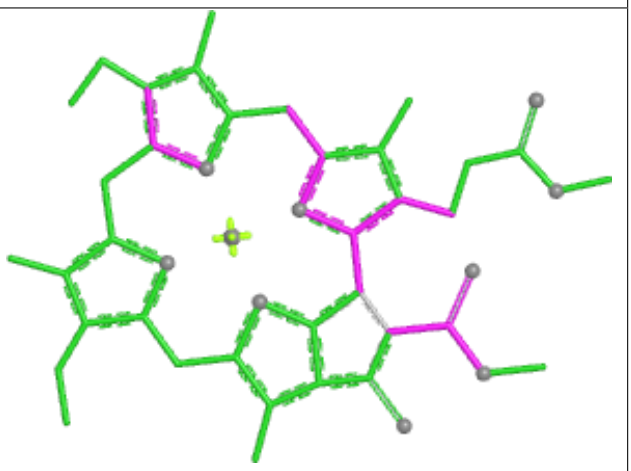


Rings

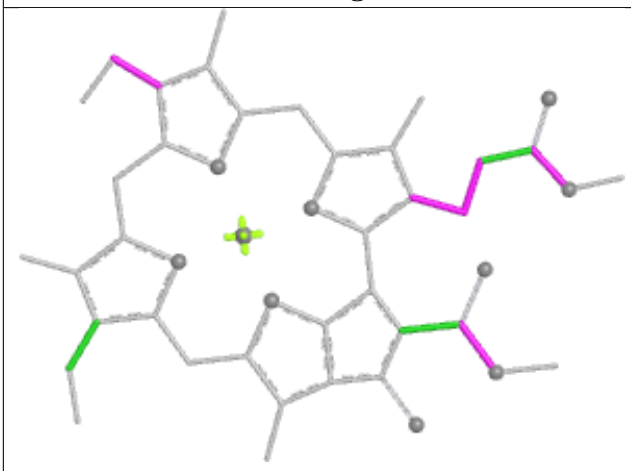
Ligand CLA O 310



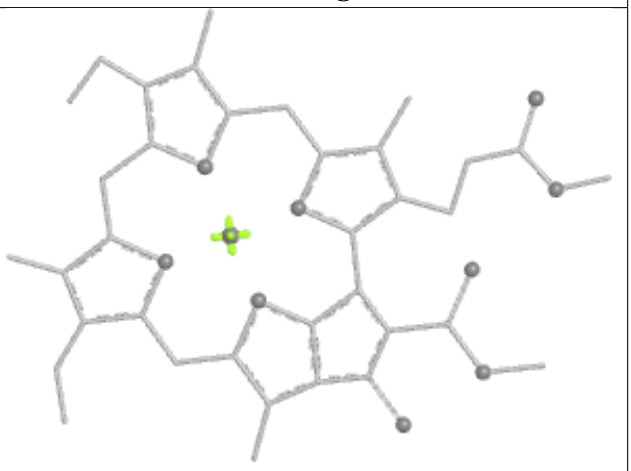
Bond lengths



Bond angles

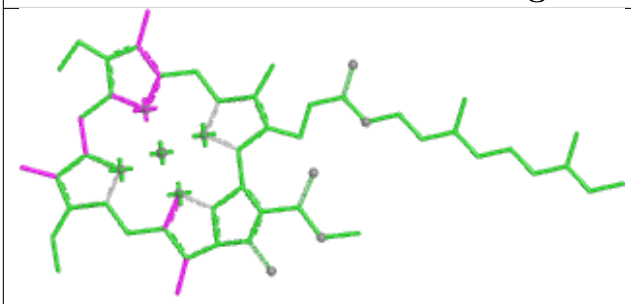


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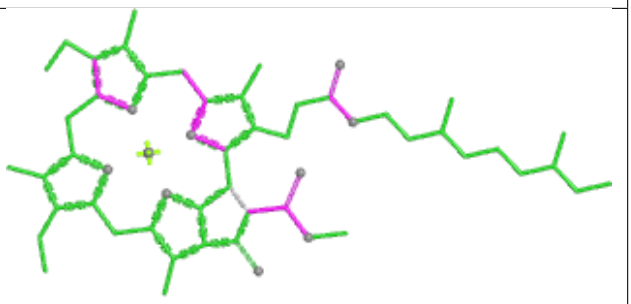


Rings

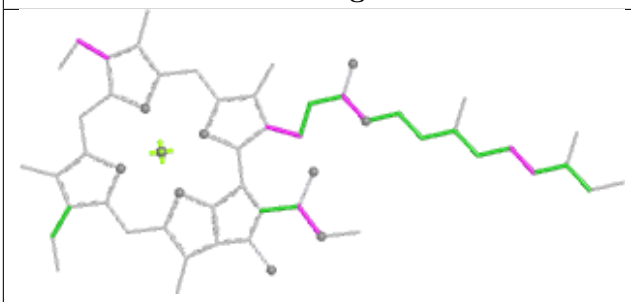
Ligand CLA a 809



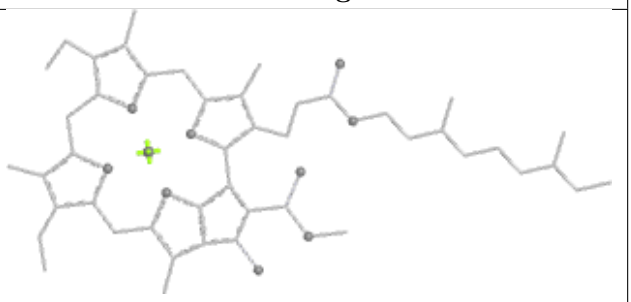
Bond lengths



Bond angles

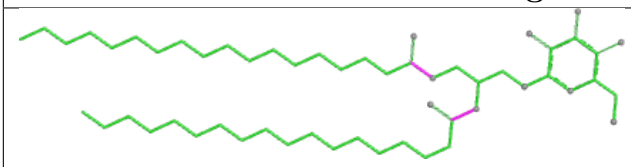


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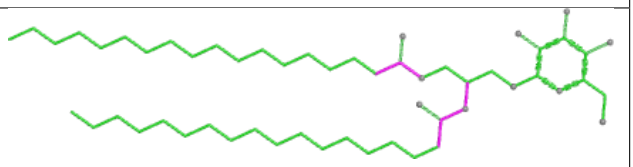


Rings

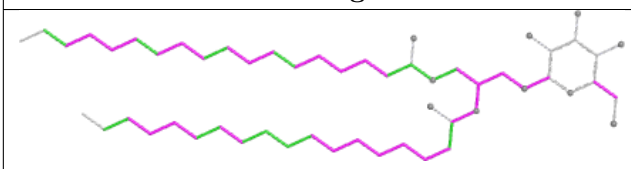
Ligand LMG I 315



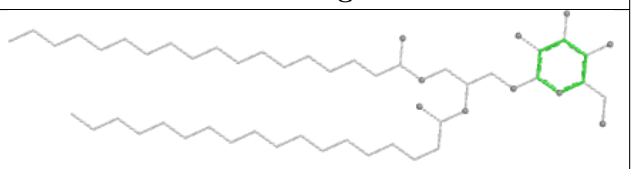
Bond lengths



Bond angles

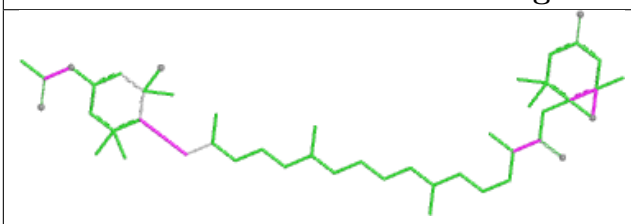


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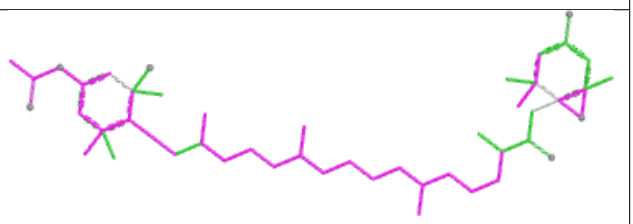


Rings

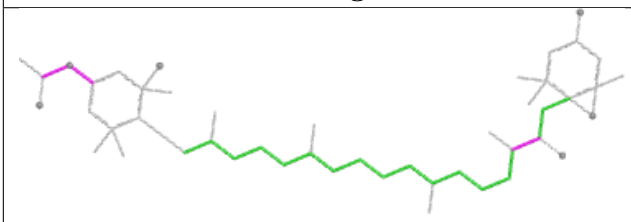
Ligand A86 S 303



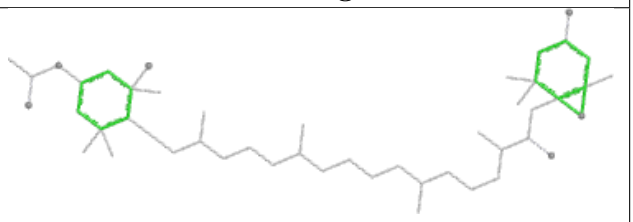
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Bond angles

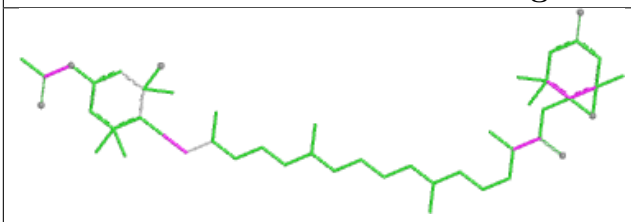


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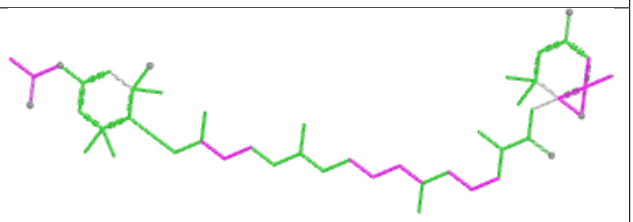


Rings

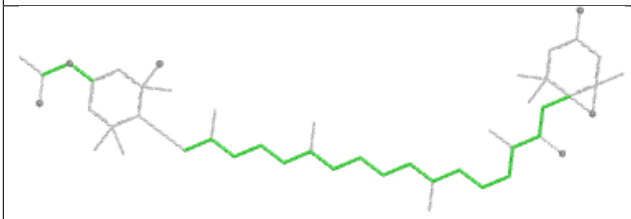
Ligand A86 T 304



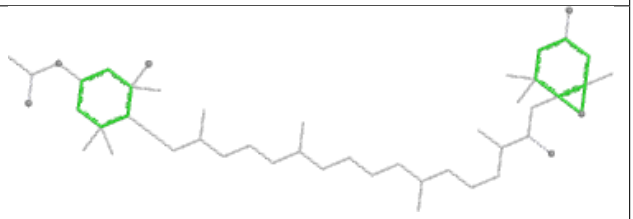
Bond lengths



Bond angles

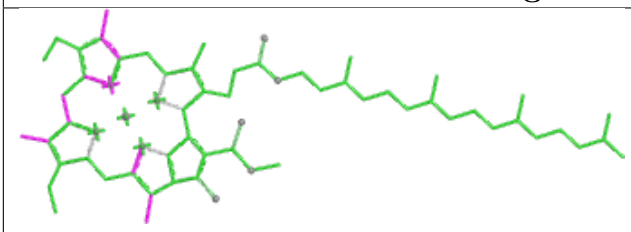


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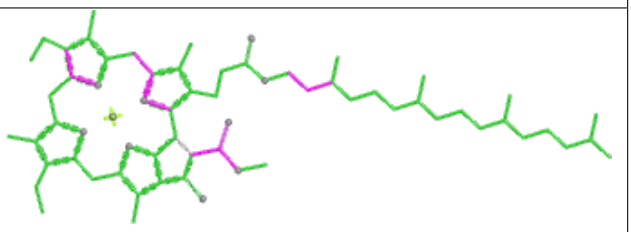


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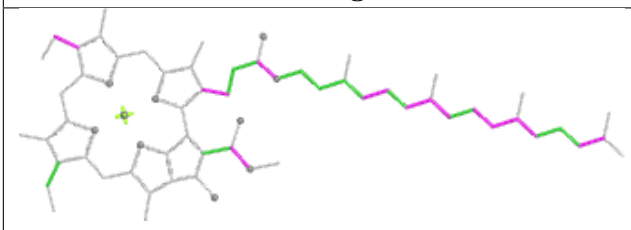
Ligand CLA A 311



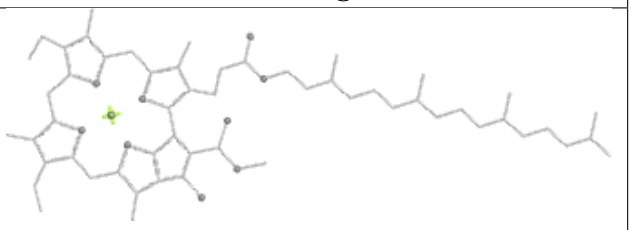
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Bond angles

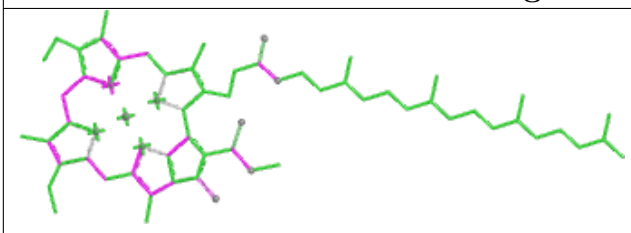


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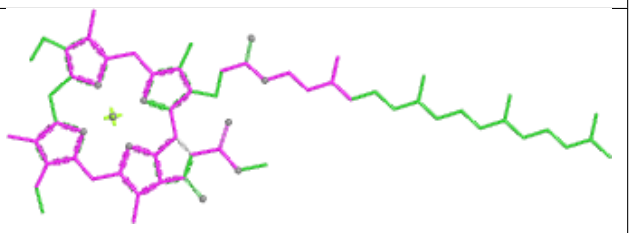


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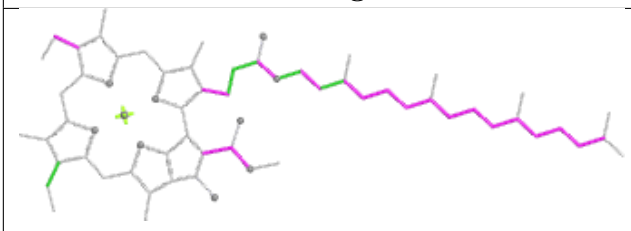
Ligand CLA O 316



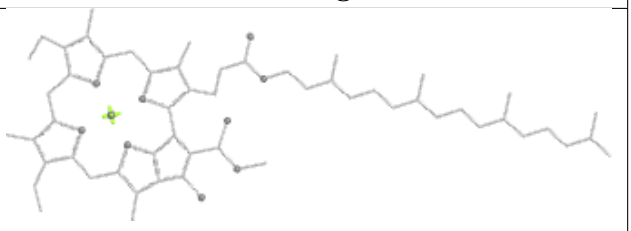
Bond lengths



Bond angles

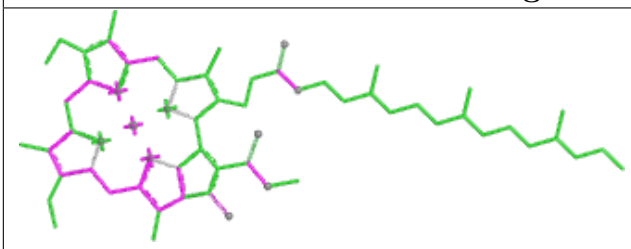


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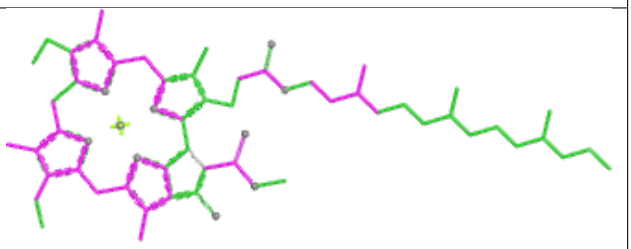


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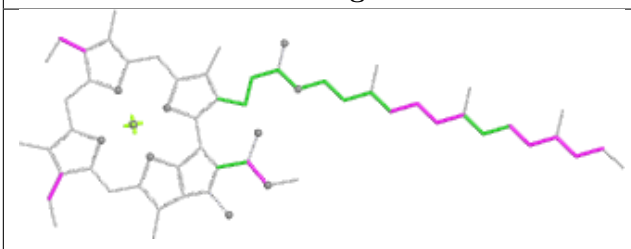
Ligand CLA K 310



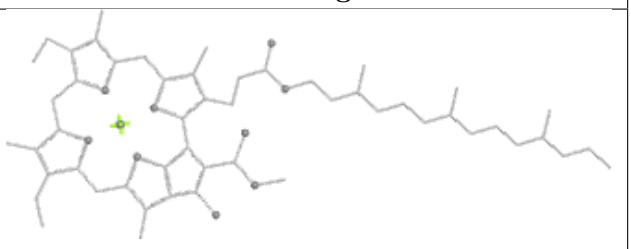
Bond lengths



Bond angles

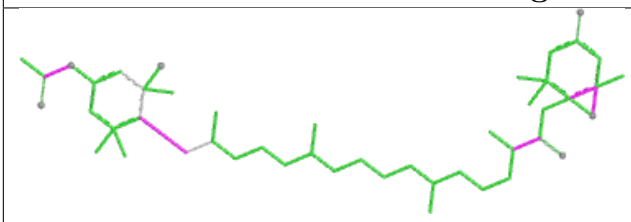


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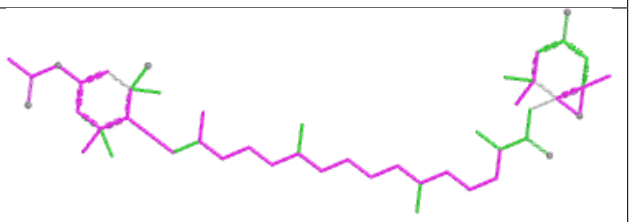


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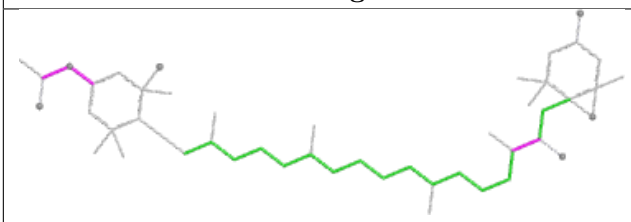
Ligand A86 T 303



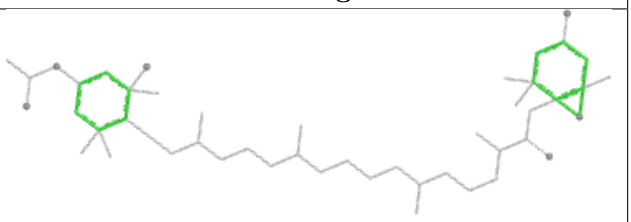
Bond lengths



Bond angles

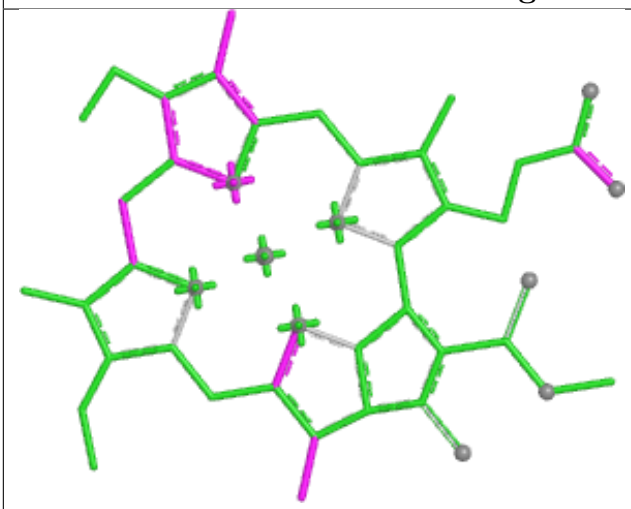


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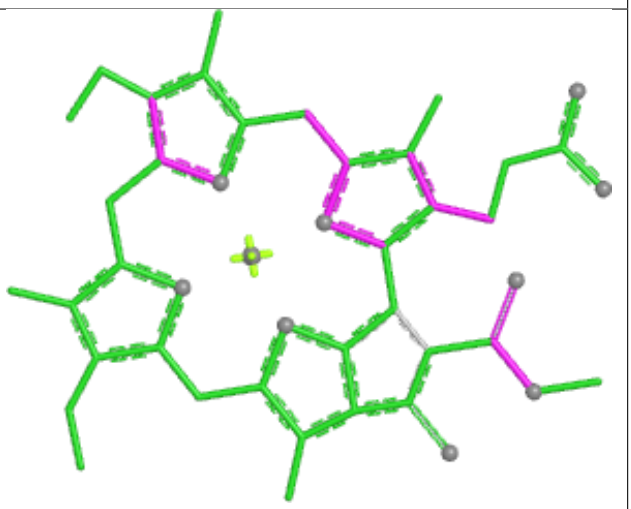


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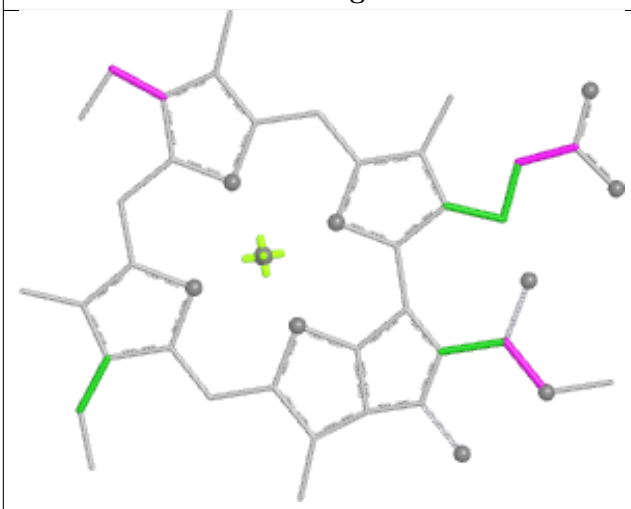
Ligand CLA W 208



Bond lengths



Bond angles

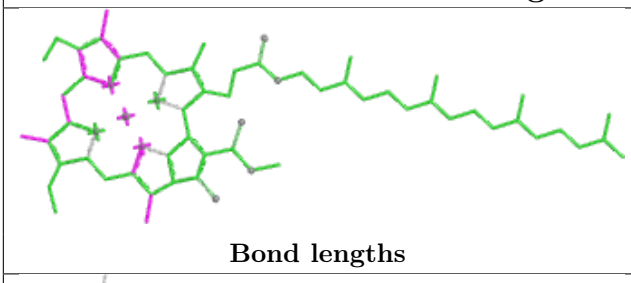


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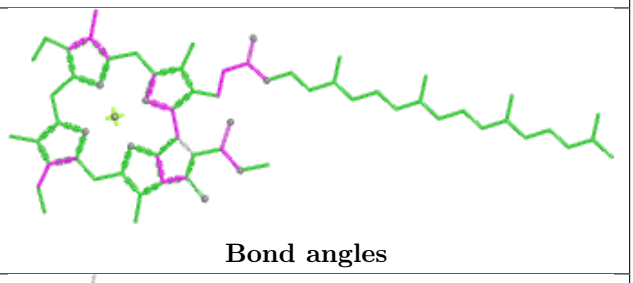


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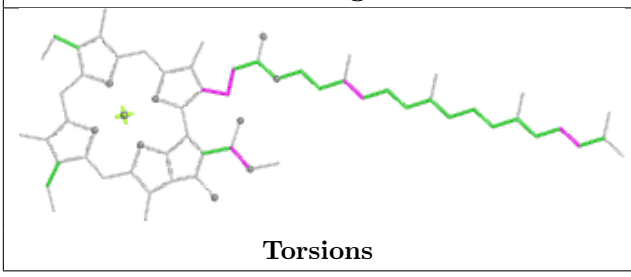
Ligand CLA b 801



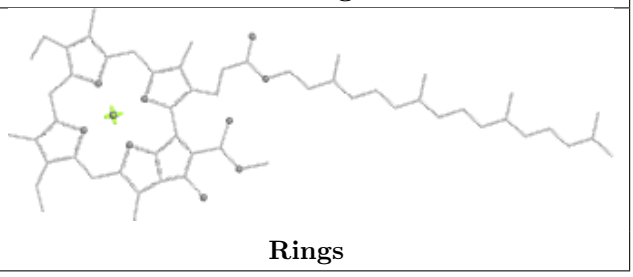
Bond lengths



Bond angles

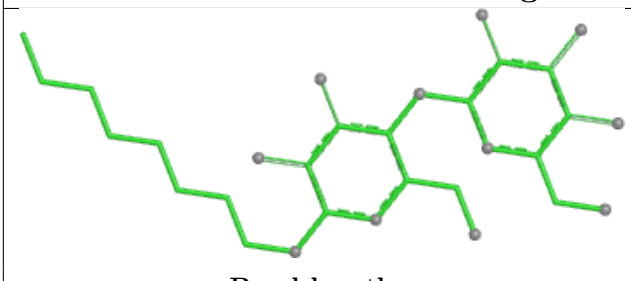


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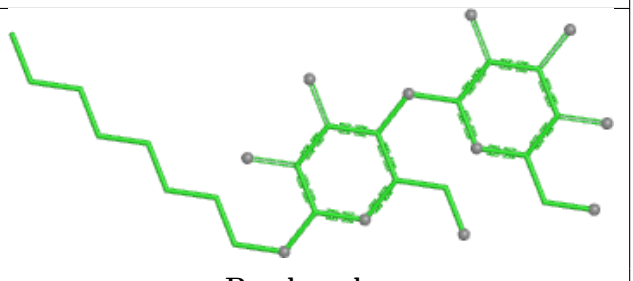


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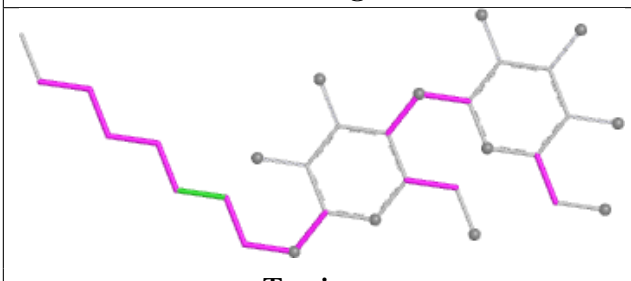
Ligand LMT K 317



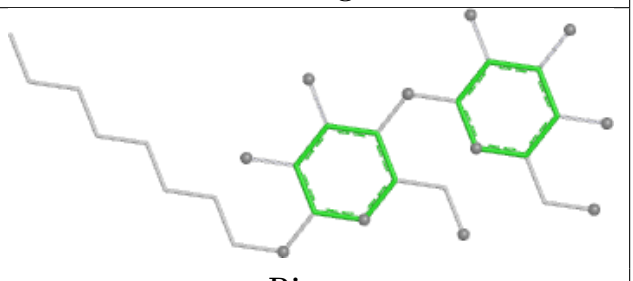
Bond lengths



Bond angles

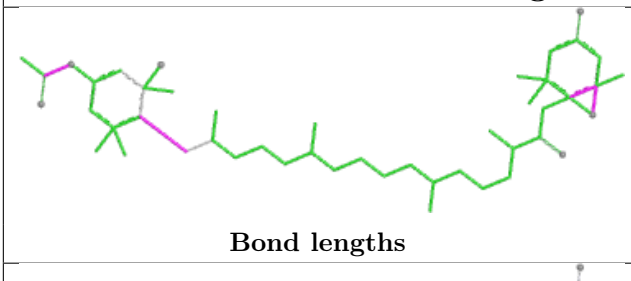


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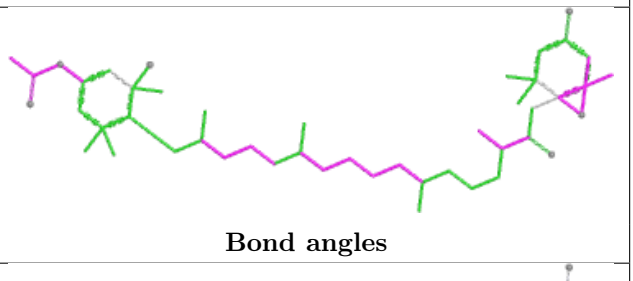


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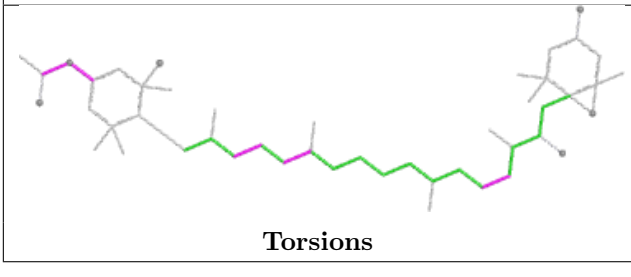
Ligand A86 G 302



Bond lengths



Bond angles

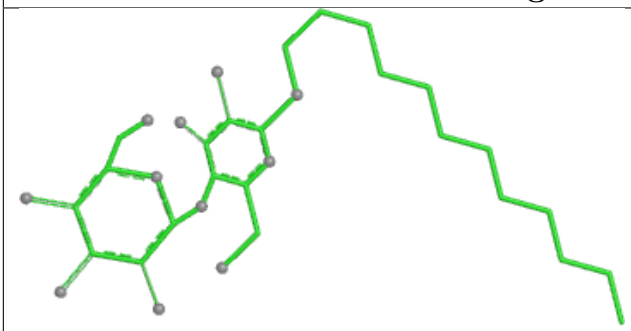


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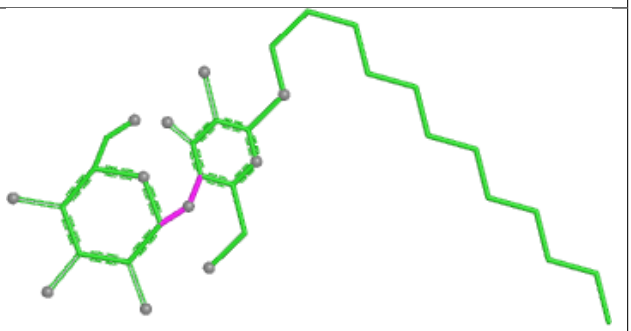


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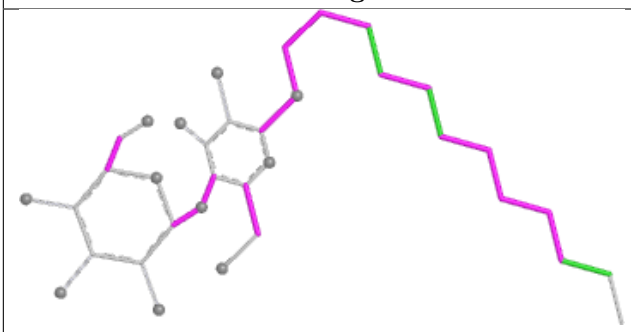
Ligand LMT I 318



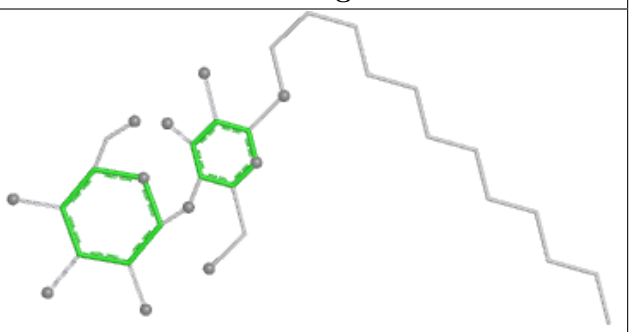
Bond lengths



Bond angles

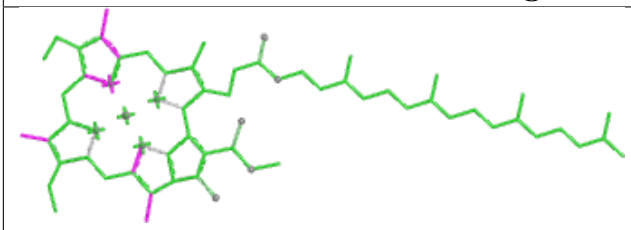


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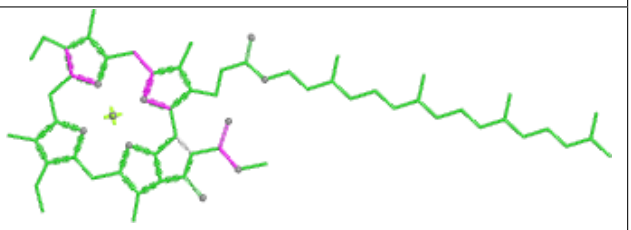


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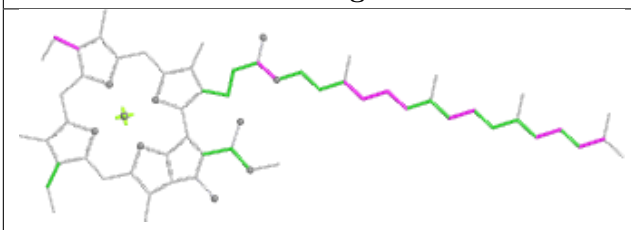
Ligand CLA K 316



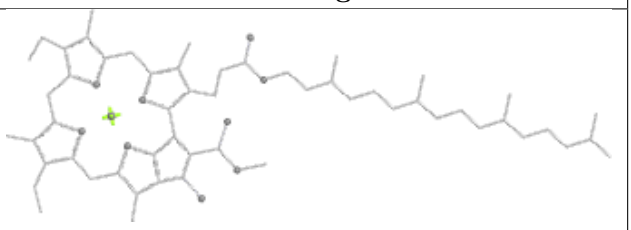
Bond lengths



Bond angles

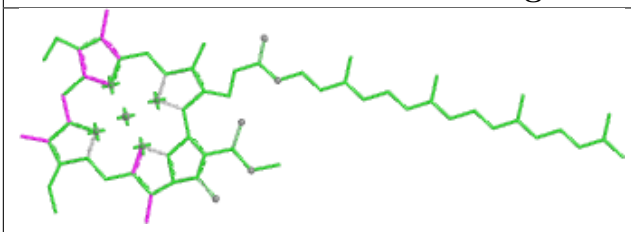


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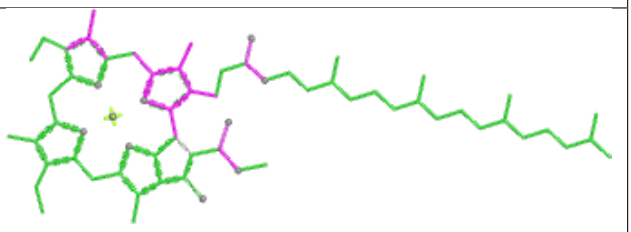


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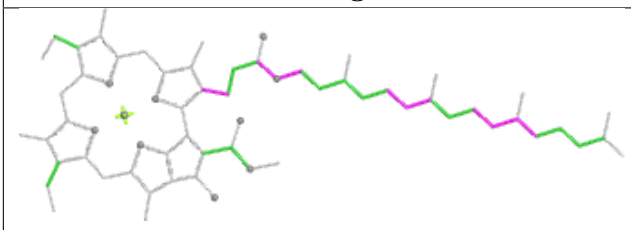
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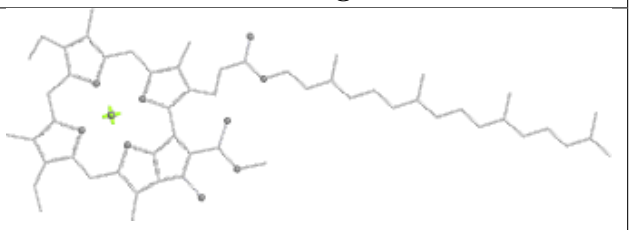
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Bond angles

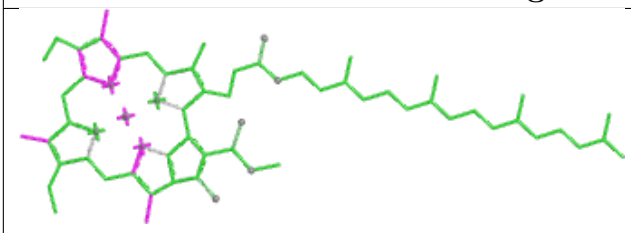


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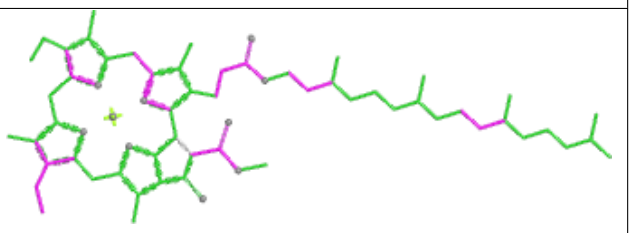


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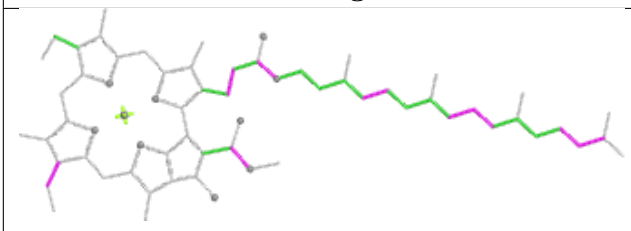
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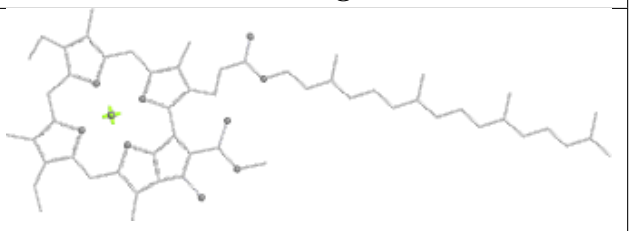
Bond lengths



Bond angles

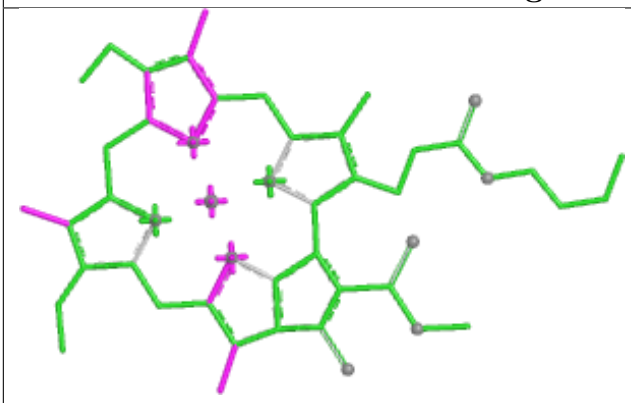


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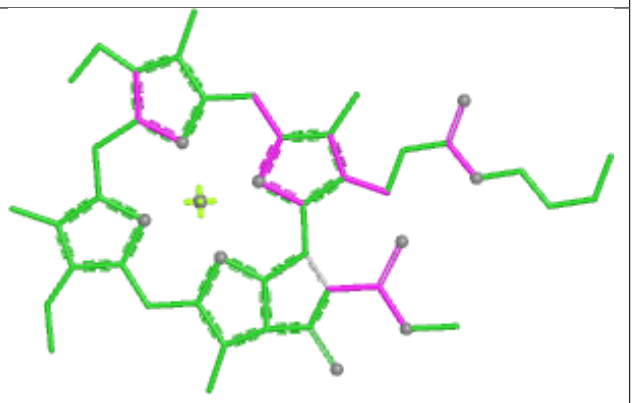


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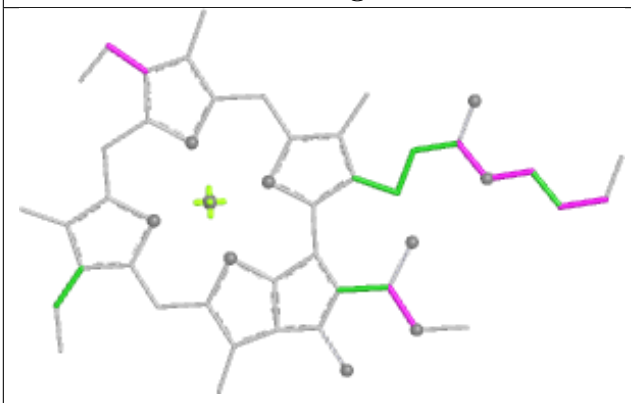
Ligand CLA E 308



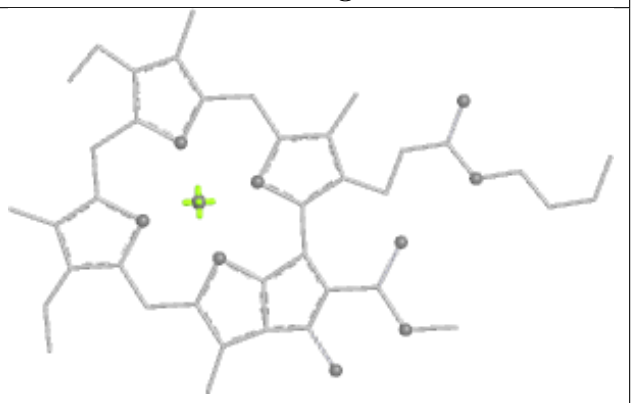
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Bond angles

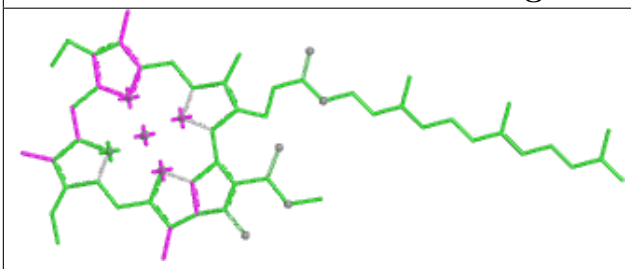


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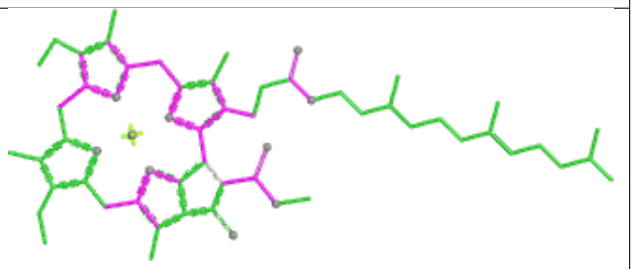


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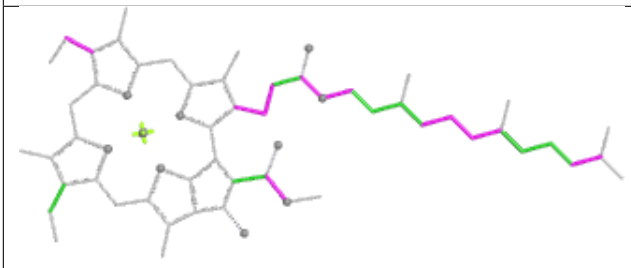
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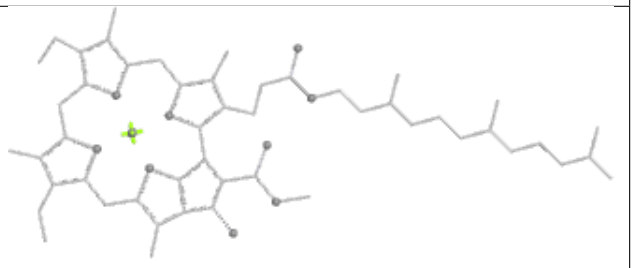
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Bond angles

