Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:42 AM UTC

PDB ID	:	7YCA / pdb_00007yca
EMDB ID	:	EMD-33737
Title	:	Cryo-EM structure of the PSI-LHCI-Lhcp supercomplex from Ostreococcus tauri
Authors	:	Shan, J.; Sheng, X.; Ishii, A.; Watanabe, A.; Song, C.; Murata, K.; Minagawa, J.; Liu, Z.
Deposited on	:	2022-07-01
Resolution	:	2.94 Å(reported)
Based on initial models	:	5ZJI, 7D0J

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

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

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

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

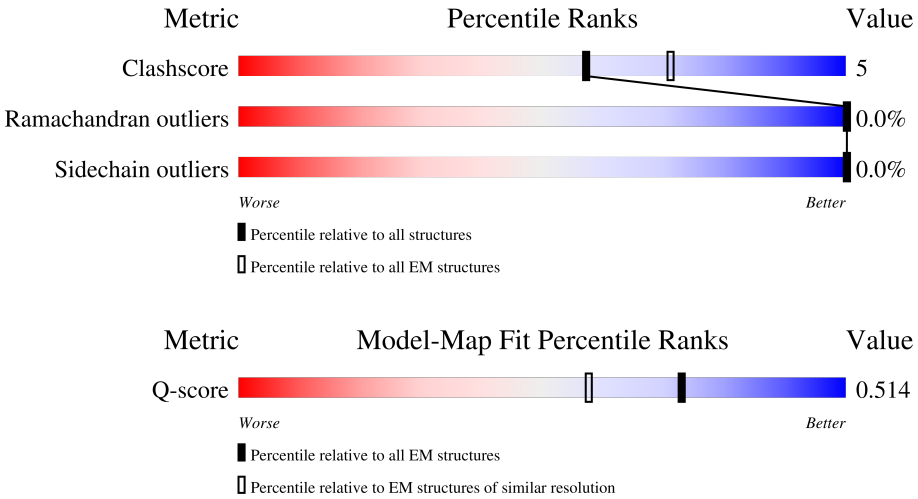
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.94 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	225	53% 61% 9% 29%
2	2	242	31% 77% 7% 15%
3	3	272	21% 75% 9% 17%

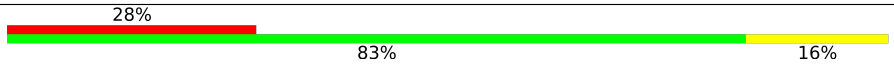
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Mol	Chain	Length	Quality of chain
4	4	236	44% 73% 13% 14%
5	5	217	21% 69% 7% 24%
6	6	249	8% 71% 6% 22%
7	A	751	89% 10%
8	B	733	92% 8%
9	C	81	7% 94% 5%
10	D	188	14% 69% 7% 24%
11	E	101	10% 59% 39%
12	F	231	13% 63% 9% 29%
13	G	132	38% 51% 21% 28%
14	H	166	13% 53% 5% 42%
15	I	35	11% 91% 9%
16	J	42	7% 81% 17%
17	K	131	6% 61% 5% 34%
18	L	204	72% 6% 23%
19	M	31	6% 94% 6%
20	N	139	45% 54% 12% 35%
21	O	136	6% 67% 29%
22	P	233	71% 78% 8% 14%
22	R	233	55% 70% 16% 14%
22	S	233	68% 71% 15% 13%
22	T	233	50% 76% 11% 14%
22	U	233	80% 80% 6% 14%
22	V	233	78% 68% 16% 15%
22	W	233	58% 73% 13% 14%

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Mol	Chain	Length	Quality of chain
22	X	233	
23	Q	226	

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
24	CHL	1	601	X	-	-	-
24	CHL	1	604	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	605	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	615	X	-	-	-
24	CHL	3	306	X	-	-	-
24	CHL	4	302	X	-	-	-
24	CHL	4	306	X	-	-	-
24	CHL	4	307	X	-	-	-
24	CHL	4	308	X	-	-	-
24	CHL	5	605	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	605	X	-	-	-
24	CHL	6	606	X	-	-	-
24	CHL	P	304	X	-	-	-
24	CHL	P	305	X	-	-	-
24	CHL	P	306	X	-	-	-
24	CHL	P	307	X	-	-	-
24	CHL	P	314	X	-	-	-
24	CHL	Q	307	X	-	-	-
24	CHL	Q	308	X	-	-	-
24	CHL	Q	309	X	-	-	-
24	CHL	Q	316	X	-	-	-
24	CHL	R	302	X	-	-	-
24	CHL	R	308	X	-	-	-
24	CHL	R	309	X	-	-	-
24	CHL	R	310	X	-	-	-
24	CHL	R	311	X	-	-	-
24	CHL	R	318	X	-	-	-
24	CHL	S	304	X	-	-	-
24	CHL	S	305	X	-	-	-
24	CHL	S	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	S	307	X	-	-	-
24	CHL	S	314	X	-	-	-
24	CHL	T	304	X	-	-	-
24	CHL	T	305	X	-	-	-
24	CHL	T	306	X	-	-	-
24	CHL	T	307	X	-	-	-
24	CHL	T	314	X	-	-	-
24	CHL	T	320	X	-	-	-
24	CHL	U	304	X	-	-	-
24	CHL	U	305	X	-	-	-
24	CHL	U	306	X	-	-	-
24	CHL	U	313	X	-	-	-
24	CHL	V	304	X	-	-	-
24	CHL	V	305	X	-	-	-
24	CHL	V	306	X	-	-	-
24	CHL	V	307	X	-	-	-
24	CHL	V	314	X	-	-	-
24	CHL	W	304	X	-	-	-
24	CHL	W	305	X	-	-	-
24	CHL	W	306	X	-	-	-
24	CHL	W	307	X	-	-	-
24	CHL	W	314	X	-	-	-
24	CHL	X	305	X	-	-	-
24	CHL	X	306	X	-	-	-
24	CHL	X	307	X	-	-	-
24	CHL	X	308	X	-	-	-
24	CHL	X	315	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	605	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	608	X	-	-	-
25	CLA	1	609	X	-	-	-
25	CLA	1	613	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	606	X	-	-	-
25	CLA	2	608	X	-	-	-
25	CLA	2	609	X	-	-	-
25	CLA	2	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	613	X	-	-	-
25	CLA	2	614	X	-	-	-
25	CLA	3	301	X	-	-	-
25	CLA	3	302	X	-	-	-
25	CLA	3	303	X	-	-	-
25	CLA	3	304	X	-	-	-
25	CLA	3	305	X	-	-	-
25	CLA	3	307	X	-	-	-
25	CLA	3	308	X	-	-	-
25	CLA	3	309	X	-	-	-
25	CLA	3	310	X	-	-	-
25	CLA	3	311	X	-	-	-
25	CLA	3	312	X	-	-	-
25	CLA	3	313	X	-	-	-
25	CLA	4	303	X	-	-	-
25	CLA	4	304	X	-	-	-
25	CLA	4	305	X	-	-	-
25	CLA	4	309	X	-	-	-
25	CLA	4	310	X	-	-	-
25	CLA	4	311	X	-	-	-
25	CLA	4	312	X	-	-	-
25	CLA	4	314	X	-	-	-
25	CLA	4	315	X	-	-	-
25	CLA	4	316	X	-	-	-
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-
25	CLA	5	608	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	607	X	-	-	-
25	CLA	6	608	X	-	-	-
25	CLA	6	609	X	-	-	-
25	CLA	6	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	A	803	X	-	-	-
25	CLA	A	804	X	-	-	-
25	CLA	A	805	X	-	-	-
25	CLA	A	806	X	-	-	-
25	CLA	A	807	X	-	-	-
25	CLA	A	808	X	-	-	-
25	CLA	A	809	X	-	-	-
25	CLA	A	810	X	-	-	-
25	CLA	A	811	X	-	-	-
25	CLA	A	812	X	-	-	-
25	CLA	A	813	X	-	-	-
25	CLA	A	814	X	-	-	-
25	CLA	A	815	X	-	-	-
25	CLA	A	816	X	-	-	-
25	CLA	A	818	X	-	-	-
25	CLA	A	819	X	-	-	-
25	CLA	A	820	X	-	-	-
25	CLA	A	821	X	-	-	-
25	CLA	A	822	X	-	-	-
25	CLA	A	823	X	-	-	-
25	CLA	A	824	X	-	-	-
25	CLA	A	825	X	-	-	-
25	CLA	A	826	X	-	-	-
25	CLA	A	827	X	-	-	-
25	CLA	A	829	X	-	-	-
25	CLA	A	830	X	-	-	-
25	CLA	A	831	X	-	-	-
25	CLA	A	832	X	-	-	-
25	CLA	A	834	X	-	-	-
25	CLA	A	835	X	-	-	-
25	CLA	A	836	X	-	-	-
25	CLA	A	837	X	-	-	-
25	CLA	A	839	X	-	-	-
25	CLA	A	841	X	-	-	-
25	CLA	A	842	X	-	-	-
25	CLA	A	843	X	-	-	-
25	CLA	A	845	X	-	-	-
25	CLA	A	856	X	-	-	-
25	CLA	B	802	X	-	-	-
25	CLA	B	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	804	X	-	-	-
25	CLA	B	805	X	-	-	-
25	CLA	B	806	X	-	-	-
25	CLA	B	807	X	-	-	-
25	CLA	B	808	X	-	-	-
25	CLA	B	809	X	-	-	-
25	CLA	B	810	X	-	-	-
25	CLA	B	811	X	-	-	-
25	CLA	B	812	X	-	-	-
25	CLA	B	813	X	-	-	-
25	CLA	B	814	X	-	-	-
25	CLA	B	815	X	-	-	-
25	CLA	B	816	X	-	-	-
25	CLA	B	817	X	-	-	-
25	CLA	B	818	X	-	-	-
25	CLA	B	819	X	-	-	-
25	CLA	B	820	X	-	-	-
25	CLA	B	821	X	-	-	-
25	CLA	B	822	X	-	-	-
25	CLA	B	823	X	-	-	-
25	CLA	B	824	X	-	-	-
25	CLA	B	825	X	-	-	-
25	CLA	B	826	X	-	-	-
25	CLA	B	827	X	-	-	-
25	CLA	B	828	X	-	-	-
25	CLA	B	829	X	-	-	-
25	CLA	B	830	X	-	-	-
25	CLA	B	831	X	-	-	-
25	CLA	B	832	X	-	-	-
25	CLA	B	833	X	-	-	-
25	CLA	B	834	X	-	-	-
25	CLA	B	835	X	-	-	-
25	CLA	B	837	X	-	-	-
25	CLA	B	838	X	-	-	-
25	CLA	B	839	X	-	-	-
25	CLA	B	841	X	-	-	-
25	CLA	B	842	X	-	-	-
25	CLA	B	843	X	-	-	-
25	CLA	F	802	X	-	-	-
25	CLA	F	803	X	-	-	-
25	CLA	G	202	X	-	-	-
25	CLA	G	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	G	204	X	-	-	-
25	CLA	H	301	X	-	-	-
25	CLA	H	302	X	-	-	-
25	CLA	H	304	X	-	-	-
25	CLA	J	102	X	-	-	-
25	CLA	K	201	X	-	-	-
25	CLA	K	203	X	-	-	-
25	CLA	K	204	X	-	-	-
25	CLA	K	206	X	-	-	-
25	CLA	L	301	X	-	-	-
25	CLA	L	303	X	-	-	-
25	CLA	L	304	X	-	-	-
25	CLA	N	202	X	-	-	-
25	CLA	N	203	X	-	-	-
25	CLA	O	2001	X	-	-	-
25	CLA	O	2002	X	-	-	-
25	CLA	O	2003	X	-	-	-
25	CLA	O	2004	X	-	-	-
25	CLA	O	2005	X	-	-	-
25	CLA	P	301	X	-	-	-
25	CLA	P	302	X	-	-	-
25	CLA	P	303	X	-	-	-
25	CLA	P	309	X	-	-	-
25	CLA	P	310	X	-	-	-
25	CLA	P	311	X	-	-	-
25	CLA	P	312	X	-	-	-
25	CLA	Q	301	X	-	-	-
25	CLA	Q	304	X	-	-	-
25	CLA	Q	305	X	-	-	-
25	CLA	Q	306	X	-	-	-
25	CLA	Q	311	X	-	-	-
25	CLA	Q	312	X	-	-	-
25	CLA	Q	313	X	-	-	-
25	CLA	Q	314	X	-	-	-
25	CLA	Q	315	X	-	-	-
25	CLA	R	305	X	-	-	-
25	CLA	R	306	X	-	-	-
25	CLA	R	307	X	-	-	-
25	CLA	R	313	X	-	-	-
25	CLA	R	314	X	-	-	-
25	CLA	R	315	X	-	-	-
25	CLA	R	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	301	X	-	-	-
25	CLA	S	302	X	-	-	-
25	CLA	S	303	X	-	-	-
25	CLA	S	309	X	-	-	-
25	CLA	S	310	X	-	-	-
25	CLA	S	311	X	-	-	-
25	CLA	S	312	X	-	-	-
25	CLA	S	313	X	-	-	-
25	CLA	T	301	X	-	-	-
25	CLA	T	302	X	-	-	-
25	CLA	T	303	X	-	-	-
25	CLA	T	309	X	-	-	-
25	CLA	T	310	X	-	-	-
25	CLA	T	311	X	-	-	-
25	CLA	T	312	X	-	-	-
25	CLA	T	313	X	-	-	-
25	CLA	U	301	X	-	-	-
25	CLA	U	302	X	-	-	-
25	CLA	U	303	X	-	-	-
25	CLA	U	308	X	-	-	-
25	CLA	U	309	X	-	-	-
25	CLA	U	310	X	-	-	-
25	CLA	U	311	X	-	-	-
25	CLA	U	312	X	-	-	-
25	CLA	V	301	X	-	-	-
25	CLA	V	302	X	-	-	-
25	CLA	V	303	X	-	-	-
25	CLA	V	309	X	-	-	-
25	CLA	V	310	X	-	-	-
25	CLA	V	311	X	-	-	-
25	CLA	V	313	X	-	-	-
25	CLA	W	301	X	-	-	-
25	CLA	W	302	X	-	-	-
25	CLA	W	303	X	-	-	-
25	CLA	W	309	X	-	-	-
25	CLA	W	310	X	-	-	-
25	CLA	W	311	X	-	-	-
25	CLA	W	312	X	-	-	-
25	CLA	W	313	X	-	-	-
25	CLA	X	302	X	-	-	-
25	CLA	X	303	X	-	-	-
25	CLA	X	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	X	310	X	-	-	-
25	CLA	X	311	X	-	-	-
25	CLA	X	312	X	-	-	-
25	CLA	X	313	X	-	-	-
25	CLA	X	314	X	-	-	-
33	CL0	A	802	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 64832 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 Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	159	Total	C	N	O	S	0	0
			1209	768	219	213	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1583	1023	265	286	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	227	Total	C	N	O	S	0	0
			1717	1111	279	311	16		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	203	Total	C	N	O	S	0	0
			1579	1021	267	280	11		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	166	Total	C	N	O	S	0	0
			1278	826	215	226	11		

- Molecule 6 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	194	Total	C	N	O	S	0	0
			1484	963	243	269	9		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	742	Total	C	N	O	S	0	0
			5819	3802	990	1000	27		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	732	Total	C	N	O	S	0	0
			5773	3793	966	996	18		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	80	Total	C	N	O	S	0	0
			593	364	103	115	11		

- Molecule 10 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	143	Total	C	N	O	S	0	0
			1116	717	197	196	6		

- Molecule 11 is a protein called Photosystem I reaction centre subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	62	Total	C	N	O	S	0	0
			503	324	84	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	165	Total	C	N	O	S	0	0
			1259	808	212	235	4		

- Molecule 13 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	95	Total	C	N	O	S	0	0
			717	453	124	137	3		

- Molecule 14 is a protein called Photosystem I PsaH, reaction centre subunit VI.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	H	96	Total 721	C 456	N 122	O 143	0	0

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total 264	C 181	N 37	O 44	S 2	0	0

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	41	Total 328	C 225	N 49	O 53	S 1	0	0

- Molecule 17 is a protein called Photosystem I PsaG/PsaK protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	87	Total 625	C 393	N 106	O 121	S 5	0	0

- Molecule 18 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	158	Total 1169	C 759	N 190	O 217	S 3	0	0

- Molecule 19 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	31	Total 239	C 159	N 37	O 42	S 1	0	0

- Molecule 20 is a protein called Photosystem I PsaN, reaction centre subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	91	Total 676	C 415	N 118	O 138	S 5	0	0

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	96	Total	C	N	O	S	0	0
			759	498	123	132	6		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	R	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	S	202	Total	C	N	O	S	0	0
			1512	971	247	288	6		
22	T	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	U	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	V	197	Total	C	N	O	S	0	0
			1484	956	242	280	6		
22	W	200	Total	C	N	O	S	0	0
			1499	964	245	284	6		
22	X	196	Total	C	N	O	S	0	0
			1474	949	241	278	6		

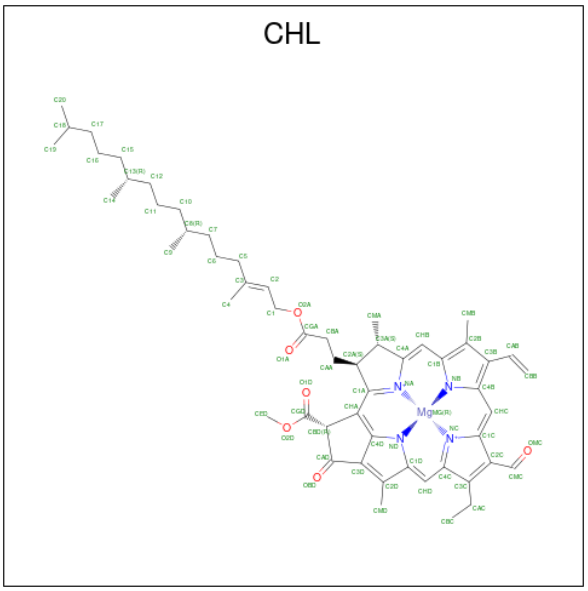
- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Q	226	Total	C	N	O	P	S	0	0
			1706	1100	285	313	1	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	28	ACE	-	acetylation	UNP A0A090LYE8

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	P	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	P	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	P	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	Q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	Q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	S	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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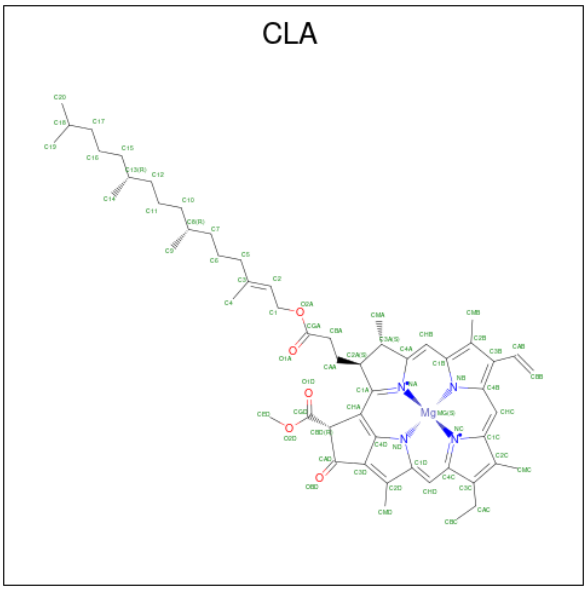
Mol	Chain	Residues	Atoms					AltConf
24	T	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	T	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
24	T	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	T	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	T	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	T	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	U	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	U	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	V	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	W	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	W	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	W	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	W	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	X	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	X	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	X	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
25	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	O	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	P	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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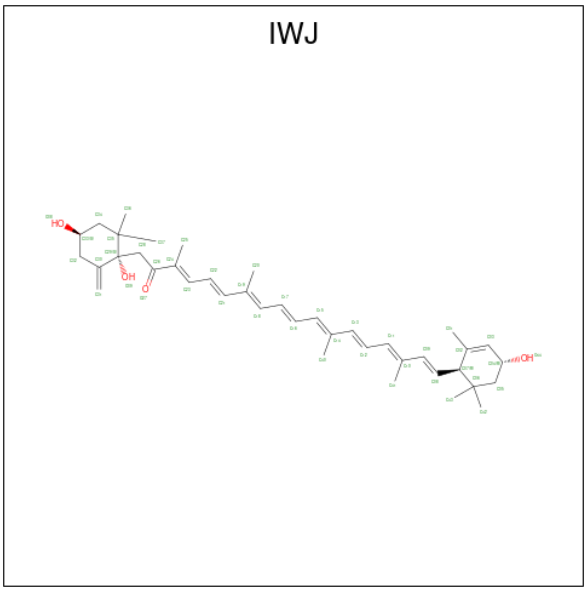
Mol	Chain	Residues	Atoms					AltConf
25	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	V	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	V	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	V	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	V	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	W	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 26 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methylidene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-2-one (CCD ID: IWJ) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



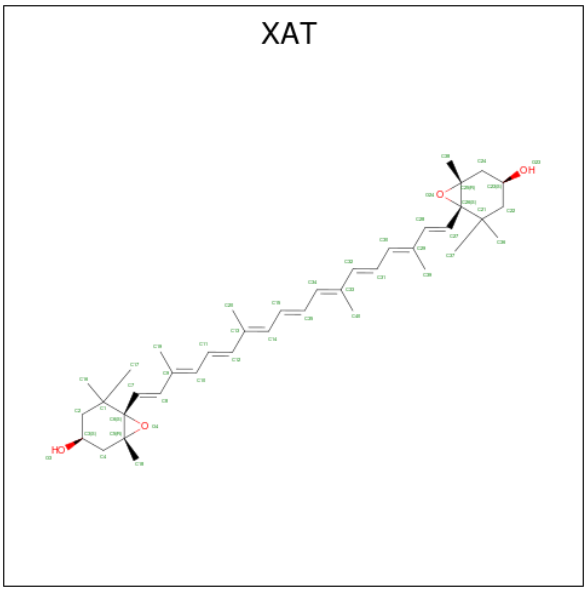
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			44	40	4	
26	3	1	Total	C	O	0
			44	40	4	
26	4	1	Total	C	O	0
			44	40	4	

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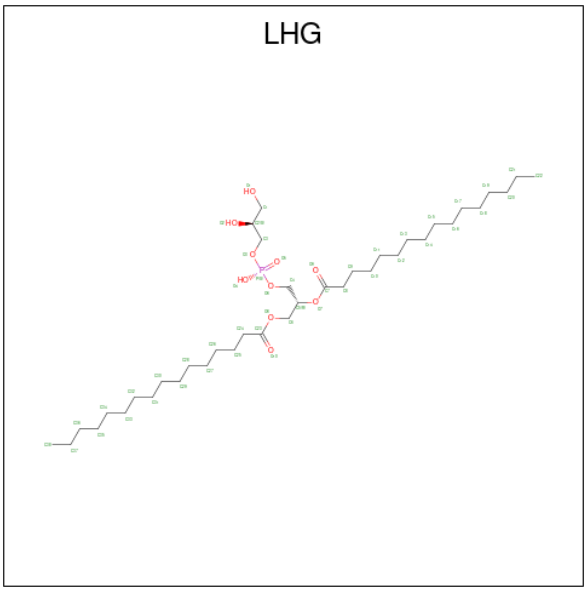
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	
26	6	1	Total	C	O	0
			44	40	4	
26	P	1	Total	C	O	0
			44	40	4	
26	P	1	Total	C	O	0
			44	40	4	
26	Q	1	Total	C	O	0
			44	40	4	
26	Q	1	Total	C	O	0
			44	40	4	
26	R	1	Total	C	O	0
			44	40	4	
26	R	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	T	1	Total	C	O	0
			44	40	4	
26	T	1	Total	C	O	0
			44	40	4	
26	U	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	W	1	Total	C	O	0
			44	40	4	
26	X	1	Total	C	O	0
			44	40	4	

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



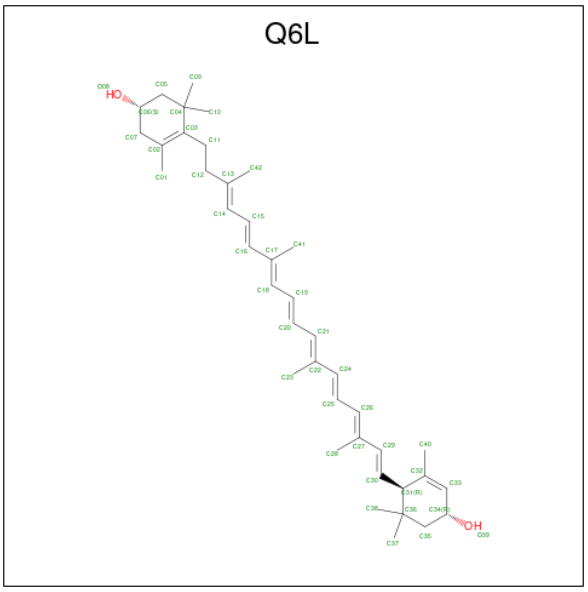
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total 35	C 24	O 10	P 1	0
28	2	1	Total 33	C 22	O 10	P 1	0
28	3	1	Total 23	C 13	O 9	P 1	0
28	3	1	Total 43	C 32	O 10	P 1	0
28	3	1	Total 36	C 25	O 10	P 1	0
28	3	1	Total 43	C 32	O 10	P 1	0
28	6	1	Total 46	C 35	O 10	P 1	0
28	A	1	Total 49	C 38	O 10	P 1	0
28	A	1	Total 30	C 19	O 10	P 1	0
28	Q	1	Total 35	C 24	O 10	P 1	0

- Molecule 29 is (1 {S})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaenyl]cyclohex-3-en-1-ol (CCD ID: Q6L) (formula: $C_{40}H_{58}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	

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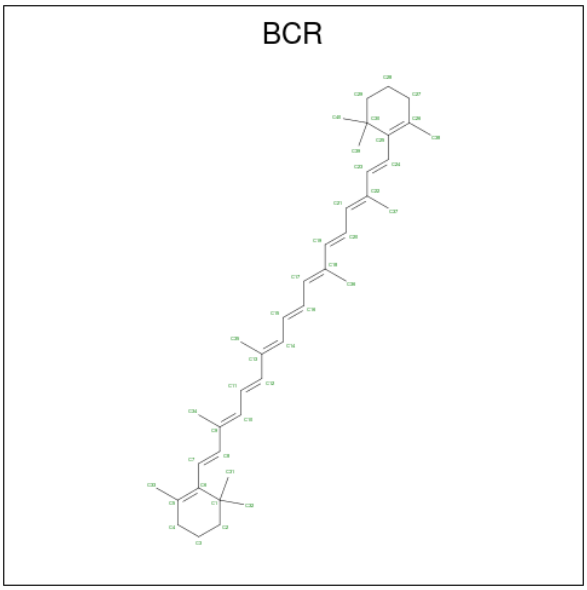
Mol	Chain	Residues	Atoms			AltConf
29	R	1	Total	C	O	0
			42	40	2	
29	S	1	Total	C	O	0
			42	40	2	
29	S	1	Total	C	O	0
			42	40	2	
29	S	1	Total	C	O	0
			42	40	2	
29	S	1	Total	C	O	0
			42	40	2	
29	S	1	Total	C	O	0
			42	40	2	
29	T	1	Total	C	O	0
			42	40	2	
29	T	1	Total	C	O	0
			42	40	2	
29	T	1	Total	C	O	0
			42	40	2	
29	T	1	Total	C	O	0
			42	40	2	
29	U	1	Total	C	O	0
			42	40	2	
29	U	1	Total	C	O	0
			42	40	2	
29	U	1	Total	C	O	0
			42	40	2	
29	V	1	Total	C	O	0
			42	40	2	
29	V	1	Total	C	O	0
			42	40	2	
29	V	1	Total	C	O	0
			42	40	2	
29	V	1	Total	C	O	0
			42	40	2	
29	W	1	Total	C	O	0
			42	40	2	
29	W	1	Total	C	O	0
			42	40	2	
29	W	1	Total	C	O	0
			42	40	2	
29	W	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
29	X	1	Total C O 42 40 2	0
29	X	1	Total C 40 40	0
29	X	1	Total C O 42 40 2	0
29	X	1	Total C O 42 40 2	0

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
30	2	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	4	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0

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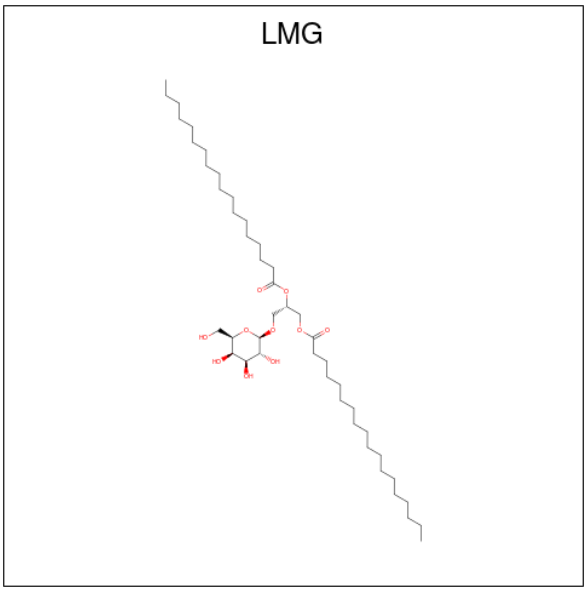
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	I	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
30	L	1	Total C 40 40	0
30	M	1	Total C 40 40	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



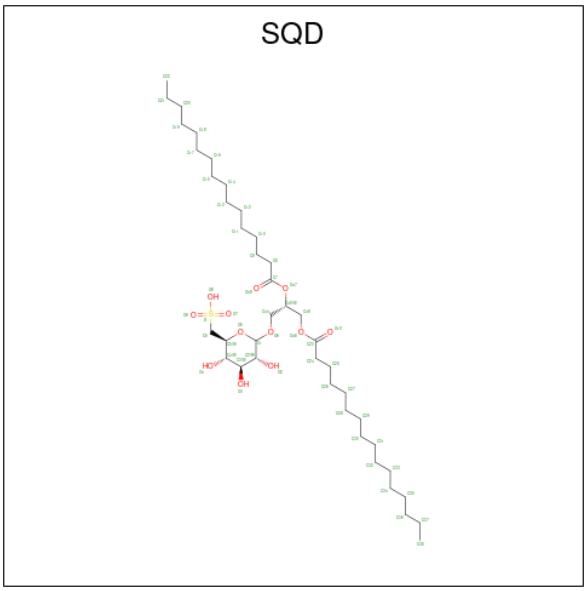
Mol	Chain	Residues	Atoms	AltConf
31	2	1	Total C O 31 21 10	0
31	5	1	Total C O 54 44 10	0
31	A	1	Total C O 31 21 10	0
31	A	1	Total C O 27 17 10	0
31	A	1	Total C O 46 36 10	0
31	B	1	Total C O 38 28 10	0
31	F	1	Total C O 31 21 10	0
31	J	1	Total C O 46 36 10	0
31	L	1	Total C O 31 21 10	0

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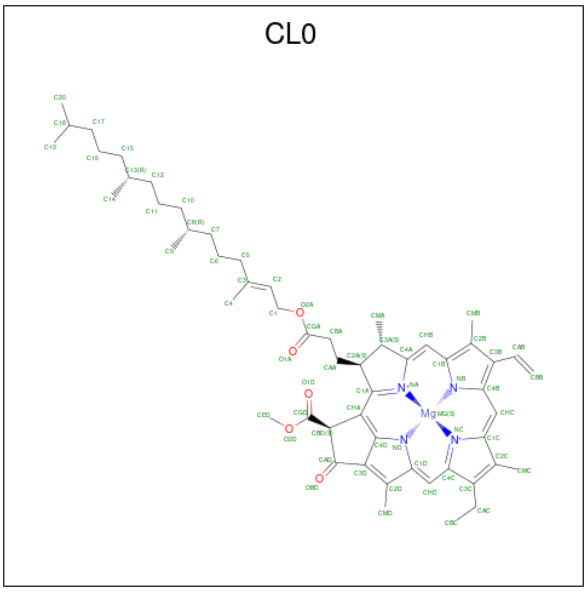
Mol	Chain	Residues	Atoms	AltConf
31	N	1	Total C O 55 45 10	0
31	O	1	Total C O 39 29 10	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



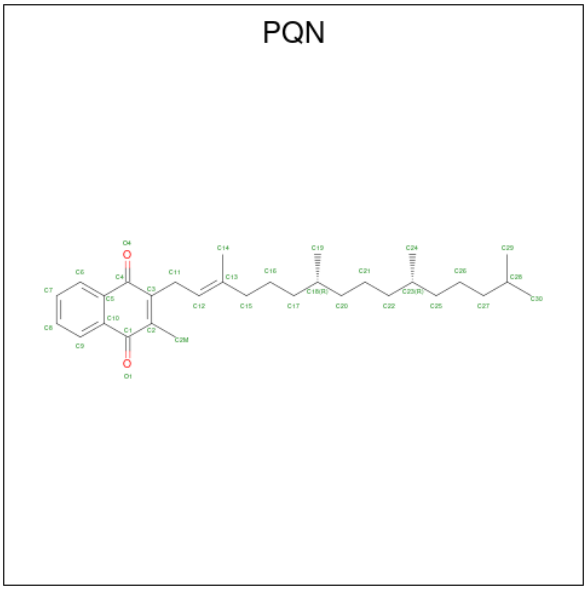
Mol	Chain	Residues	Atoms	AltConf
32	6	1	Total C O S 54 41 12 1	0
32	H	1	Total C O S 48 35 12 1	0

- Molecule 33 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



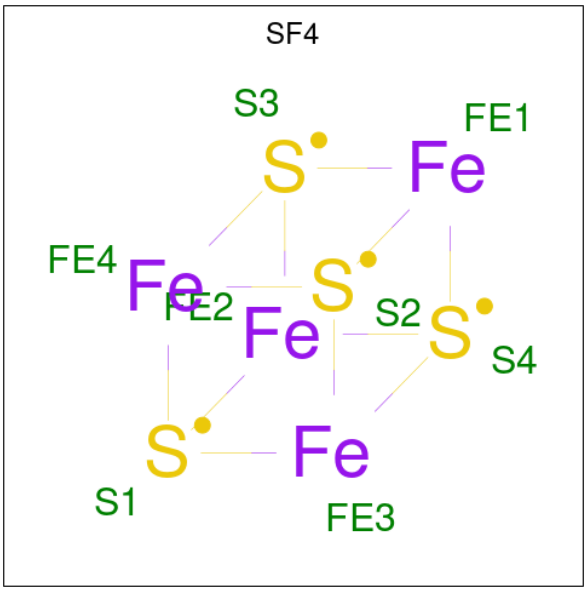
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 34 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



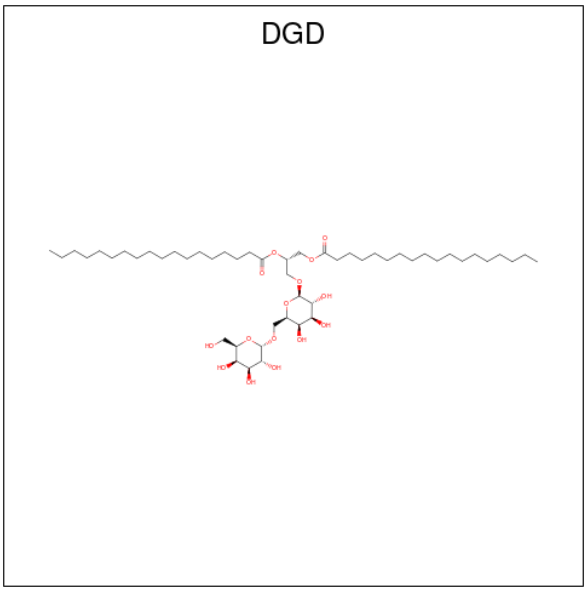
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			33	31	2	
34	B	1	Total	C	O	0
			33	31	2	

- Molecule 35 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



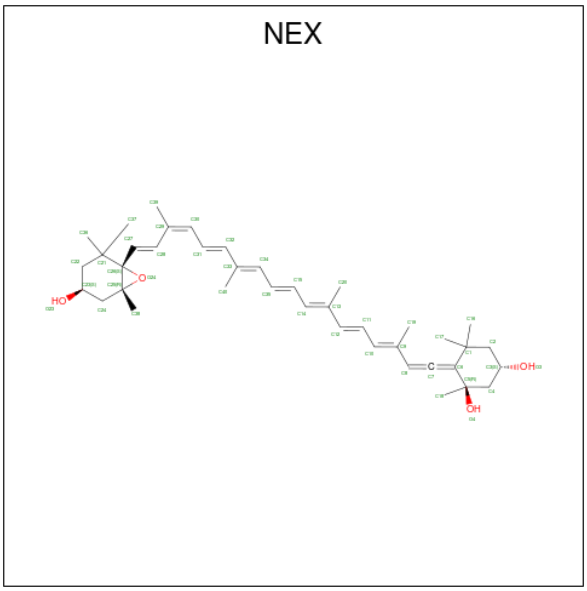
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total Fe S 8 4 4	0
35	C	1	Total Fe S 8 4 4	0
35	C	1	Total Fe S 8 4 4	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



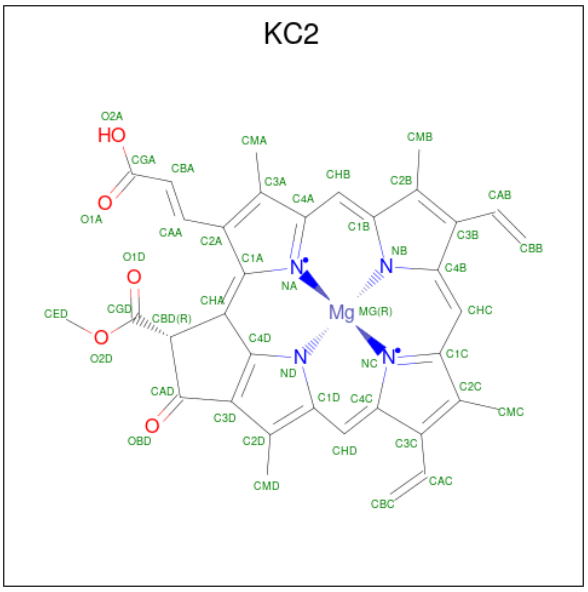
Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total C O 51 36 15	0
36	B	1	Total C O 59 44 15	0

- Molecule 37 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
37	H	1	Total C O 44 40 4	0
37	P	1	Total C O 44 40 4	0
37	R	1	Total C O 44 40 4	0
37	S	1	Total C O 44 40 4	0
37	T	1	Total C O 44 40 4	0
37	W	1	Total C O 44 40 4	0

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	3	Total	O	0
			3	3	
39	Q	1	Total	O	0
			1	1	

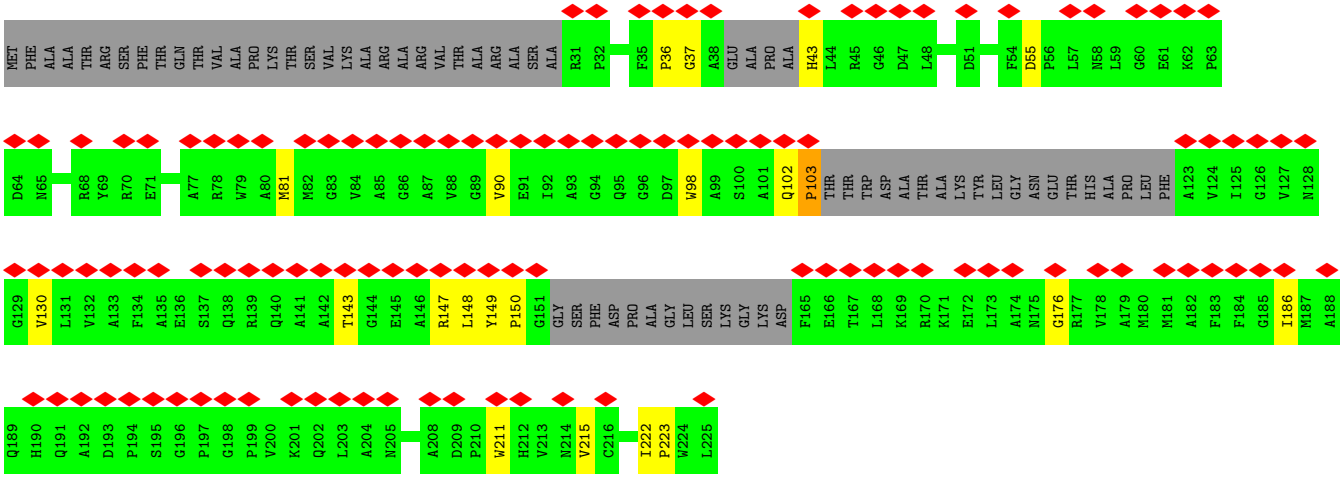
3 Residue-property plots (i)

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

• Molecule 1: Lhca1

Chain 1:

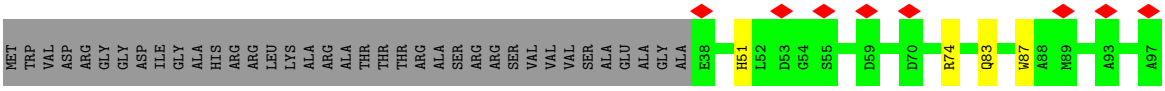


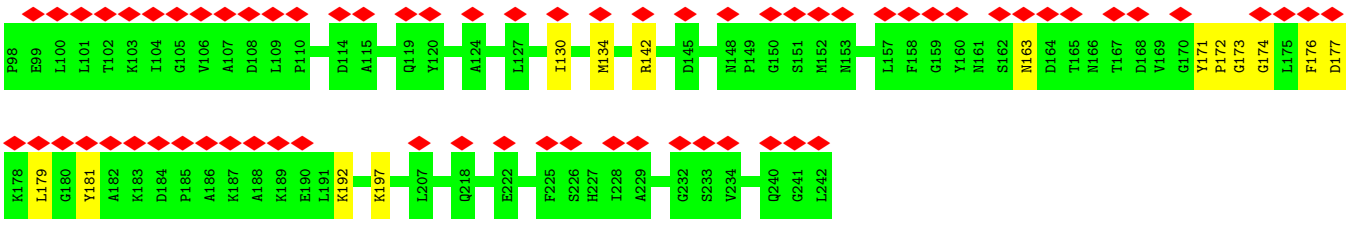


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



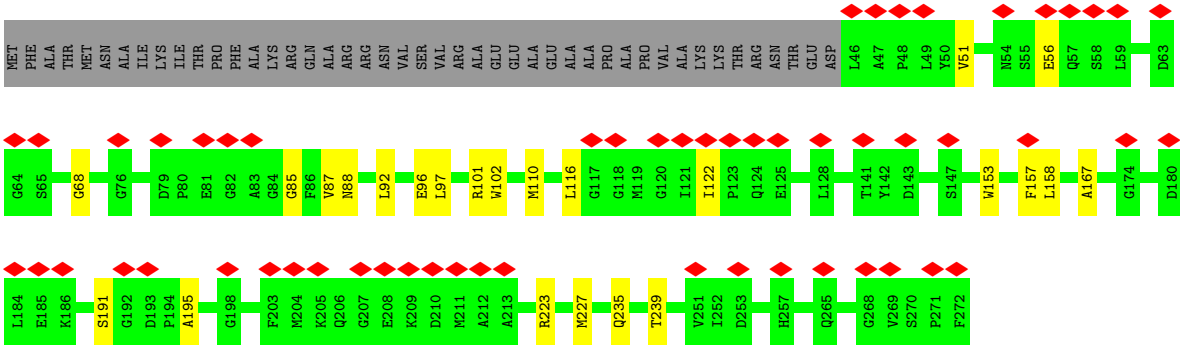




• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

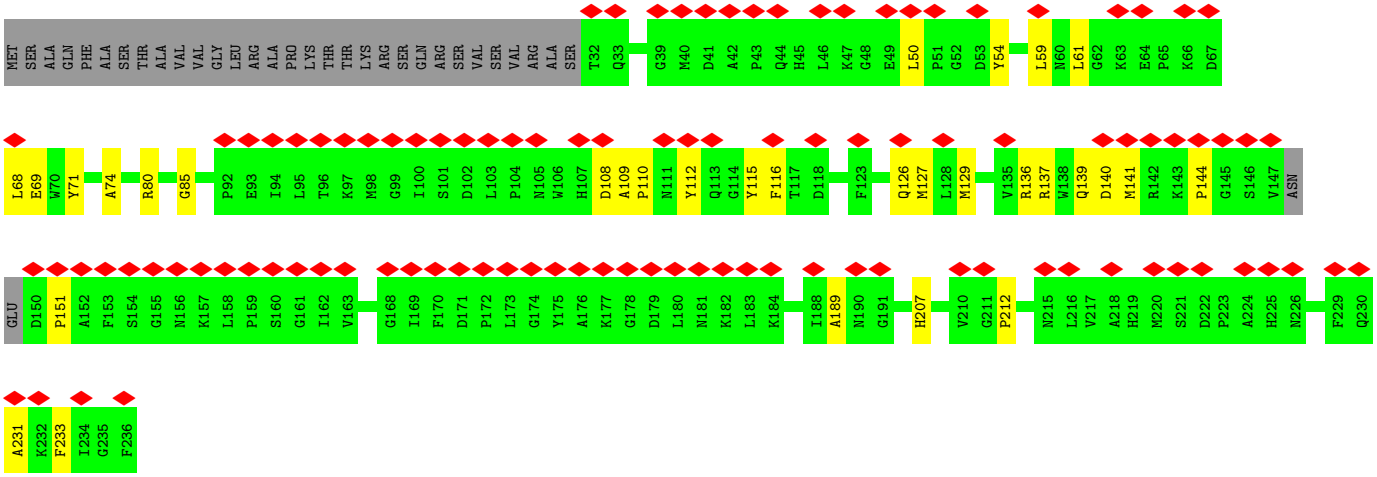
Chain 3:





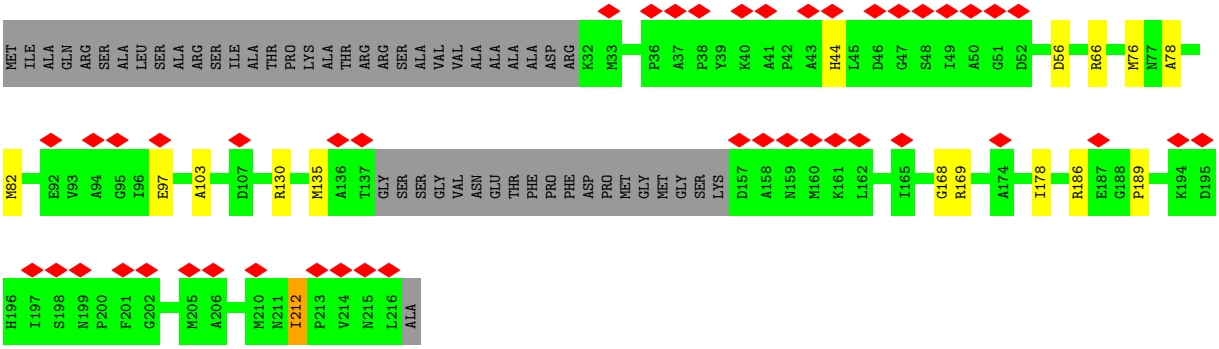
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic





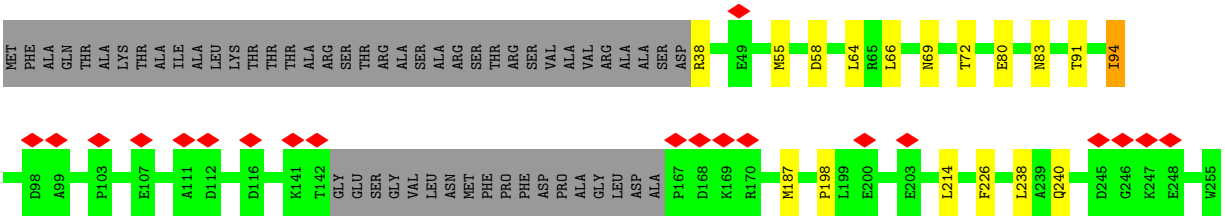
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic



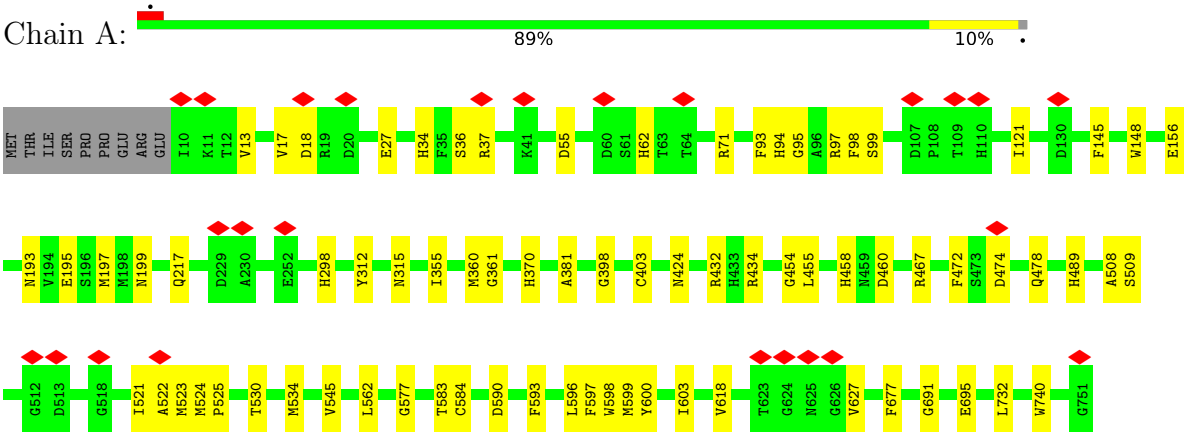


• Molecule 6: Lhca6

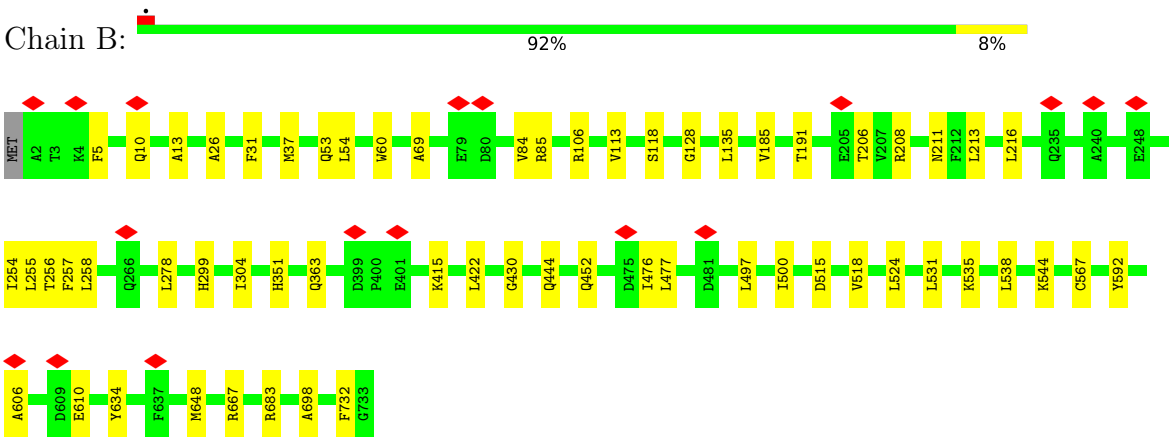




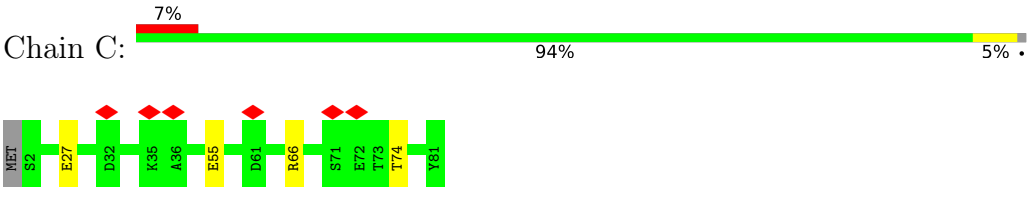
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

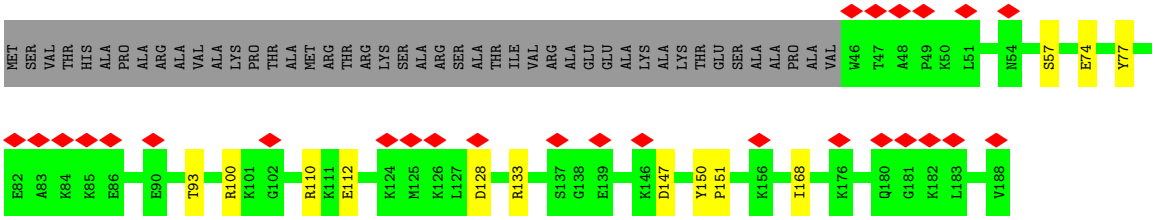


• Molecule 9: Photosystem I iron-sulfur center



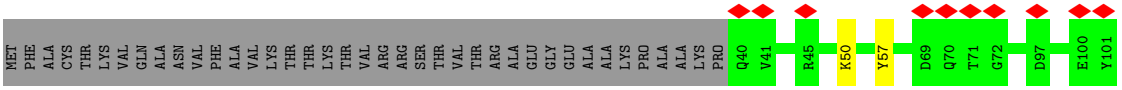
• Molecule 10: Photosystem I reaction center subunit II, chloroplastic





• Molecule 11: Photosystem I reaction centre subunit IV

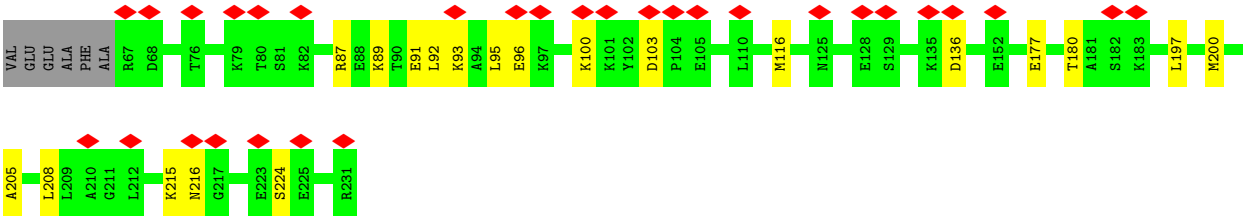




• Molecule 12: Photosystem I reaction center subunit III

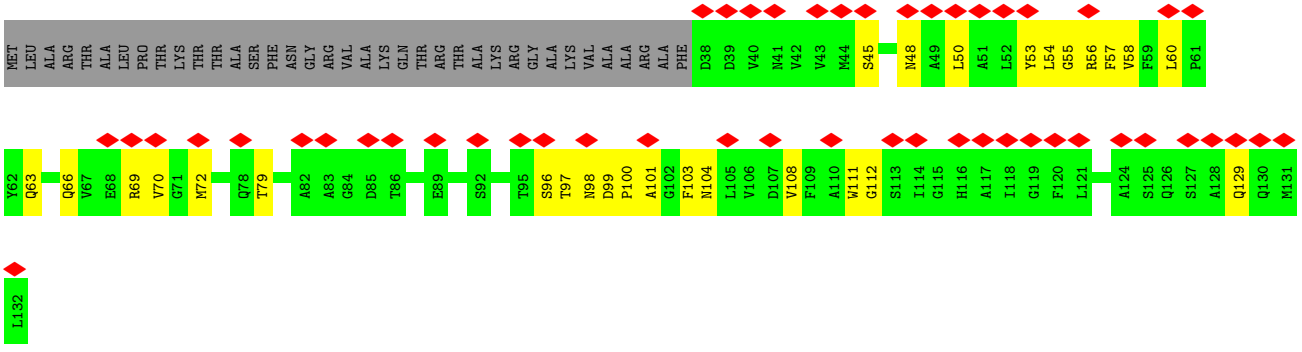






• Molecule 13: PsaG

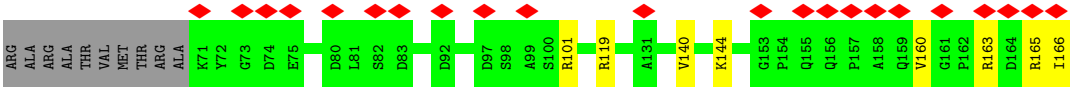




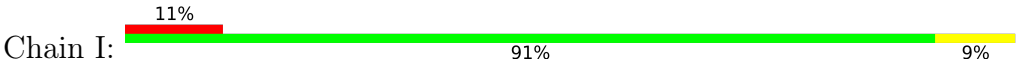
• Molecule 14: Photosystem I PsaH, reaction centre subunit VI

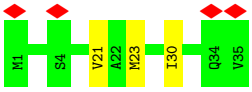




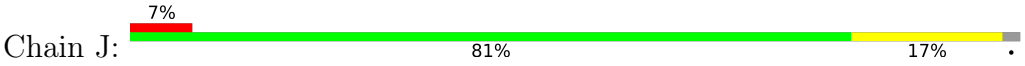


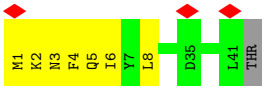
• Molecule 15: Photosystem I reaction center subunit VIII





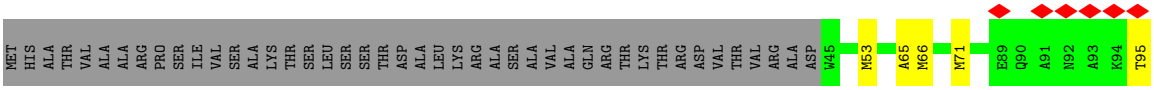
• Molecule 16: Photosystem I reaction center subunit IX

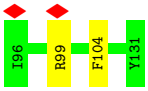




• Molecule 17: Photosystem I PsaG/PsaK protein

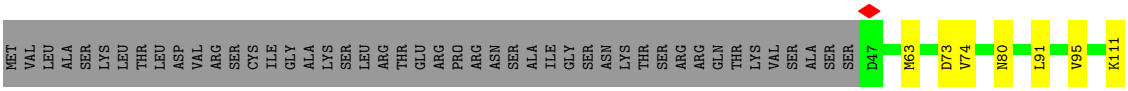


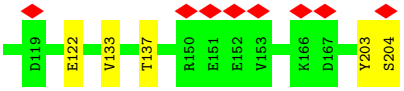




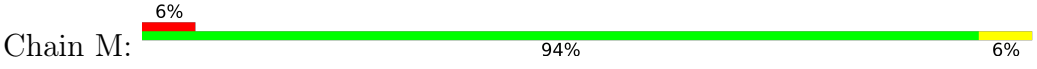
• Molecule 18: PSI subunit V

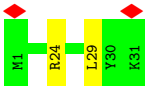






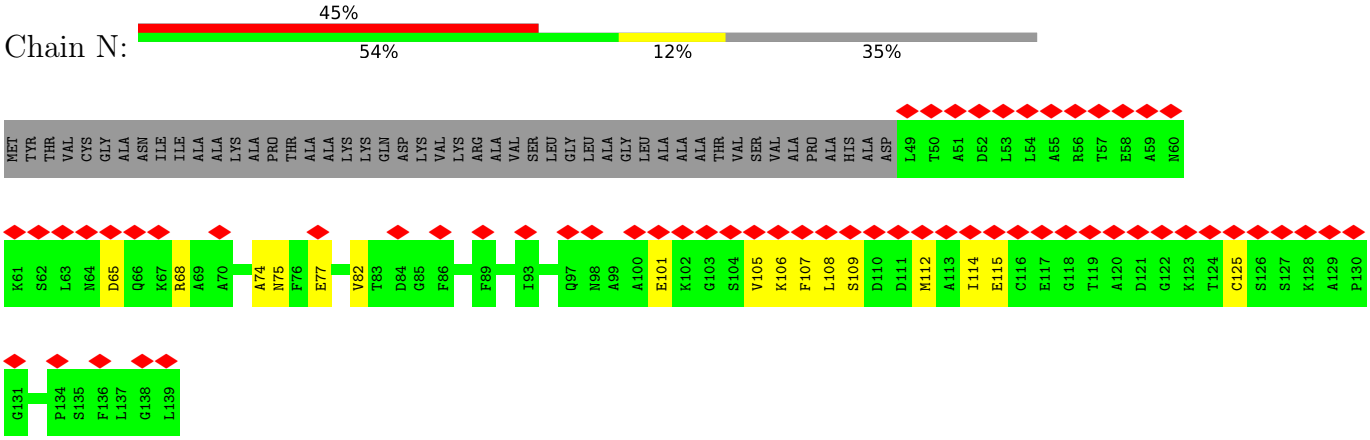
• Molecule 19: Photosystem I reaction center subunit XII





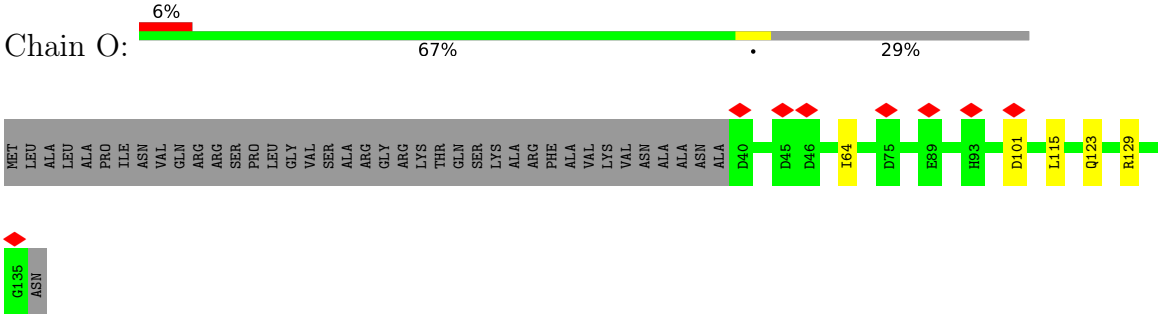
• Molecule 20: Photosystem I PsaN, reaction centre subunit N

Chain N:



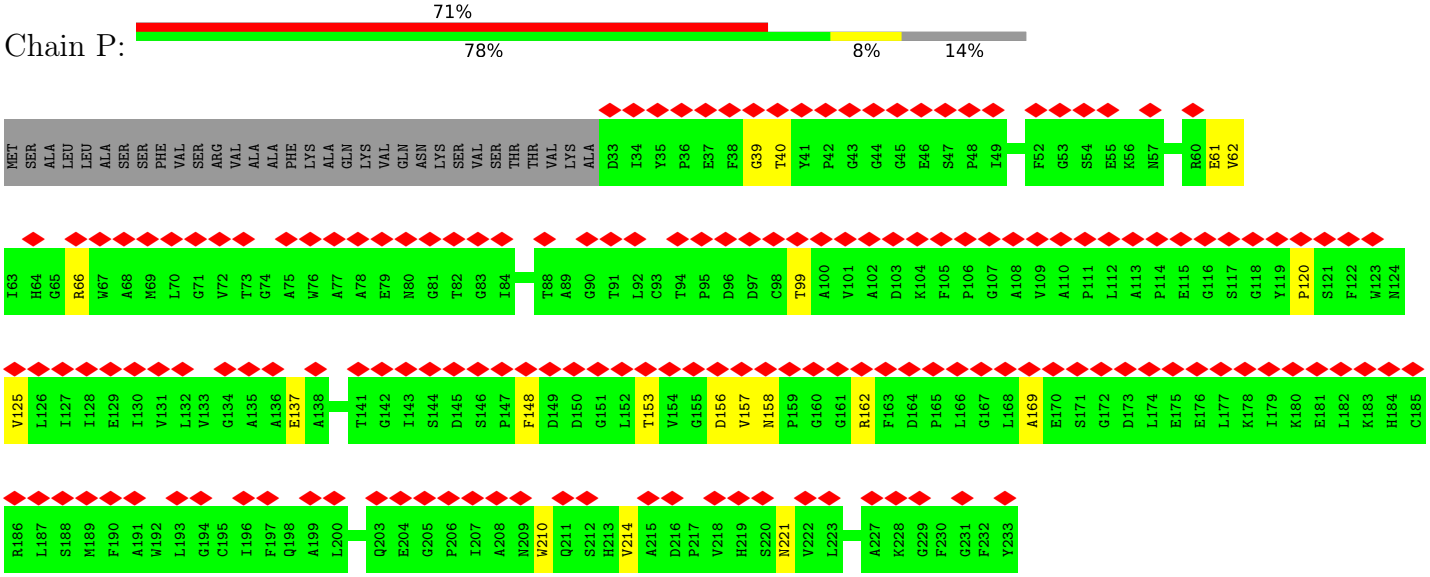
• Molecule 21: PsaO

Chain O:



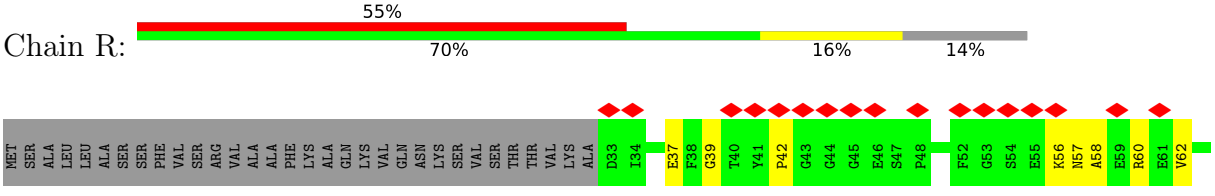
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

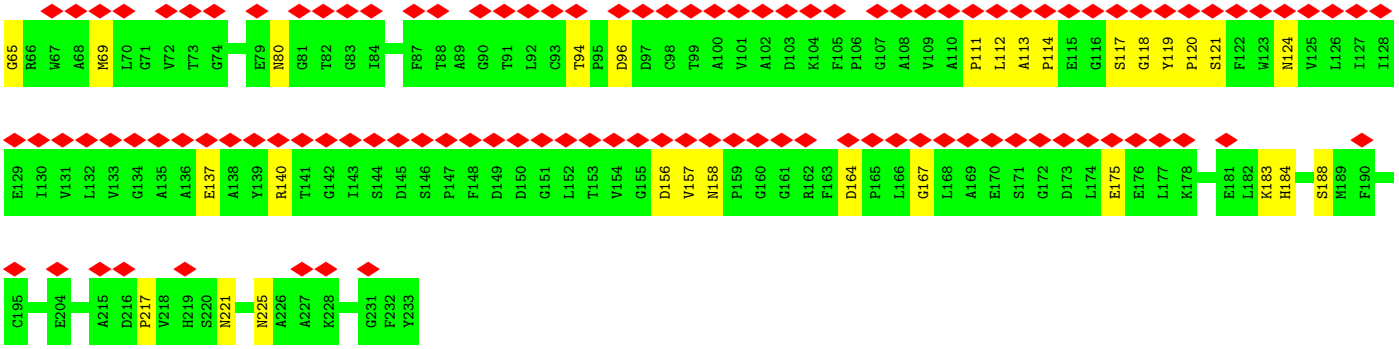
Chain P:



• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain R:



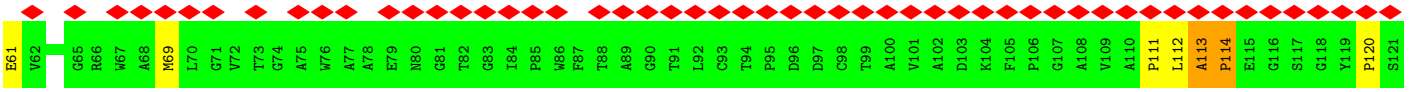


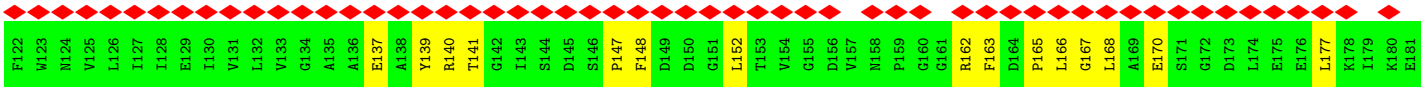
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

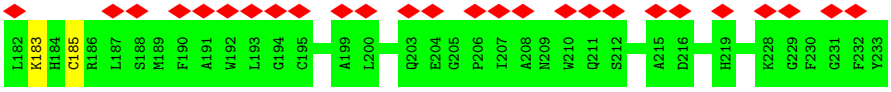
Chain S:







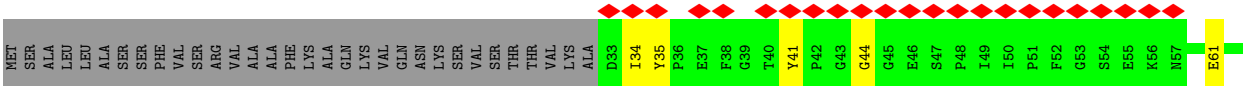


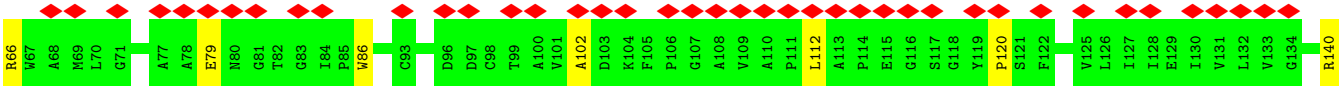


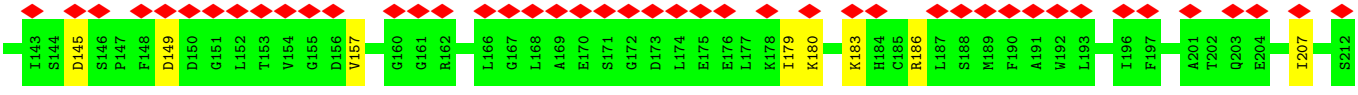
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

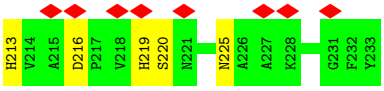
Chain T:



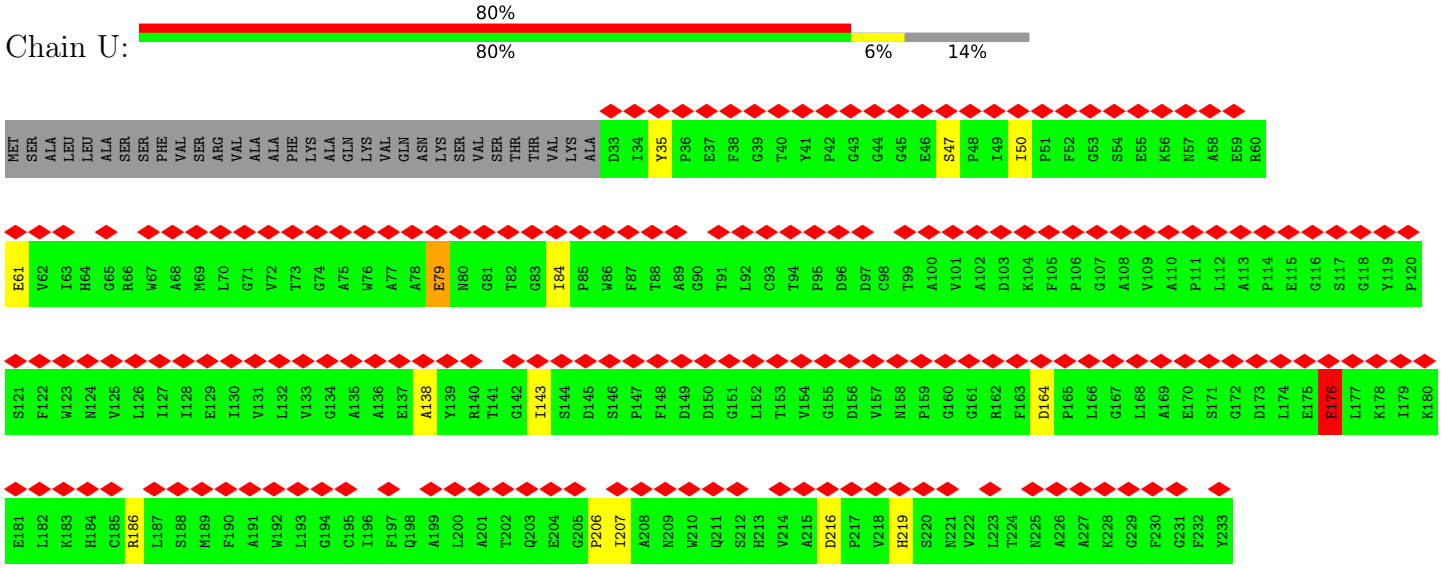




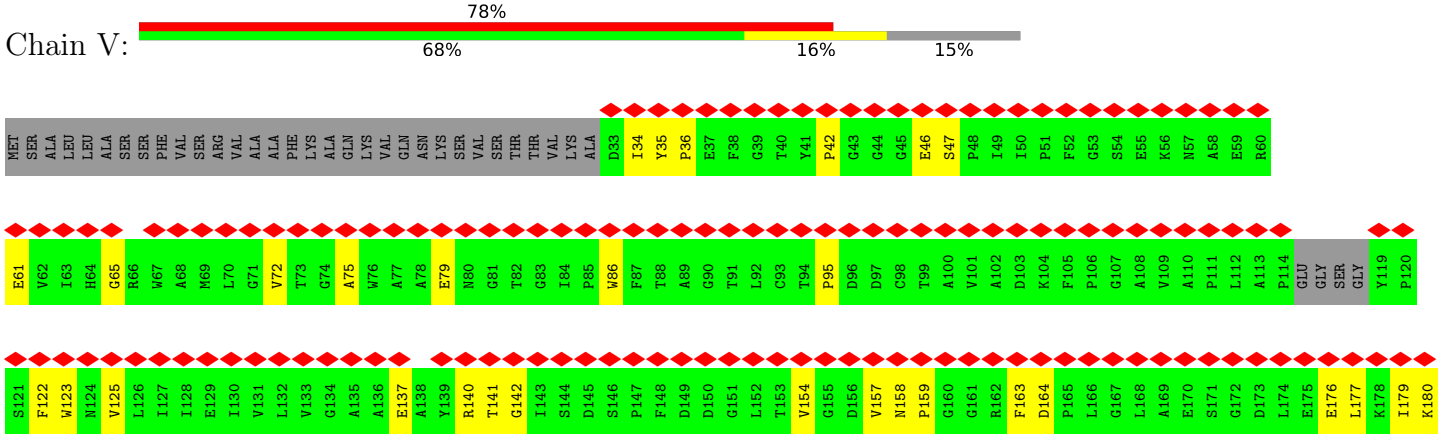




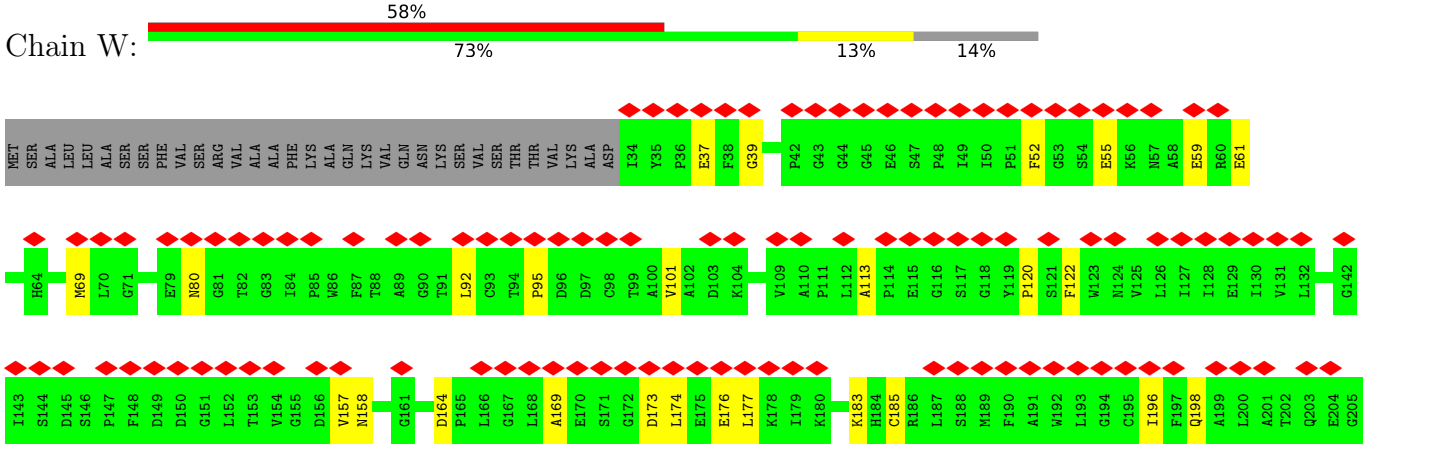
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

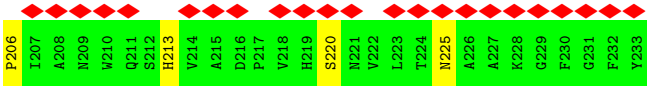


• Molecule 22: Chlorophyll a-b binding protein, chloroplastic



• Molecule 22: Chlorophyll a-b binding protein, chloroplastic



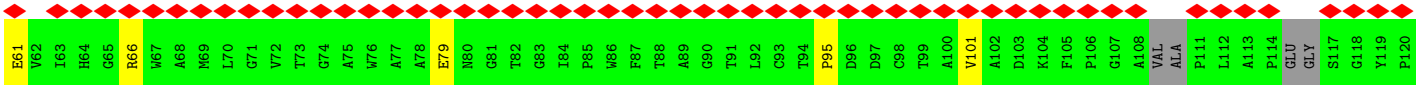


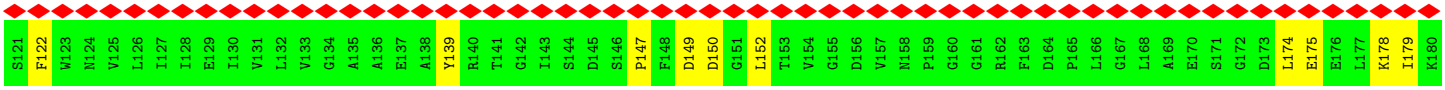
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain X:









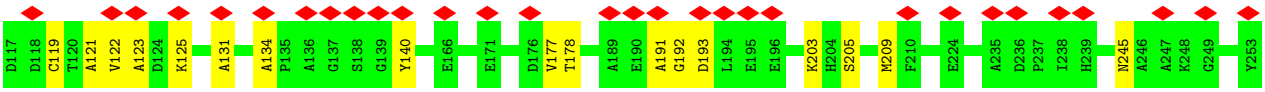


• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain Q:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IWJ, KC2, TPO, BCR, PQN, SF4, CLA, CHL, SQD, XAT, LMG, DGD, ACE, LHG, NEX, Q6L, CL0

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	1	0.59	1/1242 (0.1%)	0.71	2/1686 (0.1%)
2	2	0.48	0/1634	0.63	0/2224
3	3	0.51	0/1768	0.70	0/2394
4	4	0.47	0/1630	0.65	1/2215 (0.0%)
5	5	0.50	1/1312 (0.1%)	0.64	0/1783
6	6	0.41	1/1522 (0.1%)	0.56	0/2068
7	A	0.41	0/6017	0.55	0/8202
8	B	0.41	0/5981	0.54	0/8166
9	C	0.43	0/603	0.64	0/818
10	D	0.46	0/1142	0.66	1/1537 (0.1%)
11	E	0.35	0/516	0.57	0/703
12	F	0.40	0/1286	0.57	0/1739
13	G	0.49	0/732	0.70	0/995
14	H	0.35	0/736	0.52	0/1001
15	I	0.57	0/270	0.69	0/368
16	J	0.43	0/338	0.58	0/462
17	K	0.40	0/635	0.55	0/860
18	L	0.41	0/1197	0.52	0/1635
19	M	0.43	0/242	0.46	0/328
20	N	0.47	0/685	0.75	1/921 (0.1%)
21	O	0.45	1/787 (0.1%)	0.52	0/1070
22	P	0.46	0/1553	0.69	0/2122
22	R	0.47	0/1553	0.77	2/2122 (0.1%)
22	S	0.46	0/1558	0.72	2/2129 (0.1%)
22	T	0.43	1/1553 (0.1%)	0.62	0/2122
22	U	0.46	1/1553 (0.1%)	0.67	1/2122 (0.0%)
22	V	0.54	2/1529 (0.1%)	0.70	1/2089 (0.0%)
22	W	0.45	0/1545	0.66	1/2111 (0.0%)
22	X	0.44	0/1518	0.69	2/2070 (0.1%)
23	Q	0.50	1/1746 (0.1%)	0.72	1/2379 (0.0%)
All	All	0.45	9/44383 (0.0%)	0.63	15/60441 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
22	U	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	103	PRO	CB-CG	9.42	1.96	1.49
22	T	35	TYR	C-O	7.19	1.27	1.23
21	O	64	ILE	CA-CB	-7.08	1.50	1.54
22	V	164	ASP	N-CA	6.34	1.50	1.46
5	5	212	ILE	CA-CB	-6.25	1.50	1.54
22	U	79	GLU	CG-CD	-5.98	1.37	1.52
22	V	164	ASP	C-O	5.66	1.26	1.23
6	6	94	ILE	CG1-CD1	-5.59	1.29	1.51
23	Q	80	GLU	CD-OE1	-5.16	1.15	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	111	PRO	CA-N-CD	-8.52	100.07	112.00
1	1	103	PRO	CB-CG-CD	-7.69	81.50	106.10
22	S	114	PRO	CA-N-CD	-7.23	101.88	112.00
22	X	149	ASP	CA-C-N	6.53	133.24	122.73
22	X	149	ASP	C-N-CA	6.53	133.24	122.73
22	U	176	GLU	CG-CD-OE1	5.97	132.12	118.40
20	N	125	CYS	CA-CB-SG	5.85	127.85	114.40
22	W	55	GLU	CB-CG-CD	5.79	122.45	112.60
22	V	36	PRO	CA-N-CD	-5.63	104.11	112.00
4	4	69	GLU	OE1-CD-OE2	-5.59	109.47	122.90
22	R	175	GLU	CG-CD-OE2	5.56	131.19	118.40
1	1	102	GLN	C-N-CD	5.39	147.10	125.00
23	Q	80	GLU	CB-CG-CD	5.31	121.63	112.60
10	D	147	ASP	OD1-CG-OD2	-5.02	110.86	122.90
22	S	113	ALA	CA-C-O	-5.01	115.88	120.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	U	176	GLU	Mainchain

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	1	1209	0	1167	16	0
2	2	1583	0	1529	17	0
3	3	1717	0	1657	19	0
4	4	1579	0	1521	27	0
5	5	1278	0	1267	16	0
6	6	1484	0	1465	13	0
7	A	5819	0	5655	60	0
8	B	5773	0	5540	45	0
9	C	593	0	573	4	0
10	D	1116	0	1151	9	0
11	E	503	0	489	2	0
12	F	1259	0	1285	16	0
13	G	717	0	685	35	0
14	H	721	0	698	8	0
15	I	264	0	286	8	0
16	J	328	0	341	6	0
17	K	625	0	625	10	0
18	L	1169	0	1186	7	0
19	M	239	0	262	2	0
20	N	676	0	650	13	0
21	O	759	0	722	7	0
22	P	1507	0	1429	20	0
22	R	1507	0	1429	40	0
22	S	1512	0	1434	35	0
22	T	1507	0	1429	20	0
22	U	1507	0	1429	11	0
22	V	1484	0	1411	33	0
22	W	1499	0	1425	25	0
22	X	1474	0	1401	26	0
23	Q	1706	0	1649	33	0
24	1	96	0	68	1	0
24	2	177	0	115	0	0
24	3	45	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4	181	0	117	4	0
24	5	41	0	24	0	0
24	6	127	0	77	0	0
24	P	233	0	163	1	0
24	Q	185	0	130	1	0
24	R	284	0	200	9	0
24	S	223	0	151	7	0
24	T	282	0	199	2	0
24	U	175	0	118	1	0
24	V	221	0	153	3	0
24	W	243	0	189	1	0
24	X	225	0	155	2	0
25	1	424	0	334	5	0
25	2	530	0	430	6	0
25	3	602	0	470	5	0
25	4	510	0	396	4	0
25	5	430	0	345	2	0
25	6	494	0	412	5	0
25	A	2557	0	2585	16	0
25	B	2465	0	2485	25	0
25	F	83	0	60	1	0
25	G	132	0	97	3	0
25	H	154	0	138	0	0
25	J	42	0	31	1	0
25	K	218	0	201	3	0
25	L	188	0	152	0	0
25	N	87	0	61	0	0
25	O	247	0	217	2	0
25	P	467	0	454	5	0
25	Q	458	0	387	8	0
25	R	467	0	454	5	0
25	S	443	0	414	13	0
25	T	438	0	411	3	0
25	U	378	0	296	1	0
25	V	412	0	347	13	0
25	W	427	0	379	11	0
25	X	373	0	290	9	0
26	1	44	0	0	0	0
26	3	44	0	0	1	0
26	4	88	0	0	2	0
26	5	44	0	0	0	0
26	6	44	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	88	0	0	2	0
26	Q	88	0	0	1	0
26	R	88	0	0	1	0
26	S	132	0	0	2	0
26	T	88	0	0	2	0
26	U	44	0	0	0	0
26	V	132	0	0	2	0
26	W	44	0	0	2	0
26	X	44	0	0	0	0
27	1	44	0	56	0	0
27	2	44	0	56	0	0
27	3	44	0	56	1	0
27	4	44	0	56	1	0
27	5	44	0	56	0	0
27	6	44	0	56	1	0
28	1	35	0	40	1	0
28	2	33	0	36	1	0
28	3	145	0	180	0	0
28	6	46	0	65	1	0
28	A	79	0	104	0	0
28	Q	35	0	40	0	0
29	2	42	0	0	1	0
29	O	84	0	0	1	0
29	P	168	0	0	1	0
29	Q	126	0	0	1	0
29	R	210	0	0	0	0
29	S	210	0	0	1	0
29	T	168	0	0	1	0
29	U	126	0	0	2	0
29	V	168	0	0	1	0
29	W	168	0	0	2	0
29	X	166	0	0	1	0
30	2	40	0	56	0	0
30	3	120	0	168	1	0
30	4	40	0	56	2	0
30	A	200	0	280	3	0
30	B	200	0	280	2	0
30	F	80	0	112	1	0
30	G	80	0	112	4	0
30	H	40	0	56	0	0
30	I	40	0	56	0	0
30	J	80	0	112	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	K	120	0	168	2	0
30	L	120	0	168	2	0
30	M	40	0	56	1	0
31	2	31	0	32	0	0
31	5	54	0	81	0	0
31	A	104	0	121	0	0
31	B	38	0	46	0	0
31	F	31	0	32	1	0
31	J	46	0	65	0	0
31	L	31	0	32	0	0
31	N	55	0	86	0	0
31	O	39	0	48	0	0
32	6	54	0	78	0	0
32	H	48	0	60	1	0
33	A	65	0	72	0	0
34	A	33	0	46	1	0
34	B	33	0	46	0	0
35	A	8	0	0	0	0
35	C	16	0	0	0	0
36	A	51	0	60	1	0
36	B	59	0	79	1	0
37	H	44	0	56	0	0
37	P	44	0	56	1	0
37	R	44	0	56	0	0
37	S	44	0	56	0	0
37	T	44	0	56	0	0
37	W	44	0	56	0	0
38	P	45	0	0	1	0
38	Q	45	0	0	0	0
38	R	45	0	0	2	0
38	S	45	0	0	1	0
38	T	45	0	0	1	0
38	U	45	0	0	0	0
38	V	45	0	0	1	0
38	W	45	0	0	0	0
38	X	45	0	0	0	0
39	A	3	0	0	0	0
39	Q	1	0	0	0	0
All	All	64832	0	59326	584	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 5.

All (584) 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)
1:1:103:PRO:CG	1:1:103:PRO:CB	1.96	1.39
7:A:489:HIS:NE2	21:O:101:ASP:OD1	1.65	1.30
5:5:97:GLU:OE2	5:5:103:ALA:HB2	1.12	1.28
5:5:97:GLU:OE2	5:5:103:ALA:CB	1.84	1.25
15:I:23:MET:HE2	30:L:305:BCR:H352	1.23	1.15
25:B:842:CLA:C7	15:I:23:MET:HE1	1.78	1.14
13:G:53:TYR:CE1	13:G:57:PHE:CE2	2.38	1.12
23:Q:209:MET:HE1	25:Q:304:CLA:HAB	1.18	1.12
13:G:53:TYR:CD1	13:G:57:PHE:CE2	2.38	1.11
23:Q:209:MET:CE	25:Q:304:CLA:HAB	1.81	1.10
13:G:53:TYR:CD1	13:G:57:PHE:HE2	1.70	1.08
25:B:842:CLA:H72	15:I:23:MET:CE	1.83	1.08
25:B:842:CLA:H72	15:I:23:MET:HE1	1.04	1.01
22:P:66:ARG:HH22	22:P:158:ASN:HB3	1.23	1.01
22:S:39:GLY:HA3	25:S:301:CLA:HMD1	1.53	0.90
13:G:66:GLN:O	13:G:70:VAL:HG12	1.72	0.88
15:I:23:MET:CE	30:L:305:BCR:H352	2.03	0.88
22:R:114:PRO:HB2	22:R:117:SER:HB3	1.56	0.87
13:G:53:TYR:CE1	13:G:57:PHE:CD2	2.62	0.86
7:A:197:MET:HG2	25:A:815:CLA:HBC2	1.59	0.83
22:V:177:LEU:HG	25:V:309:CLA:H3A	1.62	0.80
7:A:508:ALA:HB3	7:A:523:MET:HG3	1.62	0.80
22:R:114:PRO:HG3	24:R:308:CHL:C3B	2.12	0.80
22:W:174:LEU:HD12	25:W:309:CLA:HMA2	1.65	0.78
23:Q:121:ALA:O	23:Q:125:LYS:NZ	2.11	0.78
23:Q:209:MET:HE1	25:Q:304:CLA:CAB	2.07	0.77
22:R:114:PRO:HG2	22:R:119:TYR:HD1	1.51	0.76
25:B:824:CLA:HED3	13:G:69:ARG:HH12	1.50	0.76
22:U:47:SER:OG	22:U:50:ILE:O	1.99	0.76
17:K:65:ALA:HB1	17:K:71:MET:HG3	1.68	0.76
22:R:94:THR:OG1	22:R:96:ASP:OD1	2.03	0.76
22:S:52:PHE:HZ	22:S:55:GLU:HA	1.48	0.76
13:G:53:TYR:HD1	13:G:57:PHE:HE2	1.32	0.75
23:Q:85:HIS:HB3	23:Q:209:MET:HE3	1.68	0.75
12:F:215:LYS:NZ	12:F:216:ASN:OD1	2.19	0.75
13:G:63:GLN:HE22	30:G:201:BCR:H313	1.51	0.75
8:B:363:GLN:O	14:H:163:ARG:NH1	2.20	0.74
22:P:66:ARG:NH2	22:P:158:ASN:HB3	2.01	0.74
7:A:489:HIS:NE2	21:O:101:ASP:CG	2.46	0.73
22:V:137:GLU:OE1	38:V:308:KC2:C4C	2.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:71:MET:HE3	25:K:206:CLA:HAB	1.71	0.72
22:W:169:ALA:HB1	22:W:174:LEU:HD13	1.70	0.72
22:S:52:PHE:CD1	25:S:301:CLA:HMA2	2.24	0.72
22:R:65:GLY:O	22:R:69:MET:HG3	1.89	0.72
13:G:63:GLN:NE2	30:G:201:BCR:H313	2.05	0.71
13:G:97:THR:HG22	13:G:99:ASP:H	1.55	0.70
10:D:128:ASP:OD1	10:D:150:TYR:OH	2.08	0.70
13:G:53:TYR:CD1	13:G:57:PHE:CD2	2.79	0.70
5:5:130:ARG:NH2	25:5:607:CLA:O1D	2.25	0.70
8:B:256:THR:HA	25:B:818:CLA:HED1	1.74	0.70
1:1:36:PRO:O	4:4:139:GLN:NE2	2.24	0.69
17:K:71:MET:HG2	25:K:206:CLA:CHC	2.22	0.69
8:B:732:PHE:O	14:H:163:ARG:NE	2.26	0.69
17:K:65:ALA:HB3	17:K:71:MET:SD	2.34	0.68
22:R:80:ASN:ND2	26:R:322:IWJ:O44	2.26	0.68
5:5:97:GLU:OE2	5:5:103:ALA:CA	2.40	0.68
22:U:84:ILE:O	22:U:84:ILE:HD12	1.94	0.68
13:G:63:GLN:NE2	30:G:201:BCR:C31	2.57	0.68
7:A:509:SER:HA	7:A:525:PRO:HA	1.76	0.68
22:X:36:PRO:HD2	22:X:183:LYS:NZ	2.09	0.68
22:W:169:ALA:CB	22:W:174:LEU:HD13	2.24	0.67
7:A:94:HIS:HA	7:A:98:PHE:HD2	1.58	0.67
7:A:18:ASP:OD2	7:A:71:ARG:NH2	2.28	0.67
25:B:824:CLA:CED	13:G:69:ARG:HH12	2.08	0.66
12:F:95:LEU:HD13	12:F:116:MET:HA	1.77	0.66
14:H:140:VAL:O	14:H:144:LYS:NZ	2.28	0.66
22:V:180:LYS:HZ1	25:V:311:CLA:HBD	1.59	0.66
4:4:116:PHE:HD1	24:4:306:CHL:HMD1	1.61	0.66
3:3:96:GLU:OE1	25:3:301:CLA:C4A	2.43	0.65
5:5:97:GLU:CD	5:5:103:ALA:HB2	2.14	0.65
22:X:39:GLY:HA3	25:X:302:CLA:HMD1	1.78	0.65
22:W:92:LEU:CD2	25:W:303:CLA:H2A	2.26	0.65
22:X:36:PRO:HD2	22:X:183:LYS:HZ1	1.60	0.65
22:S:52:PHE:HD1	25:S:301:CLA:HMA2	1.60	0.65
13:G:56:ARG:HH22	13:G:100:PRO:HD2	1.62	0.65
7:A:695:GLU:OE1	8:B:535:LYS:NZ	2.29	0.65
22:X:36:PRO:HG3	25:X:311:CLA:HMA1	1.79	0.65
22:V:198:GLN:HE21	22:V:209:ASN:HD22	1.44	0.64
13:G:66:GLN:OE1	13:G:69:ARG:NH2	2.30	0.64
22:P:66:ARG:HH22	22:P:158:ASN:CB	2.07	0.64
22:R:137:GLU:OE1	38:R:312:KC2:NB	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:34:ILE:O	22:S:36:PRO:HD3	1.98	0.64
22:R:62:VAL:HG11	22:R:157:VAL:HG11	1.81	0.63
2:2:177:ASP:OD1	25:2:609:CLA:HBD	1.98	0.63
23:Q:177:VAL:HG23	23:Q:178:THR:HG23	1.79	0.63
6:6:38:ARG:NH1	6:6:58:ASP:O	2.32	0.63
22:W:61:GLU:OE1	25:W:301:CLA:C4A	2.46	0.63
7:A:467:ARG:NH2	25:A:836:CLA:O1D	2.32	0.63
20:N:106:LYS:HD2	20:N:107:PHE:CE2	2.33	0.63
22:X:35:TYR:CD2	22:X:183:LYS:HE2	2.34	0.63
22:S:39:GLY:HA3	25:S:301:CLA:CMD	2.28	0.63
21:O:101:ASP:OD1	21:O:101:ASP:O	2.17	0.62
22:X:35:TYR:HD2	22:X:183:LYS:HE2	1.64	0.62
22:R:69:MET:HE3	22:R:184:HIS:HB3	1.80	0.62
25:V:301:CLA:H72	25:V:302:CLA:HMD1	1.82	0.62
7:A:489:HIS:CD2	21:O:101:ASP:OD1	2.51	0.62
22:R:113:ALA:HB1	22:R:118:GLY:HA2	1.81	0.62
22:V:163:PHE:CD2	25:V:309:CLA:HMD1	2.34	0.62
26:P:320:IWJ:O27	26:P:320:IWJ:O39	2.17	0.62
13:G:63:GLN:HE22	30:G:201:BCR:C31	2.13	0.62
8:B:53:GLN:OE1	25:B:808:CLA:NC	2.33	0.62
17:K:71:MET:HG2	25:K:206:CLA:C4B	2.30	0.61
7:A:524:MET:HE1	7:A:627:VAL:HG21	1.81	0.61
22:S:168:LEU:HD13	25:S:309:CLA:H42	1.81	0.61
22:U:35:TYR:OH	22:U:186:ARG:NH1	2.34	0.61
23:Q:58:GLU:OE1	23:Q:203:LYS:NZ	2.34	0.61
22:R:69:MET:HG2	22:R:188:SER:OG	2.01	0.61
22:R:56:LYS:HB3	22:R:60:ARG:NH1	2.16	0.60
13:G:56:ARG:HE	13:G:101:ALA:HB3	1.65	0.60
26:T:318:IWJ:O27	26:T:318:IWJ:O39	2.16	0.60
21:O:123:GLN:OE1	29:O:2006:Q6L:O39	2.19	0.60
22:S:52:PHE:CZ	22:S:55:GLU:HA	2.34	0.60
4:4:212:PRO:O	26:4:317:IWJ:O38	2.20	0.60
26:W:318:IWJ:O27	26:W:318:IWJ:O39	2.15	0.60
22:X:174:LEU:HG	22:X:178:LYS:HZ2	1.67	0.59
22:S:167:GLY:O	22:S:170:GLU:HG2	2.02	0.59
7:A:600:TYR:HB2	7:A:732:LEU:HD11	1.84	0.59
22:R:39:GLY:HA3	25:R:305:CLA:HMD1	1.83	0.59
22:W:92:LEU:HG	22:W:101:VAL:HG22	1.84	0.59
22:T:41:TYR:CE1	22:T:44:GLY:N	2.71	0.59
1:1:148:LEU:O	25:1:607:CLA:HBB2	2.03	0.59
7:A:197:MET:CG	25:A:815:CLA:HBC2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:209:MET:HE2	25:Q:304:CLA:HAB	1.82	0.59
22:V:194:GLY:O	22:V:198:GLN:HG3	2.03	0.58
22:R:114:PRO:HD2	22:R:119:TYR:H	1.69	0.58
7:A:381:ALA:HB1	7:A:522:ALA:O	2.03	0.58
22:R:164:ASP:OD1	22:R:167:GLY:N	2.36	0.58
8:B:254:ILE:HG13	8:B:255:LEU:HG	1.84	0.58
22:W:39:GLY:HA3	25:W:301:CLA:HMD1	1.85	0.58
3:3:85:GLY:O	3:3:88:ASN:ND2	2.37	0.58
30:B:847:BCR:H313	30:B:848:BCR:H272	1.85	0.57
22:W:173:ASP:HB2	22:W:176:GLU:HB2	1.85	0.57
8:B:256:THR:HA	25:B:818:CLA:CED	2.34	0.57
4:4:109:ALA:O	4:4:112:TYR:HB3	2.04	0.57
13:G:98:ASN:HB2	25:G:204:CLA:CAD	2.34	0.57
22:W:206:PRO:O	29:W:315:Q6L:O08	2.23	0.57
22:X:34:ILE:HG12	22:X:36:PRO:HD3	1.87	0.57
7:A:521:ILE:HD11	7:A:627:VAL:HG13	1.86	0.56
22:X:209:ASN:N	22:X:209:ASN:OD1	2.36	0.56
1:1:43:HIS:NE2	1:1:55:ASP:OD2	2.38	0.56
3:3:56:GLU:OE2	17:K:95:THR:OG1	2.24	0.56
12:F:197:LEU:HD23	12:F:200:MET:HE2	1.87	0.56
13:G:129:GLN:HE21	25:G:202:CLA:CAD	2.17	0.56
20:N:65:ASP:OD1	20:N:68:ARG:NH2	2.38	0.56
22:P:39:GLY:HA3	25:P:301:CLA:HMD1	1.87	0.56
25:V:301:CLA:H3A	25:V:301:CLA:O1A	2.06	0.56
22:X:61:GLU:OE1	25:X:302:CLA:C4A	2.53	0.56
22:R:112:LEU:HD21	24:R:308:CHL:CHD	2.36	0.56
8:B:683:ARG:HE	18:L:63:MET:HB2	1.71	0.56
3:3:235:GLN:O	3:3:239:THR:OG1	2.21	0.56
22:P:158:ASN:HB2	25:P:309:CLA:CGD	2.36	0.56
1:1:215:VAL:HG21	25:1:610:CLA:HMD2	1.86	0.56
22:U:206:PRO:O	29:U:314:Q6L:O08	2.24	0.56
8:B:106:ARG:NH2	8:B:113:VAL:O	2.38	0.56
22:V:86:TRP:CH2	22:V:196:ILE:HG22	2.41	0.56
25:X:304:CLA:H2A	25:X:304:CLA:HED3	1.87	0.56
4:4:137:ARG:O	4:4:141:MET:HG3	2.06	0.55
7:A:156:GLU:OE2	20:N:75:ASN:ND2	2.38	0.55
22:X:101:VAL:HG11	24:X:306:CHL:HBC1	1.88	0.55
22:W:80:ASN:ND2	26:W:318:IWJ:O44	2.39	0.55
22:X:218:VAL:O	22:X:221:ASN:ND2	2.39	0.55
4:4:71:TYR:HH	12:F:208:LEU:HD11	1.71	0.55
23:Q:60:GLY:HA3	25:Q:304:CLA:HMD1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:61:GLU:OE2	22:T:186:ARG:NH2	2.39	0.55
16:J:1:MET:O	16:J:5:GLN:HG3	2.06	0.55
4:4:74:ALA:HB2	25:4:309:CLA:HED3	1.89	0.55
14:H:101:ARG:NH2	18:L:80:ASN:O	2.40	0.55
26:6:614:IWJ:O27	26:6:614:IWJ:O39	2.21	0.55
23:Q:40:SER:HB3	23:Q:43:LYS:HB2	1.88	0.55
23:Q:57:PRO:HG2	23:Q:58:GLU:OE2	2.06	0.55
23:Q:85:HIS:HB3	23:Q:209:MET:CE	2.37	0.55
22:V:86:TRP:HH2	22:V:196:ILE:HG22	1.70	0.54
4:4:50:LEU:HD21	4:4:68:LEU:HD11	1.88	0.54
31:F:805:LMG:HC61	16:J:2:LYS:HD2	1.89	0.54
7:A:600:TYR:HB2	7:A:732:LEU:CD1	2.37	0.54
25:B:842:CLA:C8	15:I:23:MET:HE1	2.37	0.54
13:G:55:GLY:O	13:G:60:LEU:HB2	2.07	0.54
23:Q:49:SER:HB3	23:Q:193:ASP:HB3	1.90	0.54
22:V:61:GLU:OE2	22:V:186:ARG:NE	2.40	0.54
26:S:322:IWJ:O27	26:S:322:IWJ:O39	2.26	0.53
11:E:50:LYS:NZ	12:F:224:SER:O	2.41	0.53
22:R:37:GLU:OE1	22:R:183:LYS:NZ	2.42	0.53
17:K:65:ALA:CB	17:K:71:MET:SD	2.96	0.53
22:R:42:PRO:HA	25:R:305:CLA:HED3	1.90	0.53
22:V:35:TYR:OH	22:V:186:ARG:NH1	2.41	0.53
10:D:110:ARG:NH2	10:D:112:GLU:OE1	2.40	0.53
22:R:114:PRO:CD	22:R:119:TYR:H	2.22	0.53
22:S:139:TYR:CD2	22:S:147:PRO:HD3	2.43	0.53
7:A:34:HIS:NE2	25:A:813:CLA:O1A	2.39	0.53
7:A:562:LEU:O	10:D:110:ARG:NH1	2.42	0.53
7:A:577:GLY:O	7:A:583:THR:OG1	2.27	0.53
22:S:112:LEU:O	24:S:304:CHL:C4D	2.56	0.53
22:U:216:ASP:OD2	22:U:219:HIS:CD2	2.61	0.53
12:F:87:ARG:NH2	12:F:136:ASP:OD1	2.42	0.53
22:V:177:LEU:CG	25:V:309:CLA:H3A	2.35	0.53
22:W:52:PHE:HA	25:W:301:CLA:HBA1	1.90	0.53
23:Q:101:ASN:ND2	26:Q:320:IWJ:O44	2.41	0.53
8:B:54:LEU:HD11	25:B:815:CLA:HBA2	1.91	0.52
8:B:444:GLN:NE2	8:B:452:GLN:OE1	2.41	0.52
2:2:83:GLN:OE1	2:2:142:ARG:NH1	2.41	0.52
22:U:79:GLU:HB2	22:U:207:ILE:HD13	1.92	0.52
2:2:176:PHE:CD2	25:2:609:CLA:HMD1	2.43	0.52
7:A:193:ASN:O	7:A:197:MET:HG3	2.10	0.52
8:B:128:GLY:O	8:B:208:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:56:ARG:NE	13:G:101:ALA:HB3	2.25	0.52
22:P:61:GLU:OE1	25:P:301:CLA:C4A	2.56	0.52
22:P:137:GLU:OE1	38:P:308:KC2:C4A	2.55	0.52
23:Q:123:ALA:HB1	23:Q:134:ALA:H	1.75	0.52
22:R:62:VAL:CG1	22:R:157:VAL:HG11	2.40	0.52
22:R:120:PRO:HG3	24:R:308:CHL:C4C	2.39	0.52
4:4:116:PHE:CD1	24:4:306:CHL:HMD1	2.43	0.52
22:R:69:MET:CG	22:R:188:SER:OG	2.58	0.52
2:2:87:TRP:CD1	25:2:608:CLA:HMD3	2.45	0.52
8:B:5:PHE:HB2	15:I:30:ILE:HA	1.91	0.52
22:V:79:GLU:OE1	22:V:207:ILE:HB	2.10	0.52
4:4:112:TYR:HD1	4:4:115:TYR:CE2	2.28	0.52
6:6:240:GLN:OE1	19:M:24:ARG:NH2	2.43	0.52
17:K:53:MET:HG2	24:W:314:CHL:H3A	1.92	0.52
22:T:140:ARG:NH1	38:T:308:KC2:O1D	2.39	0.51
3:3:87:VAL:HA	3:3:92:LEU:HD11	1.93	0.51
7:A:36:SER:OG	7:A:37:ARG:N	2.44	0.51
5:5:78:ALA:HB1	5:5:168:GLY:HA3	1.92	0.51
8:B:257:PHE:CD1	25:B:819:CLA:HMB1	2.46	0.51
23:Q:245:ASN:ND2	25:Q:314:CLA:OBD	2.42	0.51
7:A:455:LEU:HB3	7:A:534:MET:HE3	1.92	0.51
13:G:96:SER:O	13:G:96:SER:OG	2.27	0.51
23:Q:46:LYS:HD2	23:Q:191:ALA:O	2.11	0.51
2:2:51:HIS:O	2:2:74:ARG:NH1	2.44	0.51
22:P:66:ARG:NH1	22:P:157:VAL:HG12	2.25	0.51
7:A:97:ARG:HG2	36:A:854:DGD:O5E	2.11	0.51
13:G:48:ASN:OD1	13:G:112:GLY:HA2	2.11	0.51
22:V:176:GLU:O	22:V:180:LYS:HG3	2.11	0.51
25:B:825:CLA:HAB	25:B:832:CLA:HMD2	1.91	0.51
4:4:109:ALA:N	4:4:110:PRO:HD2	2.26	0.50
7:A:27:GLU:HA	16:J:3:ASN:HD22	1.76	0.50
16:J:4:PHE:O	16:J:8:LEU:HG	2.10	0.50
23:Q:39:ARG:NE	22:T:149:ASP:OD1	2.43	0.50
4:4:129:MET:HE2	24:4:306:CHL:HMA2	1.92	0.50
22:R:156:ASP:OD1	22:R:158:ASN:N	2.41	0.50
30:A:852:BCR:H24C	25:B:835:CLA:HMC1	1.94	0.50
22:R:114:PRO:HG2	22:R:119:TYR:CD1	2.40	0.50
22:W:69:MET:HE2	22:W:185:CYS:HA	1.93	0.50
4:4:126:GLN:OE1	4:4:127:MET:SD	2.69	0.50
7:A:434:ARG:NH2	10:D:93:THR:O	2.43	0.50
8:B:54:LEU:HD12	25:B:815:CLA:HED1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:95:LEU:HB3	12:F:116:MET:HG2	1.94	0.50
22:V:198:GLN:HG2	25:V:312:CLA:ND	2.26	0.50
26:P:318:IWJ:O27	26:P:318:IWJ:O39	2.29	0.50
22:R:114:PRO:HG3	24:R:308:CHL:C2B	2.41	0.50
1:1:130:VAL:HG11	13:G:50:LEU:HD21	1.93	0.50
2:2:172:PRO:HG2	2:2:176:PHE:CE2	2.47	0.50
7:A:199:ASN:HB3	25:A:822:CLA:HMD2	1.92	0.50
22:V:34:ILE:HD11	22:V:179:ILE:HG21	1.94	0.50
1:1:148:LEU:HA	25:1:605:CLA:HMD1	1.94	0.50
3:3:235:GLN:NE2	26:3:315:IWJ:O38	2.45	0.50
21:O:129:ARG:NH1	25:O:2002:CLA:OBD	2.44	0.50
22:P:153:THR:O	22:P:156:ASP:HB3	2.11	0.50
22:T:216:ASP:OD1	22:T:219:HIS:ND1	2.45	0.50
25:X:311:CLA:H2A	25:X:311:CLA:HED3	1.93	0.50
9:C:55:GLU:OE2	9:C:66:ARG:NH1	2.45	0.49
12:F:92:LEU:O	12:F:96:GLU:HG2	2.12	0.49
23:Q:71:ILE:HG22	25:Q:304:CLA:HBA2	1.93	0.49
22:S:137:GLU:OE1	38:S:308:KC2:NB	2.45	0.49
5:5:82:MET:HE2	5:5:168:GLY:HA2	1.94	0.49
22:V:42:PRO:HD3	22:V:186:ARG:NH2	2.27	0.49
22:V:46:GLU:OE2	22:V:47:SER:OG	2.30	0.49
10:D:77:TYR:OH	10:D:133:ARG:NH1	2.45	0.49
8:B:667:ARG:NH1	8:B:698:ALA:O	2.45	0.49
25:A:824:CLA:HMA1	30:K:207:BCR:H343	1.95	0.49
8:B:84:VAL:HA	14:H:166:ILE:HG12	1.94	0.49
22:U:61:GLU:OE1	25:U:301:CLA:C4A	2.56	0.49
26:V:317:IWJ:O27	26:V:317:IWJ:O39	2.30	0.49
1:1:37:GLY:O	4:4:139:GLN:NE2	2.43	0.49
22:T:66:ARG:NH2	22:T:157:VAL:O	2.45	0.49
25:W:309:CLA:O1D	25:W:309:CLA:H2A	2.12	0.49
7:A:195:GLU:OE1	7:A:312:TYR:HB3	2.12	0.49
22:P:210:TRP:CZ3	22:P:214:VAL:HG21	2.48	0.49
22:T:225:ASN:ND2	25:T:312:CLA:OBD	2.45	0.49
24:V:307:CHL:HMB1	24:V:307:CHL:HBB1	1.95	0.49
3:3:101:ARG:NH1	24:3:306:CHL:OBD	2.44	0.49
12:F:92:LEU:HA	12:F:95:LEU:HD12	1.94	0.49
22:R:140:ARG:HG3	24:R:311:CHL:C1D	2.43	0.49
2:2:179:LEU:HB3	2:2:181:TYR:CE1	2.48	0.48
8:B:206:THR:O	8:B:211:ASN:ND2	2.38	0.48
4:4:71:TYR:OH	12:F:208:LEU:HD11	2.12	0.48
13:G:54:LEU:HD12	13:G:58:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:606:ALA:O	8:B:610:GLU:HG3	2.14	0.48
22:R:69:MET:HG2	22:R:188:SER:CB	2.43	0.48
22:T:79:GLU:HG2	22:T:207:ILE:HB	1.95	0.48
4:4:54:TYR:N	25:4:303:CLA:OBD	2.45	0.48
22:T:102:ALA:HA	22:T:112:LEU:HD23	1.95	0.48
7:A:584:CYS:N	8:B:667:ARG:O	2.46	0.48
22:U:138:ALA:HA	22:U:143:ILE:HD12	1.95	0.48
7:A:596:LEU:O	7:A:599:MET:HE2	2.14	0.48
13:G:55:GLY:HA3	13:G:111:TRP:CE2	2.48	0.48
22:W:158:ASN:HB2	25:W:309:CLA:CGD	2.44	0.48
2:2:173:GLY:O	2:2:177:ASP:HB2	2.12	0.48
7:A:370:HIS:ND1	25:A:820:CLA:OBD	2.46	0.48
23:Q:48:GLY:N	23:Q:192:GLY:HA2	2.28	0.48
22:R:140:ARG:HG3	24:R:311:CHL:CHD	2.44	0.48
22:S:147:PRO:CD	22:S:148:PHE:H	2.27	0.48
7:A:508:ALA:HB3	7:A:523:MET:CG	2.37	0.48
8:B:351:HIS:ND1	25:B:819:CLA:OBD	2.44	0.48
20:N:77:GLU:HG2	20:N:107:PHE:HD2	1.78	0.48
22:X:66:ARG:NH1	24:X:308:CHL:OBD	2.45	0.48
26:4:301:IWJ:O27	26:4:301:IWJ:O39	2.29	0.47
25:B:808:CLA:HBC3	25:B:808:CLA:HHD	1.95	0.47
22:R:58:ALA:HA	25:R:305:CLA:HMA1	1.95	0.47
22:T:66:ARG:NH1	24:T:307:CHL:OBD	2.44	0.47
5:5:82:MET:HE2	5:5:168:GLY:CA	2.44	0.47
22:S:47:SER:OG	22:S:51:PRO:HA	2.13	0.47
22:U:176:GLU:C	22:U:176:GLU:OE1	2.57	0.47
2:2:197:LYS:NZ	28:2:619:LHG:O5	2.44	0.47
16:J:2:LYS:O	16:J:6:ILE:HG13	2.14	0.47
22:S:114:PRO:HD2	24:S:304:CHL:C1B	2.45	0.47
22:T:86:TRP:O	29:T:316:Q6L:O39	2.32	0.47
22:S:137:GLU:O	22:S:141:THR:HG22	2.15	0.47
22:V:125:VAL:HG21	24:V:305:CHL:C3D	2.44	0.47
22:V:142:GLY:HA2	22:V:154:VAL:HG11	1.95	0.47
5:5:76:MET:SD	5:5:130:ARG:NE	2.88	0.47
8:B:60:TRP:NE1	25:B:829:CLA:OBD	2.48	0.47
22:R:121:SER:H	22:R:124:ASN:HB2	1.80	0.47
1:1:222:ILE:HD12	1:1:223:PRO:O	2.14	0.47
22:U:164:ASP:OD1	29:U:314:Q6L:O39	2.33	0.47
25:B:815:CLA:O1A	25:B:815:CLA:H3A	2.15	0.47
20:N:112:MET:O	20:N:115:GLU:HG2	2.15	0.47
22:S:163:PHE:HZ	24:S:307:CHL:NB	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:180:LYS:HD3	25:T:311:CLA:HBD	1.96	0.47
22:V:61:GLU:OE1	25:V:301:CLA:C4A	2.57	0.47
22:V:142:GLY:CA	22:V:154:VAL:HG11	2.45	0.47
22:P:148:PHE:HB3	22:P:162:ARG:NH1	2.30	0.46
4:4:80:ARG:NH1	24:4:308:CHL:OBD	2.44	0.46
5:5:44:HIS:NE2	5:5:56:ASP:OD2	2.49	0.46
7:A:599:MET:O	7:A:603:ILE:HG12	2.15	0.46
22:V:72:VAL:O	22:V:75:ALA:HB3	2.15	0.46
22:W:198:GLN:HG2	25:W:312:CLA:ND	2.30	0.46
14:H:160:VAL:HG12	14:H:166:ILE:HG22	1.97	0.46
18:L:111:LYS:NZ	18:L:204:SER:O	2.41	0.46
22:W:113:ALA:HB3	22:W:120:PRO:HG3	1.96	0.46
22:W:164:ASP:OD1	29:W:315:Q6L:O39	2.33	0.46
2:2:130:ILE:HG12	2:2:134:MET:HE2	1.98	0.46
5:5:186:ARG:HH22	8:B:213:LEU:HB3	1.81	0.46
22:S:52:PHE:CE1	25:S:301:CLA:HMA2	2.51	0.46
1:1:90:VAL:HG23	1:1:98:TRP:HA	1.97	0.46
37:P:317:NEX:H162	37:P:317:NEX:H193	1.96	0.46
22:R:56:LYS:NZ	38:R:312:KC2:O2A	2.47	0.46
22:S:61:GLU:OE1	25:S:301:CLA:C4A	2.63	0.46
26:V:320:IWJ:O27	26:V:320:IWJ:O39	2.34	0.46
7:A:454:GLY:O	7:A:458:HIS:HB3	2.16	0.46
13:G:53:TYR:HE1	13:G:57:PHE:CE2	2.21	0.46
13:G:104:ASN:O	13:G:108:VAL:HG23	2.15	0.46
18:L:133:VAL:O	18:L:137:THR:OG1	2.30	0.46
25:P:301:CLA:HMC1	29:P:316:Q6L:C15	2.46	0.46
22:W:213:HIS:HA	22:W:220:SER:HB2	1.98	0.46
25:A:816:CLA:HAC2	25:A:817:CLA:HMB2	1.98	0.46
8:B:26:ALA:HB2	36:B:850:DGD:HA31	1.97	0.46
22:S:177:LEU:HG	25:S:309:CLA:H3A	1.98	0.46
1:1:81:MET:HE2	1:1:176:GLY:CA	2.46	0.46
9:C:27:GLU:HA	10:D:151:PRO:HB2	1.98	0.46
23:Q:56:TYR:HE1	23:Q:59:PHE:O	1.98	0.46
6:6:80:GLU:OE1	25:6:602:CLA:C4A	2.63	0.46
22:W:95:PRO:HA	22:W:122:PHE:HB3	1.97	0.46
4:4:140:ASP:CG	4:4:144:PRO:HA	2.40	0.45
16:J:4:PHE:CZ	16:J:8:LEU:HD21	2.51	0.45
25:J:102:CLA:HMD1	20:N:82:VAL:HG21	1.99	0.45
22:S:168:LEU:CD1	25:S:309:CLA:H42	2.46	0.45
25:A:825:CLA:HAA1	30:K:207:BCR:H342	1.97	0.45
25:A:856:CLA:HMC2	30:F:801:BCR:H381	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:422:LEU:HD13	8:B:531:LEU:HA	1.97	0.45
17:K:66:MET:HG3	17:K:104:PHE:HE1	1.82	0.45
23:Q:47:PHE:CE2	23:Q:191:ALA:HB3	2.52	0.45
6:6:55:MET:HE3	25:6:602:CLA:HED2	1.99	0.45
20:N:106:LYS:O	20:N:106:LYS:HD3	2.16	0.45
22:V:157:VAL:C	22:V:159:PRO:HD3	2.42	0.45
22:X:34:ILE:N	22:X:179:ILE:HG21	2.31	0.45
22:X:79:GLU:OE2	22:X:207:ILE:N	2.46	0.45
7:A:596:LEU:HD21	25:A:832:CLA:HBC1	1.98	0.45
8:B:518:VAL:HG21	8:B:592:TYR:HB2	1.97	0.45
22:V:123:TRP:HZ2	22:X:218:VAL:HG21	1.82	0.45
22:V:137:GLU:HA	22:V:140:ARG:HG2	1.98	0.45
2:2:171:TYR:CZ	2:2:192:LYS:HG2	2.52	0.45
3:3:102:TRP:CD1	25:3:307:CLA:HMD3	2.52	0.45
13:G:72:MET:HG2	13:G:79:THR:CG2	2.47	0.45
23:Q:43:LYS:HD2	22:T:145:ASP:HB2	1.99	0.45
22:X:174:LEU:HD11	25:X:310:CLA:HED2	1.98	0.45
2:2:163:ASN:ND2	2:2:174:GLY:HA3	2.30	0.45
18:L:91:LEU:O	18:L:95:VAL:HG23	2.17	0.45
22:P:66:ARG:HH12	22:P:157:VAL:HG12	1.81	0.45
22:S:168:LEU:HD22	25:S:309:CLA:H11	1.99	0.45
26:T:321:IWJ:O27	26:T:321:IWJ:O39	2.35	0.45
23:Q:49:SER:HB3	23:Q:193:ASP:CB	2.47	0.45
3:3:191:SER:O	3:3:191:SER:OG	2.32	0.45
6:6:226:PHE:HB2	25:6:612:CLA:HMC3	1.99	0.45
22:T:213:HIS:HA	22:T:220:SER:HB2	1.99	0.45
13:G:56:ARG:HH22	13:G:100:PRO:CD	2.29	0.45
13:G:56:ARG:NH1	13:G:99:ASP:OD1	2.50	0.45
20:N:105:VAL:HB	20:N:109:SER:H	1.82	0.45
22:R:57:ASN:OD1	25:R:306:CLA:HED3	2.17	0.45
5:5:135:MET:HE1	6:6:238:LEU:HD11	1.99	0.44
8:B:185:VAL:HG11	30:B:845:BCR:H341	1.98	0.44
22:P:62:VAL:CG1	22:P:157:VAL:HG11	2.47	0.44
22:P:153:THR:HG23	22:P:156:ASP:CB	2.47	0.44
23:Q:119:CYS:O	23:Q:122:VAL:HG12	2.17	0.44
25:Q:312:CLA:C4B	25:S:310:CLA:H43	2.47	0.44
4:4:108:ASP:O	4:4:112:TYR:N	2.49	0.44
7:A:360:MET:HE3	25:A:808:CLA:CBB	2.47	0.44
7:A:472:PHE:O	7:A:530:THR:HG21	2.17	0.44
22:R:120:PRO:HG3	24:R:308:CHL:C3C	2.47	0.44
22:S:49:ILE:O	22:S:50:ILE:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:424:ASN:OD1	7:A:432:ARG:NH1	2.46	0.44
13:G:50:LEU:C	13:G:50:LEU:HD23	2.42	0.44
3:3:227:MET:SD	25:3:301:CLA:HMC1	2.57	0.44
7:A:355:ILE:HD11	30:A:850:BCR:H24C	1.97	0.44
22:X:46:GLU:HA	25:X:302:CLA:HED1	1.99	0.44
6:6:64:LEU:HB2	6:6:66:LEU:CD2	2.47	0.44
12:F:91:GLU:O	12:F:95:LEU:HG	2.18	0.44
22:S:162:ARG:O	22:S:165:PRO:HD3	2.17	0.44
3:3:68:GLY:O	3:3:223:ARG:NH2	2.48	0.44
28:6:616:LHG:H151	15:I:21:VAL:HG12	1.99	0.44
22:V:65:GLY:HA2	22:V:189:MET:HG3	1.99	0.44
22:W:59:GLU:OE2	22:W:157:VAL:HG13	2.18	0.44
2:2:177:ASP:CG	25:2:609:CLA:HBD	2.43	0.44
3:3:157:PHE:CE1	3:3:158:LEU:HD22	2.52	0.44
5:5:169:ARG:HB3	25:5:602:CLA:HBC3	1.98	0.44
12:F:89:LYS:O	12:F:93:LYS:HG3	2.18	0.44
23:Q:48:GLY:CA	23:Q:192:GLY:HA2	2.47	0.44
22:X:36:PRO:HG3	25:X:311:CLA:CMA	2.45	0.44
22:X:139:TYR:CE2	22:X:147:PRO:HB3	2.53	0.44
7:A:474:ASP:O	7:A:478:GLN:NE2	2.50	0.44
22:S:37:GLU:OE2	22:S:183:LYS:HD3	2.17	0.44
22:X:175:GLU:HA	22:X:178:LYS:NZ	2.33	0.44
7:A:13:VAL:N	7:A:315:ASN:OD1	2.47	0.44
7:A:95:GLY:HA3	7:A:148:TRP:CH2	2.53	0.44
7:A:677:PHE:CG	30:A:852:BCR:H363	2.53	0.44
18:L:122:GLU:OE2	18:L:203:TYR:OH	2.34	0.44
25:V:301:CLA:H3A	25:V:301:CLA:CGA	2.48	0.43
3:3:51:VAL:HG21	17:K:99:ARG:HB2	2.00	0.43
28:1:614:LHG:O4	25:B:843:CLA:NB	2.52	0.43
7:A:197:MET:HE1	25:A:827:CLA:H71	2.01	0.43
7:A:403:CYS:SG	7:A:596:LEU:HA	2.58	0.43
12:F:96:GLU:O	12:F:100:LYS:HG3	2.18	0.43
22:W:37:GLU:OE2	22:W:183:LYS:NZ	2.49	0.43
22:X:175:GLU:HA	22:X:178:LYS:HZ3	1.84	0.43
7:A:593:PHE:CE1	7:A:597:PHE:HE2	2.36	0.43
22:S:163:PHE:CZ	24:S:307:CHL:NC	2.86	0.43
22:W:225:ASN:ND2	25:W:312:CLA:OBD	2.51	0.43
3:3:110:MET:HG3	27:3:316:XAT:H163	2.00	0.43
7:A:545:VAL:HG11	7:A:598:TRP:CE2	2.54	0.43
7:A:590:ASP:O	7:A:593:PHE:HB3	2.18	0.43
8:B:191:THR:HG21	8:B:278:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:99:ASP:OD2	13:G:103:PHE:HB3	2.17	0.43
22:V:158:ASN:ND2	25:V:309:CLA:O1D	2.51	0.43
22:V:193:LEU:O	22:V:196:ILE:HG12	2.18	0.43
22:T:34:ILE:HD11	22:T:179:ILE:HG13	2.01	0.43
7:A:121:ILE:HD13	30:J:101:BCR:H332	2.01	0.43
20:N:77:GLU:HG2	20:N:107:PHE:CD2	2.54	0.43
22:P:125:VAL:HG11	24:P:305:CHL:HMD2	2.00	0.43
22:S:166:LEU:HD22	29:S:315:Q6L:C35	2.48	0.43
8:B:430:GLY:HA2	8:B:524:LEU:HD22	2.00	0.43
25:B:806:CLA:H3A	19:M:29:LEU:HD13	2.01	0.43
22:P:99:THR:HG22	22:P:120:PRO:HG2	2.01	0.43
25:2:613:CLA:OBD	3:3:153:TRP:NE1	2.50	0.43
7:A:55:ASP:O	7:A:62:HIS:NE2	2.45	0.43
18:L:73:ASP:OD1	18:L:74:VAL:N	2.52	0.43
23:Q:86:GLY:HA3	23:Q:205:SER:HB3	2.00	0.43
29:V:321:Q6L:C28	22:W:196:ILE:HG23	2.48	0.43
2:2:172:PRO:HG2	2:2:176:PHE:HE2	1.84	0.42
6:6:198:PRO:O	26:6:614:IWJ:O44	2.37	0.42
22:V:95:PRO:HA	22:V:122:PHE:CD2	2.54	0.42
7:A:740:TRP:NE1	25:A:830:CLA:O1A	2.48	0.42
3:3:97:LEU:HD23	3:3:195:ALA:HB1	2.02	0.42
8:B:497:LEU:HA	8:B:500:ILE:HG22	2.01	0.42
22:P:210:TRP:CH2	22:P:214:VAL:HG11	2.54	0.42
8:B:69:ALA:HB2	8:B:135:LEU:HB2	2.01	0.42
8:B:648:MET:HE1	25:B:810:CLA:HBC3	2.01	0.42
12:F:103:ASP:OD1	12:F:103:ASP:N	2.52	0.42
21:O:115:LEU:HD21	25:O:2001:CLA:C3B	2.49	0.42
22:S:52:PHE:CE1	22:S:58:ALA:HB2	2.54	0.42
22:W:157:VAL:HG23	22:W:158:ASN:CG	2.44	0.42
2:2:171:TYR:CE2	2:2:192:LYS:HG2	2.54	0.42
4:4:189:ALA:HB3	25:4:311:CLA:HMB3	2.01	0.42
4:4:207:HIS:HB3	4:4:231:ALA:HB1	2.01	0.42
23:Q:131:ALA:HB1	24:Q:307:CHL:HMA3	2.01	0.42
23:Q:134:ALA:HA	23:Q:140:TYR:HA	2.01	0.42
22:R:58:ALA:O	22:R:62:VAL:HG23	2.19	0.42
22:S:111:PRO:HB2	22:S:113:ALA:O	2.20	0.42
22:V:140:ARG:HG3	22:V:141:THR:HG23	2.01	0.42
22:X:150:ASP:HB3	22:X:152:LEU:HD23	2.02	0.42
6:6:214:LEU:HD13	25:6:610:CLA:HMD2	2.01	0.42
7:A:93:PHE:CZ	7:A:97:ARG:HD2	2.54	0.42
8:B:118:SER:HA	25:B:829:CLA:HMA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:74:ALA:HB1	20:N:108:LEU:HD23	2.02	0.42
22:P:169:ALA:HB2	25:P:309:CLA:HAA2	2.01	0.42
22:S:140:ARG:HA	24:S:307:CHL:C4C	2.50	0.42
22:X:95:PRO:HA	22:X:122:PHE:HB3	2.01	0.42
5:5:66:ARG:NH2	25:B:813:CLA:OBD	2.53	0.42
30:M:101:BCR:H15C	30:M:101:BCR:H351	1.87	0.42
22:R:225:ASN:ND2	25:R:316:CLA:OBD	2.51	0.42
22:S:35:TYR:CE1	22:S:37:GLU:HB2	2.54	0.42
22:T:102:ALA:HB2	22:T:120:PRO:HG2	2.00	0.42
7:A:99:SER:HB2	7:A:145:PHE:HZ	1.84	0.42
22:U:79:GLU:CB	22:U:207:ILE:HD13	2.49	0.42
22:V:198:GLN:HG2	25:V:312:CLA:C1D	2.50	0.42
14:H:119:ARG:NH2	32:H:303:SQD:O10	2.53	0.42
20:N:101:GLU:HA	20:N:112:MET:HG2	2.01	0.42
22:R:120:PRO:HG3	24:R:308:CHL:C1C	2.50	0.42
22:S:47:SER:HB3	25:S:301:CLA:OBD	2.19	0.42
22:S:152:LEU:HB3	24:S:307:CHL:HBC3	2.01	0.42
8:B:256:THR:CG2	8:B:258:LEU:HG	2.50	0.42
9:C:74:THR:HG21	10:D:74:GLU:OE2	2.20	0.42
10:D:57:SER:O	10:D:100:ARG:NH1	2.53	0.42
24:U:304:CHL:HBB1	24:V:314:CHL:HHB	2.02	0.42
22:V:180:LYS:NZ	25:V:311:CLA:HAA2	2.35	0.42
1:1:98:TRP:CZ2	1:1:186:ILE:HG22	2.55	0.41
24:1:601:CHL:OBD	4:4:136:ARG:NH1	2.52	0.41
5:5:212:ILE:HG22	8:B:216:LEU:HD21	2.02	0.41
7:A:524:MET:HB3	7:A:618:VAL:HG13	2.02	0.41
25:S:310:CLA:H2A	25:S:310:CLA:O2D	2.20	0.41
22:T:41:TYR:CD1	22:T:44:GLY:N	2.88	0.41
24:3:306:CHL:HMB3	30:3:319:BCR:H24C	2.02	0.41
25:A:803:CLA:H161	25:B:803:CLA:H151	2.02	0.41
8:B:31:PHE:HB3	8:B:37:MET:HE3	2.01	0.41
25:X:313:CLA:O2D	25:X:313:CLA:H2A	2.20	0.41
8:B:515:ASP:HA	8:B:518:VAL:HG12	2.03	0.41
26:S:319:IWJ:O27	26:S:319:IWJ:O39	2.38	0.41
30:4:319:BCR:H15C	30:4:319:BCR:H351	1.96	0.41
7:A:460:ASP:OD2	8:B:634:TYR:OH	2.35	0.41
7:A:691:GLY:N	8:B:567:CYS:O	2.48	0.41
30:J:101:BCR:H351	30:J:101:BCR:H15C	1.88	0.41
22:R:217:PRO:O	22:R:221:ASN:ND2	2.53	0.41
1:1:211:TRP:CE3	4:4:116:PHE:HE2	2.38	0.41
4:4:151:PRO:HB2	30:4:319:BCR:H401	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:476:ILE:HG13	8:B:477:LEU:N	2.36	0.41
23:Q:107:TRP:O	29:Q:319:Q6L:O08	2.38	0.41
22:W:177:LEU:HD13	25:W:309:CLA:O1A	2.21	0.41
22:R:114:PRO:HG3	24:R:308:CHL:CAB	2.51	0.41
22:X:38:PHE:O	29:X:319:Q6L:O39	2.38	0.41
1:1:149:TYR:CD1	25:1:607:CLA:HHC	2.56	0.41
2:2:176:PHE:CG	25:2:609:CLA:HMD1	2.56	0.41
8:B:10:GLN:O	8:B:13:ALA:N	2.54	0.41
22:P:39:GLY:C	22:P:40:THR:HG23	2.45	0.41
23:Q:115:THR:CG2	23:Q:116:PRO:HD2	2.51	0.41
22:R:65:GLY:O	22:R:69:MET:CG	2.65	0.41
22:S:163:PHE:HE1	24:S:307:CHL:NA	2.19	0.41
6:6:94:ILE:HD11	27:6:615:XAT:O4	2.21	0.41
25:B:824:CLA:CED	13:G:69:ARG:NH1	2.81	0.41
22:R:96:ASP:OD1	22:R:96:ASP:N	2.54	0.41
3:3:116:LEU:HB3	3:3:122:ILE:HG12	2.02	0.41
4:4:85:GLY:HA2	27:4:318:XAT:H181	2.02	0.41
8:B:544:LYS:HD2	11:E:57:TYR:HA	2.03	0.41
9:C:66:ARG:HG3	10:D:168:ILE:CD1	2.51	0.41
22:S:69:MET:HE2	22:S:185:CYS:HA	2.02	0.41
22:W:177:LEU:HB3	25:W:309:CLA:H3A	2.03	0.41
22:X:55:GLU:O	22:X:58:ALA:N	2.54	0.41
7:A:17:VAL:HG21	25:A:812:CLA:HED2	2.01	0.41
8:B:299:HIS:HB3	8:B:304:ILE:HD11	2.02	0.41
20:N:105:VAL:H	20:N:109:SER:CB	2.34	0.41
20:N:114:ILE:O	20:N:114:ILE:HG12	2.20	0.41
22:P:221:ASN:OD1	22:P:221:ASN:N	2.53	0.41
1:1:143:THR:C	1:1:147:ARG:HE	2.29	0.40
2:2:179:LEU:HB2	29:2:616:Q6L:O08	2.21	0.40
3:3:102:TRP:HD1	25:3:307:CLA:HMD3	1.86	0.40
3:3:167:ALA:HB2	25:3:307:CLA:CMA	2.51	0.40
4:4:59:LEU:O	4:4:61:LEU:N	2.54	0.40
8:B:85:ARG:HG3	14:H:165:ARG:HB3	2.03	0.40
23:Q:43:LYS:C	23:Q:43:LYS:HD3	2.46	0.40
1:1:149:TYR:HD1	25:1:607:CLA:HAB	1.85	0.40
5:5:178:ILE:HG23	5:5:189:PRO:HG3	2.04	0.40
13:G:45:SER:OG	25:G:203:CLA:HBD	2.21	0.40
23:Q:39:ARG:NH2	22:T:149:ASP:HA	2.37	0.40
6:6:83:ASN:ND2	25:6:607:CLA:OBD	2.53	0.40
7:A:361:GLY:HA2	7:A:398:GLY:HA2	2.03	0.40
34:A:844:PQN:H291	25:F:802:CLA:HMC1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:177:GLU:O	12:F:180:THR:OG1	2.39	0.40
4:4:207:HIS:HA	4:4:233:PHE:HA	2.03	0.40
6:6:69:ASN:HB3	6:6:72:THR:HG22	2.03	0.40
22:T:112:LEU:HD12	24:T:304:CHL:HMD2	2.02	0.40
22:V:180:LYS:NZ	25:V:311:CLA:HBD	2.30	0.40
25:4:303:CLA:H93	12:F:205:ALA:HB2	2.03	0.40
6:6:91:THR:HG23	6:6:187:MET:HE1	2.04	0.40
7:A:217:GLN:OE1	7:A:298:HIS:ND1	2.52	0.40
7:A:524:MET:HE3	7:A:524:MET:HB2	1.98	0.40
8:B:415:LYS:HB2	8:B:538:LEU:HD13	2.03	0.40
22:T:183:LYS:HD2	25:T:310:CLA:C3D	2.52	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	1	151/225 (67%)	144 (95%)	6 (4%)	1 (1%)	18	40
2	2	203/242 (84%)	197 (97%)	6 (3%)	0	100	100
3	3	225/272 (83%)	215 (96%)	10 (4%)	0	100	100
4	4	199/236 (84%)	190 (96%)	9 (4%)	0	100	100
5	5	162/217 (75%)	158 (98%)	4 (2%)	0	100	100
6	6	190/249 (76%)	187 (98%)	3 (2%)	0	100	100
7	A	740/751 (98%)	724 (98%)	16 (2%)	0	100	100
8	B	730/733 (100%)	706 (97%)	24 (3%)	0	100	100
9	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
10	D	141/188 (75%)	135 (96%)	6 (4%)	0	100	100
11	E	60/101 (59%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	F	163/231 (71%)	159 (98%)	4 (2%)	0	100	100
13	G	93/132 (70%)	89 (96%)	4 (4%)	0	100	100
14	H	94/166 (57%)	93 (99%)	1 (1%)	0	100	100
15	I	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
16	J	39/42 (93%)	37 (95%)	2 (5%)	0	100	100
17	K	85/131 (65%)	84 (99%)	1 (1%)	0	100	100
18	L	156/204 (76%)	153 (98%)	3 (2%)	0	100	100
19	M	29/31 (94%)	29 (100%)	0	0	100	100
20	N	89/139 (64%)	83 (93%)	6 (7%)	0	100	100
21	O	94/136 (69%)	93 (99%)	1 (1%)	0	100	100
22	P	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
22	R	199/233 (85%)	185 (93%)	14 (7%)	0	100	100
22	S	200/233 (86%)	190 (95%)	9 (4%)	1 (0%)	24	49
22	T	199/233 (85%)	189 (95%)	10 (5%)	0	100	100
22	U	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
22	V	193/233 (83%)	188 (97%)	5 (3%)	0	100	100
22	W	198/233 (85%)	188 (95%)	10 (5%)	0	100	100
22	X	190/233 (82%)	184 (97%)	6 (3%)	0	100	100
23	Q	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
All	All	5554/6632 (84%)	5362 (96%)	190 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	S	120	PRO
1	1	150	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	118/166 (71%)	118 (100%)	0	100	100
2	2	160/186 (86%)	160 (100%)	0	100	100
3	3	173/208 (83%)	173 (100%)	0	100	100
4	4	159/186 (86%)	159 (100%)	0	100	100
5	5	127/163 (78%)	127 (100%)	0	100	100
6	6	148/188 (79%)	148 (100%)	0	100	100
7	A	600/609 (98%)	600 (100%)	0	100	100
8	B	584/585 (100%)	584 (100%)	0	100	100
9	C	66/67 (98%)	66 (100%)	0	100	100
10	D	118/150 (79%)	118 (100%)	0	100	100
11	E	55/85 (65%)	55 (100%)	0	100	100
12	F	130/176 (74%)	130 (100%)	0	100	100
13	G	73/99 (74%)	73 (100%)	0	100	100
14	H	72/128 (56%)	72 (100%)	0	100	100
15	I	29/29 (100%)	29 (100%)	0	100	100
16	J	35/36 (97%)	35 (100%)	0	100	100
17	K	66/101 (65%)	66 (100%)	0	100	100
18	L	125/165 (76%)	125 (100%)	0	100	100
19	M	27/27 (100%)	27 (100%)	0	100	100
20	N	72/103 (70%)	72 (100%)	0	100	100
21	O	80/110 (73%)	80 (100%)	0	100	100
22	P	153/179 (86%)	153 (100%)	0	100	100
22	R	153/179 (86%)	153 (100%)	0	100	100
22	S	153/179 (86%)	153 (100%)	0	100	100
22	T	153/179 (86%)	153 (100%)	0	100	100
22	U	153/179 (86%)	153 (100%)	0	100	100
22	V	151/179 (84%)	151 (100%)	0	100	100
22	W	152/179 (85%)	152 (100%)	0	100	100
22	X	150/179 (84%)	150 (100%)	0	100	100
23	Q	167/167 (100%)	166 (99%)	1 (1%)	78	89
All	All	4402/5166 (85%)	4401 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Q	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	223	ASN
4	4	77	GLN
4	4	113	GLN
4	4	156	ASN
7	A	653	GLN
8	B	98	GLN
8	B	236	ASN
8	B	266	GLN
8	B	629	GLN
12	F	149	HIS
13	G	63	GLN
13	G	129	GLN
16	J	3	ASN
16	J	5	GLN
16	J	30	ASN
21	O	76	ASN
22	P	211	GLN
23	Q	229	ASN
22	U	219	HIS
22	V	209	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$
23	TPO	Q	31	23	8,10,11	1.75	1 (12%)	10,14,16	1.21	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	TPO	Q	31	23	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Q	31	TPO	P-O1P	3.60	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Q	31	TPO	P-OG1-CB	-2.57	116.33	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Q	31	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