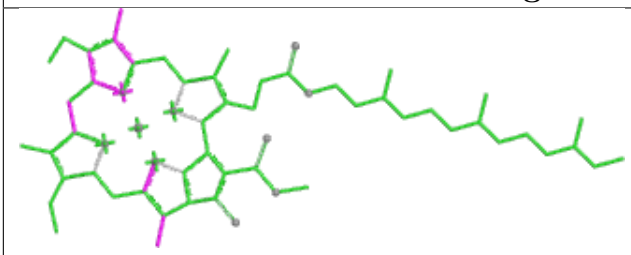


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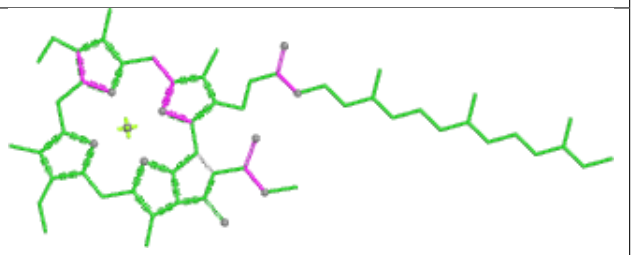


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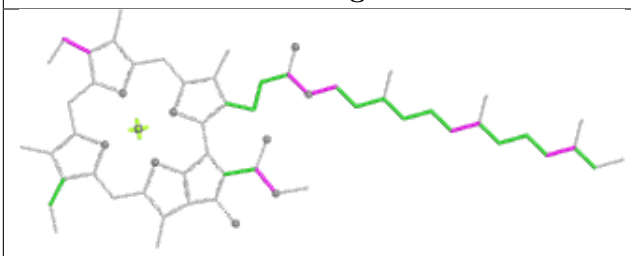
Ligand CLA U 305



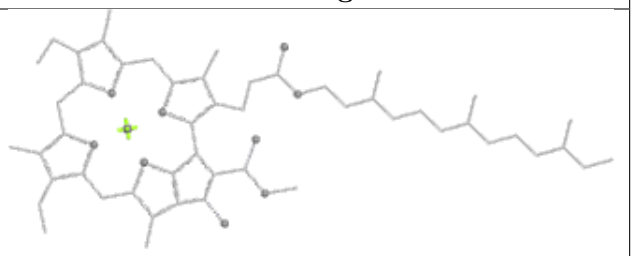
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Bond angles

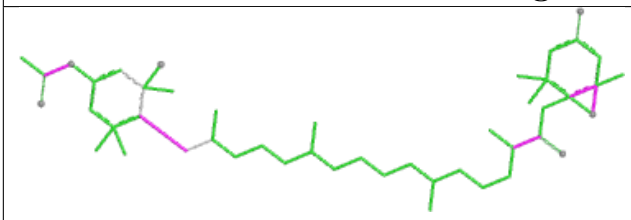


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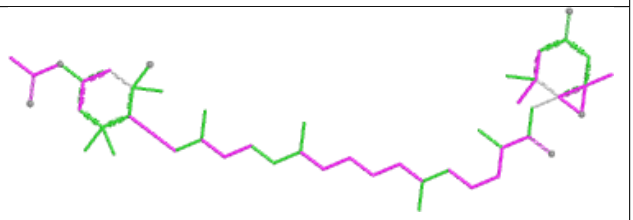


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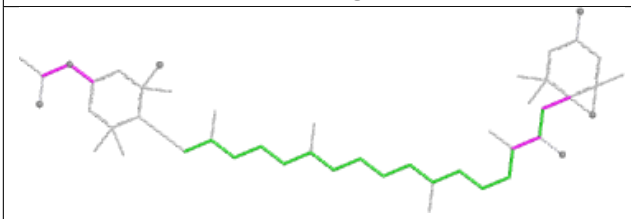
Ligand A86 L 304



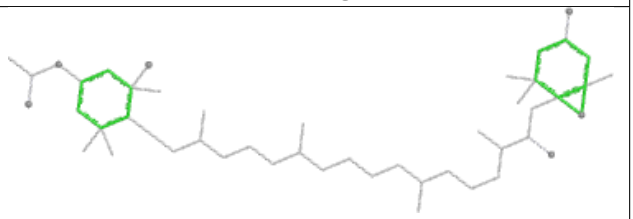
Bond lengths



Bond angles

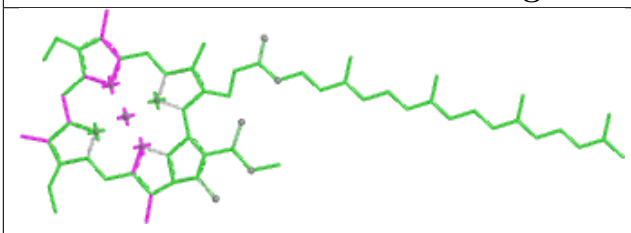


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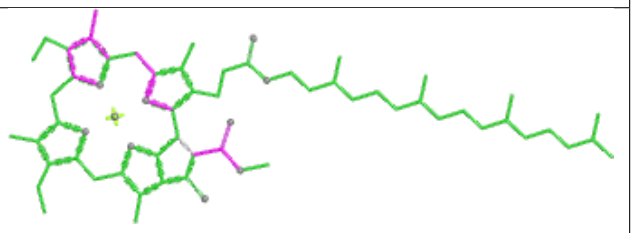


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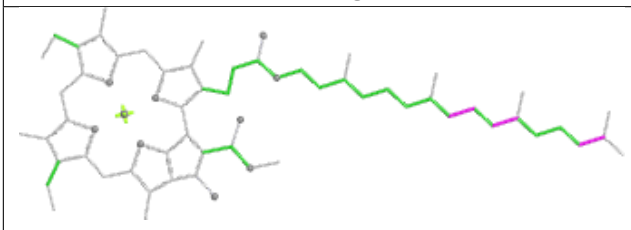
Ligand CLA G 310



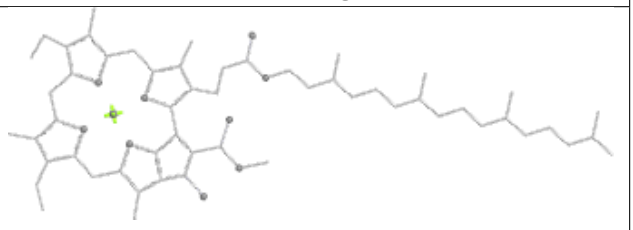
Bond lengths



Bond angles

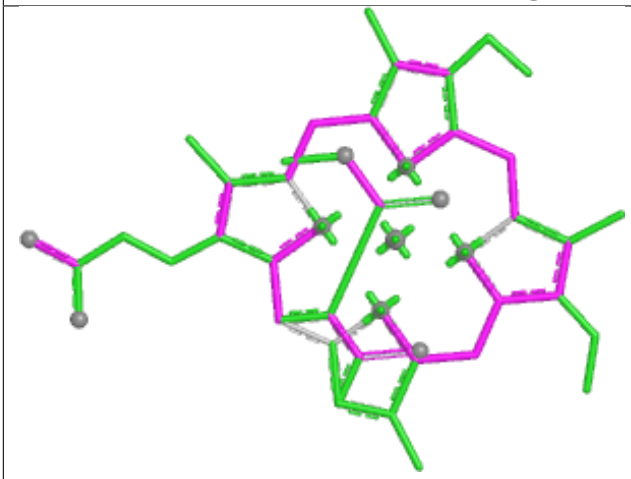


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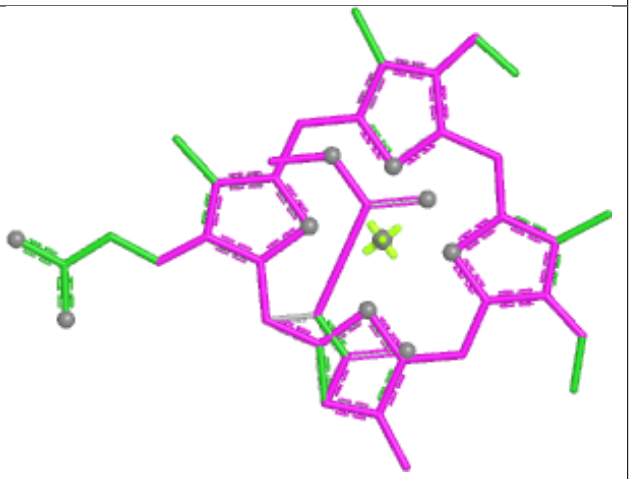


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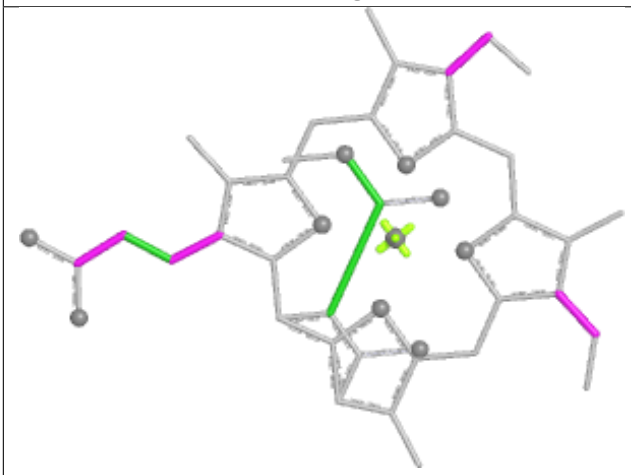
Ligand KC1 G 308



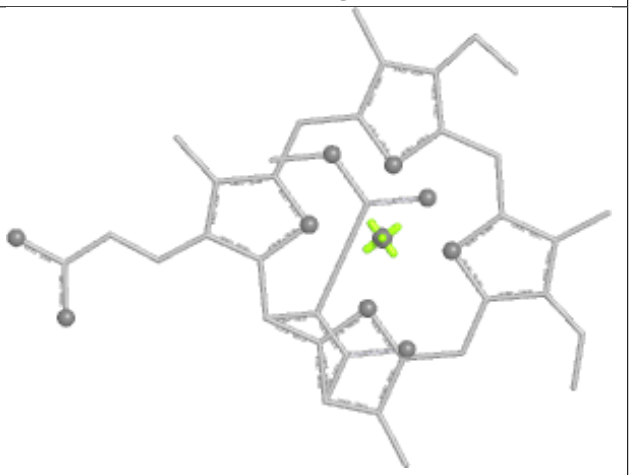
Bond lengths



Bond angles

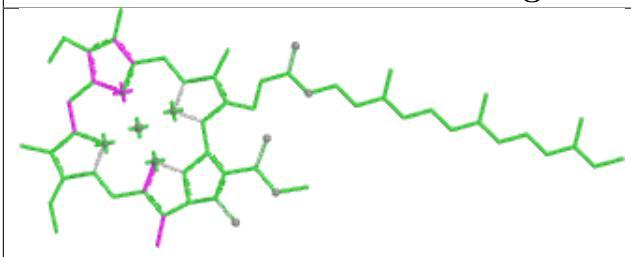


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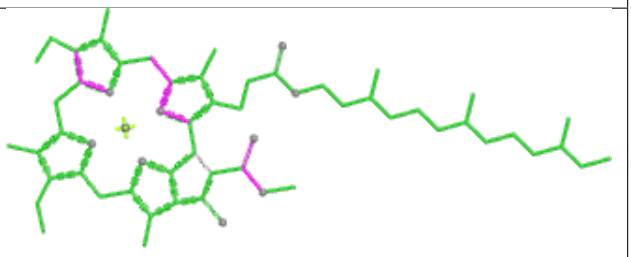


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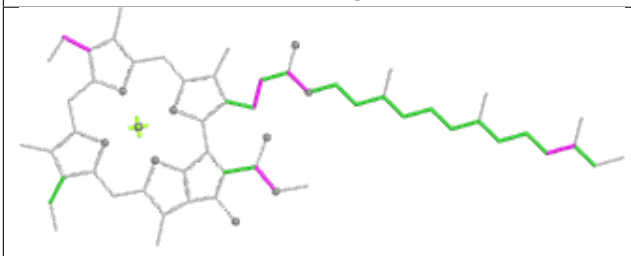
Ligand CLA N 307



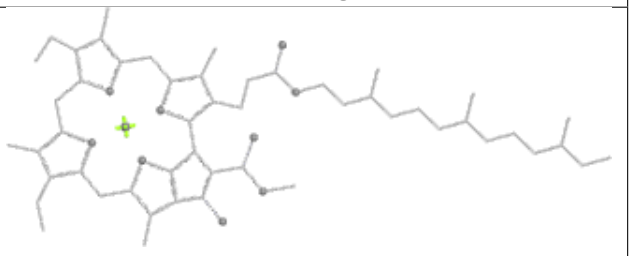
Bond lengths



Bond angles

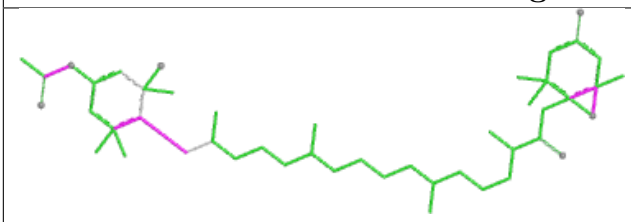


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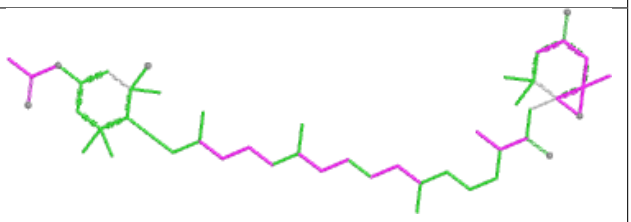


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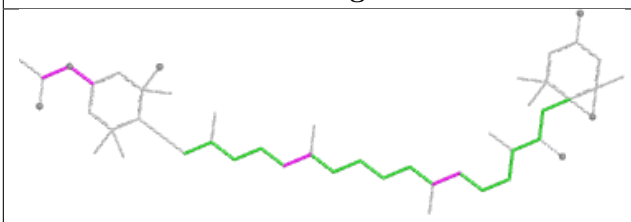
Ligand A86 D 302



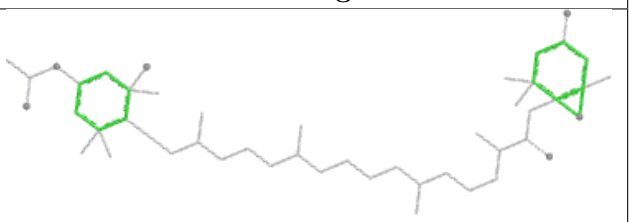
Bond lengths



Bond angles

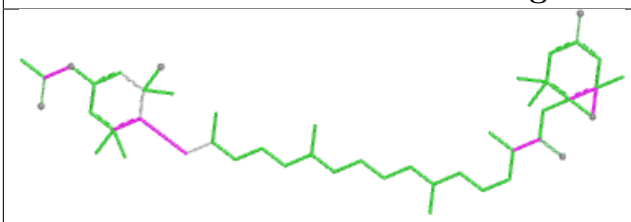


Torsions

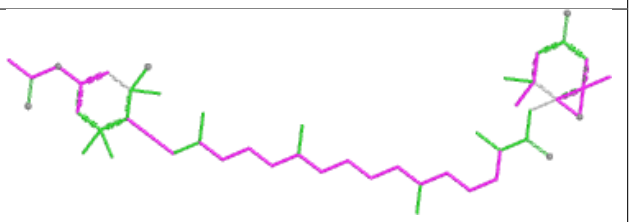


Rings

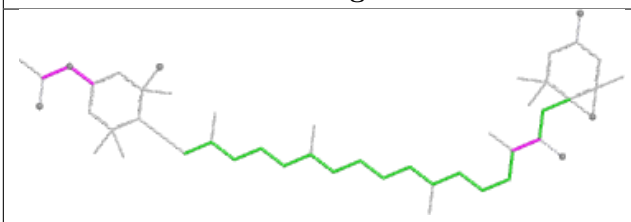
Ligand A86 R 302



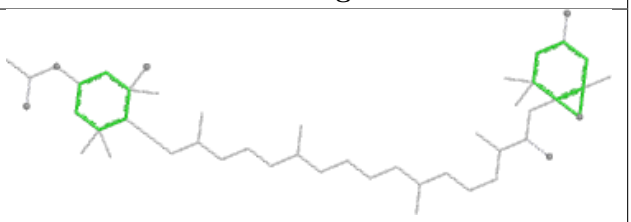
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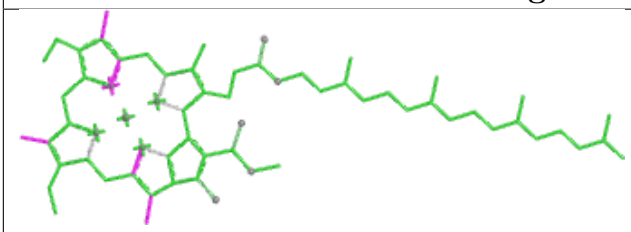


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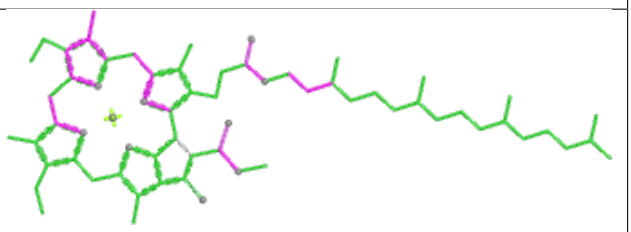


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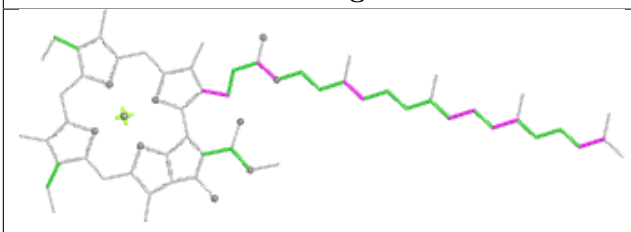
Ligand CLA a 818



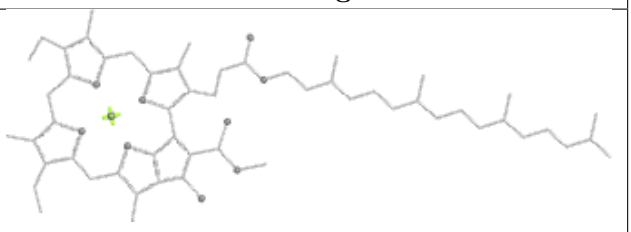
Bond lengths



Bond angles

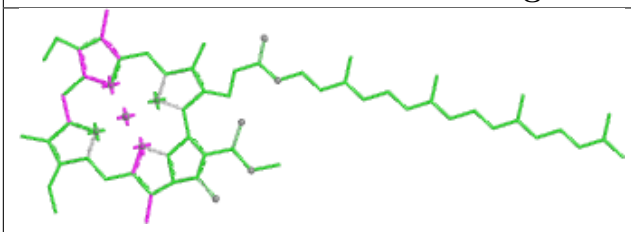


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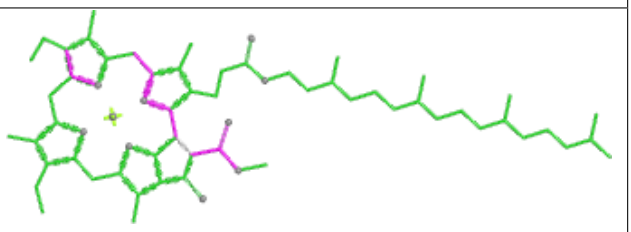


Rings

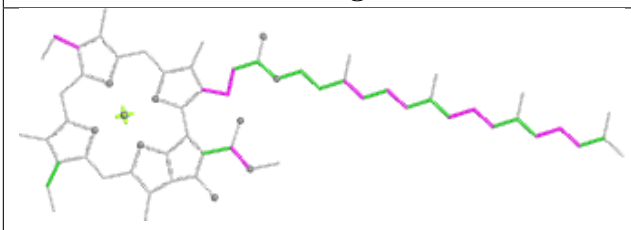
Ligand CLA V 313



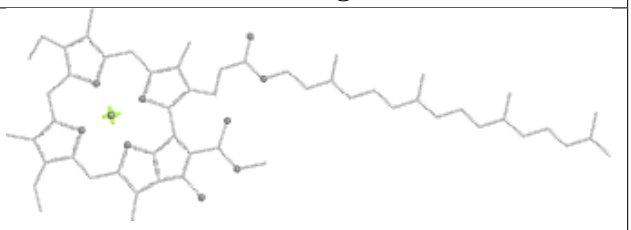
Bond lengths



Bond angles

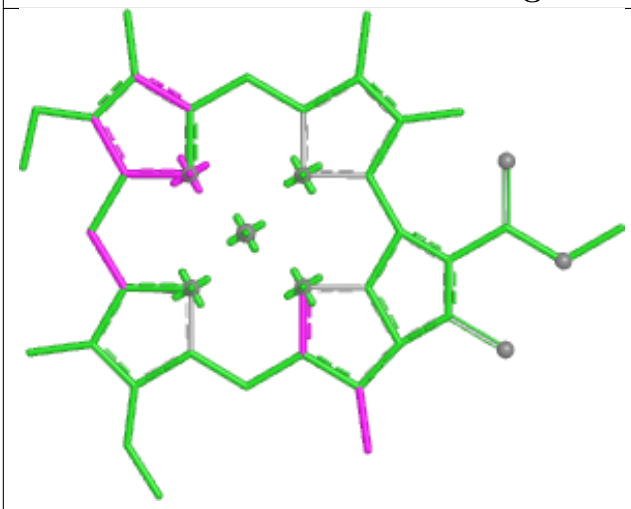


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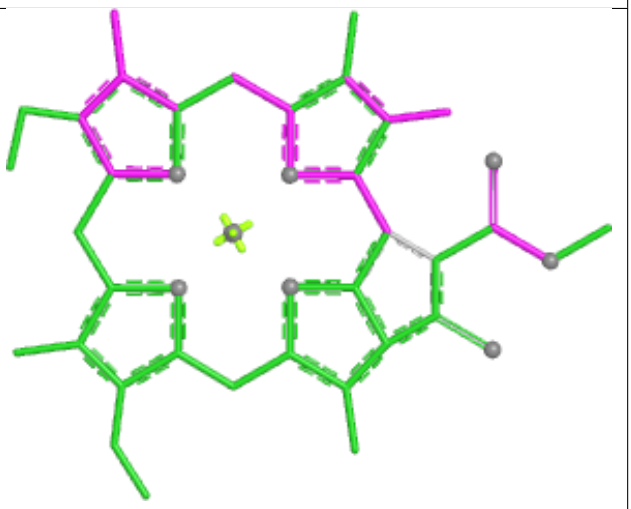


Rings

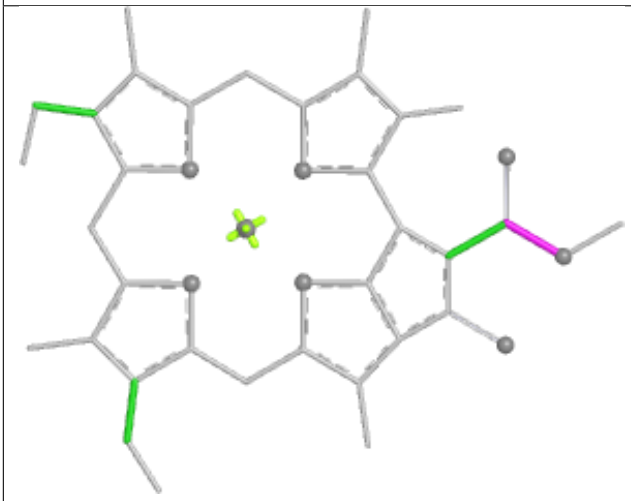
Ligand CLA X 315



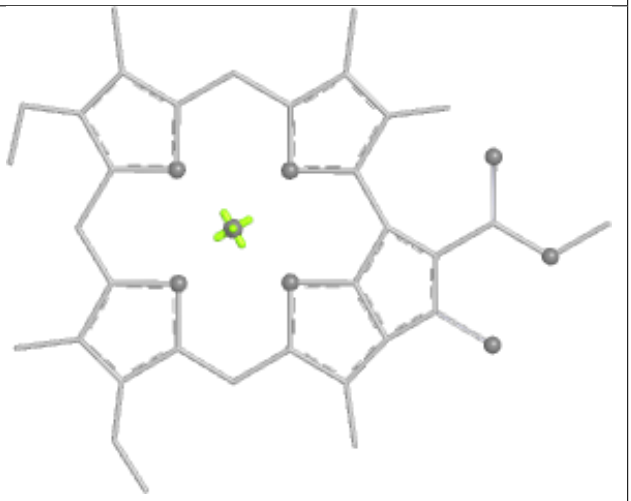
Bond lengths



Bond angles

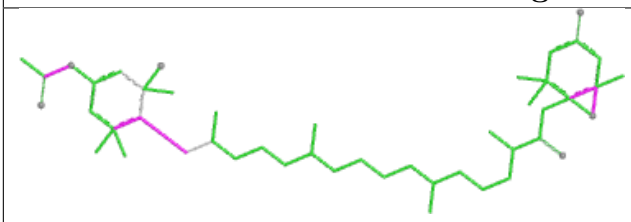


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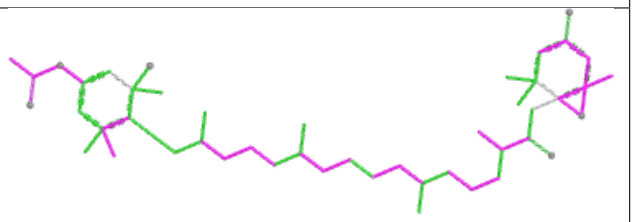


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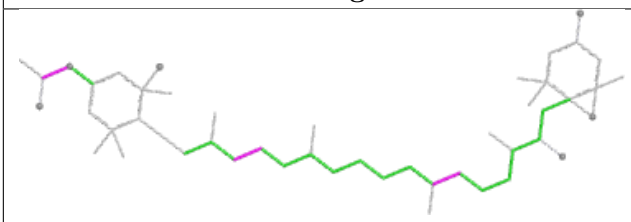
Ligand A86 E 305



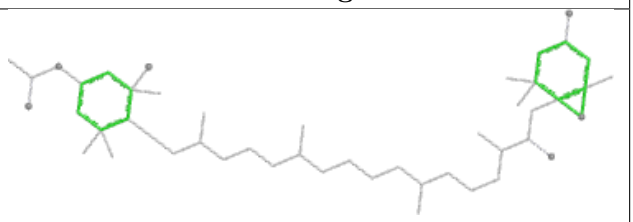
Bond lengths



Bond angles

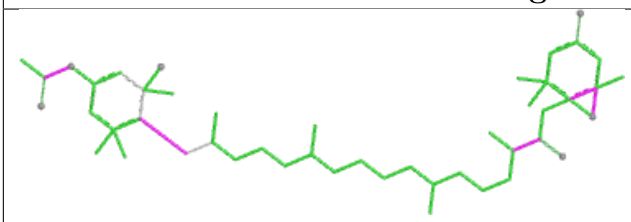


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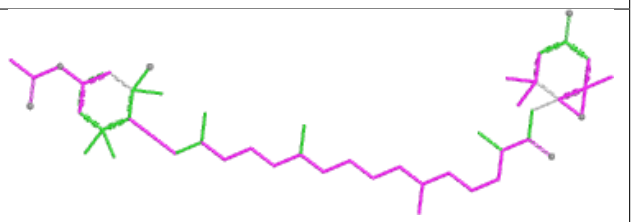


Rings

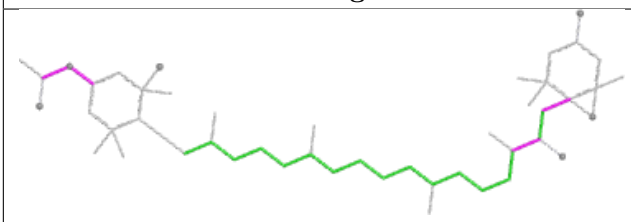
Ligand A86 X 303



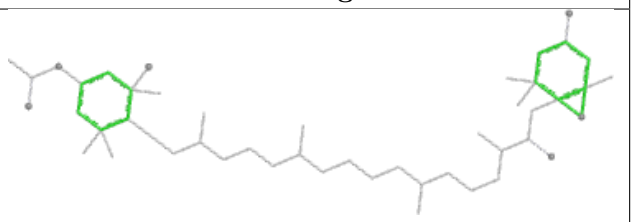
Bond lengths



Bond angles

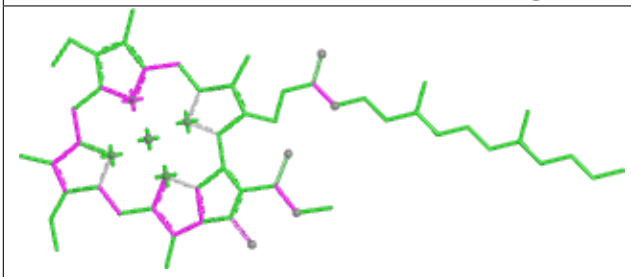


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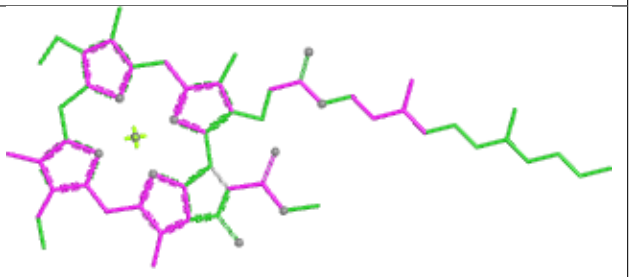


Rings

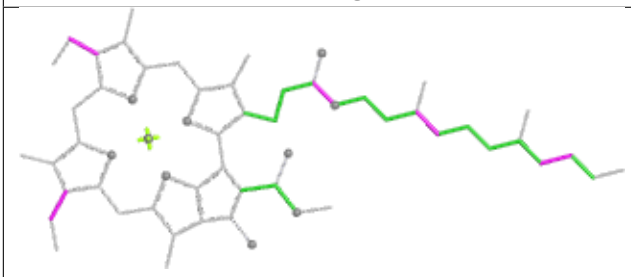
Ligand CLA b 836



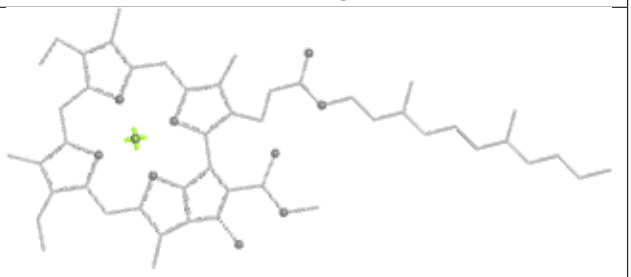
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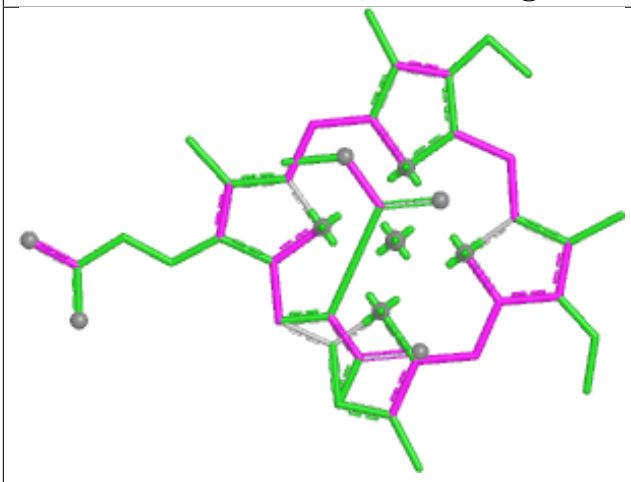


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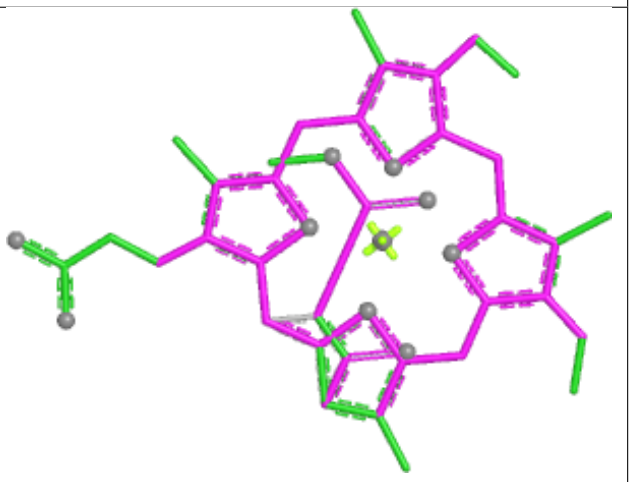


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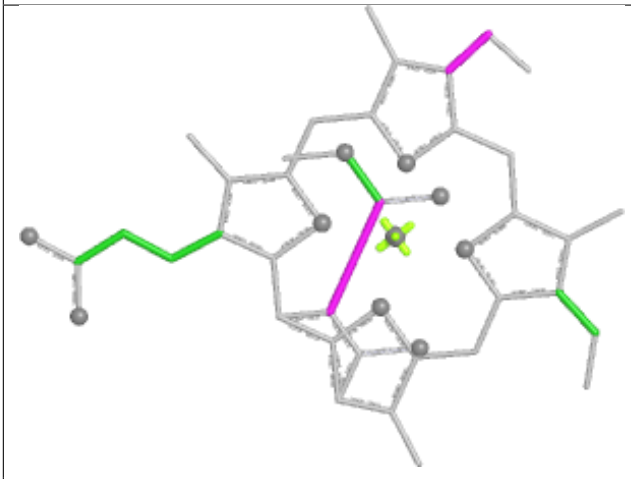
Ligand KC1 W 217



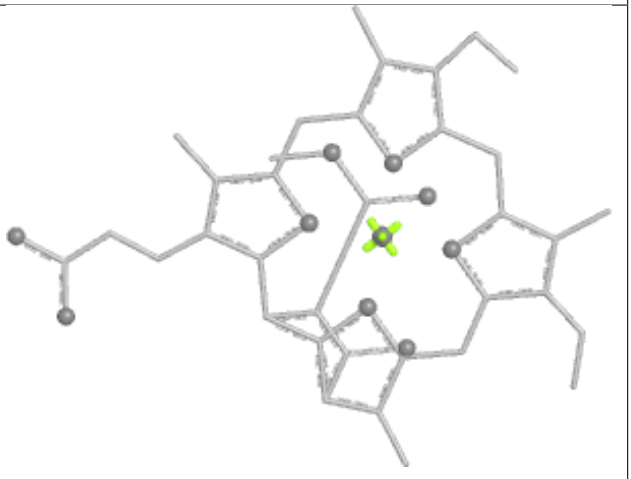
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Bond angles

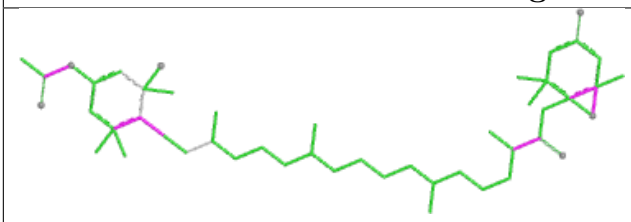


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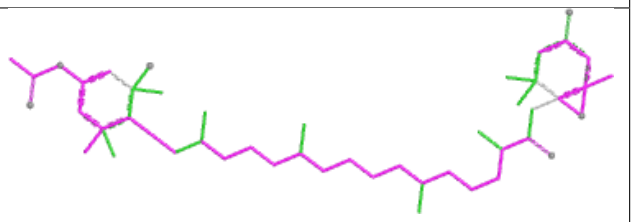


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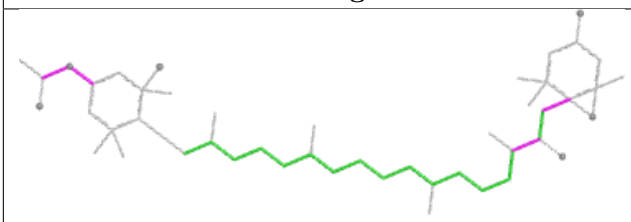
Ligand A86 N 301



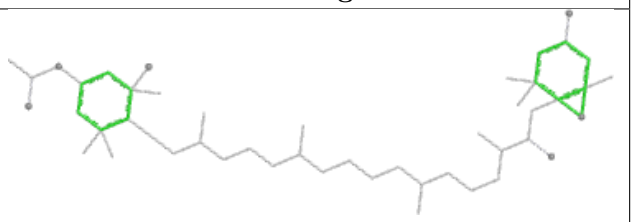
Bond lengths



Bond angles

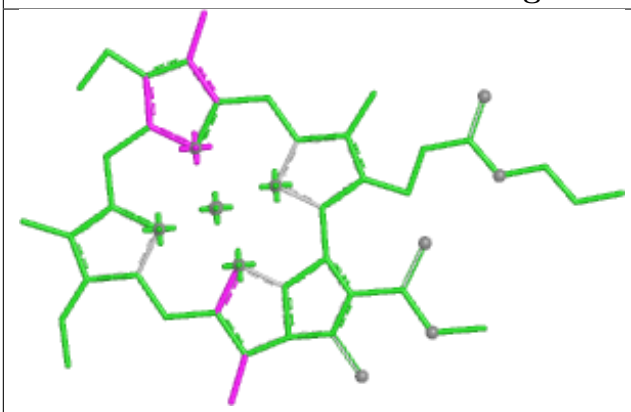


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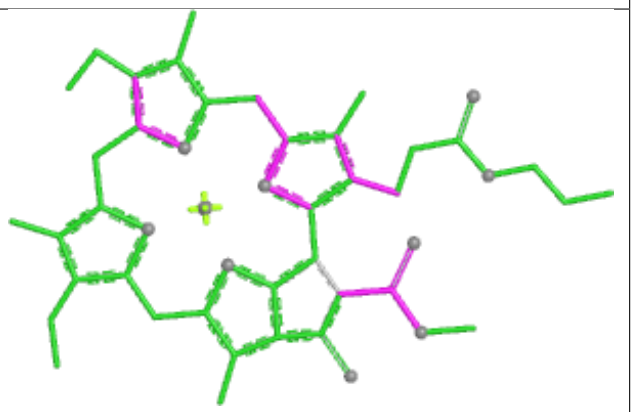


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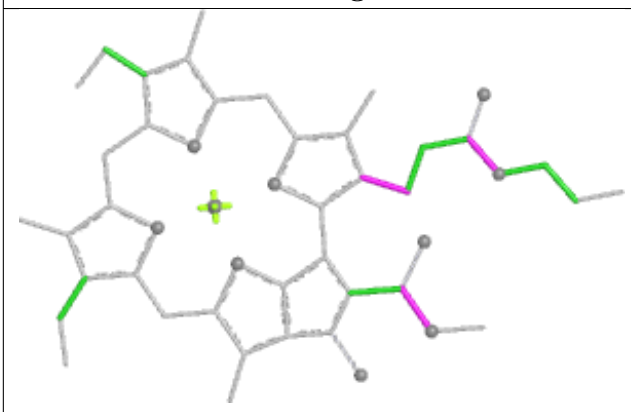
Ligand CLA H 305



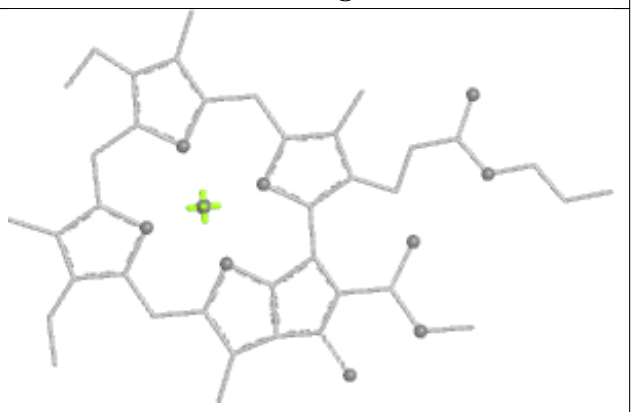
Bond lengths



Bond angles

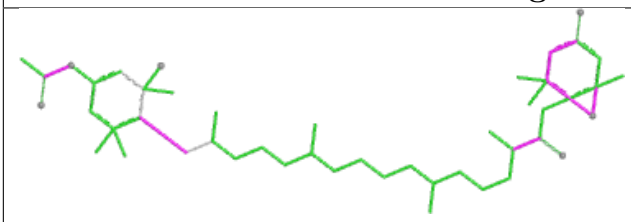


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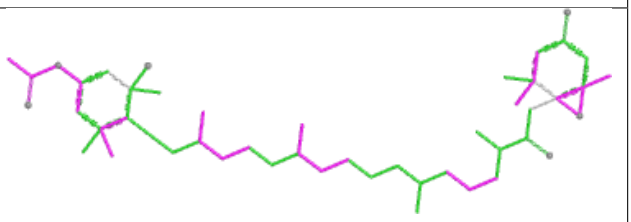


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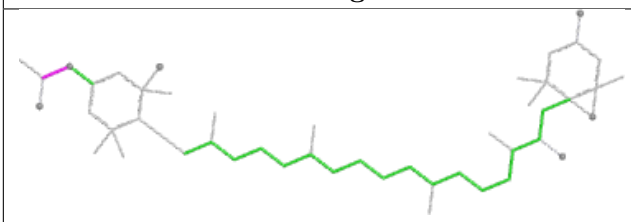
Ligand A86 N 305



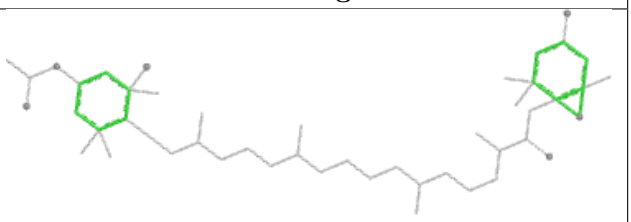
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Bond angles

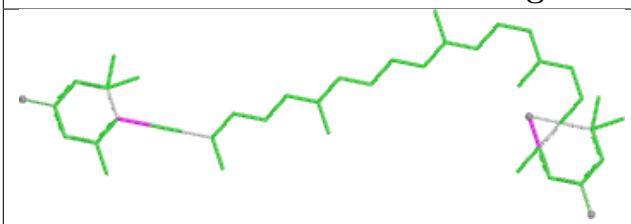


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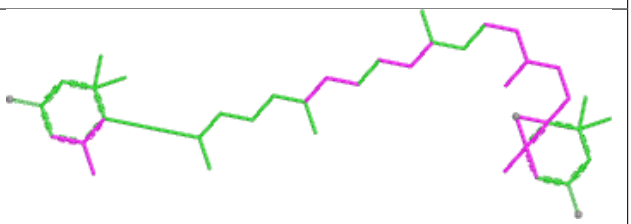


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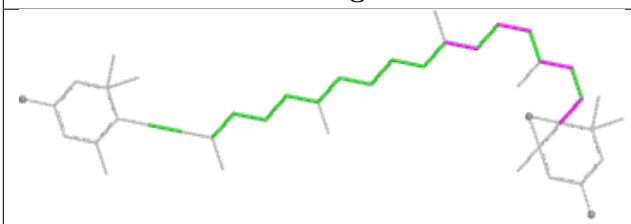
Ligand DD6 F 303



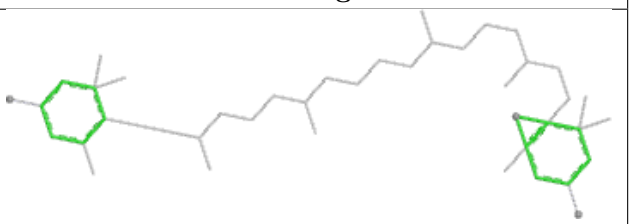
Bond lengths



Bond angles

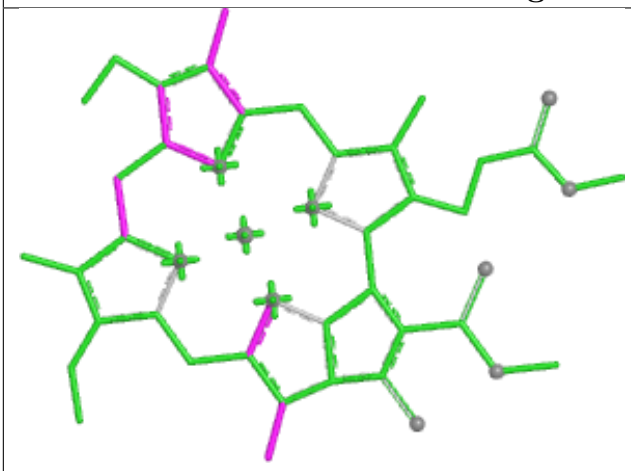


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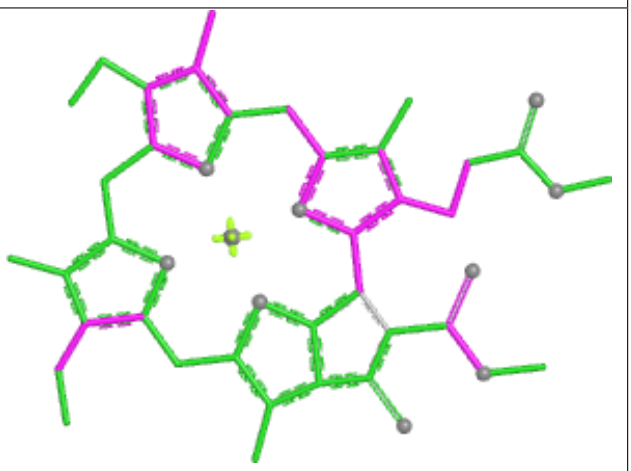


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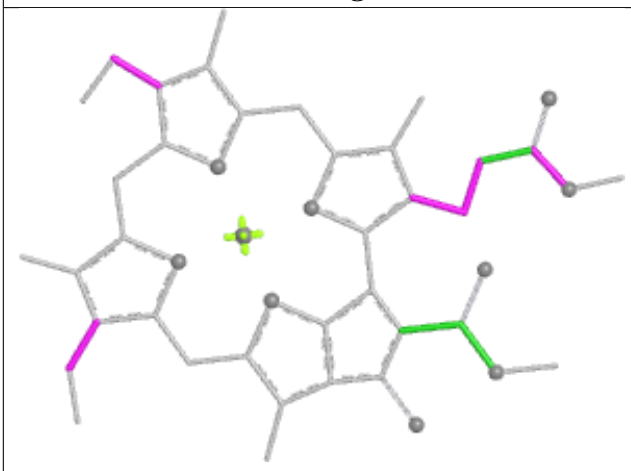
Ligand CLA S 313



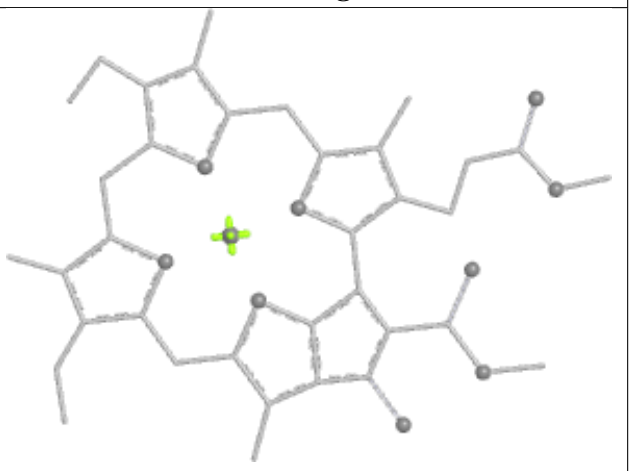
Bond lengths



Bond angles

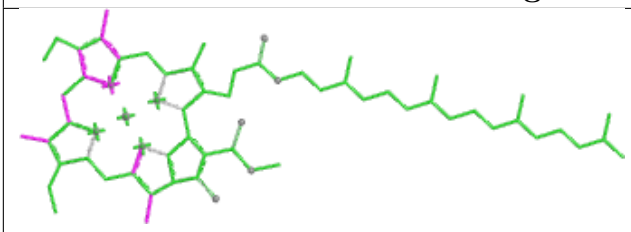


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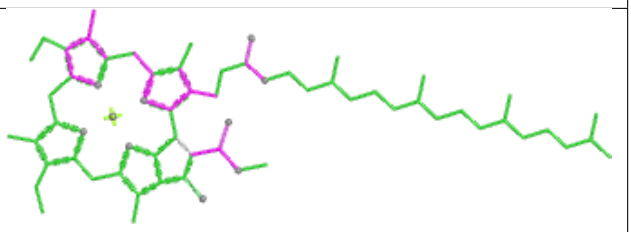


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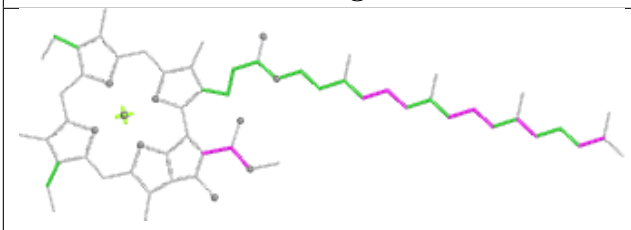
Ligand CLA A 308



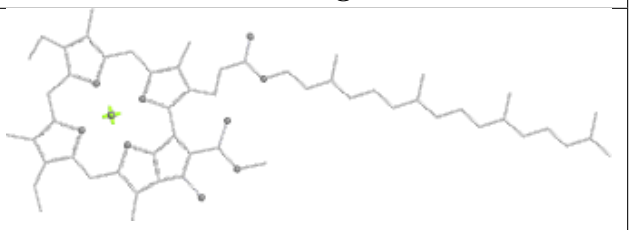
Bond lengths



Bond angles

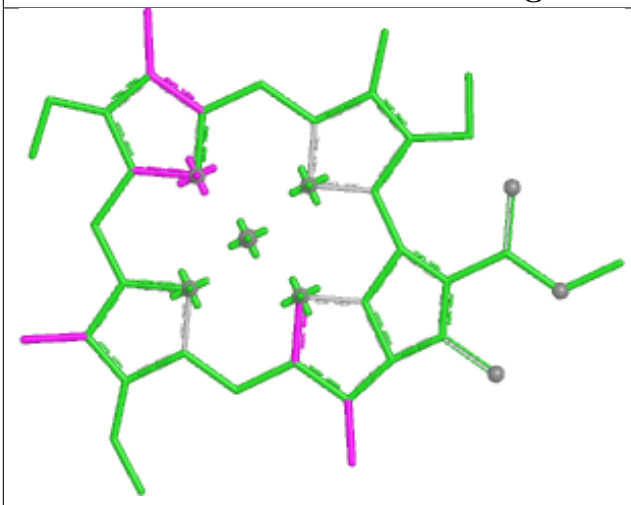


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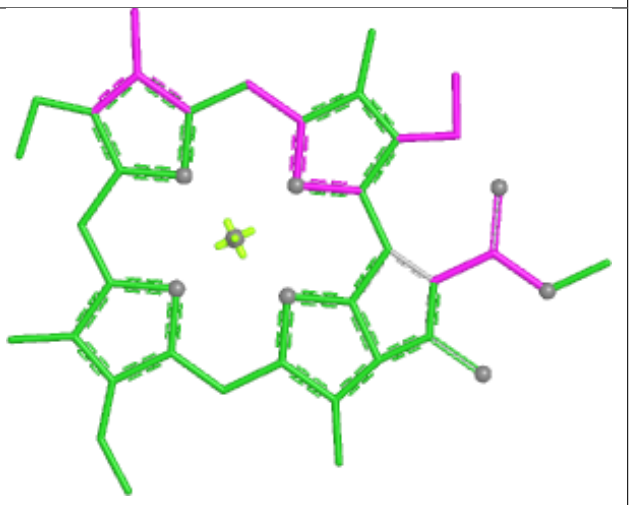


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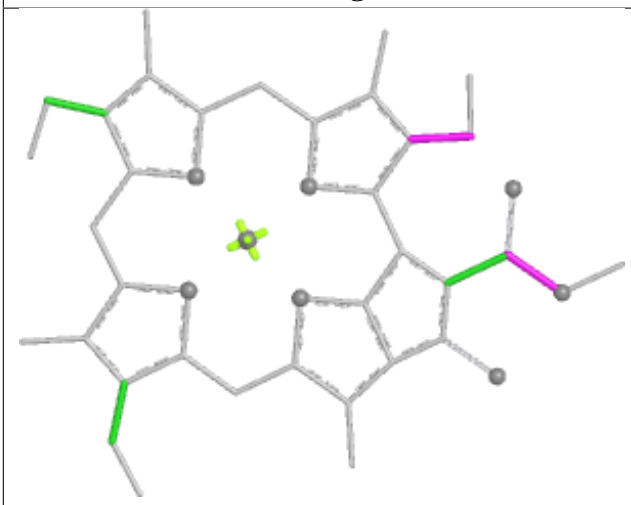
Ligand CLA P 302



Bond lengths



Bond angles

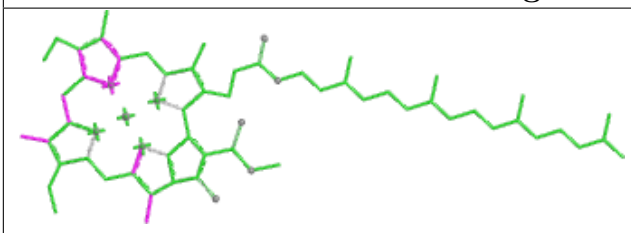


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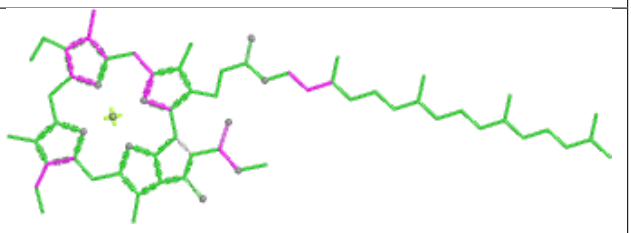


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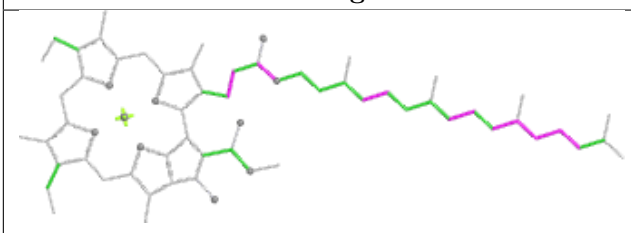
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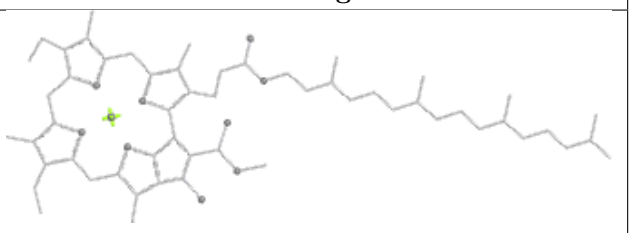
Bond lengths



Bond angles

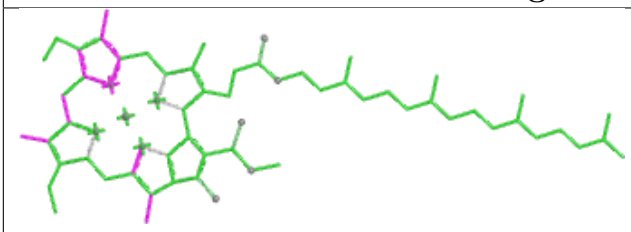


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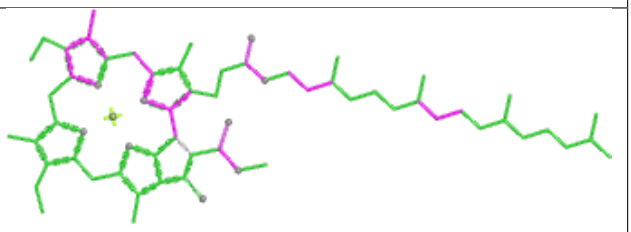


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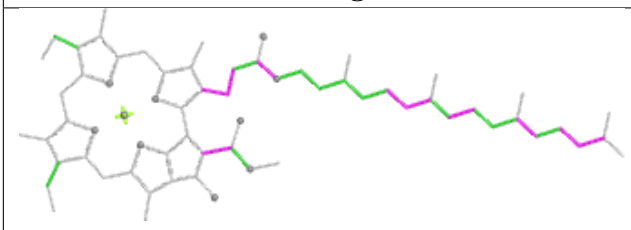
Ligand CLA a 807



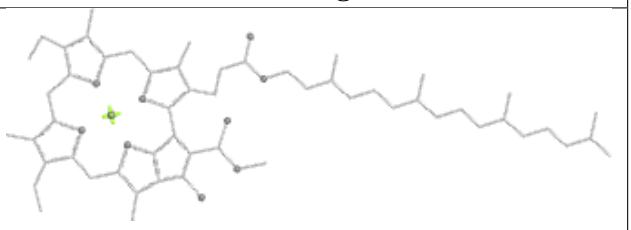
Bond lengths



Bond angles

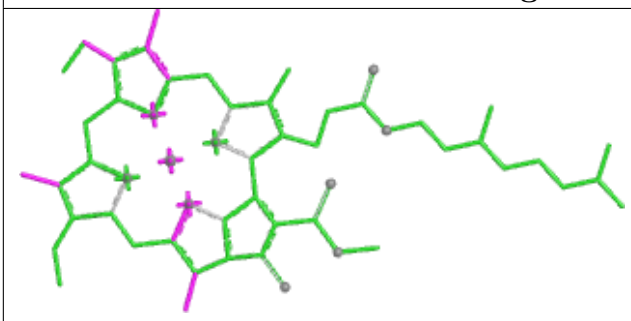


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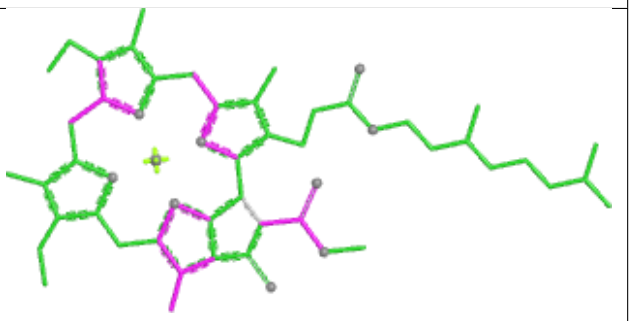


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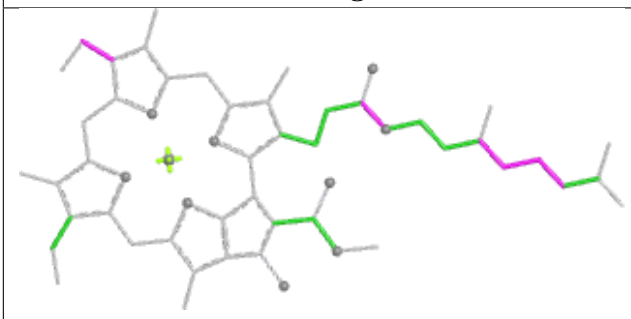
Ligand CLA M 306



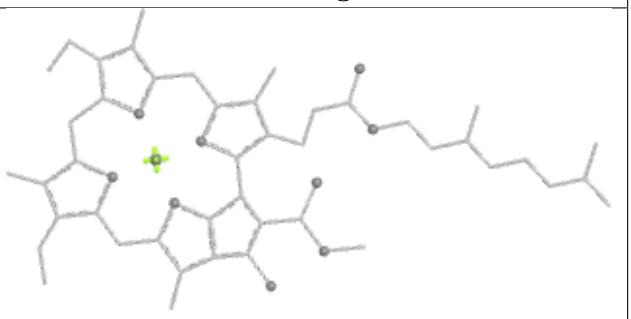
Bond lengths



Bond angles

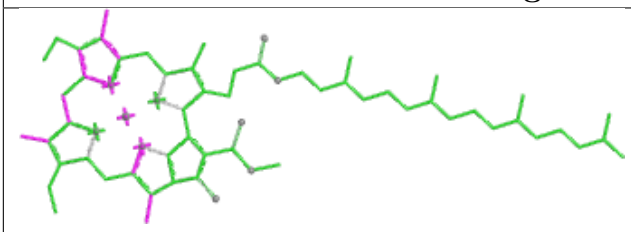


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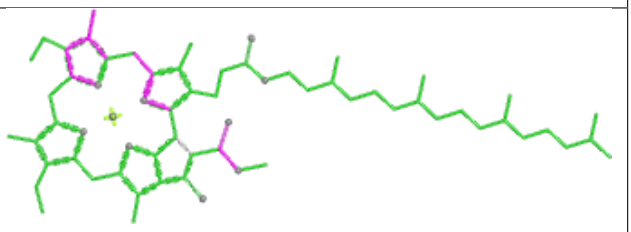


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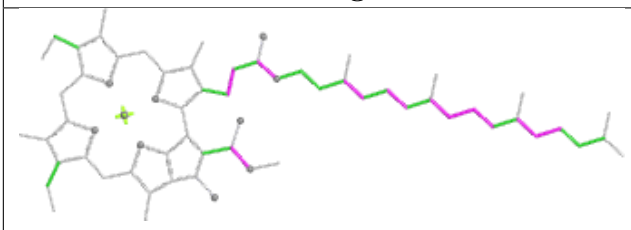
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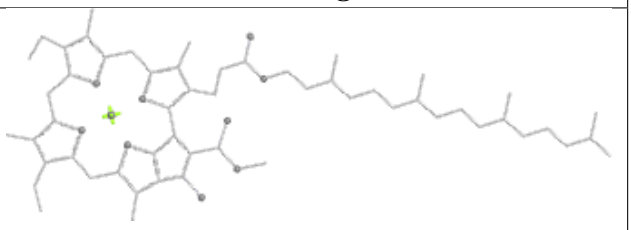
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Bond angles

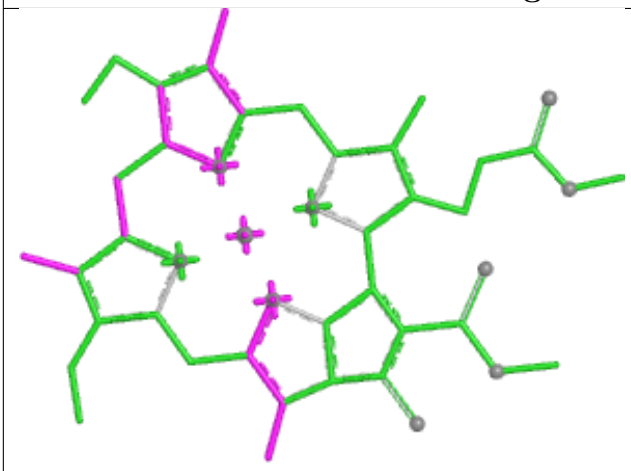


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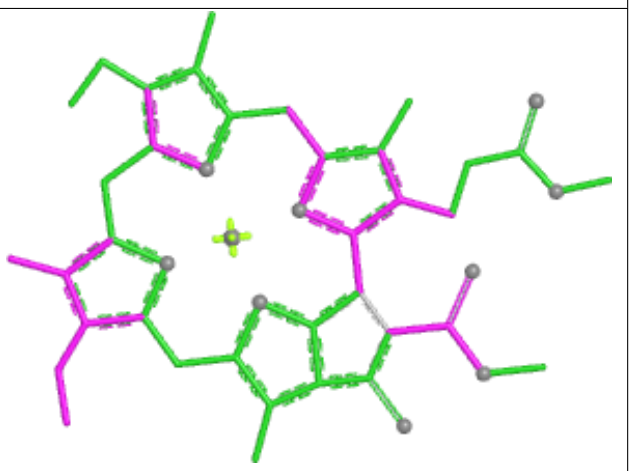


Rings

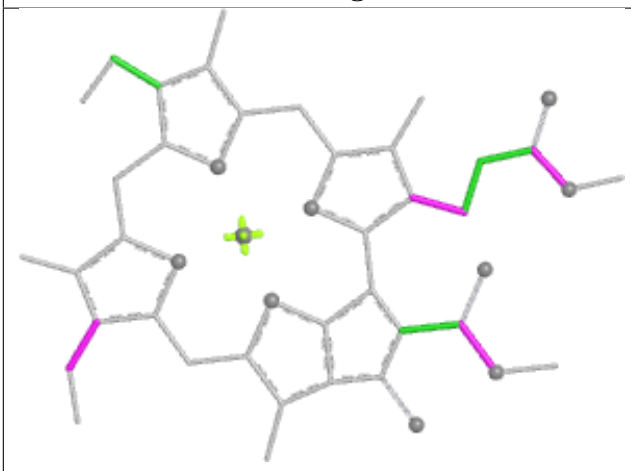
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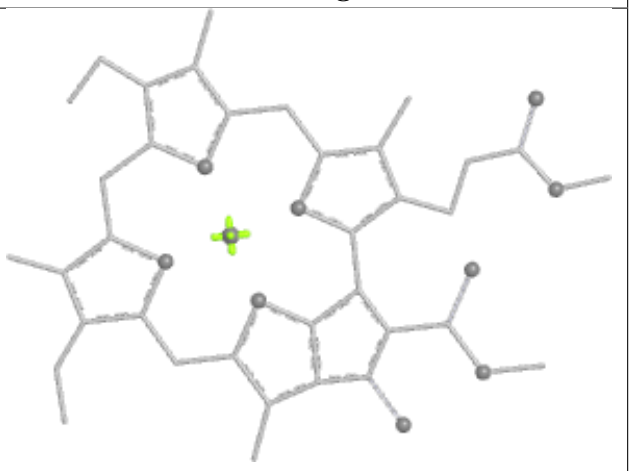
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Bond angles

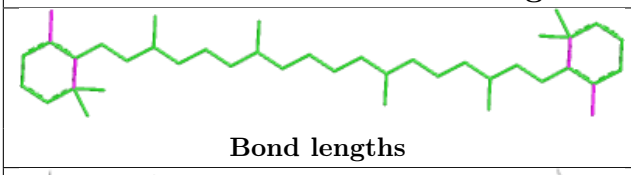


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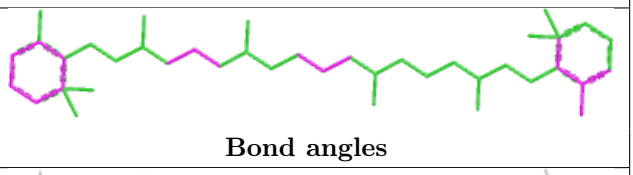


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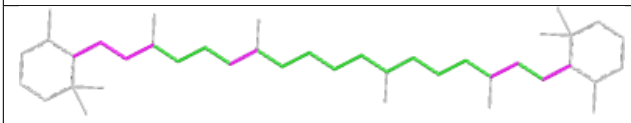
Ligand BCR b 847



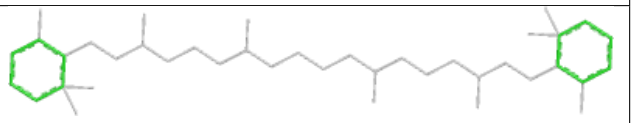
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Bond angles

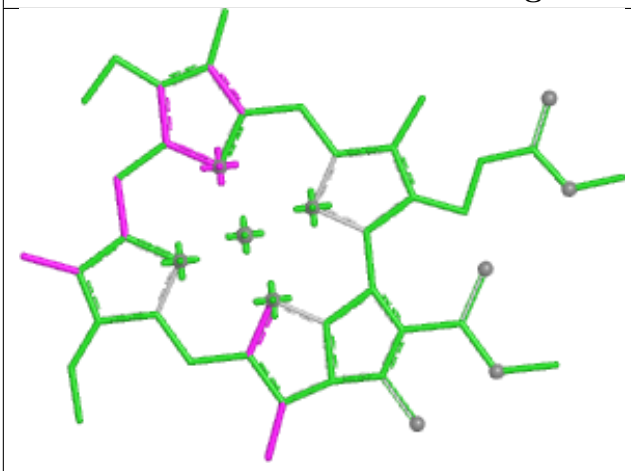


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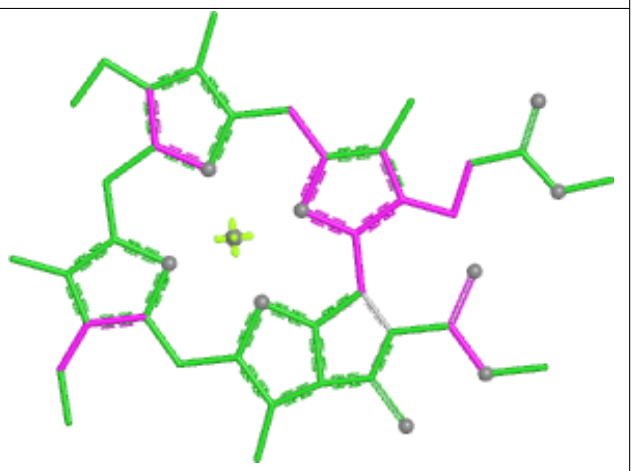


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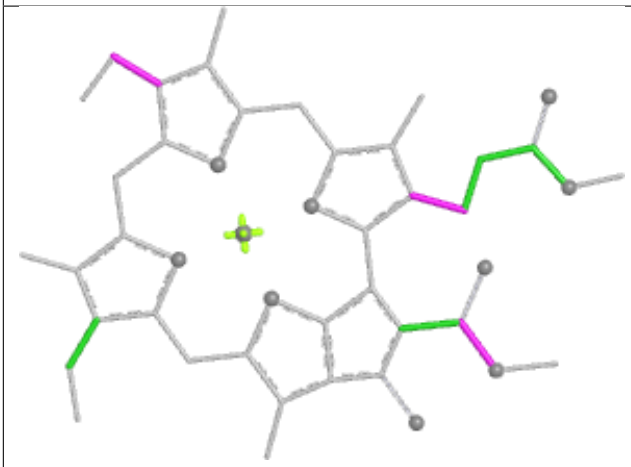
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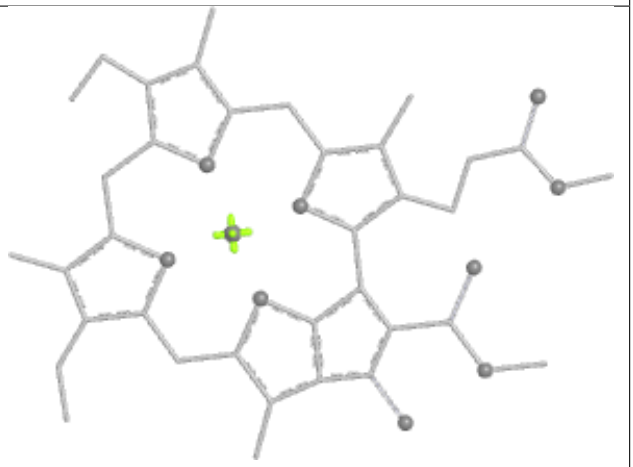
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Bond angles

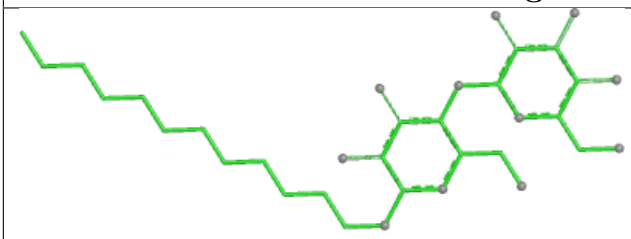


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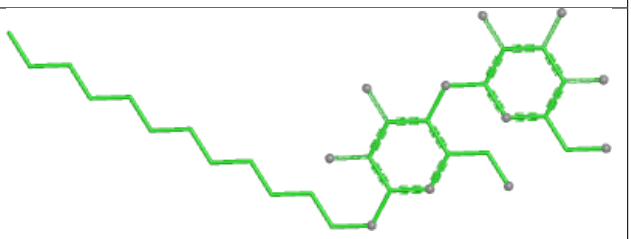


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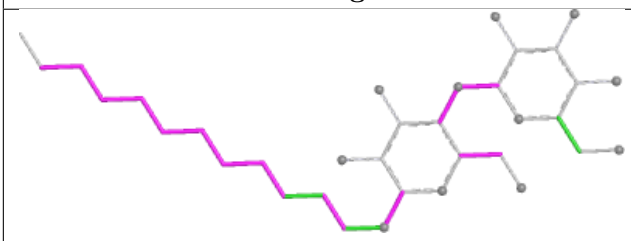
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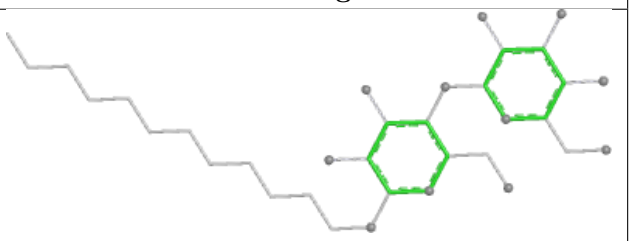
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Bond angles

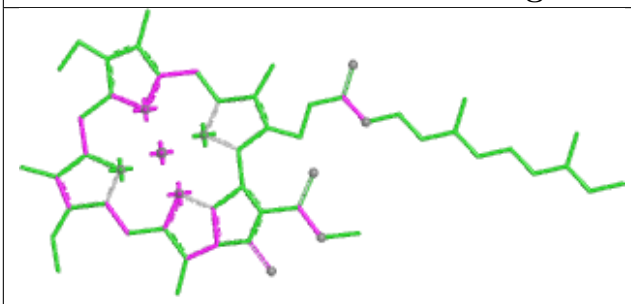


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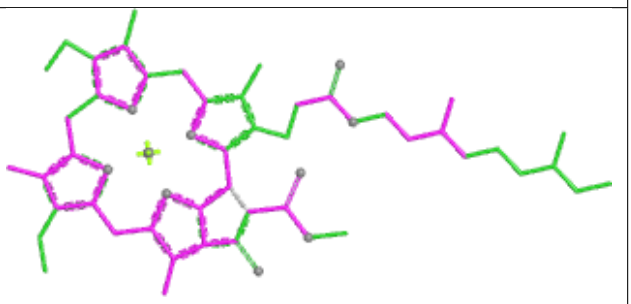


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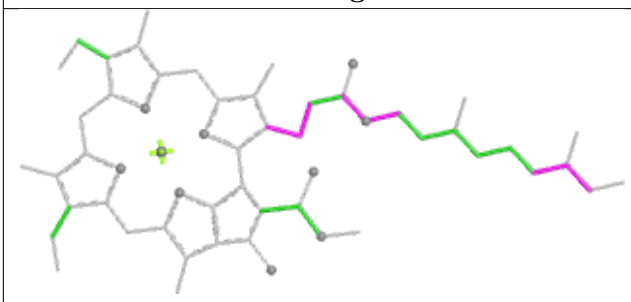
Ligand CLA F 317



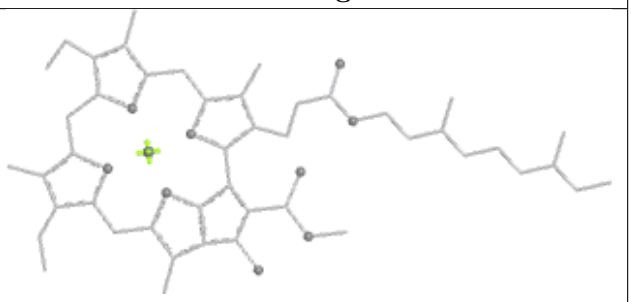
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Bond angles

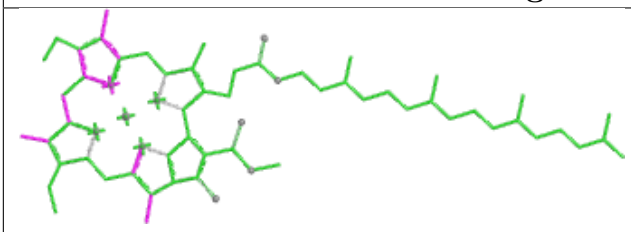


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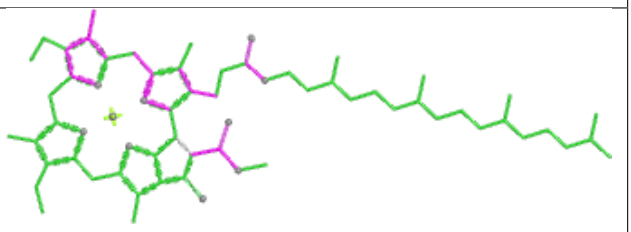


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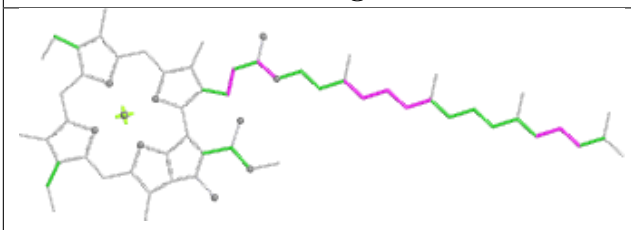
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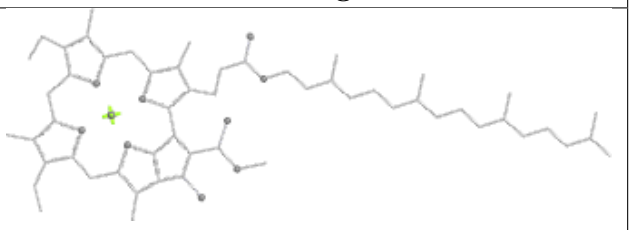
Bond lengths



Bond angles

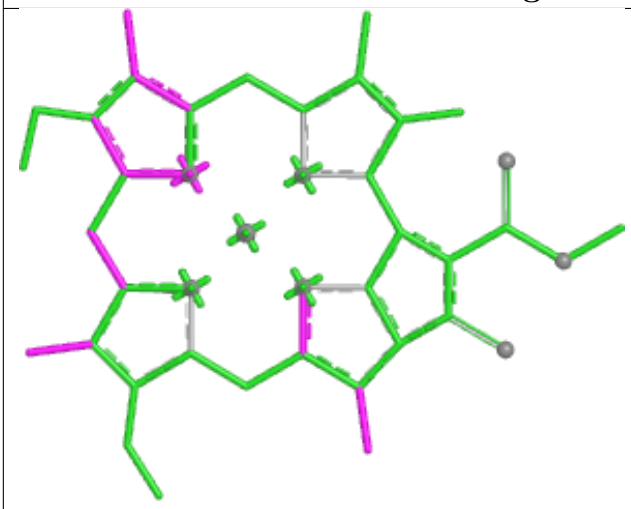


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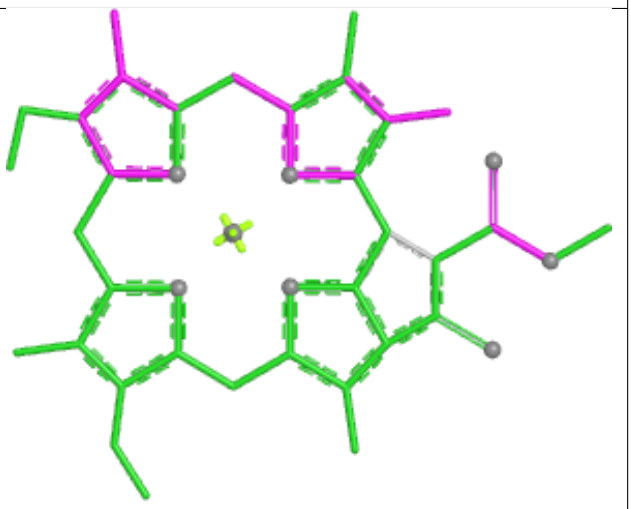


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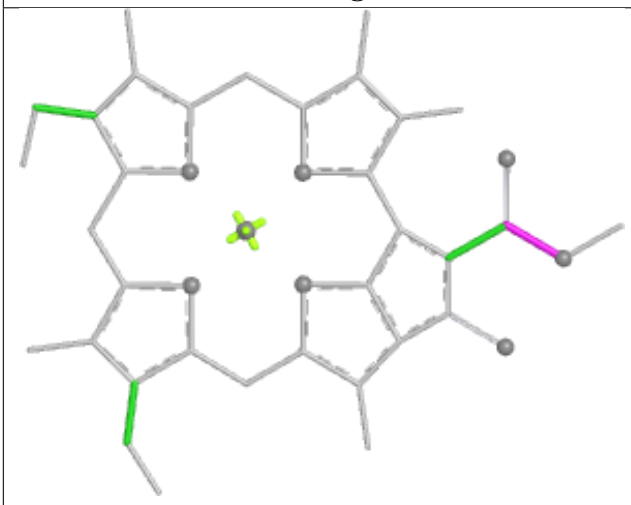
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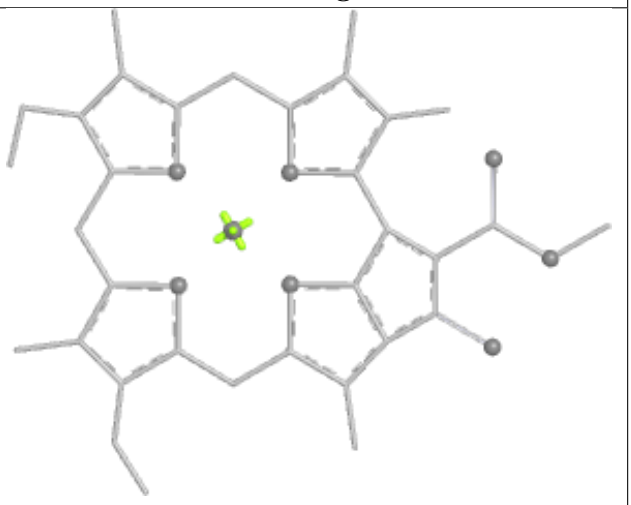
Bond lengths



Bond angles

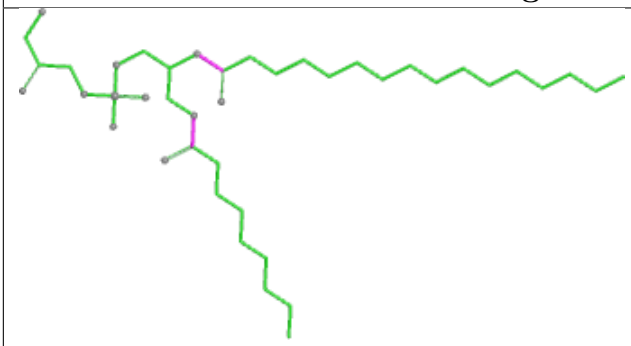


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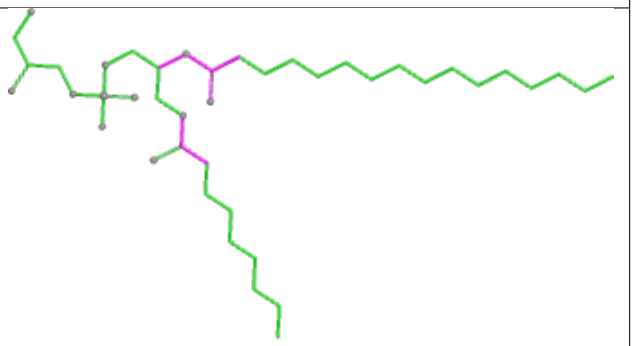


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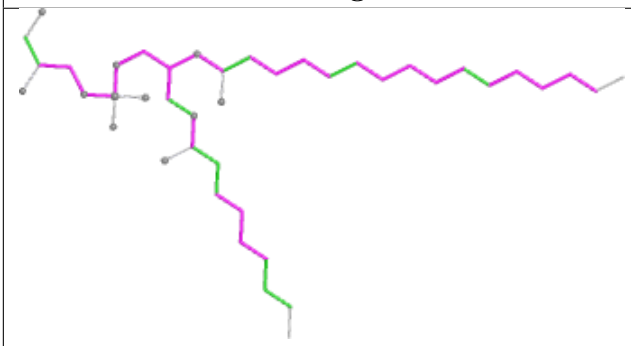
Ligand LHG O 317



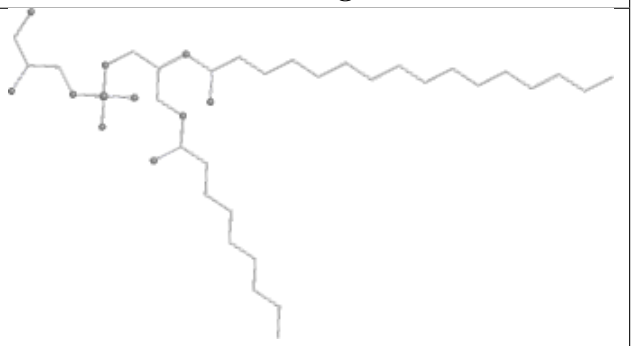
Bond lengths



Bond angles

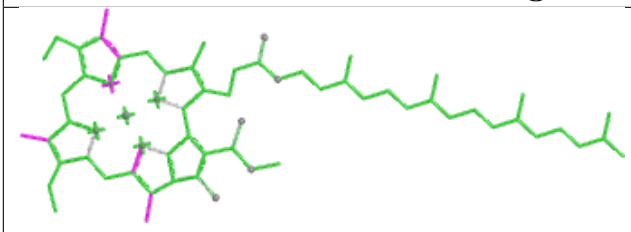


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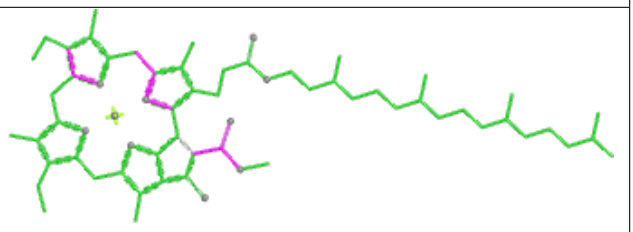


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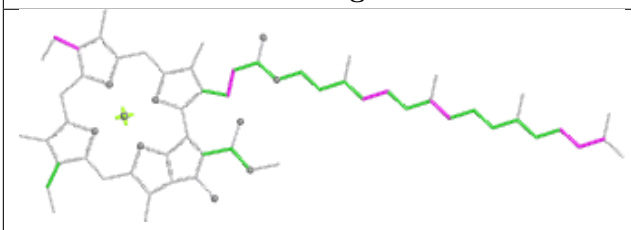
Ligand CLA b 810



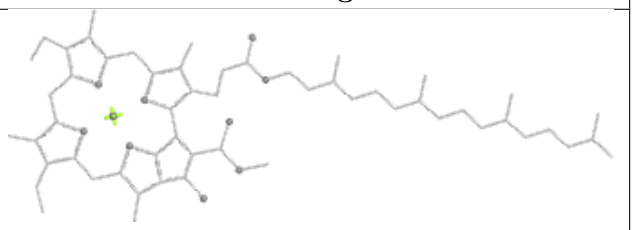
Bond lengths



Bond angles

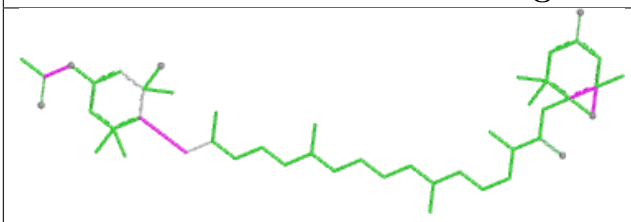


Torsions

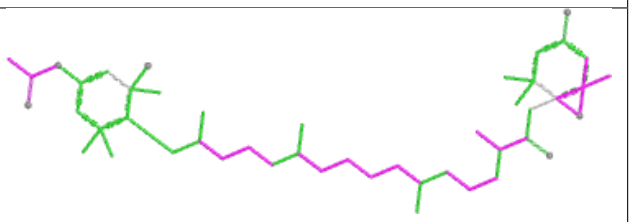


Rings

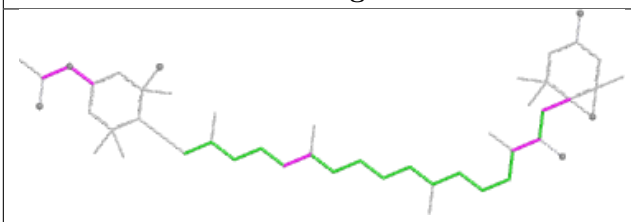
Ligand A86 J 306



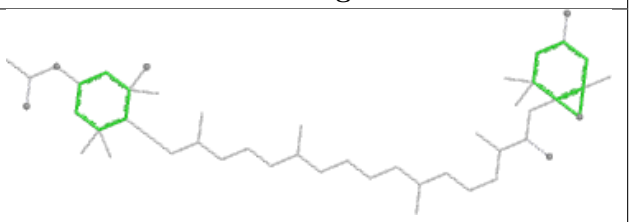
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Bond angles