449 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	$\#\|Z\| > 2$
24	CHL	6	601	6	36,50,74	2.84	9 (25%)	31,85,114	1.93	11 (35%)
25	CLA	A	828	-	63,67,73	1.25	8 (12%)	74,105,113	1.27	9 (12%)
25	CLA	A	829	-	69,73,73	1.16	6 (8%)	82,113,113	1.42	15 (18%)
25	CLA	B	803	-	69,73,73	1.22	9 (13%)	82,113,113	1.46	14 (17%)
25	CLA	A	833	-	54,58,73	1.38	8 (14%)	64,95,113	1.32	9 (14%)
25	CLA	A	810	7	69,73,73	1.17	10 (14%)	82,113,113	1.31	9 (10%)
25	CLA	Q	301	14	59,63,73	1.30	8 (13%)	70,101,113	1.56	11 (15%)
24	CHL	1	601	1	49,63,74	2.67	12 (24%)	45,101,114	1.76	11 (24%)
24	CHL	S	314	22	38,53,74	2.96	9 (23%)	31,88,114	1.87	10 (32%)
25	CLA	L	301	18	45,49,73	1.40	7 (15%)	54,84,113	1.35	5 (9%)
25	CLA	B	843	28	69,73,73	1.14	8 (11%)	82,113,113	1.44	10 (12%)
31	LMG	N	201	-	55,55,55	0.91	2 (3%)	63,63,63	1.16	4 (6%)
31	LMG	L	308	-	31,31,55	1.21	2 (6%)	39,39,63	1.04	2 (5%)
25	CLA	U	310	-	47,52,73	1.38	7 (14%)	55,87,113	1.32	8 (14%)
26	IWJ	5	611	-	43,45,45	1.56	4 (9%)	47,65,65	1.41	6 (12%)
37	NEX	T	317	-	40,46,46	1.35	6 (15%)	50,70,70	2.40	16 (32%)
24	CHL	U	306	-	38,52,74	3.04	11 (28%)	31,87,114	1.73	9 (29%)
30	BCR	H	305	-	41,41,41	1.18	3 (7%)	56,56,56	1.80	18 (32%)
25	CLA	X	314	-	45,49,73	1.41	6 (13%)	54,84,113	1.32	5 (9%)
25	CLA	J	102	16	46,50,73	1.35	8 (17%)	53,85,113	1.46	5 (9%)
25	CLA	A	831	-	69,73,73	1.21	10 (14%)	82,113,113	1.40	8 (9%)
29	Q6L	R	323	-	42,43,43	1.93	7 (16%)	51,60,60	1.94	10 (19%)
26	IWJ	Q	303	-	43,45,45	1.58	6 (13%)	47,65,65	1.50	9 (19%)
29	Q6L	T	315	-	42,43,43	1.89	8 (19%)	51,60,60	1.63	7 (13%)
25	CLA	5	608	5	45,49,73	1.43	7 (15%)	54,84,113	1.44	5 (9%)
38	KC2	X	309	22	49,53,53	2.21	16 (32%)	60,89,89	2.28	21 (35%)
38	KC2	R	312	22	49,53,53	2.16	14 (28%)	60,89,89	2.18	19 (31%)
28	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	0.98	2 (3%)
25	CLA	A	832	-	69,73,73	1.19	5 (7%)	82,113,113	1.15	5 (6%)
35	SF4	C	102	9	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	P	310	22	64,68,73	1.22	6 (9%)	76,107,113	1.28	8 (10%)
30	BCR	2	618	-	41,41,41	1.14	3 (7%)	56,56,56	2.18	14 (25%)
38	KC2	S	308	22	49,53,53	2.17	14 (28%)	60,89,89	2.22	15 (25%)
24	CHL	2	615	2	37,51,74	3.07	11 (29%)	30,86,114	2.08	12 (40%)
25	CLA	A	805	-	69,73,73	1.20	5 (7%)	82,113,113	1.49	10 (12%)
25	CLA	A	822	-	49,53,73	1.36	8 (16%)	58,89,113	1.26	7 (12%)
25	CLA	N	202	20	48,53,73	1.37	6 (12%)	56,89,113	1.33	5 (8%)
29	Q6L	U	317	-	42,43,43	1.90	8 (19%)	51,60,60	1.82	8 (15%)
25	CLA	P	311	-	64,68,73	1.18	4 (6%)	76,107,113	1.39	12 (15%)
24	CHL	P	305	-	40,54,74	3.09	12 (30%)	34,90,114	1.97	11 (32%)
25	CLA	3	312	-	43,48,73	1.45	8 (18%)	51,83,113	1.33	8 (15%)
25	CLA	X	311	22	54,58,73	1.31	6 (11%)	64,95,113	1.21	5 (7%)
25	CLA	T	312	22	59,63,73	1.25	8 (13%)	70,101,113	1.32	7 (10%)
29	Q6L	S	316	-	42,43,43	1.90	7 (16%)	51,60,60	1.96	9 (17%)
24	CHL	R	308	22	40,54,74	2.89	11 (27%)	34,90,114	1.83	13 (38%)
24	CHL	S	307	-	36,50,74	3.15	11 (30%)	29,85,114	2.07	12 (41%)
25	CLA	4	313	4	61,65,73	1.25	7 (11%)	72,103,113	1.45	8 (11%)
25	CLA	B	838	-	54,58,73	1.28	8 (14%)	64,95,113	1.40	5 (7%)
25	CLA	B	840	-	51,55,73	1.35	7 (13%)	60,91,113	1.41	6 (10%)
29	Q6L	W	320	-	42,43,43	1.91	7 (16%)	51,60,60	1.77	7 (13%)
25	CLA	T	301	22	69,73,73	1.19	9 (13%)	82,113,113	1.50	14 (17%)
25	CLA	W	310	22	64,68,73	1.21	6 (9%)	76,107,113	1.11	4 (5%)
24	CHL	R	310	-	46,60,74	2.73	13 (28%)	40,97,114	1.93	14 (35%)
24	CHL	X	307	-	46,60,74	2.76	11 (23%)	40,97,114	2.63	16 (40%)
25	CLA	6	609	-	48,52,73	1.43	4 (8%)	57,88,113	1.62	10 (17%)
24	CHL	P	306	-	46,60,74	2.68	14 (30%)	40,97,114	1.77	15 (37%)
27	XAT	4	318	-	41,47,47	1.17	5 (12%)	54,74,74	3.04	24 (44%)
25	CLA	2	606	-	49,53,73	1.36	7 (14%)	58,89,113	1.39	7 (12%)
25	CLA	V	309	22	46,50,73	1.57	8 (17%)	53,85,113	1.79	13 (24%)
25	CLA	B	839	-	69,73,73	1.20	8 (11%)	82,113,113	1.24	5 (6%)
25	CLA	B	804	-	69,73,73	1.19	9 (13%)	82,113,113	1.29	7 (8%)
26	IWJ	P	320	-	43,45,45	1.61	6 (13%)	47,65,65	1.70	7 (14%)
25	CLA	P	313	-	52,56,73	1.33	6 (11%)	61,92,113	1.24	6 (9%)
25	CLA	X	303	-	55,59,73	1.27	5 (9%)	64,96,113	1.18	4 (6%)
26	IWJ	S	318	-	43,45,45	1.51	5 (11%)	47,65,65	1.63	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	6	607	6	49,53,73	1.45	11 (22%)	58,89,113	1.46	8 (13%)
25	CLA	S	301	22	69,73,73	1.23	9 (13%)	82,113,113	1.30	13 (15%)
25	CLA	6	612	6	49,53,73	1.37	7 (14%)	58,89,113	1.23	5 (8%)
25	CLA	A	827	39	69,73,73	1.26	10 (14%)	82,113,113	1.57	16 (19%)
25	CLA	1	602	1	60,64,73	1.32	7 (11%)	71,102,113	1.26	9 (12%)
27	XAT	3	316	-	41,47,47	1.22	6 (14%)	54,74,74	3.02	23 (42%)
25	CLA	U	301	22	49,53,73	1.40	7 (14%)	58,89,113	1.44	10 (17%)
25	CLA	B	841	-	69,73,73	1.23	10 (14%)	82,113,113	1.36	11 (13%)
29	Q6L	W	319	-	42,43,43	1.91	7 (16%)	51,60,60	1.75	7 (13%)
38	KC2	U	307	22	49,53,53	2.15	13 (26%)	60,89,89	2.12	14 (23%)
30	BCR	L	306	-	41,41,41	1.15	4 (9%)	56,56,56	2.07	20 (35%)
24	CHL	V	305	22	37,51,74	2.85	12 (32%)	30,86,114	2.07	13 (43%)
25	CLA	A	803	-	69,73,73	1.15	6 (8%)	82,113,113	1.39	11 (13%)
25	CLA	B	828	-	69,73,73	1.19	8 (11%)	82,113,113	1.28	9 (10%)
24	CHL	X	305	22	36,50,74	3.03	13 (36%)	29,85,114	1.81	11 (37%)
25	CLA	B	829	-	69,73,73	1.20	8 (11%)	82,113,113	1.44	10 (12%)
25	CLA	F	802	-	46,50,73	1.42	10 (21%)	53,85,113	1.38	7 (13%)
35	SF4	A	853	8,7	0,12,12	-	-	-		
25	CLA	B	830	-	69,73,73	1.18	7 (10%)	82,113,113	1.22	8 (9%)
30	BCR	A	849	-	41,41,41	1.10	3 (7%)	56,56,56	2.24	19 (33%)
27	XAT	1	612	-	41,47,47	1.31	7 (17%)	54,74,74	3.02	28 (51%)
24	CHL	T	305	-	43,57,74	2.88	12 (27%)	37,93,114	2.15	13 (35%)
27	XAT	2	617	-	41,47,47	1.16	4 (9%)	54,74,74	2.80	27 (50%)
25	CLA	O	2003	-	45,49,73	1.39	6 (13%)	54,84,113	1.19	5 (9%)
25	CLA	U	312	-	45,49,73	1.41	6 (13%)	54,84,113	1.23	5 (9%)
25	CLA	O	2004	-	45,49,73	1.40	7 (15%)	54,84,113	1.43	6 (11%)
25	CLA	T	313	-	46,50,73	1.39	8 (17%)	53,85,113	1.20	3 (5%)
25	CLA	T	310	22	46,50,73	1.42	7 (15%)	53,85,113	1.18	3 (5%)
25	CLA	B	815	-	69,73,73	1.20	9 (13%)	82,113,113	1.68	11 (13%)
25	CLA	P	301	22	69,73,73	1.16	8 (11%)	82,113,113	1.36	10 (12%)
32	SQD	H	303	-	46,48,54	1.23	3 (6%)	56,59,65	1.11	3 (5%)
25	CLA	W	311	-	49,53,73	1.34	7 (14%)	58,89,113	1.39	7 (12%)
25	CLA	P	309	22	68,72,73	1.12	7 (10%)	80,111,113	1.47	11 (13%)
31	LMG	O	2008	-	39,39,55	1.06	2 (5%)	47,47,63	1.15	3 (6%)
30	BCR	K	207	-	41,41,41	1.26	5 (12%)	56,56,56	2.10	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	Q	304	23	69,73,73	1.21	8 (11%)	82,113,113	1.54	6 (7%)
25	CLA	V	311	-	64,68,73	1.21	6 (9%)	76,107,113	1.27	7 (9%)
25	CLA	6	603	6	47,52,73	1.51	9 (19%)	55,88,113	1.43	11 (20%)
24	CHL	R	311	-	38,52,74	3.12	14 (36%)	31,87,114	1.86	7 (22%)
30	BCR	L	307	-	41,41,41	1.12	2 (4%)	56,56,56	2.59	19 (33%)
24	CHL	2	605	-	36,50,74	3.00	12 (33%)	31,85,114	1.86	8 (25%)
25	CLA	B	818	-	59,63,73	1.28	7 (11%)	70,101,113	1.47	12 (17%)
29	Q6L	T	319	-	42,43,43	1.89	7 (16%)	51,60,60	1.96	7 (13%)
24	CHL	R	302	-	41,55,74	2.87	12 (29%)	35,91,114	1.95	12 (34%)
24	CHL	4	308	-	40,54,74	3.04	11 (27%)	34,90,114	2.15	12 (35%)
25	CLA	T	311	-	64,68,73	1.20	6 (9%)	76,107,113	1.34	8 (10%)
29	Q6L	O	2007	-	42,43,43	1.97	9 (21%)	51,60,60	1.71	8 (15%)
25	CLA	F	803	12	45,49,73	1.42	7 (15%)	54,84,113	1.54	9 (16%)
25	CLA	Q	305	-	47,52,73	1.39	6 (12%)	55,87,113	1.22	4 (7%)
25	CLA	2	604	-	46,51,73	1.39	4 (8%)	54,86,113	1.28	8 (14%)
24	CHL	V	307	-	38,52,74	3.05	10 (26%)	31,87,114	1.83	9 (29%)
26	IWJ	Q	320	-	43,45,45	1.44	4 (9%)	47,65,65	1.67	9 (19%)
25	CLA	L	304	-	46,50,73	1.37	8 (17%)	53,85,113	1.42	5 (9%)
25	CLA	B	813	-	69,73,73	1.21	8 (11%)	82,113,113	1.57	17 (20%)
25	CLA	1	608	1	69,73,73	1.23	8 (11%)	82,113,113	1.24	8 (9%)
24	CHL	4	302	4	46,60,74	2.77	15 (32%)	40,97,114	2.07	15 (37%)
26	IWJ	4	301	-	43,45,45	1.56	4 (9%)	47,65,65	1.26	4 (8%)
29	Q6L	X	301	-	42,43,43	1.94	8 (19%)	51,60,60	1.74	8 (15%)
24	CHL	3	306	-	38,53,74	2.90	15 (39%)	36,89,114	1.72	9 (25%)
24	CHL	T	306	-	46,60,74	2.57	12 (26%)	40,97,114	1.73	15 (37%)
25	CLA	4	314	-	45,49,73	1.38	6 (13%)	54,84,113	1.39	6 (11%)
24	CHL	R	309	-	44,58,74	2.82	13 (29%)	37,94,114	2.16	15 (40%)
25	CLA	A	823	39	69,73,73	1.23	8 (11%)	82,113,113	1.36	12 (14%)
25	CLA	W	303	-	54,58,73	1.30	9 (16%)	64,95,113	1.38	10 (15%)
24	CHL	6	605	-	36,50,74	2.98	9 (25%)	31,85,114	1.79	8 (25%)
25	CLA	B	814	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	8 (9%)
25	CLA	2	614	2	47,52,73	1.31	6 (12%)	55,87,113	1.45	7 (12%)
25	CLA	B	812	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	9 (10%)
25	CLA	A	821	-	69,73,73	1.23	8 (11%)	82,113,113	1.35	12 (14%)
31	LMG	B	801	-	38,38,55	1.15	3 (7%)	46,46,63	1.13	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	BCR	I	101	-	41,41,41	1.00	4 (9%)	56,56,56	2.46	21 (37%)
24	CHL	4	307	-	37,50,74	2.97	14 (37%)	31,85,114	2.47	12 (38%)
25	CLA	B	825	-	49,53,73	1.36	7 (14%)	58,89,113	1.30	9 (15%)
25	CLA	3	302	-	59,63,73	1.39	10 (16%)	70,101,113	1.73	17 (24%)
25	CLA	R	306	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	3 (3%)
25	CLA	T	302	-	69,73,73	1.21	7 (10%)	82,113,113	1.19	5 (6%)
37	NEX	W	317	-	40,46,46	1.22	5 (12%)	50,70,70	2.44	14 (28%)
25	CLA	U	303	-	54,58,73	1.34	6 (11%)	64,95,113	1.28	6 (9%)
25	CLA	A	830	-	69,73,73	1.22	7 (10%)	82,113,113	1.60	13 (15%)
25	CLA	G	204	13	49,53,73	1.50	8 (16%)	58,89,113	1.49	10 (17%)
30	BCR	M	101	-	41,41,41	1.33	8 (19%)	56,56,56	2.33	23 (41%)
25	CLA	6	604	-	46,51,73	1.38	6 (13%)	54,86,113	1.28	6 (11%)
29	Q6L	R	319	-	42,43,43	1.93	8 (19%)	51,60,60	1.68	6 (11%)
26	IWJ	R	322	-	43,45,45	1.52	4 (9%)	47,65,65	1.19	4 (8%)
25	CLA	4	305	-	47,51,73	1.54	10 (21%)	58,87,113	1.26	5 (8%)
24	CHL	Q	308	23	44,58,74	3.00	16 (36%)	37,94,114	1.79	5 (13%)
25	CLA	A	843	-	69,73,73	1.17	6 (8%)	82,113,113	1.48	8 (9%)
25	CLA	T	303	-	54,58,73	1.33	7 (12%)	64,95,113	1.27	6 (9%)
24	CHL	2	601	2	41,55,74	3.00	14 (34%)	35,91,114	1.66	9 (25%)
24	CHL	P	314	22	38,53,74	3.02	10 (26%)	31,88,114	1.81	10 (32%)
25	CLA	A	825	-	69,73,73	1.23	6 (8%)	82,113,113	1.61	16 (19%)
25	CLA	N	203	-	46,50,73	1.52	8 (17%)	53,85,113	1.33	10 (18%)
24	CHL	W	306	-	46,60,74	2.72	15 (32%)	40,97,114	1.96	15 (37%)
26	IWJ	U	316	-	43,45,45	1.50	7 (16%)	47,65,65	2.05	7 (14%)
31	LMG	5	613	-	54,54,55	0.92	2 (3%)	62,62,63	0.84	1 (1%)
25	CLA	6	610	-	65,69,73	1.18	6 (9%)	77,108,113	1.17	5 (6%)
25	CLA	A	809	-	54,58,73	1.27	8 (14%)	64,95,113	1.40	9 (14%)
26	IWJ	T	321	-	43,45,45	1.58	6 (13%)	47,65,65	1.36	5 (10%)
25	CLA	1	607	1	40,44,73	1.61	8 (20%)	48,74,113	2.24	10 (20%)
24	CHL	2	607	-	38,53,74	3.08	15 (39%)	31,88,114	1.87	9 (29%)
25	CLA	P	312	22	59,63,73	1.26	5 (8%)	70,101,113	1.34	8 (11%)
30	BCR	F	801	-	41,41,41	1.14	4 (9%)	56,56,56	1.98	17 (30%)
25	CLA	A	815	-	69,73,73	1.21	6 (8%)	82,113,113	1.56	10 (12%)
25	CLA	H	302	-	69,73,73	1.14	7 (10%)	82,113,113	1.42	9 (10%)
24	CHL	X	315	22	38,53,74	2.93	8 (21%)	31,88,114	1.81	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	Q6L	X	319	-	42,43,43	1.96	8 (19%)	51,60,60	2.05	9 (17%)
31	LMG	J	104	-	46,46,55	0.98	2 (4%)	54,54,63	0.89	2 (3%)
24	CHL	S	304	22	36,50,74	3.01	14 (38%)	29,85,114	2.06	14 (48%)
24	CHL	Q	309	-	38,52,74	3.01	10 (26%)	31,87,114	1.96	12 (38%)
36	DGD	B	850	-	60,60,67	0.95	3 (5%)	74,74,81	0.96	4 (5%)
24	CHL	W	307	-	60,74,74	2.41	8 (13%)	58,114,114	1.72	15 (25%)
25	CLA	A	806	-	56,60,73	1.31	6 (10%)	65,97,113	1.47	10 (15%)
29	Q6L	R	301	-	42,43,43	1.91	7 (16%)	51,60,60	2.04	8 (15%)
29	Q6L	S	321	-	42,43,43	2.00	10 (23%)	51,60,60	1.78	10 (19%)
25	CLA	U	311	22	59,63,73	1.27	8 (13%)	70,101,113	1.47	10 (14%)
28	LHG	2	619	25	32,32,48	1.13	2 (6%)	35,38,54	1.08	4 (11%)
25	CLA	5	602	5	64,68,73	1.21	5 (7%)	76,107,113	1.35	10 (13%)
25	CLA	B	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.36	6 (9%)
25	CLA	A	834	-	60,64,73	1.25	6 (10%)	71,102,113	1.25	8 (11%)
25	CLA	2	602	2	65,69,73	1.27	6 (9%)	77,108,113	1.61	15 (19%)
30	BCR	J	101	-	41,41,41	1.19	4 (9%)	56,56,56	2.57	22 (39%)
25	CLA	B	805	-	69,73,73	1.21	8 (11%)	82,113,113	1.30	10 (12%)
28	LHG	1	614	25	34,34,48	1.12	2 (5%)	37,40,54	1.19	3 (8%)
25	CLA	P	303	-	54,58,73	1.31	5 (9%)	64,95,113	1.31	9 (14%)
29	Q6L	V	321	-	42,43,43	1.90	8 (19%)	51,60,60	1.71	7 (13%)
25	CLA	A	840	-	59,63,73	1.26	6 (10%)	70,101,113	1.45	6 (8%)
29	Q6L	P	321	-	42,43,43	1.92	8 (19%)	51,60,60	1.58	7 (13%)
33	CL0	A	802	-	58,73,73	2.15	13 (22%)	60,113,113	1.55	11 (18%)
25	CLA	2	608	2	49,53,73	1.36	4 (8%)	58,89,113	1.36	9 (15%)
25	CLA	2	611	2	47,52,73	1.38	4 (8%)	55,88,113	1.40	4 (7%)
29	Q6L	U	314	-	42,43,43	1.89	7 (16%)	51,60,60	1.87	8 (15%)
24	CHL	T	320	-	46,60,74	2.64	10 (21%)	40,97,114	2.10	15 (37%)
26	IWJ	X	318	-	43,45,45	1.63	7 (16%)	47,65,65	1.72	10 (21%)
25	CLA	O	2001	-	63,67,73	1.20	5 (7%)	74,105,113	1.44	7 (9%)
25	CLA	B	835	-	49,53,73	1.40	6 (12%)	58,89,113	1.20	4 (6%)
25	CLA	S	309	22	64,68,73	1.22	9 (14%)	76,107,113	1.16	6 (7%)
29	Q6L	Q	318	-	42,43,43	1.81	6 (14%)	51,60,60	1.63	7 (13%)
25	CLA	A	820	-	63,67,73	1.28	9 (14%)	74,105,113	1.41	11 (14%)
32	SQD	6	617	-	52,54,54	1.12	3 (5%)	62,65,65	1.09	4 (6%)
25	CLA	5	607	5	69,73,73	1.16	6 (8%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	3	305	3	45,49,73	1.51	10 (22%)	54,84,113	1.32	7 (12%)
37	NEX	S	317	-	40,46,46	1.42	5 (12%)	50,70,70	2.44	17 (34%)
38	KC2	P	308	22	49,53,53	2.13	15 (30%)	60,89,89	2.40	17 (28%)
28	LHG	A	847	25	29,29,48	1.18	2 (6%)	32,35,54	1.06	2 (6%)
25	CLA	B	809	-	69,73,73	1.23	9 (13%)	82,113,113	1.37	10 (12%)
25	CLA	O	2005	-	45,49,73	1.39	6 (13%)	54,84,113	1.39	5 (9%)
24	CHL	T	314	22	36,50,74	2.97	9 (25%)	29,85,114	2.01	9 (31%)
25	CLA	B	802	-	69,73,73	1.18	7 (10%)	82,113,113	1.44	11 (13%)
30	BCR	4	319	-	41,41,41	1.30	5 (12%)	56,56,56	2.34	23 (41%)
25	CLA	2	609	2	59,63,73	1.22	6 (10%)	70,101,113	1.32	8 (11%)
30	BCR	G	205	-	41,41,41	1.21	5 (12%)	56,56,56	2.00	14 (25%)
25	CLA	B	831	-	69,73,73	1.23	8 (11%)	82,113,113	1.47	10 (12%)
25	CLA	1	613	-	56,60,73	1.30	5 (8%)	65,97,113	1.25	8 (12%)
25	CLA	B	816	-	55,59,73	1.28	7 (12%)	64,96,113	1.27	7 (10%)
24	CHL	V	304	22	40,54,74	2.84	11 (27%)	34,90,114	1.79	10 (29%)
25	CLA	B	817	-	47,51,73	1.39	9 (19%)	55,86,113	1.30	4 (7%)
25	CLA	L	302	-	64,68,73	1.24	7 (10%)	76,107,113	1.41	7 (9%)
24	CHL	W	305	-	36,50,74	3.07	14 (38%)	29,85,114	2.09	11 (37%)
28	LHG	3	323	-	42,42,48	1.00	2 (4%)	45,48,54	0.93	3 (6%)
25	CLA	A	811	7	54,58,73	1.29	4 (7%)	64,95,113	1.48	7 (10%)
24	CHL	U	313	22	37,51,74	2.96	10 (27%)	30,86,114	1.88	10 (33%)
30	BCR	K	205	-	41,41,41	1.21	4 (9%)	56,56,56	2.09	16 (28%)
37	NEX	P	317	-	40,46,46	1.33	8 (20%)	50,70,70	2.45	16 (32%)
25	CLA	6	608	6	46,50,73	1.37	5 (10%)	53,85,113	1.47	6 (11%)
25	CLA	5	609	-	57,62,73	1.27	7 (12%)	67,100,113	1.31	5 (7%)
25	CLA	2	610	28	46,50,73	1.38	6 (13%)	53,85,113	1.36	6 (11%)
25	CLA	S	302	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	6 (7%)
38	KC2	V	308	22	49,53,53	2.29	13 (26%)	60,89,89	2.09	19 (31%)
25	CLA	A	856	-	61,65,73	1.21	5 (8%)	72,103,113	1.65	13 (18%)
25	CLA	4	309	4	49,53,73	1.40	7 (14%)	58,89,113	1.66	11 (18%)
25	CLA	A	842	-	69,73,73	1.20	9 (13%)	82,113,113	1.42	12 (14%)
29	Q6L	S	315	-	42,43,43	1.78	5 (11%)	51,60,60	1.72	10 (19%)
25	CLA	5	604	-	41,46,73	1.61	10 (24%)	51,81,113	1.29	6 (11%)
25	CLA	A	818	-	49,53,73	1.37	5 (10%)	58,89,113	1.39	7 (12%)
26	IWJ	T	318	-	43,45,45	1.58	4 (9%)	47,65,65	1.37	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	W	309	22	68,72,73	1.16	7 (10%)	80,111,113	1.44	9 (11%)
30	BCR	B	848	-	41,41,41	1.29	4 (9%)	56,56,56	2.23	19 (33%)
25	CLA	B	832	-	47,51,73	1.50	10 (21%)	55,86,113	1.54	12 (21%)
24	CHL	Q	316	23	38,53,74	3.04	10 (26%)	31,88,114	2.12	13 (41%)
25	CLA	3	311	3	57,62,73	1.33	8 (14%)	67,100,113	1.66	12 (17%)
25	CLA	B	806	-	69,73,73	1.19	8 (11%)	82,113,113	1.53	12 (14%)
25	CLA	S	310	22	64,68,73	1.19	8 (12%)	76,107,113	1.25	7 (9%)
24	CHL	5	605	-	35,49,74	2.98	9 (25%)	28,84,114	1.88	9 (32%)
28	LHG	3	322	-	35,35,48	1.04	2 (5%)	38,41,54	1.08	3 (7%)
30	BCR	A	850	-	41,41,41	1.26	5 (12%)	56,56,56	2.40	22 (39%)
29	Q6L	R	304	-	42,43,43	1.94	8 (19%)	51,60,60	1.68	7 (13%)
30	BCR	L	305	-	41,41,41	1.04	1 (2%)	56,56,56	2.31	20 (35%)
30	BCR	A	852	-	41,41,41	1.16	4 (9%)	56,56,56	2.17	13 (23%)
25	CLA	X	310	22	46,50,73	1.39	7 (15%)	53,85,113	1.34	7 (13%)
24	CHL	W	304	22	36,50,74	3.02	10 (27%)	29,85,114	1.80	9 (31%)
25	CLA	R	314	22	64,68,73	1.24	6 (9%)	76,107,113	1.43	9 (11%)
25	CLA	A	816	-	49,53,73	1.36	7 (14%)	58,89,113	1.52	8 (13%)
29	Q6L	P	316	-	42,43,43	1.96	9 (21%)	51,60,60	1.77	9 (17%)
25	CLA	A	807	-	68,72,73	1.23	8 (11%)	80,111,113	1.33	8 (10%)
31	LMG	A	801	-	31,31,55	1.15	2 (6%)	39,39,63	0.93	1 (2%)
30	BCR	K	202	-	41,41,41	1.20	6 (14%)	56,56,56	2.61	26 (46%)
38	KC2	Q	310	23	49,53,53	2.20	13 (26%)	60,89,89	2.26	13 (21%)
29	Q6L	V	315	-	42,43,43	1.93	7 (16%)	51,60,60	1.91	7 (13%)
25	CLA	Q	315	-	52,56,73	1.32	7 (13%)	61,92,113	1.41	8 (13%)
24	CHL	P	307	-	38,52,74	3.26	11 (28%)	31,87,114	1.99	10 (32%)
25	CLA	3	309	28	46,50,73	1.40	6 (13%)	53,85,113	1.33	6 (11%)
24	CHL	6	606	-	37,51,74	3.08	8 (21%)	30,86,114	2.11	11 (36%)
30	BCR	B	849	-	41,41,41	1.07	2 (4%)	56,56,56	2.31	17 (30%)
30	BCR	A	851	-	41,41,41	0.95	2 (4%)	56,56,56	2.45	22 (39%)
25	CLA	K	203	-	66,70,73	1.19	7 (10%)	78,109,113	1.42	7 (8%)
25	CLA	2	613	-	45,50,73	1.39	6 (13%)	52,85,113	1.31	8 (15%)
25	CLA	B	823	-	51,55,73	1.37	5 (9%)	60,91,113	1.20	4 (6%)
25	CLA	H	301	14	47,52,73	1.34	5 (10%)	55,87,113	1.36	7 (12%)
26	IWJ	V	317	-	43,45,45	1.58	4 (9%)	47,65,65	1.38	4 (8%)
30	BCR	F	804	-	41,41,41	1.17	3 (7%)	56,56,56	2.37	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	V	314	22	38,52,74	2.90	11 (28%)	31,87,114	1.80	10 (32%)
25	CLA	A	813	-	69,73,73	1.19	7 (10%)	82,113,113	1.13	5 (6%)
24	CHL	S	305	22	36,50,74	2.91	12 (33%)	29,85,114	2.18	15 (51%)
25	CLA	R	305	22	69,73,73	1.20	5 (7%)	82,113,113	1.37	8 (9%)
25	CLA	B	807	-	69,73,73	1.20	8 (11%)	82,113,113	1.44	9 (10%)
25	CLA	S	313	-	45,49,73	1.43	6 (13%)	54,84,113	1.29	5 (9%)
24	CHL	X	306	-	36,50,74	2.95	12 (33%)	29,85,114	2.46	12 (41%)
29	Q6L	P	319	-	42,43,43	1.91	7 (16%)	51,60,60	1.76	9 (17%)
25	CLA	K	201	17	49,53,73	1.40	4 (8%)	58,89,113	1.70	12 (20%)
25	CLA	X	313	22	45,49,73	1.40	8 (17%)	54,84,113	1.33	7 (12%)
25	CLA	A	838	7	69,73,73	1.19	7 (10%)	82,113,113	1.42	11 (13%)
26	IWJ	S	322	-	43,45,45	1.60	5 (11%)	47,65,65	1.49	5 (10%)
25	CLA	A	812	-	68,72,73	1.17	7 (10%)	80,111,113	1.30	6 (7%)
25	CLA	B	821	-	59,63,73	1.31	7 (11%)	70,101,113	1.33	10 (14%)
25	CLA	3	307	3	65,69,73	1.26	9 (13%)	77,108,113	1.53	10 (12%)
25	CLA	6	611	-	47,51,73	1.36	5 (10%)	55,86,113	1.37	8 (14%)
31	LMG	A	857	-	46,46,55	0.97	2 (4%)	54,54,63	0.89	2 (3%)
25	CLA	5	606	-	44,48,73	1.50	7 (15%)	55,83,113	1.51	8 (14%)
25	CLA	A	808	7	69,73,73	1.18	7 (10%)	82,113,113	1.44	9 (10%)
25	CLA	A	839	-	69,73,73	1.13	6 (8%)	82,113,113	1.38	11 (13%)
26	IWJ	S	319	-	43,45,45	1.57	6 (13%)	47,65,65	1.54	8 (17%)
25	CLA	Q	314	23	57,61,73	1.24	5 (8%)	67,98,113	1.37	7 (10%)
25	CLA	X	302	22	59,63,73	1.25	10 (16%)	70,101,113	1.36	11 (15%)
28	LHG	3	320	25	22,22,48	1.10	1 (4%)	24,27,54	1.08	1 (4%)
38	KC2	W	308	22	49,53,53	2.18	15 (30%)	60,89,89	2.07	18 (30%)
25	CLA	2	603	-	47,52,73	1.42	7 (14%)	55,88,113	1.42	7 (12%)
29	Q6L	O	2006	-	42,43,43	1.94	8 (19%)	51,60,60	1.79	7 (13%)
24	CHL	U	305	-	40,54,74	2.97	10 (25%)	34,90,114	2.25	11 (32%)
25	CLA	B	826	-	69,73,73	1.26	11 (15%)	82,113,113	1.49	14 (17%)
25	CLA	5	601	5	50,54,73	1.35	7 (14%)	59,90,113	1.64	12 (20%)
25	CLA	4	312	4	44,49,73	1.43	6 (13%)	50,84,113	1.41	7 (14%)
29	Q6L	T	322	-	42,43,43	1.94	8 (19%)	51,60,60	1.99	8 (15%)
25	CLA	R	316	22	59,63,73	1.27	6 (10%)	70,101,113	1.54	9 (12%)
30	BCR	A	848	-	41,41,41	1.34	5 (12%)	56,56,56	2.14	19 (33%)
24	CHL	R	318	22	38,53,74	3.02	9 (23%)	31,88,114	1.85	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LHG	6	616	-	45,45,48	0.96	2 (4%)	48,51,54	1.09	3 (6%)
24	CHL	V	306	-	38,52,74	2.96	13 (34%)	31,87,114	1.93	10 (32%)
28	LHG	3	321	-	42,42,48	1.00	2 (4%)	45,48,54	0.90	1 (2%)
29	Q6L	X	317	-	42,43,43	1.90	8 (19%)	51,60,60	2.02	8 (15%)
25	CLA	B	837	-	46,50,73	1.42	6 (13%)	53,85,113	1.43	7 (13%)
29	Q6L	T	316	-	42,43,43	1.89	7 (16%)	51,60,60	2.02	12 (23%)
25	CLA	S	311	-	51,55,73	1.31	5 (9%)	60,91,113	1.47	8 (13%)
29	Q6L	2	616	-	42,43,43	1.85	7 (16%)	51,60,60	2.24	14 (27%)
25	CLA	3	314	3	43,48,73	1.44	5 (11%)	51,83,113	1.34	7 (13%)
29	Q6L	Q	317	-	42,43,43	1.85	6 (14%)	51,60,60	1.76	9 (17%)
25	CLA	K	204	-	50,54,73	1.34	8 (16%)	59,90,113	1.56	8 (13%)
26	IWJ	R	303	-	43,45,45	1.55	5 (11%)	47,65,65	1.40	7 (14%)
29	Q6L	X	316	-	40,41,43	1.90	6 (15%)	50,56,60	1.93	10 (20%)
30	BCR	B	845	-	41,41,41	1.30	4 (9%)	56,56,56	2.74	25 (44%)
25	CLA	A	826	-	59,63,73	1.23	5 (8%)	70,101,113	1.35	7 (10%)
24	CHL	X	308	-	38,52,74	2.94	10 (26%)	31,87,114	1.97	11 (35%)
29	Q6L	Q	319	-	42,43,43	1.91	7 (16%)	51,60,60	1.86	12 (23%)
29	Q6L	W	315	-	42,43,43	1.86	8 (19%)	51,60,60	1.74	8 (15%)
25	CLA	Q	311	23	59,63,73	1.22	5 (8%)	70,101,113	1.25	8 (11%)
27	XAT	6	615	-	41,47,47	1.11	3 (7%)	54,74,74	2.77	25 (46%)
25	CLA	U	302	-	60,64,73	1.28	8 (13%)	71,102,113	1.36	8 (11%)
25	CLA	V	310	22	51,55,73	1.35	6 (11%)	60,91,113	1.25	8 (13%)
25	CLA	B	810	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	8 (9%)
25	CLA	B	836	8	64,68,73	1.22	8 (12%)	76,107,113	1.34	6 (7%)
25	CLA	4	304	-	48,52,73	1.48	8 (16%)	59,88,113	1.64	9 (15%)
25	CLA	B	827	-	54,58,73	1.30	4 (7%)	64,95,113	1.42	9 (14%)
24	CHL	Q	307	23	40,54,74	3.01	8 (20%)	34,90,114	2.07	12 (35%)
38	KC2	T	308	22	49,53,53	2.14	13 (26%)	60,89,89	2.20	16 (26%)
26	IWJ	V	318	-	43,45,45	1.60	4 (9%)	47,65,65	1.70	9 (19%)
25	CLA	U	308	22	45,49,73	1.35	7 (15%)	54,84,113	1.67	10 (18%)
25	CLA	A	837	-	69,73,73	1.21	7 (10%)	82,113,113	1.32	9 (10%)
25	CLA	6	602	6	66,70,73	1.16	4 (6%)	78,109,113	1.39	10 (12%)
30	BCR	3	319	-	41,41,41	1.25	5 (12%)	56,56,56	2.04	15 (26%)
25	CLA	R	313	22	68,72,73	1.20	7 (10%)	80,111,113	1.31	10 (12%)
25	CLA	V	302	-	54,58,73	1.29	7 (12%)	64,95,113	1.29	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	IWJ	1	611	-	43,45,45	1.73	5 (11%)	47,65,65	1.27	5 (10%)
29	Q6L	V	319	-	42,43,43	1.83	8 (19%)	51,60,60	2.12	16 (31%)
25	CLA	K	206	17	69,73,73	1.18	6 (8%)	82,113,113	1.35	10 (12%)
25	CLA	O	2002	-	69,73,73	1.23	8 (11%)	82,113,113	1.60	17 (20%)
25	CLA	Q	312	23	46,50,73	1.41	7 (15%)	53,85,113	1.18	4 (7%)
25	CLA	P	302	-	69,73,73	1.14	7 (10%)	82,113,113	1.34	10 (12%)
29	Q6L	R	320	-	42,43,43	1.92	7 (16%)	51,60,60	1.74	10 (19%)
29	Q6L	S	323	-	42,43,43	1.89	6 (14%)	51,60,60	1.78	12 (23%)
25	CLA	H	304	18	49,53,73	1.33	8 (16%)	58,89,113	1.41	8 (13%)
25	CLA	A	814	-	58,62,73	1.34	9 (15%)	68,99,113	1.32	11 (16%)
25	CLA	5	603	5	49,53,73	1.42	7 (14%)	58,89,113	1.39	6 (10%)
25	CLA	4	310	4	58,62,73	1.23	5 (8%)	68,99,113	1.34	11 (16%)
37	NEX	H	306	-	40,46,46	1.42	9 (22%)	50,70,70	2.32	18 (36%)
24	CHL	T	307	-	38,52,74	3.04	11 (28%)	31,87,114	1.94	10 (32%)
25	CLA	G	203	-	46,50,73	1.42	6 (13%)	53,85,113	1.49	5 (9%)
25	CLA	A	836	-	69,73,73	1.18	9 (13%)	82,113,113	1.38	5 (6%)
25	CLA	A	817	-	69,73,73	1.21	6 (8%)	82,113,113	1.27	8 (9%)
25	CLA	V	303	-	54,58,73	1.34	7 (12%)	64,95,113	1.50	8 (12%)
25	CLA	A	804	39	69,73,73	1.28	8 (11%)	82,113,113	1.46	15 (18%)
30	BCR	J	103	-	41,41,41	1.09	4 (9%)	56,56,56	2.22	19 (33%)
25	CLA	A	835	-	69,73,73	1.21	7 (10%)	82,113,113	1.27	6 (7%)
25	CLA	4	315	-	45,49,73	1.41	5 (11%)	54,84,113	1.28	7 (12%)
24	CHL	U	304	22	36,50,74	2.94	13 (36%)	29,85,114	1.93	10 (34%)
25	CLA	R	315	-	64,68,73	1.26	7 (10%)	76,107,113	1.37	8 (10%)
25	CLA	U	309	22	50,54,73	1.31	6 (12%)	59,90,113	1.24	4 (6%)
26	IWJ	V	320	-	43,45,45	1.57	5 (11%)	47,65,65	1.40	4 (8%)
25	CLA	4	311	-	46,50,73	1.57	6 (13%)	53,85,113	1.68	11 (20%)
25	CLA	V	313	-	52,56,73	1.31	6 (11%)	61,92,113	1.20	5 (8%)
37	NEX	R	321	-	40,46,46	1.43	8 (20%)	50,70,70	2.42	17 (34%)
25	CLA	R	307	-	54,58,73	1.32	7 (12%)	64,95,113	1.26	6 (9%)
25	CLA	Q	306	39	54,58,73	1.35	9 (16%)	64,95,113	1.52	12 (18%)
24	CHL	T	304	22	37,51,74	3.09	11 (29%)	30,86,114	2.06	11 (36%)
25	CLA	2	612	2	69,73,73	1.20	6 (8%)	82,113,113	1.34	12 (14%)
29	Q6L	V	316	-	42,43,43	1.98	7 (16%)	51,60,60	1.99	9 (17%)
30	BCR	G	201	-	41,41,41	1.08	3 (7%)	56,56,56	2.22	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	1	605	-	44,49,73	1.44	7 (15%)	50,84,113	1.22	3 (6%)
25	CLA	B	811	8	69,73,73	1.21	9 (13%)	82,113,113	1.30	6 (7%)
25	CLA	3	304	3	44,49,73	1.45	9 (20%)	50,84,113	1.46	7 (14%)
25	CLA	1	609	-	41,46,73	1.52	6 (14%)	51,81,113	1.47	8 (15%)
24	CHL	P	304	22	40,54,74	3.03	10 (25%)	34,90,114	2.19	16 (47%)
25	CLA	A	845	28	54,58,73	1.25	6 (11%)	64,95,113	1.35	7 (10%)
24	CHL	4	306	-	35,49,74	3.11	10 (28%)	30,84,114	1.68	8 (26%)
25	CLA	W	302	-	59,63,73	1.26	7 (11%)	70,101,113	1.17	5 (7%)
25	CLA	3	310	-	47,51,73	1.38	5 (10%)	55,86,113	1.30	7 (12%)
25	CLA	1	606	1	44,48,73	1.49	6 (13%)	55,83,113	1.39	9 (16%)
26	IWJ	4	317	-	43,45,45	1.64	6 (13%)	47,65,65	1.51	9 (19%)
36	DGD	A	854	-	52,52,67	1.05	3 (5%)	66,66,81	1.21	6 (9%)
25	CLA	B	842	-	69,73,73	1.22	8 (11%)	82,113,113	1.56	11 (13%)
25	CLA	X	312	-	55,59,73	1.29	7 (12%)	64,96,113	1.40	7 (10%)
31	LMG	2	620	-	31,31,55	1.18	2 (6%)	39,39,63	1.29	4 (10%)
25	CLA	3	303	-	47,51,73	1.53	9 (19%)	58,87,113	1.38	6 (10%)
25	CLA	B	833	-	47,51,73	1.36	5 (10%)	55,86,113	1.50	5 (9%)
25	CLA	V	301	22	64,68,73	1.16	5 (7%)	76,107,113	1.47	10 (13%)
25	CLA	X	304	-	46,50,73	1.44	8 (17%)	53,85,113	1.45	8 (15%)
25	CLA	A	841	-	54,58,73	1.34	6 (11%)	64,95,113	1.36	5 (7%)
24	CHL	W	314	22	35,49,74	3.11	11 (31%)	30,83,114	2.11	12 (40%)
26	IWJ	W	318	-	43,45,45	1.59	4 (9%)	47,65,65	1.51	8 (17%)
25	CLA	W	313	-	47,51,73	1.37	7 (14%)	55,86,113	1.17	4 (7%)
31	LMG	A	855	-	27,27,55	1.27	2 (7%)	35,35,63	1.32	4 (11%)
25	CLA	B	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.32	8 (9%)
25	CLA	4	303	4	64,68,73	1.26	9 (14%)	76,107,113	1.25	11 (14%)
25	CLA	L	303	-	49,53,73	1.40	6 (12%)	58,89,113	1.56	13 (22%)
28	LHG	Q	302	-	34,34,48	1.10	2 (5%)	37,40,54	1.07	2 (5%)
25	CLA	Q	313	-	50,54,73	1.33	7 (14%)	59,90,113	1.45	6 (10%)
29	Q6L	U	315	-	42,43,43	1.93	8 (19%)	51,60,60	2.04	12 (23%)
25	CLA	1	610	1	44,48,73	1.51	7 (15%)	53,83,113	1.48	12 (22%)
25	CLA	5	610	-	45,49,73	1.42	7 (15%)	54,84,113	1.23	5 (9%)
25	CLA	W	312	22	59,63,73	1.21	7 (11%)	70,101,113	1.56	12 (17%)
25	CLA	A	819	-	64,68,73	1.17	5 (7%)	76,107,113	1.47	8 (10%)
25	CLA	V	312	22	59,63,73	1.26	7 (11%)	70,101,113	1.30	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	IWJ	6	614	-	43,45,45	1.53	4 (9%)	47,65,65	1.43	5 (10%)
30	BCR	3	318	-	41,41,41	1.28	6 (14%)	56,56,56	2.19	19 (33%)
25	CLA	6	613	6	69,73,73	1.22	6 (8%)	82,113,113	1.30	9 (10%)
30	BCR	B	846	-	41,41,41	1.09	5 (12%)	56,56,56	2.35	19 (33%)
25	CLA	B	820	-	64,68,73	1.24	10 (15%)	76,107,113	1.43	13 (17%)
26	IWJ	3	315	-	43,45,45	1.46	7 (16%)	47,65,65	1.93	5 (10%)
26	IWJ	P	318	-	43,45,45	1.49	5 (11%)	47,65,65	1.27	4 (8%)
29	Q6L	S	320	-	42,43,43	1.96	7 (16%)	51,60,60	1.83	12 (23%)
25	CLA	3	313	-	45,49,73	1.40	6 (13%)	54,84,113	1.30	5 (9%)
34	PQN	B	844	-	34,34,34	2.99	11 (32%)	43,45,45	2.01	9 (20%)
25	CLA	S	303	-	54,58,73	1.35	8 (14%)	64,95,113	1.37	8 (12%)
27	XAT	5	612	-	41,47,47	1.07	2 (4%)	54,74,74	2.84	24 (44%)
29	Q6L	W	316	-	42,43,43	1.95	9 (21%)	51,60,60	2.04	13 (25%)
25	CLA	B	808	8	69,73,73	1.20	10 (14%)	82,113,113	1.31	11 (13%)
25	CLA	1	603	-	59,63,73	1.28	7 (11%)	70,101,113	1.63	13 (18%)
25	CLA	T	309	22	63,67,73	1.22	8 (12%)	74,105,113	1.32	8 (10%)
25	CLA	B	819	-	63,67,73	1.25	6 (9%)	74,105,113	1.27	9 (12%)
35	SF4	C	101	9	0,12,12	-	-	-		
30	BCR	B	847	-	41,41,41	1.33	6 (14%)	56,56,56	2.52	22 (39%)
25	CLA	3	308	3	45,49,73	1.40	7 (15%)	54,84,113	1.37	8 (14%)
34	PQN	A	844	-	34,34,34	3.02	10 (29%)	43,45,45	1.93	8 (18%)
24	CHL	S	306	-	46,60,74	2.78	12 (26%)	40,97,114	2.19	14 (35%)
25	CLA	R	317	-	52,56,73	1.32	6 (11%)	61,92,113	1.36	8 (13%)
30	BCR	3	317	-	41,41,41	1.10	3 (7%)	56,56,56	1.90	17 (30%)
25	CLA	B	824	-	64,68,73	1.29	10 (15%)	76,107,113	1.29	9 (11%)
24	CHL	1	604	1	35,49,74	3.05	10 (28%)	28,84,114	1.72	10 (35%)
25	CLA	S	312	22	59,63,73	1.25	8 (13%)	70,101,113	1.26	7 (10%)
25	CLA	G	202	-	49,53,73	1.40	7 (14%)	58,89,113	1.25	6 (10%)
29	Q6L	P	315	-	42,43,43	1.96	8 (19%)	51,60,60	1.63	7 (13%)
25	CLA	3	301	3	64,68,73	1.28	8 (12%)	76,107,113	1.41	5 (6%)
25	CLA	W	301	22	59,63,73	1.24	7 (11%)	70,101,113	1.33	4 (5%)
31	LMG	F	805	-	31,31,55	1.15	2 (6%)	39,39,63	1.13	3 (7%)
25	CLA	A	824	-	46,50,73	1.45	6 (13%)	53,85,113	1.38	6 (11%)
25	CLA	4	316	4	46,50,73	1.36	5 (10%)	53,85,113	1.33	7 (13%)