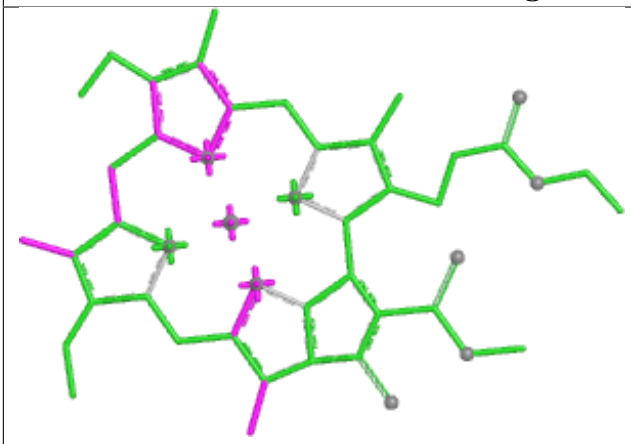


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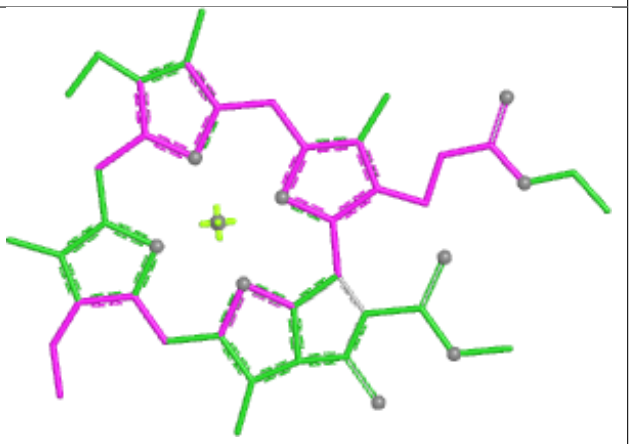


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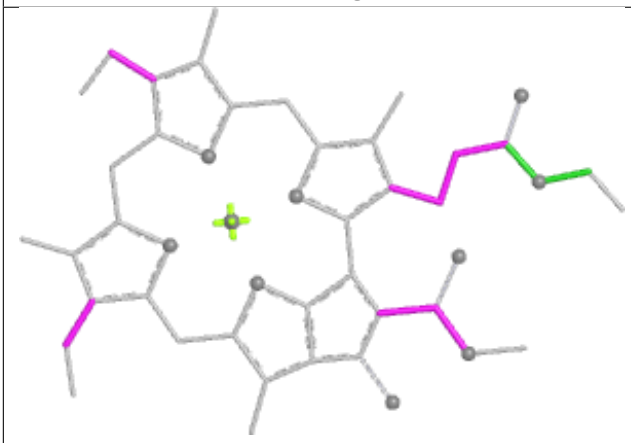
Ligand CLA X 308



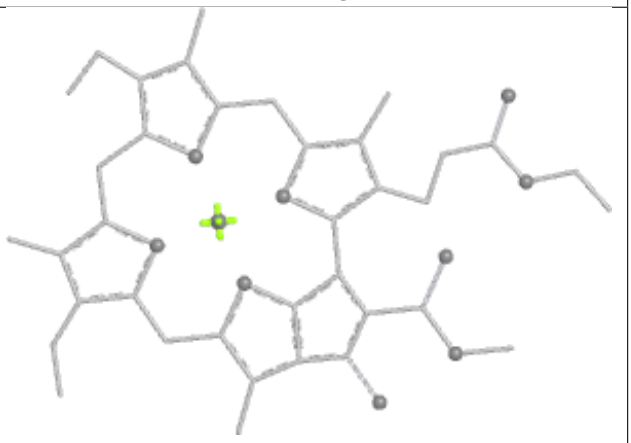
Bond lengths



Bond angles

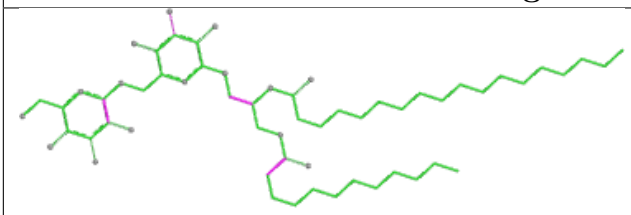


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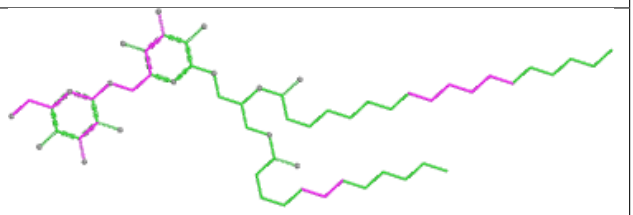


Rings

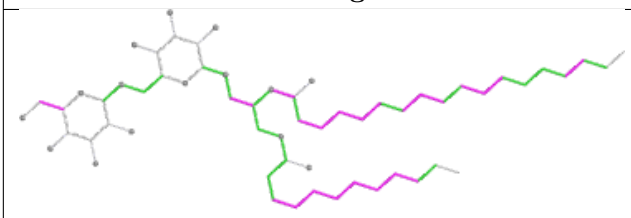
Ligand DGD b 849



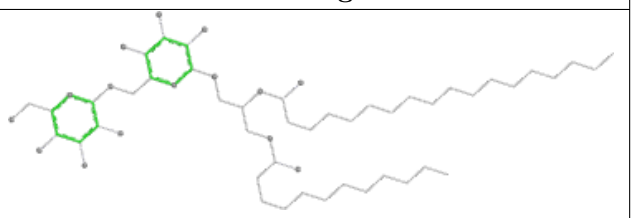
Bond lengths



Bond angles

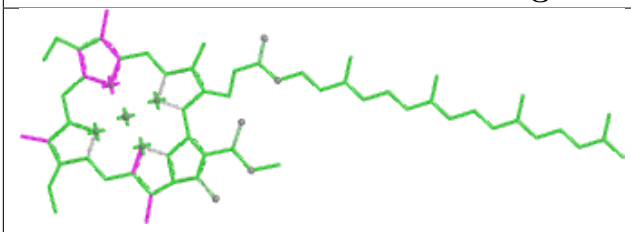


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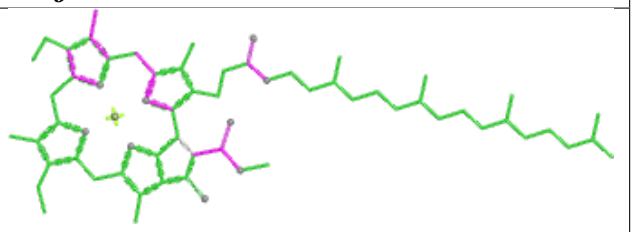


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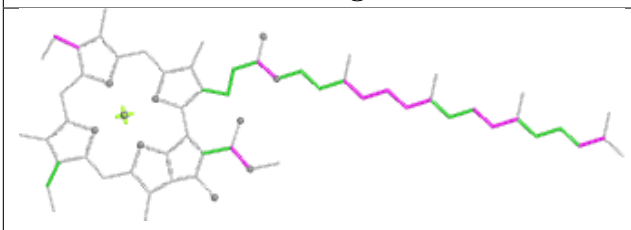
Ligand CLA j 101



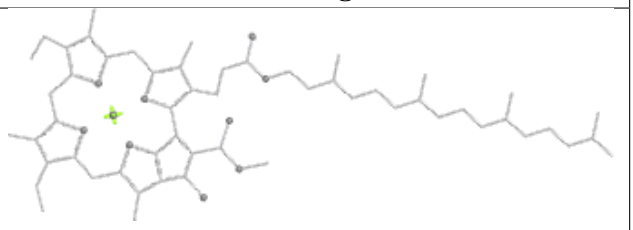
Bond lengths



Bond angles

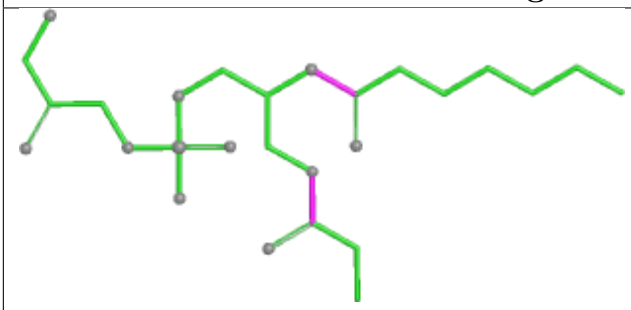


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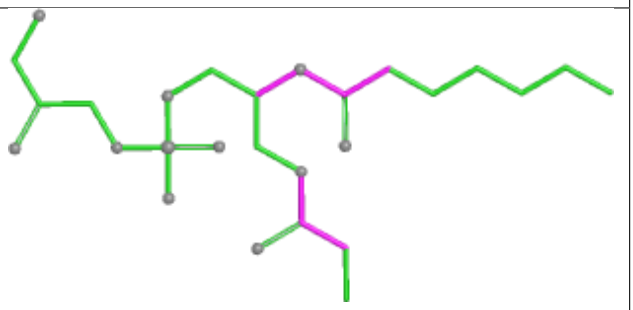


Rings

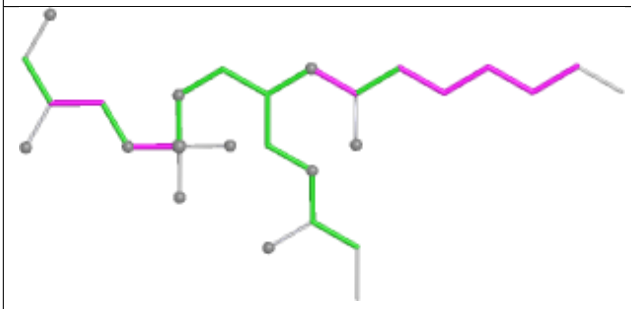
Ligand LHG a 843



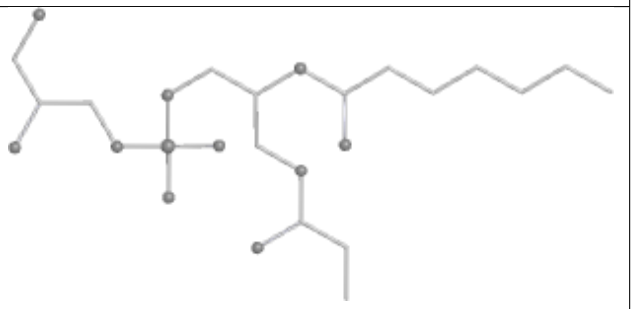
Bond lengths



Bond angles

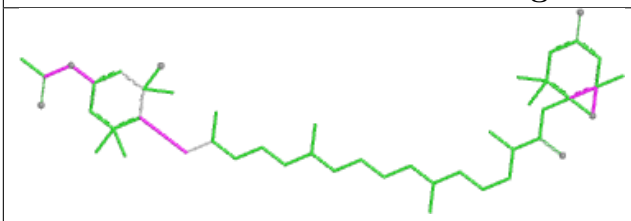


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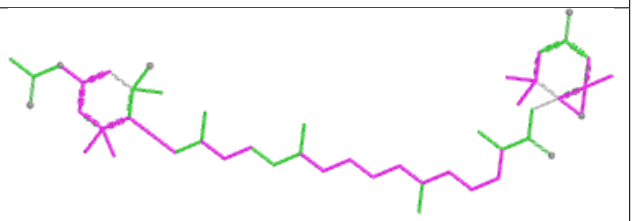


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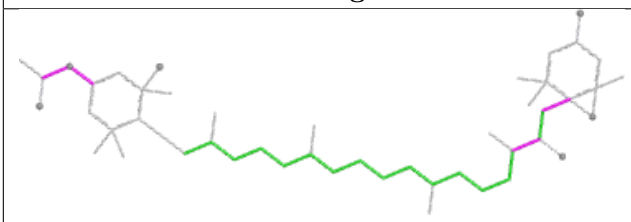
Ligand A86 T 307



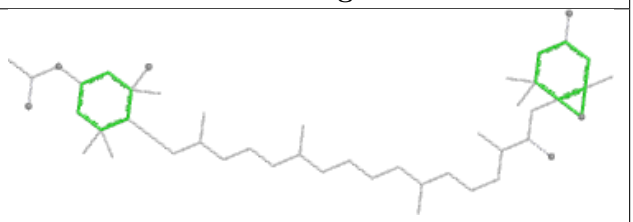
Bond lengths



Bond angles

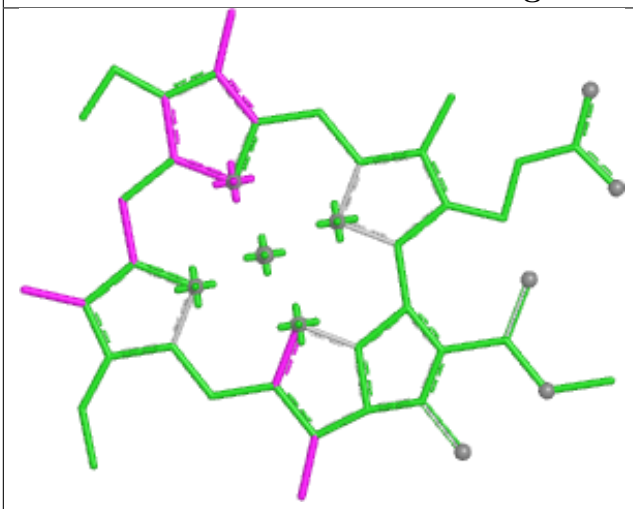


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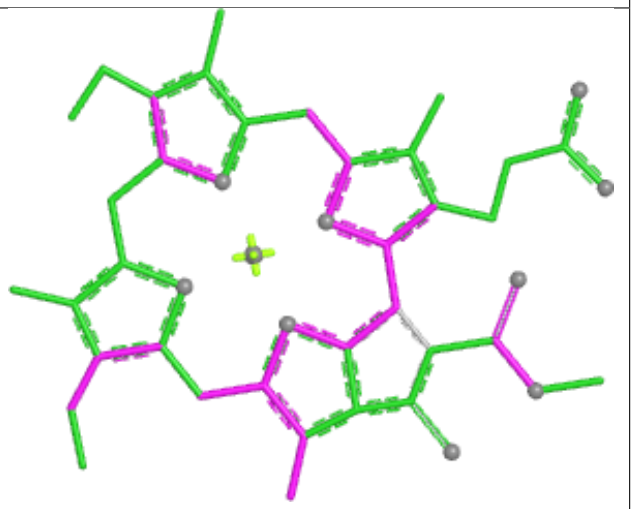


Rings

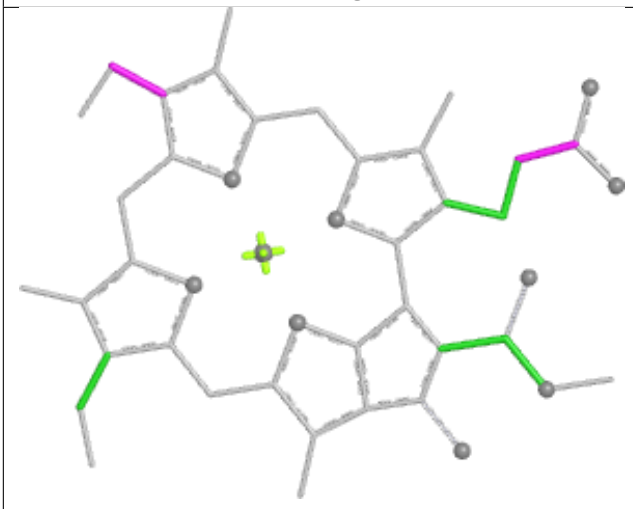
Ligand CLA R 320



Bond lengths



Bond angles

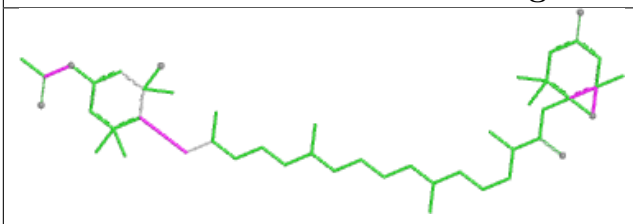


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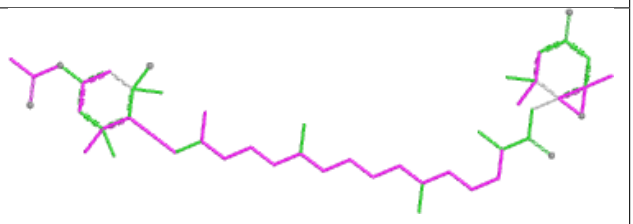


Rings

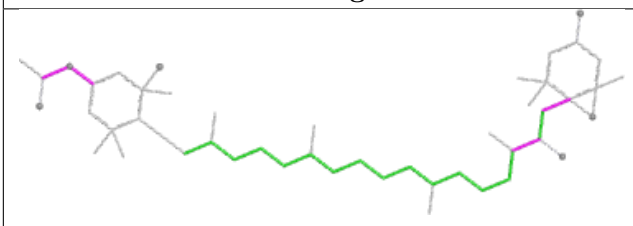
Ligand A86 N 306



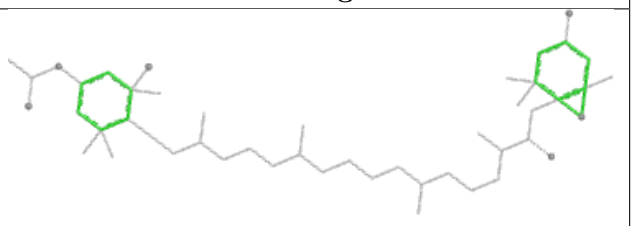
Bond lengths



Bond angles

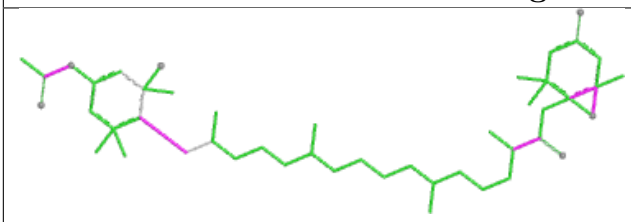


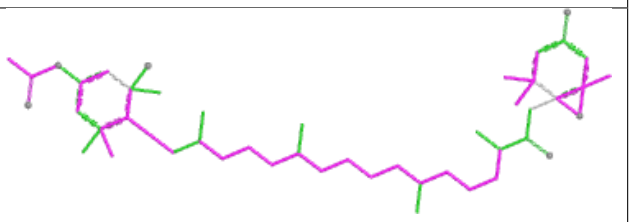
Torsions

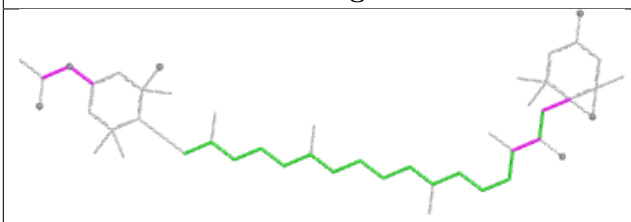


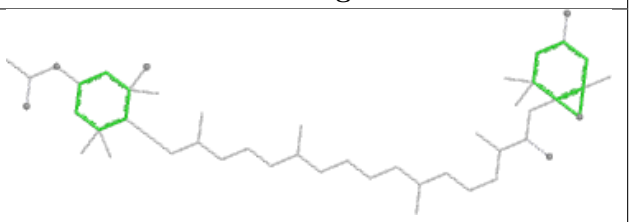
Rings

Ligand A86 U 302

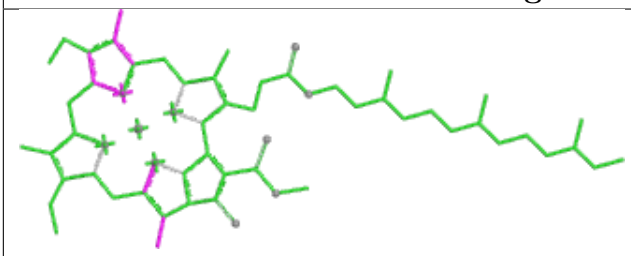

Bond lengths

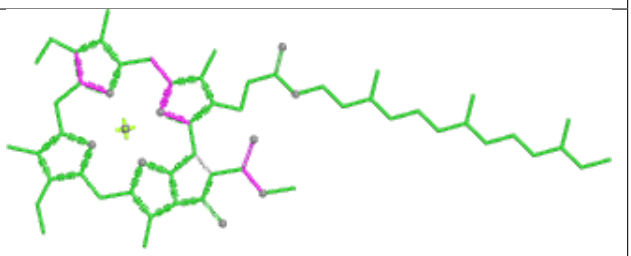

Bond angles

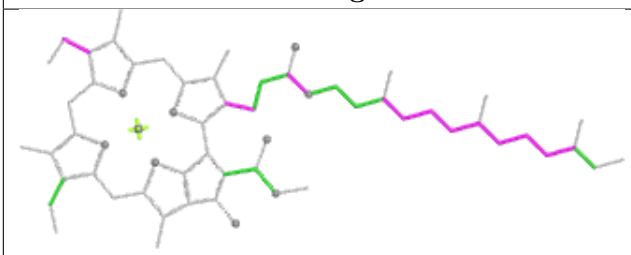

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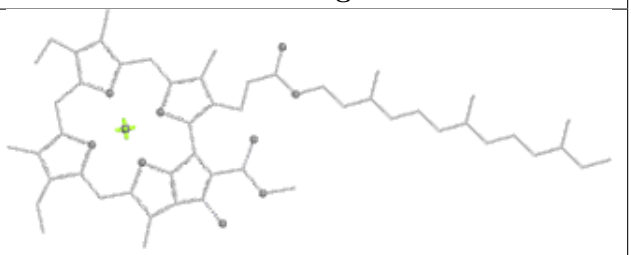

Rings

Ligand CLA C 206

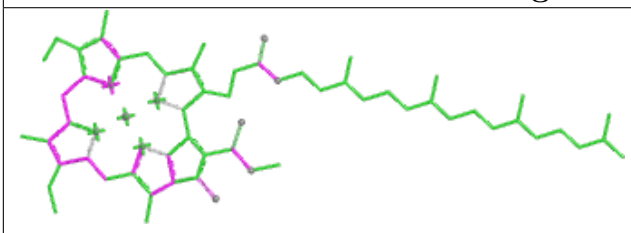

Bond lengths

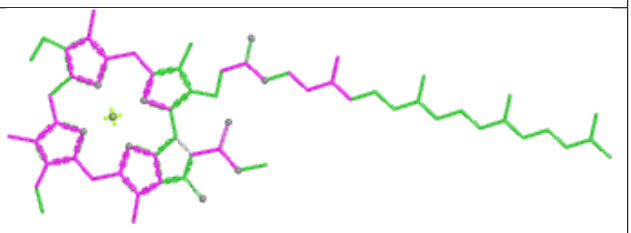

Bond angles

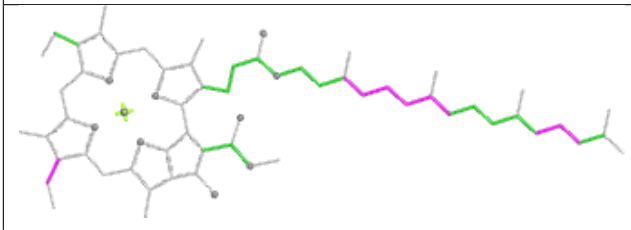

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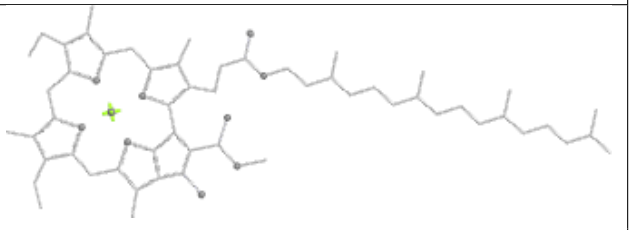

Rings

Ligand CLA f 803

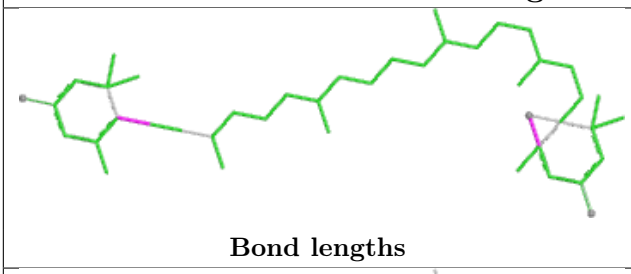

Bond lengths


Bond angles

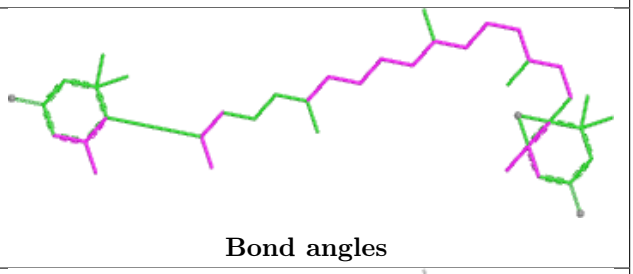

Torsions


Rings

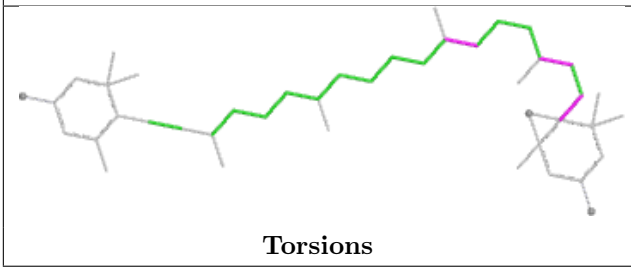
Ligand DD6 E 303



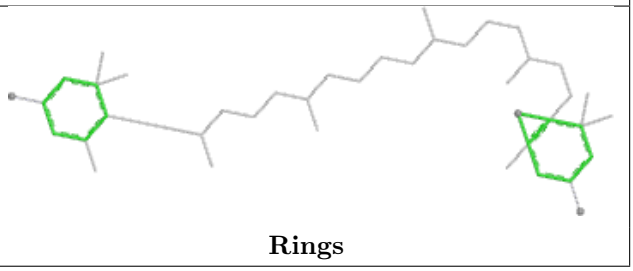
Bond lengths



Bond angles

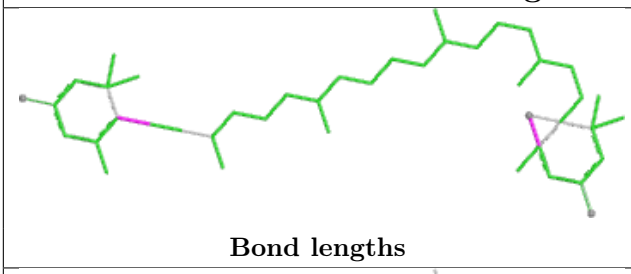


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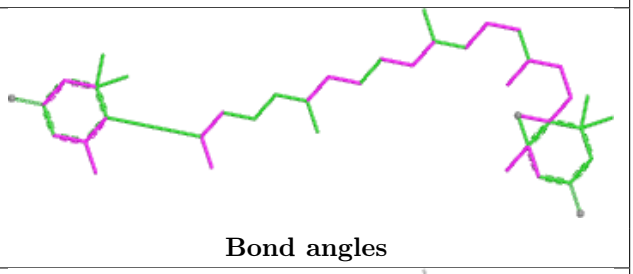


Rings

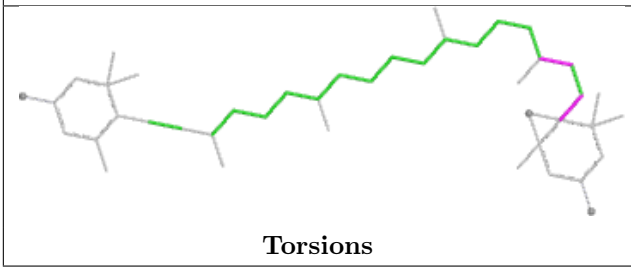
Ligand DD6 G 303



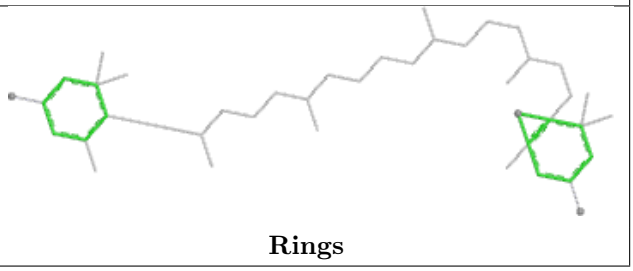
Bond lengths



Bond angles

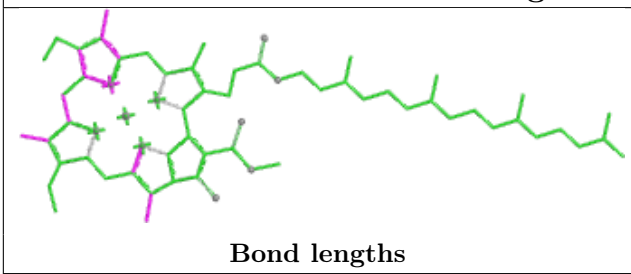


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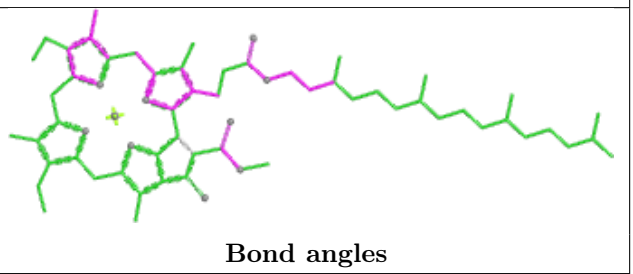


Rings

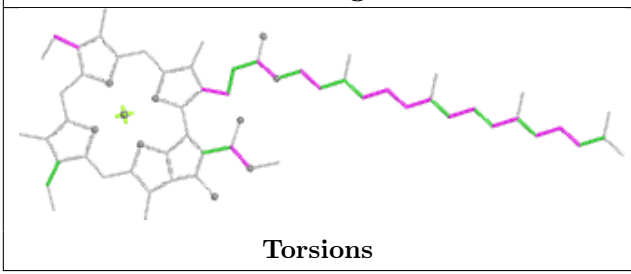
Ligand CLA S 310



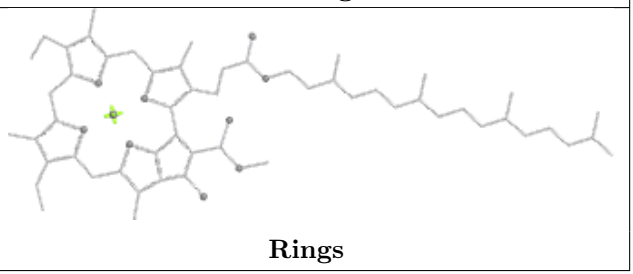
Bond lengths



Bond angles

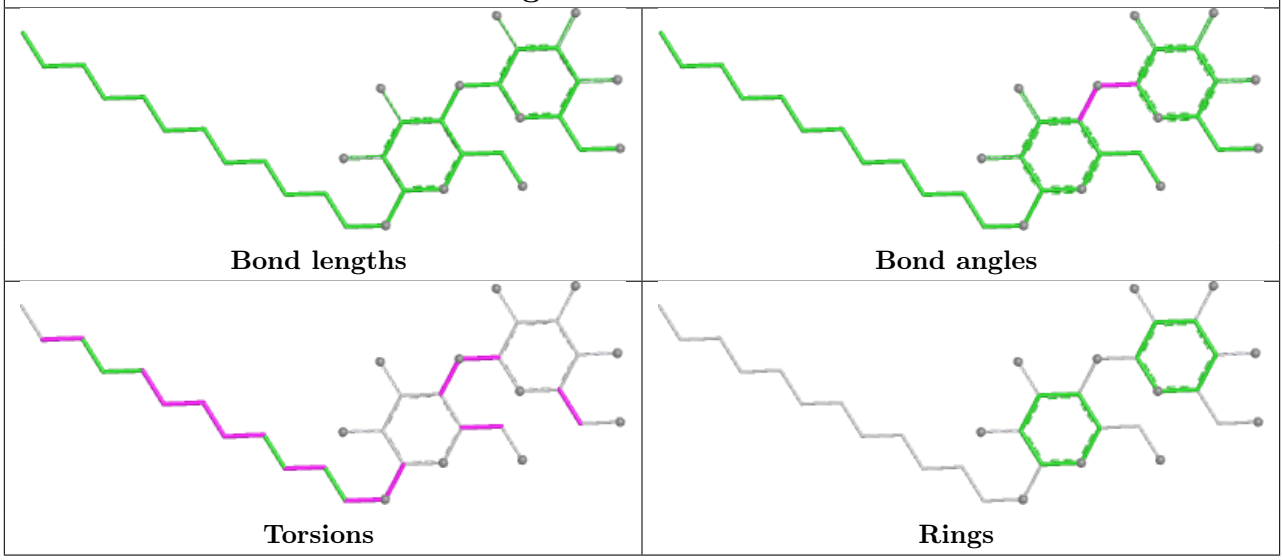


Torsions

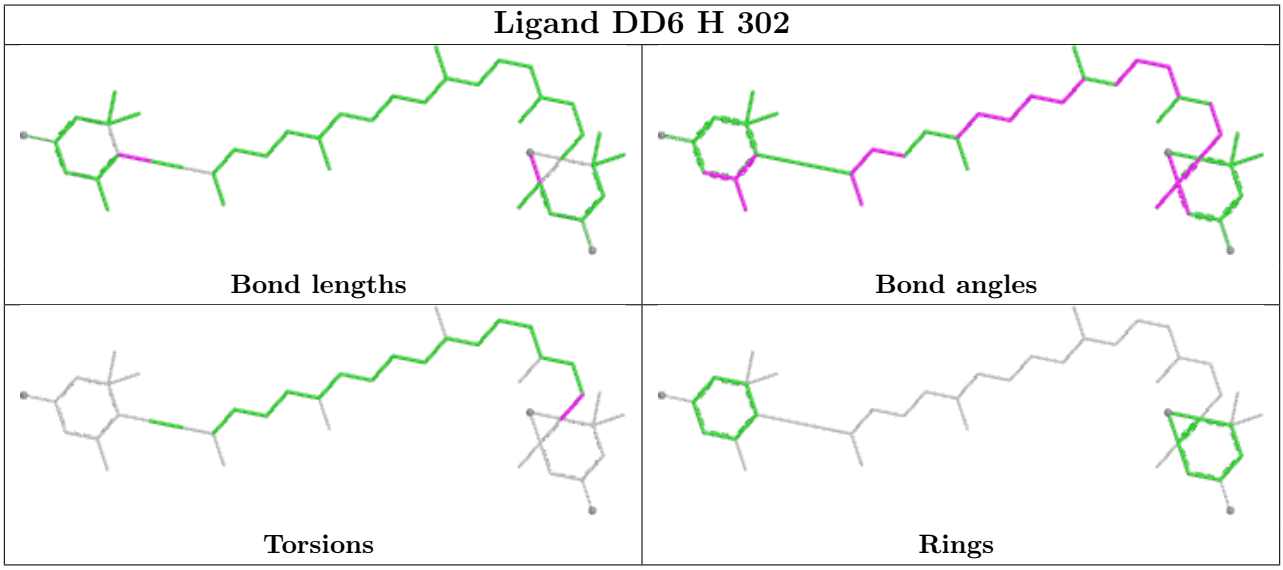


Rings

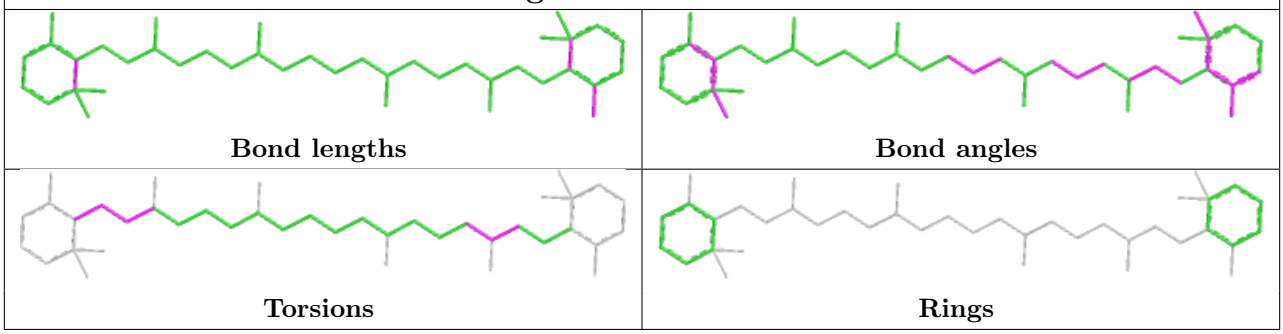
Ligand LMT B 313



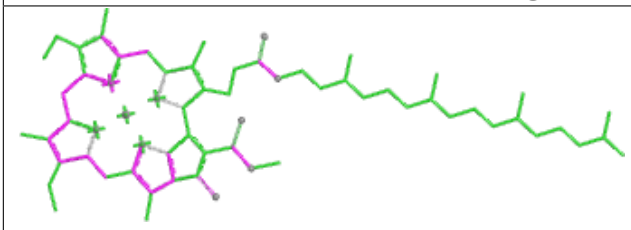
Ligand DD6 H 302



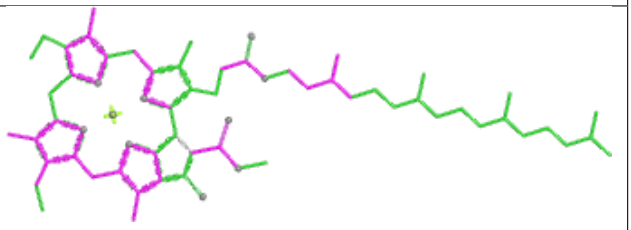
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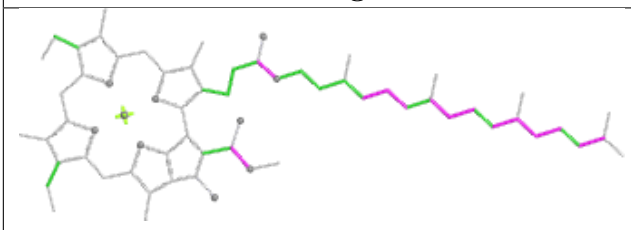
Ligand CLA C 207



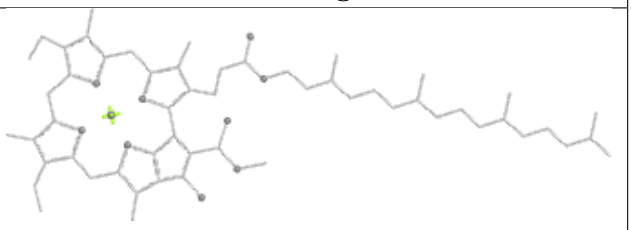
Bond lengths



Bond angles

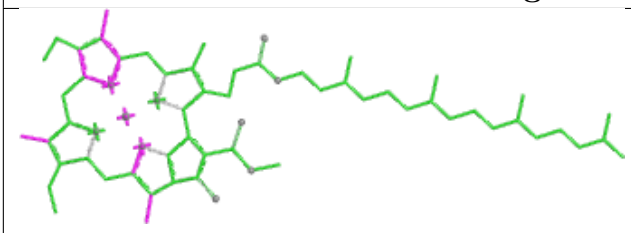


Torsions

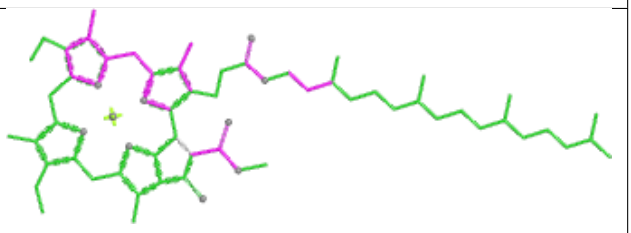


Rings

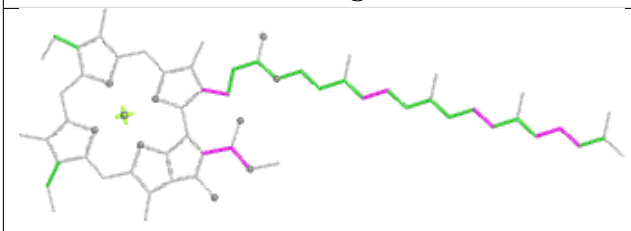
Ligand CLA R 321



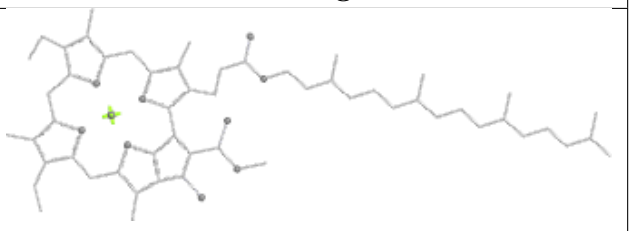
Bond lengths



Bond angles

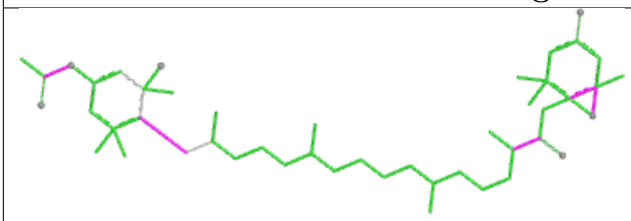


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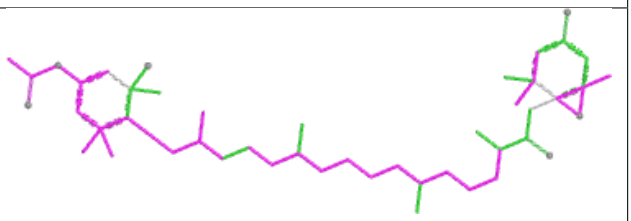