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
24	CHL	6	601	6	3/3/15/26	1/10/108/137	-
25	CLA	A	828	-	-	5/32/108/115	-
25	CLA	A	829	-	1/1/15/20	14/39/115/115	-
25	CLA	B	803	-	1/1/15/20	10/39/115/115	-
25	CLA	A	833	-	-	5/21/97/115	-
25	CLA	A	810	7	1/1/15/20	7/39/115/115	-
25	CLA	Q	301	14	1/1/13/20	11/27/103/115	-
24	CHL	1	601	1	3/3/18/26	5/25/123/137	-
24	CHL	S	314	22	3/3/15/26	3/14/112/137	-
25	CLA	L	301	18	1/1/10/20	2/10/86/115	-
25	CLA	B	843	28	1/1/15/20	12/39/115/115	-
31	LMG	N	201	-	-	3/50/70/70	0/1/1/1
31	LMG	L	308	-	-	7/26/46/70	0/1/1/1
25	CLA	U	310	-	1/1/10/20	9/14/90/115	-
26	IWJ	5	611	-	-	5/33/76/76	1/2/2/2
37	NEX	T	317	-	-	3/27/83/83	0/3/3/3
24	CHL	U	306	-	3/3/15/26	5/13/111/137	-
30	BCR	H	305	-	-	6/29/63/63	0/2/2/2
25	CLA	X	314	-	1/1/10/20	6/10/86/115	-
25	CLA	J	102	16	1/1/10/20	7/12/88/115	-
25	CLA	A	831	-	1/1/15/20	15/39/115/115	-
29	Q6L	R	323	-	-	9/29/67/67	0/2/2/2
26	IWJ	Q	303	-	-	4/33/76/76	0/2/2/2
29	Q6L	T	315	-	-	6/29/67/67	0/2/2/2
25	CLA	5	608	5	1/1/10/20	4/10/86/115	-
38	KC2	X	309	22	-	9/15/71/71	-
38	KC2	R	312	22	-	7/15/71/71	-
28	LHG	A	846	-	-	10/53/53/53	-
25	CLA	A	832	-	1/1/15/20	12/39/115/115	-
35	SF4	C	102	9	-	-	0/6/5/5
25	CLA	P	310	22	1/1/14/20	8/33/109/115	-
30	BCR	2	618	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC2	S	308	22	-	7/15/71/71	-
24	CHL	2	615	2	3/3/15/26	4/12/110/137	-
25	CLA	A	805	-	1/1/15/20	13/39/115/115	-
25	CLA	A	822	-	1/1/11/20	3/15/91/115	-
25	CLA	N	202	20	1/1/11/20	2/15/91/115	-
29	Q6L	U	317	-	-	5/29/67/67	0/2/2/2
25	CLA	P	311	-	1/1/14/20	9/33/109/115	-
24	CHL	P	305	-	3/3/16/26	4/15/113/137	-
25	CLA	3	312	-	1/1/10/20	2/8/84/115	-
25	CLA	X	311	22	1/1/12/20	10/21/97/115	-
25	CLA	T	312	22	1/1/13/20	12/27/103/115	-
29	Q6L	S	316	-	-	2/29/67/67	0/2/2/2
24	CHL	R	308	22	3/3/16/26	3/15/113/137	-
24	CHL	S	307	-	3/3/15/26	5/10/108/137	-
25	CLA	4	313	4	-	7/30/106/115	-
25	CLA	B	838	-	1/1/12/20	2/21/97/115	-
25	CLA	B	840	-	-	9/18/94/115	-
29	Q6L	W	320	-	-	7/29/67/67	0/2/2/2
25	CLA	T	301	22	1/1/15/20	12/39/115/115	-
25	CLA	W	310	22	1/1/14/20	9/33/109/115	-
24	CHL	R	310	-	3/3/17/26	8/23/121/137	-
24	CHL	X	307	-	3/3/17/26	10/23/121/137	-
25	CLA	6	609	-	1/1/11/20	4/13/89/115	-
24	CHL	P	306	-	3/3/17/26	8/23/121/137	-
27	XAT	4	318	-	-	5/31/93/93	0/4/4/4
25	CLA	2	606	-	1/1/11/20	7/15/91/115	-
25	CLA	V	309	22	1/1/10/20	3/12/88/115	-
25	CLA	B	839	-	1/1/15/20	16/39/115/115	-
25	CLA	B	804	-	1/1/15/20	14/39/115/115	-
26	IWJ	P	320	-	-	3/33/76/76	0/2/2/2
25	CLA	P	313	-	-	6/19/95/115	-
25	CLA	X	303	-	1/1/12/20	8/23/99/115	-
26	IWJ	S	318	-	-	5/33/76/76	0/2/2/2
25	CLA	6	607	6	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	301	22	1/1/15/20	7/39/115/115	-
25	CLA	6	612	6	1/1/11/20	6/15/91/115	-
25	CLA	A	827	39	1/1/15/20	9/39/115/115	-
25	CLA	1	602	1	1/1/13/20	4/29/105/115	-
27	XAT	3	316	-	-	3/31/93/93	0/4/4/4
25	CLA	U	301	22	1/1/11/20	7/15/91/115	-
25	CLA	B	841	-	1/1/15/20	6/39/115/115	-
29	Q6L	W	319	-	-	9/29/67/67	0/2/2/2
38	KC2	U	307	22	-	10/15/71/71	-
30	BCR	L	306	-	-	2/29/63/63	0/2/2/2
24	CHL	V	305	22	3/3/15/26	4/12/110/137	-
25	CLA	A	803	-	1/1/15/20	6/39/115/115	-
25	CLA	B	828	-	1/1/15/20	4/39/115/115	-
24	CHL	X	305	22	3/3/15/26	0/10/108/137	-
25	CLA	B	829	-	1/1/15/20	16/39/115/115	-
25	CLA	F	802	-	1/1/10/20	3/12/88/115	-
35	SF4	A	853	8,7	-	-	0/6/5/5
25	CLA	B	830	-	1/1/15/20	12/39/115/115	-
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
27	XAT	1	612	-	-	6/31/93/93	0/4/4/4
24	CHL	T	305	-	3/3/16/26	5/19/117/137	-
27	XAT	2	617	-	-	0/31/93/93	0/4/4/4
25	CLA	O	2003	-	1/1/10/20	2/10/86/115	-
25	CLA	U	312	-	1/1/10/20	2/10/86/115	-
25	CLA	O	2004	-	1/1/10/20	6/10/86/115	-
25	CLA	T	313	-	1/1/10/20	5/12/88/115	-
25	CLA	T	310	22	1/1/10/20	3/12/88/115	-
25	CLA	B	815	-	1/1/15/20	12/39/115/115	-
25	CLA	P	301	22	1/1/15/20	10/39/115/115	-
32	SQD	H	303	-	-	10/43/63/69	0/1/1/1
25	CLA	W	311	-	1/1/11/20	5/15/91/115	-
25	CLA	P	309	22	1/1/14/20	15/38/114/115	-
31	LMG	O	2008	-	-	2/34/54/70	0/1/1/1
30	BCR	K	207	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Q	304	23	1/1/15/20	11/39/115/115	-
25	CLA	V	311	-	1/1/14/20	12/33/109/115	-
25	CLA	6	603	6	1/1/11/20	3/13/89/115	-
24	CHL	R	311	-	3/3/15/26	2/13/111/137	-
30	BCR	L	307	-	-	4/29/63/63	0/2/2/2
24	CHL	2	605	-	3/3/15/26	6/10/108/137	-
25	CLA	B	818	-	1/1/13/20	10/27/103/115	-
29	Q6L	T	319	-	-	8/29/67/67	0/2/2/2
24	CHL	R	302	-	3/3/16/26	7/17/115/137	-
24	CHL	4	308	-	3/3/16/26	3/15/113/137	-
25	CLA	T	311	-	1/1/14/20	12/33/109/115	-
29	Q6L	O	2007	-	-	6/29/67/67	0/2/2/2
25	CLA	F	803	12	1/1/10/20	4/10/86/115	-
25	CLA	Q	305	-	1/1/10/20	0/14/90/115	-
25	CLA	2	604	-	1/1/10/20	4/12/88/115	-
24	CHL	V	307	-	3/3/15/26	4/13/111/137	-
26	IWJ	Q	320	-	-	11/33/76/76	0/2/2/2
25	CLA	L	304	-	1/1/10/20	5/12/88/115	-
25	CLA	B	813	-	1/1/15/20	14/39/115/115	-
25	CLA	1	608	1	1/1/15/20	12/39/115/115	-
24	CHL	4	302	4	3/3/17/26	4/23/121/137	-
26	IWJ	4	301	-	-	6/33/76/76	0/2/2/2
29	Q6L	X	301	-	-	9/29/67/67	0/2/2/2
24	CHL	3	306	-	3/3/16/26	7/13/111/137	-
24	CHL	T	306	-	3/3/17/26	9/23/121/137	-
25	CLA	4	314	-	1/1/10/20	4/10/86/115	-
24	CHL	R	309	-	3/3/16/26	6/20/118/137	-
25	CLA	A	823	39	1/1/15/20	11/39/115/115	-
25	CLA	W	303	-	1/1/12/20	4/21/97/115	-
24	CHL	6	605	-	3/3/15/26	3/10/108/137	-
25	CLA	B	814	-	1/1/15/20	11/39/115/115	-
25	CLA	2	614	2	1/1/10/20	8/14/90/115	-
25	CLA	B	812	-	1/1/15/20	12/39/115/115	-
25	CLA	A	821	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	B	801	-	-	4/33/53/70	0/1/1/1
30	BCR	I	101	-	-	9/29/63/63	0/2/2/2
24	CHL	4	307	-	3/3/15/26	6/12/108/137	-
25	CLA	B	825	-	1/1/11/20	4/15/91/115	-
25	CLA	3	302	-	1/1/13/20	7/27/103/115	-
25	CLA	R	306	-	1/1/15/20	13/39/115/115	-
25	CLA	T	302	-	1/1/15/20	10/39/115/115	-
37	NEX	W	317	-	-	2/27/83/83	0/3/3/3
25	CLA	U	303	-	1/1/12/20	5/21/97/115	-
25	CLA	A	830	-	1/1/15/20	19/39/115/115	-
25	CLA	G	204	13	1/1/11/20	8/15/91/115	-
30	BCR	M	101	-	-	6/29/63/63	0/2/2/2
25	CLA	6	604	-	1/1/10/20	3/12/88/115	-
29	Q6L	R	319	-	-	10/29/67/67	0/2/2/2
26	IWJ	R	322	-	-	7/33/76/76	1/2/2/2
25	CLA	4	305	-	1/1/11/20	0/11/87/115	-
24	CHL	Q	308	23	3/3/16/26	6/20/118/137	-
25	CLA	A	843	-	1/1/15/20	7/39/115/115	-
25	CLA	T	303	-	1/1/12/20	4/21/97/115	-
24	CHL	2	601	2	3/3/16/26	2/17/115/137	-
24	CHL	P	314	22	3/3/15/26	4/14/112/137	-
25	CLA	A	825	-	1/1/15/20	17/39/115/115	-
25	CLA	N	203	-	1/1/10/20	4/12/88/115	-
24	CHL	W	306	-	3/3/17/26	3/23/121/137	-
26	IWJ	U	316	-	-	2/33/76/76	0/2/2/2
31	LMG	5	613	-	-	6/49/69/70	0/1/1/1
25	CLA	6	610	-	1/1/14/20	12/35/111/115	-
25	CLA	A	809	-	1/1/12/20	5/21/97/115	-
26	IWJ	T	321	-	-	4/33/76/76	1/2/2/2
25	CLA	1	607	1	1/1/7/20	2/8/68/115	-
24	CHL	2	607	-	3/3/15/26	5/14/112/137	-
25	CLA	P	312	22	1/1/13/20	10/27/103/115	-
30	BCR	F	801	-	-	4/29/63/63	0/2/2/2
25	CLA	A	815	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	H	302	-	1/1/15/20	11/39/115/115	-
24	CHL	X	315	22	3/3/15/26	6/14/112/137	-
29	Q6L	X	319	-	-	10/29/67/67	0/2/2/2
31	LMG	J	104	-	-	6/41/61/70	0/1/1/1
24	CHL	S	304	22	3/3/15/26	2/10/108/137	-
24	CHL	Q	309	-	3/3/15/26	2/13/111/137	-
36	DGD	B	850	-	-	12/48/88/95	0/2/2/2
24	CHL	W	307	-	3/3/20/26	13/39/137/137	-
25	CLA	A	806	-	1/1/12/20	5/24/100/115	-
29	Q6L	R	301	-	-	10/29/67/67	0/2/2/2
29	Q6L	S	321	-	-	11/29/67/67	0/2/2/2
25	CLA	U	311	22	1/1/13/20	5/27/103/115	-
28	LHG	2	619	25	-	7/37/37/53	-
25	CLA	5	602	5	1/1/14/20	10/33/109/115	-
25	CLA	B	822	-	1/1/12/20	2/21/97/115	-
25	CLA	A	834	-	1/1/13/20	4/29/105/115	-
25	CLA	2	602	2	1/1/14/20	15/35/111/115	-
30	BCR	J	101	-	-	4/29/63/63	0/2/2/2
25	CLA	B	805	-	1/1/15/20	15/39/115/115	-
28	LHG	1	614	25	-	11/39/39/53	-
25	CLA	P	303	-	1/1/12/20	9/21/97/115	-
29	Q6L	V	321	-	-	6/29/67/67	0/2/2/2
25	CLA	A	840	-	-	6/27/103/115	-
29	Q6L	P	321	-	-	7/29/67/67	0/2/2/2
33	CL0	A	802	-	3/3/20/25	10/37/135/135	-
25	CLA	2	608	2	1/1/11/20	6/15/91/115	-
25	CLA	2	611	2	1/1/11/20	5/13/89/115	-
29	Q6L	U	314	-	-	7/29/67/67	0/2/2/2
24	CHL	T	320	-	3/3/17/26	6/23/121/137	-
26	IWJ	X	318	-	-	7/33/76/76	1/2/2/2
25	CLA	O	2001	-	1/1/13/20	8/32/108/115	-
25	CLA	B	835	-	1/1/11/20	4/15/91/115	-
25	CLA	S	309	22	1/1/14/20	12/33/109/115	-
29	Q6L	Q	318	-	-	6/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	820	-	1/1/13/20	11/32/108/115	-
32	SQD	6	617	-	-	13/49/69/69	0/1/1/1
25	CLA	5	607	5	1/1/15/20	14/39/115/115	-
25	CLA	3	305	3	1/1/10/20	1/10/86/115	-
37	NEX	S	317	-	-	3/27/83/83	0/3/3/3
38	KC2	P	308	22	-	8/15/71/71	-
28	LHG	A	847	25	-	7/34/34/53	-
25	CLA	B	809	-	1/1/15/20	10/39/115/115	-
25	CLA	O	2005	-	1/1/10/20	2/10/86/115	-
24	CHL	T	314	22	3/3/15/26	2/10/108/137	-
25	CLA	B	802	-	1/1/15/20	9/39/115/115	-
30	BCR	4	319	-	-	2/29/63/63	0/2/2/2
25	CLA	2	609	2	1/1/13/20	7/27/103/115	-
30	BCR	G	205	-	-	2/29/63/63	0/2/2/2
25	CLA	B	831	-	1/1/15/20	13/39/115/115	-
25	CLA	1	613	-	1/1/12/20	7/24/100/115	-
25	CLA	B	816	-	1/1/12/20	4/23/99/115	-
24	CHL	V	304	22	3/3/16/26	6/15/113/137	-
25	CLA	B	817	-	1/1/10/20	3/13/89/115	-
25	CLA	L	302	-	-	12/33/109/115	-
24	CHL	W	305	-	3/3/15/26	2/10/108/137	-
28	LHG	3	323	-	-	13/47/47/53	-
25	CLA	A	811	7	1/1/12/20	2/21/97/115	-
24	CHL	U	313	22	3/3/15/26	2/12/110/137	-
30	BCR	K	205	-	-	2/29/63/63	0/2/2/2
37	NEX	P	317	-	-	2/27/83/83	0/3/3/3
25	CLA	6	608	6	1/1/10/20	4/12/88/115	-
25	CLA	5	609	-	1/1/13/20	9/25/101/115	-
25	CLA	2	610	28	1/1/10/20	4/12/88/115	-
25	CLA	S	302	-	1/1/15/20	12/39/115/115	-
38	KC2	V	308	22	-	11/15/71/71	-
25	CLA	A	856	-	1/1/13/20	12/30/106/115	-
25	CLA	4	309	4	1/1/11/20	6/15/91/115	-
25	CLA	A	842	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	Q6L	S	315	-	-	5/29/67/67	0/2/2/2
25	CLA	5	604	-	1/1/10/20	0/4/80/115	-
25	CLA	A	818	-	1/1/11/20	4/15/91/115	-
26	IWJ	T	318	-	-	6/33/76/76	0/2/2/2
25	CLA	W	309	22	1/1/14/20	9/38/114/115	-
30	BCR	B	848	-	-	2/29/63/63	0/2/2/2
25	CLA	B	832	-	1/1/10/20	5/13/89/115	-
24	CHL	Q	316	23	3/3/15/26	5/14/112/137	-
25	CLA	3	311	3	1/1/13/20	10/25/101/115	-
25	CLA	B	806	-	1/1/15/20	12/39/115/115	-
25	CLA	S	310	22	1/1/14/20	11/33/109/115	-
24	CHL	5	605	-	3/3/15/26	1/8/106/137	-
28	LHG	3	322	-	-	8/40/40/53	-
30	BCR	A	850	-	-	1/29/63/63	0/2/2/2
29	Q6L	R	304	-	-	5/29/67/67	0/2/2/2
30	BCR	L	305	-	-	3/29/63/63	0/2/2/2
30	BCR	A	852	-	-	4/29/63/63	0/2/2/2
25	CLA	X	310	22	1/1/10/20	2/12/88/115	-
24	CHL	W	304	22	3/3/15/26	1/10/108/137	-
25	CLA	R	314	22	1/1/14/20	12/33/109/115	-
25	CLA	A	816	-	1/1/11/20	7/15/91/115	-
29	Q6L	P	316	-	-	2/29/67/67	0/2/2/2
25	CLA	A	807	-	1/1/14/20	17/38/114/115	-
31	LMG	A	801	-	-	1/26/46/70	0/1/1/1
30	BCR	K	202	-	-	0/29/63/63	0/2/2/2
38	KC2	Q	310	23	-	6/15/71/71	-
29	Q6L	V	315	-	-	11/29/67/67	0/2/2/2
25	CLA	Q	315	-	1/1/11/20	4/19/95/115	-
24	CHL	P	307	-	3/3/15/26	2/13/111/137	-
25	CLA	3	309	28	1/1/10/20	5/12/88/115	-
24	CHL	6	606	-	3/3/15/26	6/12/110/137	-
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
30	BCR	A	851	-	-	5/29/63/63	0/2/2/2
25	CLA	K	203	-	1/1/14/20	6/36/112/115	-
25	CLA	2	613	-	1/1/10/20	5/11/87/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	823	-	1/1/11/20	6/18/94/115	-
25	CLA	H	301	14	1/1/10/20	8/14/90/115	-
26	IWJ	V	317	-	-	5/33/76/76	0/2/2/2
30	BCR	F	804	-	-	6/29/63/63	0/2/2/2
24	CHL	V	314	22	3/3/15/26	4/13/111/137	-
25	CLA	A	813	-	1/1/15/20	15/39/115/115	-
24	CHL	S	305	22	3/3/15/26	3/10/108/137	-
25	CLA	R	305	22	1/1/15/20	11/39/115/115	-
25	CLA	B	807	-	1/1/15/20	11/39/115/115	-
25	CLA	S	313	-	1/1/10/20	2/10/86/115	-
24	CHL	X	306	-	3/3/15/26	2/10/108/137	-
29	Q6L	P	319	-	-	6/29/67/67	0/2/2/2
25	CLA	K	201	17	1/1/11/20	4/15/91/115	-
25	CLA	X	313	22	1/1/10/20	2/10/86/115	-
25	CLA	A	838	7	-	18/39/115/115	-
26	IWJ	S	322	-	-	5/33/76/76	0/2/2/2
25	CLA	A	812	-	1/1/14/20	9/38/114/115	-
25	CLA	B	821	-	1/1/13/20	9/27/103/115	-
25	CLA	3	307	3	1/1/14/20	11/35/111/115	-
25	CLA	6	611	-	1/1/10/20	6/13/89/115	-
31	LMG	A	857	-	-	9/41/61/70	0/1/1/1
25	CLA	5	606	-	1/1/10/20	0/8/84/115	-
25	CLA	A	808	7	1/1/15/20	9/39/115/115	-
25	CLA	A	839	-	1/1/15/20	16/39/115/115	-
26	IWJ	S	319	-	-	7/33/76/76	1/2/2/2
25	CLA	Q	314	23	1/1/12/20	10/25/101/115	-
25	CLA	X	302	22	1/1/13/20	9/27/103/115	-
28	LHG	3	320	25	-	3/26/26/53	-
38	KC2	W	308	22	-	9/15/71/71	-
25	CLA	2	603	-	1/1/11/20	4/13/89/115	-
29	Q6L	O	2006	-	-	9/29/67/67	0/2/2/2
24	CHL	U	305	-	3/3/16/26	8/15/113/137	-
25	CLA	B	826	-	1/1/15/20	8/39/115/115	-
25	CLA	5	601	5	1/1/11/20	11/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	4	312	4	1/1/10/20	2/10/86/115	-
29	Q6L	T	322	-	-	7/29/67/67	0/2/2/2
25	CLA	R	316	22	1/1/13/20	9/27/103/115	-
30	BCR	A	848	-	-	2/29/63/63	0/2/2/2
24	CHL	R	318	22	3/3/15/26	3/14/112/137	-
28	LHG	6	616	-	-	10/50/50/53	-
24	CHL	V	306	-	3/3/15/26	0/13/111/137	-
28	LHG	3	321	-	-	9/47/47/53	-
29	Q6L	X	317	-	-	2/29/67/67	0/2/2/2
25	CLA	B	837	-	1/1/10/20	2/12/88/115	-
29	Q6L	T	316	-	-	1/29/67/67	0/2/2/2
25	CLA	S	311	-	1/1/11/20	6/18/94/115	-
29	Q6L	2	616	-	-	11/29/67/67	0/2/2/2
25	CLA	3	314	3	-	0/8/84/115	-
29	Q6L	Q	317	-	-	7/29/67/67	0/2/2/2
25	CLA	K	204	-	1/1/11/20	7/17/93/115	-
26	IWJ	R	303	-	-	4/33/76/76	0/2/2/2
29	Q6L	X	316	-	-	7/29/63/67	0/2/2/2
30	BCR	B	845	-	-	2/29/63/63	0/2/2/2
25	CLA	A	826	-	1/1/13/20	9/27/103/115	-
24	CHL	X	308	-	3/3/15/26	6/13/111/137	-
29	Q6L	Q	319	-	-	5/29/67/67	0/2/2/2
29	Q6L	W	315	-	-	4/29/67/67	0/2/2/2
25	CLA	Q	311	23	1/1/13/20	7/27/103/115	-
27	XAT	6	615	-	-	0/31/93/93	0/4/4/4
25	CLA	U	302	-	1/1/13/20	9/29/105/115	-
25	CLA	V	310	22	1/1/11/20	8/18/94/115	-
25	CLA	B	810	-	1/1/15/20	18/39/115/115	-
25	CLA	B	836	8	-	7/33/109/115	-
25	CLA	4	304	-	1/1/11/20	4/13/89/115	-
25	CLA	B	827	-	1/1/12/20	4/21/97/115	-
24	CHL	Q	307	23	3/3/16/26	8/15/113/137	-
38	KC2	T	308	22	-	7/15/71/71	-
26	IWJ	V	318	-	-	4/33/76/76	0/2/2/2
25	CLA	U	308	22	1/1/10/20	0/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	837	-	1/1/15/20	11/39/115/115	-
25	CLA	6	602	6	1/1/14/20	11/36/112/115	-
30	BCR	3	319	-	-	1/29/63/63	0/2/2/2
25	CLA	R	313	22	1/1/14/20	16/38/114/115	-
25	CLA	V	302	-	1/1/12/20	9/21/97/115	-
26	IWJ	1	611	-	-	4/33/76/76	0/2/2/2
29	Q6L	V	319	-	-	9/29/67/67	0/2/2/2
25	CLA	K	206	17	1/1/15/20	13/39/115/115	-
25	CLA	O	2002	-	1/1/15/20	8/39/115/115	-
25	CLA	Q	312	23	1/1/10/20	3/12/88/115	-
25	CLA	P	302	-	1/1/15/20	15/39/115/115	-
29	Q6L	R	320	-	-	0/29/67/67	0/2/2/2
29	Q6L	S	323	-	-	9/29/67/67	0/2/2/2
25	CLA	H	304	18	1/1/11/20	5/15/91/115	-
25	CLA	A	814	-	1/1/12/20	6/26/102/115	-
25	CLA	5	603	5	1/1/11/20	5/15/91/115	-
25	CLA	4	310	4	1/1/12/20	4/26/102/115	-
37	NEX	H	306	-	-	3/27/83/83	0/3/3/3
24	CHL	T	307	-	3/3/15/26	3/13/111/137	-
25	CLA	G	203	-	1/1/10/20	4/12/88/115	-
25	CLA	A	836	-	1/1/15/20	5/39/115/115	-
25	CLA	A	817	-	-	11/39/115/115	-
25	CLA	V	303	-	1/1/12/20	4/21/97/115	-
25	CLA	A	804	39	1/1/15/20	14/39/115/115	-
30	BCR	J	103	-	-	1/29/63/63	0/2/2/2
25	CLA	A	835	-	1/1/15/20	13/39/115/115	-
25	CLA	4	315	-	1/1/10/20	4/10/86/115	-
24	CHL	U	304	22	3/3/15/26	3/10/108/137	-
25	CLA	R	315	-	1/1/14/20	10/33/109/115	-
25	CLA	U	309	22	1/1/11/20	8/17/93/115	-
26	IWJ	V	320	-	-	5/33/76/76	1/2/2/2
25	CLA	4	311	-	1/1/10/20	6/12/88/115	-
25	CLA	V	313	-	1/1/11/20	6/19/95/115	-
37	NEX	R	321	-	-	3/27/83/83	0/3/3/3
25	CLA	R	307	-	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Q	306	39	1/1/12/20	7/21/97/115	-
24	CHL	T	304	22	3/3/15/26	4/12/110/137	-
25	CLA	2	612	2	1/1/15/20	15/39/115/115	-
29	Q6L	V	316	-	-	7/29/67/67	0/2/2/2
30	BCR	G	201	-	-	2/29/63/63	0/2/2/2
25	CLA	1	605	-	1/1/10/20	4/10/86/115	-
25	CLA	B	811	8	1/1/15/20	12/39/115/115	-
25	CLA	3	304	3	1/1/10/20	2/10/86/115	-
25	CLA	1	609	-	1/1/10/20	1/4/80/115	-
24	CHL	P	304	22	3/3/16/26	5/15/113/137	-
25	CLA	A	845	28	1/1/12/20	5/21/97/115	-
24	CHL	4	306	-	3/3/15/26	0/8/106/137	-
25	CLA	W	302	-	1/1/13/20	5/27/103/115	-
25	CLA	3	310	-	1/1/10/20	5/13/89/115	-
25	CLA	1	606	1	1/1/10/20	2/8/84/115	-
26	IWJ	4	317	-	-	8/33/76/76	0/2/2/2
36	DGD	A	854	-	-	4/40/80/95	0/2/2/2
25	CLA	B	842	-	1/1/15/20	17/39/115/115	-
25	CLA	X	312	-	1/1/12/20	6/23/99/115	-
31	LMG	2	620	-	-	3/26/46/70	0/1/1/1
25	CLA	3	303	-	1/1/11/20	0/11/87/115	-
25	CLA	B	833	-	1/1/10/20	0/13/89/115	-
25	CLA	V	301	22	1/1/14/20	10/33/109/115	-
25	CLA	X	304	-	1/1/10/20	3/12/88/115	-
25	CLA	A	841	-	1/1/12/20	4/21/97/115	-
24	CHL	W	314	22	3/3/14/26	3/10/104/137	-
26	IWJ	W	318	-	-	9/33/76/76	0/2/2/2
25	CLA	W	313	-	1/1/10/20	3/13/89/115	-
31	LMG	A	855	-	-	3/22/42/70	0/1/1/1
25	CLA	B	834	-	1/1/15/20	11/39/115/115	-
25	CLA	4	303	4	1/1/14/20	17/33/109/115	-
25	CLA	L	303	-	1/1/11/20	5/15/91/115	-
28	LHG	Q	302	-	-	5/39/39/53	-
25	CLA	Q	313	-	1/1/11/20	11/17/93/115	-
29	Q6L	U	315	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	1	610	1	-	6/8/84/115	-
25	CLA	5	610	-	1/1/10/20	4/10/86/115	-
25	CLA	W	312	22	1/1/13/20	7/27/103/115	-
25	CLA	A	819	-	1/1/14/20	13/33/109/115	-
25	CLA	V	312	22	-	7/27/103/115	-
26	IWJ	6	614	-	-	3/33/76/76	0/2/2/2
30	BCR	3	318	-	-	2/29/63/63	0/2/2/2
25	CLA	6	613	6	-	8/39/115/115	-
30	BCR	B	846	-	-	4/29/63/63	0/2/2/2
25	CLA	B	820	-	1/1/14/20	10/33/109/115	-
26	IWJ	3	315	-	-	3/33/76/76	1/2/2/2
26	IWJ	P	318	-	-	2/33/76/76	0/2/2/2
29	Q6L	S	320	-	-	7/29/67/67	0/2/2/2
25	CLA	3	313	-	1/1/10/20	2/10/86/115	-
34	PQN	B	844	-	-	6/23/43/43	0/2/2/2
25	CLA	S	303	-	1/1/12/20	2/21/97/115	-
27	XAT	5	612	-	-	0/31/93/93	0/4/4/4
29	Q6L	W	316	-	-	6/29/67/67	0/2/2/2
25	CLA	B	808	8	1/1/15/20	23/39/115/115	-
25	CLA	1	603	-	1/1/13/20	6/27/103/115	-
25	CLA	T	309	22	1/1/13/20	10/32/108/115	-
25	CLA	B	819	-	1/1/13/20	11/32/108/115	-
35	SF4	C	101	9	-	-	0/6/5/5
30	BCR	B	847	-	-	0/29/63/63	0/2/2/2
25	CLA	3	308	3	1/1/10/20	3/10/86/115	-
34	PQN	A	844	-	-	13/23/43/43	0/2/2/2
24	CHL	S	306	-	3/3/17/26	9/23/121/137	-
25	CLA	R	317	-	-	5/19/95/115	-
30	BCR	3	317	-	-	2/29/63/63	0/2/2/2
25	CLA	B	824	-	1/1/14/20	4/33/109/115	-
24	CHL	1	604	1	3/3/15/26	0/8/106/137	-
25	CLA	S	312	22	1/1/13/20	7/27/103/115	-
25	CLA	G	202	-	1/1/11/20	8/15/91/115	-
29	Q6L	P	315	-	-	6/29/67/67	0/2/2/2
25	CLA	3	301	3	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	W	301	22	1/1/13/20	9/27/103/115	-
31	LMG	F	805	-	-	2/26/46/70	0/1/1/1
25	CLA	A	824	-	1/1/10/20	5/12/88/115	-
25	CLA	4	316	4	1/1/10/20	3/12/88/115	-