Rings

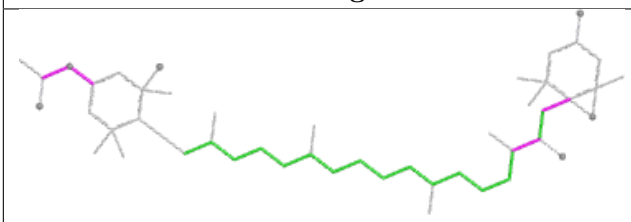
Ligand A86 L 319



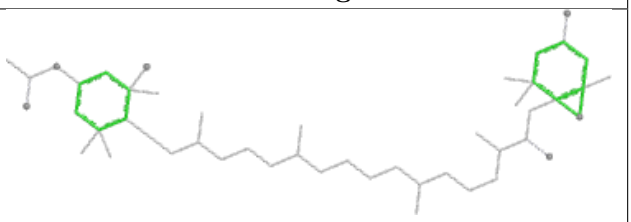
Bond lengths



Bond angles

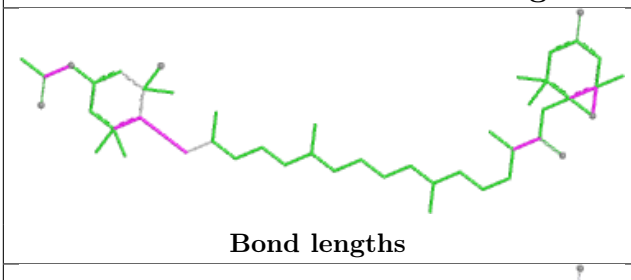


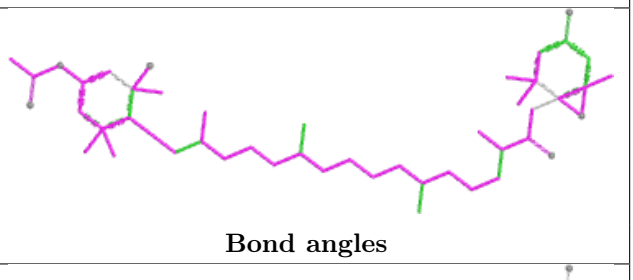
Torsions

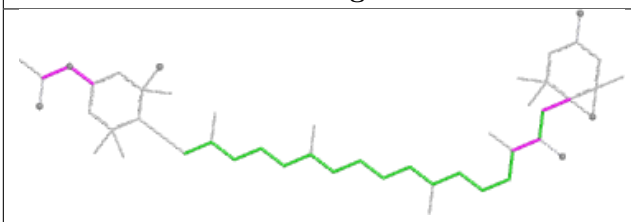


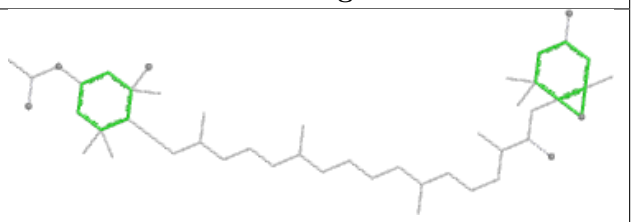
Rings

Ligand A86 X 301

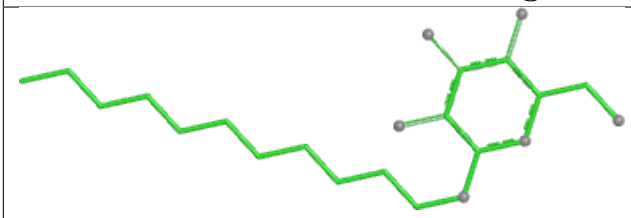

Bond lengths

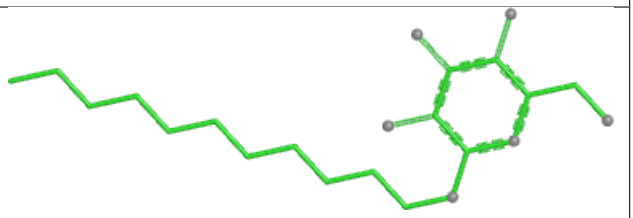

Bond angles

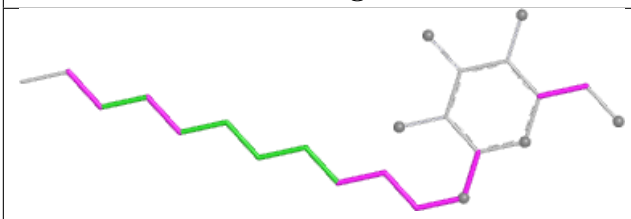

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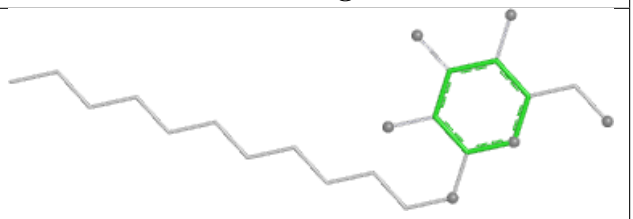

Rings

Ligand LMT P 320

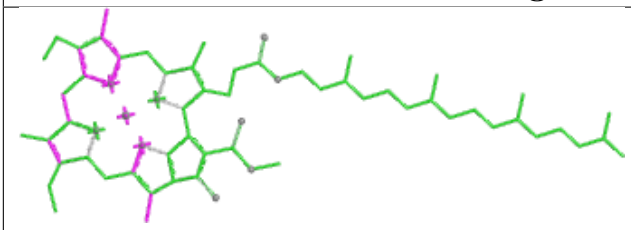

Bond lengths

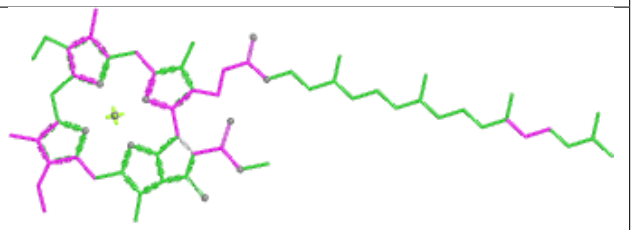

Bond angles

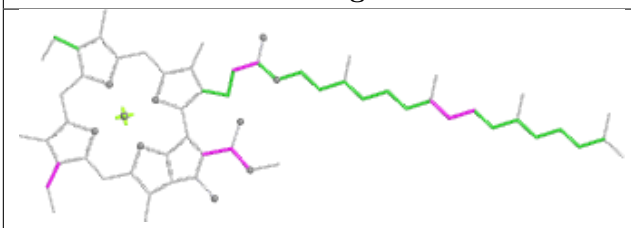

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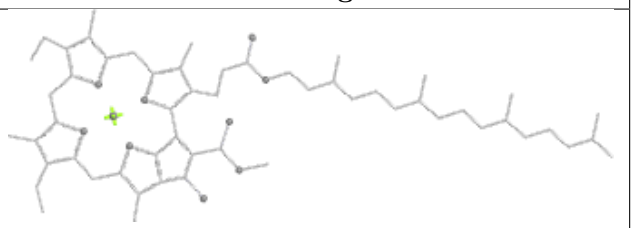

Rings

Ligand CLA a 824

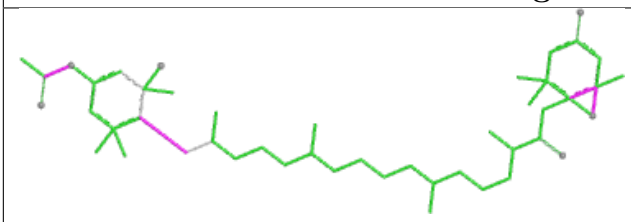

Bond lengths


Bond angles

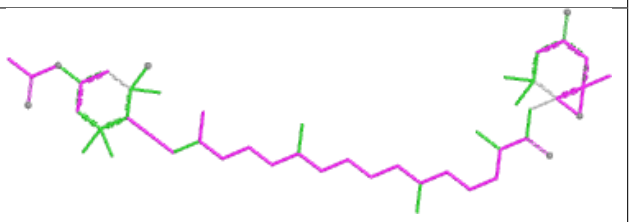

Torsions


Rings

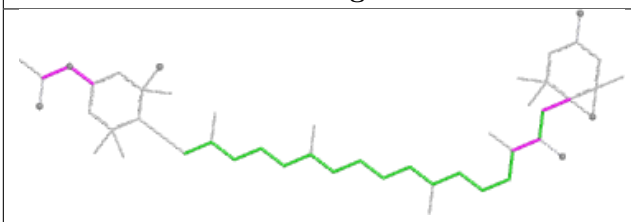
Ligand A86 S 305



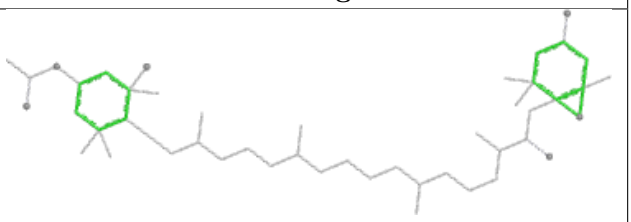
Bond lengths



Bond angles

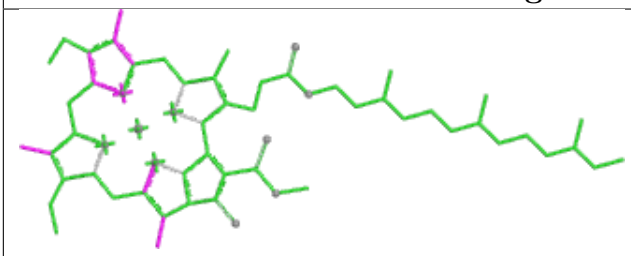


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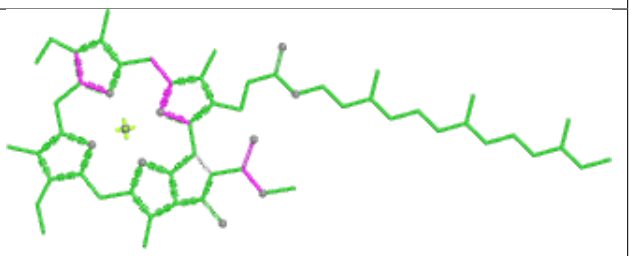


Rings

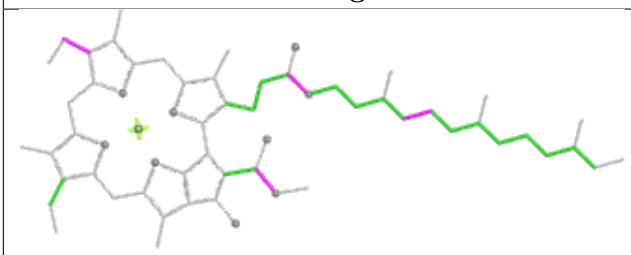
Ligand CLA P 308



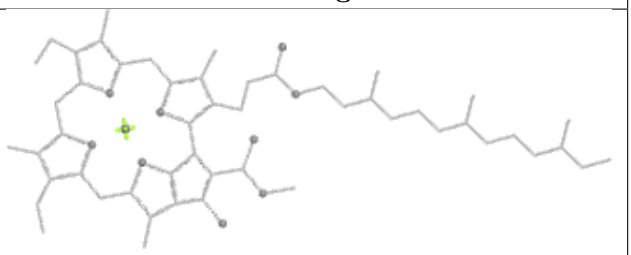
Bond lengths



Bond angles

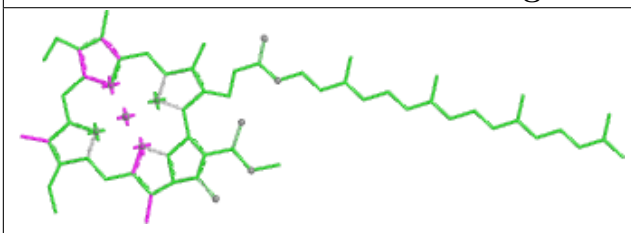


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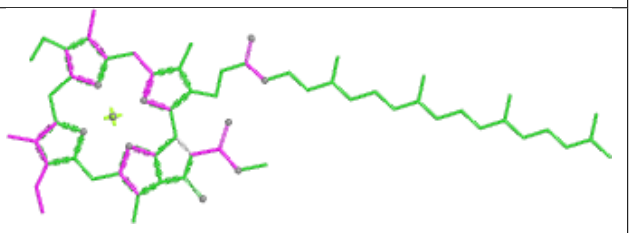


Rings

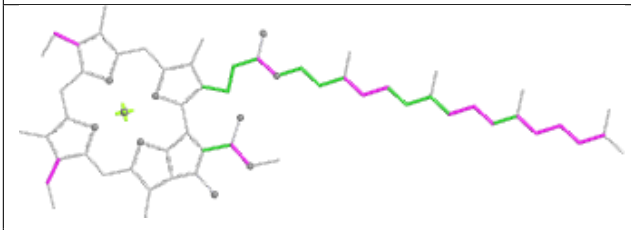
Ligand CLA U 310



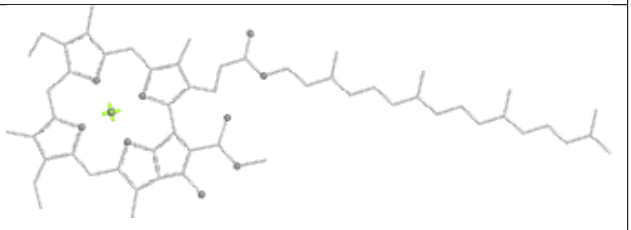
Bond lengths



Bond angles

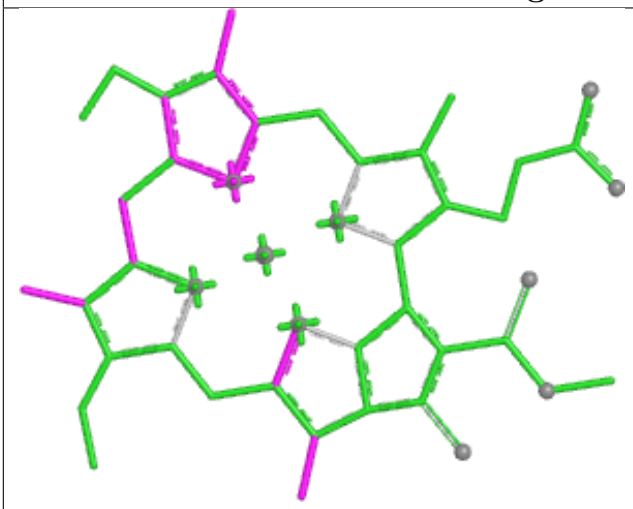


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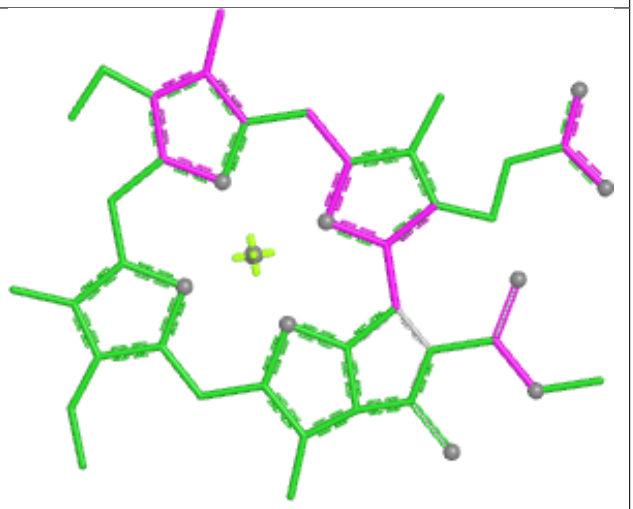


Rings

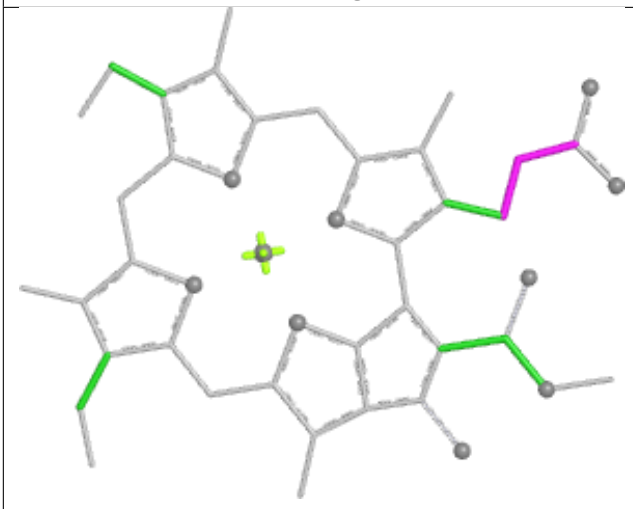
Ligand CLA b 807



Bond lengths



Bond angles

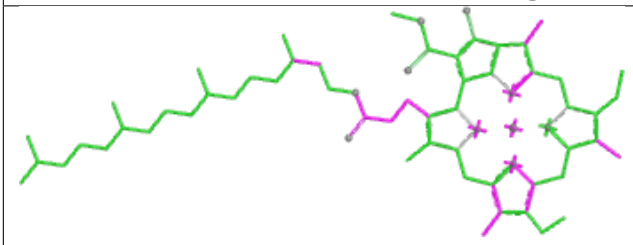


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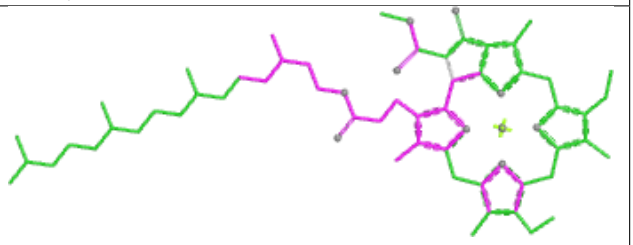


Rings

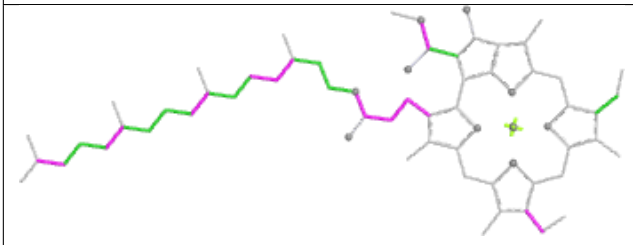
Ligand CLA Q 310



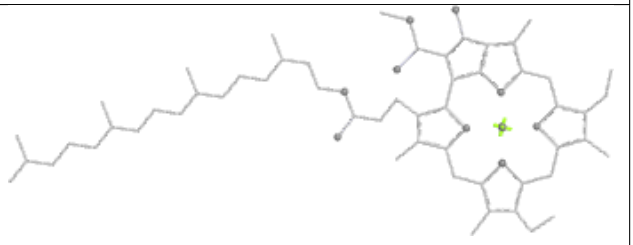
Bond lengths



Bond angles

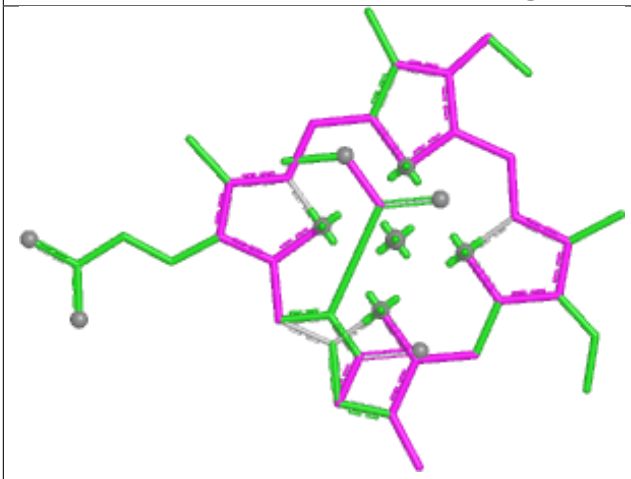


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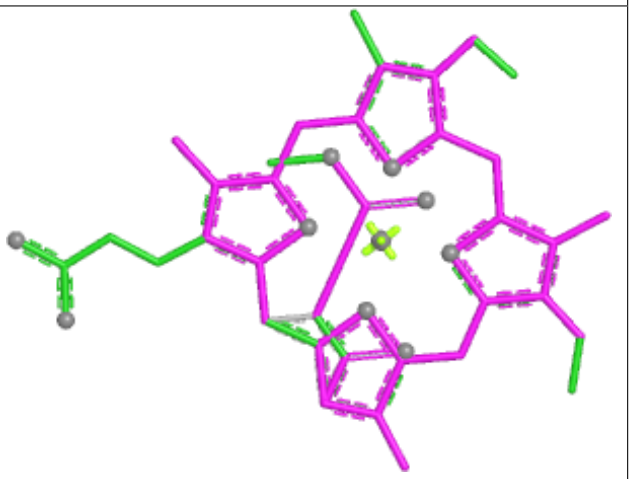


Rings

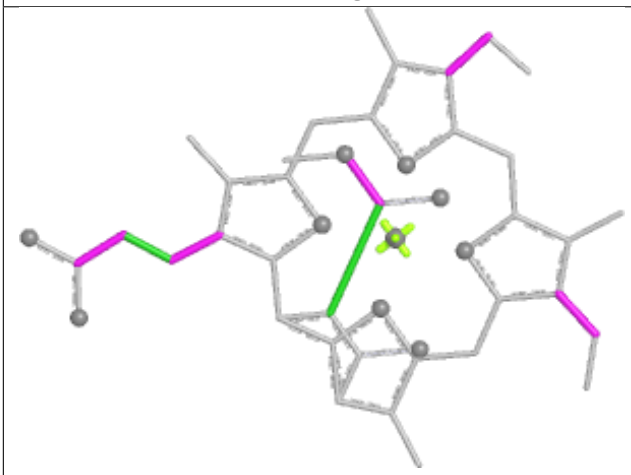
Ligand KC1 M 318



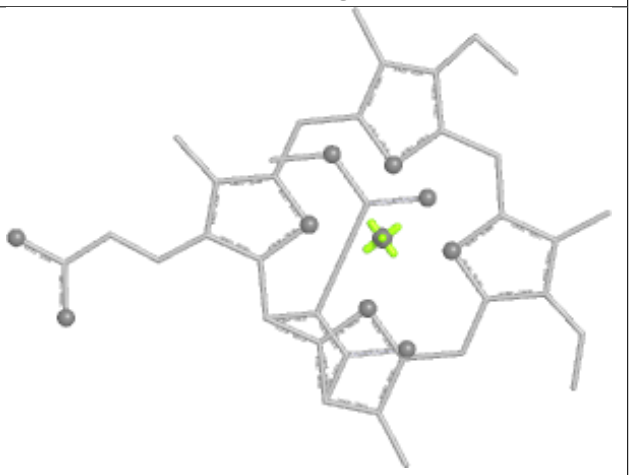
Bond lengths



Bond angles

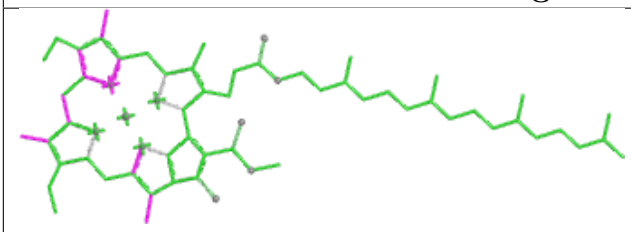


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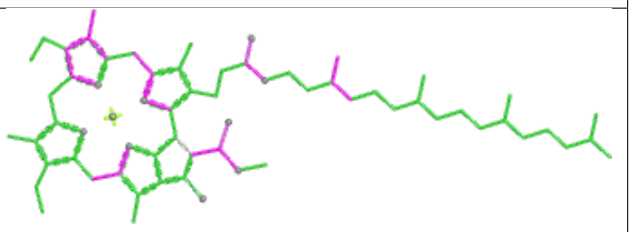


Rings

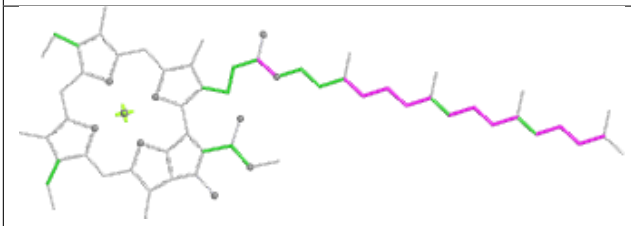
Ligand CLA l 201



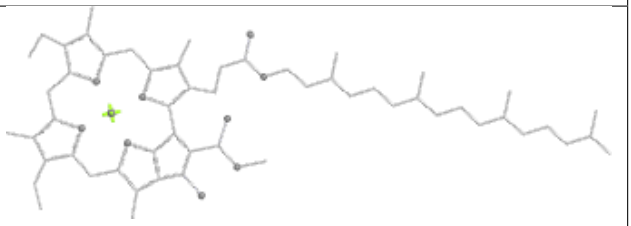
Bond lengths



Bond angles

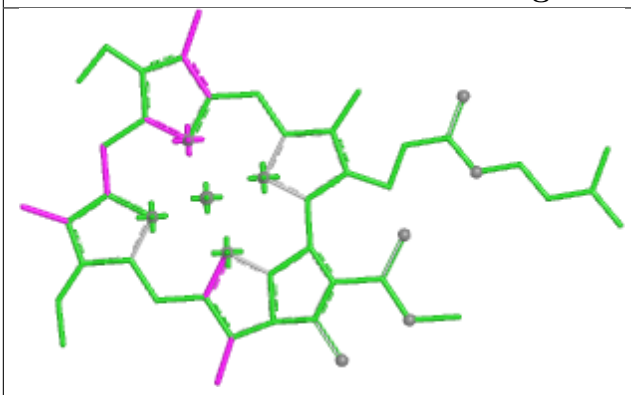


Torsions

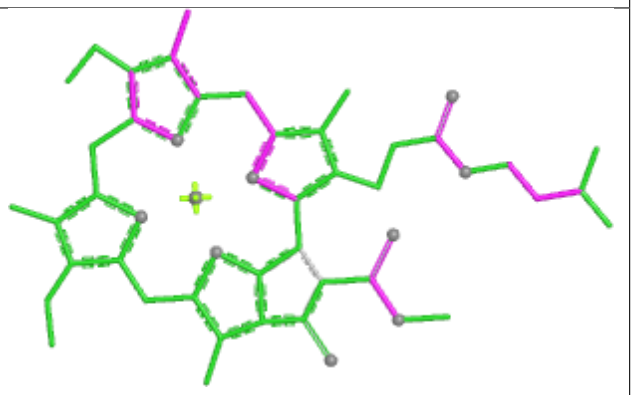


Rings

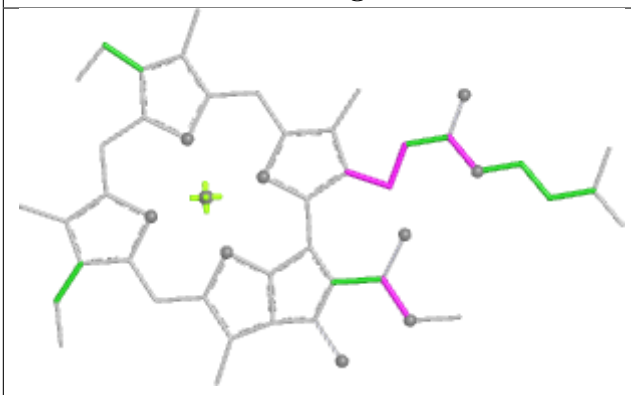
Ligand CLA l 206



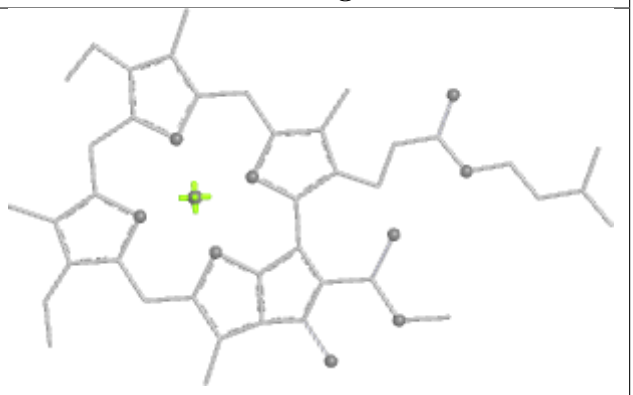
Bond lengths



Bond angles

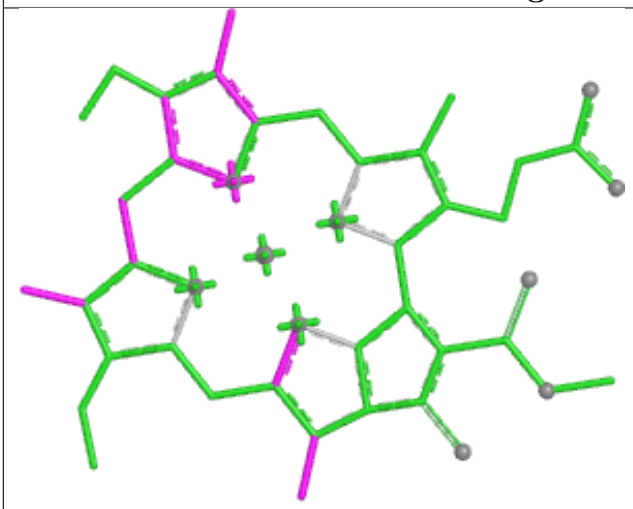


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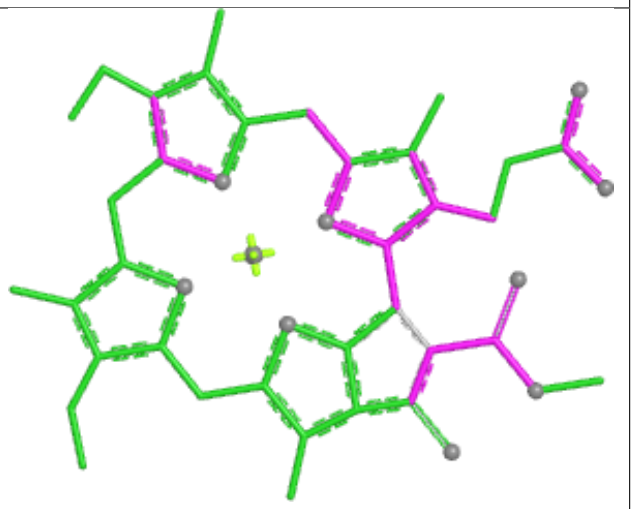


Rings

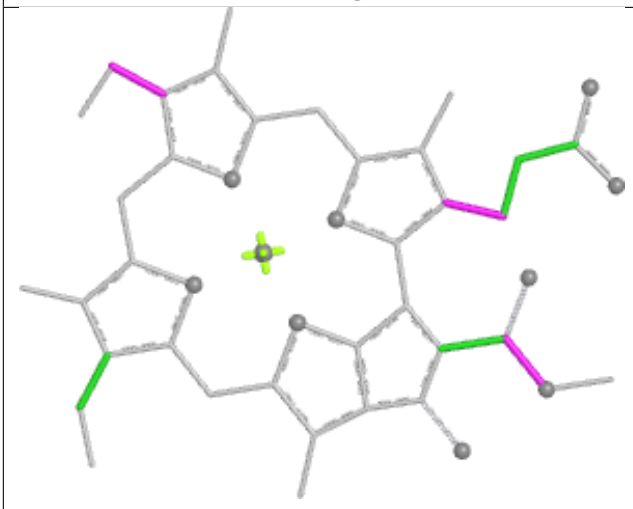
Ligand CLA b 835



Bond lengths



Bond angles

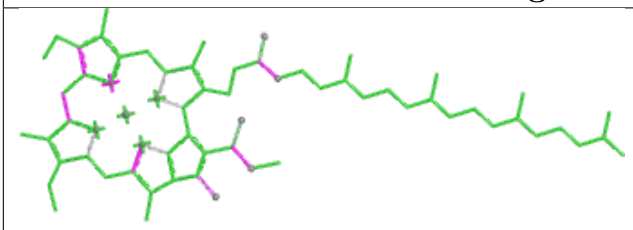


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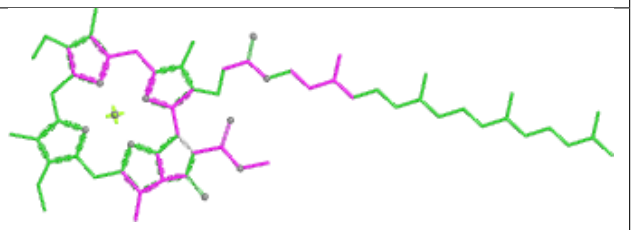


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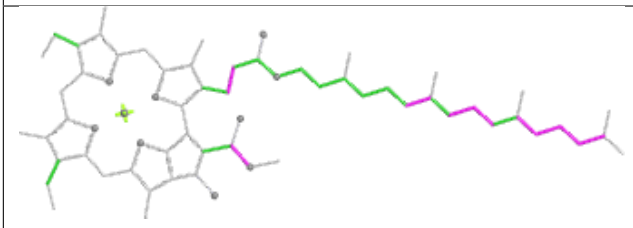
Ligand CLA a 802



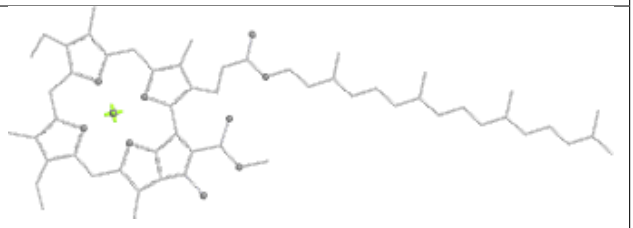
Bond lengths



Bond angles

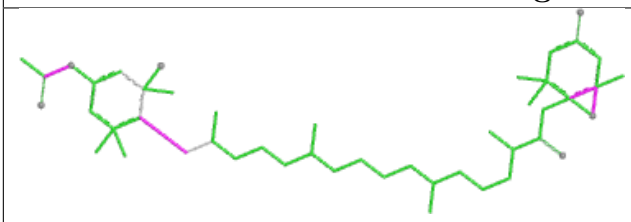


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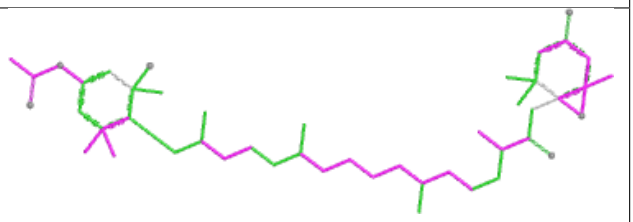


Rings

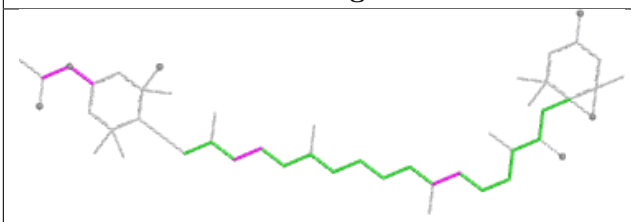
Ligand A86 J 305



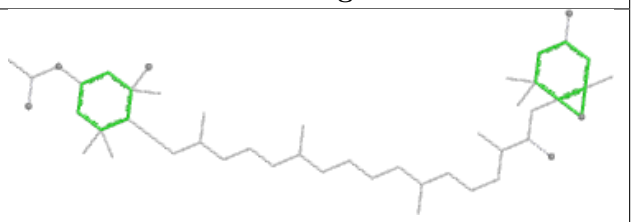
Bond lengths



Bond angles

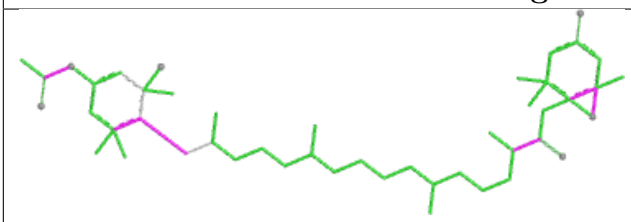


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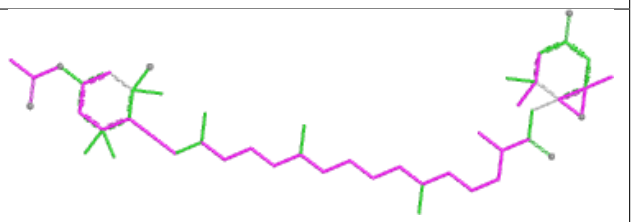


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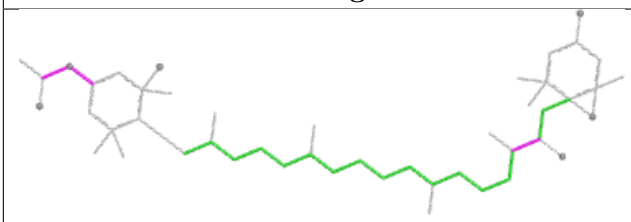
Ligand A86 P 304



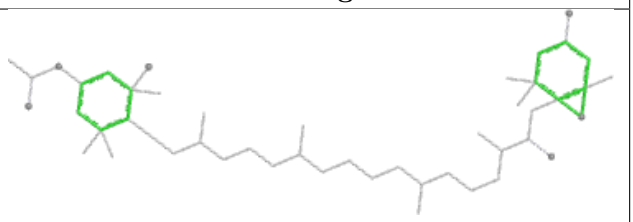
Bond lengths



Bond angles

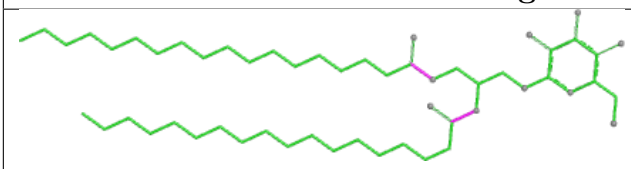


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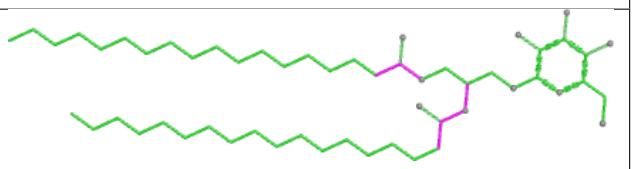


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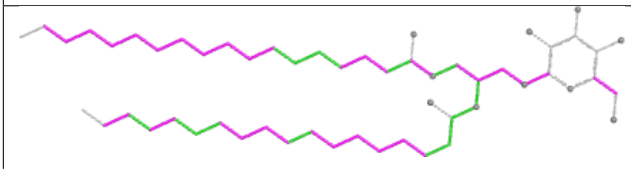
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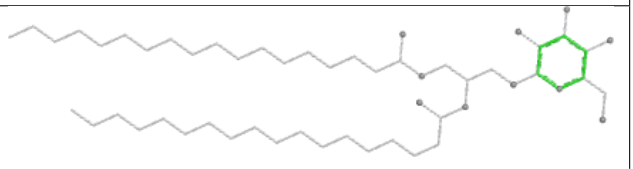
Bond lengths



Bond angles

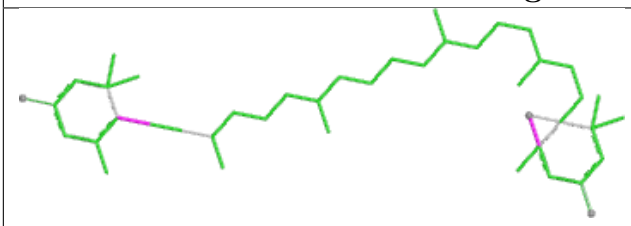


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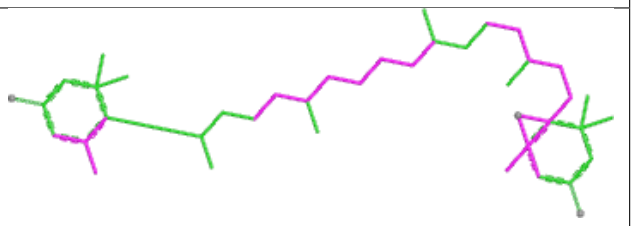


Rings

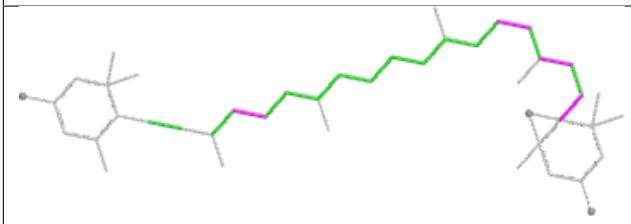
Ligand DD6 A 301



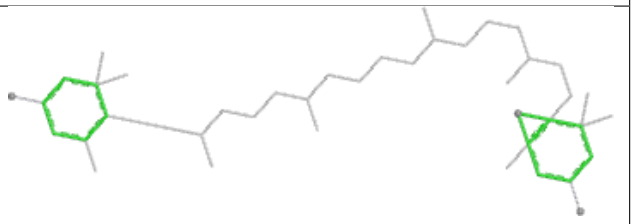
Bond lengths



Bond angles

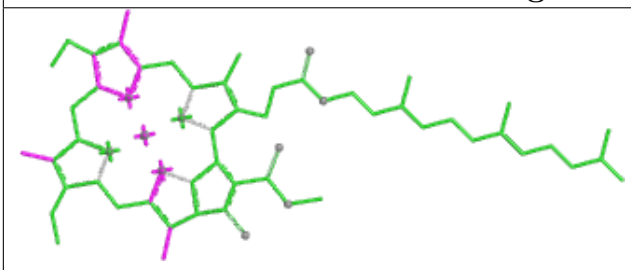


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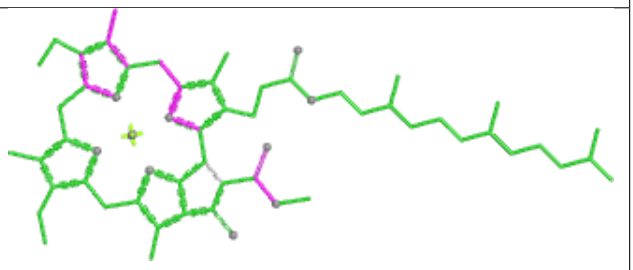


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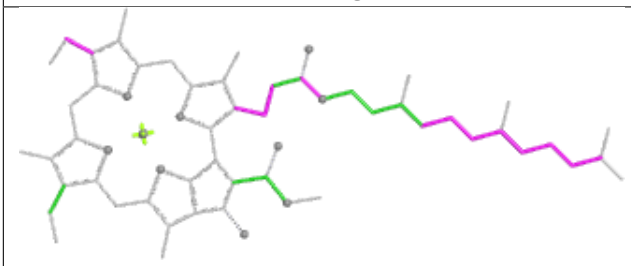
Ligand CLA b 820



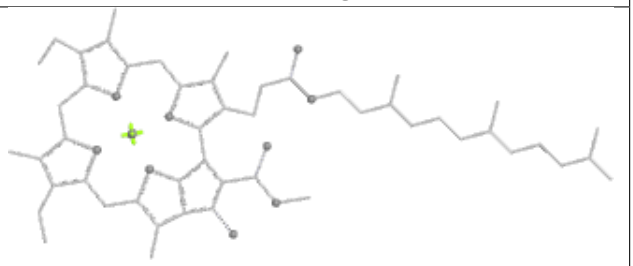
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Bond angles

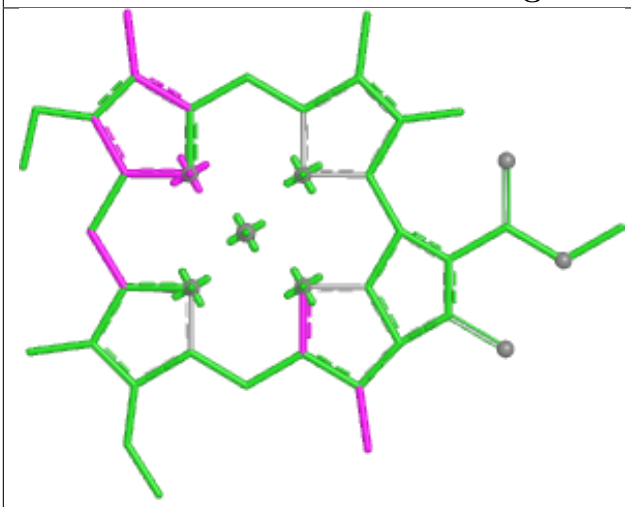


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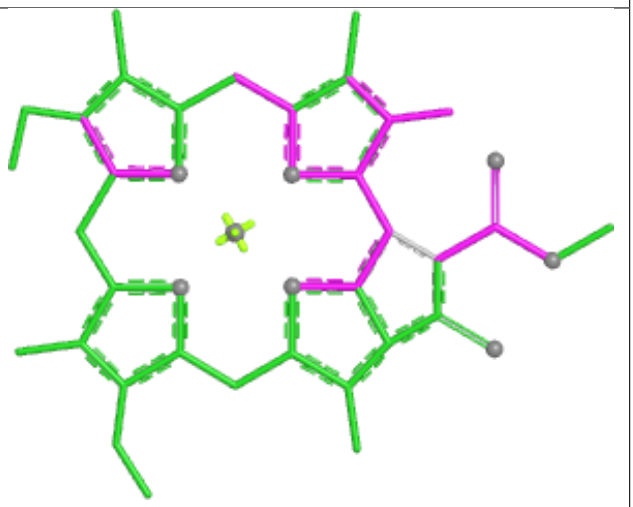


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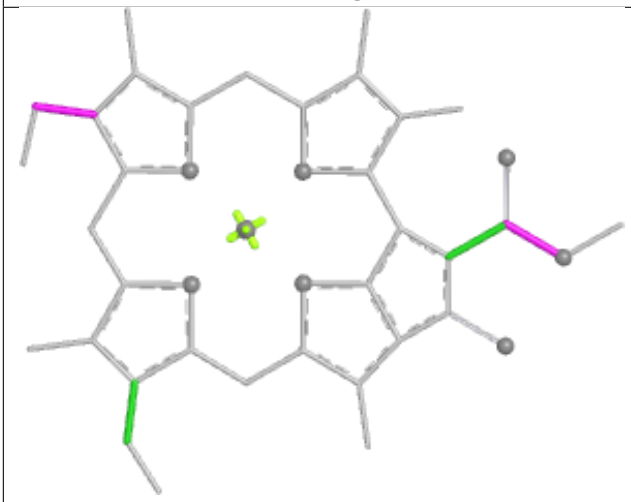
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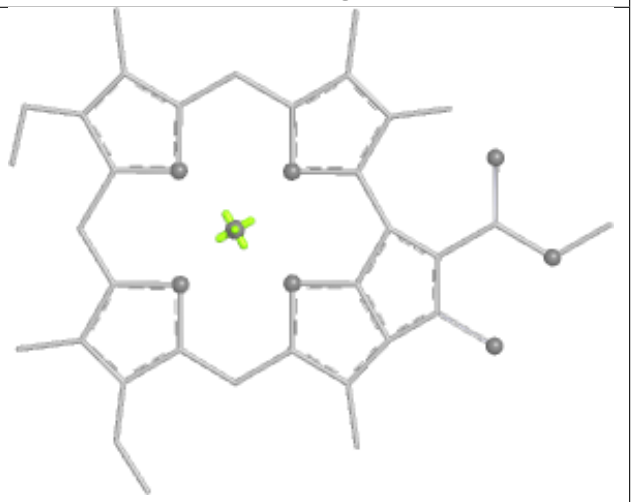
Bond lengths



Bond angles

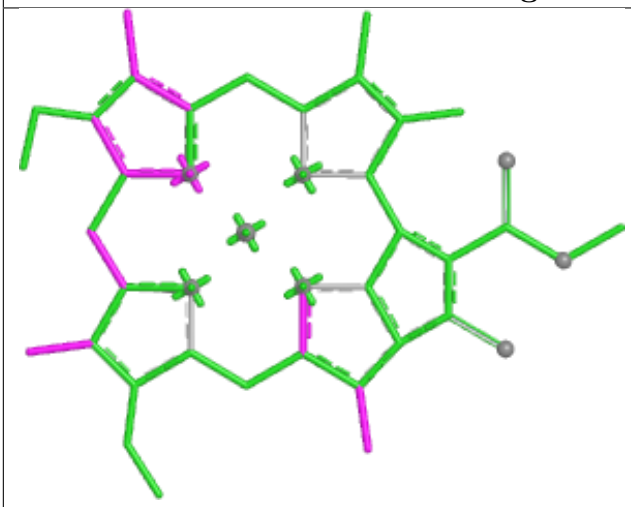


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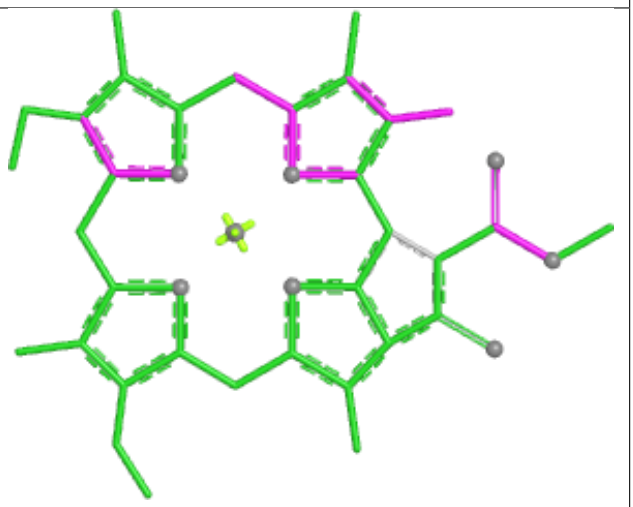


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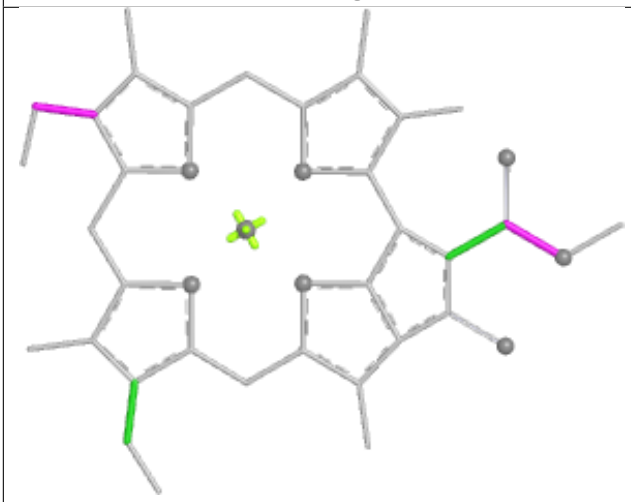
Ligand CLA M 314



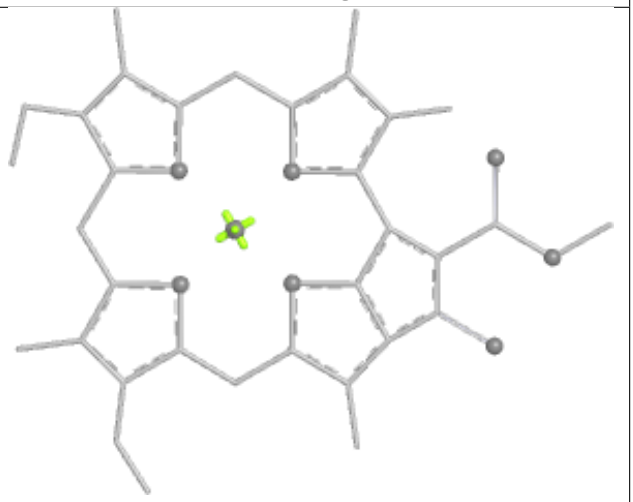
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Bond angles

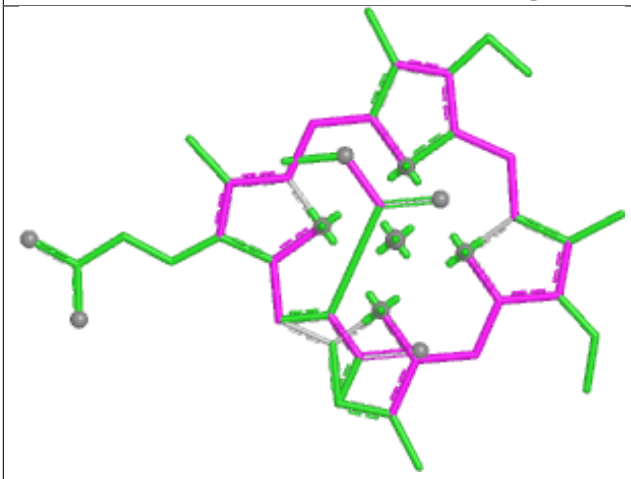


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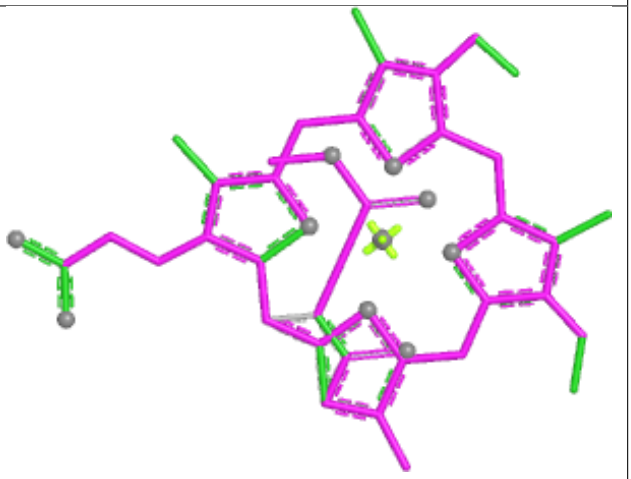


Rings

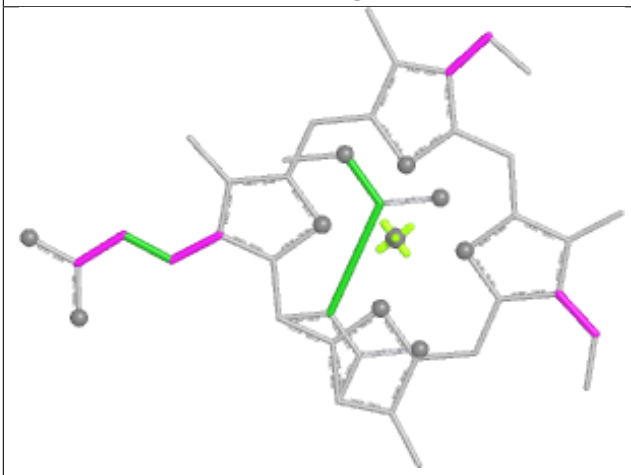
Ligand KC1 N 314



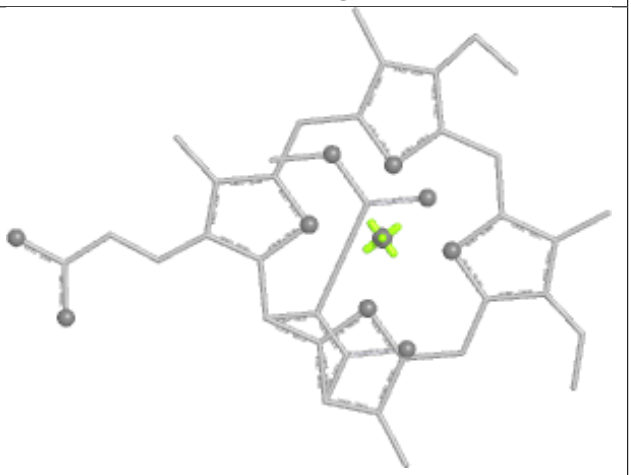
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Bond angles

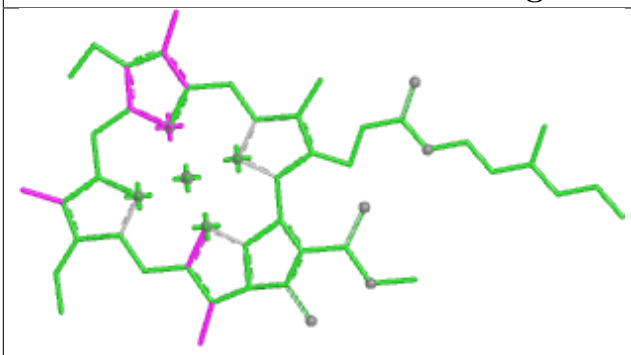


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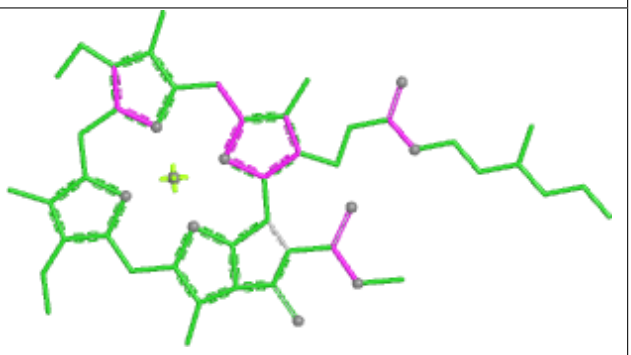


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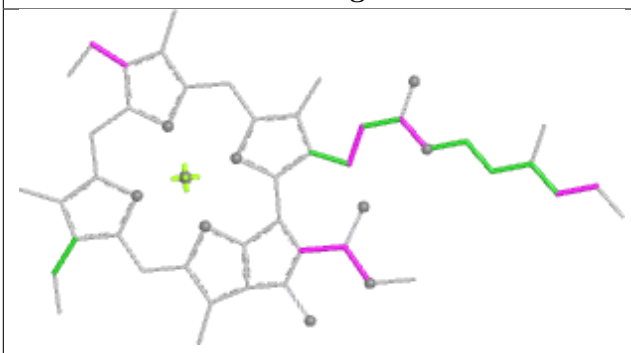
Ligand CLA F 311



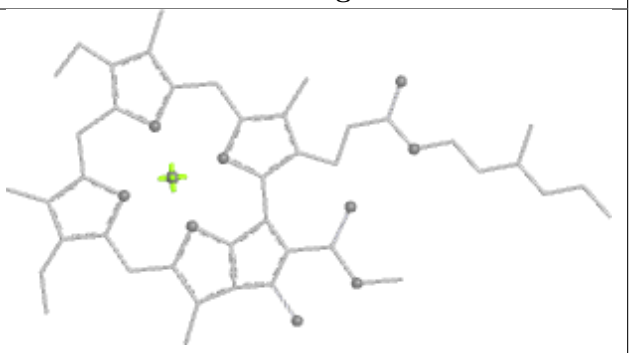
Bond lengths



Bond angles

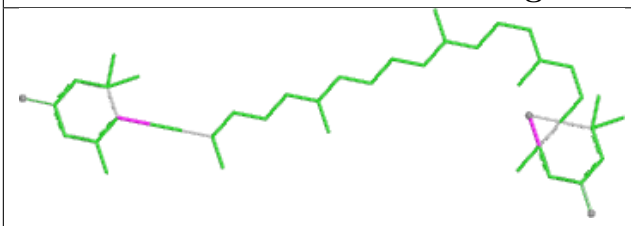


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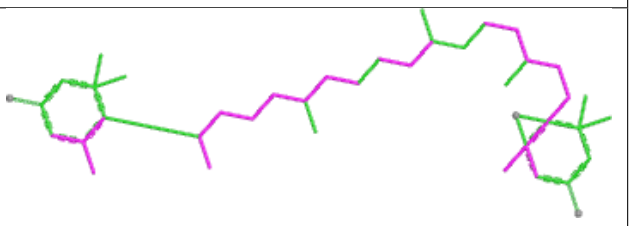


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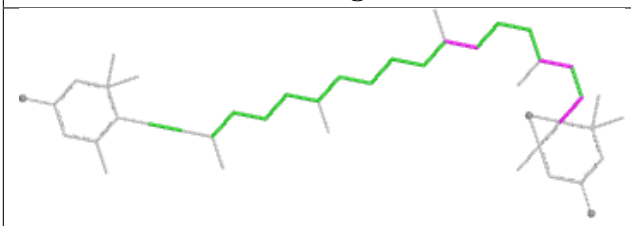
Ligand DD6 C 201



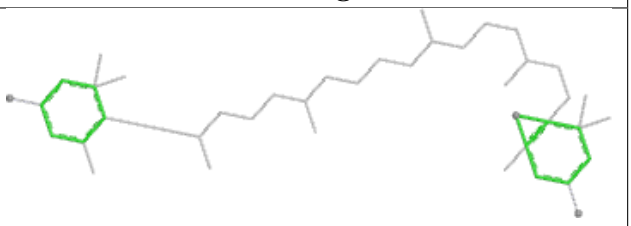
Bond lengths



Bond angles

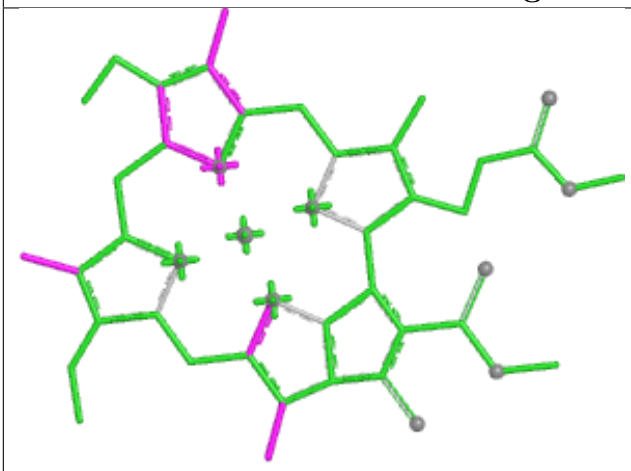


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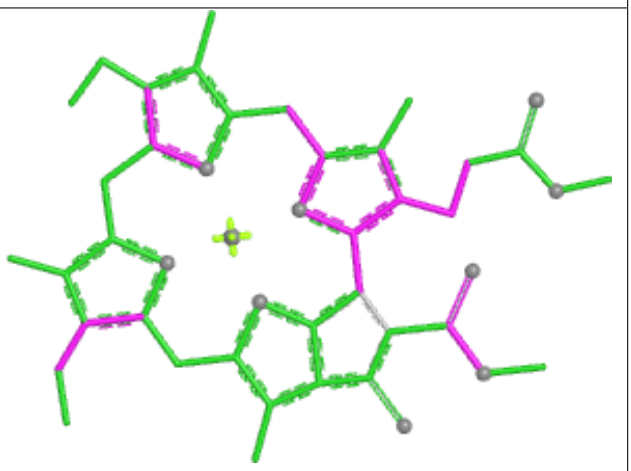


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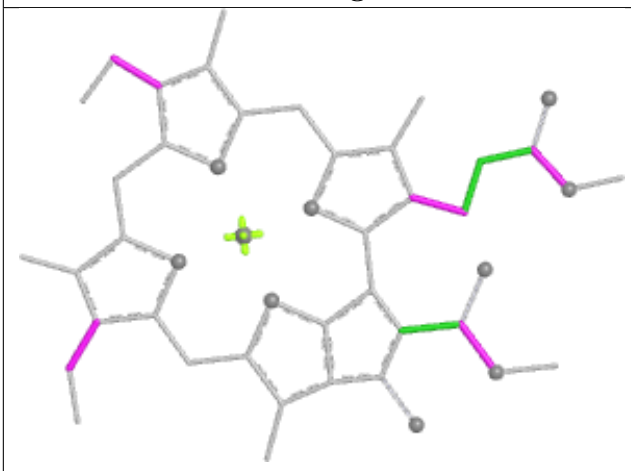
Ligand CLA R 314



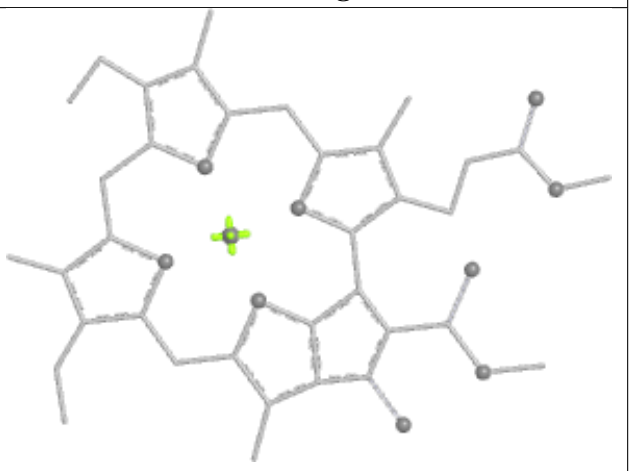
Bond lengths



Bond angles



Torsions

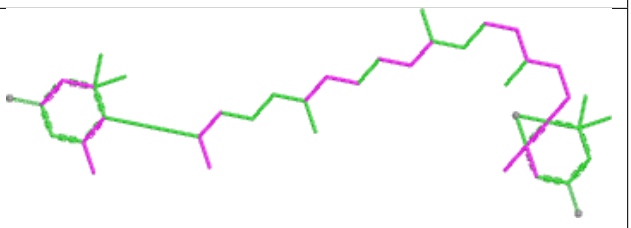


Rings

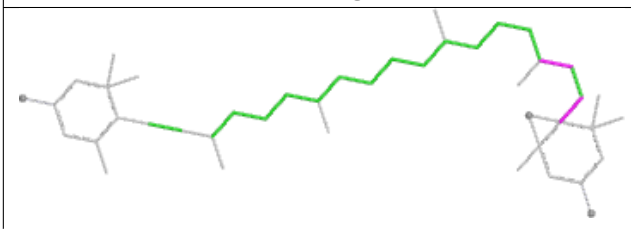
Ligand DD6 E 304



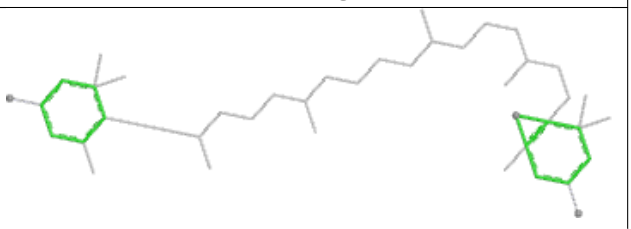
Bond lengths



Bond angles

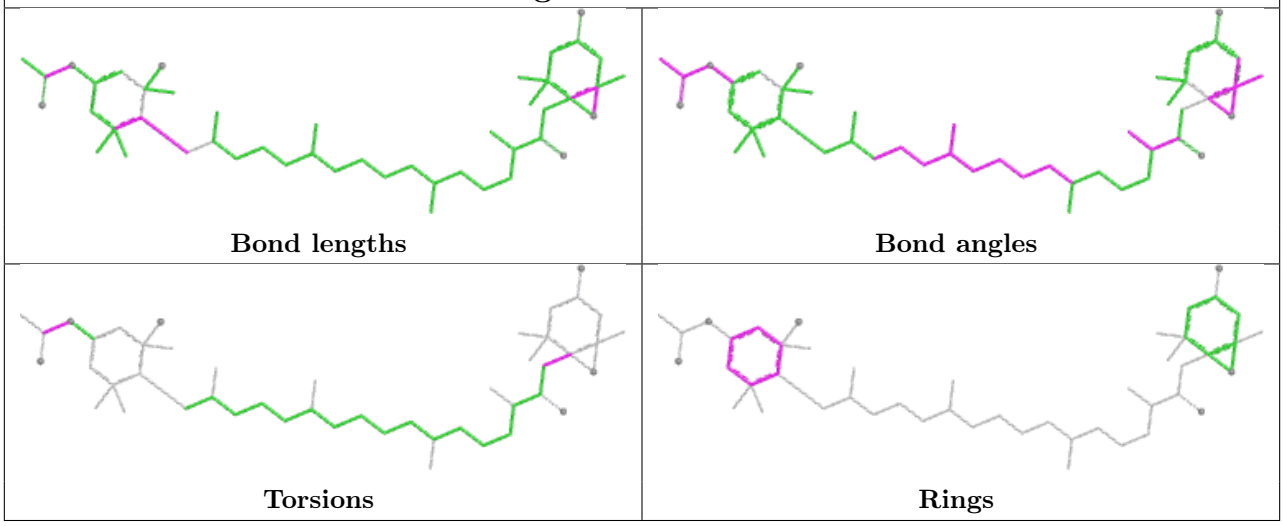


Torsions

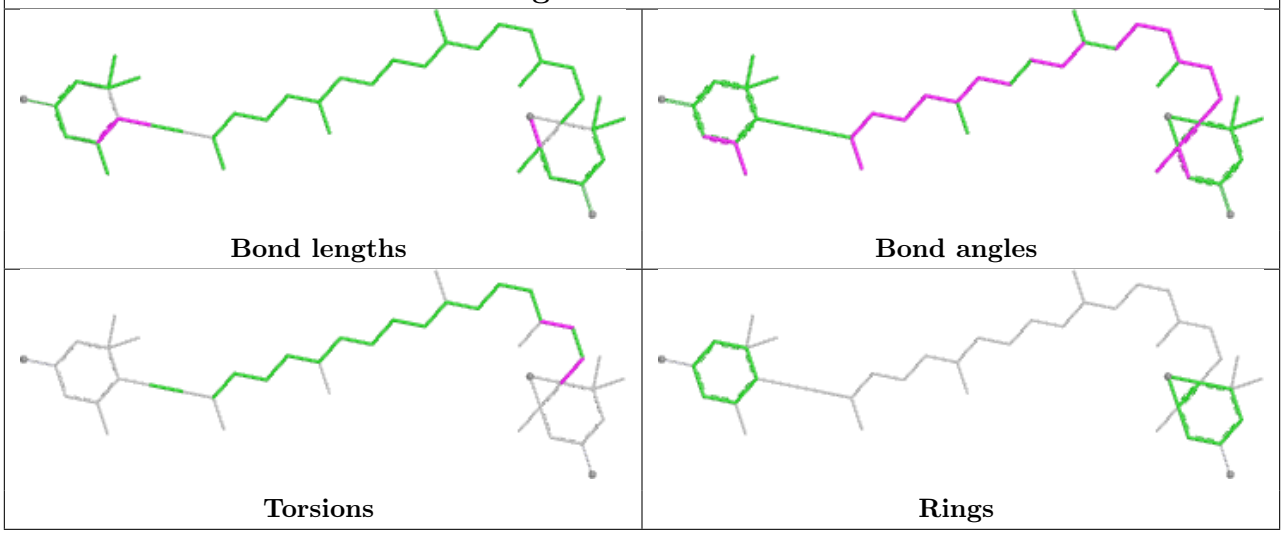


Rings

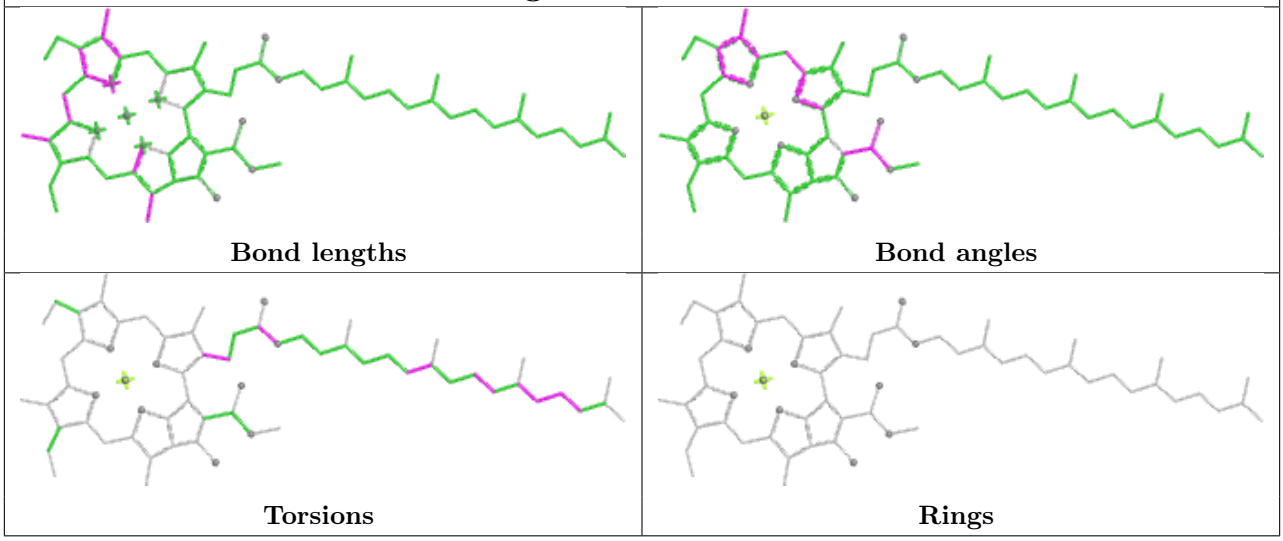
Ligand A86 h 202



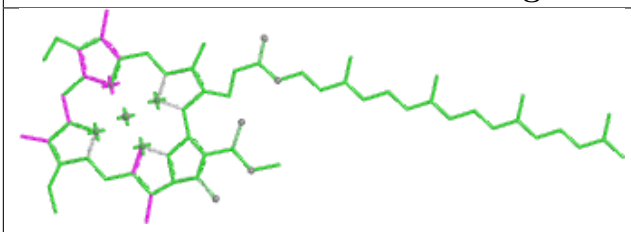
Ligand DD6 I 303



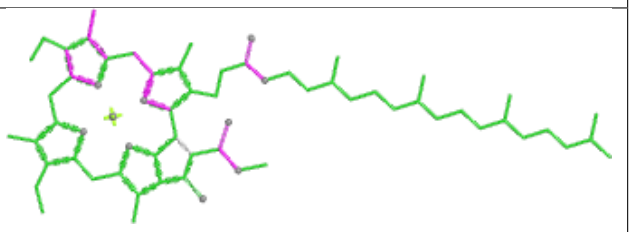
Ligand CLA H 311



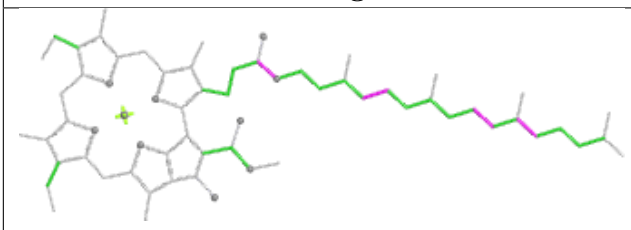
Ligand CLA K 312



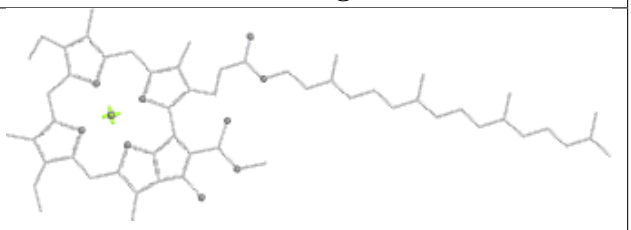
Bond lengths



Bond angles

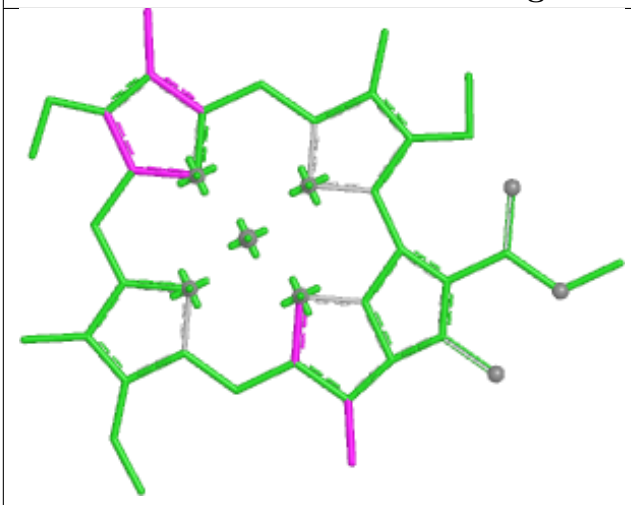


Torsions

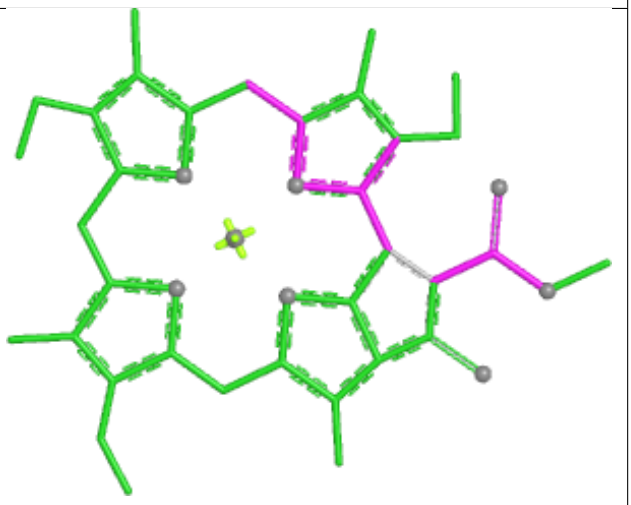


Rings

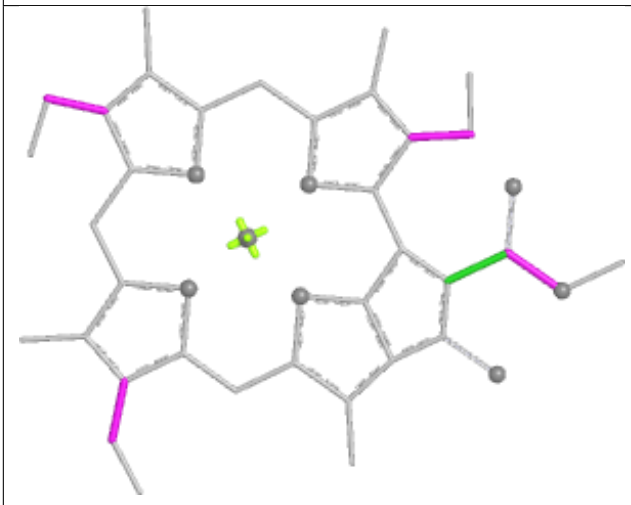
Ligand CLA S 318



Bond lengths



Bond angles

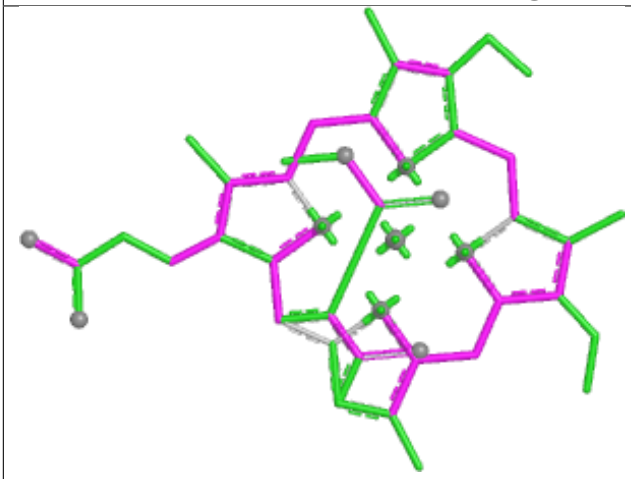


Torsions

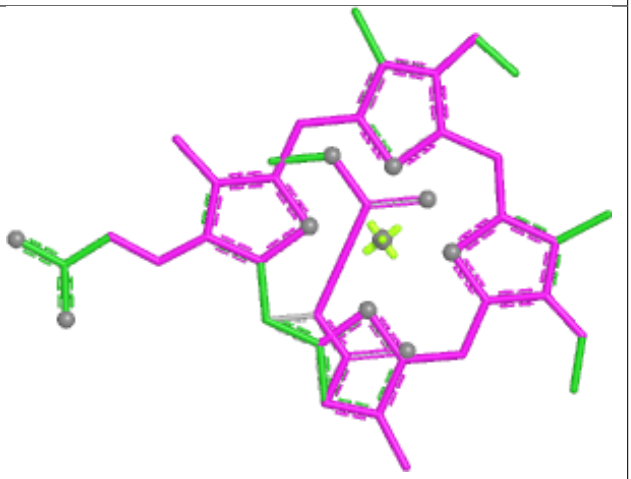


Rings

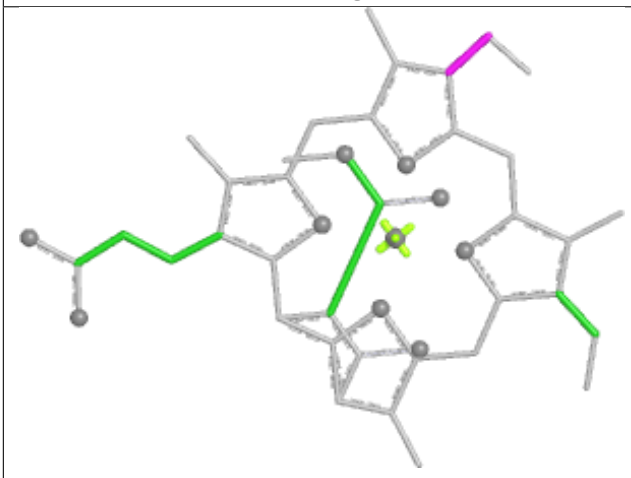
Ligand KC1 O 315



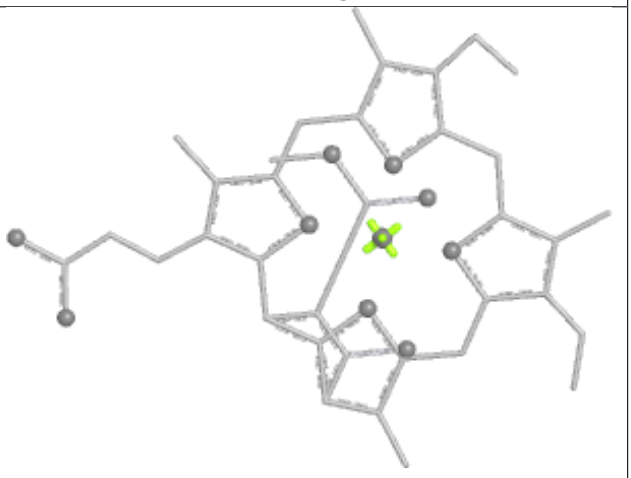
Bond lengths



Bond angles

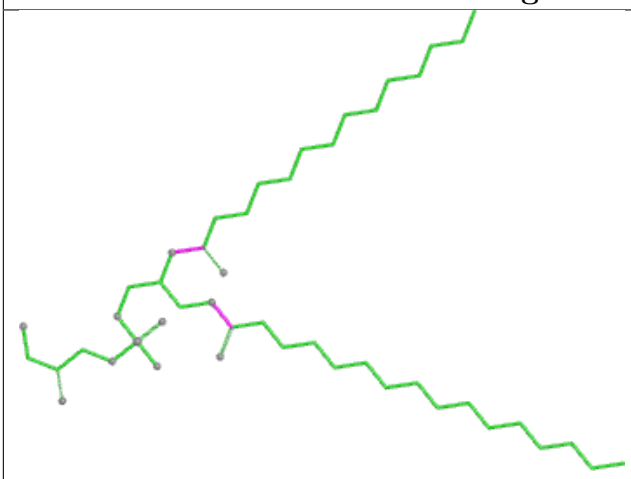


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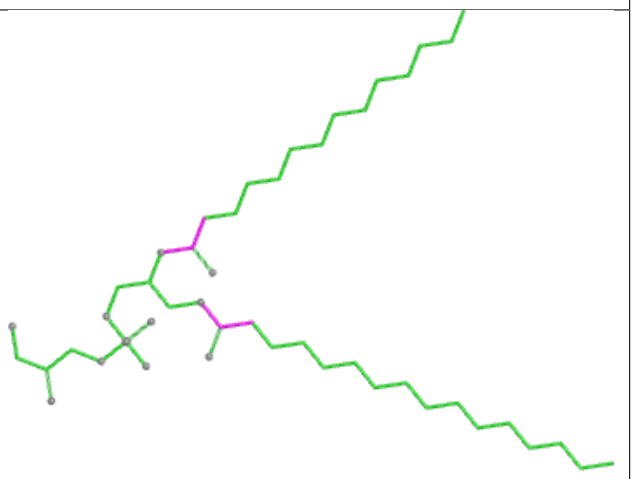


Rings

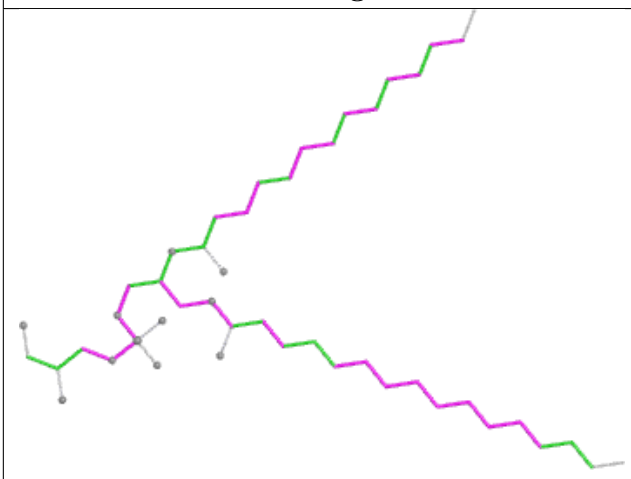
Ligand LHG G 321



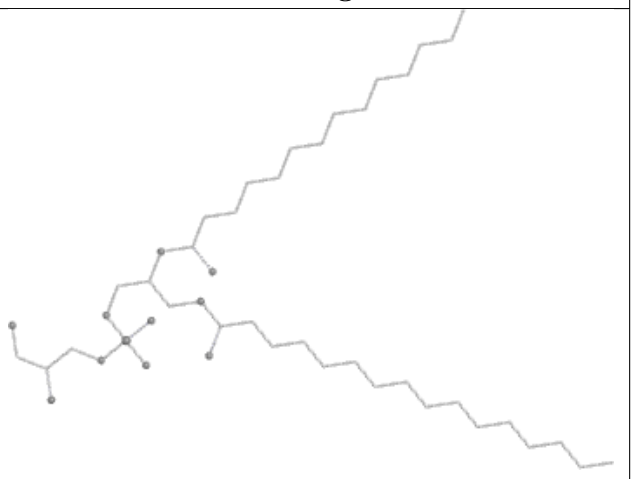
Bond lengths



Bond angles

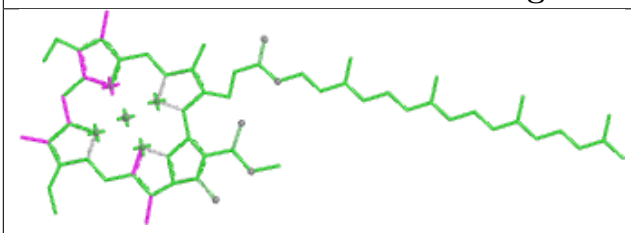


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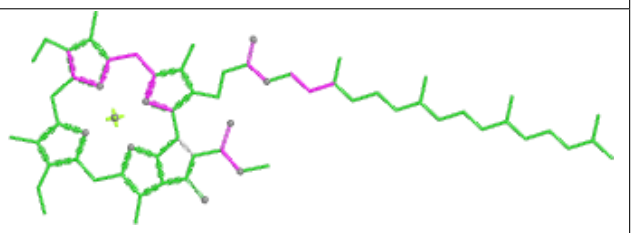


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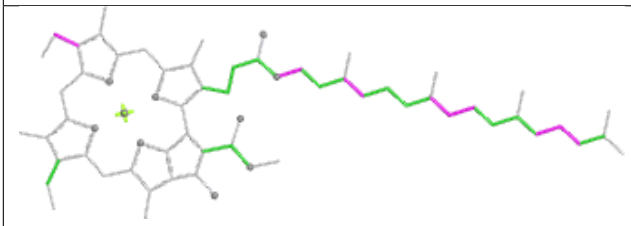
Ligand CLA b 802



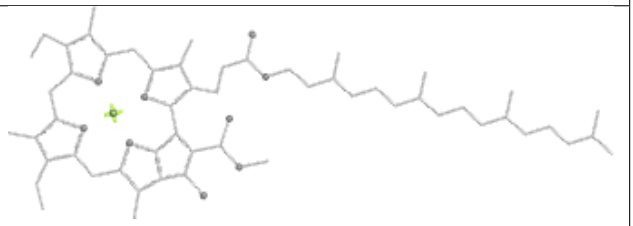
Bond lengths



Bond angles

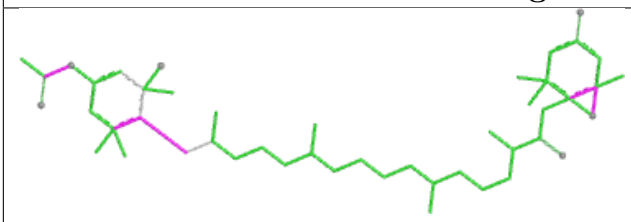


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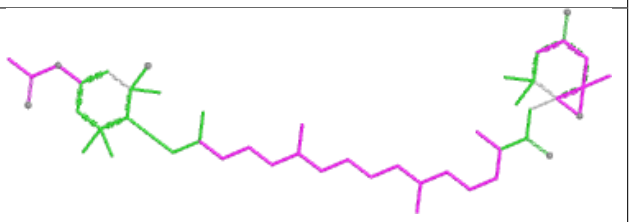