All (3209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	307	CHL	C3B-C4B	11.68	1.52	1.41
24	T	304	CHL	C3B-C4B	11.25	1.52	1.41
24	P	304	CHL	C3B-C4B	11.21	1.52	1.41
24	Q	308	CHL	C3B-C4B	11.02	1.52	1.41
24	T	305	CHL	C3B-C4B	10.96	1.52	1.41
24	U	306	CHL	C3B-C4B	10.89	1.52	1.41
24	6	606	CHL	C3B-C4B	10.83	1.51	1.41
24	W	314	CHL	C3B-C4B	10.78	1.51	1.41
24	T	307	CHL	C3B-C4B	10.64	1.51	1.41
24	R	318	CHL	C3B-C4B	10.59	1.51	1.41
24	U	305	CHL	C3B-C4B	10.59	1.51	1.41
24	S	307	CHL	C3B-C4B	10.53	1.51	1.41
24	Q	316	CHL	C3B-C4B	10.48	1.51	1.41
24	X	308	CHL	C3B-C4B	10.46	1.51	1.41
24	W	307	CHL	C3B-C4B	10.45	1.51	1.41
24	R	311	CHL	C3B-C4B	10.45	1.51	1.41
24	P	305	CHL	C3B-C4B	10.43	1.51	1.41
24	4	308	CHL	C3B-C4B	10.42	1.51	1.41
24	Q	307	CHL	C3B-C4B	10.34	1.51	1.41
24	S	314	CHL	C3B-C4B	10.33	1.51	1.41
24	4	306	CHL	C3B-C4B	10.28	1.51	1.41
24	R	309	CHL	C3B-C4B	10.25	1.51	1.41
24	V	307	CHL	C3B-C4B	10.23	1.51	1.41
24	W	305	CHL	C3B-C4B	10.16	1.51	1.41
24	W	304	CHL	C3B-C4B	10.15	1.51	1.41
24	P	314	CHL	C3B-C4B	10.15	1.51	1.41
24	2	601	CHL	C3B-C4B	10.12	1.51	1.41
24	2	615	CHL	C3B-C4B	10.00	1.51	1.41
24	P	305	CHL	C1B-C2B	10.00	1.50	1.39
24	1	604	CHL	C3B-C4B	9.95	1.51	1.41
24	1	601	CHL	C3B-C4B	9.94	1.51	1.41
24	4	302	CHL	C3B-C4B	9.94	1.51	1.41
24	R	302	CHL	C3B-C4B	9.89	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	309	CHL	C3B-C4B	9.88	1.51	1.41
24	R	308	CHL	C3B-C4B	9.84	1.51	1.41
24	V	306	CHL	C3B-C4B	9.82	1.51	1.41
24	X	315	CHL	C3B-C4B	9.78	1.50	1.41
24	2	607	CHL	C3B-C4B	9.75	1.50	1.41
24	X	305	CHL	C3B-C4B	9.73	1.50	1.41
24	R	311	CHL	C1B-C2B	9.66	1.50	1.39
24	V	304	CHL	C3B-C4B	9.65	1.50	1.41
24	4	308	CHL	C1B-C2B	9.64	1.50	1.39
24	T	320	CHL	C3B-C4B	9.61	1.50	1.41
24	Q	307	CHL	C1B-C2B	9.59	1.50	1.39
24	R	309	CHL	C1B-C2B	9.58	1.50	1.39
24	P	307	CHL	C1B-C2B	9.58	1.50	1.39
24	Q	309	CHL	C1B-C2B	9.56	1.50	1.39
34	A	844	PQN	C12-C13	9.53	1.55	1.33
24	S	306	CHL	C1D-C2D	9.53	1.50	1.39
24	5	605	CHL	C3B-C4B	9.47	1.50	1.41
24	R	310	CHL	C3B-C4B	9.41	1.50	1.41
24	W	306	CHL	C3B-C4B	9.41	1.50	1.41
34	B	844	PQN	C12-C13	9.40	1.54	1.33
24	V	314	CHL	C3B-C4B	9.38	1.50	1.41
24	6	606	CHL	C1B-C2B	9.37	1.50	1.39
24	T	314	CHL	C3B-C4B	9.36	1.50	1.41
24	U	313	CHL	C3B-C4B	9.34	1.50	1.41
24	X	306	CHL	C3B-C4B	9.33	1.50	1.41
24	U	313	CHL	C1B-C2B	9.33	1.50	1.39
24	T	305	CHL	C1B-C2B	9.33	1.50	1.39
24	X	306	CHL	C1B-C2B	9.32	1.50	1.39
24	W	307	CHL	C1B-C2B	9.31	1.50	1.39
24	6	605	CHL	C3B-C4B	9.29	1.50	1.41
24	U	304	CHL	C3B-C4B	9.26	1.50	1.41
24	S	305	CHL	C3B-C4B	9.25	1.50	1.41
24	6	605	CHL	C1B-C2B	9.25	1.50	1.39
24	S	304	CHL	C1B-C2B	9.24	1.50	1.39
24	4	302	CHL	C1B-C2B	9.24	1.50	1.39
24	X	307	CHL	C1B-C2B	9.21	1.50	1.39
29	V	316	Q6L	C29-C30	9.21	1.53	1.32
24	Q	308	CHL	C1B-C2B	9.20	1.50	1.39
24	P	306	CHL	C1B-C2B	9.20	1.50	1.39
24	V	307	CHL	C1B-C2B	9.19	1.50	1.39
24	1	604	CHL	C1B-C2B	9.18	1.50	1.39
24	X	305	CHL	C1B-C2B	9.18	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	615	CHL	C1B-C2B	9.16	1.50	1.39
24	R	302	CHL	C1B-C2B	9.15	1.50	1.39
24	W	305	CHL	C1B-C2B	9.14	1.50	1.39
24	S	304	CHL	C3B-C4B	9.13	1.50	1.41
24	Q	316	CHL	C1B-C2B	9.12	1.49	1.39
24	T	314	CHL	C1B-C2B	9.11	1.49	1.39
24	V	305	CHL	C3B-C4B	9.10	1.50	1.41
24	X	307	CHL	C3B-C4B	9.10	1.50	1.41
24	T	307	CHL	C1B-C2B	9.10	1.49	1.39
24	S	314	CHL	C1B-C2B	9.07	1.49	1.39
24	S	306	CHL	C3B-C4B	9.05	1.50	1.41
29	P	321	Q6L	C29-C30	9.05	1.52	1.32
24	R	310	CHL	C1B-C2B	9.03	1.49	1.39
29	O	2007	Q6L	C29-C30	9.02	1.52	1.32
24	X	308	CHL	C1B-C2B	9.02	1.49	1.39
29	S	321	Q6L	C29-C30	9.02	1.52	1.32
24	2	605	CHL	C3B-C4B	9.01	1.50	1.41
24	P	314	CHL	C1B-C2B	9.00	1.49	1.39
24	S	307	CHL	C1B-C2B	9.00	1.49	1.39
24	W	314	CHL	C1B-C2B	8.97	1.49	1.39
24	W	306	CHL	C1B-C2B	8.95	1.49	1.39
24	4	307	CHL	C4B-C3B	8.94	1.49	1.39
29	P	316	Q6L	C29-C30	8.94	1.52	1.32
24	2	607	CHL	C1B-C2B	8.93	1.49	1.39
24	R	318	CHL	C1B-C2B	8.93	1.49	1.39
29	X	319	Q6L	C29-C30	8.92	1.52	1.32
29	R	304	Q6L	C29-C30	8.91	1.52	1.32
24	5	605	CHL	C1B-C2B	8.89	1.49	1.39
29	O	2006	Q6L	C29-C30	8.89	1.52	1.32
29	R	301	Q6L	C29-C30	8.89	1.52	1.32
24	U	305	CHL	C1B-C2B	8.89	1.49	1.39
29	R	319	Q6L	C29-C30	8.88	1.52	1.32
29	U	315	Q6L	C29-C30	8.87	1.52	1.32
29	S	316	Q6L	C29-C30	8.87	1.52	1.32
29	P	319	Q6L	C29-C30	8.86	1.52	1.32
24	V	314	CHL	C1B-C2B	8.85	1.49	1.39
29	P	315	Q6L	C29-C30	8.85	1.52	1.32
29	T	322	Q6L	C29-C30	8.85	1.52	1.32
29	R	323	Q6L	C29-C30	8.85	1.52	1.32
29	X	301	Q6L	C29-C30	8.84	1.52	1.32
29	R	320	Q6L	C29-C30	8.83	1.52	1.32
29	W	319	Q6L	C29-C30	8.83	1.52	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	U	317	Q6L	C29-C30	8.82	1.52	1.32
29	T	319	Q6L	C29-C30	8.82	1.52	1.32
24	R	308	CHL	C1B-C2B	8.81	1.49	1.39
29	W	316	Q6L	C29-C30	8.81	1.52	1.32
24	6	601	CHL	C3B-C4B	8.81	1.50	1.41
24	S	306	CHL	C1B-C2B	8.80	1.49	1.39
29	X	316	Q6L	C29-C30	8.79	1.52	1.32
29	X	317	Q6L	C29-C30	8.79	1.52	1.32
24	T	306	CHL	C1B-C2B	8.77	1.49	1.39
24	V	305	CHL	C1B-C2B	8.75	1.49	1.39
29	T	316	Q6L	C29-C30	8.75	1.51	1.32
29	S	320	Q6L	C29-C30	8.73	1.51	1.32
24	1	601	CHL	C1B-C2B	8.72	1.49	1.39
29	W	320	Q6L	C29-C30	8.72	1.51	1.32
29	V	321	Q6L	C29-C30	8.70	1.51	1.32
24	4	306	CHL	C1B-C2B	8.70	1.49	1.39
24	X	315	CHL	C1B-C2B	8.68	1.49	1.39
29	Q	317	Q6L	C29-C30	8.68	1.51	1.32
38	V	308	KC2	C2A-C3A	8.67	1.54	1.37
29	T	315	Q6L	C29-C30	8.66	1.51	1.32
29	S	323	Q6L	C29-C30	8.65	1.51	1.32
38	X	309	KC2	C2A-C3A	8.64	1.54	1.37
24	U	306	CHL	C1B-C2B	8.64	1.49	1.39
29	Q	319	Q6L	C29-C30	8.64	1.51	1.32
24	2	605	CHL	C1B-C2B	8.64	1.49	1.39
24	W	304	CHL	C1B-C2B	8.64	1.49	1.39
38	S	308	KC2	C2A-C3A	8.59	1.54	1.37
29	V	315	Q6L	C29-C30	8.58	1.51	1.32
29	U	314	Q6L	C29-C30	8.57	1.51	1.32
24	P	304	CHL	C1B-C2B	8.56	1.49	1.39
24	V	304	CHL	C1B-C2B	8.55	1.49	1.39
24	U	304	CHL	C1B-C2B	8.54	1.49	1.39
24	V	306	CHL	C1B-C2B	8.54	1.49	1.39
24	6	601	CHL	C1B-C2B	8.52	1.49	1.39
24	S	305	CHL	C1B-C2B	8.46	1.49	1.39
29	Q	318	Q6L	C29-C30	8.46	1.51	1.32
24	T	320	CHL	C1B-C2B	8.46	1.49	1.39
29	W	315	Q6L	C29-C30	8.46	1.51	1.32
24	P	306	CHL	C3B-C4B	8.44	1.49	1.41
24	4	306	CHL	C1D-C2D	8.43	1.49	1.39
29	2	616	Q6L	C29-C30	8.41	1.51	1.32
24	2	601	CHL	C1B-C2B	8.36	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	611	IWJ	C29-C30	-8.36	1.44	1.53
34	A	844	PQN	O1-C1	8.34	1.40	1.23
24	X	307	CHL	C1D-C2D	8.33	1.49	1.39
24	T	304	CHL	C1B-C2B	8.32	1.49	1.39
29	S	315	Q6L	C29-C30	8.32	1.51	1.32
38	Q	310	KC2	C2A-C3A	8.32	1.54	1.37
38	T	308	KC2	C2A-C3A	8.32	1.54	1.37
38	R	312	KC2	C2A-C3A	8.28	1.54	1.37
24	T	304	CHL	C1D-C2D	8.19	1.48	1.39
24	T	306	CHL	C3B-C4B	8.17	1.49	1.41
38	U	307	KC2	C2A-C3A	8.16	1.53	1.37
24	2	601	CHL	C1D-C2D	8.14	1.48	1.39
24	3	306	CHL	C1B-C2B	8.11	1.48	1.39
34	B	844	PQN	O4-C4	8.00	1.39	1.23
24	3	306	CHL	C3B-C4B	7.98	1.49	1.41
34	A	844	PQN	O4-C4	7.97	1.39	1.23
29	V	319	Q6L	C29-C30	7.97	1.50	1.32
38	W	308	KC2	C2A-C3A	7.94	1.53	1.37
24	V	306	CHL	C1D-C2D	7.94	1.48	1.39
24	4	307	CHL	C1B-C2B	7.93	1.48	1.39
24	V	304	CHL	C1D-C2D	7.92	1.48	1.39
24	V	307	CHL	C1D-C2D	7.90	1.48	1.39
24	Q	316	CHL	C1D-C2D	7.89	1.48	1.39
24	P	307	CHL	C1D-C2D	7.89	1.48	1.39
26	4	317	IWJ	C29-C30	-7.86	1.45	1.53
38	P	308	KC2	C2A-C3A	7.86	1.53	1.37
24	W	304	CHL	C1D-C2D	7.83	1.48	1.39
24	4	308	CHL	C1D-C2D	7.81	1.48	1.39
24	Q	307	CHL	C1D-C2D	7.78	1.48	1.39
34	B	844	PQN	O1-C1	7.78	1.39	1.23
26	X	318	IWJ	C29-C30	-7.77	1.45	1.53
24	4	307	CHL	C1D-C2D	7.74	1.48	1.39
24	6	606	CHL	C1D-C2D	7.73	1.48	1.39
24	1	601	CHL	C1D-C2D	7.70	1.48	1.39
24	P	306	CHL	C1D-C2D	7.69	1.48	1.39
24	U	313	CHL	C1D-C2D	7.67	1.48	1.39
26	V	318	IWJ	C29-C30	-7.65	1.45	1.53
24	U	304	CHL	C1D-C2D	7.65	1.48	1.39
24	6	601	CHL	C1D-C2D	7.64	1.48	1.39
24	P	314	CHL	C1D-C2D	7.61	1.48	1.39
24	W	306	CHL	C1D-C2D	7.60	1.48	1.39
33	A	802	CL0	C1B-C2B	7.59	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W	318	IWJ	C29-C30	-7.59	1.45	1.53
24	3	306	CHL	C1D-C2D	7.58	1.48	1.39
24	R	310	CHL	C1D-C2D	7.58	1.48	1.39
24	T	314	CHL	C1D-C2D	7.57	1.48	1.39
24	R	308	CHL	C1D-C2D	7.54	1.48	1.39
24	R	302	CHL	C1D-C2D	7.53	1.48	1.39
24	X	305	CHL	C1D-C2D	7.52	1.48	1.39
26	V	317	IWJ	C29-C30	-7.51	1.45	1.53
24	W	314	CHL	C1D-C2D	7.49	1.48	1.39
24	2	607	CHL	C1D-C2D	7.49	1.48	1.39
24	5	605	CHL	C1D-C2D	7.49	1.48	1.39
24	S	314	CHL	C1D-C2D	7.48	1.48	1.39
24	Q	309	CHL	C1D-C2D	7.45	1.48	1.39
24	2	605	CHL	C1D-C2D	7.44	1.48	1.39
24	R	318	CHL	C1D-C2D	7.43	1.48	1.39
24	U	306	CHL	C1D-C2D	7.43	1.48	1.39
24	P	305	CHL	C1D-C2D	7.42	1.48	1.39
24	U	305	CHL	C1D-C2D	7.42	1.48	1.39
24	P	304	CHL	C1D-C2D	7.37	1.47	1.39
26	S	322	IWJ	C29-C30	-7.37	1.45	1.53
26	P	320	IWJ	C29-C30	-7.35	1.45	1.53
24	X	315	CHL	C1D-C2D	7.31	1.47	1.39
24	2	615	CHL	C1D-C2D	7.31	1.47	1.39
24	T	306	CHL	C1D-C2D	7.28	1.47	1.39
26	T	318	IWJ	C29-C30	-7.28	1.45	1.53
33	A	802	CL0	C1D-C2D	7.26	1.47	1.39
24	W	307	CHL	C1D-C2D	7.21	1.47	1.39
24	6	605	CHL	C1D-C2D	7.20	1.47	1.39
24	S	307	CHL	C1D-C2D	7.16	1.47	1.39
26	V	320	IWJ	C29-C30	-7.13	1.46	1.53
24	X	308	CHL	C1D-C2D	7.08	1.47	1.39
24	V	314	CHL	C1D-C2D	7.05	1.47	1.39
24	T	320	CHL	C1D-C2D	7.04	1.47	1.39
24	T	307	CHL	C1D-C2D	7.00	1.47	1.39
24	1	604	CHL	C1D-C2D	6.99	1.47	1.39
26	T	321	IWJ	C29-C30	-6.99	1.46	1.53
26	S	319	IWJ	C29-C30	-6.94	1.46	1.53
26	4	301	IWJ	C29-C30	-6.94	1.46	1.53
24	R	309	CHL	C1D-C2D	6.91	1.47	1.39
26	5	611	IWJ	C29-C30	-6.90	1.46	1.53
24	S	304	CHL	C1D-C2D	6.88	1.47	1.39
26	P	318	IWJ	C29-C30	-6.86	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	303	IWJ	C29-C30	-6.85	1.46	1.53
24	V	305	CHL	C1D-C2D	6.81	1.47	1.39
26	Q	303	IWJ	C29-C30	-6.80	1.46	1.53
26	6	614	IWJ	C29-C30	-6.78	1.46	1.53
24	X	306	CHL	C1D-C2D	6.77	1.47	1.39
26	R	322	IWJ	C29-C30	-6.76	1.46	1.53
24	4	302	CHL	C1D-C2D	6.74	1.47	1.39
24	S	305	CHL	C1D-C2D	6.67	1.47	1.39
24	W	305	CHL	C1D-C2D	6.60	1.47	1.39
26	S	318	IWJ	C29-C30	-6.55	1.46	1.53
38	Q	310	KC2	CBA-CAA	6.41	1.52	1.33
24	Q	308	CHL	C1D-C2D	6.37	1.46	1.39
38	V	308	KC2	CBA-CAA	6.36	1.52	1.33
26	Q	320	IWJ	C29-C30	-6.30	1.46	1.53
26	U	316	IWJ	C29-C30	-6.29	1.46	1.53
24	T	305	CHL	C1D-C2D	6.24	1.46	1.39
26	3	315	IWJ	C29-C30	-6.21	1.47	1.53
38	U	307	KC2	CBA-CAA	6.17	1.51	1.33
38	W	308	KC2	CBA-CAA	6.13	1.51	1.33
38	P	308	KC2	CBA-CAA	6.08	1.51	1.33
24	R	311	CHL	C1D-C2D	6.08	1.46	1.39
38	R	312	KC2	CBA-CAA	6.07	1.51	1.33
38	X	309	KC2	CBA-CAA	6.06	1.51	1.33
38	T	308	KC2	CBA-CAA	6.05	1.51	1.33
38	S	308	KC2	CBA-CAA	5.98	1.50	1.33
33	A	802	CL0	C3B-C4B	5.73	1.47	1.41
29	V	315	Q6L	C12-C11	-5.24	1.33	1.51
29	R	301	Q6L	C12-C11	-5.14	1.34	1.51
29	R	323	Q6L	C12-C11	-5.08	1.34	1.51
24	Q	308	CHL	CMD-C2D	-5.06	1.41	1.51
29	P	315	Q6L	C12-C11	-5.06	1.34	1.51
24	R	311	CHL	C2C-C3C	5.06	1.41	1.36
29	W	320	Q6L	C12-C11	-5.06	1.34	1.51
29	W	315	Q6L	C12-C11	-5.04	1.34	1.51
29	X	319	Q6L	C12-C11	-5.04	1.34	1.51
29	S	320	Q6L	C12-C11	-5.03	1.34	1.51
29	S	321	Q6L	C12-C11	-5.01	1.34	1.51
29	T	315	Q6L	C12-C11	-5.00	1.34	1.51
29	U	314	Q6L	C12-C11	-5.00	1.34	1.51
24	2	601	CHL	C2C-C3C	5.00	1.41	1.36
29	V	316	Q6L	C12-C11	-5.00	1.34	1.51
29	W	316	Q6L	C12-C11	-5.00	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Q	317	Q6L	C12-C11	-4.99	1.34	1.51
29	V	321	Q6L	C12-C11	-4.98	1.34	1.51
29	V	319	Q6L	C12-C11	-4.98	1.34	1.51
29	2	616	Q6L	C12-C11	-4.97	1.34	1.51
29	W	319	Q6L	C12-C11	-4.94	1.34	1.51
29	X	301	Q6L	C12-C11	-4.93	1.34	1.51
29	T	322	Q6L	C12-C11	-4.93	1.34	1.51
29	S	323	Q6L	C12-C11	-4.92	1.34	1.51
29	R	319	Q6L	C12-C11	-4.92	1.34	1.51
29	P	321	Q6L	C12-C11	-4.91	1.34	1.51
29	Q	319	Q6L	C12-C11	-4.91	1.34	1.51
29	O	2006	Q6L	C12-C11	-4.88	1.35	1.51
29	Q	318	Q6L	C12-C11	-4.87	1.35	1.51
29	S	315	Q6L	C12-C11	-4.86	1.35	1.51
29	R	304	Q6L	C12-C11	-4.85	1.35	1.51
29	R	320	Q6L	C12-C11	-4.82	1.35	1.51
29	U	317	Q6L	C12-C11	-4.82	1.35	1.51
29	U	315	Q6L	C12-C11	-4.82	1.35	1.51
29	O	2007	Q6L	C12-C11	-4.79	1.35	1.51
29	X	316	Q6L	C12-C11	-4.79	1.35	1.51
25	V	309	CLA	C4B-NB	4.79	1.44	1.37
29	T	319	Q6L	C12-C11	-4.79	1.35	1.51
25	4	311	CLA	CMB-C2B	-4.79	1.41	1.50
29	P	316	Q6L	C12-C11	-4.78	1.35	1.51
29	P	319	Q6L	C12-C11	-4.77	1.35	1.51
29	S	316	Q6L	C12-C11	-4.73	1.35	1.51
29	X	317	Q6L	C12-C11	-4.72	1.35	1.51
29	T	316	Q6L	C12-C11	-4.68	1.35	1.51
24	2	615	CHL	C2C-C3C	4.62	1.40	1.36
24	R	318	CHL	C2C-C3C	4.60	1.40	1.36
36	A	854	DGD	O1G-C1A	4.59	1.46	1.33
24	Q	307	CHL	C3D-C4D	4.57	1.48	1.41
24	S	307	CHL	C2C-C3C	4.56	1.40	1.36
24	W	304	CHL	C3D-C4D	4.55	1.48	1.41
28	3	320	LHG	O7-C7	4.54	1.47	1.34
24	1	601	CHL	C2C-C3C	4.51	1.40	1.36
34	B	844	PQN	C2-C1	-4.51	1.37	1.47
32	H	303	SQD	O47-C7	4.49	1.47	1.34
24	P	305	CHL	C3D-C4D	4.47	1.48	1.41
24	R	308	CHL	C3D-C4D	4.46	1.48	1.41
32	H	303	SQD	O8-S	4.45	1.64	1.47
24	P	304	CHL	C3D-C4D	4.44	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	320	CHL	C3D-C4D	4.44	1.48	1.41
24	P	307	CHL	C3D-C4D	4.43	1.48	1.41
28	1	614	LHG	O8-C23	4.42	1.46	1.33
24	X	305	CHL	C3D-C4D	4.42	1.48	1.41
32	6	617	SQD	O8-S	4.38	1.63	1.47
28	3	321	LHG	O7-C7	4.38	1.46	1.34
36	B	850	DGD	O2G-C1B	4.38	1.46	1.34
28	2	619	LHG	O7-C7	4.38	1.46	1.34
24	6	606	CHL	C3D-C4D	4.37	1.48	1.41
32	H	303	SQD	O48-C23	4.37	1.46	1.33
31	O	2008	LMG	O7-C10	4.37	1.46	1.34
36	B	850	DGD	O1G-C1A	4.35	1.46	1.33
24	P	314	CHL	C3D-C4D	4.35	1.48	1.41
24	T	306	CHL	C3D-C4D	4.34	1.48	1.41
32	6	617	SQD	O47-C7	4.34	1.46	1.34
31	N	201	LMG	O7-C10	4.33	1.46	1.34
31	A	855	LMG	O7-C10	4.30	1.46	1.34
28	Q	302	LHG	O7-C7	4.30	1.46	1.34
36	A	854	DGD	O2G-C1B	4.30	1.46	1.34
24	P	314	CHL	C2C-C3C	4.30	1.40	1.36
24	R	310	CHL	C2C-C3C	4.30	1.40	1.36
24	4	302	CHL	C3D-C4D	4.29	1.48	1.41
24	Q	309	CHL	C3D-C4D	4.27	1.48	1.41
38	V	308	KC2	MG-ND	-4.26	1.97	2.05
24	5	605	CHL	C3D-C4D	4.25	1.48	1.41
31	5	613	LMG	O8-C28	4.24	1.45	1.33
24	W	307	CHL	C3D-C4D	4.24	1.48	1.41
24	1	601	CHL	C3D-C4D	4.24	1.48	1.41
24	P	306	CHL	C3D-C4D	4.24	1.48	1.41
31	A	857	LMG	O8-C28	4.23	1.45	1.33
24	4	307	CHL	C3D-C4D	4.23	1.48	1.41
24	U	304	CHL	C3D-C4D	4.23	1.48	1.41
24	4	306	CHL	C3D-C4D	4.23	1.48	1.41
28	A	846	LHG	O8-C23	4.23	1.45	1.33
24	T	307	CHL	C3D-C4D	4.22	1.48	1.41
31	L	308	LMG	O8-C28	4.22	1.45	1.33
28	A	847	LHG	O8-C23	4.22	1.45	1.33
24	S	304	CHL	C3D-C4D	4.22	1.48	1.41
24	R	311	CHL	CMD-C2D	-4.21	1.43	1.51
32	6	617	SQD	O48-C23	4.21	1.45	1.33
34	B	844	PQN	C3-C2	4.21	1.42	1.35
24	R	310	CHL	C3D-C4D	4.20	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	203	CLA	CMD-C2D	-4.20	1.42	1.50
24	V	307	CHL	C3D-C4D	4.20	1.47	1.41
24	2	615	CHL	C3D-C4D	4.19	1.47	1.41
24	4	308	CHL	C3D-C4D	4.19	1.47	1.41
24	6	601	CHL	C3D-C4D	4.19	1.47	1.41
31	L	308	LMG	O7-C10	4.18	1.46	1.34
31	2	620	LMG	O8-C28	4.18	1.45	1.33
31	B	801	LMG	O7-C10	4.18	1.46	1.34
24	P	305	CHL	C2C-C3C	4.17	1.40	1.36
24	V	304	CHL	C3D-C4D	4.16	1.47	1.41
31	F	805	LMG	O7-C10	4.16	1.46	1.34
24	S	307	CHL	C3D-C4D	4.15	1.47	1.41
24	Q	307	CHL	C2C-C3C	4.15	1.40	1.36
24	U	306	CHL	C3D-C4D	4.15	1.47	1.41
34	A	844	PQN	C3-C2	4.14	1.42	1.35
37	R	321	NEX	C7-C6	-4.12	1.25	1.30
38	R	312	KC2	C4A-C3A	4.12	1.52	1.44
31	A	855	LMG	O8-C28	4.12	1.45	1.33
24	U	305	CHL	C3D-C4D	4.11	1.47	1.41
24	4	302	CHL	C2C-C3C	4.11	1.40	1.36
24	Q	308	CHL	C2C-C3C	4.10	1.40	1.36
24	U	313	CHL	C3D-C4D	4.10	1.47	1.41
24	S	305	CHL	C2C-C3C	4.09	1.40	1.36
24	2	607	CHL	C3D-C4D	4.09	1.47	1.41
28	3	322	LHG	O7-C7	4.09	1.45	1.34
24	X	308	CHL	C3D-C4D	4.08	1.47	1.41
28	3	323	LHG	O7-C7	4.08	1.45	1.34
24	R	318	CHL	C3D-C4D	4.08	1.47	1.41
24	P	307	CHL	C2C-C3C	4.07	1.40	1.36
28	A	846	LHG	O7-C7	4.07	1.45	1.34
24	T	305	CHL	C2C-C3C	4.07	1.40	1.36
24	2	605	CHL	C3D-C4D	4.07	1.47	1.41
31	O	2008	LMG	O8-C28	4.07	1.45	1.33
31	J	104	LMG	O8-C28	4.06	1.45	1.33
24	Q	316	CHL	C3D-C4D	4.06	1.47	1.41
24	X	315	CHL	C3D-C4D	4.05	1.47	1.41
24	R	302	CHL	C3D-C4D	4.05	1.47	1.41
31	5	613	LMG	O7-C10	4.05	1.45	1.34
38	Q	310	KC2	MG-ND	-4.05	1.97	2.05
24	6	606	CHL	C2C-C3C	4.04	1.40	1.36
24	X	307	CHL	C3D-C4D	4.04	1.47	1.41
24	X	315	CHL	C2C-C3C	4.04	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	605	CHL	C1A-CHA	-4.03	1.35	1.40
31	B	801	LMG	O8-C28	4.02	1.45	1.33
24	3	306	CHL	CMB-C2B	-4.01	1.43	1.51
31	A	857	LMG	O7-C10	4.00	1.45	1.34
24	T	305	CHL	C3D-C4D	3.99	1.47	1.41
28	6	616	LHG	O8-C23	3.98	1.44	1.33
28	6	616	LHG	O7-C7	3.98	1.45	1.34
24	3	306	CHL	C3D-C4D	3.98	1.47	1.41
24	V	306	CHL	C3D-C4D	3.97	1.47	1.41
28	Q	302	LHG	O8-C23	3.97	1.44	1.33
24	W	307	CHL	C2C-C3C	3.97	1.40	1.36
31	A	801	LMG	O7-C10	3.96	1.45	1.34
31	A	801	LMG	O8-C28	3.95	1.44	1.33
24	T	304	CHL	C3D-C4D	3.95	1.47	1.41
24	W	306	CHL	C3D-C4D	3.95	1.47	1.41
38	S	308	KC2	C4A-C3A	3.95	1.52	1.44
38	W	308	KC2	C4A-C3A	3.94	1.52	1.44
24	2	607	CHL	C1A-CHA	-3.94	1.35	1.40
24	4	307	CHL	CAB-C3B	-3.94	1.43	1.51
31	2	620	LMG	O7-C10	3.94	1.45	1.34
31	J	104	LMG	O7-C10	3.93	1.45	1.34
24	1	604	CHL	C3D-C4D	3.92	1.47	1.41
24	2	601	CHL	C3D-C4D	3.92	1.47	1.41
28	3	321	LHG	O8-C23	3.91	1.44	1.33
38	P	308	KC2	C4A-C3A	3.91	1.52	1.44
37	S	317	NEX	C7-C8	-3.91	1.25	1.31
33	A	802	CL0	CMD-C2D	-3.90	1.43	1.51
24	P	306	CHL	C2C-C3C	3.90	1.40	1.36
25	6	609	CLA	C1D-ND	3.89	1.43	1.37
24	W	306	CHL	CAC-C3C	-3.89	1.44	1.51
30	K	207	BCR	C8-C9	3.89	1.54	1.46
28	A	847	LHG	O7-C7	3.89	1.45	1.34
24	W	305	CHL	C3D-C4D	3.89	1.47	1.41
24	V	306	CHL	C2C-C3C	3.89	1.40	1.36
24	P	304	CHL	C2C-C3C	3.89	1.40	1.36
25	G	203	CLA	C1D-ND	3.87	1.42	1.37
24	S	314	CHL	C3D-C4D	3.86	1.47	1.41
24	S	306	CHL	C2C-C3C	3.86	1.40	1.36
31	N	201	LMG	O8-C28	3.84	1.44	1.33
24	P	304	CHL	C3A-C2A	3.84	1.58	1.54
24	T	314	CHL	C3D-C4D	3.84	1.47	1.41
28	1	614	LHG	O7-C7	3.83	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	309	KC2	CMD-C2D	-3.83	1.42	1.50
24	Q	309	CHL	C2C-C3C	3.83	1.40	1.36
25	5	603	CLA	C1D-ND	3.82	1.42	1.37
24	Q	316	CHL	C2C-C3C	3.81	1.40	1.36
37	R	321	NEX	C7-C8	-3.81	1.25	1.31
24	V	305	CHL	C3D-C4D	3.81	1.47	1.41
28	3	323	LHG	O8-C23	3.80	1.44	1.33
24	Q	308	CHL	C1A-CHA	-3.79	1.35	1.40
37	S	317	NEX	C7-C6	-3.78	1.26	1.30
25	B	833	CLA	C1D-ND	3.78	1.42	1.37
24	6	605	CHL	CMD-C2D	-3.77	1.44	1.51
24	S	314	CHL	C2C-C3C	3.77	1.40	1.36
25	G	204	CLA	CMB-C2B	-3.77	1.43	1.50
25	5	604	CLA	CAB-C3B	-3.77	1.43	1.50
25	G	204	CLA	C1D-ND	3.77	1.42	1.37
24	V	314	CHL	C2C-C3C	3.77	1.40	1.36
24	R	308	CHL	C2C-C3C	3.77	1.40	1.36
31	F	805	LMG	O8-C28	3.77	1.44	1.33
28	3	322	LHG	O8-C23	3.76	1.44	1.33
24	W	314	CHL	C3D-C4D	3.76	1.47	1.41
25	1	613	CLA	C1D-ND	3.76	1.42	1.37
24	U	305	CHL	C2C-C3C	3.76	1.40	1.36
38	T	308	KC2	C4A-C3A	3.76	1.52	1.44
38	U	307	KC2	C4A-C3A	3.76	1.52	1.44
25	K	206	CLA	C1D-ND	3.75	1.42	1.37
25	A	833	CLA	CMB-C2B	-3.74	1.43	1.50
25	B	827	CLA	C1D-ND	3.73	1.42	1.37
30	A	850	BCR	C30-C25	-3.73	1.49	1.53
25	A	823	CLA	CMB-C2B	-3.73	1.43	1.50
25	2	610	CLA	C1D-ND	3.73	1.42	1.37
24	R	311	CHL	C3D-C4D	3.73	1.47	1.41
25	K	201	CLA	C1D-ND	3.72	1.42	1.37
24	S	306	CHL	C3D-C4D	3.72	1.47	1.41
26	Q	303	IWJ	C09-C10	3.71	1.53	1.46
25	5	608	CLA	C1D-ND	3.71	1.42	1.37
25	R	313	CLA	C1D-ND	3.71	1.42	1.37
24	S	305	CHL	C3D-C4D	3.71	1.47	1.41
25	P	310	CLA	C1D-ND	3.71	1.42	1.37
38	V	308	KC2	CMD-C2D	-3.71	1.43	1.50
24	V	314	CHL	C3D-C4D	3.71	1.47	1.41
24	1	604	CHL	C2C-C3C	3.70	1.40	1.36
24	R	309	CHL	C3D-C4D	3.70	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	309	CLA	C1D-ND	3.69	1.42	1.37
24	4	308	CHL	C2C-C3C	3.69	1.39	1.36
25	3	301	CLA	C1D-ND	3.68	1.42	1.37
25	B	823	CLA	C1D-ND	3.67	1.42	1.37
24	U	313	CHL	C2C-C3C	3.67	1.39	1.36
24	T	304	CHL	C2C-C3C	3.66	1.39	1.36
38	V	308	KC2	C4A-C3A	3.65	1.51	1.44
25	1	606	CLA	C1D-ND	3.65	1.42	1.37
24	2	605	CHL	C3B-C2B	-3.64	1.35	1.40
24	2	605	CHL	CMB-C2B	-3.64	1.44	1.51
25	S	302	CLA	C1D-ND	3.63	1.42	1.37
24	T	320	CHL	C2C-C3C	3.63	1.39	1.36
25	X	303	CLA	C1D-ND	3.63	1.42	1.37
25	A	820	CLA	C1D-ND	3.62	1.42	1.37
37	H	306	NEX	C7-C6	-3.62	1.26	1.30
25	2	602	CLA	C1D-ND	3.62	1.42	1.37
24	T	305	CHL	CMD-C2D	-3.62	1.44	1.51
25	A	825	CLA	C1D-ND	3.62	1.42	1.37
25	L	301	CLA	C1D-ND	3.61	1.42	1.37
24	4	308	CHL	C1A-CHA	-3.60	1.35	1.40
25	6	607	CLA	CMB-C2B	-3.60	1.43	1.50
38	X	309	KC2	C4A-C3A	3.60	1.51	1.44
25	B	821	CLA	CMB-C2B	-3.60	1.43	1.50
25	5	610	CLA	C1D-ND	3.59	1.42	1.37
25	W	302	CLA	C1D-ND	3.59	1.42	1.37
24	R	309	CHL	C2C-C3C	3.59	1.39	1.36
24	X	307	CHL	CAC-C3C	-3.59	1.45	1.51
25	5	609	CLA	C1D-ND	3.58	1.42	1.37
25	O	2001	CLA	C1D-ND	3.58	1.42	1.37
25	Q	312	CLA	C4B-NB	3.57	1.42	1.37
28	2	619	LHG	O8-C23	3.57	1.43	1.33
25	5	601	CLA	C1D-ND	3.56	1.42	1.37
25	6	603	CLA	CMB-C2B	-3.56	1.43	1.50
24	T	314	CHL	C2C-C3C	3.56	1.39	1.36
25	A	813	CLA	C1D-ND	3.55	1.42	1.37
25	K	204	CLA	C1D-ND	3.55	1.42	1.37
25	R	314	CLA	C1D-ND	3.55	1.42	1.37
25	4	312	CLA	C1D-ND	3.55	1.42	1.37
38	Q	310	KC2	C4A-C3A	3.55	1.51	1.44
33	A	802	CL0	CBD-CGD	-3.55	1.48	1.52
33	A	802	CL0	C3D-C4D	3.55	1.46	1.41
25	3	314	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	311	CLA	C1D-ND	3.54	1.42	1.37
24	4	307	CHL	CAC-C3C	-3.54	1.45	1.51
37	T	317	NEX	C7-C8	-3.54	1.26	1.31
25	2	611	CLA	C1D-ND	3.54	1.42	1.37
25	W	310	CLA	C1D-ND	3.53	1.42	1.37
25	4	315	CLA	C1D-ND	3.53	1.42	1.37
25	A	834	CLA	C1D-ND	3.53	1.42	1.37
25	T	302	CLA	C1D-ND	3.53	1.42	1.37
25	B	842	CLA	C1D-ND	3.52	1.42	1.37
25	V	311	CLA	C1D-ND	3.52	1.42	1.37
25	G	202	CLA	C1D-ND	3.52	1.42	1.37
24	X	306	CHL	C3D-C4D	3.51	1.46	1.41
25	B	828	CLA	C1D-ND	3.51	1.42	1.37
24	R	311	CHL	C1A-CHA	-3.51	1.36	1.40
25	1	607	CLA	C4D-CHA	3.50	1.44	1.39
25	S	301	CLA	CMC-C2C	-3.50	1.43	1.50
25	W	313	CLA	C1D-ND	3.50	1.42	1.37
25	2	604	CLA	C1D-ND	3.50	1.42	1.37
25	A	839	CLA	C1D-ND	3.50	1.42	1.37
25	X	314	CLA	C1D-ND	3.50	1.42	1.37
25	6	604	CLA	C1D-ND	3.50	1.42	1.37
25	6	611	CLA	C1D-ND	3.49	1.42	1.37
25	A	832	CLA	C1D-ND	3.49	1.42	1.37
25	W	301	CLA	C1D-ND	3.49	1.42	1.37
24	R	310	CHL	CMD-C2D	-3.49	1.44	1.51
25	4	313	CLA	C1D-ND	3.49	1.42	1.37
25	4	316	CLA	C1D-ND	3.48	1.42	1.37
25	1	605	CLA	C1D-ND	3.48	1.42	1.37
25	5	606	CLA	C1D-ND	3.47	1.42	1.37
24	V	305	CHL	C2C-C3C	3.47	1.39	1.36
26	5	611	IWJ	C09-C10	3.47	1.53	1.46
24	X	305	CHL	C2C-C3C	3.47	1.39	1.36
24	6	605	CHL	C3D-C4D	3.47	1.46	1.41
24	X	306	CHL	C1A-CHA	-3.46	1.36	1.40
25	B	829	CLA	CMD-C2D	-3.46	1.43	1.50
25	X	304	CLA	CMB-C2B	-3.46	1.43	1.50
25	R	305	CLA	C1D-ND	3.46	1.42	1.37
25	O	2004	CLA	C1D-ND	3.46	1.42	1.37
24	V	307	CHL	C2C-C3C	3.45	1.39	1.36
26	4	301	IWJ	C09-C10	3.45	1.53	1.46
25	B	817	CLA	C1D-ND	3.45	1.42	1.37
25	P	302	CLA	C1D-ND	3.45	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	303	CLA	C1D-ND	3.45	1.42	1.37
26	T	321	IWJ	C09-C10	3.45	1.53	1.46
25	6	608	CLA	C1D-ND	3.45	1.42	1.37
25	P	313	CLA	C1D-ND	3.45	1.42	1.37
24	S	307	CHL	C1A-CHA	-3.44	1.36	1.40
30	M	101	BCR	C12-C13	3.44	1.53	1.46
26	1	611	IWJ	C09-C10	3.44	1.53	1.46
25	Q	301	CLA	C1D-ND	3.44	1.42	1.37
25	U	311	CLA	C1D-ND	3.44	1.42	1.37
25	4	305	CLA	C1D-ND	3.43	1.42	1.37
25	4	311	CLA	C4B-NB	3.43	1.42	1.37
26	6	614	IWJ	C09-C10	3.43	1.53	1.46
25	2	613	CLA	C1D-ND	3.43	1.42	1.37
30	B	845	BCR	C12-C13	3.43	1.53	1.46
24	P	307	CHL	C1A-CHA	-3.43	1.36	1.40
37	T	317	NEX	C7-C6	-3.43	1.26	1.30
24	X	307	CHL	CHC-C4B	-3.42	1.34	1.39
25	B	818	CLA	C1D-ND	3.41	1.42	1.37
25	5	604	CLA	C1D-ND	3.41	1.42	1.37
25	V	310	CLA	C1D-ND	3.41	1.42	1.37
25	V	309	CLA	CHC-C1C	3.40	1.45	1.38
25	T	310	CLA	C4B-NB	3.40	1.42	1.37
25	4	309	CLA	C1D-ND	3.40	1.42	1.37
26	R	303	IWJ	C09-C10	3.40	1.53	1.46
25	B	832	CLA	CMB-C2B	-3.40	1.43	1.50
24	2	601	CHL	C1A-CHA	-3.40	1.36	1.40
25	O	2005	CLA	C1D-ND	3.39	1.42	1.37
25	A	815	CLA	C1D-ND	3.39	1.42	1.37
24	X	307	CHL	C3A-C2A	3.39	1.57	1.54
25	B	824	CLA	CMB-C2B	-3.39	1.43	1.50
26	T	318	IWJ	C09-C10	3.39	1.53	1.46
26	V	317	IWJ	C09-C10	3.39	1.53	1.46
25	U	302	CLA	C1D-ND	3.39	1.42	1.37
26	R	322	IWJ	C09-C10	3.38	1.53	1.46
29	V	315	Q6L	C12-C13	-3.38	1.44	1.51
25	U	310	CLA	C1D-ND	3.38	1.42	1.37
24	U	306	CHL	C2C-C3C	3.38	1.39	1.36
25	O	2002	CLA	C1B-NB	-3.38	1.33	1.37
25	W	309	CLA	C1D-ND	3.38	1.42	1.37
37	H	306	NEX	C7-C8	-3.38	1.26	1.31
26	S	322	IWJ	C09-C10	3.37	1.53	1.46
26	S	319	IWJ	C09-C10	3.37	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	803	CLA	C1D-ND	3.37	1.42	1.37
26	V	320	IWJ	C09-C10	3.36	1.53	1.46
24	W	305	CHL	C2C-C3C	3.36	1.39	1.36
25	A	845	CLA	C1D-ND	3.36	1.42	1.37
25	3	302	CLA	CMD-C2D	-3.36	1.43	1.50
25	1	603	CLA	C1D-ND	3.36	1.42	1.37
25	R	315	CLA	C4B-NB	3.36	1.42	1.37
25	U	303	CLA	C1D-ND	3.36	1.42	1.37
25	3	304	CLA	C1D-ND	3.35	1.42	1.37
25	R	316	CLA	C1D-ND	3.35	1.42	1.37
24	V	307	CHL	C1A-CHA	-3.35	1.36	1.40
25	R	313	CLA	C4B-NB	3.34	1.42	1.37
33	A	802	CL0	CMB-C2B	-3.34	1.44	1.51
26	V	318	IWJ	C09-C10	3.34	1.53	1.46
25	O	2003	CLA	C1D-ND	3.34	1.42	1.37
25	3	312	CLA	C1D-ND	3.34	1.42	1.37
25	A	821	CLA	C1D-ND	3.33	1.42	1.37
25	2	609	CLA	C1D-ND	3.33	1.42	1.37
25	R	317	CLA	C1D-ND	3.33	1.42	1.37
26	U	316	IWJ	C09-C10	3.33	1.53	1.46
25	3	310	CLA	C1D-ND	3.33	1.42	1.37
25	L	302	CLA	CMB-C2B	-3.32	1.44	1.50
25	Q	311	CLA	C1D-ND	3.32	1.42	1.37
30	L	307	BCR	C8-C9	3.32	1.53	1.46
34	A	844	PQN	C2-C1	-3.31	1.40	1.47
25	X	311	CLA	C1D-ND	3.31	1.42	1.37
25	A	810	CLA	C1D-ND	3.31	1.42	1.37
25	K	203	CLA	C1D-ND	3.31	1.42	1.37
25	B	841	CLA	CMB-C2B	-3.31	1.44	1.50
26	S	318	IWJ	C09-C10	3.31	1.53	1.46
25	1	602	CLA	C4B-NB	3.31	1.42	1.37
26	W	318	IWJ	C09-C10	3.30	1.53	1.46
25	3	311	CLA	C1D-ND	3.30	1.42	1.37
25	T	309	CLA	C1D-ND	3.30	1.42	1.37
25	2	603	CLA	C1D-ND	3.30	1.42	1.37
25	P	311	CLA	C1D-ND	3.30	1.42	1.37
25	1	607	CLA	C1D-ND	3.30	1.42	1.37
25	A	826	CLA	C1D-ND	3.30	1.42	1.37
25	V	301	CLA	C1D-ND	3.30	1.42	1.37
25	A	840	CLA	C1D-ND	3.29	1.42	1.37
25	B	837	CLA	C1D-ND	3.29	1.42	1.37
24	1	604	CHL	CMD-C2D	-3.29	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	612	CLA	C1D-ND	3.29	1.42	1.37
25	V	313	CLA	C1D-ND	3.28	1.42	1.37
25	3	313	CLA	C1D-ND	3.28	1.42	1.37
25	Q	305	CLA	C1D-ND	3.28	1.42	1.37
25	P	301	CLA	C1D-ND	3.28	1.42	1.37
25	T	310	CLA	C1D-ND	3.28	1.42	1.37
24	X	308	CHL	C2C-C3C	3.28	1.39	1.36
25	X	312	CLA	C1D-ND	3.28	1.42	1.37
25	Q	306	CLA	C1D-ND	3.28	1.42	1.37
25	Q	315	CLA	C1D-ND	3.28	1.42	1.37
25	R	315	CLA	C1D-ND	3.27	1.42	1.37
25	A	806	CLA	C1D-ND	3.27	1.42	1.37
25	A	838	CLA	C1D-ND	3.27	1.42	1.37
29	S	320	Q6L	C34-C33	3.27	1.54	1.50
25	P	312	CLA	C1D-ND	3.26	1.42	1.37
25	Q	312	CLA	C1D-ND	3.26	1.42	1.37
25	N	202	CLA	C1D-ND	3.26	1.42	1.37
25	U	309	CLA	C1D-ND	3.26	1.42	1.37
25	Q	304	CLA	C1D-ND	3.26	1.42	1.37
24	T	307	CHL	C2C-C3C	3.25	1.39	1.36
38	W	308	KC2	CMD-C2D	-3.25	1.44	1.50
25	6	609	CLA	C4B-NB	3.25	1.42	1.37
25	L	303	CLA	C1D-ND	3.25	1.42	1.37
25	A	835	CLA	C1D-ND	3.25	1.42	1.37
25	A	805	CLA	C1D-ND	3.25	1.42	1.37
24	W	305	CHL	CMD-C2D	-3.24	1.45	1.51
25	A	829	CLA	C1D-ND	3.24	1.42	1.37
25	A	837	CLA	C4B-NB	3.24	1.42	1.37
25	A	824	CLA	C4B-NB	3.24	1.42	1.37
26	P	320	IWJ	C09-C10	3.24	1.52	1.46
24	V	305	CHL	CMD-C2D	-3.24	1.45	1.51
25	5	606	CLA	CAB-C3B	-3.24	1.44	1.50
25	5	607	CLA	C4B-NB	3.24	1.42	1.37
25	3	314	CLA	C4B-NB	3.24	1.42	1.37
26	3	315	IWJ	C09-C10	3.24	1.52	1.46
24	U	304	CHL	C2C-C3C	3.23	1.39	1.36
24	3	306	CHL	CBD-CGD	-3.23	1.48	1.52
25	B	830	CLA	CMD-C2D	-3.23	1.44	1.50
24	U	305	CHL	CBD-CGD	-3.23	1.48	1.52
37	P	317	NEX	C7-C6	-3.23	1.26	1.30
25	U	312	CLA	C1D-ND	3.23	1.42	1.37
25	4	310	CLA	C1D-ND	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	818	CLA	C1D-ND	3.23	1.42	1.37
25	2	608	CLA	C1D-ND	3.23	1.42	1.37
25	A	817	CLA	C1D-ND	3.22	1.42	1.37
26	Q	320	IWJ	C09-C10	3.22	1.52	1.46
25	6	609	CLA	C3B-C4B	3.22	1.52	1.42
25	S	313	CLA	C1D-ND	3.22	1.42	1.37
25	B	837	CLA	CMB-C2B	-3.21	1.44	1.50
25	B	838	CLA	C1D-ND	3.21	1.42	1.37
25	A	843	CLA	CMD-C2D	-3.21	1.44	1.50
25	3	305	CLA	CAB-C3B	-3.21	1.44	1.50
26	4	317	IWJ	C09-C10	3.21	1.52	1.46
25	A	812	CLA	C1D-ND	3.21	1.42	1.37
25	L	304	CLA	C1D-ND	3.21	1.42	1.37
24	3	306	CHL	CAC-C3C	-3.21	1.46	1.51
25	A	827	CLA	C1D-ND	3.20	1.42	1.37
25	6	603	CLA	C1D-ND	3.20	1.42	1.37
25	H	302	CLA	C1D-ND	3.20	1.42	1.37
26	P	318	IWJ	C09-C10	3.20	1.52	1.46
25	H	301	CLA	C1D-ND	3.20	1.42	1.37
24	3	306	CHL	CMD-C2D	-3.20	1.45	1.51
25	T	311	CLA	C1D-ND	3.20	1.42	1.37
25	A	814	CLA	CMB-C2B	-3.19	1.44	1.50
38	V	308	KC2	MG-NA	3.19	2.13	2.06
25	U	308	CLA	C4B-NB	3.19	1.42	1.37
25	A	830	CLA	C1D-ND	3.19	1.42	1.37
25	A	819	CLA	C1D-ND	3.19	1.42	1.37
25	Q	313	CLA	C1D-ND	3.18	1.42	1.37
24	V	314	CHL	CMD-C2D	-3.18	1.45	1.51
25	R	316	CLA	C4B-NB	3.18	1.42	1.37
25	S	309	CLA	C4B-NB	3.18	1.42	1.37
25	V	309	CLA	C1B-C2B	3.17	1.50	1.43
25	A	833	CLA	C1D-ND	3.17	1.42	1.37
25	B	827	CLA	C1B-C2B	3.17	1.50	1.43
24	T	307	CHL	C1A-CHA	-3.17	1.36	1.40
25	2	608	CLA	C4B-NB	3.17	1.42	1.37
25	1	606	CLA	CAB-C3B	-3.17	1.44	1.50
24	R	302	CHL	CAC-C3C	-3.17	1.46	1.51
25	4	304	CLA	CAB-C3B	-3.17	1.44	1.50
25	5	608	CLA	CMC-C2C	-3.17	1.44	1.50
25	1	609	CLA	C4B-NB	3.17	1.42	1.37
25	3	303	CLA	CAB-C3B	-3.17	1.44	1.50
25	3	307	CLA	C1D-ND	3.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	302	CLA	C4B-NB	3.17	1.42	1.37
25	U	301	CLA	CMD-C2D	-3.17	1.44	1.50
25	S	312	CLA	C1D-ND	3.17	1.42	1.37
25	X	313	CLA	C1D-ND	3.17	1.42	1.37
25	S	309	CLA	CMD-C2D	-3.16	1.44	1.50
25	B	820	CLA	C1D-ND	3.16	1.42	1.37
25	W	311	CLA	C1D-ND	3.16	1.42	1.37
25	A	807	CLA	C1D-ND	3.16	1.42	1.37
25	A	808	CLA	C1D-ND	3.16	1.42	1.37
37	W	317	NEX	C7-C6	-3.16	1.26	1.30
38	P	308	KC2	C1D-ND	3.15	1.42	1.37
25	5	602	CLA	C3B-C4B	3.15	1.51	1.42
25	V	302	CLA	C1D-ND	3.15	1.42	1.37
25	A	811	CLA	C1D-ND	3.15	1.42	1.37
24	W	314	CHL	C2C-C3C	3.15	1.39	1.36
25	A	841	CLA	C1D-ND	3.15	1.42	1.37
25	1	613	CLA	C4B-NB	3.14	1.42	1.37
25	4	314	CLA	C1D-ND	3.14	1.42	1.37
25	5	602	CLA	C1D-ND	3.14	1.42	1.37
25	B	807	CLA	C1D-ND	3.14	1.42	1.37
25	4	304	CLA	C1D-ND	3.14	1.42	1.37
25	S	313	CLA	C4B-NB	3.13	1.42	1.37
25	B	827	CLA	C3B-C4B	3.13	1.51	1.42
25	B	810	CLA	C1B-C2B	3.13	1.50	1.43
25	A	825	CLA	C1B-C2B	3.13	1.50	1.43
25	S	303	CLA	C4B-NB	3.13	1.42	1.37
25	2	610	CLA	C4B-NB	3.13	1.42	1.37
25	A	827	CLA	CMD-C2D	-3.13	1.44	1.50
25	2	602	CLA	C4B-NB	3.12	1.42	1.37
25	R	307	CLA	C1D-ND	3.12	1.42	1.37
25	3	303	CLA	CMC-C2C	-3.12	1.44	1.50
34	A	844	PQN	C2M-C2	3.12	1.57	1.50
25	T	312	CLA	C4B-NB	3.12	1.42	1.37
25	1	610	CLA	CAB-C3B	-3.12	1.44	1.50
25	6	610	CLA	C1D-ND	3.12	1.42	1.37
25	4	310	CLA	C4B-NB	3.11	1.42	1.37
25	A	841	CLA	C4B-NB	3.11	1.41	1.37
25	1	608	CLA	C1D-ND	3.11	1.41	1.37
25	A	818	CLA	C4B-NB	3.11	1.41	1.37
25	A	824	CLA	C1D-ND	3.11	1.41	1.37
25	T	312	CLA	C1D-ND	3.11	1.41	1.37
25	N	202	CLA	C4B-NB	3.11	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	609	CLA	CAB-C3B	-3.10	1.44	1.50
25	A	825	CLA	C4B-NB	3.10	1.41	1.37
30	A	848	BCR	C12-C13	3.10	1.52	1.46
25	B	810	CLA	C1D-ND	3.10	1.41	1.37
25	S	310	CLA	C1D-ND	3.10	1.41	1.37
25	X	304	CLA	C1D-ND	3.10	1.41	1.37
25	B	840	CLA	C1D-ND	3.10	1.41	1.37
25	S	303	CLA	C1D-ND	3.10	1.41	1.37
25	3	309	CLA	C4B-NB	3.09	1.41	1.37
25	S	311	CLA	C1D-ND	3.09	1.41	1.37
25	A	806	CLA	C4B-NB	3.09	1.41	1.37
25	K	201	CLA	C4B-NB	3.09	1.41	1.37
25	1	610	CLA	C4B-NB	3.09	1.41	1.37
25	A	804	CLA	C1D-ND	3.09	1.41	1.37
25	A	843	CLA	C4B-NB	3.09	1.41	1.37
25	B	813	CLA	C1B-C2B	3.09	1.50	1.43
25	P	309	CLA	C1D-ND	3.08	1.41	1.37
25	1	608	CLA	CMB-C2B	-3.08	1.44	1.50
25	T	313	CLA	C4B-NB	3.08	1.41	1.37
25	6	613	CLA	C1D-ND	3.08	1.41	1.37
25	X	313	CLA	C4B-NB	3.08	1.41	1.37
25	4	313	CLA	C1B-C2B	3.08	1.50	1.43
25	U	310	CLA	C4B-NB	3.08	1.41	1.37
25	6	613	CLA	C4B-NB	3.07	1.41	1.37
25	T	303	CLA	C4B-NB	3.07	1.41	1.37
25	A	837	CLA	CMB-C2B	-3.07	1.44	1.50
24	2	607	CHL	CMA-C3A	-3.07	1.48	1.53
25	1	602	CLA	C1D-ND	3.07	1.41	1.37
25	4	305	CLA	CAB-C3B	-3.07	1.44	1.50
25	Q	305	CLA	CMD-C2D	-3.07	1.44	1.50
25	A	809	CLA	C1D-ND	3.07	1.41	1.37
25	B	831	CLA	C4B-NB	3.07	1.41	1.37
25	G	204	CLA	MG-NB	-3.07	1.99	2.05
30	H	305	BCR	C8-C9	3.07	1.52	1.46
25	A	828	CLA	C1D-ND	3.07	1.41	1.37
25	G	202	CLA	C1B-C2B	3.07	1.50	1.43
25	4	316	CLA	C4B-NB	3.07	1.41	1.37
25	B	819	CLA	C1D-ND	3.07	1.41	1.37
24	2	605	CHL	CMD-C2D	-3.07	1.45	1.51
24	S	304	CHL	C1A-CHA	-3.06	1.36	1.40
25	3	305	CLA	C4B-NB	3.06	1.41	1.37
24	V	304	CHL	C2C-C3C	3.06	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	814	CLA	C1D-ND	3.06	1.41	1.37
25	U	312	CLA	C4B-NB	3.06	1.41	1.37
25	3	303	CLA	C1D-ND	3.06	1.41	1.37
25	B	804	CLA	C4B-NB	3.06	1.41	1.37
26	X	318	IWJ	C09-C10	3.06	1.52	1.46
25	6	603	CLA	CMD-C2D	-3.06	1.44	1.50
24	T	306	CHL	CBD-CGD	-3.06	1.48	1.52
24	2	615	CHL	CMD-C2D	-3.06	1.45	1.51
29	O	2006	Q6L	C02-C03	3.05	1.38	1.34
25	R	306	CLA	C1D-ND	3.05	1.41	1.37
38	S	308	KC2	C1D-ND	3.05	1.41	1.37
25	W	309	CLA	C4B-NB	3.05	1.41	1.37
25	B	823	CLA	C4B-NB	3.05	1.41	1.37
25	R	305	CLA	CMA-C3A	-3.05	1.46	1.53
25	P	312	CLA	C4B-NB	3.05	1.41	1.37
25	W	312	CLA	C4B-NB	3.05	1.41	1.37
25	6	613	CLA	CMD-C2D	-3.05	1.44	1.50
29	U	317	Q6L	C02-C03	3.05	1.38	1.34
25	A	815	CLA	C3B-C4B	3.05	1.51	1.42
25	L	303	CLA	C4B-NB	3.05	1.41	1.37
25	A	805	CLA	CMD-C2D	-3.04	1.44	1.50
25	R	307	CLA	C4B-NB	3.04	1.41	1.37
24	2	615	CHL	CHC-C4B	-3.04	1.34	1.39
24	Q	308	CHL	C3D-C2D	-3.04	1.34	1.39
25	1	610	CLA	C1D-ND	3.04	1.41	1.37
24	V	307	CHL	CAC-C3C	-3.04	1.46	1.51
25	4	314	CLA	C4B-NB	3.04	1.41	1.37
25	A	822	CLA	C1D-ND	3.04	1.41	1.37
25	6	612	CLA	C1D-ND	3.04	1.41	1.37
24	X	315	CHL	C1A-CHA	-3.03	1.36	1.40
25	1	607	CLA	C4B-NB	3.03	1.41	1.37
25	V	309	CLA	C1D-ND	3.03	1.41	1.37
30	B	847	BCR	C19-C18	3.03	1.52	1.46
30	G	205	BCR	C12-C13	3.03	1.52	1.46
25	2	614	CLA	C1D-ND	3.03	1.41	1.37
25	V	309	CLA	C3B-C4B	3.03	1.51	1.42
25	O	2002	CLA	CMB-C2B	-3.03	1.44	1.50
25	B	831	CLA	C1D-ND	3.03	1.41	1.37
25	X	310	CLA	C1D-ND	3.03	1.41	1.37
25	A	824	CLA	C1B-C2B	3.02	1.50	1.43
24	U	306	CHL	C1A-CHA	-3.02	1.36	1.40
25	B	819	CLA	CMB-C2B	-3.02	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	814	CLA	C1D-ND	3.02	1.41	1.37
24	W	314	CHL	CMD-C2D	-3.02	1.45	1.51
25	S	310	CLA	C4B-NB	3.02	1.41	1.37
25	B	814	CLA	C4B-NB	3.02	1.41	1.37
29	P	316	Q6L	C02-C03	3.02	1.38	1.34
25	O	2002	CLA	C1D-ND	3.02	1.41	1.37
25	T	301	CLA	C4B-NB	3.02	1.41	1.37
24	4	307	CHL	C1A-CHA	-3.02	1.36	1.40
25	3	308	CLA	C1D-ND	3.01	1.41	1.37
25	B	832	CLA	C1D-ND	3.01	1.41	1.37
25	B	826	CLA	CMB-C2B	-3.01	1.44	1.50
25	3	301	CLA	C1B-C2B	3.01	1.50	1.43
24	W	305	CHL	CAC-C3C	-3.01	1.46	1.51
25	N	203	CLA	CMB-C2B	-3.01	1.44	1.50
25	1	608	CLA	CMD-C2D	-3.01	1.44	1.50
24	T	304	CHL	C1A-CHA	-3.01	1.36	1.40
25	B	840	CLA	C4B-NB	3.01	1.41	1.37
25	B	842	CLA	CMB-C2B	-3.01	1.44	1.50
25	A	821	CLA	CMB-C2B	-3.00	1.44	1.50
25	A	842	CLA	C1B-C2B	3.00	1.50	1.43
25	A	836	CLA	C1D-ND	3.00	1.41	1.37
24	4	302	CHL	CMA-C3A	-3.00	1.48	1.53
24	Q	308	CHL	C3D-C4D	3.00	1.46	1.41
25	2	603	CLA	CMB-C2B	-3.00	1.44	1.50
25	4	309	CLA	C4B-NB	3.00	1.41	1.37
25	4	312	CLA	C4B-NB	3.00	1.41	1.37
38	X	309	KC2	MG-ND	-3.00	1.99	2.05
25	T	301	CLA	C1D-ND	3.00	1.41	1.37
25	O	2002	CLA	C3B-C4B	2.99	1.51	1.42
25	S	312	CLA	C4B-NB	2.99	1.41	1.37
25	B	824	CLA	C4B-NB	2.99	1.41	1.37
25	U	309	CLA	C4B-NB	2.99	1.41	1.37
25	3	312	CLA	C4B-NB	2.99	1.41	1.37
25	A	815	CLA	C4B-NB	2.99	1.41	1.37
25	T	313	CLA	C1D-ND	2.99	1.41	1.37
25	6	609	CLA	C1B-C2B	2.98	1.50	1.43
38	Q	310	KC2	C2A-C1A	2.98	1.53	1.44
25	A	824	CLA	CMB-C2B	-2.98	1.44	1.50
25	A	825	CLA	C3B-C4B	2.98	1.51	1.42
25	B	805	CLA	C1D-ND	2.98	1.41	1.37
26	1	611	IWJ	C04-C03	2.98	1.54	1.50
25	U	303	CLA	C4B-NB	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	322	IWJ	C04-C03	2.97	1.54	1.50
30	B	847	BCR	C1-C6	-2.97	1.50	1.53
25	B	815	CLA	C1B-C2B	2.97	1.50	1.43
25	2	606	CLA	C1D-ND	2.97	1.41	1.37
25	4	305	CLA	C4B-NB	2.97	1.41	1.37
38	U	307	KC2	C1D-ND	2.97	1.41	1.37
25	N	202	CLA	C1B-C2B	2.97	1.50	1.43
25	6	607	CLA	C4B-NB	2.97	1.41	1.37
25	B	837	CLA	C4B-NB	2.97	1.41	1.37
25	5	610	CLA	C4B-NB	2.97	1.41	1.37
25	P	313	CLA	C4B-NB	2.96	1.41	1.37
24	2	607	CHL	CAC-C3C	-2.96	1.46	1.51
25	B	831	CLA	C3B-C4B	2.96	1.51	1.42
25	3	307	CLA	CMB-C2B	-2.96	1.44	1.50
25	B	816	CLA	C1D-ND	2.96	1.41	1.37
25	5	609	CLA	C1B-C2B	2.96	1.50	1.43
38	T	308	KC2	C1D-ND	2.96	1.41	1.37
29	T	316	Q6L	C02-C03	2.96	1.38	1.34
25	T	311	CLA	C4B-NB	2.96	1.41	1.37
25	B	830	CLA	MG-NB	-2.96	1.99	2.05
25	U	311	CLA	C4B-NB	2.96	1.41	1.37
24	S	306	CHL	CHC-C4B	-2.96	1.34	1.39
30	F	804	BCR	C12-C13	2.96	1.52	1.46
25	X	310	CLA	C4B-NB	2.96	1.41	1.37
25	1	607	CLA	C4D-ND	-2.96	1.34	1.37
25	A	840	CLA	C4B-NB	2.96	1.41	1.37
25	B	841	CLA	C1D-ND	2.96	1.41	1.37
24	P	305	CHL	CBD-CGD	-2.95	1.48	1.52
25	6	604	CLA	C4B-NB	2.95	1.41	1.37
24	T	314	CHL	C1A-CHA	-2.95	1.36	1.40
25	S	311	CLA	C4B-NB	2.95	1.41	1.37
24	S	305	CHL	CMD-C2D	-2.95	1.45	1.51
25	K	201	CLA	C3B-C4B	2.95	1.51	1.42
25	1	606	CLA	C4B-NB	2.95	1.41	1.37
25	A	830	CLA	C3B-C4B	2.95	1.51	1.42
30	K	207	BCR	C12-C13	2.95	1.52	1.46
25	3	304	CLA	CMB-C2B	-2.95	1.44	1.50
24	R	309	CHL	C1A-CHA	-2.95	1.36	1.40
25	Q	314	CLA	C1D-ND	2.95	1.41	1.37
25	W	310	CLA	C4B-NB	2.95	1.41	1.37
30	4	319	BCR	C8-C9	2.95	1.52	1.46
25	A	837	CLA	C1D-ND	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	315	CLA	C4B-NB	2.95	1.41	1.37
25	T	309	CLA	C4B-NB	2.95	1.41	1.37
24	T	307	CHL	CBD-CGD	-2.94	1.48	1.52
25	B	812	CLA	C1D-ND	2.94	1.41	1.37
24	4	306	CHL	CAC-C3C	-2.94	1.46	1.50
26	5	611	IWJ	C04-C03	2.94	1.54	1.50
25	A	856	CLA	C1D-ND	2.94	1.41	1.37
25	R	313	CLA	C3B-C4B	2.94	1.51	1.42
29	S	320	Q6L	C33-C32	2.94	1.36	1.33
25	R	314	CLA	C4B-NB	2.94	1.41	1.37
29	V	319	Q6L	C34-C33	2.93	1.54	1.50
25	5	603	CLA	C4B-NB	2.93	1.41	1.37
24	P	314	CHL	C1A-CHA	-2.93	1.36	1.40
33	A	802	CL0	C1A-CHA	-2.93	1.36	1.40
25	A	838	CLA	CMB-C2B	-2.93	1.44	1.50
25	P	310	CLA	C4B-NB	2.93	1.41	1.37
24	P	306	CHL	CMD-C2D	-2.93	1.45	1.51
37	W	317	NEX	C7-C8	-2.93	1.27	1.31
25	K	201	CLA	C1B-C2B	2.93	1.50	1.43
29	X	319	Q6L	C34-C33	2.92	1.54	1.50
25	1	602	CLA	MG-NC	2.92	2.13	2.06
25	B	806	CLA	C1D-ND	2.92	1.41	1.37
25	B	809	CLA	C1B-C2B	2.92	1.50	1.43
24	V	314	CHL	C1A-CHA	-2.92	1.36	1.40
25	B	826	CLA	C1D-ND	2.92	1.41	1.37
38	X	309	KC2	C2A-C1A	2.92	1.53	1.44
29	R	301	Q6L	C12-C13	-2.92	1.45	1.51
25	6	607	CLA	CMD-C2D	-2.92	1.44	1.50
25	B	821	CLA	C1D-ND	2.92	1.41	1.37
25	3	304	CLA	C4B-NB	2.92	1.41	1.37
25	2	602	CLA	C1B-C2B	2.92	1.50	1.43
25	3	313	CLA	CMB-C2B	-2.92	1.44	1.50
24	S	307	CHL	CMB-C2B	-2.91	1.45	1.51
25	H	302	CLA	C1B-C2B	2.91	1.50	1.43
25	3	305	CLA	C1D-ND	2.91	1.41	1.37
25	4	303	CLA	C1D-ND	2.91	1.41	1.37
24	R	318	CHL	CMD-C2D	-2.91	1.45	1.51
25	3	301	CLA	CHC-C4B	-2.91	1.32	1.39
29	P	315	Q6L	C34-C33	2.91	1.54	1.50
30	2	618	BCR	C23-C22	2.90	1.52	1.46
26	R	322	IWJ	C04-C03	2.90	1.54	1.50
29	P	315	Q6L	C12-C13	-2.90	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	311	CLA	C4B-NB	2.90	1.41	1.37
25	A	840	CLA	C1B-C2B	2.90	1.49	1.43
25	H	302	CLA	C4B-NB	2.90	1.41	1.37
25	O	2003	CLA	C4B-NB	2.90	1.41	1.37
29	R	323	Q6L	C34-C33	2.90	1.54	1.50
25	A	838	CLA	C4B-NB	2.90	1.41	1.37
25	B	809	CLA	C1D-ND	2.90	1.41	1.37
25	3	303	CLA	C1B-C2B	2.90	1.49	1.43
29	Q	319	Q6L	C34-C33	2.90	1.54	1.50
25	P	303	CLA	C4B-NB	2.90	1.41	1.37
25	A	814	CLA	C4B-NB	2.90	1.41	1.37
24	4	302	CHL	CMD-C2D	-2.89	1.45	1.51
25	4	304	CLA	C4B-NB	2.89	1.41	1.37
25	Q	314	CLA	CMD-C2D	-2.89	1.44	1.50
30	3	318	BCR	C8-C9	2.89	1.52	1.46
25	B	809	CLA	C1B-NB	-2.89	1.34	1.37
29	R	319	Q6L	C02-C03	2.89	1.38	1.34
29	X	319	Q6L	C12-C13	-2.89	1.45	1.51
24	5	605	CHL	CAC-C3C	-2.89	1.46	1.51
25	5	607	CLA	C1D-ND	2.89	1.41	1.37
37	T	317	NEX	C22-C21	-2.89	1.50	1.54
24	W	306	CHL	C1A-CHA	-2.89	1.36	1.40
25	B	811	CLA	CMB-C2B	-2.89	1.44	1.50
26	T	321	IWJ	C04-C03	2.89	1.54	1.50
38	W	308	KC2	CMC-C2C	-2.89	1.44	1.50
25	F	802	CLA	C1D-ND	2.88	1.41	1.37
24	S	304	CHL	C2C-C3C	2.88	1.39	1.36
25	K	206	CLA	C4B-NB	2.88	1.41	1.37
26	Q	320	IWJ	C04-C03	2.88	1.54	1.50
25	B	835	CLA	C4B-NB	2.88	1.41	1.37
25	U	301	CLA	C1D-ND	2.88	1.41	1.37
25	S	301	CLA	C4B-NB	2.88	1.41	1.37
24	Q	308	CHL	CBD-CGD	-2.88	1.48	1.52
25	3	302	CLA	C1D-ND	2.88	1.41	1.37
25	3	303	CLA	CMD-C2D	-2.87	1.44	1.50
25	B	813	CLA	C1D-ND	2.87	1.41	1.37
25	P	301	CLA	C3B-C4B	2.87	1.51	1.42
26	X	318	IWJ	C04-C03	2.87	1.54	1.50
25	A	836	CLA	C1B-C2B	2.87	1.49	1.43
24	R	311	CHL	CMB-C2B	-2.87	1.45	1.51
25	5	602	CLA	C4B-NB	2.87	1.41	1.37
25	K	206	CLA	C3B-C4B	2.87	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	604	CLA	C4B-NB	2.86	1.41	1.37
25	6	602	CLA	C1B-C2B	2.86	1.49	1.43
25	B	829	CLA	C1D-ND	2.86	1.41	1.37
25	Q	301	CLA	C1B-C2B	2.86	1.49	1.43
26	U	316	IWJ	C04-C03	2.86	1.54	1.50
25	B	826	CLA	C1B-NB	-2.86	1.34	1.37
25	A	842	CLA	C4B-NB	2.86	1.41	1.37
25	B	836	CLA	C1D-ND	2.86	1.41	1.37
30	B	847	BCR	C31-C1	-2.86	1.48	1.53
25	Q	314	CLA	C1B-C2B	2.86	1.49	1.43
29	S	323	Q6L	C12-C13	-2.86	1.45	1.51
25	2	612	CLA	C4B-NB	2.86	1.41	1.37
29	W	316	Q6L	C12-C13	-2.85	1.45	1.51
25	B	835	CLA	CMD-C2D	-2.85	1.44	1.50
24	T	307	CHL	CMB-C2B	-2.85	1.45	1.51
29	T	322	Q6L	C34-C33	2.85	1.54	1.50
26	T	318	IWJ	C04-C03	2.85	1.54	1.50
24	Q	309	CHL	CMD-C2D	-2.85	1.45	1.51
25	N	203	CLA	C1D-ND	2.85	1.41	1.37
38	P	308	KC2	C4B-NB	2.85	1.41	1.37
25	X	314	CLA	C4B-NB	2.85	1.41	1.37
25	B	804	CLA	CMC-C2C	-2.85	1.44	1.50
25	5	606	CLA	C4B-NB	2.85	1.41	1.37
25	S	303	CLA	C3B-C4B	2.85	1.51	1.42
24	U	306	CHL	CBD-CGD	-2.85	1.48	1.52
26	P	320	IWJ	C04-C03	2.84	1.54	1.50
38	V	308	KC2	C2A-C1A	2.84	1.53	1.44
25	A	831	CLA	CMB-C2B	-2.84	1.44	1.50
25	G	202	CLA	C4B-NB	2.84	1.41	1.37
25	4	303	CLA	C3B-C4B	2.84	1.51	1.42
24	4	307	CHL	C2C-C3C	2.84	1.39	1.36
37	P	317	NEX	C7-C8	-2.84	1.27	1.31
25	A	830	CLA	CMB-C2B	-2.84	1.45	1.50
24	4	306	CHL	CMB-C2B	-2.84	1.46	1.51
25	A	815	CLA	C1B-C2B	2.84	1.49	1.43
25	B	816	CLA	C4B-NB	2.84	1.41	1.37
25	A	831	CLA	C1D-ND	2.83	1.41	1.37
25	B	817	CLA	CMB-C2B	-2.83	1.45	1.50
24	4	307	CHL	CMA-C3A	-2.83	1.48	1.53
25	3	310	CLA	C4B-NB	2.83	1.41	1.37
25	S	313	CLA	CMD-C2D	-2.83	1.45	1.50
25	R	316	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	318	CHL	C1A-CHA	-2.83	1.36	1.40
25	3	313	CLA	C4B-NB	2.83	1.41	1.37
25	B	839	CLA	C1D-ND	2.83	1.41	1.37
26	S	319	IWJ	C04-C03	2.83	1.54	1.50
30	A	848	BCR	C8-C9	2.83	1.52	1.46
24	W	305	CHL	C1A-CHA	-2.83	1.36	1.40
25	B	841	CLA	C4B-NB	2.83	1.41	1.37
25	O	2005	CLA	C4B-NB	2.82	1.41	1.37
25	2	613	CLA	C1B-C2B	2.82	1.49	1.43
27	4	318	XAT	O24-C25	-2.82	1.42	1.46
25	A	805	CLA	C1B-C2B	2.82	1.49	1.43
25	L	301	CLA	C1B-C2B	2.82	1.49	1.43
24	R	310	CHL	C1A-CHA	-2.82	1.36	1.40
25	4	315	CLA	C4B-NB	2.82	1.41	1.37
25	A	832	CLA	C1B-C2B	2.82	1.49	1.43
25	U	308	CLA	MG-NC	2.82	2.13	2.06
24	U	306	CHL	CMD-C2D	-2.82	1.46	1.51
25	4	312	CLA	C1B-C2B	2.82	1.49	1.43
25	3	307	CLA	CHC-C4B	-2.82	1.33	1.39
25	O	2004	CLA	C4B-NB	2.82	1.41	1.37
29	O	2007	Q6L	C02-C03	2.82	1.37	1.34
25	4	310	CLA	C3B-C4B	2.82	1.50	1.42
26	R	303	IWJ	C04-C03	2.82	1.54	1.50
25	L	301	CLA	CMC-C2C	-2.82	1.45	1.50
26	Q	303	IWJ	C04-C03	2.82	1.54	1.50
24	T	314	CHL	CMD-C2D	-2.82	1.46	1.51
25	G	204	CLA	C1B-NB	-2.82	1.34	1.37
29	S	321	Q6L	C12-C13	-2.82	1.45	1.51
30	A	850	BCR	C1-C6	-2.82	1.50	1.53
25	F	802	CLA	CMB-C2B	-2.81	1.45	1.50
24	3	306	CHL	C1A-CHA	-2.81	1.36	1.40
26	S	318	IWJ	C04-C03	2.81	1.54	1.50
24	S	307	CHL	CMD-C2D	-2.81	1.46	1.51
25	B	824	CLA	C1D-ND	2.81	1.41	1.37
25	V	302	CLA	C4B-NB	2.81	1.41	1.37
25	X	312	CLA	C4B-NB	2.81	1.41	1.37
29	O	2006	Q6L	C34-C33	2.81	1.54	1.50
25	B	834	CLA	C1B-C2B	2.81	1.49	1.43
25	P	311	CLA	C4B-NB	2.81	1.41	1.37
29	S	320	Q6L	C12-C13	-2.81	1.45	1.51
25	3	314	CLA	C3B-C4B	2.81	1.50	1.42
30	A	848	BCR	C19-C18	2.81	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	811	CLA	CMC-C2C	-2.81	1.45	1.50
29	R	323	Q6L	C12-C13	-2.81	1.45	1.51
25	5	604	CLA	C4B-NB	2.81	1.41	1.37
29	X	316	Q6L	C02-C03	2.81	1.37	1.34
26	V	320	IWJ	C04-C03	2.81	1.54	1.50
29	X	317	Q6L	C02-C03	2.80	1.37	1.34
37	P	317	NEX	C12-C13	2.80	1.52	1.46
25	P	309	CLA	C4B-NB	2.80	1.41	1.37
30	J	101	BCR	C19-C18	2.80	1.51	1.46
25	A	832	CLA	C4B-NB	2.80	1.41	1.37
38	U	307	KC2	C2A-C1A	2.80	1.53	1.44
25	X	302	CLA	C1D-ND	2.80	1.41	1.37
24	P	306	CHL	CHC-C4B	-2.80	1.35	1.39
25	A	818	CLA	C3B-C4B	2.80	1.50	1.42
30	A	852	BCR	C37-C22	2.80	1.56	1.50
25	1	602	CLA	C1B-C2B	2.80	1.49	1.43
38	W	308	KC2	C2A-C1A	2.80	1.53	1.44
25	2	606	CLA	C4B-NB	2.80	1.41	1.37
25	Q	315	CLA	C1B-C2B	2.80	1.49	1.43
25	3	301	CLA	CMC-C2C	-2.79	1.45	1.50
30	K	202	BCR	C19-C18	2.79	1.51	1.46
25	B	821	CLA	C4B-NB	2.79	1.41	1.37
25	1	609	CLA	C1B-C2B	2.79	1.49	1.43
25	6	602	CLA	C1D-ND	2.79	1.41	1.37
25	V	312	CLA	C1D-ND	2.79	1.41	1.37
25	B	831	CLA	CMD-C2D	-2.79	1.45	1.50
25	5	603	CLA	C3B-C4B	2.79	1.50	1.42
29	O	2007	Q6L	C34-C33	2.79	1.54	1.50
25	L	303	CLA	C3B-C4B	2.79	1.50	1.42
24	S	304	CHL	CMD-C2D	-2.79	1.46	1.51
25	K	203	CLA	C1B-C2B	2.79	1.49	1.43
38	R	312	KC2	C3D-C4D	2.79	1.47	1.40
25	B	811	CLA	C1D-ND	2.79	1.41	1.37
24	2	607	CHL	CBD-CGD	-2.79	1.49	1.52
30	A	850	BCR	C12-C13	2.78	1.51	1.46
25	R	306	CLA	CMD-C2D	-2.78	1.45	1.50
25	A	827	CLA	C3B-C4B	2.78	1.50	1.42
34	B	844	PQN	C10-C5	-2.78	1.36	1.40
24	U	313	CHL	CMD-C2D	-2.78	1.46	1.51
26	T	321	IWJ	C03-C02	2.78	1.36	1.33
25	A	827	CLA	C1B-C2B	2.78	1.49	1.43
25	V	303	CLA	C4B-NB	2.78	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	607	CLA	CMB-C2B	-2.78	1.45	1.50
25	P	311	CLA	C1B-C2B	2.78	1.49	1.43
24	2	605	CHL	C1A-CHA	-2.78	1.36	1.40
29	X	301	Q6L	C33-C32	2.78	1.36	1.33
30	B	845	BCR	C34-C9	2.78	1.56	1.50
25	O	2005	CLA	C1B-C2B	2.78	1.49	1.43
29	S	323	Q6L	C02-C03	2.77	1.37	1.34
25	R	313	CLA	C1B-C2B	2.77	1.49	1.43
25	A	814	CLA	CMD-C2D	-2.77	1.45	1.50
25	P	302	CLA	C4B-NB	2.77	1.41	1.37
26	5	611	IWJ	C03-C02	2.77	1.36	1.33
24	U	305	CHL	CMD-C2D	-2.77	1.46	1.51
26	Q	303	IWJ	C03-C02	2.77	1.36	1.33
25	B	815	CLA	C3B-C4B	2.77	1.50	1.42
38	W	308	KC2	C4B-NB	2.77	1.41	1.37
25	A	826	CLA	C1B-C2B	2.77	1.49	1.43
25	A	823	CLA	C4B-NB	2.77	1.41	1.37
25	3	310	CLA	C1B-C2B	2.77	1.49	1.43
25	6	602	CLA	C3B-C4B	2.77	1.50	1.42
25	4	310	CLA	C1B-C2B	2.77	1.49	1.43
25	6	611	CLA	C4B-NB	2.77	1.41	1.37
25	A	842	CLA	C1D-ND	2.77	1.41	1.37
25	Q	304	CLA	C3B-C4B	2.77	1.50	1.42
25	T	303	CLA	C1D-ND	2.77	1.41	1.37
26	4	317	IWJ	C04-C03	2.77	1.54	1.50
25	A	835	CLA	C4B-NB	2.77	1.41	1.37
29	P	319	Q6L	C02-C03	2.77	1.37	1.34
37	S	317	NEX	C22-C21	-2.77	1.50	1.54
30	4	319	BCR	C12-C13	2.77	1.51	1.46
25	U	312	CLA	C1B-C2B	2.77	1.49	1.43
38	T	308	KC2	C2A-C1A	2.76	1.53	1.44
24	V	306	CHL	CMD-C2D	-2.76	1.46	1.51
29	R	320	Q6L	C34-C33	2.76	1.54	1.50
25	A	803	CLA	C4B-NB	2.76	1.41	1.37
25	V	313	CLA	C4B-NB	2.76	1.41	1.37
25	W	303	CLA	C1D-ND	2.76	1.41	1.37
29	V	321	Q6L	C12-C13	-2.76	1.45	1.51
25	G	203	CLA	C1B-C2B	2.76	1.49	1.43
34	B	844	PQN	C2M-C2	2.76	1.56	1.50
30	K	205	BCR	C8-C9	2.76	1.51	1.46
24	1	604	CHL	C1A-CHA	-2.76	1.36	1.40
25	B	820	CLA	CMB-C2B	-2.76	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	304	CHL	CMB-C2B	-2.76	1.46	1.51
29	U	314	Q6L	C02-C03	2.76	1.37	1.34
24	P	304	CHL	CHC-C1C	2.76	1.44	1.39
25	A	841	CLA	C1B-C2B	2.76	1.49	1.43
25	2	612	CLA	C1B-C2B	2.76	1.49	1.43
29	W	315	Q6L	C12-C13	-2.76	1.45	1.51
25	U	312	CLA	CMD-C2D	-2.76	1.45	1.50
25	X	303	CLA	C4B-NB	2.76	1.41	1.37
25	3	302	CLA	CMC-C2C	-2.75	1.45	1.50
25	4	305	CLA	CMB-C2B	-2.75	1.45	1.50
29	W	320	Q6L	C12-C13	-2.75	1.45	1.51
29	Q	319	Q6L	C33-C32	2.75	1.36	1.33
25	6	612	CLA	CMB-C2B	-2.75	1.45	1.50
25	U	303	CLA	CMB-C2B	-2.75	1.45	1.50
26	S	319	IWJ	C03-C02	2.75	1.36	1.33
29	S	321	Q6L	C34-C33	2.75	1.54	1.50
24	X	315	CHL	CMD-C2D	-2.75	1.46	1.51
24	W	307	CHL	CMD-C2D	-2.75	1.46	1.51
25	1	602	CLA	CMD-C2D	-2.75	1.45	1.50
29	S	321	Q6L	C33-C32	2.75	1.36	1.33
25	A	817	CLA	C4B-NB	2.75	1.41	1.37
25	1	613	CLA	C1B-C2B	2.75	1.49	1.43
24	5	605	CHL	CMB-C2B	-2.74	1.46	1.51
24	X	307	CHL	CMD-C2D	-2.74	1.46	1.51
24	X	307	CHL	CMB-C2B	-2.74	1.46	1.51
25	A	830	CLA	CMC-C2C	-2.74	1.45	1.50
25	A	845	CLA	C1B-C2B	2.74	1.49	1.43
25	K	206	CLA	C1B-C2B	2.74	1.49	1.43
25	B	823	CLA	C1B-C2B	2.74	1.49	1.43
29	O	2007	Q6L	C33-C32	2.74	1.36	1.33
25	5	602	CLA	C1B-C2B	2.74	1.49	1.43
24	W	306	CHL	CMD-C2D	-2.74	1.46	1.51
38	P	308	KC2	C3D-C4D	2.74	1.47	1.40
25	B	802	CLA	C4B-NB	2.74	1.41	1.37
25	B	827	CLA	C4B-NB	2.74	1.41	1.37
25	Q	313	CLA	C4B-NB	2.74	1.41	1.37
25	A	843	CLA	C1B-C2B	2.74	1.49	1.43
25	B	835	CLA	C1B-C2B	2.74	1.49	1.43
25	V	312	CLA	CMD-C2D	-2.74	1.45	1.50
29	T	322	Q6L	C12-C13	-2.74	1.45	1.51
25	A	830	CLA	CMD-C2D	-2.74	1.45	1.50
25	A	819	CLA	C3B-C4B	2.74	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	313	CLA	C4B-NB	2.74	1.41	1.37
25	A	804	CLA	CMA-C3A	-2.74	1.47	1.53
24	S	306	CHL	CMC-C2C	2.74	1.50	1.44
29	T	315	Q6L	C12-C13	-2.74	1.45	1.51
30	K	202	BCR	C16-C15	-2.74	1.28	1.36
34	B	844	PQN	C3-C4	-2.74	1.40	1.47
25	B	836	CLA	CMD-C2D	-2.73	1.45	1.50
24	W	304	CHL	C1A-CHA	-2.73	1.36	1.40
25	S	312	CLA	C1B-C2B	2.73	1.49	1.43
25	B	835	CLA	C1D-ND	2.73	1.41	1.37
25	H	304	CLA	C1D-ND	2.73	1.41	1.37
30	M	101	BCR	C34-C9	2.73	1.56	1.50
25	A	827	CLA	CMB-C2B	-2.73	1.45	1.50
25	B	810	CLA	CMC-C2C	-2.73	1.45	1.50
25	B	822	CLA	C4B-NB	2.73	1.41	1.37
25	T	303	CLA	C3B-C4B	2.73	1.50	1.42
24	P	306	CHL	CAC-C3C	-2.73	1.46	1.51
25	T	310	CLA	C1B-C2B	2.73	1.49	1.43
34	A	844	PQN	C3-C4	-2.73	1.40	1.47
25	2	611	CLA	C1B-C2B	2.73	1.49	1.43
25	R	315	CLA	C1B-C2B	2.73	1.49	1.43
25	B	830	CLA	MG-ND	-2.73	2.00	2.05
38	U	307	KC2	MG-ND	-2.73	2.00	2.05
25	B	804	CLA	C1D-ND	2.73	1.41	1.37
29	W	319	Q6L	C12-C13	-2.73	1.45	1.51
25	K	204	CLA	C1B-C2B	2.73	1.49	1.43
38	X	309	KC2	CMC-C2C	-2.72	1.45	1.50
38	R	312	KC2	C2A-C1A	2.72	1.53	1.44
25	A	806	CLA	CHC-C1C	2.72	1.43	1.38
25	A	816	CLA	CMD-C2D	-2.72	1.45	1.50
25	U	301	CLA	C3B-C4B	2.72	1.50	1.42
25	X	314	CLA	C1B-C2B	2.72	1.49	1.43
38	Q	310	KC2	C3D-C4D	2.72	1.47	1.40
25	6	602	CLA	C4B-NB	2.72	1.41	1.37
26	P	318	IWJ	C04-C03	2.72	1.54	1.50
25	A	827	CLA	C4B-NB	2.72	1.41	1.37
29	Q	317	Q6L	C12-C13	-2.72	1.45	1.51
24	P	305	CHL	CMD-C2D	-2.72	1.46	1.51
24	P	307	CHL	CAC-C3C	-2.72	1.46	1.51
25	G	203	CLA	C4B-NB	2.72	1.41	1.37
29	U	315	Q6L	C02-C03	2.72	1.37	1.34
29	U	315	Q6L	C34-C33	2.72	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	802	CL0	MG-NB	-2.72	2.00	2.05
25	3	311	CLA	C1B-C2B	2.71	1.49	1.43
24	S	306	CHL	CMB-C2B	-2.71	1.46	1.51
25	3	309	CLA	C1B-C2B	2.71	1.49	1.43
29	T	319	Q6L	C34-C33	2.71	1.54	1.50
25	B	842	CLA	C1B-C2B	2.71	1.49	1.43
25	R	317	CLA	C4B-NB	2.71	1.41	1.37
24	W	304	CHL	C2C-C3C	2.71	1.39	1.36
25	S	302	CLA	C4B-NB	2.71	1.41	1.37
25	P	313	CLA	C1B-C2B	2.71	1.49	1.43
29	W	316	Q6L	C02-C03	2.71	1.37	1.34
25	S	309	CLA	C1D-ND	2.71	1.41	1.37
25	B	829	CLA	CMB-C2B	-2.71	1.45	1.50
25	W	312	CLA	C1B-C2B	2.71	1.49	1.43
26	6	614	IWJ	C04-C03	2.70	1.54	1.50
25	3	305	CLA	CMB-C2B	-2.70	1.45	1.50
25	W	313	CLA	C1B-C2B	2.70	1.49	1.43
25	1	605	CLA	C4B-NB	2.70	1.41	1.37
25	A	831	CLA	MG-NB	-2.70	2.00	2.05
26	U	316	IWJ	C03-C02	2.70	1.36	1.33
27	4	318	XAT	C32-C33	2.70	1.51	1.46
25	B	838	CLA	C3B-C4B	2.70	1.50	1.42
25	B	826	CLA	CMC-C2C	-2.70	1.45	1.50
26	4	301	IWJ	C04-C03	2.70	1.54	1.50
25	B	803	CLA	CMB-C2B	-2.70	1.45	1.50
25	3	314	CLA	C1B-C2B	2.70	1.49	1.43
24	6	601	CHL	CMD-C2D	-2.70	1.46	1.51
29	V	319	Q6L	C02-C03	2.70	1.37	1.34
25	S	301	CLA	CMD-C2D	-2.70	1.45	1.50
25	3	303	CLA	C4B-NB	2.69	1.41	1.37
38	V	308	KC2	CMC-C2C	-2.69	1.45	1.50
24	P	314	CHL	CMD-C2D	-2.69	1.46	1.51
24	V	304	CHL	CMD-C2D	-2.69	1.46	1.51
26	1	611	IWJ	C03-C02	2.69	1.36	1.33
24	X	306	CHL	C2C-C3C	2.69	1.39	1.36
25	Q	305	CLA	C4B-NB	2.69	1.41	1.37
25	B	812	CLA	CMD-C2D	-2.69	1.45	1.50
26	S	322	IWJ	C03-C02	2.69	1.36	1.33
25	A	811	CLA	C3B-C4B	2.69	1.50	1.42
29	T	315	Q6L	C34-C33	2.69	1.54	1.50
26	W	318	IWJ	C03-C02	2.69	1.36	1.33
25	Q	301	CLA	CHC-C4B	-2.69	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	606	CLA	C4B-C3B	2.69	1.49	1.43
24	6	601	CHL	C1A-CHA	-2.69	1.36	1.40
24	Q	309	CHL	C1A-CHA	-2.69	1.36	1.40
25	6	603	CLA	MG-NB	-2.69	2.00	2.05
30	F	801	BCR	C19-C18	2.69	1.51	1.46
26	4	301	IWJ	C03-C02	2.69	1.36	1.33
29	U	314	Q6L	C12-C13	-2.69	1.45	1.51
29	R	320	Q6L	C12-C13	-2.69	1.45	1.51
25	1	606	CLA	C1B-C2B	2.69	1.49	1.43
25	2	610	CLA	C1B-C2B	2.69	1.49	1.43
25	V	303	CLA	C3B-C4B	2.69	1.50	1.42
25	U	302	CLA	C4B-NB	2.69	1.41	1.37
24	Q	309	CHL	CMB-C2B	-2.69	1.46	1.51
29	V	319	Q6L	C12-C13	-2.68	1.45	1.51
25	3	307	CLA	CMA-C3A	-2.68	1.47	1.53
26	V	318	IWJ	C04-C03	2.68	1.54	1.50
24	T	305	CHL	CBD-CGD	-2.68	1.49	1.52
25	A	816	CLA	C1D-ND	2.68	1.41	1.37
38	W	308	KC2	MG-ND	-2.68	2.00	2.05
30	4	319	BCR	C30-C25	-2.68	1.50	1.53
27	1	612	XAT	C35-C15	-2.68	1.28	1.36
29	S	320	Q6L	C02-C03	2.68	1.37	1.34
25	S	303	CLA	CMD-C2D	-2.68	1.45	1.50
25	B	822	CLA	C1B-C2B	2.68	1.49	1.43
25	T	312	CLA	C1B-C2B	2.68	1.49	1.43
25	A	806	CLA	C3B-C4B	2.68	1.50	1.42
27	1	612	XAT	O24-C25	-2.68	1.42	1.46
25	O	2003	CLA	C1B-C2B	2.68	1.49	1.43
29	P	319	Q6L	C33-C32	2.68	1.36	1.33
24	U	304	CHL	CMD-C2D	-2.68	1.46	1.51
24	X	308	CHL	CMD-C2D	-2.68	1.46	1.51
25	J	102	CLA	C1D-ND	2.68	1.41	1.37
24	1	601	CHL	C3B-C2B	-2.68	1.36	1.40
25	F	803	CLA	C1B-C2B	2.68	1.49	1.43
24	2	607	CHL	CHB-C4A	-2.67	1.35	1.38
29	Q	318	Q6L	C02-C03	2.67	1.37	1.34
25	B	815	CLA	C1D-ND	2.67	1.41	1.37
25	5	606	CLA	C1B-C2B	2.67	1.49	1.43
25	R	317	CLA	C1B-C2B	2.67	1.49	1.43
25	X	303	CLA	C1B-C2B	2.67	1.49	1.43
24	2	615	CHL	C1A-CHA	-2.67	1.37	1.40
25	A	819	CLA	C4B-NB	2.67	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	304	CLA	C1B-C2B	2.67	1.49	1.43
25	2	602	CLA	C3B-C4B	2.67	1.50	1.42
25	5	608	CLA	C4B-NB	2.67	1.41	1.37
29	R	304	Q6L	C34-C33	2.67	1.54	1.50
25	A	813	CLA	C1B-C2B	2.67	1.49	1.43
24	S	314	CHL	C1A-CHA	-2.67	1.37	1.40
25	1	603	CLA	C4B-NB	2.67	1.41	1.37
34	A	844	PQN	C10-C5	-2.67	1.36	1.40
24	T	306	CHL	C2C-C3C	2.66	1.39	1.36
25	4	303	CLA	CMB-C2B	-2.66	1.45	1.50
29	S	316	Q6L	C02-C03	2.66	1.37	1.34
25	5	609	CLA	C4B-NB	2.66	1.41	1.37
25	L	304	CLA	C1B-C2B	2.66	1.49	1.43
24	2	607	CHL	CMB-C2B	-2.66	1.46	1.51
25	A	813	CLA	CMD-C2D	-2.66	1.45	1.50
37	H	306	NEX	C22-C21	-2.66	1.50	1.54
25	K	203	CLA	C4B-NB	2.66	1.41	1.37
33	A	802	CL0	CHC-C4B	-2.66	1.35	1.39
24	Q	308	CHL	CMB-C2B	-2.66	1.46	1.51
26	R	322	IWJ	C03-C02	2.66	1.36	1.33
25	A	828	CLA	CMB-C2B	-2.66	1.45	1.50
38	R	312	KC2	C4B-NB	2.66	1.41	1.37
30	3	318	BCR	C12-C13	2.66	1.51	1.46
24	2	607	CHL	C3B-C2B	-2.66	1.36	1.40
30	A	849	BCR	C19-C18	2.66	1.51	1.46
25	A	842	CLA	CMD-C2D	-2.66	1.45	1.50
29	2	616	Q6L	C02-C03	2.66	1.37	1.34
25	A	821	CLA	C4B-NB	2.66	1.41	1.37
25	P	312	CLA	C1B-C2B	2.66	1.49	1.43
24	T	306	CHL	CMD-C2D	-2.65	1.46	1.51
25	U	310	CLA	C1B-C2B	2.65	1.49	1.43
25	3	311	CLA	C4-C3	-2.65	1.44	1.50
25	O	2004	CLA	C1B-C2B	2.65	1.49	1.43
25	N	203	CLA	MG-ND	-2.65	2.00	2.05
26	3	315	IWJ	C04-C03	2.65	1.54	1.50
24	T	320	CHL	C3B-C2B	-2.65	1.36	1.40
25	B	842	CLA	C4B-NB	2.65	1.41	1.37
24	T	307	CHL	CAC-C3C	-2.65	1.47	1.51
24	R	302	CHL	CMA-C3A	-2.65	1.48	1.53
25	4	314	CLA	C1B-C2B	2.65	1.49	1.43
38	R	312	KC2	MG-ND	-2.65	2.00	2.05
24	S	305	CHL	C1A-CHA	-2.65	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	X	306	CHL	CMD-C2D	-2.65	1.46	1.51
25	3	302	CLA	C4B-NB	2.65	1.41	1.37
25	B	839	CLA	C4B-NB	2.65	1.41	1.37
24	V	306	CHL	C1A-CHA	-2.65	1.37	1.40
30	2	618	BCR	C19-C18	2.65	1.51	1.46
25	A	805	CLA	C4B-NB	2.65	1.41	1.37
29	T	316	Q6L	C34-C33	2.65	1.54	1.50
29	W	320	Q6L	C34-C33	2.65	1.54	1.50
25	2	613	CLA	C4B-NB	2.65	1.41	1.37
24	V	314	CHL	CBD-CGD	-2.65	1.49	1.52
25	A	811	CLA	C1B-C2B	2.64	1.49	1.43
24	V	304	CHL	C3B-C2B	-2.64	1.36	1.40
25	B	832	CLA	MG-NB	-2.64	2.00	2.05
25	T	303	CLA	CMD-C2D	-2.64	1.45	1.50
24	S	306	CHL	CMD-C2D	-2.64	1.46	1.51
38	V	308	KC2	C4B-NB	2.64	1.41	1.37
24	T	307	CHL	CMD-C2D	-2.64	1.46	1.51
25	6	611	CLA	C1B-C2B	2.64	1.49	1.43
25	B	825	CLA	C1B-C2B	2.64	1.49	1.43
29	R	319	Q6L	C12-C13	-2.64	1.45	1.51
25	4	316	CLA	C1B-C2B	2.64	1.49	1.43
25	3	308	CLA	C1B-C2B	2.64	1.49	1.43
38	R	312	KC2	CMC-C2C	-2.64	1.45	1.50
24	4	308	CHL	CMD-C2D	-2.64	1.46	1.51
25	5	607	CLA	C1B-C2B	2.64	1.49	1.43
25	V	303	CLA	CMB-C2B	-2.64	1.45	1.50
25	A	807	CLA	CMB-C2B	-2.64	1.45	1.50
26	V	317	IWJ	C04-C03	2.63	1.54	1.50
25	T	301	CLA	C3B-C4B	2.63	1.50	1.42
25	B	810	CLA	CMD-C2D	-2.63	1.45	1.50
25	Q	312	CLA	C1B-C2B	2.63	1.49	1.43
25	O	2001	CLA	C1B-C2B	2.63	1.49	1.43
25	B	802	CLA	CMD-C2D	-2.63	1.45	1.50
24	4	306	CHL	C1A-CHA	-2.63	1.37	1.40
25	T	302	CLA	C1B-C2B	2.63	1.49	1.43
25	W	303	CLA	CMB-C2B	-2.63	1.45	1.50
25	X	304	CLA	C4B-NB	2.63	1.41	1.37
25	A	833	CLA	MG-NB	-2.63	2.00	2.05
25	T	311	CLA	C3B-C4B	2.63	1.50	1.42
25	5	610	CLA	C1B-C2B	2.63	1.49	1.43
25	Q	306	CLA	C4B-NB	2.63	1.41	1.37
29	R	304	Q6L	C02-C03	2.63	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	305	CLA	C1B-C2B	2.63	1.49	1.43
26	T	318	IWJ	C03-C02	2.63	1.36	1.33
25	2	614	CLA	C4B-NB	2.63	1.41	1.37
25	3	311	CLA	CMB-C2B	-2.63	1.45	1.50
25	B	805	CLA	CMB-C2B	-2.63	1.45	1.50
25	1	605	CLA	C1B-C2B	2.63	1.49	1.43
29	V	316	Q6L	C34-C33	2.63	1.54	1.50
25	B	825	CLA	C1D-ND	2.63	1.41	1.37
30	K	205	BCR	C12-C13	2.62	1.51	1.46
29	X	319	Q6L	C02-C03	2.62	1.37	1.34
25	Q	305	CLA	C1B-C2B	2.62	1.49	1.43
30	J	101	BCR	C16-C15	-2.62	1.29	1.36
25	R	317	CLA	CMC-C2C	-2.62	1.45	1.50
25	B	834	CLA	C4B-NB	2.62	1.41	1.37
25	S	302	CLA	CMD-C2D	-2.62	1.45	1.50
29	W	320	Q6L	C02-C03	2.62	1.37	1.34
25	A	822	CLA	C4B-NB	2.62	1.41	1.37
29	P	316	Q6L	C12-C13	-2.62	1.45	1.51
37	H	306	NEX	C12-C13	2.62	1.51	1.46
25	6	610	CLA	CMD-C2D	-2.62	1.45	1.50
25	Q	306	CLA	CMB-C2B	-2.62	1.45	1.50
29	T	322	Q6L	C02-C03	2.61	1.37	1.34
25	2	611	CLA	C4B-NB	2.61	1.41	1.37
29	P	316	Q6L	C34-C33	2.61	1.54	1.50
24	2	605	CHL	CBD-CGD	-2.61	1.49	1.52
25	R	305	CLA	C3B-C4B	2.61	1.50	1.42
29	X	301	Q6L	C12-C13	-2.61	1.45	1.51
25	F	802	CLA	C4B-NB	2.61	1.41	1.37
25	4	315	CLA	C1B-C2B	2.61	1.49	1.43
25	B	803	CLA	C3B-C4B	2.61	1.50	1.42
25	R	305	CLA	C4B-NB	2.61	1.41	1.37
25	L	304	CLA	C4B-NB	2.61	1.41	1.37
26	P	320	IWJ	C03-C02	2.61	1.36	1.33
24	3	306	CHL	C3B-C2B	-2.61	1.36	1.40
24	4	302	CHL	CBD-CGD	-2.61	1.49	1.52
24	X	315	CHL	CMB-C2B	-2.61	1.46	1.51
25	B	806	CLA	CMD-C2D	-2.61	1.45	1.50
25	A	830	CLA	C4B-NB	2.61	1.41	1.37
29	V	315	Q6L	C02-C03	2.61	1.37	1.34
24	4	307	CHL	CMB-C2B	-2.61	1.46	1.51
25	3	308	CLA	C1B-NB	-2.61	1.34	1.37
25	R	305	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	613	CLA	CMB-C2B	-2.61	1.45	1.50
29	W	315	Q6L	C02-C03	2.61	1.37	1.34
24	5	605	CHL	C1A-CHA	-2.60	1.37	1.40
30	L	306	BCR	C12-C13	2.60	1.51	1.46
25	6	603	CLA	MG-ND	-2.60	2.00	2.05
25	A	819	CLA	C1B-C2B	2.60	1.49	1.43
25	B	833	CLA	C1B-C2B	2.60	1.49	1.43
25	B	803	CLA	CMC-C2C	-2.60	1.45	1.50
29	V	316	Q6L	C02-C03	2.60	1.37	1.34
24	Q	308	CHL	C3D-CAD	-2.60	1.42	1.47
24	P	307	CHL	CMD-C2D	-2.60	1.46	1.51
25	A	842	CLA	CMB-C2B	-2.60	1.45	1.50
24	W	306	CHL	CMB-C2B	-2.60	1.46	1.51
24	Q	308	CHL	CAC-C3C	-2.60	1.47	1.51
29	V	316	Q6L	C12-C13	-2.60	1.45	1.51
25	T	310	CLA	CMD-C2D	-2.60	1.45	1.50
24	2	607	CHL	CHC-C4B	-2.60	1.35	1.39
24	W	304	CHL	CMB-C2B	-2.60	1.46	1.51
29	W	316	Q6L	C34-C33	2.60	1.54	1.50
24	P	307	CHL	CMB-C2B	-2.60	1.46	1.51
38	S	308	KC2	C4B-NB	2.60	1.41	1.37
38	S	308	KC2	C2A-C1A	2.60	1.52	1.44
25	U	302	CLA	CMD-C2D	-2.60	1.45	1.50
24	4	308	CHL	CAC-C3C	-2.60	1.47	1.51
25	Q	311	CLA	C1B-C2B	2.59	1.49	1.43
26	R	303	IWJ	C03-C02	2.59	1.36	1.33
25	S	313	CLA	C1B-C2B	2.59	1.49	1.43
25	A	837	CLA	C3B-C4B	2.59	1.50	1.42
25	X	310	CLA	CMD-C2D	-2.59	1.45	1.50
25	V	313	CLA	C1B-C2B	2.59	1.49	1.43
26	4	317	IWJ	C03-C02	2.59	1.36	1.33
25	L	301	CLA	C4B-NB	2.59	1.41	1.37
25	Q	301	CLA	CMB-C2B	-2.59	1.45	1.50
24	5	605	CHL	CMD-C2D	-2.59	1.46	1.51
25	A	812	CLA	C1B-C2B	2.59	1.49	1.43
29	U	314	Q6L	C34-C33	2.59	1.54	1.50
26	W	318	IWJ	C04-C03	2.59	1.54	1.50
25	B	825	CLA	C1B-NB	-2.59	1.34	1.37
25	J	102	CLA	CMC-C2C	-2.59	1.45	1.50
25	V	310	CLA	CHC-C4B	-2.59	1.33	1.39
25	V	311	CLA	C4B-NB	2.59	1.41	1.37
27	2	617	XAT	C22-C21	-2.59	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	807	CLA	C1B-C2B	2.59	1.49	1.43
25	L	303	CLA	CMB-C2B	-2.59	1.45	1.50
25	B	808	CLA	C3B-C4B	2.59	1.50	1.42
25	H	304	CLA	C1B-C2B	2.59	1.49	1.43
25	A	808	CLA	MG-NB	-2.58	2.00	2.05
29	X	301	Q6L	C34-C33	2.58	1.54	1.50
38	Q	310	KC2	C4B-NB	2.58	1.41	1.37
25	3	305	CLA	C1B-C2B	2.58	1.49	1.43
25	W	313	CLA	C4B-NB	2.58	1.41	1.37
25	A	824	CLA	C3B-C4B	2.58	1.50	1.42
25	B	814	CLA	C3B-C4B	2.58	1.50	1.42
24	2	615	CHL	CAC-C3C	-2.58	1.47	1.51
25	W	302	CLA	C4B-NB	2.58	1.41	1.37
25	B	824	CLA	C1B-C2B	2.58	1.49	1.43
25	4	311	CLA	CHC-C4B	-2.58	1.33	1.39
25	6	603	CLA	C4B-NB	2.58	1.41	1.37
25	6	613	CLA	C3B-C4B	2.58	1.50	1.42
38	S	308	KC2	CMD-C2D	-2.58	1.45	1.50
25	3	302	CLA	CMB-C2B	-2.58	1.45	1.50
29	Q	319	Q6L	C02-C03	2.58	1.37	1.34
26	V	320	IWJ	C03-C02	2.57	1.36	1.33
25	3	307	CLA	CMC-C2C	-2.57	1.45	1.50
25	B	807	CLA	C4B-NB	2.57	1.41	1.37
26	P	320	IWJ	O39-C29	-2.57	1.39	1.43
24	4	307	CHL	CMD-C2D	-2.57	1.46	1.51
24	R	309	CHL	C3D-CAD	-2.57	1.42	1.47
25	B	832	CLA	C4B-NB	2.57	1.41	1.37
25	S	301	CLA	C3B-C4B	2.57	1.50	1.42
25	A	820	CLA	CAB-C3B	-2.57	1.40	1.47
25	W	301	CLA	C1B-C2B	2.57	1.49	1.43
25	T	311	CLA	C1B-C2B	2.57	1.49	1.43
25	1	610	CLA	C1B-C2B	2.57	1.49	1.43
25	2	608	CLA	C1B-C2B	2.57	1.49	1.43
24	S	306	CHL	C1A-CHA	-2.57	1.37	1.40
25	X	304	CLA	C1B-NB	-2.57	1.34	1.37
25	A	822	CLA	C3B-C4B	2.57	1.50	1.42
29	S	316	Q6L	C34-C33	2.57	1.53	1.50
25	H	301	CLA	C4B-NB	2.57	1.41	1.37
24	T	306	CHL	CMB-C2B	-2.57	1.46	1.51
25	A	820	CLA	CMC-C2C	-2.57	1.45	1.50
29	R	304	Q6L	C12-C13	-2.57	1.46	1.51
25	5	603	CLA	C1B-C2B	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	309	CLA	C1B-C2B	2.57	1.49	1.43
26	V	318	IWJ	C03-C02	2.56	1.36	1.33
25	A	837	CLA	CMD-C2D	-2.56	1.45	1.50
38	X	309	KC2	CMB-C2B	-2.56	1.45	1.50
33	A	802	CL0	CAC-C3C	-2.56	1.47	1.51
24	P	307	CHL	CBD-CGD	-2.56	1.49	1.52
24	T	320	CHL	CMB-C2B	-2.56	1.46	1.51
25	4	304	CLA	C4B-C3B	2.56	1.49	1.43
25	S	311	CLA	C3B-C4B	2.56	1.50	1.42
25	B	817	CLA	C4B-NB	2.56	1.41	1.37
26	6	614	IWJ	C03-C02	2.56	1.36	1.33
25	B	824	CLA	C1B-NB	-2.56	1.34	1.37
25	V	310	CLA	C1B-C2B	2.56	1.49	1.43
25	B	831	CLA	C1B-C2B	2.56	1.49	1.43
24	V	306	CHL	CAC-C3C	-2.56	1.47	1.51
25	A	841	CLA	CMD-C2D	-2.56	1.45	1.50
30	J	103	BCR	C23-C22	2.56	1.51	1.46
25	B	813	CLA	CMD-C2D	-2.55	1.45	1.50
25	L	303	CLA	C1B-C2B	2.55	1.49	1.43
24	P	306	CHL	CMB-C2B	-2.55	1.46	1.51
27	3	316	XAT	C12-C13	2.55	1.51	1.46
25	4	303	CLA	C4B-NB	2.55	1.41	1.37
30	4	319	BCR	C16-C15	-2.55	1.29	1.36
24	X	305	CHL	CMB-C2B	-2.55	1.46	1.51
25	Q	304	CLA	CAA-C2A	-2.55	1.49	1.54
25	B	812	CLA	MG-NB	-2.55	2.00	2.05
25	B	808	CLA	C1B-C2B	2.55	1.49	1.43
29	S	315	Q6L	C02-C03	2.55	1.37	1.34
25	1	608	CLA	C4B-NB	2.55	1.41	1.37
29	V	315	Q6L	C11-C03	-2.55	1.47	1.51
24	P	304	CHL	CMD-C2D	-2.55	1.46	1.51
38	U	307	KC2	CMC-C2C	-2.55	1.45	1.50
24	1	601	CHL	CMD-C2D	-2.55	1.46	1.51
25	3	302	CLA	MG-ND	-2.55	2.00	2.05
29	2	616	Q6L	C12-C13	-2.55	1.46	1.51
25	S	311	CLA	C1B-C2B	2.55	1.49	1.43
29	2	616	Q6L	C34-C33	2.55	1.53	1.50
24	V	304	CHL	C1A-CHA	-2.55	1.37	1.40
25	W	311	CLA	C1B-C2B	2.55	1.49	1.43
30	3	319	BCR	C19-C18	2.54	1.51	1.46
30	3	319	BCR	C12-C13	2.54	1.51	1.46
29	R	301	Q6L	C33-C32	2.54	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	301	CLA	C1D-ND	2.54	1.41	1.37
25	5	608	CLA	C3B-C4B	2.54	1.50	1.42
25	6	613	CLA	C1B-C2B	2.54	1.49	1.43
29	R	320	Q6L	C02-C03	2.54	1.37	1.34
25	Q	313	CLA	C1B-C2B	2.54	1.49	1.43
25	T	301	CLA	CMC-C2C	-2.54	1.45	1.50
29	Q	318	Q6L	C12-C13	-2.54	1.46	1.51
25	A	810	CLA	C1B-C2B	2.54	1.49	1.43
25	B	807	CLA	CMB-C2B	-2.54	1.45	1.50
25	R	307	CLA	C1B-C2B	2.54	1.49	1.43
25	6	603	CLA	C1B-NB	-2.54	1.34	1.37
25	A	835	CLA	C1B-C2B	2.54	1.49	1.43
24	R	310	CHL	CBD-CGD	-2.54	1.49	1.52
25	B	814	CLA	C1B-C2B	2.54	1.49	1.43
25	A	811	CLA	C4B-NB	2.54	1.41	1.37
25	A	843	CLA	C1D-ND	2.54	1.41	1.37
25	A	822	CLA	C1B-C2B	2.53	1.49	1.43
38	S	308	KC2	CMB-C2B	-2.53	1.45	1.50
29	P	321	Q6L	C12-C13	-2.53	1.46	1.51
38	X	309	KC2	C3D-C4D	2.53	1.46	1.40
24	P	306	CHL	CBD-CGD	-2.53	1.49	1.52
29	X	317	Q6L	C34-C33	2.53	1.53	1.50
37	H	306	NEX	C38-C25	2.53	1.55	1.51
25	B	838	CLA	C1B-C2B	2.53	1.49	1.43
24	S	314	CHL	CMD-C2D	-2.53	1.46	1.51
25	L	302	CLA	CMC-C2C	-2.53	1.45	1.50
25	V	312	CLA	C4B-NB	2.53	1.41	1.37
30	3	319	BCR	C8-C9	2.53	1.51	1.46
25	R	317	CLA	CHC-C1C	2.53	1.43	1.38
25	A	845	CLA	CMC-C2C	-2.53	1.45	1.50
25	1	609	CLA	C1D-ND	2.53	1.41	1.37
25	S	309	CLA	C1B-C2B	2.53	1.49	1.43
27	3	316	XAT	O4-C5	-2.53	1.43	1.46
29	S	315	Q6L	C12-C13	-2.53	1.46	1.51
26	S	318	IWJ	C03-C02	2.53	1.36	1.33
25	W	312	CLA	C1D-ND	2.53	1.41	1.37
25	A	835	CLA	CMB-C2B	-2.53	1.45	1.50
25	A	805	CLA	C3B-C4B	2.52	1.50	1.42
25	6	612	CLA	C4B-NB	2.52	1.41	1.37
26	4	317	IWJ	C26-C24	-2.52	1.45	1.49
26	Q	320	IWJ	C03-C02	2.52	1.36	1.33
27	4	318	XAT	O4-C5	-2.52	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	310	CLA	C1B-C2B	2.52	1.49	1.43
25	2	603	CLA	C1B-C2B	2.52	1.49	1.43
25	3	314	CLA	CHC-C1C	2.52	1.43	1.38
38	U	307	KC2	CMB-C2B	-2.52	1.45	1.50
38	Q	310	KC2	CMC-C2C	-2.52	1.45	1.50
29	X	301	Q6L	C02-C03	2.52	1.37	1.34
24	S	304	CHL	C3B-C2B	-2.52	1.37	1.40
25	A	845	CLA	C3B-C4B	2.52	1.50	1.42
25	A	804	CLA	MG-NB	-2.52	2.00	2.05
29	S	321	Q6L	C02-C03	2.52	1.37	1.34
25	R	306	CLA	C1B-C2B	2.52	1.49	1.43
25	W	310	CLA	C1B-C2B	2.52	1.49	1.43
25	3	308	CLA	CHC-C4B	-2.52	1.33	1.39
38	T	308	KC2	MG-ND	-2.52	2.00	2.05
25	B	840	CLA	C1B-C2B	2.52	1.49	1.43
38	W	308	KC2	C1D-ND	2.52	1.41	1.37
25	B	839	CLA	CMB-C2B	-2.52	1.45	1.50
30	B	846	BCR	C8-C9	2.52	1.51	1.46
25	A	817	CLA	C1B-C2B	2.52	1.49	1.43
25	B	812	CLA	C1B-C2B	2.52	1.49	1.43
25	2	610	CLA	C3B-C4B	2.52	1.50	1.42
25	A	831	CLA	MG-ND	-2.52	2.00	2.05
30	L	307	BCR	C19-C18	2.52	1.51	1.46
25	B	826	CLA	CHC-C4B	-2.51	1.33	1.39
24	T	320	CHL	CMD-C2D	-2.51	1.46	1.51
25	A	806	CLA	C1B-C2B	2.51	1.49	1.43
25	X	311	CLA	C1B-C2B	2.51	1.49	1.43
38	V	308	KC2	O2A-CGA	2.51	1.36	1.30
25	B	843	CLA	C4B-NB	2.51	1.41	1.37
25	A	817	CLA	C3B-C4B	2.51	1.50	1.42
25	A	823	CLA	MG-NB	-2.51	2.00	2.05
25	2	606	CLA	CMB-C2B	-2.51	1.45	1.50
29	T	322	Q6L	C33-C32	2.51	1.36	1.33
25	6	608	CLA	C4B-NB	2.51	1.41	1.37
25	A	803	CLA	CMB-C2B	-2.51	1.45	1.50
24	R	309	CHL	OBD-CAD	-2.51	1.19	1.22
25	3	312	CLA	CMB-C2B	-2.51	1.45	1.50
30	3	318	BCR	C30-C25	-2.51	1.50	1.53
38	P	308	KC2	C2A-C1A	2.51	1.52	1.44
25	T	313	CLA	C1B-C2B	2.51	1.49	1.43
25	6	610	CLA	C4B-NB	2.51	1.41	1.37
25	T	309	CLA	CMD-C2D	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	303	CLA	CHC-C1C	2.51	1.43	1.38
25	B	810	CLA	C4B-NB	2.51	1.41	1.37
25	Q	314	CLA	C3B-C4B	2.50	1.50	1.42
25	6	608	CLA	C1B-C2B	2.50	1.49	1.43
25	B	809	CLA	CHC-C4B	-2.50	1.33	1.39
33	A	802	CL0	MG-ND	-2.50	2.00	2.05
38	Q	310	KC2	C1D-ND	2.50	1.41	1.37
29	T	319	Q6L	C02-C03	2.50	1.37	1.34
25	F	802	CLA	CMD-C2D	-2.50	1.45	1.50
25	R	317	CLA	C3B-C4B	2.50	1.50	1.42
25	6	607	CLA	C1B-NB	-2.50	1.34	1.37
24	T	304	CHL	CMD-C2D	-2.50	1.46	1.51
25	H	304	CLA	CMB-C2B	-2.50	1.45	1.50
24	R	311	CHL	CMC-C2C	2.50	1.50	1.44
25	V	310	CLA	C4B-NB	2.50	1.41	1.37
25	A	832	CLA	C3B-C4B	2.50	1.50	1.42
29	V	321	Q6L	C02-C03	2.50	1.37	1.34
25	1	608	CLA	C1B-C2B	2.49	1.49	1.43
25	1	603	CLA	C3B-C4B	2.49	1.50	1.42
25	U	309	CLA	C1B-C2B	2.49	1.49	1.43
29	W	319	Q6L	C34-C33	2.49	1.53	1.50
25	A	823	CLA	C1D-ND	2.49	1.41	1.37
25	V	312	CLA	CMB-C2B	-2.49	1.45	1.50
25	Q	314	CLA	C4B-NB	2.49	1.41	1.37
25	V	311	CLA	C1B-C2B	2.49	1.49	1.43
25	A	836	CLA	C3B-C4B	2.49	1.50	1.42
38	T	308	KC2	CMC-C2C	-2.49	1.45	1.50
27	5	612	XAT	O4-C5	-2.49	1.43	1.46
25	B	834	CLA	CMB-C2B	-2.49	1.45	1.50
24	Q	308	CHL	CMA-C3A	-2.49	1.49	1.53
25	R	314	CLA	C1B-C2B	2.49	1.49	1.43
25	2	602	CLA	CMB-C2B	-2.49	1.45	1.50
25	O	2001	CLA	C4B-NB	2.49	1.41	1.37
25	6	604	CLA	C1B-C2B	2.49	1.49	1.43
24	X	308	CHL	C1A-CHA	-2.49	1.37	1.40
30	F	801	BCR	C37-C22	2.49	1.55	1.50
25	3	305	CLA	C4B-C3B	2.49	1.49	1.43
38	P	308	KC2	CMC-C2C	-2.49	1.45	1.50
25	B	807	CLA	C3B-C4B	2.49	1.50	1.42
25	U	301	CLA	CMC-C2C	-2.48	1.45	1.50
25	2	603	CLA	C4B-NB	2.48	1.41	1.37
25	6	607	CLA	C1D-ND	2.48	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	319	Q6L	C33-C32	2.48	1.36	1.33
25	A	813	CLA	CHC-C4B	-2.48	1.33	1.39
25	V	301	CLA	CMB-C2B	-2.48	1.45	1.50
24	T	314	CHL	CMB-C2B	-2.48	1.46	1.51
29	P	315	Q6L	C02-C03	2.48	1.37	1.34
25	A	836	CLA	CHC-C4B	-2.48	1.33	1.39
25	A	809	CLA	C1B-C2B	2.48	1.49	1.43
29	Q	319	Q6L	C12-C13	-2.48	1.46	1.51
26	X	318	IWJ	C03-C02	2.48	1.36	1.33
29	R	301	Q6L	C34-C33	2.48	1.53	1.50
29	V	315	Q6L	C34-C33	2.48	1.53	1.50
25	V	301	CLA	C1B-C2B	2.48	1.49	1.43
30	J	103	BCR	C19-C18	2.48	1.51	1.46
25	B	802	CLA	C1B-C2B	2.48	1.49	1.43
25	A	820	CLA	CHC-C1C	2.48	1.43	1.38
29	O	2006	Q6L	C12-C13	-2.48	1.46	1.51
25	A	856	CLA	C4B-NB	2.48	1.41	1.37
38	T	308	KC2	CMB-C2B	-2.48	1.45	1.50
38	Q	310	KC2	C1B-C2B	2.48	1.50	1.45
25	B	836	CLA	CMB-C2B	-2.48	1.45	1.50
25	1	607	CLA	C3D-C4D	2.48	1.48	1.42
26	3	315	IWJ	C03-C02	2.48	1.36	1.33
38	T	308	KC2	C3D-C4D	2.48	1.46	1.40
38	Q	310	KC2	O2A-CGA	2.48	1.36	1.30
25	3	302	CLA	C3B-C4B	2.47	1.49	1.42
25	B	822	CLA	CMD-C2D	-2.47	1.45	1.50
24	W	307	CHL	CMB-C2B	-2.47	1.46	1.51
25	A	818	CLA	CMB-C2B	-2.47	1.45	1.50
25	B	809	CLA	CMD-C2D	-2.47	1.45	1.50
38	S	308	KC2	CMC-C2C	-2.47	1.45	1.50
24	Q	307	CHL	CMD-C2D	-2.47	1.46	1.51
24	V	306	CHL	CMB-C2B	-2.47	1.46	1.51
25	4	305	CLA	C4B-C3B	2.47	1.48	1.43
25	N	202	CLA	C3B-C4B	2.47	1.49	1.42
25	B	828	CLA	CMB-C2B	-2.47	1.45	1.50
25	3	303	CLA	C4B-C3B	2.47	1.48	1.43
24	U	313	CHL	C1A-CHA	-2.47	1.37	1.40
24	V	305	CHL	C1A-CHA	-2.47	1.37	1.40
25	1	610	CLA	C4B-C3B	2.47	1.48	1.43
25	B	836	CLA	C4B-NB	2.47	1.41	1.37
25	Q	311	CLA	C3B-C4B	2.47	1.49	1.42
25	P	301	CLA	C1B-C2B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	802	CLA	C3B-C4B	2.47	1.49	1.42
25	5	604	CLA	CMB-C2B	-2.47	1.45	1.50
25	B	815	CLA	C4B-NB	2.47	1.41	1.37
25	B	809	CLA	CMB-C2B	-2.47	1.45	1.50
25	B	839	CLA	CHC-C1C	2.47	1.43	1.38
25	V	309	CLA	C1A-CHA	-2.47	1.32	1.43
24	4	306	CHL	CMD-C2D	-2.47	1.46	1.51
29	V	316	Q6L	C33-C32	2.47	1.36	1.33
25	1	613	CLA	C3B-C4B	2.47	1.49	1.42
25	B	843	CLA	C1D-ND	2.47	1.41	1.37
29	V	315	Q6L	C01-C02	2.46	1.54	1.50
25	V	310	CLA	CMB-C2B	-2.46	1.45	1.50
38	P	308	KC2	CMB-C2B	-2.46	1.45	1.50
24	W	304	CHL	CAC-C3C	-2.46	1.47	1.51
24	X	306	CHL	MG-NB	-2.46	2.00	2.05
29	X	316	Q6L	C12-C13	-2.46	1.46	1.51
30	A	851	BCR	C8-C9	2.46	1.51	1.46
25	1	603	CLA	C1B-NB	-2.46	1.34	1.37
25	V	312	CLA	C1B-C2B	2.46	1.48	1.43
29	R	304	Q6L	C33-C32	2.46	1.36	1.33
25	3	305	CLA	CMD-C2D	-2.46	1.45	1.50
24	Q	307	CHL	CHC-C4B	-2.46	1.35	1.39
24	6	606	CHL	C1A-CHA	-2.46	1.37	1.40
24	2	601	CHL	CMA-C3A	-2.46	1.49	1.53
25	B	826	CLA	MG-NB	-2.46	2.00	2.05
25	A	829	CLA	CMD-C2D	-2.46	1.45	1.50
25	F	803	CLA	CMB-C2B	-2.46	1.45	1.50
24	R	308	CHL	CMD-C2D	-2.46	1.46	1.51
25	5	609	CLA	CHC-C1C	2.46	1.43	1.38
24	U	304	CHL	CMB-C2B	-2.46	1.46	1.51
25	A	828	CLA	CMD-C2D	-2.46	1.45	1.50
25	A	804	CLA	MG-ND	-2.46	2.00	2.05
25	T	312	CLA	CMD-C2D	-2.46	1.45	1.50
29	W	319	Q6L	C01-C02	2.46	1.54	1.50
25	B	808	CLA	CMD-C2D	-2.45	1.45	1.50
25	6	612	CLA	CMD-C2D	-2.45	1.45	1.50
25	2	602	CLA	C2-C3	2.45	1.38	1.33
25	6	607	CLA	C3B-C4B	2.45	1.49	1.42
25	A	818	CLA	C1B-C2B	2.45	1.48	1.43
30	4	319	BCR	C19-C18	2.45	1.51	1.46
25	S	303	CLA	CMB-C2B	-2.45	1.45	1.50
25	A	831	CLA	C4B-NB	2.45	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	612	CLA	C1B-C2B	2.45	1.48	1.43
24	W	304	CHL	CHC-C1C	2.45	1.44	1.39
25	A	816	CLA	C1B-C2B	2.45	1.48	1.43
25	1	607	CLA	C3B-C4B	2.45	1.49	1.42
30	K	207	BCR	C19-C18	2.45	1.51	1.46
25	S	312	CLA	CMC-C2C	-2.45	1.45	1.50
24	R	309	CHL	CMD-C2D	-2.45	1.46	1.51
30	A	851	BCR	C16-C15	-2.45	1.29	1.36
25	N	203	CLA	C4B-NB	2.45	1.41	1.37
38	W	308	KC2	C3D-C4D	2.45	1.46	1.40
24	R	311	CHL	MG-NB	-2.45	2.00	2.05
25	B	818	CLA	C4B-NB	2.45	1.41	1.37
25	R	315	CLA	C3B-C4B	2.45	1.49	1.42
25	A	843	CLA	C3B-C4B	2.45	1.49	1.42
25	B	816	CLA	C1B-C2B	2.45	1.48	1.43
30	M	101	BCR	C1-C6	-2.45	1.50	1.53
29	P	319	Q6L	C01-C02	2.45	1.54	1.50
25	A	812	CLA	CAA-C2A	-2.44	1.49	1.54
25	5	608	CLA	C1B-C2B	2.44	1.48	1.43
25	J	102	CLA	MG-NB	-2.44	2.00	2.05
25	V	301	CLA	C3B-C4B	2.44	1.49	1.42
29	W	319	Q6L	C02-C03	2.44	1.37	1.34
29	W	315	Q6L	C34-C33	2.44	1.53	1.50
25	B	806	CLA	MG-NB	-2.44	2.00	2.05
30	B	845	BCR	C30-C25	-2.44	1.50	1.53
25	B	824	CLA	CMD-C2D	-2.44	1.45	1.50
25	3	302	CLA	MG-NB	-2.44	2.00	2.05
24	W	307	CHL	CBD-CGD	-2.44	1.49	1.52
25	A	828	CLA	MG-NB	-2.44	2.01	2.05
25	J	102	CLA	C1B-C2B	2.44	1.48	1.43
24	4	302	CHL	CHC-C4B	-2.44	1.35	1.39
25	5	604	CLA	C4B-C3B	2.44	1.48	1.43
24	6	606	CHL	CMD-C2D	-2.44	1.46	1.51
25	X	312	CLA	C1B-C2B	2.44	1.48	1.43
38	T	308	KC2	CMD-C2D	-2.44	1.45	1.50
24	U	304	CHL	C1A-CHA	-2.44	1.37	1.40
25	P	303	CLA	C1B-C2B	2.44	1.48	1.43
25	A	803	CLA	C3B-C4B	2.44	1.49	1.42
30	J	103	BCR	C12-C13	2.43	1.51	1.46
25	B	830	CLA	C1D-ND	2.43	1.41	1.37
25	B	842	CLA	CHC-C4B	-2.43	1.34	1.39
24	4	302	CHL	CAC-C3C	-2.43	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	302	CLA	C3B-C4B	2.43	1.49	1.42
25	W	311	CLA	C4B-NB	2.43	1.41	1.37
38	U	307	KC2	O2A-CGA	2.43	1.36	1.30
25	3	302	CLA	C1B-C2B	2.43	1.48	1.43
25	U	301	CLA	CHC-C1C	2.43	1.43	1.38
25	W	303	CLA	O2D-CED	-2.43	1.39	1.45
25	X	313	CLA	C1B-C2B	2.43	1.48	1.43
25	4	303	CLA	CMD-C2D	-2.43	1.45	1.50
25	O	2002	CLA	CMD-C2D	-2.43	1.45	1.50
29	R	319	Q6L	C34-C33	2.43	1.53	1.50
24	P	305	CHL	C1A-CHA	-2.43	1.37	1.40
25	B	816	CLA	CHC-C1C	2.43	1.43	1.38
24	X	308	CHL	CAC-C3C	-2.43	1.47	1.51
29	R	319	Q6L	C01-C02	2.43	1.54	1.50
25	1	609	CLA	C4B-C3B	2.43	1.48	1.43
25	1	606	CLA	C4B-C3B	2.43	1.48	1.43
25	Q	301	CLA	C1B-NB	-2.43	1.34	1.37
29	S	316	Q6L	C12-C13	-2.43	1.46	1.51
25	B	804	CLA	C1B-C2B	2.43	1.48	1.43
25	B	817	CLA	C1B-C2B	2.43	1.48	1.43
25	B	803	CLA	MG-NB	-2.42	2.01	2.05
25	T	303	CLA	CMB-C2B	-2.42	1.45	1.50
30	G	205	BCR	C8-C9	2.42	1.51	1.46
30	A	852	BCR	C8-C9	2.42	1.51	1.46
25	B	833	CLA	C4B-NB	2.42	1.41	1.37
25	B	826	CLA	CMD-C2D	-2.42	1.45	1.50
25	A	834	CLA	C3B-C4B	2.42	1.49	1.42
25	A	810	CLA	C4B-NB	2.42	1.41	1.37
38	R	312	KC2	C1D-ND	2.42	1.41	1.37
25	B	830	CLA	CMB-C2B	-2.42	1.45	1.50
25	X	313	CLA	CMB-C2B	-2.42	1.45	1.50
29	P	316	Q6L	C33-C32	2.42	1.36	1.33
25	V	302	CLA	C1B-C2B	2.42	1.48	1.43
25	B	840	CLA	CMB-C2B	-2.42	1.45	1.50
29	U	317	Q6L	C34-C33	2.42	1.53	1.50
25	1	603	CLA	CMB-C2B	-2.42	1.45	1.50
25	6	610	CLA	C1B-C2B	2.42	1.48	1.43
25	F	803	CLA	C4B-NB	2.42	1.41	1.37
25	A	808	CLA	CMD-C2D	-2.42	1.45	1.50
24	S	304	CHL	MG-ND	-2.42	2.01	2.05
38	U	307	KC2	CMD-C2D	-2.42	1.45	1.50
24	P	304	CHL	CHB-C4A	-2.42	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	320	CHL	CBD-CGD	-2.42	1.49	1.52
29	R	323	Q6L	C01-C02	2.42	1.54	1.50
25	4	313	CLA	C3B-C4B	2.42	1.49	1.42
24	1	601	CHL	CMA-C3A	-2.42	1.49	1.53
38	V	308	KC2	CAA-C2A	2.41	1.53	1.46
29	Q	317	Q6L	C02-C03	2.41	1.37	1.34
24	T	306	CHL	C1A-CHA	-2.41	1.37	1.40
25	B	818	CLA	CHC-C1C	2.41	1.43	1.38
25	B	803	CLA	C1B-C2B	2.41	1.48	1.43
25	A	831	CLA	C3B-C4B	2.41	1.49	1.42
25	T	309	CLA	C3B-C4B	2.41	1.49	1.42
25	B	834	CLA	C1D-ND	2.41	1.41	1.37
24	W	306	CHL	CBD-CGD	-2.41	1.49	1.52
29	U	315	Q6L	C12-C13	-2.41	1.46	1.51
25	P	309	CLA	C3B-C4B	2.41	1.49	1.42
25	A	833	CLA	C4B-NB	2.41	1.41	1.37
24	6	605	CHL	CMB-C2B	-2.41	1.46	1.51
38	X	309	KC2	C4B-NB	2.41	1.41	1.37
24	U	304	CHL	C3B-C2B	-2.41	1.37	1.40
25	B	839	CLA	CMD-C2D	-2.41	1.45	1.50
27	3	316	XAT	C35-C15	-2.41	1.29	1.36
30	K	202	BCR	C36-C18	2.41	1.55	1.50
25	A	822	CLA	CMD-C2D	-2.41	1.45	1.50
29	P	321	Q6L	C01-C02	2.41	1.54	1.50
29	R	304	Q6L	C01-C02	2.41	1.54	1.50
25	B	829	CLA	MG-ND	-2.41	2.01	2.05
25	B	802	CLA	C1D-ND	2.40	1.41	1.37
38	T	308	KC2	C4B-NB	2.40	1.41	1.37
38	U	307	KC2	C4B-NB	2.40	1.41	1.37
25	2	606	CLA	C1B-C2B	2.40	1.48	1.43
25	N	203	CLA	MG-NB	-2.40	2.01	2.05
29	P	315	Q6L	C01-C02	2.40	1.54	1.50
25	B	839	CLA	C3B-C4B	2.40	1.49	1.42
24	V	305	CHL	CMB-C2B	-2.40	1.46	1.51
24	R	302	CHL	CHC-C4B	-2.40	1.35	1.39
25	L	302	CLA	C4B-NB	2.40	1.41	1.37
25	F	802	CLA	C1B-C2B	2.40	1.48	1.43
24	2	601	CHL	CBD-CGD	-2.40	1.49	1.52
24	5	605	CHL	C2C-C3C	2.40	1.38	1.36
25	R	316	CLA	C3B-C4B	2.40	1.49	1.42
25	T	301	CLA	CMD-C2D	-2.40	1.45	1.50
25	5	601	CLA	C4B-NB	2.40	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	304	CHL	CHC-C1C	2.40	1.43	1.39
25	B	815	CLA	CMD-C2D	-2.40	1.45	1.50
25	X	311	CLA	C4B-NB	2.40	1.41	1.37
29	U	315	Q6L	C33-C32	2.40	1.36	1.33
27	2	617	XAT	O24-C25	-2.40	1.43	1.46
25	A	821	CLA	C3B-C4B	2.40	1.49	1.42
25	U	310	CLA	C3B-C4B	2.40	1.49	1.42
25	B	803	CLA	C4B-NB	2.40	1.41	1.37
38	U	307	KC2	C3D-C4D	2.40	1.46	1.40
29	W	316	Q6L	C33-C32	2.40	1.36	1.33
29	V	321	Q6L	C34-C33	2.40	1.53	1.50
24	W	306	CHL	C2C-C3C	2.39	1.38	1.36
25	2	604	CLA	C1B-C2B	2.39	1.48	1.43
25	S	309	CLA	C3B-C4B	2.39	1.49	1.42
25	A	821	CLA	C1B-C2B	2.39	1.48	1.43
30	M	101	BCR	C8-C9	2.39	1.51	1.46
29	X	301	Q6L	C01-C02	2.39	1.54	1.50
38	P	308	KC2	O2A-CGA	2.39	1.36	1.30
25	4	311	CLA	MG-NB	-2.39	2.01	2.05
25	X	310	CLA	C1B-C2B	2.39	1.48	1.43
30	J	101	BCR	C40-C30	-2.39	1.49	1.53
25	A	842	CLA	C5-C3	-2.39	1.46	1.51
25	2	614	CLA	C1B-C2B	2.39	1.48	1.43
25	T	301	CLA	C1B-C2B	2.39	1.48	1.43
38	R	312	KC2	CMB-C2B	-2.39	1.45	1.50
24	W	305	CHL	CMB-C2B	-2.39	1.46	1.51
25	2	604	CLA	CMB-C2B	-2.39	1.45	1.50
25	Q	315	CLA	C3B-C4B	2.39	1.49	1.42
29	U	317	Q6L	C12-C13	-2.39	1.46	1.51
24	S	307	CHL	CBD-CGD	-2.39	1.49	1.52
38	X	309	KC2	O2A-CGA	2.39	1.36	1.30
25	B	806	CLA	CAB-C3B	-2.39	1.41	1.47
25	B	811	CLA	C1B-C2B	2.39	1.48	1.43
25	B	802	CLA	CMB-C2B	-2.39	1.45	1.50
25	A	836	CLA	C4B-NB	2.38	1.41	1.37
25	B	819	CLA	C4B-NB	2.38	1.41	1.37
25	Q	306	CLA	MG-NB	-2.38	2.01	2.05
25	B	831	CLA	CMB-C2B	-2.38	1.45	1.50
25	W	309	CLA	C1B-C2B	2.38	1.48	1.43
30	A	849	BCR	C12-C13	2.38	1.51	1.46
29	X	317	Q6L	C12-C13	-2.38	1.46	1.51
25	4	312	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	837	CLA	C1B-C2B	2.38	1.48	1.43
25	A	833	CLA	CMD-C2D	-2.38	1.45	1.50
25	B	816	CLA	C3B-C4B	2.38	1.49	1.42
38	R	312	KC2	CMD-C2D	-2.38	1.45	1.50
29	Q	317	Q6L	C34-C33	2.38	1.53	1.50
25	5	609	CLA	C3B-C4B	2.38	1.49	1.42
25	Q	311	CLA	C4B-NB	2.38	1.41	1.37
25	S	310	CLA	MG-NA	2.38	2.11	2.06
38	S	308	KC2	O2A-CGA	2.38	1.36	1.30
38	S	308	KC2	C3D-C4D	2.38	1.46	1.40
25	6	608	CLA	C3B-C4B	2.38	1.49	1.42
38	W	308	KC2	O2A-CGA	2.38	1.36	1.30
25	V	302	CLA	CMB-C2B	-2.38	1.45	1.50
25	S	302	CLA	CMC-C2C	-2.38	1.45	1.50
37	R	321	NEX	C28-C29	2.38	1.51	1.46
25	B	813	CLA	C4B-NB	2.38	1.41	1.37
25	A	841	CLA	CMB-C2B	-2.38	1.45	1.50
29	V	316	Q6L	C29-C27	2.38	1.51	1.46
34	B	844	PQN	C10-C1	-2.38	1.43	1.48
25	H	304	CLA	C4B-NB	2.37	1.41	1.37
25	3	309	CLA	C3B-C4B	2.37	1.49	1.42
25	P	311	CLA	C3B-C4B	2.37	1.49	1.42
29	P	316	Q6L	C04-C03	2.37	1.56	1.53
25	A	808	CLA	MG-ND	-2.37	2.01	2.05
25	U	311	CLA	C3B-C4B	2.37	1.49	1.42
25	1	605	CLA	CMD-C2D	-2.37	1.45	1.50
25	3	303	CLA	CMB-C2B	-2.37	1.45	1.50
24	U	306	CHL	C3B-C2B	-2.37	1.37	1.40
25	B	822	CLA	MG-NB	-2.37	2.01	2.05
25	B	832	CLA	MG-ND	-2.37	2.01	2.05
25	A	841	CLA	C3B-C4B	2.37	1.49	1.42
24	P	305	CHL	CAC-C3C	-2.37	1.47	1.51
25	L	302	CLA	C1D-ND	2.37	1.41	1.37
25	B	823	CLA	MG-NC	2.37	2.11	2.06
24	2	607	CHL	CHD-C1D	-2.37	1.35	1.39
24	4	302	CHL	CMB-C2B	-2.37	1.46	1.51
25	B	840	CLA	MG-NB	-2.37	2.01	2.05
25	B	815	CLA	CMC-C2C	-2.37	1.45	1.50
38	R	312	KC2	MG-NB	-2.37	2.01	2.05
38	Q	310	KC2	CMD-C2D	-2.37	1.45	1.50
24	V	306	CHL	CBD-CGD	-2.37	1.49	1.52
25	B	803	CLA	C1D-ND	2.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	818	CLA	C1B-C2B	2.36	1.48	1.43
24	Q	316	CHL	C1A-CHA	-2.36	1.37	1.40
34	A	844	PQN	C6-C5	2.36	1.43	1.39
29	V	319	Q6L	C01-C02	2.36	1.54	1.50
37	S	317	NEX	O24-C25	-2.36	1.43	1.46
25	B	831	CLA	CMC-C2C	-2.36	1.45	1.50
25	P	303	CLA	C3B-C4B	2.36	1.49	1.42
25	1	610	CLA	CMB-C2B	-2.36	1.45	1.50
24	R	302	CHL	CMB-C2B	-2.36	1.46	1.51
24	T	306	CHL	CHC-C4B	-2.36	1.35	1.39
29	T	316	Q6L	C33-C32	2.36	1.36	1.33
30	B	848	BCR	C16-C15	-2.36	1.29	1.36
24	X	305	CHL	CMD-C2D	-2.36	1.46	1.51
25	2	603	CLA	MG-NB	-2.36	2.01	2.05
25	3	307	CLA	C4B-NB	2.36	1.41	1.37
25	B	833	CLA	C3B-C4B	2.36	1.49	1.42
24	R	308	CHL	CBD-CGD	-2.36	1.49	1.52
25	B	811	CLA	CAC-C3C	-2.36	1.45	1.51
24	R	311	CHL	CBD-CGD	-2.35	1.49	1.52
25	B	822	CLA	C1D-ND	2.35	1.41	1.37
25	W	302	CLA	C1B-C2B	2.35	1.48	1.43
24	2	607	CHL	CMD-C2D	-2.35	1.46	1.51
24	U	313	CHL	CMB-C2B	-2.35	1.46	1.51
25	A	810	CLA	CMB-C2B	-2.35	1.45	1.50
25	F	802	CLA	MG-NB	-2.35	2.01	2.05
25	B	840	CLA	CMD-C2D	-2.35	1.45	1.50
29	T	315	Q6L	C02-C03	2.35	1.37	1.34
25	B	818	CLA	C3B-C4B	2.35	1.49	1.42
25	A	807	CLA	CMD-C2D	-2.35	1.46	1.50
25	B	806	CLA	C4B-NB	2.35	1.40	1.37
37	W	317	NEX	O24-C25	-2.35	1.43	1.46
25	B	841	CLA	CMC-C2C	-2.35	1.46	1.50
31	B	801	LMG	O1-C1	2.35	1.44	1.40
25	V	303	CLA	C1D-ND	2.35	1.40	1.37
24	W	305	CHL	CBD-CGD	-2.35	1.49	1.52
24	Q	316	CHL	CMD-C2D	-2.35	1.46	1.51
29	S	320	Q6L	C01-C02	2.35	1.54	1.50
29	X	316	Q6L	C01-C02	2.35	1.54	1.50
25	4	303	CLA	MG-ND	-2.35	2.01	2.05
29	O	2007	Q6L	C12-C13	-2.35	1.46	1.51
25	B	807	CLA	C1B-NB	-2.35	1.34	1.37
25	2	609	CLA	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	313	CLA	CMB-C2B	-2.34	1.46	1.50
27	4	318	XAT	C8-C9	2.34	1.51	1.46
25	A	817	CLA	CMB-C2B	-2.34	1.46	1.50
25	3	301	CLA	C4B-NB	2.34	1.40	1.37
24	S	304	CHL	CHC-C4B	-2.34	1.35	1.39
24	T	305	CHL	C3D-CAD	-2.34	1.43	1.47
29	T	319	Q6L	C12-C13	-2.34	1.46	1.51
25	3	313	CLA	C1B-C2B	2.34	1.48	1.43
25	B	824	CLA	CHC-C4B	-2.34	1.34	1.39
25	R	306	CLA	C4B-NB	2.34	1.40	1.37
25	B	826	CLA	C1B-C2B	2.34	1.48	1.43
24	2	601	CHL	CAC-C3C	-2.34	1.47	1.51
33	A	802	CL0	C3B-C2B	-2.34	1.37	1.40
38	R	312	KC2	O2A-CGA	2.34	1.36	1.30
29	S	321	Q6L	C29-C27	2.33	1.50	1.46
30	B	848	BCR	C19-C18	2.33	1.50	1.46
38	W	308	KC2	CMB-C2B	-2.33	1.46	1.50
24	X	306	CHL	C3D-CAD	-2.33	1.43	1.47
25	B	820	CLA	MG-NB	-2.33	2.01	2.05
37	T	317	NEX	O24-C25	-2.33	1.43	1.46
25	1	607	CLA	C1B-C2B	2.33	1.48	1.43
24	2	607	CHL	OMC-CMC	-2.33	1.16	1.22
25	P	302	CLA	C1B-C2B	2.33	1.48	1.43
24	2	601	CHL	MG-NB	-2.33	2.01	2.05
29	P	319	Q6L	C34-C33	2.33	1.53	1.50
24	W	314	CHL	CMB-C2B	-2.33	1.47	1.51
30	3	319	BCR	C1-C6	-2.33	1.50	1.53
29	T	319	Q6L	C33-C32	2.33	1.35	1.33
25	Q	313	CLA	CMD-C2D	-2.33	1.46	1.50
24	R	310	CHL	CMB-C2B	-2.33	1.47	1.51
34	A	844	PQN	C9-C10	2.33	1.43	1.39
25	A	845	CLA	CMD-C2D	-2.33	1.46	1.50
24	V	304	CHL	CMB-C2B	-2.33	1.47	1.51
30	K	202	BCR	C12-C13	2.33	1.50	1.46
25	A	803	CLA	MG-NB	-2.33	2.01	2.05
25	4	309	CLA	C1B-C2B	2.33	1.48	1.43
25	R	307	CLA	C3B-C4B	2.33	1.49	1.42
37	R	321	NEX	C32-C33	2.33	1.50	1.46
25	P	301	CLA	CHC-C1C	2.33	1.43	1.38
29	O	2006	Q6L	C01-C02	2.32	1.54	1.50
25	A	838	CLA	CMD-C2D	-2.32	1.46	1.50
25	3	304	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	303	CLA	CHC-C1C	2.32	1.43	1.38
25	A	856	CLA	CMB-C2B	-2.32	1.46	1.50
25	B	838	CLA	C4B-NB	2.32	1.40	1.37
37	S	317	NEX	C35-C15	-2.32	1.29	1.36
25	A	830	CLA	C1B-C2B	2.32	1.48	1.43
24	S	305	CHL	CMB-C2B	-2.32	1.47	1.51
25	B	820	CLA	CMD-C2D	-2.32	1.46	1.50
25	X	314	CLA	CMB-C2B	-2.32	1.46	1.50
24	S	304	CHL	CAC-C3C	-2.32	1.47	1.51
25	X	302	CLA	C1B-C2B	2.32	1.48	1.43