Rings

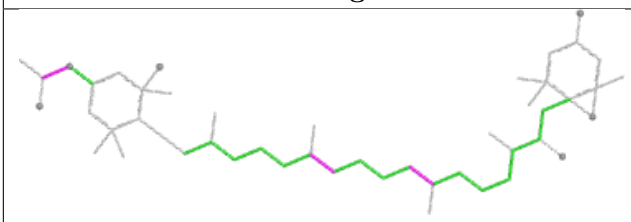
Ligand A86 G 306



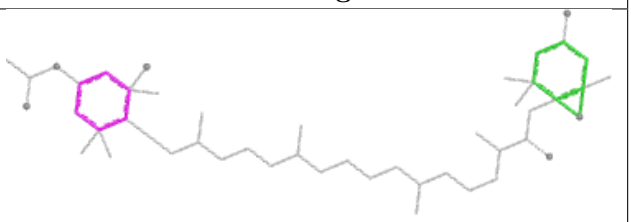
Bond lengths



Bond angles

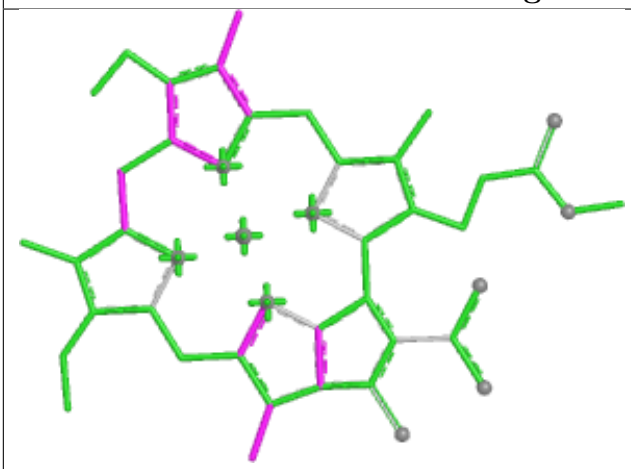


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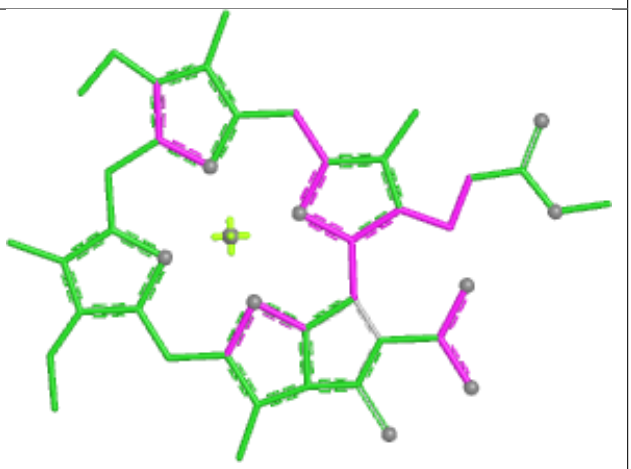


Rings

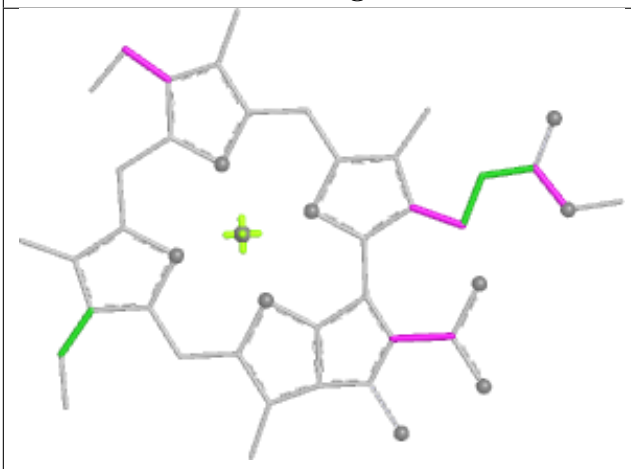
Ligand CLA X 309



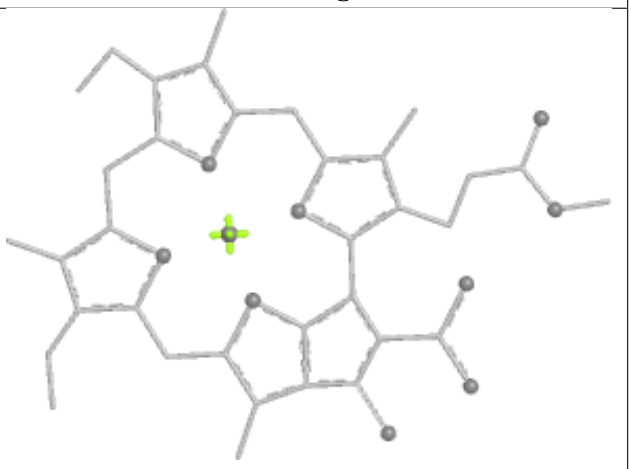
Bond lengths



Bond angles

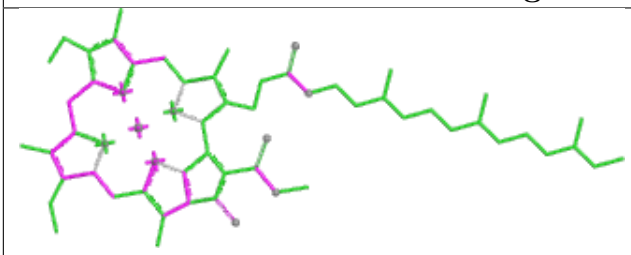


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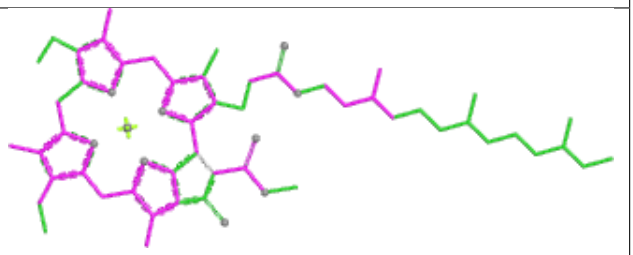


Rings

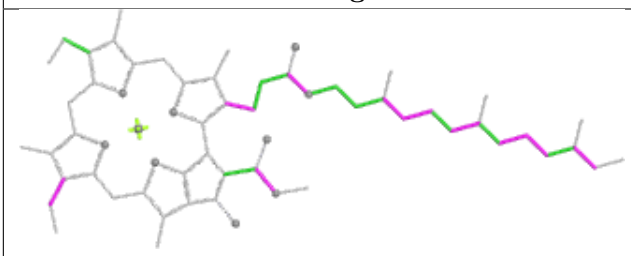
Ligand CLA A 306



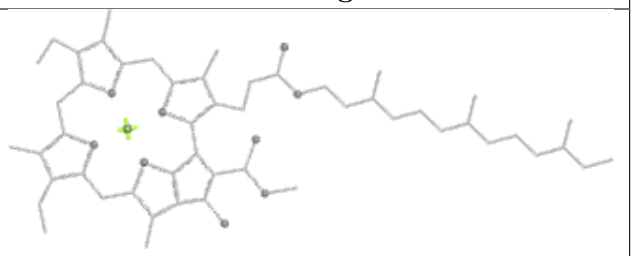
Bond lengths



Bond angles

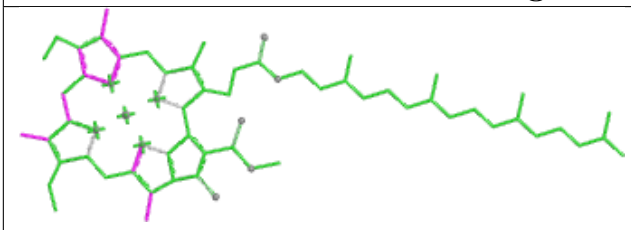


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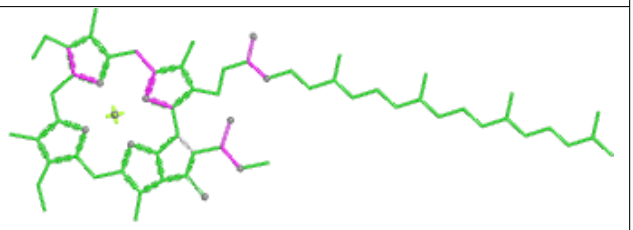


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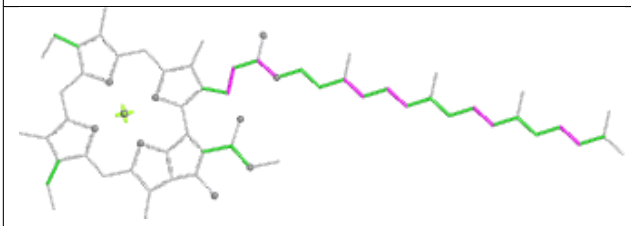
Ligand CLA b 834



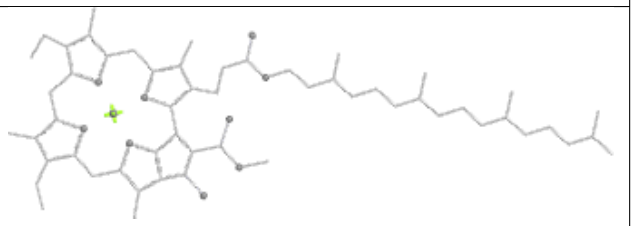
Bond lengths



Bond angles

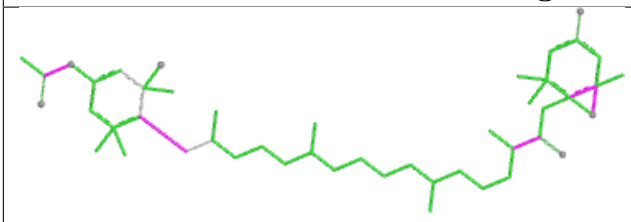


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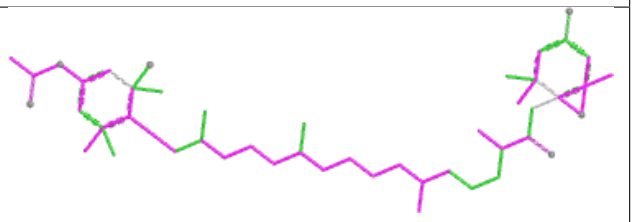


Rings

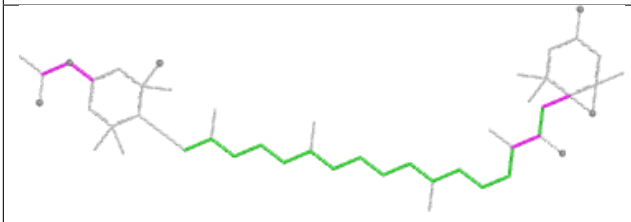
Ligand A86 I 304



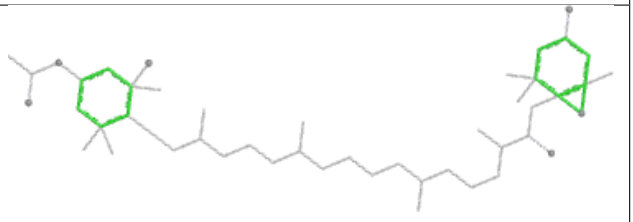
Bond lengths



Bond angles

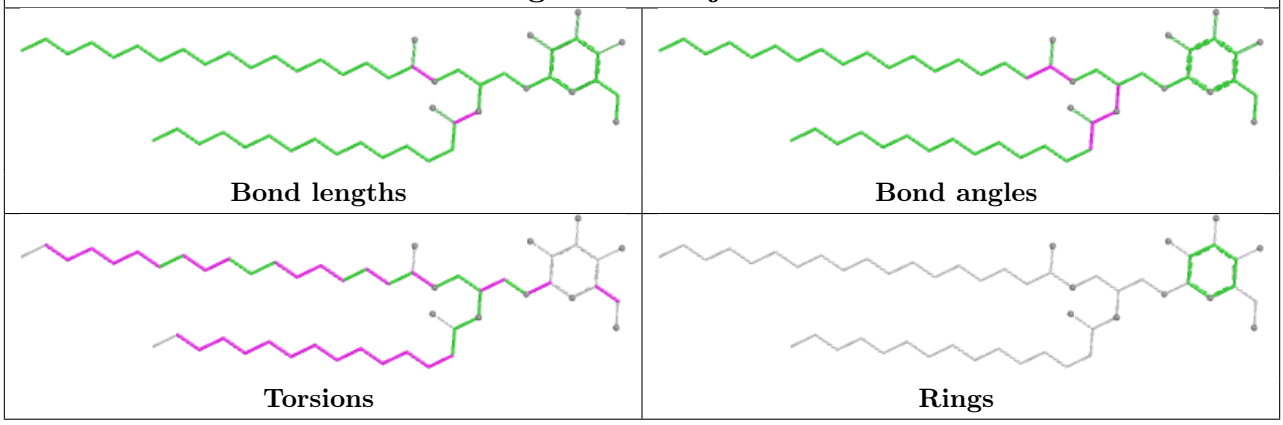


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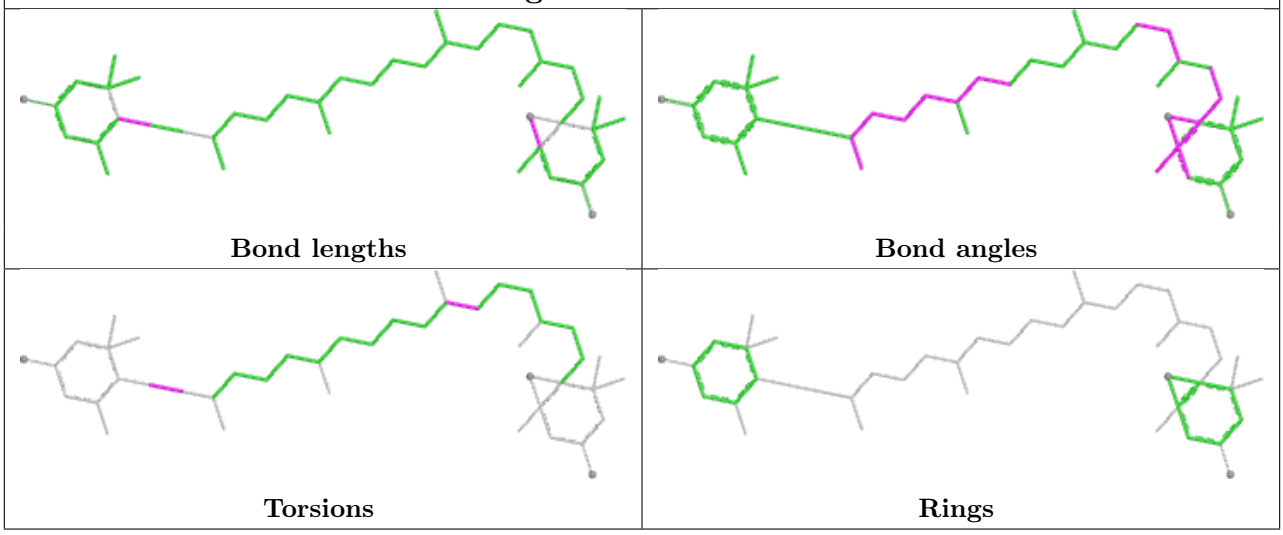


Rings

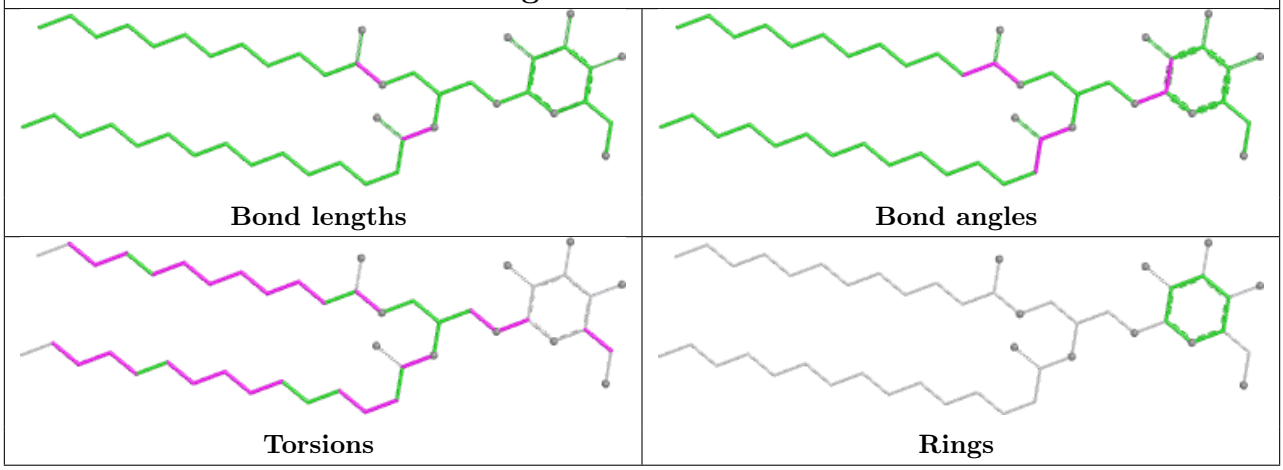
Ligand LMG j 105



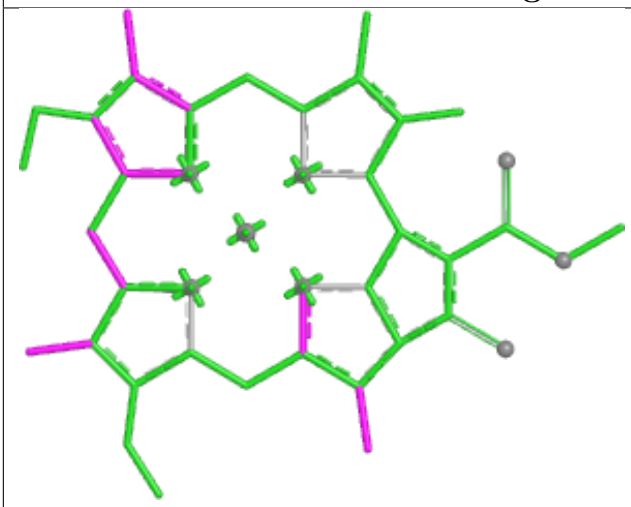
Ligand DD6 D 305



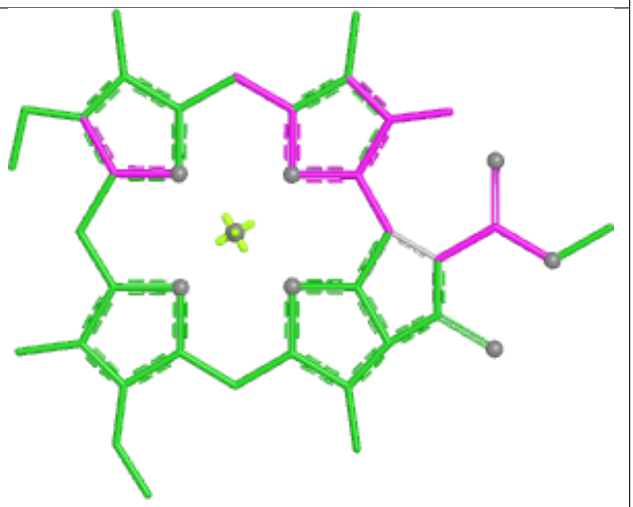
Ligand LMG E 318



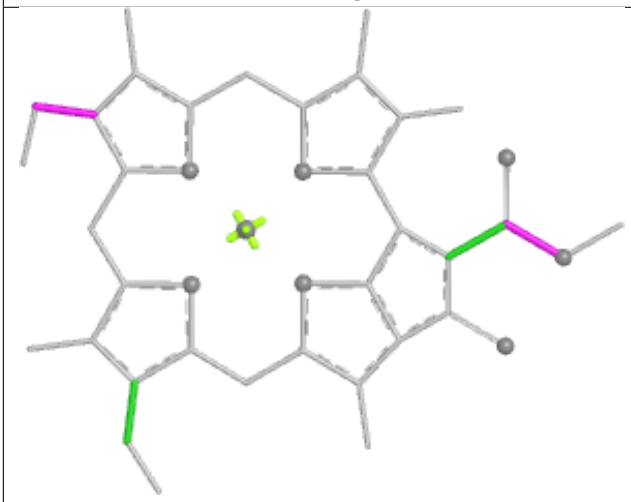
Ligand CLA U 313



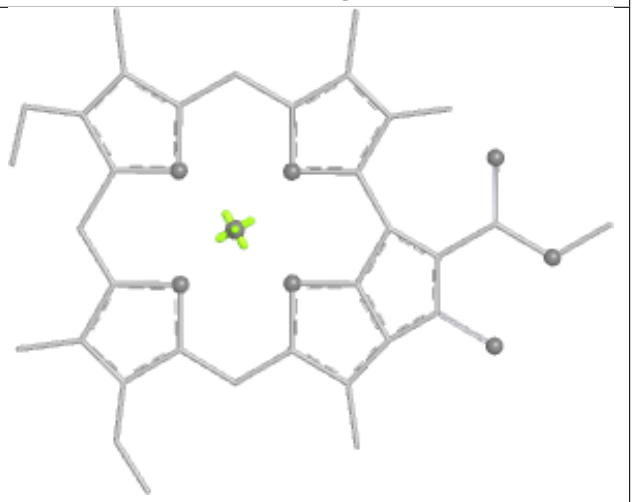
Bond lengths



Bond angles

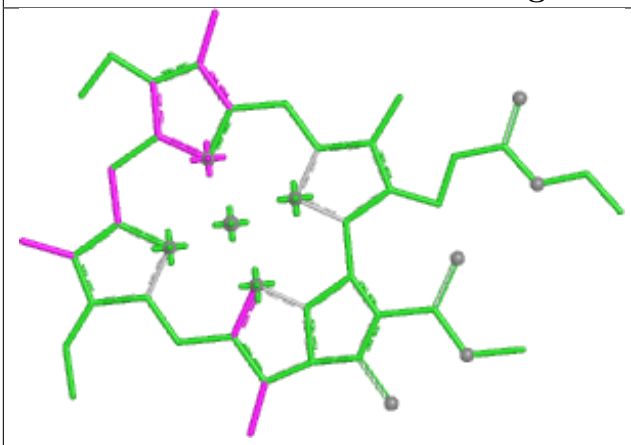


Torsions

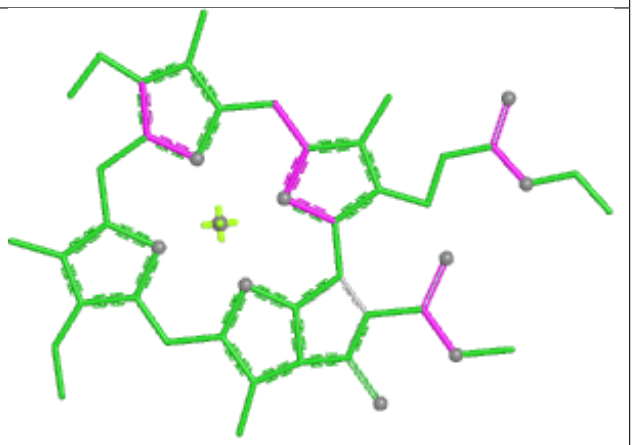


Rings

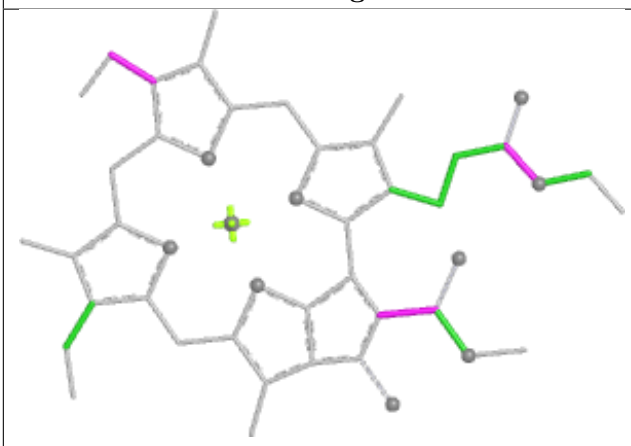
Ligand CLA J 317



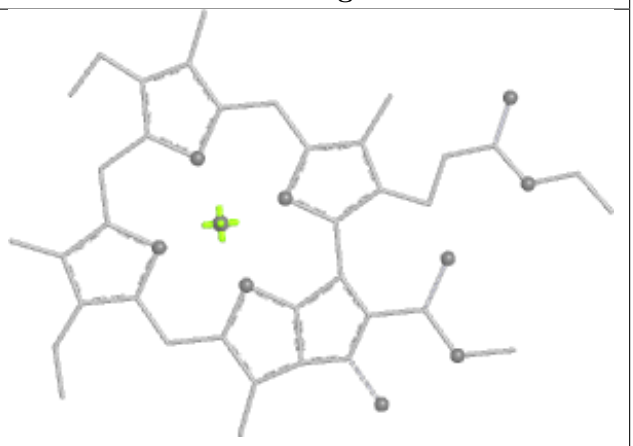
Bond lengths



Bond angles

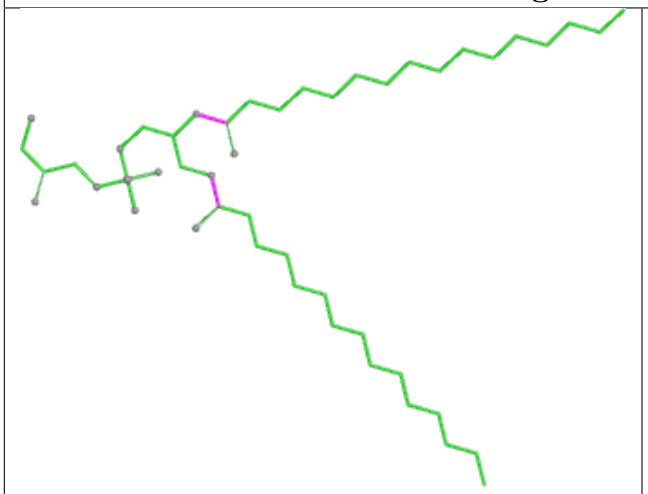


Torsions

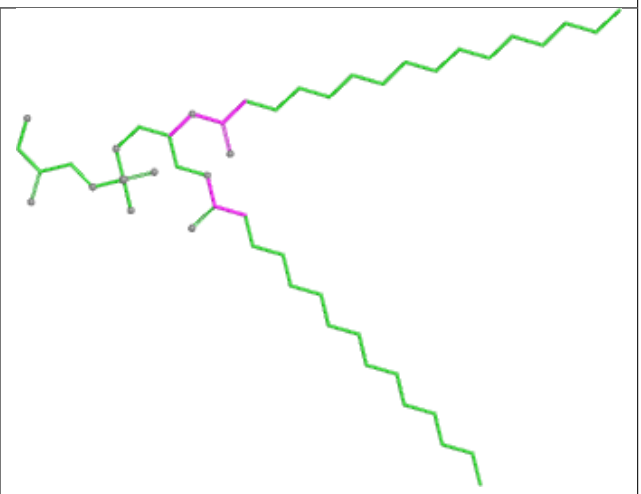


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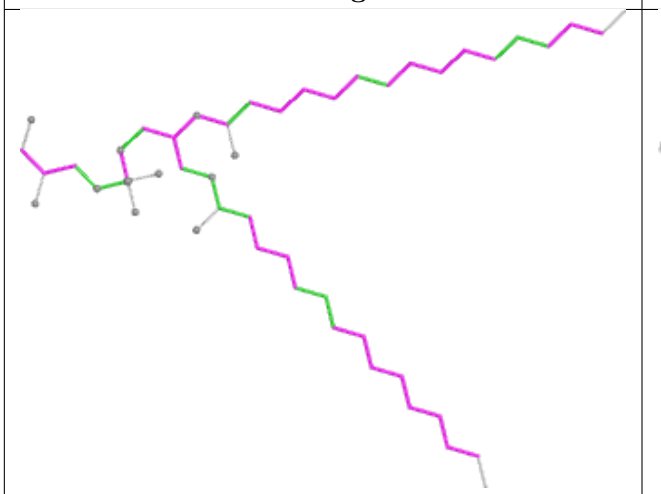
Ligand LHG l 208



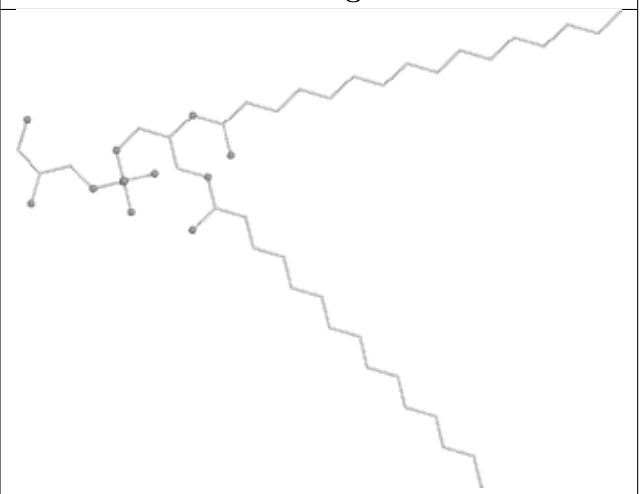
Bond lengths



Bond angles

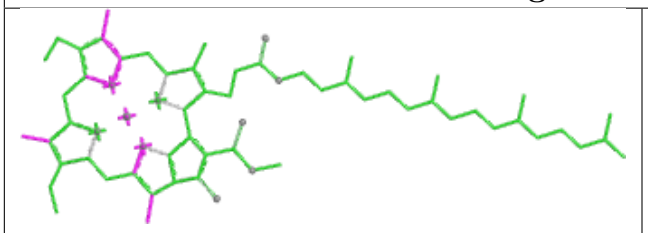


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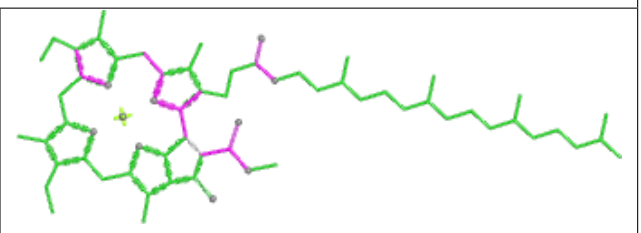


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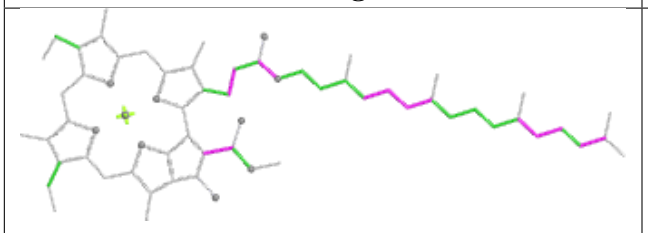
Ligand CLA b 825



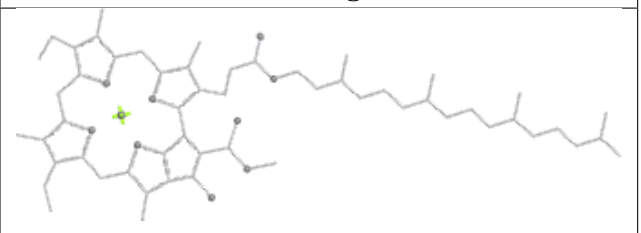
Bond lengths



Bond angles

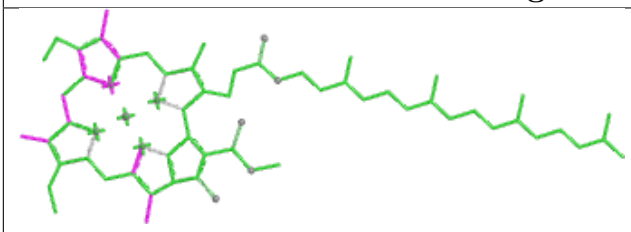


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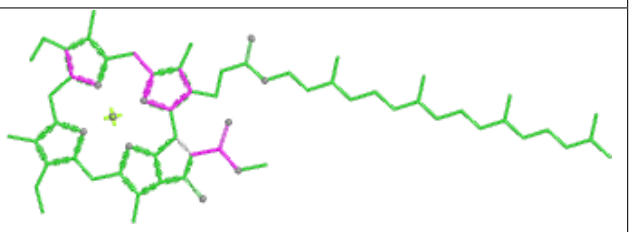


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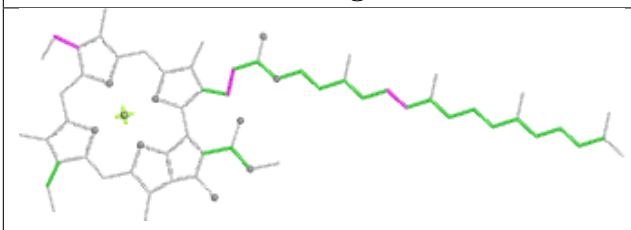
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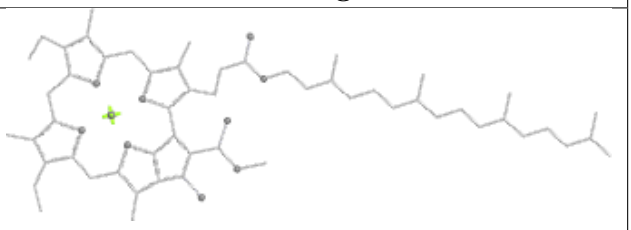
Bond lengths



Bond angles

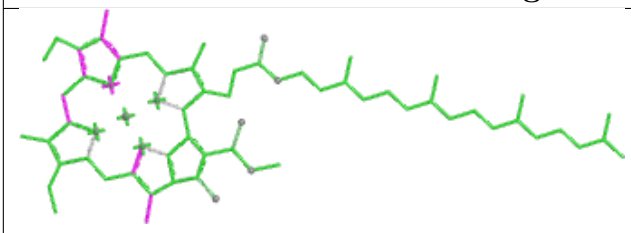


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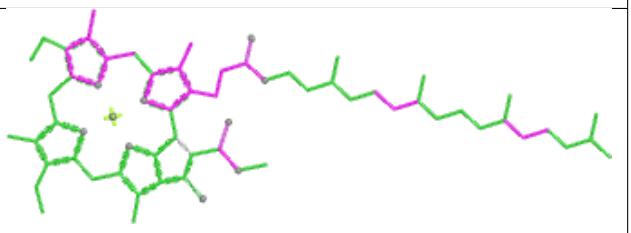


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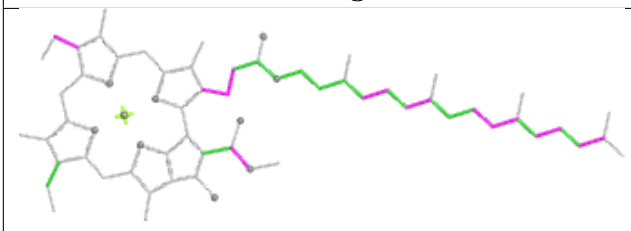
Ligand CLA G 313



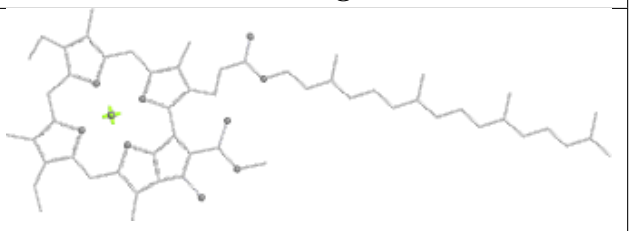
Bond lengths



Bond angles

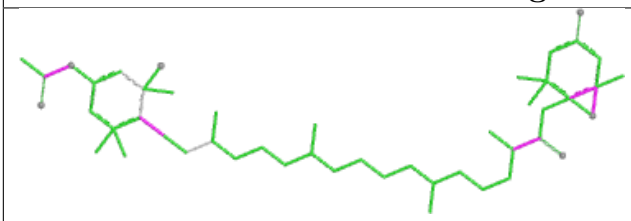


Torsions

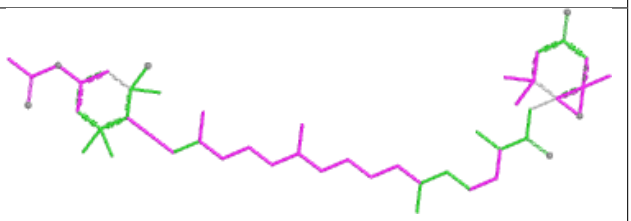


Rings

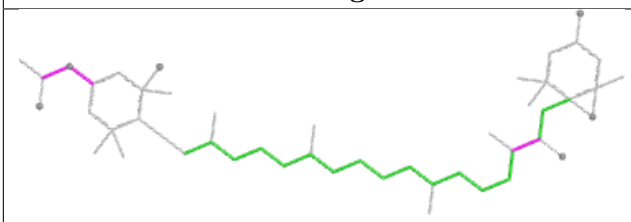
Ligand A86 H 301



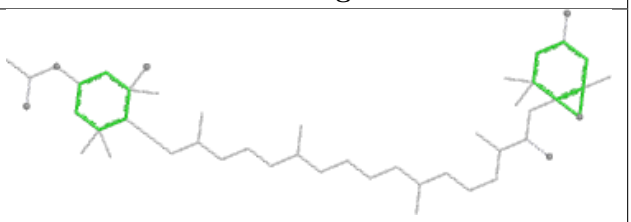
Bond lengths



Bond angles

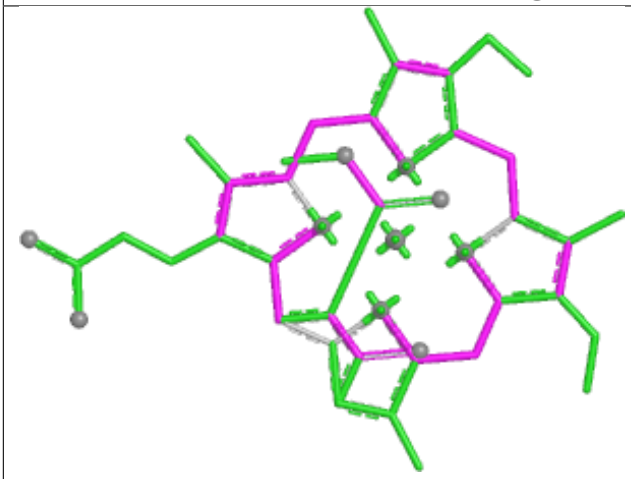


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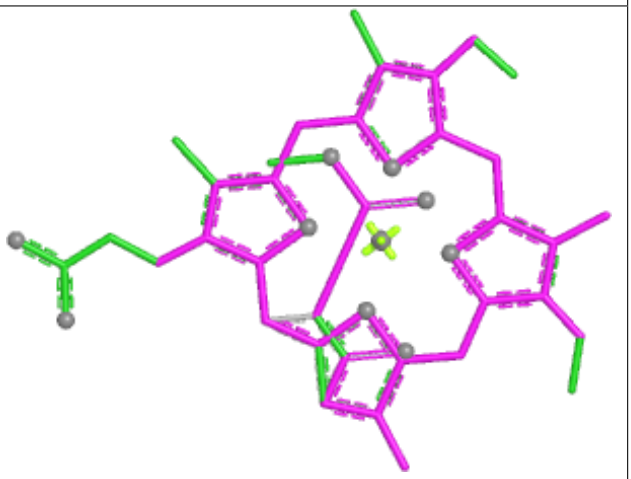


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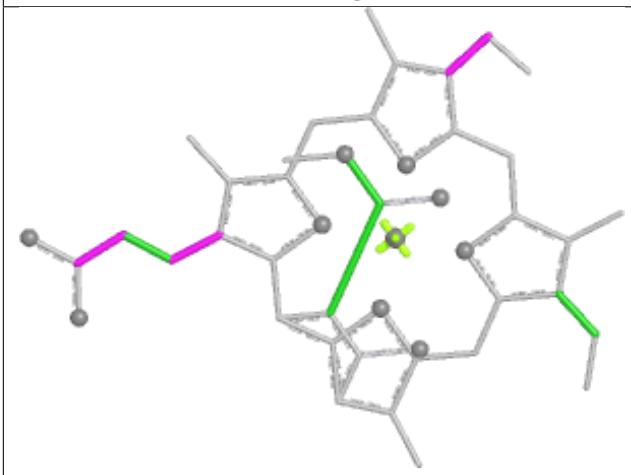
Ligand KC1 L 315



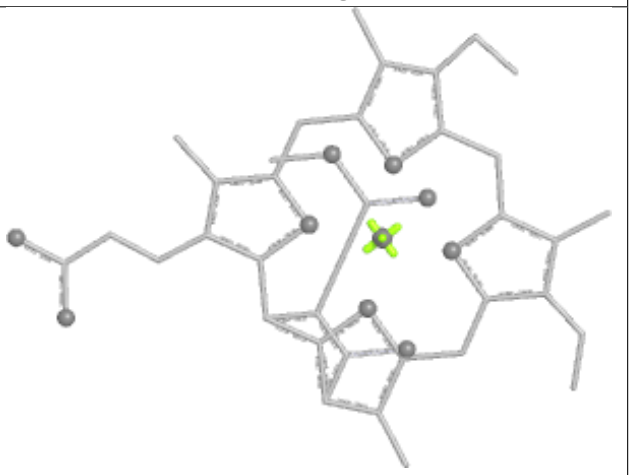
Bond lengths



Bond angles

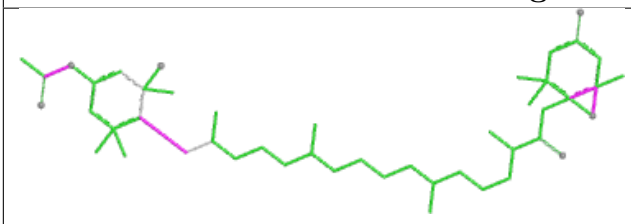


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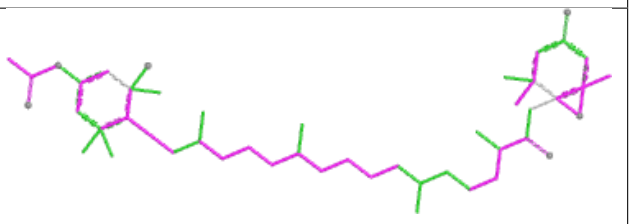


Rings

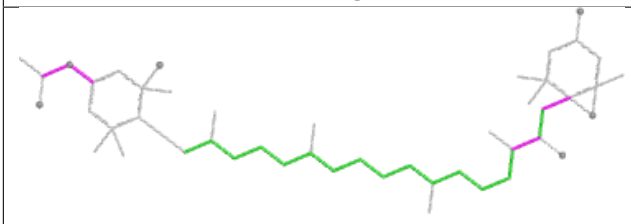
Ligand A86 R 304



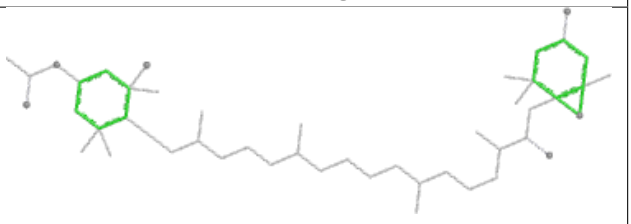
Bond lengths



Bond angles

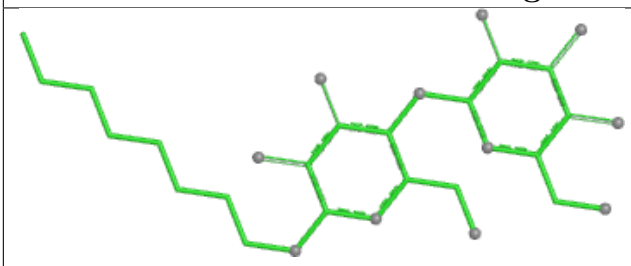


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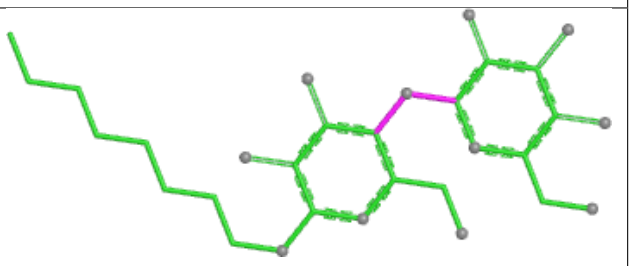


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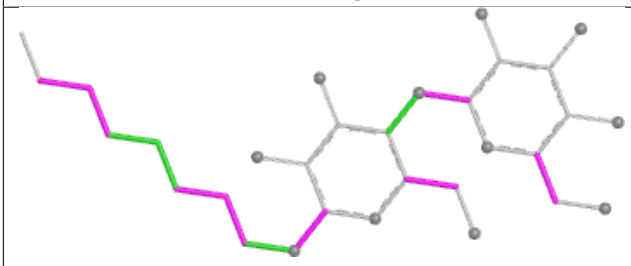
Ligand LMT L 318