25	V	301	CLA	C4B-NB	2.32	1.40	1.37
29	W	316	Q6L	C01-C02	2.32	1.54	1.50
25	B	808	CLA	MG-ND	-2.32	2.01	2.05
25	4	314	CLA	CMB-C2B	-2.32	1.46	1.50
25	T	313	CLA	CMD-C2D	-2.32	1.46	1.50
25	S	313	CLA	CHC-C1C	2.32	1.43	1.38
25	P	312	CLA	C3B-C4B	2.32	1.49	1.42
25	X	304	CLA	C3B-C4B	2.32	1.49	1.42
25	A	809	CLA	C4B-NB	2.32	1.40	1.37
25	A	831	CLA	C1B-NB	-2.32	1.34	1.37
24	6	601	CHL	CBD-CGD	-2.32	1.49	1.52
25	R	315	CLA	CHC-C1C	2.32	1.43	1.38
25	B	825	CLA	MG-NB	-2.32	2.01	2.05
24	P	314	CHL	CMB-C2B	-2.32	1.47	1.51
24	V	307	CHL	CMD-C2D	-2.32	1.47	1.51
25	B	843	CLA	CHC-C1C	2.32	1.43	1.38
25	V	309	CLA	C1C-C2C	2.32	1.49	1.44
25	A	839	CLA	C1B-C2B	2.32	1.48	1.43
25	1	608	CLA	MG-NB	-2.32	2.01	2.05
25	3	310	CLA	C3B-C4B	2.32	1.49	1.42
25	A	813	CLA	C4B-NB	2.32	1.40	1.37
29	P	316	Q6L	C01-C02	2.32	1.54	1.50
30	B	846	BCR	C23-C22	2.32	1.50	1.46
25	T	301	CLA	CHC-C1C	2.32	1.43	1.38
30	F	801	BCR	C8-C9	2.31	1.50	1.46
25	B	834	CLA	CMD-C2D	-2.31	1.46	1.50
25	B	832	CLA	CAB-C3B	-2.31	1.41	1.47
25	G	203	CLA	CHC-C4B	-2.31	1.34	1.39
25	A	804	CLA	C3B-C4B	2.31	1.49	1.42
25	F	803	CLA	CAC-C3C	-2.31	1.45	1.51
25	6	612	CLA	MG-NB	-2.31	2.01	2.05
25	X	311	CLA	CMB-C2B	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	310	CLA	C1B-C2B	2.31	1.48	1.43
24	3	306	CHL	MG-NB	-2.31	2.01	2.05
30	A	848	BCR	C23-C22	2.31	1.50	1.46
25	B	833	CLA	CMB-C2B	-2.31	1.46	1.50
29	P	319	Q6L	C12-C13	-2.31	1.46	1.51
37	R	321	NEX	C12-C13	2.31	1.50	1.46
25	5	610	CLA	C3B-C4B	2.31	1.49	1.42
29	T	315	Q6L	C33-C32	2.31	1.35	1.33
25	W	301	CLA	CMC-C2C	-2.31	1.46	1.50
25	6	608	CLA	CMA-C3A	-2.31	1.48	1.53
24	U	306	CHL	CMB-C2B	-2.31	1.47	1.51
25	3	311	CLA	C3B-C4B	2.31	1.49	1.42
25	4	304	CLA	CMB-C2B	-2.31	1.46	1.50
25	U	302	CLA	CMC-C2C	-2.31	1.46	1.50
25	2	613	CLA	C3B-C4B	2.31	1.49	1.42
24	R	309	CHL	CAC-C3C	-2.30	1.47	1.51
24	U	305	CHL	CMB-C2B	-2.30	1.47	1.51
25	X	302	CLA	MG-NB	-2.30	2.01	2.05
25	W	303	CLA	C4B-NB	2.30	1.40	1.37
38	T	308	KC2	O2A-CGA	2.30	1.36	1.30
25	B	821	CLA	MG-NB	-2.30	2.01	2.05
25	V	309	CLA	CMD-C2D	-2.30	1.46	1.50
25	A	833	CLA	CAB-C3B	-2.30	1.41	1.47
24	S	304	CHL	CHD-C1D	-2.30	1.35	1.39
30	K	205	BCR	C19-C18	2.30	1.50	1.46
25	B	830	CLA	CAB-C3B	-2.30	1.41	1.47
29	U	314	Q6L	C01-C02	2.30	1.54	1.50
24	4	307	CHL	CHB-C4A	-2.30	1.35	1.38
25	Q	301	CLA	C4B-NB	2.30	1.40	1.37
24	Q	309	CHL	CBD-CGD	-2.30	1.49	1.52
25	B	811	CLA	MG-NB	-2.30	2.01	2.05
25	W	303	CLA	C3B-C4B	2.30	1.49	1.42
37	P	317	NEX	C28-C29	2.30	1.50	1.46
25	B	832	CLA	CMD-C2D	-2.30	1.46	1.50
24	4	308	CHL	CMB-C2B	-2.30	1.47	1.51
38	X	309	KC2	C1B-NB	-2.30	1.34	1.37
25	B	822	CLA	CMB-C2B	-2.30	1.46	1.50
25	2	611	CLA	C3B-C4B	2.30	1.49	1.42
25	S	302	CLA	CMB-C2B	-2.30	1.46	1.50
25	A	835	CLA	MG-NB	-2.30	2.01	2.05
29	T	322	Q6L	C01-C02	2.30	1.54	1.50
24	V	314	CHL	CMB-C2B	-2.30	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	310	CLA	CMD-C2D	-2.30	1.46	1.50
25	S	302	CLA	C1B-C2B	2.30	1.48	1.43
25	A	838	CLA	MG-NB	-2.30	2.01	2.05
25	A	804	CLA	CMB-C2B	-2.30	1.46	1.50
25	B	824	CLA	CMC-C2C	-2.30	1.46	1.50
25	U	308	CLA	C1B-C2B	2.30	1.48	1.43
24	T	306	CHL	CAC-C3C	-2.30	1.47	1.51
25	H	302	CLA	CMB-C2B	-2.30	1.46	1.50
25	B	814	CLA	CMD-C2D	-2.30	1.46	1.50
25	6	607	CLA	MG-NB	-2.30	2.01	2.05
24	S	304	CHL	CBD-CGD	-2.30	1.49	1.52
26	3	315	IWJ	C28-C26	2.29	1.53	1.51
38	P	308	KC2	CMD-C2D	-2.29	1.46	1.50
25	2	612	CLA	CMC-C2C	-2.29	1.46	1.50
24	1	601	CHL	CAC-C3C	-2.29	1.47	1.51
29	W	319	Q6L	C33-C32	2.29	1.35	1.33
29	P	321	Q6L	C02-C03	2.29	1.37	1.34
25	A	804	CLA	C1B-NB	-2.29	1.34	1.37
25	B	806	CLA	C1B-C2B	2.29	1.48	1.43
25	S	311	CLA	CMD-C2D	-2.29	1.46	1.50
24	S	305	CHL	MG-NB	-2.29	2.01	2.05
34	B	844	PQN	C11-C12	2.29	1.54	1.50
25	B	815	CLA	C1B-NB	-2.29	1.34	1.37
25	S	313	CLA	C3B-C4B	2.29	1.49	1.42
25	A	839	CLA	CMC-C2C	-2.29	1.46	1.50
25	5	602	CLA	CMB-C2B	-2.29	1.46	1.50
25	A	817	CLA	CHC-C1C	2.29	1.43	1.38
29	T	319	Q6L	C01-C02	2.29	1.54	1.50
24	S	314	CHL	CMB-C2B	-2.29	1.47	1.51
27	2	617	XAT	C8-C9	2.29	1.50	1.46
30	G	201	BCR	C8-C9	2.29	1.50	1.46
25	V	302	CLA	CHC-C4B	-2.29	1.34	1.39
37	R	321	NEX	O24-C25	-2.29	1.43	1.46
24	Q	308	CHL	MG-ND	-2.29	2.01	2.05
25	B	805	CLA	CMA-C3A	-2.29	1.48	1.53
25	S	301	CLA	C1B-C2B	2.28	1.48	1.43
25	X	310	CLA	C3B-C4B	2.28	1.49	1.42
25	X	310	CLA	CMB-C2B	-2.28	1.46	1.50
29	O	2007	Q6L	C01-C02	2.28	1.54	1.50
25	5	609	CLA	CMD-C2D	-2.28	1.46	1.50
25	X	302	CLA	CMD-C2D	-2.28	1.46	1.50
25	N	202	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	302	CLA	CMD-C2D	-2.28	1.46	1.50
38	U	307	KC2	MG-NB	-2.28	2.01	2.05
25	6	611	CLA	C3B-C4B	2.28	1.49	1.42
25	5	608	CLA	CHC-C1C	2.28	1.43	1.38
29	O	2006	Q6L	C04-C03	2.28	1.56	1.53
25	W	312	CLA	CMB-C2B	-2.28	1.46	1.50
24	S	305	CHL	MG-ND	-2.28	2.01	2.05
25	B	819	CLA	MG-NB	-2.28	2.01	2.05
24	P	306	CHL	CMC-C2C	2.28	1.49	1.44
24	U	305	CHL	C1A-CHA	-2.28	1.37	1.40
25	B	805	CLA	C4B-NB	2.28	1.40	1.37
24	X	306	CHL	CAC-C3C	-2.28	1.47	1.51
25	T	312	CLA	CMC-C2C	-2.28	1.46	1.50
25	B	828	CLA	C4B-NB	2.28	1.40	1.37
25	4	303	CLA	C1B-C2B	2.28	1.48	1.43
25	S	310	CLA	C3B-C4B	2.28	1.49	1.42
24	T	314	CHL	CAC-C3C	-2.28	1.47	1.51
30	H	305	BCR	C12-C13	2.28	1.50	1.46
24	1	604	CHL	CMC-C2C	2.28	1.49	1.44
25	R	306	CLA	C3B-C4B	2.28	1.49	1.42
29	T	315	Q6L	C01-C02	2.28	1.54	1.50
24	P	307	CHL	CMC-C2C	2.28	1.49	1.44
25	A	856	CLA	MG-NB	-2.28	2.01	2.05
25	A	827	CLA	C1B-NB	-2.28	1.34	1.37
25	R	316	CLA	CMB-C2B	-2.27	1.46	1.50
25	3	312	CLA	C1B-C2B	2.27	1.48	1.43
25	Q	313	CLA	C3B-C4B	2.27	1.49	1.42
25	W	309	CLA	C3B-C4B	2.27	1.49	1.42
25	6	612	CLA	CHC-C4B	-2.27	1.34	1.39
25	K	204	CLA	CHC-C4B	-2.27	1.34	1.39
25	H	301	CLA	C1B-C2B	2.27	1.48	1.43
24	3	306	CHL	CHC-C4B	-2.27	1.36	1.39
24	R	310	CHL	CHC-C4B	-2.27	1.36	1.39
29	P	321	Q6L	C33-C32	2.27	1.35	1.33
25	U	311	CLA	C1B-C2B	2.27	1.48	1.43
25	A	809	CLA	CMB-C2B	-2.27	1.46	1.50
24	T	320	CHL	CMA-C3A	-2.27	1.49	1.53
25	3	301	CLA	C3B-C4B	2.27	1.49	1.42
25	A	810	CLA	C1B-NB	-2.27	1.34	1.37
29	S	316	Q6L	C33-C32	2.27	1.35	1.33
25	1	603	CLA	C1B-C2B	2.27	1.48	1.43
29	U	317	Q6L	C01-C02	2.27	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	207	BCR	C16-C15	-2.27	1.30	1.36
26	1	611	IWJ	C26-C24	-2.27	1.45	1.49
24	W	314	CHL	C2A-C1A	2.27	1.53	1.50
25	3	311	CLA	CHC-C4B	-2.27	1.34	1.39
25	A	820	CLA	MG-NB	-2.27	2.01	2.05
25	F	803	CLA	MG-NB	-2.27	2.01	2.05
29	S	316	Q6L	C01-C02	2.27	1.54	1.50
27	1	612	XAT	C18-C5	2.27	1.55	1.51
26	P	318	IWJ	C26-C24	-2.27	1.45	1.49
25	U	308	CLA	CHC-C4B	-2.27	1.34	1.39
25	S	301	CLA	MG-NB	-2.27	2.01	2.05
25	Q	305	CLA	CMB-C2B	-2.26	1.46	1.50
25	R	307	CLA	CMB-C2B	-2.26	1.46	1.50
25	S	301	CLA	CHC-C1C	2.26	1.43	1.38
24	4	306	CHL	CHB-C4A	-2.26	1.35	1.38
30	B	845	BCR	C19-C18	2.26	1.50	1.46
25	B	818	CLA	MG-NB	-2.26	2.01	2.05
25	3	305	CLA	CMC-C2C	-2.26	1.46	1.50
25	A	834	CLA	CMB-C2B	-2.26	1.46	1.50
25	S	312	CLA	CMD-C2D	-2.26	1.46	1.50
25	J	102	CLA	C4B-NB	2.26	1.40	1.37
25	5	610	CLA	CHC-C1C	2.26	1.43	1.38
29	S	321	Q6L	C01-C02	2.26	1.54	1.50
25	P	312	CLA	CHC-C1C	2.26	1.43	1.38
24	W	314	CHL	C1A-CHA	-2.26	1.36	1.39
25	A	834	CLA	C1B-C2B	2.26	1.48	1.43
24	V	314	CHL	MG-ND	-2.26	2.01	2.05
27	6	615	XAT	O24-C25	-2.26	1.43	1.46
24	T	307	CHL	CHD-C1D	-2.26	1.36	1.39
30	F	804	BCR	C19-C18	2.26	1.50	1.46
37	P	317	NEX	C32-C33	2.26	1.50	1.46
25	B	802	CLA	MG-NB	-2.26	2.01	2.05
24	R	310	CHL	CMC-C2C	2.26	1.49	1.44
25	B	808	CLA	CMB-C2B	-2.26	1.46	1.50
38	V	308	KC2	CMB-C2B	-2.26	1.46	1.50
24	Q	316	CHL	CMB-C2B	-2.26	1.47	1.51
25	B	820	CLA	C1B-NB	-2.26	1.34	1.37
25	N	203	CLA	C3B-C4B	2.26	1.49	1.42
26	V	317	IWJ	C03-C02	2.26	1.35	1.33
24	X	308	CHL	CMB-C2B	-2.26	1.47	1.51
24	4	308	CHL	CBD-CGD	-2.26	1.49	1.52
25	U	302	CLA	C1B-C2B	2.26	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	608	CLA	MG-ND	-2.25	2.01	2.05
29	O	2006	Q6L	C33-C32	2.25	1.35	1.33
24	W	306	CHL	CMA-C3A	-2.25	1.49	1.53
25	J	102	CLA	MG-ND	-2.25	2.01	2.05
25	A	807	CLA	C4B-NB	2.25	1.40	1.37
25	B	813	CLA	CAC-C3C	-2.25	1.45	1.51
25	3	312	CLA	C3B-C4B	2.25	1.49	1.42
25	5	604	CLA	C1B-C2B	2.25	1.48	1.43
24	X	306	CHL	C4A-C3A	2.25	1.55	1.51
24	3	306	CHL	CMC-C2C	-2.25	1.47	1.50
25	A	827	CLA	MG-NB	-2.25	2.01	2.05
25	A	813	CLA	CMB-C2B	-2.25	1.46	1.50
25	B	834	CLA	C3B-C4B	2.25	1.49	1.42
24	P	305	CHL	CMB-C2B	-2.25	1.47	1.51
25	B	812	CLA	MG-ND	-2.25	2.01	2.05
29	W	320	Q6L	C01-C02	2.25	1.54	1.50
25	S	310	CLA	CMB-C2B	-2.25	1.46	1.50
25	B	811	CLA	C4B-NB	2.25	1.40	1.37
25	B	836	CLA	C3B-C4B	2.25	1.49	1.42
25	A	815	CLA	CMC-C2C	-2.25	1.46	1.50
25	B	809	CLA	C4B-NB	2.25	1.40	1.37
25	W	301	CLA	C3B-C4B	2.25	1.49	1.42
25	A	821	CLA	CMC-C2C	-2.25	1.46	1.50
25	H	304	CLA	CHC-C4B	-2.25	1.34	1.39
25	A	829	CLA	MG-NB	-2.25	2.01	2.05
24	1	601	CHL	CMB-C2B	-2.25	1.47	1.51
25	B	817	CLA	CMC-C2C	-2.25	1.46	1.50
25	3	308	CLA	C4B-NB	2.25	1.40	1.37
30	B	846	BCR	C16-C15	-2.25	1.30	1.36
24	W	304	CHL	CMD-C2D	-2.25	1.47	1.51
25	O	2001	CLA	CMD-C2D	-2.25	1.46	1.50
25	A	812	CLA	C3B-C4B	2.25	1.49	1.42
25	P	310	CLA	C3B-C4B	2.25	1.49	1.42
30	B	848	BCR	C34-C9	2.25	1.55	1.50
29	X	317	Q6L	C01-C02	2.25	1.54	1.50
25	Q	304	CLA	C1B-C2B	2.24	1.48	1.43
25	P	302	CLA	C3B-C4B	2.24	1.49	1.42
25	B	829	CLA	C1B-C2B	2.24	1.48	1.43
25	4	315	CLA	CMB-C2B	-2.24	1.46	1.50
25	T	312	CLA	C3B-C4B	2.24	1.49	1.42
29	U	314	Q6L	C33-C32	2.24	1.35	1.33
25	B	805	CLA	C1B-C2B	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	808	CLA	CHC-C4B	-2.24	1.34	1.39
25	A	842	CLA	C3B-C4B	2.24	1.49	1.42
25	W	312	CLA	CHC-C4B	-2.24	1.34	1.39
25	B	814	CLA	CMB-C2B	-2.24	1.46	1.50
37	H	306	NEX	C32-C33	2.24	1.50	1.46
25	R	307	CLA	CMD-C2D	-2.24	1.46	1.50
29	2	616	Q6L	C01-C02	2.24	1.54	1.50
24	R	302	CHL	CMD-C2D	-2.24	1.47	1.51
25	O	2004	CLA	C3B-C4B	2.24	1.49	1.42
25	J	102	CLA	CMB-C2B	-2.24	1.46	1.50
25	K	204	CLA	CMC-C2C	-2.24	1.46	1.50
25	B	824	CLA	C3B-C4B	2.24	1.49	1.42
25	2	613	CLA	CHC-C1C	2.24	1.43	1.38
25	B	807	CLA	CMD-C2D	-2.24	1.46	1.50
25	A	816	CLA	C4B-NB	2.24	1.40	1.37
27	1	612	XAT	C8-C9	2.24	1.50	1.46
24	R	308	CHL	CHC-C4B	-2.24	1.36	1.39
25	S	301	CLA	MG-ND	-2.24	2.01	2.05
25	G	204	CLA	C4B-NB	2.24	1.40	1.37
25	1	602	CLA	C3B-C4B	2.24	1.49	1.42
24	R	302	CHL	CBD-CGD	-2.24	1.49	1.52
25	A	810	CLA	CMD-C2D	-2.24	1.46	1.50
25	B	804	CLA	MG-NB	-2.24	2.01	2.05
25	X	312	CLA	CMB-C2B	-2.24	1.46	1.50
30	H	305	BCR	C23-C22	2.24	1.50	1.46
30	I	101	BCR	C12-C13	2.24	1.50	1.46
24	2	601	CHL	C3D-CAD	-2.24	1.43	1.47
24	V	306	CHL	CHC-C1C	2.24	1.43	1.39
24	S	305	CHL	C3D-CAD	-2.24	1.43	1.47
24	6	605	CHL	MG-ND	-2.24	2.01	2.05
25	F	802	CLA	CHC-C4B	-2.24	1.34	1.39
30	3	318	BCR	C19-C18	2.24	1.50	1.46
24	U	304	CHL	CAC-C3C	-2.23	1.47	1.51
29	W	315	Q6L	C01-C02	2.23	1.54	1.50
25	X	310	CLA	CHC-C1C	2.23	1.43	1.38
25	B	815	CLA	C4-C3	-2.23	1.45	1.50
25	B	843	CLA	C1B-C2B	2.23	1.48	1.43
25	V	303	CLA	C1B-NB	-2.23	1.34	1.37
25	K	203	CLA	CMB-C2B	-2.23	1.46	1.50
25	A	807	CLA	C3B-C4B	2.23	1.49	1.42
25	A	840	CLA	CMD-C2D	-2.23	1.46	1.50
25	A	826	CLA	C4B-NB	2.23	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	838	CLA	CMB-C2B	-2.23	1.46	1.50
25	B	809	CLA	MG-NB	-2.23	2.01	2.05
30	B	847	BCR	C12-C13	2.23	1.50	1.46
25	B	820	CLA	C3B-C4B	2.23	1.49	1.42
38	V	308	KC2	MG-NC	2.23	2.11	2.06
25	A	835	CLA	CHC-C4B	-2.23	1.34	1.39
25	A	808	CLA	C1B-C2B	2.23	1.48	1.43
24	V	307	CHL	CMB-C2B	-2.23	1.47	1.51
25	P	313	CLA	C3B-C4B	2.23	1.49	1.42
25	A	831	CLA	C1B-C2B	2.23	1.48	1.43
24	S	307	CHL	CHC-C1C	2.23	1.43	1.39
25	L	302	CLA	CHC-C4B	-2.23	1.34	1.39
25	B	808	CLA	CMC-C2C	-2.23	1.46	1.50
25	A	823	CLA	C1B-NB	-2.23	1.34	1.37
25	B	820	CLA	C4B-NB	2.23	1.40	1.37
25	A	820	CLA	CMB-C2B	-2.23	1.46	1.50
30	3	319	BCR	C16-C15	-2.23	1.30	1.36
24	4	307	CHL	CHC-C4B	-2.23	1.36	1.39
25	H	304	CLA	CMD-C2D	-2.23	1.46	1.50
24	X	305	CHL	CBD-CGD	-2.23	1.49	1.52
25	A	814	CLA	C3B-C4B	2.23	1.49	1.42
29	T	316	Q6L	C12-C13	-2.23	1.46	1.51
29	Q	319	Q6L	C01-C02	2.22	1.54	1.50
25	4	309	CLA	CMB-C2B	-2.22	1.46	1.50
29	V	321	Q6L	C01-C02	2.22	1.54	1.50
25	O	2005	CLA	CMD-C2D	-2.22	1.46	1.50
25	G	204	CLA	CHC-C4B	-2.22	1.34	1.39
25	4	304	CLA	CHC-C1C	2.22	1.42	1.38
29	Q	318	Q6L	C01-C02	2.22	1.54	1.50
24	U	305	CHL	CAC-C3C	-2.22	1.47	1.51
25	2	614	CLA	MG-ND	-2.22	2.01	2.05
24	X	305	CHL	C1A-CHA	-2.22	1.37	1.40
25	R	307	CLA	CHC-C1C	2.22	1.42	1.38
29	U	315	Q6L	C01-C02	2.22	1.54	1.50
29	P	321	Q6L	C34-C33	2.22	1.53	1.50
25	B	823	CLA	CMB-C2B	-2.22	1.46	1.50
25	B	811	CLA	C3B-C4B	2.22	1.49	1.42
25	T	309	CLA	C1B-C2B	2.22	1.48	1.43
27	5	612	XAT	O24-C25	-2.22	1.43	1.46
25	X	302	CLA	CMC-C2C	-2.22	1.46	1.50
25	A	814	CLA	C1B-C2B	2.22	1.48	1.43
25	U	312	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	315	Q6L	C33-C32	2.22	1.35	1.33
25	B	825	CLA	C3B-C4B	2.22	1.49	1.42
25	L	302	CLA	C1B-C2B	2.22	1.48	1.43
25	Q	312	CLA	CMD-C2D	-2.22	1.46	1.50
25	A	828	CLA	MG-ND	-2.22	2.01	2.05
25	B	818	CLA	CMD-C2D	-2.22	1.46	1.50
24	U	313	CHL	CAC-C3C	-2.22	1.47	1.51
25	O	2002	CLA	C4B-NB	2.22	1.40	1.37
29	R	323	Q6L	C33-C32	2.22	1.35	1.33
38	X	309	KC2	C1D-ND	2.21	1.40	1.37
24	6	601	CHL	MG-NB	-2.21	2.01	2.05
24	4	302	CHL	C3B-C2B	-2.21	1.37	1.40
25	2	612	CLA	CMB-C2B	-2.21	1.46	1.50
25	Q	315	CLA	CMD-C2D	-2.21	1.46	1.50
24	S	307	CHL	CAC-C3C	-2.21	1.47	1.51
25	U	303	CLA	C3B-C4B	2.21	1.49	1.42
25	4	316	CLA	CMB-C2B	-2.21	1.46	1.50
30	K	207	BCR	C8-C7	2.21	1.39	1.33
25	S	309	CLA	CHC-C1C	2.21	1.42	1.38
25	A	834	CLA	C4B-NB	2.21	1.40	1.37
29	T	316	Q6L	C01-C02	2.21	1.54	1.50
25	X	313	CLA	C3B-C4B	2.21	1.49	1.42
24	2	601	CHL	CMC-C2C	2.21	1.49	1.44
30	A	849	BCR	C16-C15	-2.21	1.30	1.36
25	X	312	CLA	C3B-C4B	2.21	1.49	1.42
25	B	842	CLA	CAC-C3C	-2.21	1.45	1.51
24	X	306	CHL	CMB-C2B	-2.21	1.47	1.51
25	W	303	CLA	CMD-C2D	-2.21	1.46	1.50
25	A	812	CLA	C4B-NB	2.21	1.40	1.37
25	T	313	CLA	C3B-C4B	2.21	1.49	1.42
25	O	2005	CLA	C3B-C4B	2.21	1.49	1.42
25	W	311	CLA	C3B-C4B	2.21	1.49	1.42
25	B	840	CLA	C3B-C4B	2.21	1.49	1.42
29	S	315	Q6L	C01-C02	2.21	1.54	1.50
24	4	302	CHL	MG-ND	-2.21	2.01	2.05
25	6	607	CLA	MG-ND	-2.21	2.01	2.05
24	2	605	CHL	CHC-C4B	-2.20	1.36	1.39
25	B	841	CLA	CMD-C2D	-2.20	1.46	1.50
25	W	309	CLA	CHC-C1C	2.20	1.42	1.38
25	4	313	CLA	CMB-C2B	-2.20	1.46	1.50
25	A	836	CLA	C3C-C2C	2.20	1.41	1.36
27	1	612	XAT	C38-C25	2.20	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	607	CLA	CMC-C2C	-2.20	1.46	1.50
25	A	821	CLA	CHC-C4B	-2.20	1.34	1.39
27	3	316	XAT	C22-C21	-2.20	1.51	1.54
25	O	2003	CLA	C3B-C4B	2.20	1.49	1.42
25	P	310	CLA	CHC-C1C	2.20	1.42	1.38
25	A	832	CLA	CMB-C2B	-2.20	1.46	1.50
25	A	810	CLA	CHC-C4B	-2.20	1.34	1.39
25	Q	304	CLA	CMA-C3A	-2.20	1.48	1.53
29	R	320	Q6L	C33-C32	2.20	1.35	1.33
25	A	837	CLA	C1B-C2B	2.20	1.48	1.43
25	2	609	CLA	C3B-C4B	2.20	1.49	1.42
25	H	304	CLA	C3B-C4B	2.20	1.49	1.42
25	B	842	CLA	C3B-C4B	2.20	1.49	1.42
29	R	319	Q6L	C33-C32	2.20	1.35	1.33
37	T	317	NEX	C35-C15	-2.20	1.30	1.36
25	P	301	CLA	C4B-NB	2.20	1.40	1.37
25	B	839	CLA	CMC-C2C	-2.20	1.46	1.50
29	R	301	Q6L	C02-C03	2.20	1.37	1.34
25	B	826	CLA	C3B-C4B	2.20	1.49	1.42
27	4	318	XAT	C6-C7	2.20	1.54	1.50
26	S	322	IWJ	C26-C24	-2.20	1.45	1.49
25	B	843	CLA	CMC-C2C	-2.20	1.46	1.50
25	Q	306	CLA	C1B-C2B	2.20	1.48	1.43
38	S	308	KC2	MG-ND	-2.20	2.01	2.05
25	A	845	CLA	C4B-NB	2.20	1.40	1.37
25	Q	306	CLA	C3B-C4B	2.20	1.49	1.42
25	5	604	CLA	MG-NB	-2.20	2.01	2.05
24	T	304	CHL	CHB-C4A	-2.20	1.36	1.38
25	A	839	CLA	MG-NB	-2.19	2.01	2.05
30	K	202	BCR	C34-C9	2.19	1.55	1.50
25	1	606	CLA	CMB-C2B	-2.19	1.46	1.50
25	X	313	CLA	CMC-C2C	-2.19	1.46	1.50
25	B	829	CLA	MG-NB	-2.19	2.01	2.05
25	F	803	CLA	CHC-C4B	-2.19	1.34	1.39
25	B	835	CLA	C3B-C4B	2.19	1.49	1.42
24	P	306	CHL	MG-NB	-2.19	2.01	2.05
30	3	317	BCR	C12-C13	2.19	1.50	1.46
25	3	308	CLA	CMD-C2D	-2.19	1.46	1.50
25	T	302	CLA	CMC-C2C	-2.19	1.46	1.50
25	V	311	CLA	CMB-C2B	-2.19	1.46	1.50
25	A	842	CLA	CHC-C4B	-2.19	1.34	1.39
26	3	315	IWJ	O39-C29	-2.19	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	309	KC2	MG-NB	-2.19	2.01	2.05
25	W	302	CLA	CMB-C2B	-2.19	1.46	1.50
25	T	309	CLA	CHC-C1C	2.19	1.42	1.38
30	3	318	BCR	C23-C22	2.19	1.50	1.46
25	X	314	CLA	C3B-C4B	2.19	1.49	1.42
38	S	308	KC2	MG-NB	-2.19	2.01	2.05
26	3	315	IWJ	C26-C24	-2.19	1.45	1.49
25	B	828	CLA	MG-NB	-2.19	2.01	2.05
25	A	843	CLA	CMB-C2B	-2.19	1.46	1.50
25	Q	312	CLA	C3B-C4B	2.19	1.49	1.42
25	A	829	CLA	C1B-C2B	2.19	1.48	1.43
24	R	318	CHL	CMB-C2B	-2.19	1.47	1.51
25	T	310	CLA	C3B-C4B	2.19	1.49	1.42
30	A	848	BCR	C16-C15	-2.19	1.30	1.36
26	S	318	IWJ	C32-C30	2.19	1.55	1.51
25	B	839	CLA	C1B-C2B	2.19	1.48	1.43
25	B	832	CLA	CMC-C2C	-2.19	1.46	1.50
26	U	316	IWJ	C28-C26	2.19	1.53	1.51
25	B	819	CLA	CMD-C2D	-2.18	1.46	1.50
25	B	807	CLA	C1B-C2B	2.18	1.48	1.43
29	O	2007	Q6L	C29-C27	2.18	1.50	1.46
25	L	303	CLA	C1B-NB	-2.18	1.35	1.37
25	U	303	CLA	CMD-C2D	-2.18	1.46	1.50
25	2	613	CLA	C1D-C2D	2.18	1.49	1.45
25	3	301	CLA	CMB-C2B	-2.18	1.46	1.50
25	6	610	CLA	C3B-C4B	2.18	1.49	1.42
25	P	302	CLA	CHC-C1C	2.18	1.42	1.38
37	W	317	NEX	C35-C15	-2.18	1.30	1.36
29	V	319	Q6L	C33-C32	2.18	1.35	1.33
25	5	604	CLA	CHC-C1C	2.18	1.42	1.38
25	T	311	CLA	CMD-C2D	-2.18	1.46	1.50
25	U	311	CLA	CMB-C2B	-2.18	1.46	1.50
25	V	311	CLA	C3B-C4B	2.18	1.49	1.42
25	U	309	CLA	C3B-C4B	2.18	1.49	1.42
30	B	846	BCR	C12-C13	2.18	1.50	1.46
24	6	601	CHL	MG-ND	-2.18	2.01	2.05
30	B	849	BCR	C8-C9	2.18	1.50	1.46
24	4	308	CHL	CHC-C4B	-2.18	1.36	1.39
27	6	615	XAT	C38-C25	2.18	1.55	1.51
24	1	604	CHL	CMB-C2B	-2.18	1.47	1.51
25	K	204	CLA	C4B-NB	2.18	1.40	1.37
24	4	306	CHL	CHC-C4B	-2.18	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	315	CLA	CMB-C2B	-2.18	1.46	1.50
37	R	321	NEX	C22-C21	-2.18	1.51	1.54
25	P	313	CLA	CMB-C2B	-2.17	1.46	1.50
25	B	820	CLA	C1B-C2B	2.17	1.48	1.43
30	K	202	BCR	C37-C22	2.17	1.55	1.50
37	P	317	NEX	C35-C15	-2.17	1.30	1.36
25	B	829	CLA	C4B-NB	2.17	1.40	1.37
25	U	311	CLA	CHC-C1C	2.17	1.42	1.38
25	2	606	CLA	C3B-C4B	2.17	1.49	1.42
24	Q	309	CHL	CHC-C4B	-2.17	1.36	1.39
25	B	828	CLA	C3B-C4B	2.17	1.49	1.42
25	L	304	CLA	CMC-C2C	-2.17	1.46	1.50
26	X	318	IWJ	C26-C24	-2.17	1.45	1.49
25	T	309	CLA	CMB-C2B	-2.17	1.46	1.50
24	U	306	CHL	CAC-C3C	-2.17	1.47	1.51
25	4	309	CLA	C3B-C4B	2.17	1.49	1.42
25	B	821	CLA	CHC-C4B	-2.17	1.34	1.39
25	B	829	CLA	C3B-C4B	2.17	1.49	1.42
24	X	308	CHL	CBD-CGD	-2.17	1.49	1.52
25	B	828	CLA	C1B-C2B	2.17	1.48	1.43
25	X	303	CLA	C3B-C4B	2.17	1.49	1.42
25	T	301	CLA	CMB-C2B	-2.17	1.46	1.50
25	W	310	CLA	C3B-C4B	2.17	1.49	1.42
27	2	617	XAT	O4-C5	-2.17	1.43	1.46
25	L	302	CLA	MG-NB	-2.17	2.01	2.05
37	P	317	NEX	C22-C21	-2.17	1.51	1.54
25	W	312	CLA	C3B-C4B	2.17	1.49	1.42
25	O	2003	CLA	CHC-C1C	2.17	1.42	1.38
25	R	315	CLA	CMD-C2D	-2.17	1.46	1.50
25	A	822	CLA	CMC-C2C	-2.17	1.46	1.50
29	Q	317	Q6L	C01-C02	2.17	1.54	1.50
25	L	301	CLA	CHC-C1C	2.17	1.42	1.38
25	A	814	CLA	C1B-NB	-2.17	1.35	1.37
29	S	321	Q6L	C04-C03	2.17	1.56	1.53
25	B	825	CLA	MG-ND	-2.17	2.01	2.05
25	S	312	CLA	C3B-C4B	2.17	1.49	1.42
29	P	315	Q6L	C11-C03	-2.17	1.48	1.51
25	R	306	CLA	CMB-C2B	-2.16	1.46	1.50
24	2	615	CHL	CMB-C2B	-2.16	1.47	1.51
25	3	307	CLA	C1B-NB	-2.16	1.35	1.37
24	W	306	CHL	MG-ND	-2.16	2.01	2.05
25	V	303	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	309	CLA	CMB-C2B	-2.16	1.46	1.50
25	B	838	CLA	C1B-NB	-2.16	1.35	1.37
25	F	802	CLA	C3B-C4B	2.16	1.49	1.42
25	A	823	CLA	C1B-C2B	2.16	1.48	1.43
25	W	312	CLA	MG-NC	2.16	2.11	2.06
25	4	309	CLA	CMD-C2D	-2.16	1.46	1.50
34	B	844	PQN	C5-C4	-2.16	1.43	1.48
24	R	302	CHL	C3D-CAD	-2.16	1.43	1.47
25	A	816	CLA	MG-NB	-2.16	2.01	2.05
30	A	850	BCR	C8-C9	2.16	1.50	1.46
25	W	310	CLA	CMB-C2B	-2.16	1.46	1.50
25	B	832	CLA	CHC-C4B	-2.16	1.34	1.39
25	A	820	CLA	CMD-C2D	-2.16	1.46	1.50
25	Q	312	CLA	CMB-C2B	-2.16	1.46	1.50
25	6	607	CLA	CHC-C4B	-2.16	1.34	1.39
30	L	306	BCR	C16-C15	-2.16	1.30	1.36
26	S	319	IWJ	C26-C24	-2.16	1.45	1.49
25	4	305	CLA	CMC-C2C	-2.16	1.46	1.50
25	B	843	CLA	C3B-C4B	2.16	1.49	1.42
25	4	313	CLA	CHC-C4B	-2.16	1.34	1.39
24	4	302	CHL	CMC-C2C	2.16	1.49	1.44
25	Q	312	CLA	CHC-C1C	2.16	1.42	1.38
25	A	807	CLA	CHC-C4B	-2.15	1.34	1.39
24	P	304	CHL	MG-ND	-2.15	2.01	2.05
25	2	612	CLA	C3B-C4B	2.15	1.49	1.42
29	S	323	Q6L	C34-C33	2.15	1.53	1.50
25	4	312	CLA	CMD-C2D	-2.15	1.46	1.50
25	G	203	CLA	CMB-C2B	-2.15	1.46	1.50
25	A	804	CLA	C1B-C2B	2.15	1.48	1.43
30	K	205	BCR	C16-C15	-2.15	1.30	1.36
25	W	301	CLA	C4B-NB	2.15	1.40	1.37
25	X	302	CLA	CAB-C3B	-2.15	1.41	1.47
27	3	316	XAT	C2-C1	-2.15	1.51	1.54
25	B	841	CLA	C1B-NB	-2.15	1.35	1.37
29	R	320	Q6L	C01-C02	2.15	1.54	1.50
25	X	311	CLA	MG-NB	-2.15	2.01	2.05
25	U	309	CLA	CMD-C2D	-2.15	1.46	1.50
25	W	313	CLA	CMB-C2B	-2.15	1.46	1.50
25	B	837	CLA	MG-NB	-2.15	2.01	2.05
25	5	603	CLA	CMB-C2B	-2.15	1.46	1.50
24	R	308	CHL	MG-ND	-2.15	2.01	2.05
25	A	838	CLA	C1B-C2B	2.15	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	822	CLA	C4-C3	-2.15	1.44	1.50
24	2	605	CHL	CMA-C3A	-2.15	1.49	1.53
24	V	306	CHL	MG-NB	-2.14	2.01	2.05
24	X	305	CHL	MG-NB	-2.14	2.01	2.05
25	S	309	CLA	C1A-CHA	-2.14	1.34	1.43
25	G	202	CLA	CMD-C2D	-2.14	1.46	1.50
25	3	301	CLA	C1B-NB	-2.14	1.35	1.37
25	U	308	CLA	CMD-C2D	-2.14	1.46	1.50
25	5	606	CLA	CMB-C2B	-2.14	1.46	1.50
30	G	201	BCR	C16-C15	-2.14	1.30	1.36
24	W	306	CHL	C3A-C2A	2.14	1.56	1.54
25	3	312	CLA	CHC-C1C	2.14	1.42	1.38
25	A	816	CLA	CHC-C1C	2.14	1.42	1.38
25	3	304	CLA	MG-NB	-2.14	2.01	2.05
25	U	301	CLA	C1B-C2B	2.14	1.48	1.43
24	V	304	CHL	CAC-C3C	-2.14	1.48	1.51
24	Q	316	CHL	CHC-C4B	-2.14	1.36	1.39
25	W	301	CLA	CHC-C1C	2.14	1.42	1.38
30	F	804	BCR	C5-C6	2.14	1.38	1.34
25	V	313	CLA	C3B-C4B	2.14	1.49	1.42
38	T	308	KC2	MG-NB	-2.14	2.01	2.05
25	B	836	CLA	MG-NB	-2.14	2.01	2.05
25	X	312	CLA	CMD-C2D	-2.14	1.46	1.50
25	1	605	CLA	CMB-C2B	-2.14	1.46	1.50
25	A	810	CLA	CMC-C2C	-2.14	1.46	1.50
25	2	606	CLA	CMD-C2D	-2.14	1.46	1.50
25	T	301	CLA	CMA-C3A	-2.14	1.48	1.53
25	6	610	CLA	CMB-C2B	-2.14	1.46	1.50
25	Q	304	CLA	CHC-C4B	-2.14	1.34	1.39
25	2	609	CLA	CMD-C2D	-2.14	1.46	1.50
25	B	806	CLA	CMB-C2B	-2.14	1.46	1.50
25	R	314	CLA	C3B-C4B	2.14	1.49	1.42
25	Q	315	CLA	CMC-C2C	-2.14	1.46	1.50
25	W	303	CLA	MG-NB	-2.14	2.01	2.05
30	I	101	BCR	C16-C15	-2.14	1.30	1.36
25	B	816	CLA	CMD-C2D	-2.13	1.46	1.50
25	S	309	CLA	CMC-C2C	-2.13	1.46	1.50
25	W	311	CLA	CMB-C2B	-2.13	1.46	1.50
24	V	305	CHL	MG-ND	-2.13	2.01	2.05
24	P	306	CHL	C1A-CHA	-2.13	1.37	1.40
25	5	608	CLA	CMB-C2B	-2.13	1.46	1.50
29	P	321	Q6L	C29-C27	2.13	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	313	CLA	CHC-C1C	2.13	1.42	1.38
38	X	309	KC2	MG-NA	2.13	2.11	2.06
24	2	605	CHL	CAC-C3C	-2.13	1.47	1.50
25	S	312	CLA	CHC-C1C	2.13	1.42	1.38
29	O	2007	Q6L	C04-C03	2.13	1.56	1.53
24	W	314	CHL	CAC-C3C	-2.13	1.48	1.51
25	1	605	CLA	C3B-C4B	2.13	1.49	1.42
25	B	841	CLA	MG-NB	-2.13	2.01	2.05
25	P	309	CLA	CHC-C1C	2.13	1.42	1.38
29	Q	318	Q6L	C34-C33	2.13	1.53	1.50
25	W	313	CLA	C3B-C4B	2.13	1.49	1.42
25	A	828	CLA	C1B-C2B	2.13	1.48	1.43
30	B	846	BCR	C30-C25	-2.13	1.51	1.53
25	Q	306	CLA	MG-ND	-2.13	2.01	2.05
24	T	305	CHL	CMB-C2B	-2.13	1.47	1.51
25	3	302	CLA	CHC-C1C	2.13	1.42	1.38
25	B	826	CLA	MG-ND	-2.13	2.01	2.05
27	1	612	XAT	O4-C5	-2.13	1.43	1.46
25	U	310	CLA	CMC-C2C	-2.13	1.46	1.50
25	F	802	CLA	C1B-NB	-2.13	1.35	1.37
25	K	203	CLA	CMD-C2D	-2.13	1.46	1.50
25	T	303	CLA	C1B-C2B	2.13	1.48	1.43
25	3	313	CLA	MG-NB	-2.13	2.01	2.05
25	A	840	CLA	CMB-C2B	-2.13	1.46	1.50
25	W	302	CLA	C3B-C4B	2.13	1.48	1.42
38	W	308	KC2	MG-NB	-2.13	2.01	2.05
25	A	826	CLA	CMB-C2B	-2.13	1.46	1.50
25	K	203	CLA	CHC-C4B	-2.13	1.34	1.39
25	A	829	CLA	MG-ND	-2.13	2.01	2.05
25	O	2003	CLA	CMB-C2B	-2.13	1.46	1.50
38	P	308	KC2	MG-ND	-2.13	2.01	2.05
25	A	839	CLA	C4B-NB	2.12	1.40	1.37
25	O	2004	CLA	CMB-C2B	-2.12	1.46	1.50
25	1	610	CLA	MG-NB	-2.12	2.01	2.05
24	R	309	CHL	CMB-C2B	-2.12	1.47	1.51
26	X	318	IWJ	C32-C30	2.12	1.55	1.51
25	3	304	CLA	C1B-NB	-2.12	1.35	1.37
25	6	604	CLA	CHC-C1C	2.12	1.42	1.38
24	V	305	CHL	CAC-C3C	-2.12	1.48	1.51
25	B	821	CLA	C1B-C2B	2.12	1.48	1.43
25	V	313	CLA	CHC-C1C	2.12	1.42	1.38
25	B	808	CLA	C1B-NB	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	303	CLA	CHC-C4B	-2.12	1.34	1.39
38	W	308	KC2	MG-NA	2.12	2.11	2.06
25	B	828	CLA	CHC-C1C	2.12	1.42	1.38
29	S	323	Q6L	C01-C02	2.12	1.54	1.50
25	Q	301	CLA	CMC-C2C	-2.12	1.46	1.50
25	B	836	CLA	C1B-C2B	2.12	1.48	1.43
29	P	316	Q6L	C29-C27	2.12	1.50	1.46
37	H	306	NEX	O24-C25	-2.12	1.43	1.46
25	K	204	CLA	C3B-C4B	2.12	1.48	1.42
25	S	310	CLA	CMD-C2D	-2.12	1.46	1.50
25	6	603	CLA	CHC-C4B	-2.12	1.34	1.39
25	4	316	CLA	C3B-C4B	2.12	1.48	1.42
25	1	608	CLA	CHC-C4B	-2.12	1.34	1.39
26	T	321	IWJ	O39-C29	-2.12	1.39	1.43
25	6	604	CLA	C3B-C4B	2.12	1.48	1.42
25	1	602	CLA	CMA-C3A	-2.12	1.48	1.53
25	J	102	CLA	CMD-C2D	-2.12	1.46	1.50
25	O	2002	CLA	C1B-C2B	2.12	1.48	1.43
25	H	301	CLA	CAB-C3B	-2.12	1.41	1.47
24	W	306	CHL	MG-NB	-2.12	2.01	2.05
29	U	317	Q6L	C33-C32	2.12	1.35	1.33
25	A	840	CLA	C3B-C4B	2.12	1.48	1.42
25	G	202	CLA	C3B-C4B	2.12	1.48	1.42
24	T	305	CHL	C3D-C2D	-2.12	1.36	1.39
25	1	613	CLA	CHC-C1C	2.12	1.42	1.38
25	U	311	CLA	CMD-C2D	-2.11	1.46	1.50
25	S	303	CLA	CHC-C1C	2.11	1.42	1.38
24	T	304	CHL	CAC-C3C	-2.11	1.48	1.51
25	A	815	CLA	CMA-C3A	-2.11	1.48	1.53
25	2	609	CLA	CMB-C2B	-2.11	1.46	1.50
25	U	303	CLA	C1B-C2B	2.11	1.48	1.43
25	G	202	CLA	CMB-C2B	-2.11	1.46	1.50
25	K	206	CLA	CHC-C1C	2.11	1.42	1.38
25	6	607	CLA	C1B-C2B	2.11	1.48	1.43
25	B	820	CLA	MG-ND	-2.11	2.01	2.05
25	H	302	CLA	C3B-C4B	2.11	1.48	1.42
25	L	301	CLA	C3B-C4B	2.11	1.48	1.42
24	2	601	CHL	C3B-C2B	-2.11	1.37	1.40
25	6	604	CLA	CMB-C2B	-2.11	1.46	1.50
25	R	306	CLA	CMC-C2C	-2.11	1.46	1.50
25	B	813	CLA	C1B-NB	-2.11	1.35	1.37
25	5	610	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	W	305	CHL	C3D-CAD	-2.11	1.43	1.47
24	T	304	CHL	CMB-C2B	-2.11	1.47	1.51
25	T	302	CLA	CMB-C2B	-2.11	1.46	1.50
30	I	101	BCR	C31-C1	-2.11	1.49	1.53
25	A	827	CLA	MG-ND	-2.11	2.01	2.05
30	A	852	BCR	C16-C15	-2.11	1.30	1.36
25	B	808	CLA	C1D-ND	2.11	1.40	1.37
25	U	308	CLA	C1D-ND	2.11	1.40	1.37
25	2	614	CLA	CMD-C2D	-2.11	1.46	1.50
25	B	826	CLA	C4B-NB	2.11	1.40	1.37
25	U	310	CLA	CHC-C1C	2.11	1.42	1.38
25	P	301	CLA	CMD-C2D	-2.11	1.46	1.50
37	W	317	NEX	C22-C21	-2.11	1.51	1.54
24	X	305	CHL	CAC-C3C	-2.11	1.48	1.51
25	5	610	CLA	CMB-C2B	-2.11	1.46	1.50
29	W	316	Q6L	C11-C03	-2.11	1.48	1.51
25	G	203	CLA	C3B-C4B	2.11	1.48	1.42
25	U	309	CLA	CMB-C2B	-2.11	1.46	1.50
25	U	311	CLA	CMC-C2C	-2.11	1.46	1.50
29	X	317	Q6L	C33-C32	2.11	1.35	1.33
25	1	607	CLA	CMB-C2B	-2.11	1.46	1.50
30	M	101	BCR	C35-C13	2.10	1.55	1.50
25	O	2001	CLA	C3B-C4B	2.10	1.48	1.42
25	A	814	CLA	CHC-C4B	-2.10	1.34	1.39
25	4	309	CLA	CHC-C1C	2.10	1.42	1.38
29	V	319	Q6L	C04-C03	2.10	1.56	1.53
25	L	304	CLA	CMD-C2D	-2.10	1.46	1.50
25	A	823	CLA	CHC-C4B	-2.10	1.34	1.39
25	B	834	CLA	CHC-C4B	-2.10	1.34	1.39
25	B	824	CLA	MG-NB	-2.10	2.01	2.05
27	3	316	XAT	O24-C25	-2.10	1.43	1.46
24	1	604	CHL	MG-ND	-2.10	2.01	2.05
25	U	301	CLA	MG-ND	-2.10	2.01	2.05
25	N	203	CLA	C1B-NB	-2.10	1.35	1.37
25	B	842	CLA	CMD-C2D	-2.10	1.46	1.50
30	I	101	BCR	C30-C25	-2.10	1.51	1.53
25	B	804	CLA	CMB-C2B	-2.10	1.46	1.50
25	L	301	CLA	CMB-C2B	-2.10	1.46	1.50
37	P	317	NEX	O24-C25	-2.10	1.43	1.46
25	A	806	CLA	CMC-C2C	-2.10	1.46	1.50
25	L	304	CLA	C3B-C4B	2.10	1.48	1.42
24	2	601	CHL	CMB-C2B	-2.10	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	847	BCR	C36-C18	2.10	1.55	1.50
29	R	304	Q6L	C04-C03	2.10	1.56	1.53
29	X	301	Q6L	C04-C03	2.10	1.56	1.53
25	2	610	CLA	CMB-C2B	-2.10	1.46	1.50
24	V	306	CHL	MG-ND	-2.10	2.01	2.05
24	T	305	CHL	CHC-C1C	2.10	1.43	1.39
24	V	305	CHL	MG-NB	-2.10	2.01	2.05
25	B	813	CLA	C3B-C4B	2.10	1.48	1.42
25	T	312	CLA	CMB-C2B	-2.10	1.46	1.50
29	2	616	Q6L	C33-C32	2.10	1.35	1.33
25	W	310	CLA	CHC-C1C	2.10	1.42	1.38
25	A	809	CLA	CMD-C2D	-2.10	1.46	1.50
26	S	319	IWJ	C32-C30	2.10	1.55	1.51
26	U	316	IWJ	C32-C30	2.10	1.55	1.51
26	V	320	IWJ	C32-C30	2.10	1.55	1.51
30	A	852	BCR	C20-C19	-2.10	1.29	1.34
25	A	807	CLA	C2-C3	2.10	1.37	1.33
25	5	601	CLA	C1B-C2B	2.10	1.48	1.43
25	1	605	CLA	CHC-C1C	2.10	1.42	1.38
25	P	313	CLA	CHC-C1C	2.10	1.42	1.38
25	A	835	CLA	MG-ND	-2.10	2.01	2.05
24	R	309	CHL	CHD-C1D	-2.10	1.36	1.39
25	A	824	CLA	C1B-NB	-2.10	1.35	1.37
25	A	820	CLA	MG-ND	-2.10	2.01	2.05
24	W	306	CHL	CHC-C4B	-2.10	1.36	1.39
25	A	810	CLA	CHC-C1C	2.09	1.42	1.38
25	B	808	CLA	C4B-NB	2.09	1.40	1.37
25	Q	304	CLA	CMD-C2D	-2.09	1.46	1.50
25	A	828	CLA	C3B-C4B	2.09	1.48	1.42
30	3	317	BCR	C8-C9	2.09	1.50	1.46
24	R	311	CHL	CHC-C1C	2.09	1.43	1.39
25	R	314	CLA	CMB-C2B	-2.09	1.46	1.50
25	G	204	CLA	CHC-C1C	2.09	1.42	1.38
30	3	318	BCR	C37-C22	2.09	1.55	1.50
25	3	309	CLA	CMB-C2B	-2.09	1.46	1.50
24	6	606	CHL	CMB-C2B	-2.09	1.47	1.51
24	Q	307	CHL	C1A-CHA	-2.09	1.37	1.40
25	A	831	CLA	CMD-C2D	-2.09	1.46	1.50
25	B	805	CLA	MG-NB	-2.09	2.01	2.05
25	B	817	CLA	C3B-C4B	2.09	1.48	1.42
25	4	303	CLA	MG-NB	-2.09	2.01	2.05
25	B	835	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	841	CLA	CHC-C1C	2.09	1.42	1.38
25	U	312	CLA	CHC-C1C	2.09	1.42	1.38
24	R	310	CHL	MG-ND	-2.09	2.01	2.05
24	P	305	CHL	CMC-C2C	2.09	1.49	1.44
24	P	305	CHL	CMA-C3A	-2.09	1.49	1.53
24	P	314	CHL	CMC-C2C	2.09	1.49	1.44
25	N	202	CLA	CAC-C3C	-2.09	1.45	1.51
24	Q	308	CHL	MG-NB	-2.09	2.01	2.05
25	A	814	CLA	MG-NB	-2.09	2.01	2.05
29	W	316	Q6L	C29-C27	2.09	1.50	1.46
25	A	810	CLA	C3B-C4B	2.09	1.48	1.42
25	A	822	CLA	CMB-C2B	-2.09	1.46	1.50
25	B	837	CLA	C3B-C4B	2.09	1.48	1.42
37	R	321	NEX	C35-C15	-2.09	1.30	1.36
38	Q	310	KC2	CMB-C2B	-2.09	1.46	1.50
25	R	313	CLA	CAA-C2A	-2.09	1.50	1.54
24	V	305	CHL	CMA-C3A	-2.09	1.49	1.53
25	R	314	CLA	CHC-C1C	2.09	1.42	1.38
25	4	303	CLA	C1B-NB	-2.09	1.35	1.37
25	Q	313	CLA	CMB-C2B	-2.09	1.46	1.50
25	A	839	CLA	C3B-C4B	2.09	1.48	1.42
25	B	841	CLA	C3B-C4B	2.09	1.48	1.42
30	F	801	BCR	C12-C13	2.09	1.50	1.46
30	L	306	BCR	C1-C6	-2.09	1.51	1.53
25	B	820	CLA	CHC-C4B	-2.09	1.34	1.39
25	2	614	CLA	CMB-C2B	-2.09	1.46	1.50
38	P	308	KC2	CHB-C1B	2.09	1.42	1.38
29	R	323	Q6L	C02-C03	2.09	1.37	1.34
25	3	305	CLA	MG-NB	-2.08	2.01	2.05
25	5	604	CLA	CMD-C2D	-2.08	1.46	1.50
24	U	313	CHL	CBD-CGD	-2.08	1.49	1.52
37	H	306	NEX	C1-C6	-2.08	1.51	1.54
25	A	834	CLA	MG-NB	-2.08	2.01	2.05
25	B	804	CLA	CMD-C2D	-2.08	1.46	1.50
38	W	308	KC2	MG-NC	2.08	2.11	2.06
24	1	601	CHL	CMC-C2C	2.08	1.49	1.44
25	B	811	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	813	CLA	CHC-C4B	-2.08	1.34	1.39
37	H	306	NEX	C35-C15	-2.08	1.30	1.36
25	B	817	CLA	CHC-C4B	-2.08	1.34	1.39
25	A	819	CLA	CMA-C3A	-2.08	1.48	1.53
24	R	311	CHL	CHB-C1B	2.08	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	825	CLA	CMD-C2D	-2.08	1.46	1.50
26	X	318	IWJ	O39-C29	-2.08	1.39	1.43
25	W	303	CLA	C1B-C2B	2.08	1.48	1.43
25	B	812	CLA	CAB-C3B	-2.08	1.41	1.47
26	Q	303	IWJ	O39-C29	-2.08	1.39	1.43
24	R	318	CHL	CMC-C2C	2.08	1.49	1.44
25	B	806	CLA	CMC-C2C	-2.08	1.46	1.50
25	X	302	CLA	O2D-CED	-2.08	1.40	1.45
25	X	302	CLA	CMA-C3A	-2.08	1.48	1.53
25	2	606	CLA	CHC-C1C	2.08	1.42	1.38
29	R	301	Q6L	C01-C02	2.08	1.54	1.50
38	X	309	KC2	MG-NC	2.08	2.11	2.06
25	V	312	CLA	MG-NB	-2.08	2.01	2.05
25	O	2005	CLA	CMB-C2B	-2.08	1.46	1.50
25	P	302	CLA	CMD-C2D	-2.08	1.46	1.50
25	X	311	CLA	CHC-C1C	2.08	1.42	1.38
25	A	836	CLA	C1B-NB	-2.08	1.35	1.37
25	X	313	CLA	CHC-C1C	2.08	1.42	1.38
25	A	808	CLA	CMC-C2C	-2.08	1.46	1.50
25	A	803	CLA	C1D-ND	2.08	1.40	1.37
25	W	303	CLA	C1B-NB	-2.08	1.35	1.37
25	A	836	CLA	CMB-C2B	-2.08	1.46	1.50
25	U	302	CLA	CMB-C2B	-2.08	1.46	1.50
25	A	833	CLA	MG-ND	-2.08	2.01	2.05
25	B	838	CLA	MG-NB	-2.08	2.01	2.05
29	U	317	Q6L	C04-C03	2.07	1.56	1.53
25	P	302	CLA	CMB-C2B	-2.07	1.46	1.50
29	V	321	Q6L	C33-C32	2.07	1.35	1.33
25	W	301	CLA	CMD-C2D	-2.07	1.46	1.50
25	3	307	CLA	CMD-C2D	-2.07	1.46	1.50
25	X	302	CLA	CMB-C2B	-2.07	1.46	1.50
26	P	320	IWJ	C26-C24	-2.07	1.45	1.49
25	1	603	CLA	CAC-C3C	-2.07	1.45	1.51
25	B	843	CLA	MG-NB	-2.07	2.01	2.05
25	A	829	CLA	CMA-C3A	-2.07	1.48	1.53
25	A	816	CLA	C1B-NB	-2.07	1.35	1.37
25	B	815	CLA	MG-ND	-2.07	2.01	2.05
25	X	302	CLA	CHC-C1C	2.07	1.42	1.38
25	B	803	CLA	MG-ND	-2.07	2.01	2.05
25	A	808	CLA	CAB-C3B	-2.07	1.41	1.47
25	4	313	CLA	CMA-C3A	-2.07	1.48	1.53
25	3	304	CLA	C1D-C2D	2.07	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	601	CLA	CAB-C3B	-2.07	1.41	1.47
25	B	841	CLA	CHC-C4B	-2.07	1.34	1.39
25	2	609	CLA	MG-NB	-2.07	2.01	2.05
25	4	311	CLA	C1B-NB	-2.07	1.35	1.37
24	4	302	CHL	C1A-CHA	-2.07	1.37	1.40
25	3	311	CLA	O2A-CGA	2.07	1.39	1.33
25	4	305	CLA	CHC-C4B	-2.07	1.34	1.39
25	A	856	CLA	CMD-C2D	-2.07	1.46	1.50
30	M	101	BCR	C19-C18	2.07	1.50	1.46
25	B	805	CLA	CMC-C2C	-2.07	1.46	1.50
25	5	603	CLA	C1B-NB	-2.07	1.35	1.37
30	G	205	BCR	C23-C22	2.07	1.50	1.46
24	X	305	CHL	CHC-C1C	2.07	1.43	1.39
25	A	831	CLA	C4-C3	-2.07	1.45	1.50
25	V	313	CLA	CMB-C2B	-2.07	1.46	1.50
25	O	2002	CLA	CMC-C2C	-2.06	1.46	1.50
25	T	310	CLA	CHC-C1C	2.06	1.42	1.38
25	5	601	CLA	CMB-C2B	-2.06	1.46	1.50
25	X	313	CLA	CMD-C2D	-2.06	1.46	1.50
25	2	608	CLA	C3B-C4B	2.06	1.48	1.42
25	W	311	CLA	MG-NB	-2.06	2.01	2.05
25	5	606	CLA	CHC-C1C	2.06	1.42	1.38
29	X	317	Q6L	C04-C03	2.06	1.56	1.53
25	Q	304	CLA	CHC-C1C	2.06	1.42	1.38
24	R	308	CHL	CMC-C2C	2.06	1.49	1.44
27	1	612	XAT	C2-C1	-2.06	1.51	1.54
25	B	810	CLA	CHC-C4B	-2.06	1.34	1.39
24	3	306	CHL	C3D-CAD	-2.06	1.43	1.47
25	T	313	CLA	CMC-C2C	-2.06	1.46	1.50
29	W	315	Q6L	C33-C32	2.06	1.35	1.33
30	B	847	BCR	C16-C15	-2.06	1.30	1.36
38	R	312	KC2	C1B-C2B	2.06	1.49	1.45
25	Q	301	CLA	C3B-C4B	2.06	1.48	1.42
25	B	816	CLA	CMC-C2C	-2.06	1.46	1.50
24	Q	308	CHL	CMC-C2C	2.06	1.49	1.44
25	S	303	CLA	C1B-C2B	2.06	1.48	1.43
25	A	827	CLA	C5-C3	-2.06	1.47	1.51
29	W	320	Q6L	C33-C32	2.06	1.35	1.33
24	X	305	CHL	CHD-C1D	-2.06	1.36	1.39
24	V	307	CHL	CBD-CGD	-2.06	1.49	1.52
25	3	305	CLA	CHC-C1C	2.06	1.42	1.38
24	1	601	CHL	C1A-CHA	-2.06	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	813	CLA	C3B-C4B	2.06	1.48	1.42
24	S	314	CHL	CAC-C3C	-2.06	1.48	1.51
25	T	310	CLA	CMB-C2B	-2.05	1.46	1.50
24	W	305	CHL	CHC-C4B	-2.05	1.36	1.39
38	P	308	KC2	C1B-C2B	2.05	1.49	1.45
25	R	313	CLA	CHC-C1C	2.05	1.42	1.38
25	K	203	CLA	C3B-C4B	2.05	1.48	1.42
25	H	301	CLA	CMB-C2B	-2.05	1.46	1.50
24	W	305	CHL	MG-NB	-2.05	2.01	2.05
24	R	310	CHL	MG-NB	-2.05	2.01	2.05
25	A	825	CLA	CAC-C3C	-2.05	1.45	1.51
29	V	321	Q6L	C35-C34	2.05	1.55	1.52
25	2	603	CLA	CHC-C4B	-2.05	1.34	1.39
25	U	310	CLA	CMD-C2D	-2.05	1.46	1.50
25	B	836	CLA	CAB-C3B	-2.05	1.41	1.47
25	4	314	CLA	C3B-C4B	2.05	1.48	1.42
24	P	314	CHL	CBD-CGD	-2.05	1.49	1.52
25	4	305	CLA	CMD-C2D	-2.05	1.46	1.50
25	5	609	CLA	CMC-C2C	-2.05	1.46	1.50
25	S	312	CLA	CMB-C2B	-2.05	1.46	1.50
30	2	618	BCR	C8-C9	2.05	1.50	1.46
25	4	315	CLA	MG-NB	-2.05	2.01	2.05
25	U	302	CLA	MG-NB	-2.05	2.01	2.05
36	A	854	DGD	O5D-C1E	2.05	1.43	1.40
25	A	837	CLA	CHC-C1C	2.05	1.42	1.38
24	W	305	CHL	CMA-C3A	-2.05	1.49	1.53
30	J	103	BCR	C8-C9	2.05	1.50	1.46
25	H	304	CLA	C3C-C2C	2.05	1.41	1.36
25	B	843	CLA	CMD-C2D	-2.05	1.46	1.50
25	W	313	CLA	CHC-C1C	2.05	1.42	1.38
25	P	301	CLA	CMB-C2B	-2.05	1.46	1.50
25	S	310	CLA	CMC-C2C	-2.05	1.46	1.50
24	4	307	CHL	CHC-C1C	2.05	1.43	1.39
25	A	809	CLA	MG-NB	-2.04	2.01	2.05
25	3	304	CLA	C3B-C4B	2.04	1.48	1.42
29	W	315	Q6L	C11-C03	-2.04	1.48	1.51
25	5	604	CLA	C3B-C2B	-2.04	1.36	1.44
25	4	305	CLA	CHC-C1C	2.04	1.42	1.38
26	4	317	IWJ	C28-C29	-2.04	1.51	1.54
25	A	833	CLA	CMC-C2C	-2.04	1.46	1.50
25	6	611	CLA	CMB-C2B	-2.04	1.46	1.50
25	L	304	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	322	Q6L	C29-C27	2.04	1.50	1.46
25	T	303	CLA	MG-ND	-2.04	2.01	2.05
25	W	313	CLA	MG-NB	-2.04	2.01	2.05
25	A	836	CLA	CMD-C2D	-2.04	1.46	1.50
30	G	205	BCR	C16-C15	-2.04	1.30	1.36
25	T	312	CLA	CHC-C1C	2.04	1.42	1.38
29	S	321	Q6L	C11-C03	-2.04	1.48	1.51
25	B	804	CLA	CHC-C1C	2.04	1.42	1.38
30	M	101	BCR	C16-C15	-2.04	1.30	1.36
25	P	309	CLA	CMB-C2B	-2.04	1.46	1.50
25	B	807	CLA	CHC-C1C	2.04	1.42	1.38
24	X	307	CHL	C3B-C2B	-2.04	1.37	1.40
24	3	306	CHL	C3D-C2D	-2.04	1.36	1.39
26	R	303	IWJ	O39-C29	-2.04	1.39	1.43
25	B	805	CLA	C3B-C4B	2.04	1.48	1.42
30	L	306	BCR	C19-C18	2.04	1.50	1.46
25	V	310	CLA	CMD-C2D	-2.04	1.46	1.50
25	6	603	CLA	C3B-C4B	2.04	1.48	1.42
25	A	820	CLA	C4B-NB	2.04	1.40	1.37
25	5	601	CLA	C3B-C4B	2.04	1.48	1.42
25	G	202	CLA	CHC-C1C	2.04	1.42	1.38
24	R	308	CHL	CAC-C3C	-2.04	1.48	1.51
25	A	812	CLA	CHC-C1C	2.04	1.42	1.38
25	H	302	CLA	CMD-C2D	-2.04	1.46	1.50
26	P	318	IWJ	C32-C30	2.04	1.55	1.51
24	T	305	CHL	CAC-C3C	-2.04	1.48	1.51
29	R	319	Q6L	C04-C03	2.04	1.56	1.53
25	X	314	CLA	CMD-C2D	-2.04	1.46	1.50
24	U	304	CHL	MG-NB	-2.04	2.01	2.05
30	B	848	BCR	C12-C13	2.04	1.50	1.46
25	B	832	CLA	CHC-C1C	2.04	1.42	1.38
25	T	309	CLA	C1A-CHA	-2.04	1.34	1.43
25	3	312	CLA	MG-NB	-2.04	2.01	2.05
24	U	304	CHL	CHC-C1C	2.03	1.43	1.39
25	U	308	CLA	C1A-CHA	-2.03	1.34	1.43
36	B	850	DGD	O3G-C1D	2.03	1.43	1.40
29	U	315	Q6L	C29-C27	2.03	1.50	1.46
25	A	803	CLA	CMD-C2D	-2.03	1.46	1.50
24	U	304	CHL	MG-ND	-2.03	2.01	2.05
25	X	304	CLA	CHC-C4B	-2.03	1.34	1.39
24	S	305	CHL	CHC-C1C	2.03	1.43	1.39
25	O	2004	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	314	CLA	MG-NB	-2.03	2.01	2.05
29	X	316	Q6L	C04-C03	2.03	1.56	1.53
25	3	313	CLA	CHC-C4B	-2.03	1.34	1.39
25	A	812	CLA	CMD-C2D	-2.03	1.46	1.50
30	G	201	BCR	C37-C22	2.03	1.54	1.50
25	W	309	CLA	CMD-C2D	-2.03	1.46	1.50
25	W	302	CLA	CHC-C4B	-2.03	1.34	1.39
25	A	838	CLA	C3B-C4B	2.03	1.48	1.42
25	A	821	CLA	CHC-C1C	2.03	1.42	1.38
25	Q	305	CLA	C3B-C4B	2.03	1.48	1.42
29	X	319	Q6L	C01-C02	2.03	1.54	1.50
25	B	817	CLA	CMA-C3A	-2.03	1.48	1.53
38	P	308	KC2	MG-NB	-2.03	2.01	2.05
38	S	308	KC2	MG-NC	2.03	2.11	2.06
26	T	321	IWJ	C26-C24	-2.03	1.45	1.49
24	V	314	CHL	CAC-C3C	-2.03	1.48	1.51
25	3	312	CLA	C1B-NB	-2.03	1.35	1.37
25	A	842	CLA	C1B-NB	-2.03	1.35	1.37
25	A	828	CLA	CMA-C3A	-2.03	1.48	1.53
25	V	302	CLA	MG-NC	2.02	2.11	2.06
25	W	302	CLA	CMD-C2D	-2.02	1.46	1.50
25	H	302	CLA	CHC-C4B	-2.02	1.34	1.39
25	Q	306	CLA	CHC-C1C	2.02	1.42	1.38
26	U	316	IWJ	C26-C24	-2.02	1.45	1.49
25	L	304	CLA	CHC-C1C	2.02	1.42	1.38
24	R	309	CHL	CMC-C2C	2.02	1.49	1.44
25	O	2004	CLA	CMC-C2C	-2.02	1.46	1.50
25	X	304	CLA	CMD-C2D	-2.02	1.46	1.50
25	S	303	CLA	CMC-C2C	-2.02	1.46	1.50
25	X	303	CLA	CMB-C2B	-2.02	1.46	1.50
29	X	319	Q6L	C11-C03	-2.02	1.48	1.51
25	3	304	CLA	CHC-C4B	-2.02	1.34	1.39
25	B	819	CLA	CHC-C4B	-2.02	1.34	1.39
25	3	308	CLA	CMB-C2B	-2.02	1.46	1.50
25	B	803	CLA	CMD-C2D	-2.02	1.46	1.50
25	5	601	CLA	CHC-C1C	2.02	1.42	1.38
24	Q	316	CHL	C3A-C2A	2.02	1.56	1.54
25	U	302	CLA	MG-ND	-2.02	2.01	2.05
25	B	804	CLA	C3B-C4B	2.02	1.48	1.42
25	K	206	CLA	CMC-C2C	-2.02	1.46	1.50
25	V	302	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	810	CLA	C4-C3	-2.02	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	607	CLA	CHC-C4B	-2.02	1.34	1.39
25	B	821	CLA	C1B-NB	-2.02	1.35	1.37
25	B	831	CLA	O2D-CED	-2.02	1.40	1.45
25	A	826	CLA	CMC-C2C	-2.02	1.46	1.50
30	L	305	BCR	C19-C18	2.02	1.50	1.46
25	F	802	CLA	MG-ND	-2.02	2.01	2.05
25	3	307	CLA	MG-NB	-2.02	2.01	2.05
25	K	204	CLA	C1B-NB	-2.02	1.35	1.37
25	S	309	CLA	CMB-C2B	-2.02	1.46	1.50
30	3	317	BCR	C19-C18	2.02	1.50	1.46
30	M	101	BCR	C10-C9	2.02	1.40	1.35
24	T	306	CHL	CMA-C3A	-2.02	1.49	1.53
25	S	302	CLA	C3B-C4B	2.02	1.48	1.42
29	T	315	Q6L	C11-C03	-2.02	1.48	1.51
25	B	830	CLA	C1B-C2B	2.02	1.47	1.43
25	Q	311	CLA	CHC-C1C	2.02	1.42	1.38
25	P	310	CLA	CMB-C2B	-2.02	1.46	1.50
25	B	817	CLA	CMD-C2D	-2.02	1.46	1.50
25	P	309	CLA	CMD-C2D	-2.02	1.46	1.50
24	6	605	CHL	MG-NB	-2.02	2.01	2.05
25	B	809	CLA	MG-ND	-2.02	2.01	2.05
25	B	812	CLA	C1B-NB	-2.02	1.35	1.37
37	T	317	NEX	C38-C25	2.02	1.54	1.51
24	S	306	CHL	MG-ND	-2.02	2.01	2.05
24	V	304	CHL	CHC-C1C	2.02	1.43	1.39
25	A	809	CLA	C3B-C4B	2.01	1.48	1.42
25	5	607	CLA	MG-NB	-2.01	2.01	2.05
25	A	823	CLA	MG-ND	-2.01	2.01	2.05
25	3	309	CLA	CHC-C1C	2.01	1.42	1.38
25	4	312	CLA	CHC-C1C	2.01	1.42	1.38
24	2	615	CHL	C3B-C2B	-2.01	1.37	1.40
25	1	609	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	825	CLA	CMC-C2C	-2.01	1.46	1.50
25	X	304	CLA	C1B-C2B	2.01	1.47	1.43
25	R	316	CLA	CHC-C1C	2.01	1.42	1.38
24	R	311	CHL	CAC-C3C	-2.01	1.48	1.51
24	S	306	CHL	C3B-C2B	-2.01	1.37	1.40
25	V	312	CLA	MG-ND	-2.01	2.01	2.05
25	A	809	CLA	CHC-C1C	2.01	1.42	1.38
30	A	850	BCR	C19-C18	2.01	1.50	1.46
25	2	603	CLA	CMD-C2D	-2.01	1.46	1.50
24	X	307	CHL	O2A-CGA	2.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	311	CLA	CMC-C2C	-2.01	1.46	1.50
25	2	610	CLA	CHC-C1C	2.01	1.42	1.38
25	R	313	CLA	MG-NA	2.01	2.11	2.06
24	P	306	CHL	C3B-C2B	-2.01	1.37	1.40
25	B	828	CLA	MG-ND	-2.01	2.01	2.05
24	R	302	CHL	C1A-C2A	2.01	1.55	1.51
25	X	312	CLA	CHC-C4B	-2.01	1.34	1.39
25	W	311	CLA	C1B-NB	-2.01	1.35	1.37
30	J	101	BCR	C16-C17	2.01	1.49	1.43
25	B	838	CLA	CMD-C2D	-2.01	1.46	1.50
25	A	822	CLA	MG-NB	-2.01	2.01	2.05
25	5	603	CLA	CMD-C2D	-2.00	1.46	1.50
25	K	204	CLA	CMB-C2B	-2.00	1.46	1.50
25	V	311	CLA	CHC-C1C	2.00	1.42	1.38
25	4	304	CLA	CMD-C2D	-2.00	1.46	1.50
25	Q	306	CLA	C1A-CHA	-2.00	1.34	1.43
25	Q	315	CLA	CHC-C1C	2.00	1.42	1.38
25	Q	313	CLA	CHC-C4B	-2.00	1.34	1.39
27	6	615	XAT	C2-C1	-2.00	1.51	1.54
30	B	849	BCR	C16-C15	-2.00	1.30	1.36
24	W	314	CHL	CBD-CGD	-2.00	1.50	1.52
25	G	204	CLA	C1B-C2B	2.00	1.47	1.43
25	P	301	CLA	CMA-C3A	-2.00	1.49	1.53
25	4	310	CLA	CHC-C1C	2.00	1.42	1.38
30	G	205	BCR	C34-C9	2.00	1.54	1.50
26	Q	303	IWJ	C09-C08	2.00	1.36	1.32