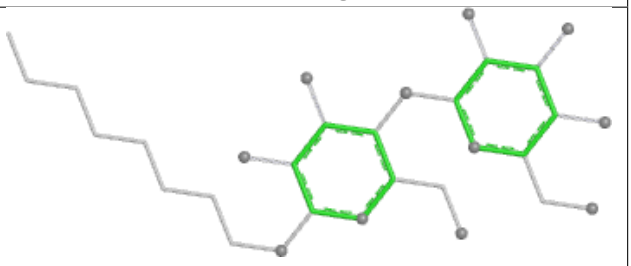
Bond lengths



Bond angles

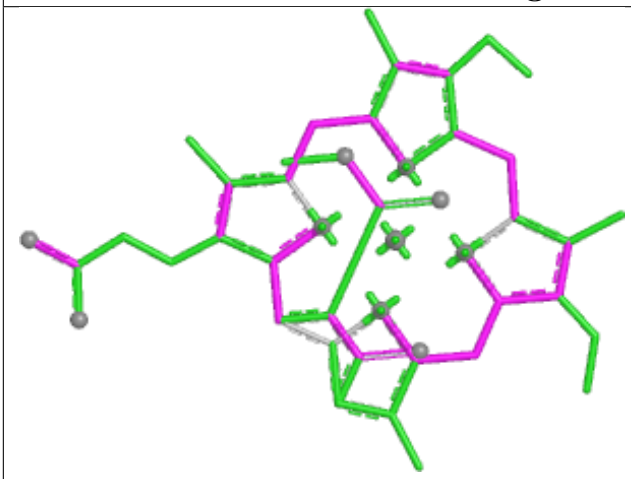


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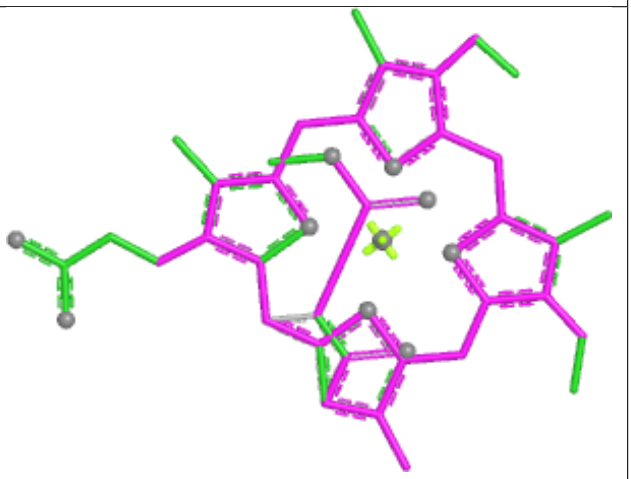


Rings

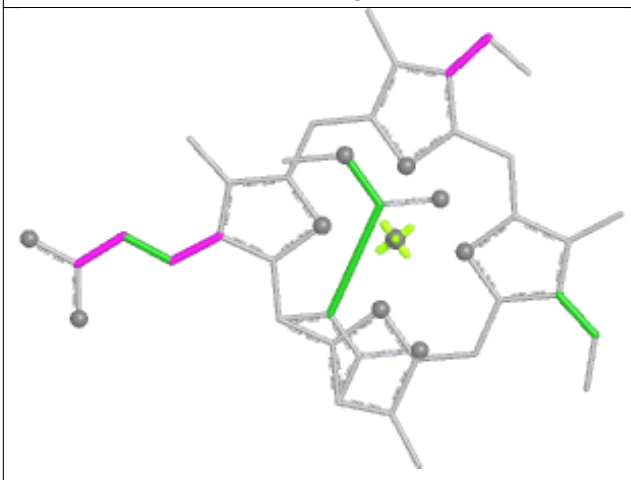
Ligand KC1 C 213



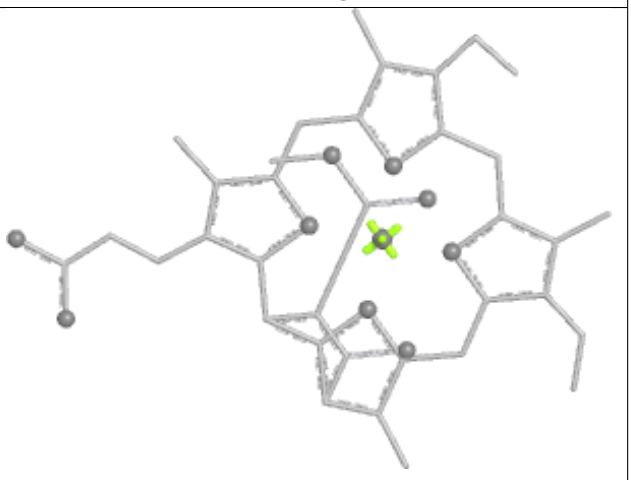
Bond lengths



Bond angles

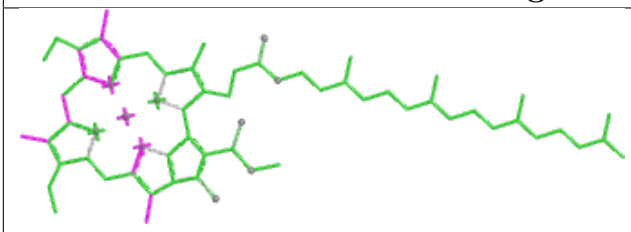


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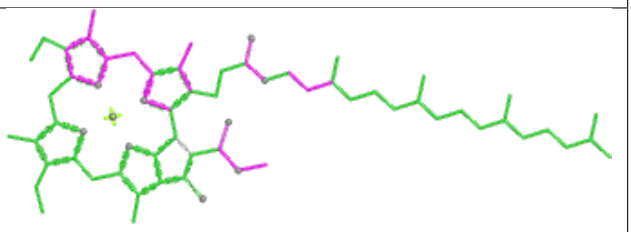


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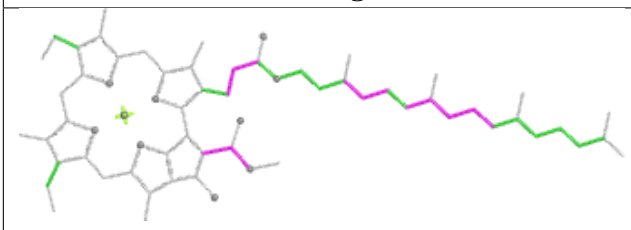
Ligand CLA S 312



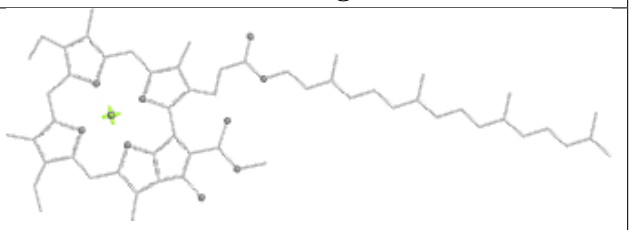
Bond lengths



Bond angles

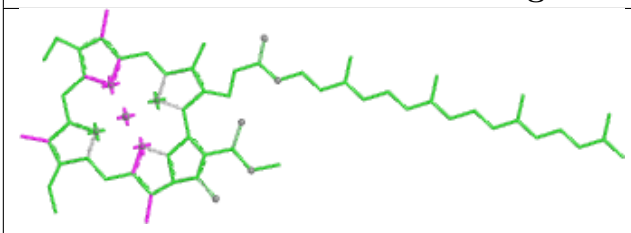


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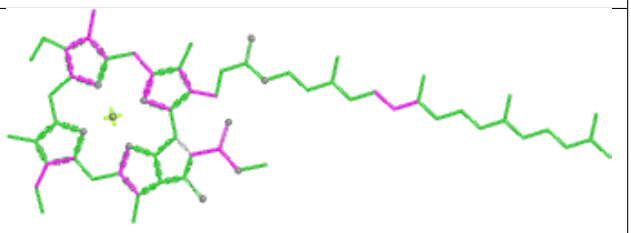


Rings

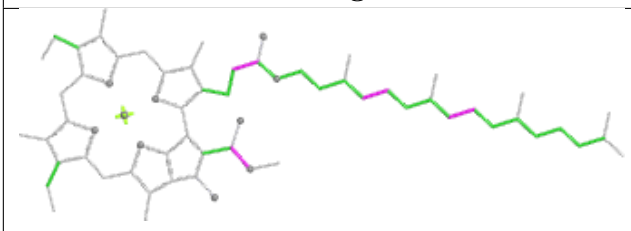
Ligand CLA b 812



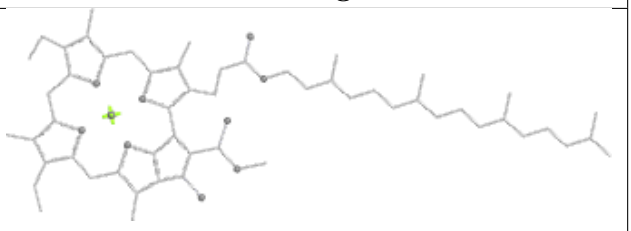
Bond lengths



Bond angles

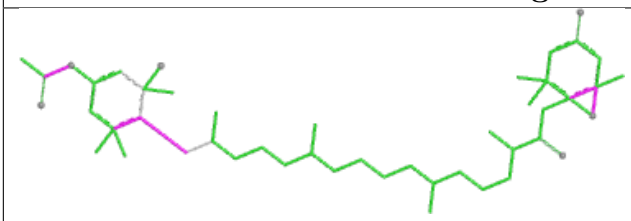


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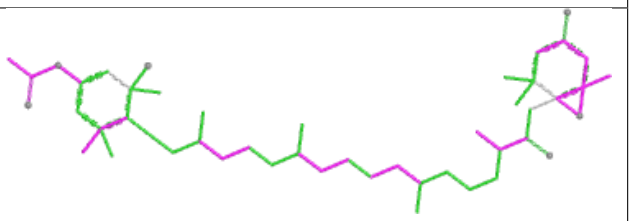


Rings

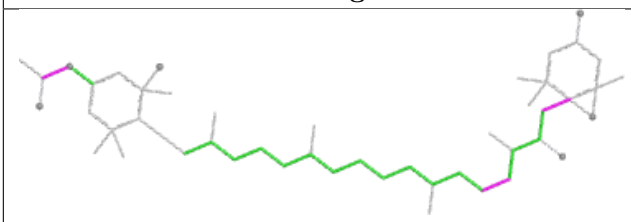
Ligand A86 E 307



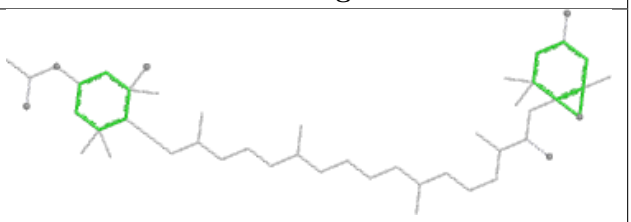
Bond lengths



Bond angles

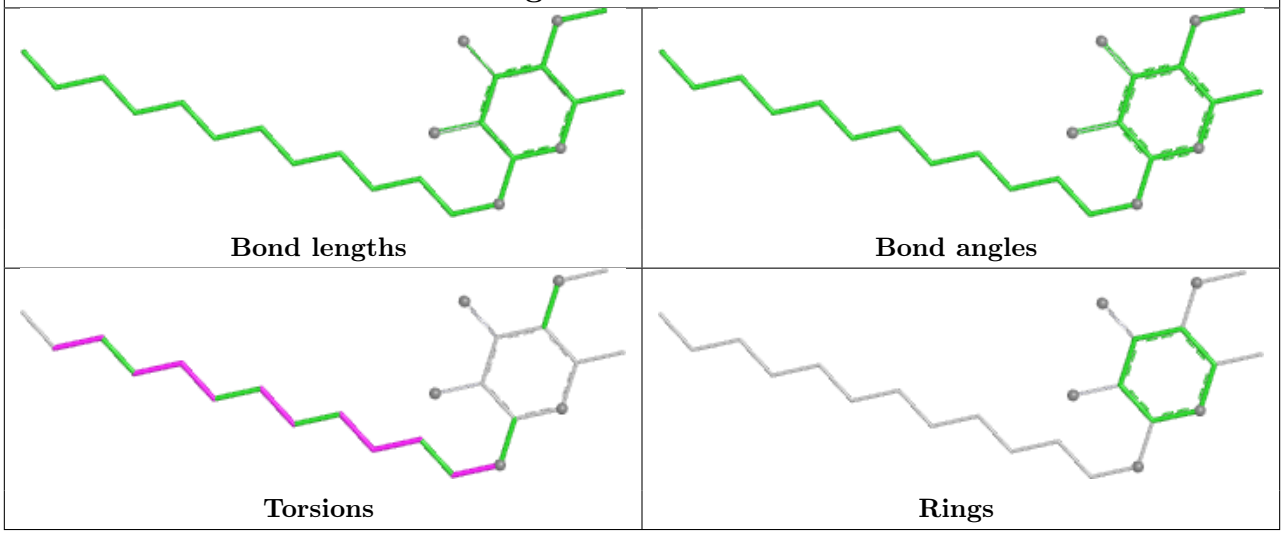


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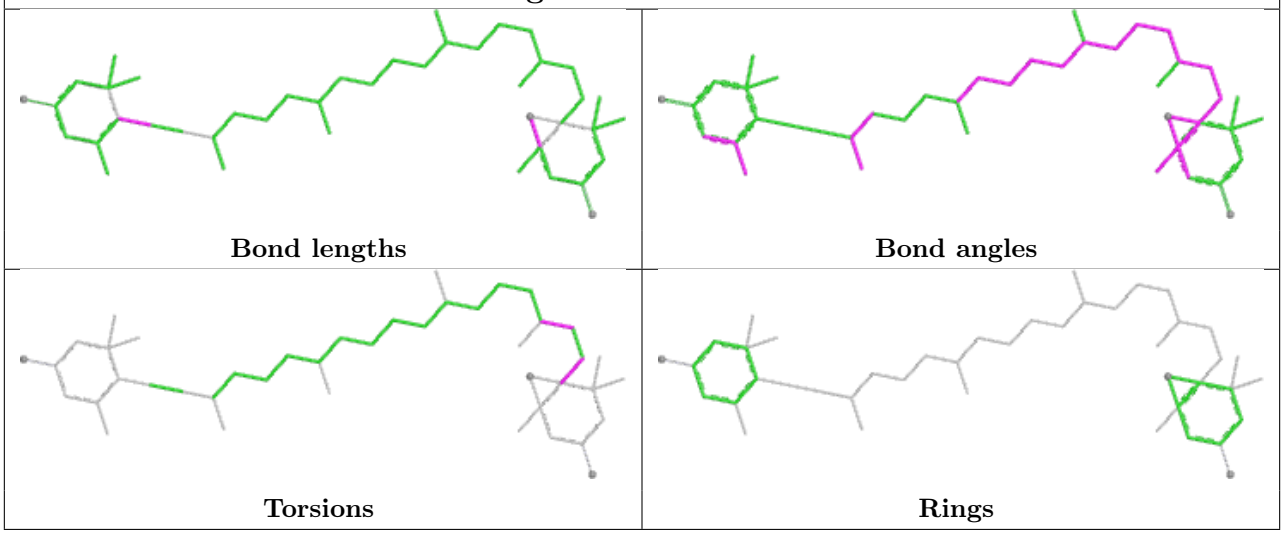


Rings

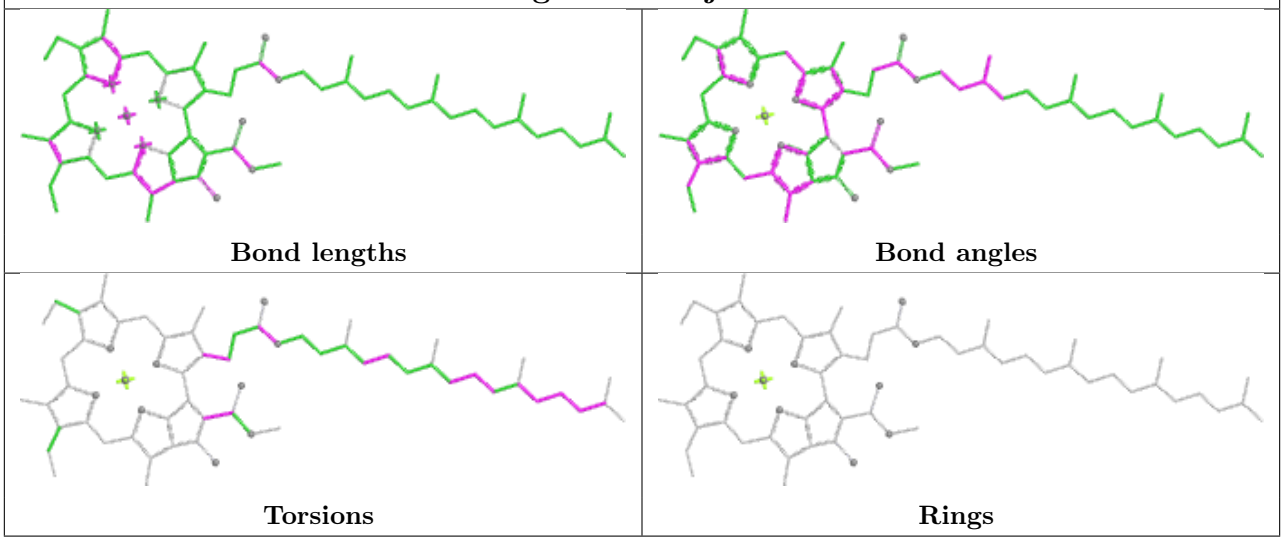
Ligand LMT b 851



Ligand DD6 B 304



Ligand CLA j 102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30012. These allow visual inspection of the internal detail of the map and identification of artifacts.

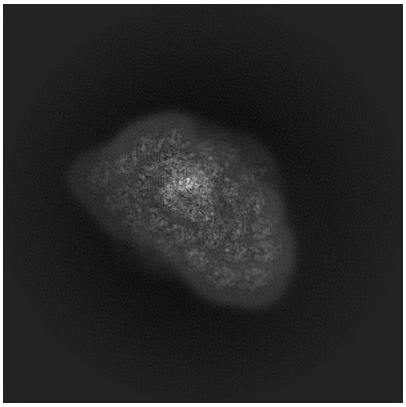
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

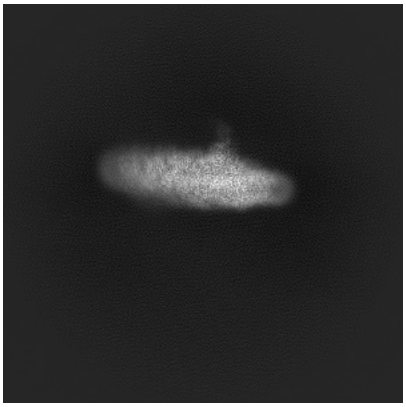
6.1.1 Primary map



X



Y

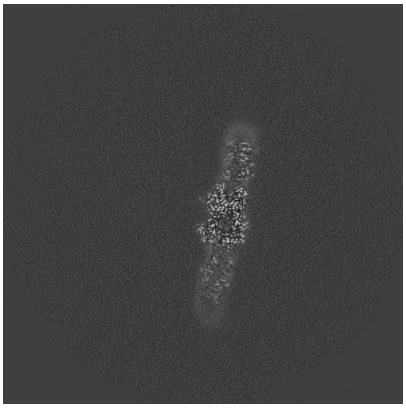


Z

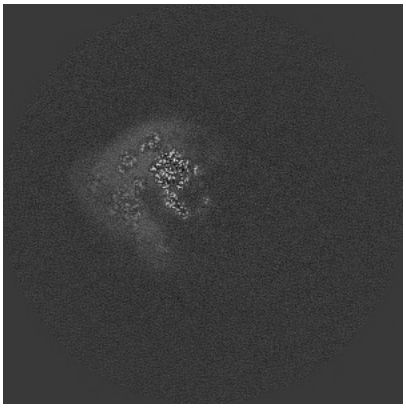
The images above show the map projected in three orthogonal directions.

6.2 Central slices

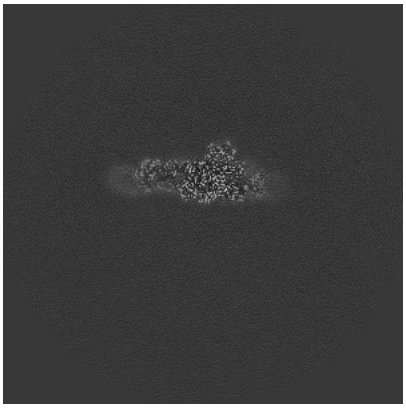
6.2.1 Primary map



X Index: 260



Y Index: 260

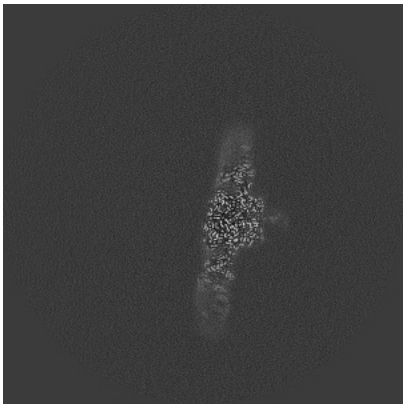


Z Index: 260

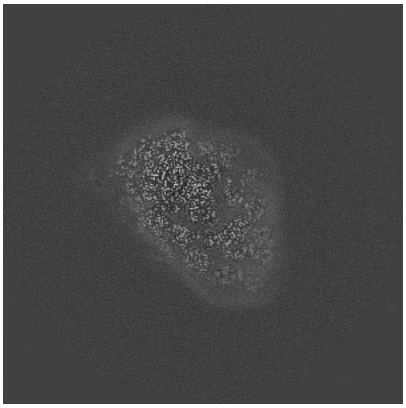
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

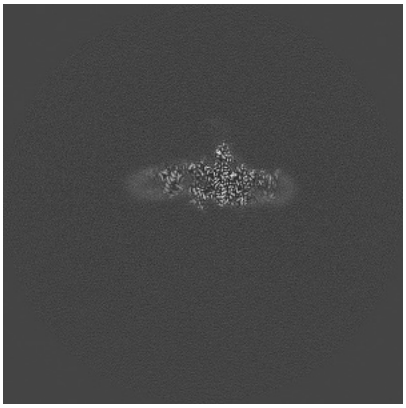
6.3.1 Primary map



X Index: 278



Y Index: 294

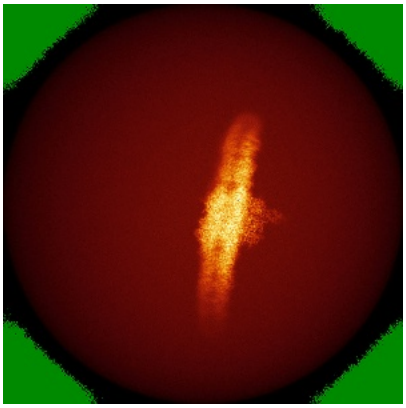


Z Index: 231

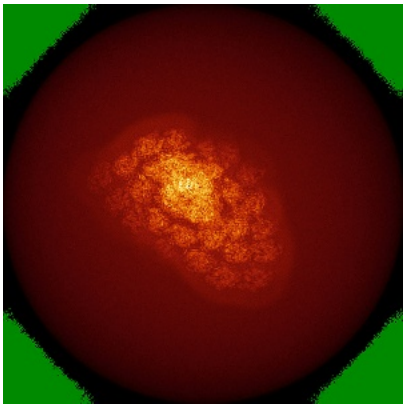
The images above show the largest variance slices of the map in three orthogonal directions.

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

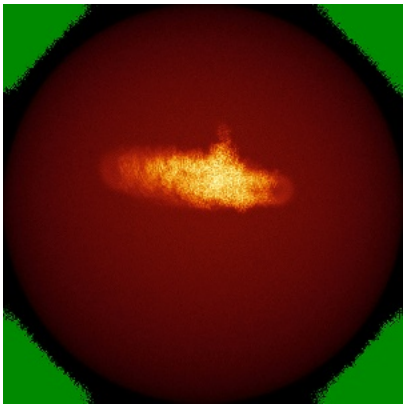
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

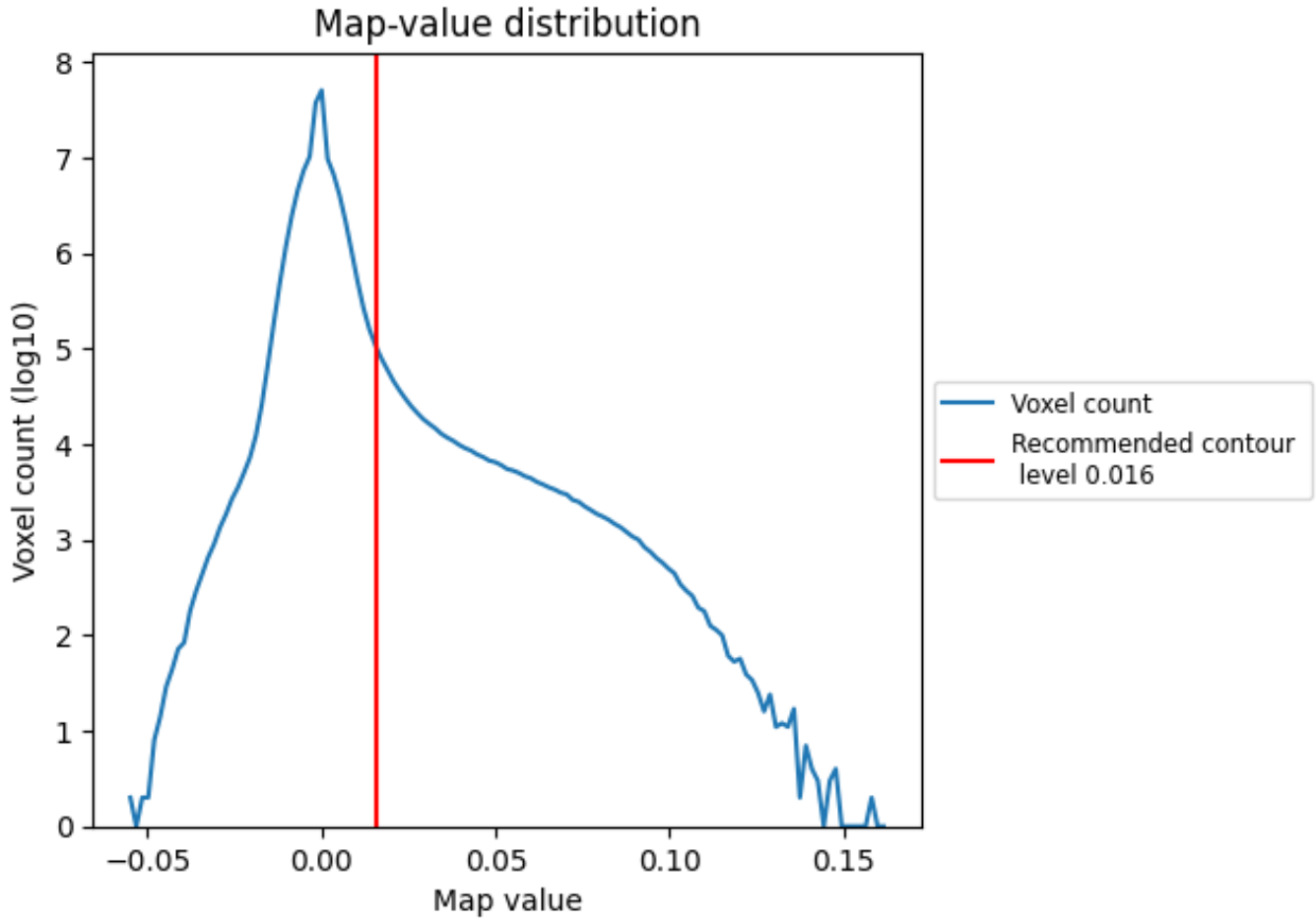
6.6 Mask visualisation (i)

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

7 Map analysis

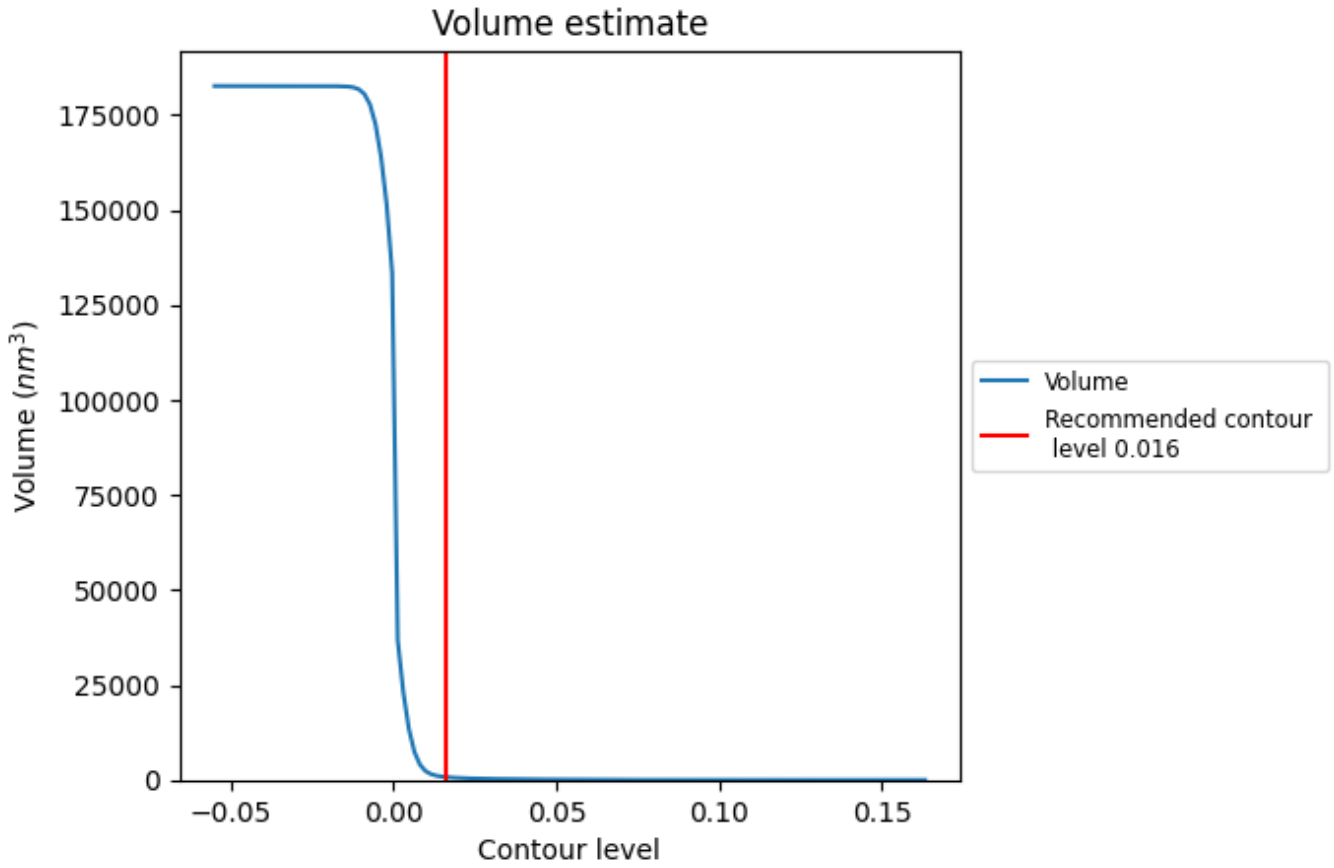
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

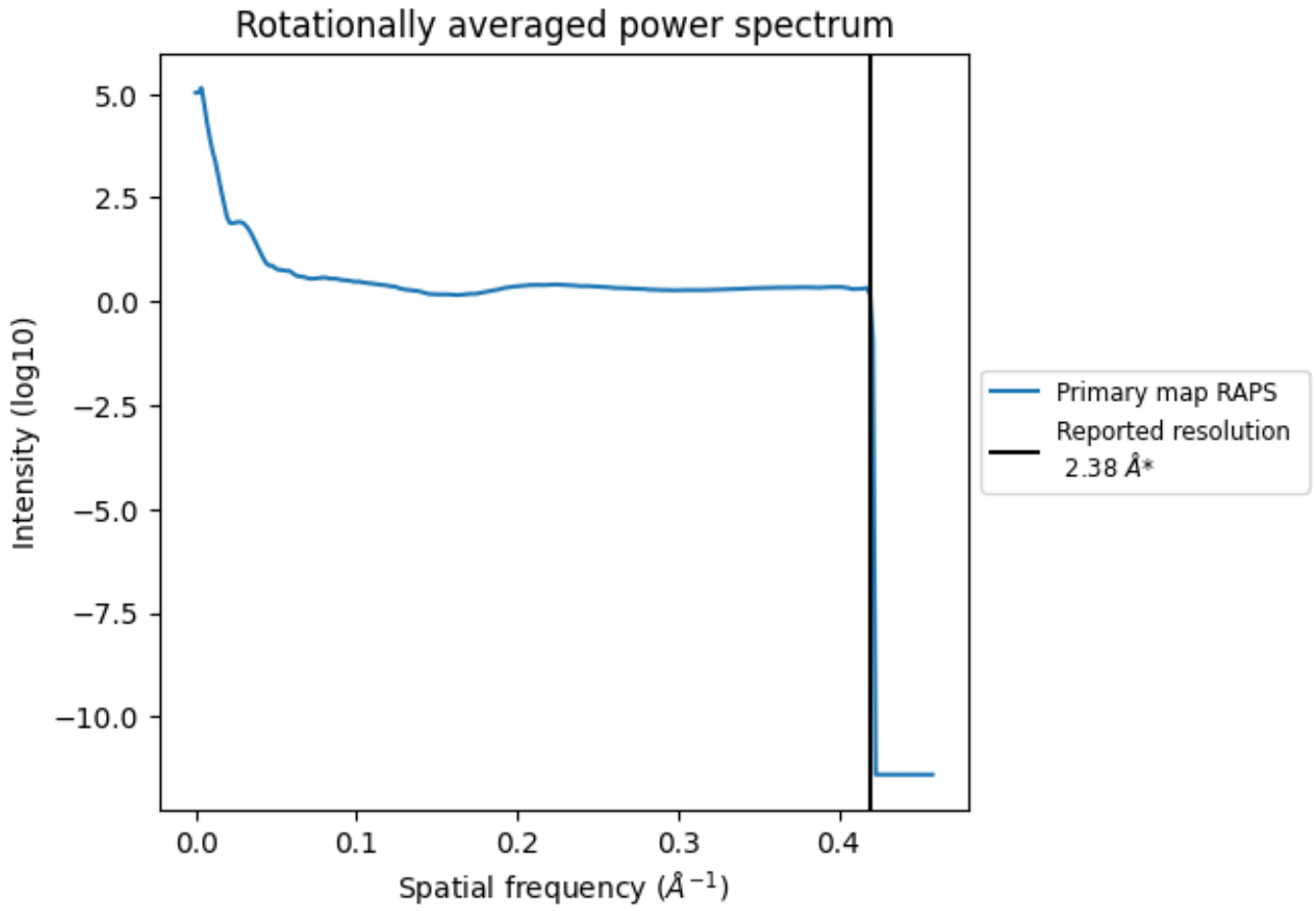
7.2 Volume estimate



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.420 $Å^{-1}$

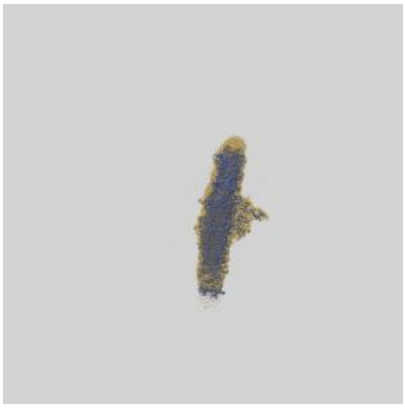
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

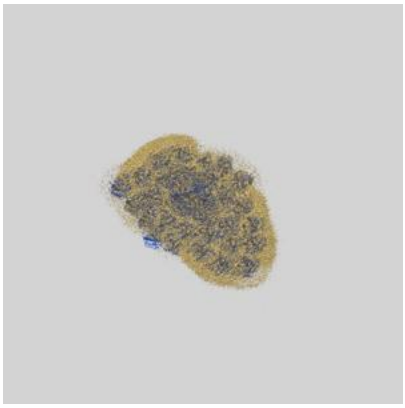
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30012 and PDB model 6LY5. Per-residue inclusion information can be found in section 3 on page 52.

9.1 Map-model overlay



X



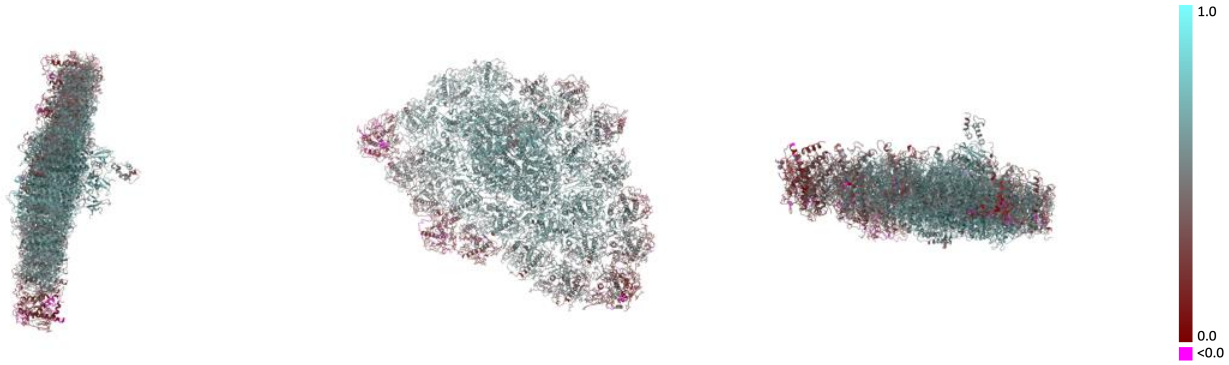
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

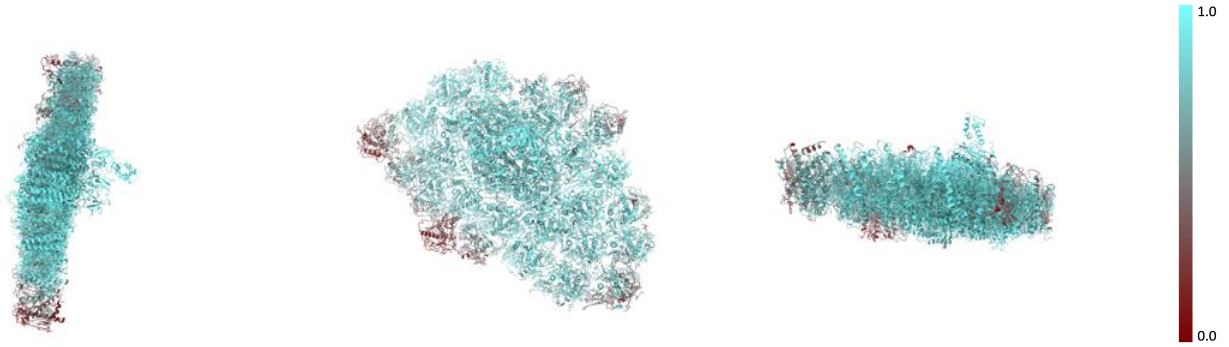
9.2 Q-score mapped to coordinate model (i)



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.

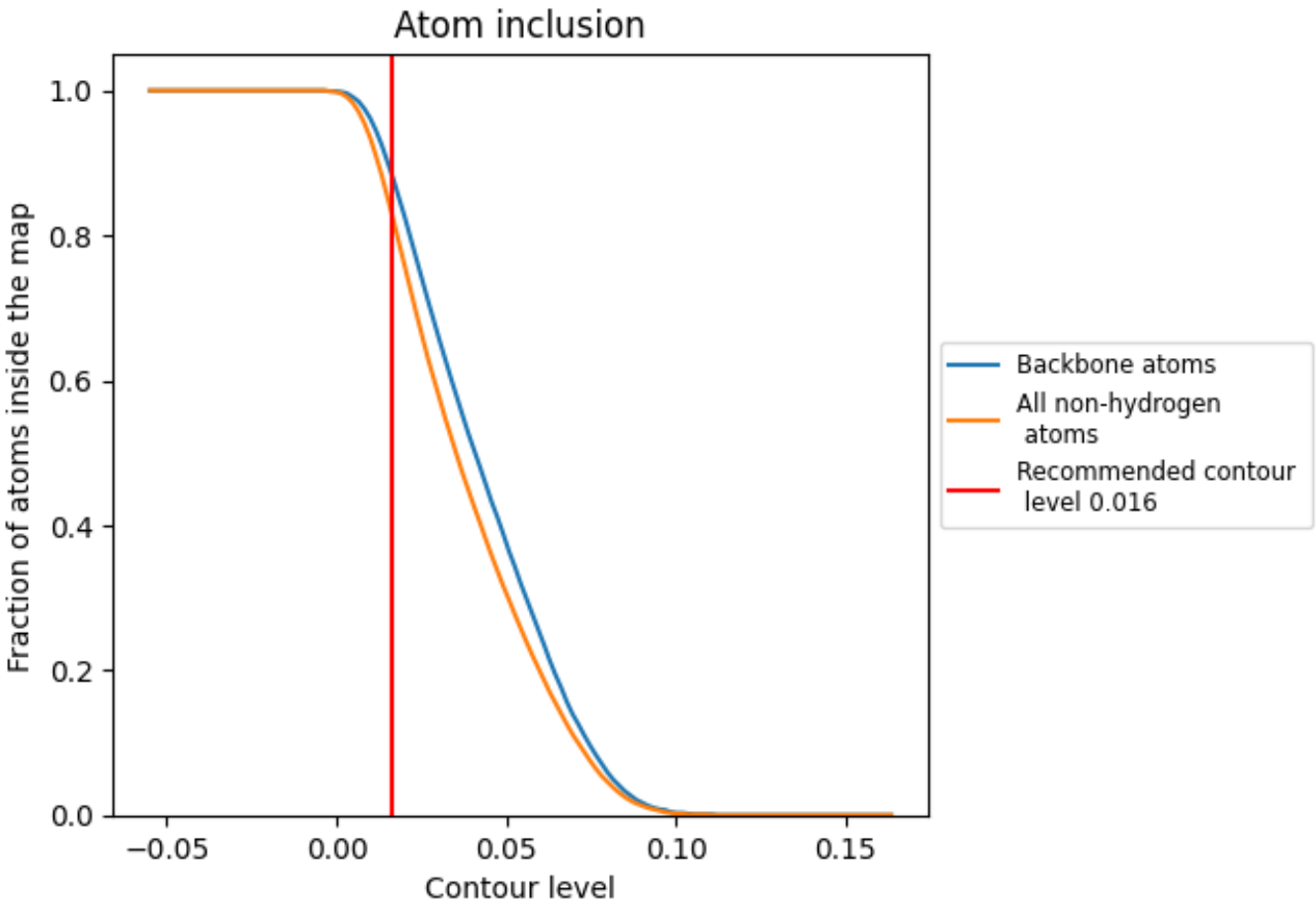
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5170
A	0.9410	0.5810
B	0.8370	0.4930
C	0.8980	0.5340
D	0.9340	0.5870
E	0.9530	0.6050
F	0.9430	0.5960
G	0.9570	0.6150
H	0.8900	0.5450
I	0.9240	0.5640
J	0.9060	0.5400
K	0.8890	0.5170
L	0.8050	0.4220
M	0.8700	0.4820
N	0.3040	0.1740
O	0.6670	0.4100
P	0.8980	0.5260
Q	0.7760	0.3880
R	0.7930	0.4220
S	0.5670	0.2610
T	0.6280	0.3920
U	0.6600	0.3880
V	0.7550	0.4470
W	0.4970	0.2640
X	0.1530	0.1400
a	0.9830	0.6690
b	0.9910	0.6730
c	0.9770	0.6620
d	0.9460	0.6200
e	0.9210	0.5940
f	0.9320	0.6150
g	0.8870	0.4480
h	0.9690	0.6040
i	0.9430	0.6250
j	0.9380	0.6250



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Chain	Atom inclusion	Q-score
l	0.9580	0.6310
m	0.9420	0.6140