All (4280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	318	XAT	O4-C5-C4	12.50	125.20	113.49
37	S	317	NEX	O24-C25-C24	10.98	123.78	113.49
25	1	607	CLA	CHA-C4D-ND	10.67	134.35	125.22
37	R	321	NEX	O24-C25-C24	10.63	123.46	113.49
27	6	615	XAT	O4-C5-C4	10.55	123.38	113.49
26	U	316	IWJ	C35-C29-C30	10.51	119.56	108.78
37	W	317	NEX	O24-C25-C24	10.45	123.28	113.49
27	2	617	XAT	O4-C5-C4	10.02	122.88	113.49
27	1	612	XAT	O4-C5-C4	9.98	122.85	113.49
30	B	849	BCR	C24-C23-C22	-9.98	111.47	126.23
26	3	315	IWJ	C32-C30-C29	-9.80	103.88	113.96
24	X	307	CHL	OMC-CMC-C2C	-9.02	109.46	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	T	317	NEX	O24-C25-C24	8.97	121.90	113.49
29	V	315	Q6L	C11-C03-C04	-8.94	111.57	116.81
38	P	308	KC2	CMA-C3A-C2A	-8.83	107.06	128.43
27	5	612	XAT	O4-C5-C18	8.76	124.84	115.05
38	P	308	KC2	C1A-NA-C4A	8.71	110.65	106.68
24	4	307	CHL	OMC-CMC-C2C	-8.69	110.03	125.12
30	K	202	BCR	C36-C18-C19	8.60	131.23	118.09
37	H	306	NEX	O24-C25-C24	8.53	121.48	113.49
29	2	616	Q6L	C11-C03-C04	-8.43	111.88	116.81
38	R	312	KC2	C1A-NA-C4A	8.37	110.50	106.68
30	B	847	BCR	C31-C1-C6	-8.31	97.21	110.24
30	J	101	BCR	C36-C18-C19	8.31	130.78	118.09
38	X	309	KC2	CMA-C3A-C4A	-8.29	112.08	125.03
37	P	317	NEX	O24-C25-C24	8.16	121.14	113.49
29	X	319	Q6L	C11-C03-C04	-8.04	112.10	116.81
25	Q	304	CLA	C4A-NA-C1A	7.99	110.32	106.68
25	3	301	CLA	C4A-NA-C1A	7.92	110.29	106.68
30	B	846	BCR	C37-C22-C21	-7.78	110.22	122.82
27	3	316	XAT	O24-C25-C24	7.70	120.70	113.49
38	T	308	KC2	CMA-C3A-C4A	-7.60	113.16	125.03
29	T	322	Q6L	C11-C03-C04	-7.53	112.40	116.81
27	3	316	XAT	O4-C5-C4	7.52	120.54	113.49
30	B	845	BCR	C33-C5-C6	7.45	132.61	124.48
30	K	207	BCR	C36-C18-C19	7.43	129.44	118.09
38	S	308	KC2	CMA-C3A-C4A	-7.40	113.47	125.03
30	A	849	BCR	C36-C18-C19	7.38	129.36	118.09
27	5	612	XAT	O4-C5-C4	7.32	120.36	113.49
38	U	307	KC2	CMA-C3A-C4A	-7.25	113.70	125.03
25	A	842	CLA	C4A-NA-C1A	7.25	109.98	106.68
29	R	323	Q6L	C11-C12-C13	7.23	133.09	112.86
25	A	830	CLA	C4A-NA-C1A	7.22	109.97	106.68
38	P	308	KC2	CMA-C3A-C4A	-7.21	113.77	125.03
29	R	301	Q6L	C11-C12-C13	7.15	132.87	112.86
25	A	815	CLA	C4A-NA-C1A	7.12	109.93	106.68
38	Q	310	KC2	CMA-C3A-C4A	-7.11	113.92	125.03
24	T	305	CHL	C1B-CHB-C4A	7.07	125.87	121.32
38	Q	310	KC2	C1A-NA-C4A	7.07	109.90	106.68
37	P	317	NEX	C16-C1-C6	7.05	116.78	110.47
30	B	848	BCR	C36-C18-C19	7.02	128.81	118.09
25	1	603	CLA	C4A-NA-C1A	6.99	109.87	106.68
25	Q	301	CLA	C4A-NA-C1A	6.93	109.84	106.68
29	W	320	Q6L	C11-C12-C13	6.93	132.26	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	318	BCR	C36-C18-C19	6.93	128.67	118.09
29	2	616	Q6L	C12-C11-C03	6.91	127.43	113.64
30	F	804	BCR	C36-C18-C19	6.89	128.61	118.09
30	A	852	BCR	C37-C22-C23	6.88	128.60	118.09
30	3	319	BCR	C36-C18-C19	6.88	128.59	118.09
30	J	103	BCR	C36-C18-C19	6.87	128.58	118.09
25	4	304	CLA	C4A-NA-C1A	6.86	109.81	106.68
27	3	316	XAT	C19-C9-C8	-6.82	107.67	118.09
34	B	844	PQN	C11-C12-C13	-6.77	115.16	126.83
29	X	319	Q6L	C11-C12-C13	6.76	131.77	112.86
30	I	101	BCR	C38-C26-C25	-6.74	117.13	124.48
26	V	318	IWJ	C32-C30-C29	-6.73	107.04	113.96
29	X	317	Q6L	C12-C11-C03	6.73	127.06	113.64
29	S	316	Q6L	C12-C11-C03	6.71	127.03	113.64
30	L	307	BCR	C36-C18-C17	-6.71	111.94	122.82
29	U	317	Q6L	C11-C12-C13	6.70	131.61	112.86
29	Q	317	Q6L	C11-C12-C13	6.70	131.59	112.86
38	W	308	KC2	C1A-C2A-C3A	-6.69	101.13	107.28
29	R	301	Q6L	C11-C03-C04	-6.69	112.89	116.81
38	X	309	KC2	C1A-NA-C4A	6.68	109.73	106.68
30	L	307	BCR	C36-C18-C19	6.68	128.29	118.09
30	L	305	BCR	C38-C26-C25	-6.67	117.20	124.48
27	4	318	XAT	O24-C25-C24	6.67	119.74	113.49
24	4	308	CHL	CBC-CAC-C3C	-6.66	103.33	112.87
27	5	612	XAT	O24-C25-C24	6.66	119.73	113.49
38	T	308	KC2	C1A-NA-C4A	6.65	109.71	106.68
27	2	617	XAT	O24-C25-C24	6.65	119.72	113.49
29	P	321	Q6L	C11-C12-C13	6.63	131.41	112.86
38	Q	310	KC2	C2A-C3A-C4A	-6.60	101.45	106.41
25	K	204	CLA	C4A-NA-C1A	6.59	109.69	106.68
30	B	845	BCR	C36-C18-C19	6.58	128.14	118.09
29	V	316	Q6L	C11-C12-C13	6.57	131.23	112.86
25	3	311	CLA	C4A-NA-C1A	6.55	109.67	106.68
25	4	313	CLA	C4A-NA-C1A	6.55	109.67	106.68
25	A	843	CLA	C4A-NA-C1A	6.53	109.66	106.68
25	B	809	CLA	C4A-NA-C1A	6.53	109.66	106.68
38	S	308	KC2	CMA-C3A-C2A	-6.51	112.68	128.43
25	A	816	CLA	C4A-NA-C1A	6.50	109.64	106.68
29	U	314	Q6L	C11-C12-C13	6.49	131.02	112.86
29	V	319	Q6L	C11-C12-C13	6.49	131.02	112.86
29	R	320	Q6L	C12-C11-C03	6.48	126.56	113.64
30	A	850	BCR	C36-C18-C19	6.48	127.98	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	V	321	Q6L	C11-C12-C13	6.48	130.98	112.86
29	T	316	Q6L	C12-C11-C03	6.47	126.54	113.64
29	P	316	Q6L	C12-C11-C03	6.47	126.53	113.64
30	B	847	BCR	C38-C26-C25	-6.46	117.44	124.48
30	L	307	BCR	C31-C1-C6	6.44	120.34	110.24
26	Q	320	IWJ	C35-C29-C30	6.43	115.37	108.78
30	A	850	BCR	C38-C26-C25	-6.41	117.50	124.48
38	R	312	KC2	CMA-C3A-C2A	-6.40	112.93	128.43
26	P	320	IWJ	C32-C30-C29	-6.40	107.38	113.96
29	W	316	Q6L	C12-C11-C03	6.39	126.39	113.64
25	B	815	CLA	C4A-NA-C1A	6.38	109.59	106.68
29	R	323	Q6L	C05-C04-C03	6.36	119.02	110.61
25	R	316	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	B	807	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	X	312	CLA	C4A-NA-C1A	6.33	109.57	106.68
27	1	612	XAT	C19-C9-C8	-6.33	108.42	118.09
29	W	319	Q6L	C12-C11-C03	6.32	126.25	113.64
30	4	319	BCR	C38-C26-C25	-6.32	117.59	124.48
29	S	320	Q6L	C11-C12-C13	6.31	130.52	112.86
30	A	851	BCR	C24-C23-C22	-6.31	116.90	126.23
25	B	843	CLA	C4A-NA-C1A	6.30	109.56	106.68
25	5	607	CLA	C4A-NA-C1A	6.30	109.55	106.68
25	A	856	CLA	O2D-CGD-O1D	-6.29	111.61	123.85
29	T	319	Q6L	C11-C03-C04	-6.28	113.13	116.81
29	R	319	Q6L	C11-C12-C13	6.27	130.41	112.86
29	S	323	Q6L	C11-C12-C13	6.27	130.41	112.86
29	T	319	Q6L	C11-C12-C13	6.26	130.37	112.86
30	4	319	BCR	C36-C18-C19	6.24	127.62	118.09
25	A	841	CLA	C4A-NA-C1A	6.24	109.52	106.68
25	Q	313	CLA	C4A-NA-C1A	6.24	109.52	106.68
26	S	318	IWJ	C35-C29-C30	6.22	115.16	108.78
29	W	315	Q6L	C11-C12-C13	6.21	130.25	112.86
38	U	307	KC2	C1A-NA-C4A	6.20	109.51	106.68
30	L	307	BCR	C34-C9-C10	-6.20	112.77	122.82
38	U	307	KC2	CMA-C3A-C2A	-6.20	113.43	128.43
30	L	307	BCR	C8-C7-C6	-6.20	110.45	127.00
25	L	304	CLA	C4A-NA-C1A	6.19	109.50	106.68
38	S	308	KC2	C1A-NA-C4A	6.18	109.50	106.68
25	B	833	CLA	C4A-NA-C1A	6.18	109.50	106.68
30	A	851	BCR	C8-C7-C6	-6.17	110.51	127.00
29	P	319	Q6L	C11-C12-C13	6.16	130.11	112.86
29	S	315	Q6L	C12-C11-C03	6.16	125.92	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	842	CLA	C4A-NA-C1A	6.16	109.49	106.68
29	O	2006	Q6L	C11-C12-C13	6.14	130.03	112.86
25	A	829	CLA	C4A-NA-C1A	6.13	109.48	106.68
30	F	801	BCR	C24-C23-C22	-6.12	117.17	126.23
24	T	320	CHL	O2D-CGD-CBD	6.11	117.66	110.95
25	A	819	CLA	C4A-NA-C1A	6.10	109.46	106.68
30	4	319	BCR	C8-C7-C6	-6.08	110.75	127.00
24	2	605	CHL	C1B-CHB-C4A	6.07	125.23	121.32
25	B	822	CLA	C4A-NA-C1A	6.06	109.44	106.68
29	Q	318	Q6L	C12-C11-C03	6.06	125.72	113.64
25	B	840	CLA	C4A-NA-C1A	6.06	109.44	106.68
30	M	101	BCR	C36-C18-C19	6.06	127.34	118.09
29	V	319	Q6L	C11-C03-C04	-6.05	113.27	116.81
25	G	203	CLA	C4A-NA-C1A	6.05	109.44	106.68
34	B	844	PQN	C15-C13-C12	-6.04	107.60	121.17
29	U	315	Q6L	C12-C11-C03	6.04	125.69	113.64
25	B	812	CLA	C4A-NA-C1A	6.04	109.43	106.68
30	B	847	BCR	C36-C18-C19	6.04	127.31	118.09
29	R	301	Q6L	C05-C04-C03	6.02	118.58	110.61
25	B	811	CLA	C4A-NA-C1A	6.01	109.42	106.68
30	B	846	BCR	C37-C22-C23	6.00	127.25	118.09
24	U	305	CHL	CBC-CAC-C3C	5.99	121.45	112.87
30	K	205	BCR	C36-C18-C19	5.99	127.24	118.09
30	G	205	BCR	C28-C27-C26	-5.98	103.39	114.06
29	O	2007	Q6L	C12-C11-C03	5.97	125.55	113.64
34	A	844	PQN	C15-C13-C12	-5.97	107.77	121.17
25	H	302	CLA	C4A-NA-C1A	5.97	109.40	106.68
30	3	317	BCR	C36-C18-C19	5.96	127.20	118.09
25	A	840	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	5	609	CLA	C4A-NA-C1A	5.96	109.40	106.68
29	X	316	Q6L	C12-C11-C03	5.95	125.52	113.64
25	W	312	CLA	C4A-NA-C1A	5.95	109.39	106.68
25	L	302	CLA	C4A-NA-C1A	5.95	109.39	106.68
24	1	601	CHL	C1B-CHB-C4A	5.95	125.15	121.32
27	2	617	XAT	O4-C5-C18	5.94	121.69	115.05
25	B	826	CLA	C4A-NA-C1A	5.94	109.39	106.68
29	O	2007	Q6L	C11-C12-C13	5.94	129.47	112.86
29	T	315	Q6L	C11-C12-C13	5.93	129.46	112.86
29	Q	319	Q6L	C11-C12-C13	5.93	129.45	112.86
30	L	305	BCR	C36-C18-C19	5.93	127.14	118.09
25	A	812	CLA	C4A-NA-C1A	5.92	109.38	106.68
25	O	2001	CLA	C4A-NA-C1A	5.91	109.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	203	CLA	C4A-NA-C1A	5.90	109.37	106.68
29	X	301	Q6L	C11-C12-C13	5.90	129.37	112.86
25	A	836	CLA	C4A-NA-C1A	5.89	109.37	106.68
38	W	308	KC2	C1A-NA-C4A	5.89	109.37	106.68
24	R	309	CHL	C1B-CHB-C4A	5.89	125.11	121.32
25	B	834	CLA	C4A-NA-C1A	5.86	109.35	106.68
25	N	202	CLA	C4A-NA-C1A	5.86	109.35	106.68
27	3	316	XAT	C6-C7-C8	-5.86	113.61	125.99
25	F	803	CLA	C4A-NA-C1A	5.85	109.35	106.68
25	T	311	CLA	C4A-NA-C1A	5.83	109.34	106.68
29	R	304	Q6L	C11-C12-C13	5.83	129.18	112.86
38	T	308	KC2	CMA-C3A-C2A	-5.82	114.33	128.43
29	T	319	Q6L	C05-C04-C03	5.82	118.31	110.61
30	A	849	BCR	C3-C4-C5	-5.80	103.72	114.06
25	A	839	CLA	C4A-NA-C1A	5.78	109.32	106.68
25	B	829	CLA	C4A-NA-C1A	5.78	109.32	106.68
25	B	832	CLA	CBA-CAA-C2A	5.77	125.98	114.05
30	3	318	BCR	C38-C26-C25	-5.75	118.21	124.48
24	X	307	CHL	O2D-CGD-CBD	5.74	117.25	110.95
25	T	301	CLA	C4-C3-C5	5.73	125.18	115.23
27	1	612	XAT	O4-C5-C18	5.73	121.45	115.05
30	2	618	BCR	C23-C24-C25	-5.73	111.69	127.00
29	T	316	Q6L	C11-C12-C13	5.73	128.89	112.86
25	4	309	CLA	O2D-CGD-CBD	5.71	121.21	111.23
25	U	311	CLA	C4A-NA-C1A	5.71	109.28	106.68
29	U	315	Q6L	C11-C12-C13	5.70	128.82	112.86
27	6	615	XAT	O4-C5-C18	5.70	121.42	115.05
30	B	845	BCR	C4-C5-C6	-5.69	115.01	122.70
25	A	810	CLA	C4A-NA-C1A	5.69	109.27	106.68
29	S	316	Q6L	C05-C04-C03	5.68	118.12	110.61
25	A	808	CLA	C4A-NA-C1A	5.65	109.26	106.68
26	S	322	IWJ	C32-C30-C29	-5.64	108.16	113.96
29	P	319	Q6L	C12-C11-C03	5.64	124.89	113.64
25	3	307	CLA	C4A-NA-C1A	5.64	109.25	106.68
25	2	611	CLA	C4A-NA-C1A	5.64	109.25	106.68
30	A	851	BCR	C36-C18-C19	5.62	126.67	118.09
25	S	312	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	L	301	CLA	C4A-NA-C1A	5.59	109.23	106.68
29	T	319	Q6L	C12-C11-C03	5.59	124.79	113.64
25	V	309	CLA	CMC-C2C-C1C	5.59	133.77	125.03
29	Q	318	Q6L	C11-C12-C13	5.58	128.48	112.86
27	1	612	XAT	C18-C5-C4	-5.58	107.97	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	827	CLA	C4A-NA-C1A	5.58	109.22	106.68
30	2	618	BCR	C36-C18-C19	5.55	126.57	118.09
25	O	2004	CLA	C4A-NA-C1A	5.54	109.21	106.68
30	B	845	BCR	C37-C22-C23	5.54	126.55	118.09
25	O	2002	CLA	C4A-NA-C1A	5.53	109.20	106.68
25	V	303	CLA	CAC-C3C-C4C	5.53	131.98	124.79
30	H	305	BCR	C37-C22-C23	5.52	126.52	118.09
25	4	309	CLA	O2D-CGD-O1D	-5.52	113.11	123.85
29	R	304	Q6L	C12-C11-C03	5.52	124.64	113.64
30	B	845	BCR	C40-C30-C25	-5.52	101.59	110.24
29	X	316	Q6L	C11-C12-C13	5.51	128.28	112.86
30	I	101	BCR	C33-C5-C6	5.50	130.49	124.48
24	T	304	CHL	CMB-C2B-C3B	5.49	135.66	124.68
37	W	317	NEX	C8-C7-C6	-5.49	171.18	177.66
25	A	807	CLA	C4A-NA-C1A	5.48	109.18	106.68
29	Q	319	Q6L	C12-C11-C03	5.47	124.55	113.64
29	P	315	Q6L	C11-C12-C13	5.47	128.15	112.86
24	S	306	CHL	O2D-CGD-CBD	5.46	116.95	110.95
29	O	2006	Q6L	C11-C03-C04	-5.45	113.62	116.81
24	R	311	CHL	C1B-CHB-C4A	5.44	124.82	121.32
30	A	848	BCR	C36-C18-C19	5.44	126.40	118.09
38	V	308	KC2	C1A-C2A-C3A	-5.44	102.28	107.28
29	S	321	Q6L	C11-C12-C13	5.44	128.07	112.86
25	X	314	CLA	C4A-NA-C1A	5.43	109.16	106.68
24	4	302	CHL	C1B-CHB-C4A	5.43	124.81	121.32
30	I	101	BCR	C8-C7-C6	-5.41	112.54	127.00
34	A	844	PQN	C14-C13-C15	-5.41	105.84	115.23
29	W	316	Q6L	C11-C03-C04	-5.39	113.65	116.81
29	T	322	Q6L	C11-C12-C13	5.38	127.92	112.86
25	O	2005	CLA	C4A-NA-C1A	5.37	109.13	106.68
30	3	317	BCR	C23-C24-C25	-5.37	112.65	127.00
27	4	318	XAT	C27-C28-C29	-5.36	117.21	125.53
29	O	2006	Q6L	C12-C11-C03	5.36	124.33	113.64
25	A	805	CLA	C4A-NA-C1A	5.35	109.12	106.68
30	L	306	BCR	C36-C18-C19	5.35	126.26	118.09
25	2	603	CLA	C4A-NA-C1A	5.35	109.12	106.68
25	R	315	CLA	C4A-NA-C1A	5.34	109.12	106.68
25	R	316	CLA	C4-C3-C5	5.34	124.50	115.23
25	A	809	CLA	C4A-NA-C1A	5.34	109.12	106.68
30	A	852	BCR	C23-C22-C21	-5.34	110.61	119.01
30	F	804	BCR	C35-C13-C14	-5.33	114.17	122.82
38	W	308	KC2	CMA-C3A-C2A	-5.33	115.52	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	810	CLA	C4A-NA-C1A	5.33	109.11	106.68
37	W	317	NEX	C26-C27-C28	-5.31	114.76	125.99
27	4	318	XAT	C39-C29-C28	-5.31	109.97	118.09
38	R	312	KC2	CMA-C3A-C4A	-5.31	116.74	125.03
27	1	612	XAT	C8-C9-C10	5.28	127.31	119.01
25	Q	314	CLA	C4A-NA-C1A	5.27	109.08	106.68
29	V	316	Q6L	C12-C11-C03	5.27	124.16	113.64
25	6	609	CLA	C4A-NA-C1A	5.26	109.08	106.68
29	S	315	Q6L	C11-C12-C13	5.26	127.58	112.86
25	Q	315	CLA	C4A-NA-C1A	5.25	109.08	106.68
30	M	101	BCR	C10-C11-C12	5.25	138.42	123.20
25	A	831	CLA	C4-C3-C5	5.25	124.34	115.23
24	W	305	CHL	C1B-CHB-C4A	5.25	124.70	121.32
29	X	301	Q6L	C12-C11-C03	5.24	124.09	113.64
25	4	305	CLA	C4A-NA-C1A	5.24	109.07	106.68
29	S	316	Q6L	C11-C12-C13	5.22	127.46	112.86
30	F	801	BCR	C40-C30-C25	5.21	118.42	110.24
25	W	311	CLA	C4A-NA-C1A	5.20	109.05	106.68
25	1	607	CLA	C4A-NA-C1A	5.19	109.05	106.68
25	J	102	CLA	C4A-NA-C1A	5.19	109.05	106.68
25	T	302	CLA	C4A-NA-C1A	5.19	109.05	106.68
24	X	306	CHL	C1B-CHB-C4A	5.19	124.66	121.32
29	U	317	Q6L	C12-C11-C03	5.19	123.99	113.64
25	U	308	CLA	C1D-ND-C4D	-5.17	102.68	106.31
24	S	306	CHL	CBC-CAC-C3C	5.16	120.26	112.87
38	V	308	KC2	CMA-C3A-C2A	-5.14	115.99	128.43
25	5	606	CLA	C4A-NA-C1A	5.14	109.02	106.68
25	G	204	CLA	C4A-NA-C1A	5.14	109.02	106.68
25	2	614	CLA	O2D-CGD-O1D	-5.13	113.85	123.85
25	A	835	CLA	C4A-NA-C1A	5.13	109.02	106.68
25	V	311	CLA	C4A-NA-C1A	5.12	109.02	106.68
24	W	307	CHL	C1B-CHB-C4A	5.11	124.61	121.32
30	B	845	BCR	C7-C8-C9	-5.11	118.68	126.23
30	A	849	BCR	C38-C26-C25	-5.09	118.94	124.48
30	G	201	BCR	C36-C18-C19	5.08	125.84	118.09
29	X	317	Q6L	C11-C12-C13	5.08	127.06	112.86
29	V	316	Q6L	C11-C03-C04	-5.07	113.84	116.81
29	S	321	Q6L	C12-C11-C03	5.07	123.76	113.64
27	1	612	XAT	C7-C8-C9	-5.07	117.66	125.53
25	A	811	CLA	CMB-C2B-C1B	-5.07	117.70	125.42
27	3	316	XAT	C19-C9-C10	5.07	131.03	122.82
30	B	846	BCR	C8-C9-C10	5.06	126.97	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	303	CLA	C4A-NA-C1A	5.05	108.98	106.68
26	W	318	IWJ	C32-C30-C29	-5.05	108.76	113.96
29	W	316	Q6L	C11-C12-C13	5.05	126.98	112.86
29	S	321	Q6L	C11-C03-C04	-5.04	113.86	116.81
29	X	317	Q6L	C11-C03-C04	-5.04	113.86	116.81
37	H	306	NEX	C26-C27-C28	-5.04	115.33	125.99
30	A	850	BCR	C3-C4-C5	-5.04	105.07	114.06
38	X	309	KC2	CMA-C3A-C2A	-5.04	116.24	128.43
37	T	317	NEX	C26-C27-C28	-5.03	115.35	125.99
25	P	312	CLA	C4A-NA-C1A	5.03	108.97	106.68
38	U	307	KC2	C1A-C2A-C3A	-5.03	102.66	107.28
25	4	314	CLA	C4A-NA-C1A	5.03	108.97	106.68
26	V	317	IWJ	C32-C30-C29	-5.03	108.79	113.96
26	4	317	IWJ	C32-C30-C29	-5.03	108.79	113.96
25	W	309	CLA	O2D-CGD-O1D	-5.03	114.07	123.85
29	T	322	Q6L	C12-C11-C03	5.02	123.66	113.64
25	3	304	CLA	C4A-NA-C1A	5.02	108.97	106.68
25	A	826	CLA	C4A-NA-C1A	5.02	108.97	106.68
25	4	312	CLA	C4A-NA-C1A	5.02	108.97	106.68
25	V	312	CLA	C4A-NA-C1A	5.02	108.97	106.68
38	Q	310	KC2	CMA-C3A-C2A	-5.01	116.31	128.43
24	2	615	CHL	C1B-CHB-C4A	5.01	124.54	121.32
25	P	309	CLA	C4A-NA-C1A	5.00	108.96	106.68
25	A	845	CLA	C4A-NA-C1A	5.00	108.96	106.68
25	B	818	CLA	C4A-NA-C1A	4.99	108.96	106.68
25	B	841	CLA	C4A-NA-C1A	4.99	108.95	106.68
24	Q	308	CHL	C1B-CHB-C4A	4.98	124.53	121.32
24	S	307	CHL	C1B-CHB-C4A	4.97	124.52	121.32
37	T	317	NEX	C8-C7-C6	-4.96	171.81	177.66
30	A	848	BCR	C8-C7-C6	-4.96	113.75	127.00
24	T	314	CHL	O2D-CGD-CBD	4.96	116.39	110.95
25	3	302	CLA	C4A-NA-C1A	4.95	108.94	106.68
25	B	823	CLA	C4A-NA-C1A	4.95	108.94	106.68
30	J	103	BCR	C27-C26-C25	-4.95	116.02	122.70
27	5	612	XAT	C18-C5-C6	-4.94	114.17	122.30
30	B	846	BCR	C34-C9-C10	-4.94	114.81	122.82
25	S	311	CLA	C4A-NA-C1A	4.94	108.93	106.68
26	X	318	IWJ	C32-C30-C29	-4.93	108.89	113.96
30	K	205	BCR	C8-C7-C6	-4.93	113.82	127.00
25	P	301	CLA	C4A-NA-C1A	4.93	108.93	106.68
25	Q	306	CLA	C4D-C3D-CAD	-4.93	102.75	108.11
26	V	320	IWJ	C32-C30-C29	-4.92	108.90	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	317	Q6L	C05-C04-C03	4.92	117.12	110.61
24	R	310	CHL	C4-C3-C5	4.91	121.91	116.13
25	A	806	CLA	C4A-NA-C1A	4.91	108.92	106.68
29	U	315	Q6L	C11-C03-C04	-4.91	113.94	116.81
27	6	615	XAT	C38-C25-C26	-4.91	114.22	122.30
30	2	618	BCR	C37-C22-C23	4.90	125.58	118.09
25	P	311	CLA	C4A-NA-C1A	4.90	108.92	106.68
34	B	844	PQN	C14-C13-C15	-4.90	106.72	115.23
25	2	612	CLA	C4A-NA-C1A	4.90	108.91	106.68
34	A	844	PQN	C11-C12-C13	-4.90	118.40	126.83
26	U	316	IWJ	C33-C32-C30	4.89	119.90	112.06
30	G	205	BCR	C36-C18-C19	4.88	125.54	118.09
30	K	205	BCR	C23-C24-C25	-4.87	113.99	127.00
25	A	825	CLA	C4-C3-C2	-4.87	111.12	123.63
25	B	824	CLA	CMB-C2B-C1B	-4.87	118.00	125.42
26	T	318	IWJ	C32-C30-C29	-4.86	108.96	113.96
26	Q	303	IWJ	C35-C29-C30	4.86	113.76	108.78
29	R	319	Q6L	C12-C11-C03	4.85	123.32	113.64
29	U	315	Q6L	C05-C04-C03	4.85	117.02	110.61
25	U	310	CLA	C4A-NA-C1A	4.85	108.89	106.68
30	K	207	BCR	C28-C27-C26	-4.84	105.42	114.06
30	A	850	BCR	C33-C5-C6	-4.83	119.21	124.48
26	5	611	IWJ	C32-C30-C29	-4.83	109.00	113.96
24	X	306	CHL	CMA-C3A-C2A	-4.82	105.17	116.23
25	U	309	CLA	C4A-NA-C1A	4.82	108.88	106.68
30	J	101	BCR	C36-C18-C17	-4.82	115.01	122.82
25	W	301	CLA	C4A-NA-C1A	4.82	108.88	106.68
37	R	321	NEX	C26-C27-C28	-4.82	115.81	125.99
27	4	318	XAT	C26-C27-C28	-4.82	115.81	125.99
24	V	307	CHL	C1B-CHB-C4A	4.81	124.42	121.32
27	4	318	XAT	C39-C29-C30	4.81	130.60	122.82
29	T	315	Q6L	C12-C11-C03	4.80	123.22	113.64
29	W	319	Q6L	C05-C04-C03	4.80	116.96	110.61
25	K	203	CLA	O2D-CGD-O1D	-4.80	114.51	123.85
29	T	322	Q6L	C05-C04-C03	4.80	116.96	110.61
25	R	317	CLA	C4A-NA-C1A	4.79	108.87	106.68
30	L	307	BCR	C8-C9-C10	4.79	126.55	119.01
29	W	315	Q6L	C11-C03-C04	-4.79	114.01	116.81
30	J	101	BCR	C34-C9-C10	4.79	130.57	122.82
25	A	811	CLA	C4A-NA-C1A	4.79	108.86	106.68
30	B	848	BCR	C8-C7-C6	-4.79	114.21	127.00
38	Q	310	KC2	CHB-C4A-C3A	-4.78	117.48	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	P	315	Q6L	C12-C11-C03	4.78	123.18	113.64
29	U	314	Q6L	C12-C11-C03	4.78	123.17	113.64
30	A	848	BCR	C23-C24-C25	-4.78	114.24	127.00
25	H	304	CLA	C4A-NA-C1A	4.78	108.86	106.68
25	T	310	CLA	C4A-NA-C1A	4.78	108.86	106.68
30	B	849	BCR	C36-C18-C19	4.77	125.38	118.09
25	3	310	CLA	C4A-NA-C1A	4.77	108.86	106.68
25	B	838	CLA	C4A-NA-C1A	4.77	108.85	106.68
37	S	317	NEX	C26-C27-C28	-4.77	115.92	125.99
25	B	804	CLA	C4A-NA-C1A	4.76	108.85	106.68
25	6	607	CLA	CMB-C2B-C1B	-4.76	118.17	125.42
25	B	828	CLA	C4A-NA-C1A	4.75	108.84	106.68
25	A	815	CLA	CMB-C2B-C1B	-4.74	118.20	125.42
29	T	316	Q6L	C11-C03-C04	-4.74	114.04	116.81
29	V	319	Q6L	C12-C11-C03	4.73	123.07	113.64
25	V	313	CLA	C4A-NA-C1A	4.73	108.83	106.68
26	S	319	IWJ	C32-C30-C29	-4.73	109.10	113.96
24	W	314	CHL	CMB-C2B-C3B	4.72	134.12	124.68
29	W	315	Q6L	C12-C11-C03	4.72	123.05	113.64
25	K	206	CLA	C4A-NA-C1A	4.71	108.83	106.68
25	B	838	CLA	CMB-C2B-C1B	-4.71	118.25	125.42
29	U	314	Q6L	C11-C03-C04	-4.71	114.05	116.81
25	6	609	CLA	CMB-C2B-C1B	-4.71	118.25	125.42
25	3	311	CLA	C1-O2A-CGA	4.71	128.05	116.65
30	A	852	BCR	C36-C18-C19	4.70	125.27	118.09
30	G	201	BCR	C33-C5-C6	4.70	129.61	124.48
25	3	305	CLA	C4A-NA-C1A	4.70	108.82	106.68
30	K	202	BCR	C37-C22-C23	4.69	125.25	118.09
25	B	817	CLA	C4A-NA-C1A	4.69	108.82	106.68
24	U	305	CHL	C1B-CHB-C4A	4.68	124.34	121.32
27	3	316	XAT	C7-C8-C9	-4.67	118.28	125.53
25	B	815	CLA	C1-C2-C3	4.67	133.85	126.20
25	B	815	CLA	CMB-C2B-C1B	-4.67	118.30	125.42
29	V	315	Q6L	C11-C12-C13	4.67	125.93	112.86
30	M	101	BCR	C24-C23-C22	-4.66	119.33	126.23
26	4	301	IWJ	C32-C30-C29	-4.66	109.16	113.96
27	3	316	XAT	C18-C5-C6	-4.66	114.63	122.30
30	B	848	BCR	C23-C24-C25	-4.66	114.56	127.00
30	J	103	BCR	C37-C22-C23	4.65	125.20	118.09
30	K	205	BCR	C33-C5-C6	4.65	129.56	124.48
25	U	302	CLA	C4A-NA-C1A	4.64	108.80	106.68
25	R	305	CLA	C4A-NA-C1A	4.64	108.80	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	616	Q6L	C11-C12-C13	4.64	125.84	112.86
30	L	305	BCR	C28-C27-C26	-4.64	105.79	114.06
25	S	303	CLA	CMB-C2B-C1B	-4.62	118.38	125.42
25	2	610	CLA	C4A-NA-C1A	4.62	108.78	106.68
25	A	818	CLA	CMB-C2B-C1B	-4.62	118.39	125.42
29	W	319	Q6L	C11-C12-C13	4.61	125.76	112.86
24	T	305	CHL	CMB-C2B-C3B	4.61	133.89	124.68
24	Q	307	CHL	O2D-CGD-CBD	4.60	116.00	110.95
25	A	817	CLA	C4A-NA-C1A	4.60	108.78	106.68
24	X	307	CHL	C1-O2A-CGA	4.60	127.79	116.65
25	B	802	CLA	CMB-C2B-C1B	-4.60	118.42	125.42
25	S	302	CLA	C4A-NA-C1A	4.59	108.77	106.68
25	L	303	CLA	CMB-C2B-C1B	-4.59	118.43	125.42
24	T	320	CHL	C4D-CHA-CBD	-4.59	104.34	108.97
25	1	609	CLA	C4A-NA-C1A	4.58	108.77	106.68
24	S	307	CHL	CMB-C2B-C3B	4.58	133.83	124.68
24	V	306	CHL	O2D-CGD-CBD	4.58	115.97	110.95
25	T	312	CLA	C4A-NA-C1A	4.57	108.76	106.68
30	F	804	BCR	C7-C8-C9	-4.56	119.48	126.23
29	V	316	Q6L	C05-C04-C03	4.56	116.64	110.61
25	B	813	CLA	C4A-NA-C1A	4.55	108.75	106.68
29	Q	319	Q6L	C05-C04-C03	4.55	116.63	110.61
25	Q	304	CLA	O2A-CGA-O1A	-4.55	112.25	123.63
25	A	825	CLA	C4A-NA-C1A	4.54	108.75	106.68
27	2	617	XAT	C18-C5-C4	-4.54	109.15	114.24
25	B	837	CLA	C4A-NA-C1A	4.53	108.75	106.68
27	1	612	XAT	O24-C25-C24	4.53	117.74	113.49
26	P	320	IWJ	C35-C29-C30	4.53	113.42	108.78
37	P	317	NEX	C26-C27-C28	-4.53	116.42	125.99
25	W	313	CLA	C4A-NA-C1A	4.52	108.74	106.68
24	T	307	CHL	C1B-CHB-C4A	4.52	124.23	121.32
26	T	321	IWJ	C32-C30-C29	-4.52	109.31	113.96
38	S	308	KC2	C2A-C3A-C4A	-4.52	103.02	106.41
25	B	839	CLA	C4A-NA-C1A	4.52	108.74	106.68
37	T	317	NEX	C28-C29-C30	4.51	126.11	119.01
25	B	816	CLA	C4A-NA-C1A	4.50	108.73	106.68
30	M	101	BCR	C31-C1-C6	-4.50	103.19	110.24
30	J	101	BCR	C15-C14-C13	-4.49	120.98	127.28
27	2	617	XAT	C38-C25-C26	-4.49	114.91	122.30
29	P	315	Q6L	C11-C03-C04	-4.49	114.18	116.81
25	A	827	CLA	C1-C2-C3	-4.48	118.85	126.20
38	R	312	KC2	C1A-C2A-C3A	-4.47	103.17	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	302	CLA	C4-C3-C2	-4.47	112.14	123.63
37	H	306	NEX	C28-C29-C30	4.47	126.04	119.01
24	P	305	CHL	CED-O2D-CGD	4.47	126.05	115.92
30	4	319	BCR	C23-C24-C25	-4.47	115.07	127.00
25	6	608	CLA	C4A-NA-C1A	4.46	108.72	106.68
25	V	301	CLA	CMB-C2B-C1B	-4.46	118.63	125.42
29	O	2007	Q6L	C05-C04-C03	4.45	116.50	110.61
25	B	803	CLA	C4A-NA-C1A	4.45	108.71	106.68
25	B	831	CLA	CMB-C2B-C1B	-4.45	118.65	125.42
24	4	308	CHL	C1B-CHB-C4A	4.44	124.18	121.32
27	2	617	XAT	C18-C5-C6	-4.43	115.01	122.30
24	X	308	CHL	CMB-C2B-C3B	4.43	133.54	124.68
30	A	851	BCR	C33-C5-C6	4.43	129.31	124.48
30	K	202	BCR	C19-C18-C17	-4.43	112.05	119.01
25	X	313	CLA	C4A-NA-C1A	4.43	108.70	106.68
25	A	837	CLA	C4A-NA-C1A	4.42	108.70	106.68
30	J	101	BCR	C23-C24-C25	-4.42	115.18	127.00
30	K	202	BCR	C23-C22-C21	-4.42	112.06	119.01
24	T	307	CHL	CMB-C2B-C3B	4.42	133.51	124.68
25	5	601	CLA	CHB-C4A-NA	4.41	130.77	124.40
25	B	827	CLA	C4A-NA-C1A	4.41	108.69	106.68
29	T	316	Q6L	C05-C04-C03	4.41	116.44	110.61
25	K	201	CLA	C4A-NA-C1A	4.41	108.69	106.68
30	B	847	BCR	C8-C7-C6	-4.40	115.23	127.00
29	P	316	Q6L	C40-C32-C33	-4.40	112.95	123.36
25	5	608	CLA	C4A-NA-C1A	4.40	108.69	106.68
37	P	317	NEX	C28-C29-C30	4.39	125.92	119.01
24	6	601	CHL	CMB-C2B-C3B	4.39	133.46	124.68
30	A	852	BCR	C34-C9-C10	-4.39	115.70	122.82
25	2	602	CLA	O2A-CGA-O1A	-4.39	112.65	123.63
29	V	319	Q6L	C05-C04-C03	4.38	116.41	110.61
30	K	202	BCR	C27-C26-C25	-4.38	116.78	122.70
26	S	319	IWJ	C35-C29-C30	4.38	113.27	108.78
29	R	304	Q6L	C05-C04-C03	4.38	116.40	110.61
38	W	308	KC2	CMA-C3A-C4A	-4.38	118.19	125.03
29	S	320	Q6L	C12-C11-C03	4.38	122.37	113.64
26	1	611	IWJ	C32-C30-C29	-4.38	109.46	113.96
29	P	321	Q6L	C12-C11-C03	4.37	122.36	113.64
25	P	302	CLA	C4A-NA-C1A	4.37	108.67	106.68
25	W	303	CLA	CMB-C2B-C1B	-4.37	118.77	125.42
24	2	607	CHL	C1B-CHB-C4A	4.37	124.13	121.32
24	P	304	CHL	C4D-CHA-CBD	-4.37	104.56	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	O	2006	Q6L	C05-C04-C03	4.36	116.39	110.61
38	S	308	KC2	CBA-CAA-C2A	-4.35	107.99	125.45
29	O	2007	Q6L	C40-C32-C33	-4.35	113.06	123.36
29	T	315	Q6L	C05-C04-C03	4.35	116.36	110.61
24	U	305	CHL	CMB-C2B-C3B	4.34	133.36	124.68
24	X	308	CHL	C1B-CHB-C4A	4.33	124.11	121.32
37	P	317	NEX	O24-C25-C38	4.33	119.89	115.05
25	B	803	CLA	CMB-C2B-C1B	-4.33	118.83	125.42
25	B	814	CLA	C4A-NA-C1A	4.33	108.65	106.68
24	S	306	CHL	O2D-CGD-O1D	-4.33	115.42	123.85
25	B	830	CLA	C3B-C4B-NB	-4.33	106.67	110.53
30	K	205	BCR	C36-C18-C17	-4.33	115.81	122.82
27	5	612	XAT	C36-C21-C22	-4.33	101.36	108.97
24	S	305	CHL	C1B-CHB-C4A	4.32	124.10	121.32
25	2	606	CLA	C4A-NA-C1A	4.32	108.65	106.68
27	6	615	XAT	C38-C25-C24	4.32	119.09	114.24
25	A	811	CLA	CMB-C2B-C3B	4.32	136.71	126.55
30	3	318	BCR	C37-C22-C23	4.32	124.68	118.09
27	5	612	XAT	C38-C25-C26	-4.31	115.20	122.30
26	R	322	IWJ	C32-C30-C29	-4.31	109.53	113.96
25	V	309	CLA	C1D-ND-C4D	-4.30	103.30	106.31
26	6	614	IWJ	C32-C30-C29	-4.30	109.54	113.96
26	R	303	IWJ	C32-C30-C29	-4.30	109.54	113.96
30	B	849	BCR	C29-C30-C25	4.29	116.67	110.44
25	U	303	CLA	C4A-NA-C1A	4.29	108.64	106.68
30	3	319	BCR	C36-C18-C17	-4.29	115.87	122.82
25	K	206	CLA	C4-C3-C5	4.29	122.67	115.23
29	X	316	Q6L	C05-C04-C03	4.29	116.28	110.61
27	4	318	XAT	C37-C21-C36	-4.28	101.15	107.37
25	K	201	CLA	O2D-CGD-CBD	4.28	118.71	111.23
29	V	321	Q6L	C40-C32-C33	-4.27	113.25	123.36
30	I	101	BCR	C24-C23-C22	-4.27	119.92	126.23
29	P	316	Q6L	C11-C12-C13	4.27	124.81	112.86
25	A	813	CLA	C4A-NA-C1A	4.27	108.62	106.68
27	3	316	XAT	C39-C29-C30	4.26	129.72	122.82
27	2	617	XAT	C26-C27-C28	-4.25	117.00	125.99
30	I	101	BCR	C4-C5-C6	-4.25	116.96	122.70
25	T	309	CLA	C4-C3-C5	4.24	122.60	115.23
24	S	305	CHL	CMB-C2B-C3B	4.24	133.16	124.68
25	P	301	CLA	C4-C3-C5	4.24	122.59	115.23
27	2	617	XAT	C38-C25-C24	4.24	119.00	114.24
25	5	603	CLA	CMB-C2B-C1B	-4.24	118.96	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	201	BCR	C37-C22-C23	4.24	124.56	118.09
24	6	606	CHL	O2D-CGD-CBD	4.24	115.60	110.95
30	B	849	BCR	C8-C7-C6	-4.24	115.68	127.00
29	P	315	Q6L	C05-C04-C03	4.24	116.21	110.61
25	F	802	CLA	C4A-NA-C1A	4.23	108.61	106.68
25	2	602	CLA	C4A-NA-C1A	4.23	108.61	106.68
25	3	302	CLA	O2A-CGA-O1A	-4.22	113.07	123.63
30	I	101	BCR	C7-C8-C9	-4.22	119.99	126.23
30	K	207	BCR	C8-C7-C6	-4.22	115.73	127.00
25	2	609	CLA	O2D-CGD-CBD	4.22	118.60	111.23
27	3	316	XAT	C26-C27-C28	-4.21	117.08	125.99
25	6	602	CLA	CMB-C2B-C1B	-4.21	119.01	125.42
25	R	307	CLA	C4A-NA-C1A	4.21	108.60	106.68
29	R	320	Q6L	C11-C12-C13	4.21	124.64	112.86
30	A	850	BCR	C35-C13-C12	4.21	124.52	118.09
25	B	842	CLA	C1C-C2C-C3C	-4.21	102.55	106.98
25	R	314	CLA	C4A-NA-C1A	4.21	108.60	106.68
24	Q	316	CHL	O2D-CGD-CBD	4.20	115.57	110.95
29	V	315	Q6L	C12-C11-C03	4.20	122.02	113.64
29	V	321	Q6L	C12-C11-C03	4.20	122.02	113.64
25	B	806	CLA	C4A-NA-C1A	4.20	108.60	106.68
30	B	848	BCR	C36-C18-C17	-4.19	116.02	122.82
30	F	801	BCR	C36-C18-C19	4.19	124.49	118.09
38	T	308	KC2	C2A-C3A-C4A	-4.19	103.26	106.41
24	1	604	CHL	C1C-CHC-C4B	4.19	131.05	116.07
38	T	308	KC2	C1A-C2A-C3A	-4.19	103.43	107.28
25	U	311	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
30	J	101	BCR	C28-C27-C26	-4.18	106.61	114.06
29	X	316	Q6L	C11-C03-C04	-4.18	114.37	116.81
25	2	609	CLA	C4A-NA-C1A	4.17	108.58	106.68
38	V	308	KC2	C2A-C3A-C4A	-4.17	103.28	106.41
24	6	606	CHL	O2D-CGD-O1D	-4.17	115.73	123.85
25	V	309	CLA	O2D-CGD-O1D	-4.17	115.74	123.85
26	X	318	IWJ	C35-C29-C30	4.17	113.05	108.78
30	I	101	BCR	C36-C18-C19	4.17	124.45	118.09
30	K	202	BCR	C28-C27-C26	-4.16	106.64	114.06
25	A	827	CLA	CMB-C2B-C1B	-4.15	119.10	125.42
25	B	831	CLA	C4A-NA-C1A	4.15	108.57	106.68
28	Q	302	LHG	O7-C7-C8	4.14	120.45	111.48
29	U	315	Q6L	C40-C32-C33	-4.14	113.55	123.36
25	5	606	CLA	O2D-CGD-CBD	4.14	118.47	111.23
30	2	618	BCR	C8-C7-C6	-4.14	115.93	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	314	CHL	CMB-C2B-C3B	4.14	132.96	124.68
25	A	832	CLA	C4A-NA-C1A	4.14	108.57	106.68
37	H	306	NEX	C16-C1-C6	4.14	114.18	110.47
30	3	319	BCR	C37-C22-C23	4.14	124.41	118.09
24	4	307	CHL	CMA-C3A-C4A	-4.13	105.70	114.61
27	4	318	XAT	C18-C5-C4	-4.13	109.60	114.24
29	U	314	Q6L	C40-C32-C33	-4.13	113.58	123.36
24	Q	316	CHL	C1B-CHB-C4A	4.13	123.98	121.32
29	P	319	Q6L	C40-C32-C33	-4.13	113.58	123.36
30	4	319	BCR	C31-C1-C6	-4.13	103.77	110.24
29	X	301	Q6L	C40-C32-C33	-4.12	113.60	123.36
27	5	612	XAT	C26-C27-C28	-4.12	117.28	125.99
30	3	319	BCR	C33-C5-C6	-4.12	119.99	124.48
29	R	304	Q6L	C40-C32-C33	-4.12	113.61	123.36
25	V	301	CLA	C4A-NA-C1A	4.12	108.56	106.68
24	Q	307	CHL	C1B-CHB-C4A	4.12	123.97	121.32
25	6	613	CLA	C4A-NA-C1A	4.11	108.55	106.68
24	P	307	CHL	CMB-C2B-C3B	4.11	132.90	124.68
37	R	321	NEX	C28-C29-C30	4.11	125.47	119.01
26	S	318	IWJ	C33-C32-C30	4.11	118.65	112.06
24	S	304	CHL	OMC-CMC-C2C	-4.10	117.99	125.12
25	K	201	CLA	CMB-C2B-C1B	-4.10	119.17	125.42
25	Q	304	CLA	CHB-C4A-NA	4.10	130.32	124.40
25	R	315	CLA	O2D-CGD-O1D	-4.10	115.86	123.85
24	P	304	CHL	O2D-CGD-CBD	4.10	115.45	110.95
26	5	611	IWJ	C01-C02-C03	-4.10	113.66	123.36
29	V	321	Q6L	C15-C14-C13	-4.10	121.93	127.69
37	P	317	NEX	C38-C25-C26	-4.09	115.56	122.30
30	K	202	BCR	C20-C21-C22	-4.09	121.54	127.28
24	P	307	CHL	C1B-CHB-C4A	4.09	123.95	121.32
24	X	306	CHL	CMA-C3A-C4A	4.09	123.42	114.61
25	T	312	CLA	C4-C3-C5	4.09	122.32	115.23
27	6	615	XAT	C18-C5-C4	-4.08	109.66	114.24
25	A	823	CLA	C6-C5-C3	4.08	123.41	113.47
30	A	852	BCR	C36-C18-C17	-4.08	116.21	122.82
29	U	317	Q6L	C11-C03-C04	-4.07	114.43	116.81
25	2	602	CLA	CMB-C2B-C1B	-4.07	119.22	125.42
29	U	314	Q6L	C05-C04-C03	4.07	116.00	110.61
27	6	615	XAT	C26-C27-C28	-4.07	117.39	125.99
25	1	606	CLA	C4A-NA-C1A	4.07	108.53	106.68
30	L	306	BCR	C24-C23-C22	-4.07	120.22	126.23
29	Q	317	Q6L	C11-C03-C04	-4.06	114.43	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	P	316	Q6L	C05-C04-C03	4.06	115.99	110.61
30	A	852	BCR	C20-C21-C22	-4.06	121.58	127.28
29	X	301	Q6L	C05-C04-C03	4.06	115.98	110.61
38	V	308	KC2	C2D-C1D-ND	-4.06	106.12	110.33
26	5	611	IWJ	C37-C35-C34	-4.05	101.84	108.97
25	R	314	CLA	O2D-CGD-O1D	-4.05	115.96	123.85
27	3	316	XAT	C11-C10-C9	-4.05	121.60	127.28
29	W	316	Q6L	C40-C32-C33	-4.05	113.78	123.36
30	G	201	BCR	C15-C16-C17	-4.04	115.25	123.52
24	P	304	CHL	CMB-C2B-C3B	4.04	132.76	124.68
25	1	613	CLA	C4A-NA-C1A	4.04	108.52	106.68
25	3	309	CLA	C4A-NA-C1A	4.04	108.52	106.68
30	B	845	BCR	C38-C26-C25	-4.03	120.08	124.48
29	Q	317	Q6L	C12-C11-C03	4.02	121.66	113.64
24	S	305	CHL	CBC-CAC-C3C	4.02	118.63	112.87
25	K	201	CLA	O2D-CGD-O1D	-4.02	116.03	123.85
30	B	845	BCR	C10-C11-C12	4.01	134.83	123.20
24	W	314	CHL	C1B-CHB-C4A	4.01	123.91	121.32
30	A	852	BCR	C24-C23-C22	-4.01	120.30	126.23
29	S	315	Q6L	C40-C32-C33	-4.01	113.86	123.36
25	2	604	CLA	C4A-NA-C1A	4.01	108.51	106.68
38	X	309	KC2	C1A-C2A-C3A	-4.01	103.59	107.28
38	Q	310	KC2	CBA-CAA-C2A	-4.01	109.36	125.45
25	B	813	CLA	O2A-CGA-O1A	-4.00	113.61	123.63
38	V	308	KC2	CMA-C3A-C4A	-4.00	118.78	125.03
25	6	607	CLA	C4A-NA-C1A	4.00	108.50	106.68
38	X	309	KC2	C2A-C3A-C4A	-4.00	103.41	106.41
25	X	304	CLA	CMB-C2B-C1B	-4.00	119.33	125.42
24	W	306	CHL	O2D-CGD-CBD	4.00	115.34	110.95
25	1	608	CLA	C4A-NA-C1A	4.00	108.50	106.68
25	B	843	CLA	C1-C2-C3	-3.99	119.66	126.20
25	6	608	CLA	CHB-C4A-NA	3.99	130.16	124.40
25	B	829	CLA	C4-C3-C5	3.99	122.15	115.23
25	6	604	CLA	C4A-NA-C1A	3.98	108.50	106.68
24	2	601	CHL	C1C-CHC-C4B	3.98	130.33	116.07
30	G	205	BCR	C23-C24-C25	-3.98	116.36	127.00
25	R	306	CLA	C4A-NA-C1A	3.98	108.50	106.68
24	W	306	CHL	CMB-C2B-C3B	3.98	132.64	124.68
24	Q	309	CHL	C1B-CHB-C4A	3.98	123.88	121.32
26	X	318	IWJ	C29-C30-C31	-3.98	119.31	124.22
29	S	321	Q6L	C05-C04-C03	3.98	115.88	110.61
37	W	317	NEX	C38-C25-C26	-3.97	115.77	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	S	317	NEX	C28-C29-C30	3.97	125.25	119.01
29	W	316	Q6L	C15-C14-C13	-3.97	122.11	127.69
25	3	309	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
30	A	848	BCR	C35-C13-C12	3.97	124.15	118.09
25	6	610	CLA	C4A-NA-C1A	3.96	108.49	106.68
30	A	849	BCR	C36-C18-C17	-3.96	116.40	122.82
30	A	848	BCR	C28-C27-C26	-3.96	106.99	114.06
25	B	843	CLA	C3A-C2A-C1A	3.96	107.27	101.34
24	W	307	CHL	CMB-C2B-C3B	3.96	132.59	124.68
29	V	316	Q6L	C38-C36-C31	-3.95	103.55	109.55
25	3	302	CLA	C6-C5-C3	3.95	123.10	113.47
30	2	618	BCR	C15-C16-C17	-3.95	115.43	123.52
25	W	309	CLA	O2D-CGD-CBD	3.95	118.14	111.23
25	A	845	CLA	C1-C2-C3	-3.95	120.37	126.76
30	L	307	BCR	C2-C1-C6	-3.95	104.70	110.44
26	R	303	IWJ	C01-C02-C03	-3.94	114.03	123.36
29	2	616	Q6L	C15-C14-C13	3.94	133.24	127.69
28	3	320	LHG	O7-C7-C8	3.94	120.01	111.48
24	V	305	CHL	C1B-CHB-C4A	3.94	123.86	121.32
30	M	101	BCR	C34-C9-C10	3.94	129.20	122.82
30	I	101	BCR	C1-C6-C5	-3.94	117.25	122.64
25	V	301	CLA	C4-C3-C5	3.94	122.06	115.23
29	W	320	Q6L	C12-C11-C03	3.94	121.49	113.64
29	X	319	Q6L	C12-C11-C03	3.94	121.49	113.64
29	X	316	Q6L	C34-C33-C32	-3.93	121.07	124.83
24	V	306	CHL	CMB-C2B-C3B	3.93	132.54	124.68
29	U	317	Q6L	C05-C04-C03	3.93	115.81	110.61
25	2	609	CLA	O2D-CGD-O1D	-3.93	116.21	123.85
30	L	306	BCR	C28-C27-C26	-3.92	107.06	114.06
30	A	851	BCR	C23-C22-C21	-3.92	112.84	119.01
30	J	101	BCR	C8-C7-C6	-3.92	116.53	127.00
25	O	2003	CLA	C4A-NA-C1A	3.92	108.47	106.68
24	Q	307	CHL	C1C-CHC-C4B	3.92	130.09	116.07
25	5	601	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
25	A	831	CLA	C4-C3-C2	-3.92	113.56	123.63
31	N	201	LMG	O7-C10-C11	3.92	119.95	111.48
25	Q	312	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
25	U	308	CLA	C4A-NA-C1A	-3.91	104.89	106.68
25	T	303	CLA	CMB-C2B-C1B	-3.91	119.46	125.42
29	R	320	Q6L	C05-C04-C03	3.91	115.79	110.61
25	2	610	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
25	5	601	CLA	C4A-NA-C1A	3.91	108.46	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	312	CLA	C4A-NA-C1A	3.91	108.46	106.68
29	W	320	Q6L	C40-C32-C33	-3.91	114.10	123.36
26	T	321	IWJ	C35-C29-C30	3.91	112.79	108.78
29	S	323	Q6L	C40-C32-C33	-3.91	114.10	123.36
29	X	319	Q6L	C05-C04-C03	3.91	115.78	110.61
25	K	203	CLA	O2D-CGD-CBD	3.91	118.06	111.23
30	F	804	BCR	C11-C10-C9	-3.90	121.80	127.28
25	A	856	CLA	O1D-CGD-CBD	3.90	132.22	124.52
25	A	830	CLA	CMB-C2B-C1B	-3.90	119.48	125.42
25	A	840	CLA	C4-C3-C2	-3.90	113.61	123.63
26	U	316	IWJ	C01-C02-C03	-3.90	114.13	123.36
25	S	313	CLA	C4A-NA-C1A	3.90	108.46	106.68
29	O	2006	Q6L	C40-C32-C33	-3.90	114.13	123.36
29	S	320	Q6L	C05-C04-C03	3.90	115.77	110.61
24	Q	308	CHL	C1C-CHC-C4B	3.90	130.01	116.07
24	T	305	CHL	C4D-CHA-CBD	-3.89	105.04	108.97
30	J	103	BCR	C4-C5-C6	-3.89	117.45	122.70
29	S	316	Q6L	C11-C03-C04	-3.89	114.54	116.81
30	L	306	BCR	C37-C22-C23	3.88	124.02	118.09
25	K	204	CLA	CBA-CAA-C2A	3.88	125.34	113.79
24	6	605	CHL	CMB-C2B-C3B	3.88	132.44	124.68
30	K	205	BCR	C3-C4-C5	-3.88	107.14	114.06
30	A	851	BCR	C28-C27-C26	-3.87	107.15	114.06
24	Q	308	CHL	CMB-C2B-C3B	3.87	132.41	124.68
24	Q	307	CHL	CMB-C2B-C3B	3.87	132.41	124.68
30	K	202	BCR	C11-C10-C9	-3.86	121.86	127.28
26	Q	303	IWJ	C32-C30-C29	-3.86	109.99	113.96
25	6	602	CLA	C4A-NA-C1A	3.86	108.44	106.68
30	I	101	BCR	C28-C27-C26	-3.86	107.18	114.06
25	W	310	CLA	C4A-NA-C1A	3.86	108.44	106.68
26	S	322	IWJ	C35-C29-C30	3.85	112.73	108.78
24	U	305	CHL	O2D-CGD-CBD	3.85	115.18	110.95
30	J	103	BCR	C36-C18-C17	-3.85	116.58	122.82
30	2	618	BCR	C3-C4-C5	-3.85	107.19	114.06
30	K	202	BCR	C36-C18-C17	-3.85	116.58	122.82
24	2	615	CHL	C1C-CHC-C4B	3.85	129.84	116.07
24	U	306	CHL	C1C-CHC-C4B	3.85	129.84	116.07
30	A	850	BCR	C31-C1-C6	-3.85	104.21	110.24
25	A	826	CLA	C4-C3-C5	3.84	121.90	115.23
25	S	310	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
30	A	852	BCR	C8-C9-C10	3.84	125.05	119.01
29	P	321	Q6L	C40-C32-C33	-3.84	114.28	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	W	301	CLA	CHB-C4A-NA	3.84	129.94	124.40
29	W	320	Q6L	C38-C36-C35	-3.83	102.26	109.41
29	W	316	Q6L	C05-C04-C03	3.83	115.68	110.61
26	V	317	IWJ	C01-C02-C03	-3.83	114.29	123.36
25	A	820	CLA	C3B-C4B-NB	-3.83	107.11	110.53
24	R	310	CHL	C1C-CHC-C4B	3.83	129.77	116.07
30	L	305	BCR	C11-C10-C9	-3.83	121.91	127.28
30	B	845	BCR	C34-C9-C10	3.82	129.01	122.82
29	T	322	Q6L	C40-C32-C33	-3.82	114.31	123.36
37	H	306	NEX	C19-C9-C10	3.82	129.01	122.82
24	P	314	CHL	C1B-CHB-C4A	3.82	123.78	121.32
29	V	316	Q6L	C40-C32-C33	-3.82	114.32	123.36
38	P	308	KC2	C1A-C2A-C3A	-3.81	103.77	107.28
27	1	612	XAT	C31-C30-C29	-3.81	121.93	127.28
24	V	314	CHL	CMB-C2B-C3B	3.81	132.30	124.68
25	B	821	CLA	CBA-CAA-C2A	3.81	125.13	113.79
30	B	846	BCR	C1-C6-C5	-3.81	117.43	122.64
29	Q	319	Q6L	C11-C03-C04	-3.81	114.58	116.81
30	G	201	BCR	C20-C19-C18	-3.81	115.93	126.36
30	L	307	BCR	C37-C22-C23	3.80	123.90	118.09
33	A	802	CL0	C1B-CHB-C4A	3.80	123.77	121.32
38	T	308	KC2	CBA-CAA-C2A	-3.80	110.20	125.45
25	A	815	CLA	C4-C3-C5	3.79	121.81	115.23
25	B	815	CLA	CMB-C2B-C3B	3.79	135.47	126.55
24	P	307	CHL	C1C-CHC-C4B	3.79	129.65	116.07
26	X	318	IWJ	C16-C15-C14	-3.79	121.96	127.28
37	S	317	NEX	C38-C25-C26	-3.79	116.06	122.30
24	6	606	CHL	CMB-C2B-C3B	3.79	132.25	124.68
26	P	318	IWJ	C32-C30-C29	-3.79	110.06	113.96
25	O	2002	CLA	C4-C3-C5	3.79	121.80	115.23
30	A	849	BCR	C28-C27-C26	-3.78	107.31	114.06
31	L	308	LMG	O7-C10-C11	3.78	119.66	111.48
25	3	313	CLA	C4A-NA-C1A	3.78	108.40	106.68
24	R	308	CHL	C1C-CHC-C4B	3.77	129.58	116.07
25	4	311	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
26	6	614	IWJ	C01-C02-C03	-3.77	114.43	123.36
25	1	602	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
26	Q	303	IWJ	C01-C02-C03	-3.77	114.44	123.36
25	Q	313	CLA	CHB-C4A-NA	3.76	129.83	124.40
31	O	2008	LMG	O7-C10-C11	3.76	119.62	111.48
25	A	833	CLA	C4A-NA-C1A	3.76	108.39	106.68
38	S	308	KC2	O2D-CGD-O1D	-3.76	116.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	323	Q6L	C11-C03-C04	-3.76	114.61	116.81
24	R	311	CHL	C1C-CHC-C4B	3.76	129.52	116.07
30	M	101	BCR	C20-C21-C22	-3.76	122.01	127.28
26	P	320	IWJ	C01-C02-C03	-3.76	114.47	123.36
26	1	611	IWJ	C01-C02-C03	-3.75	114.47	123.36
24	R	302	CHL	O2D-CGD-CBD	3.75	115.07	110.95
25	B	807	CLA	CMB-C2B-C1B	-3.75	119.71	125.42
38	X	309	KC2	CMD-C2D-C1D	-3.75	119.72	125.42
25	B	814	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
24	4	308	CHL	CHA-C1A-C2A	-3.74	124.53	133.31
25	P	309	CLA	O2D-CGD-CBD	3.74	117.77	111.23
24	6	606	CHL	C1B-CHB-C4A	3.73	123.72	121.32
27	4	318	XAT	O24-C25-C38	3.73	119.22	115.05
25	A	825	CLA	C4-C3-C5	3.73	121.70	115.23
24	R	302	CHL	C1C-CHC-C4B	3.73	129.41	116.07
26	W	318	IWJ	C01-C02-C03	-3.73	114.54	123.36
24	R	318	CHL	C1C-CHC-C4B	3.73	129.41	116.07
29	R	301	Q6L	C40-C32-C33	-3.73	114.54	123.36
29	T	315	Q6L	C11-C03-C04	-3.72	114.63	116.81
30	B	848	BCR	C11-C10-C9	-3.72	122.06	127.28
24	V	305	CHL	CMB-C2B-C3B	3.72	132.12	124.68
30	J	101	BCR	C40-C30-C25	3.72	116.08	110.24
26	4	301	IWJ	C01-C02-C03	-3.72	114.55	123.36
24	4	302	CHL	C1C-CHC-C4B	3.72	129.37	116.07
25	A	838	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
26	V	320	IWJ	C01-C02-C03	-3.72	114.56	123.36
25	4	316	CLA	C4A-NA-C1A	3.72	108.37	106.68
26	V	318	IWJ	C01-C02-C03	-3.71	114.57	123.36
25	B	806	CLA	C3B-C4B-NB	-3.71	107.21	110.53
25	P	309	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
25	A	828	CLA	C4A-NA-C1A	3.71	108.37	106.68
37	R	321	NEX	C19-C9-C10	3.71	128.83	122.82
25	W	309	CLA	C4-C3-C5	3.71	121.67	115.23
27	5	612	XAT	C6-C7-C8	-3.71	118.15	125.99
24	Q	309	CHL	O2D-CGD-CBD	3.71	115.02	110.95
25	O	2001	CLA	C4-C3-C2	-3.71	114.10	123.63
30	2	618	BCR	C15-C14-C13	-3.71	122.08	127.28
27	2	617	XAT	C39-C29-C30	3.71	128.83	122.82
25	2	613	CLA	CBA-CAA-C2A	3.71	121.71	114.05
25	A	823	CLA	C4A-NA-C1A	3.71	108.37	106.68
26	X	318	IWJ	C01-C02-C03	-3.71	114.59	123.36
27	5	612	XAT	C31-C30-C29	-3.70	122.08	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	318	CHL	O2D-CGD-O1D	-3.70	116.64	123.85
25	A	821	CLA	CHB-C4A-NA	3.70	129.74	124.40
25	2	614	CLA	O2D-CGD-CBD	3.70	117.70	111.23
27	6	615	XAT	O4-C5-C6	-3.70	56.00	58.93
25	6	612	CLA	C4A-NA-C1A	3.70	108.37	106.68
30	H	305	BCR	C38-C26-C25	-3.70	120.45	124.48
24	T	306	CHL	C4D-CHA-CBD	-3.70	105.24	108.97
25	A	827	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
25	1	610	CLA	C4A-NA-C1A	3.70	108.36	106.68
30	G	201	BCR	C28-C27-C26	-3.69	107.47	114.06
25	A	838	CLA	C4A-NA-C1A	3.69	108.36	106.68
30	B	847	BCR	C12-C13-C14	-3.69	113.20	119.01
27	3	316	XAT	C31-C30-C29	-3.69	122.10	127.28
29	S	320	Q6L	C11-C03-C04	-3.69	114.65	116.81
30	B	848	BCR	C12-C13-C14	-3.69	113.21	119.01
25	A	856	CLA	C4A-NA-C1A	3.68	108.36	106.68
24	T	314	CHL	C1B-CHB-C4A	3.68	123.69	121.32
30	A	848	BCR	C3-C4-C5	-3.68	107.49	114.06
27	4	318	XAT	C18-C5-C6	-3.68	116.24	122.30
25	B	834	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
29	W	319	Q6L	C11-C03-C04	-3.68	114.66	116.81
30	J	101	BCR	C33-C5-C6	3.68	128.50	124.48
25	B	808	CLA	CHB-C4A-NA	3.68	129.71	124.40
25	A	805	CLA	O2D-CGD-O1D	-3.67	116.69	123.85
30	K	207	BCR	C3-C4-C5	-3.67	107.50	114.06
29	S	316	Q6L	C40-C32-C33	-3.67	114.67	123.36
25	S	311	CLA	CHB-C4A-NA	3.67	129.70	124.40
29	X	317	Q6L	C19-C18-C17	-3.67	122.13	127.28
30	G	201	BCR	C8-C9-C10	-3.67	113.23	119.01
24	W	305	CHL	C1C-CHC-C4B	3.67	129.21	116.07
30	K	207	BCR	C36-C18-C17	-3.67	116.87	122.82
27	5	612	XAT	C39-C29-C30	3.67	128.76	122.82
30	L	305	BCR	C39-C30-C25	3.67	115.99	110.24
24	3	306	CHL	C4D-CHA-CBD	-3.66	105.28	108.97
24	P	305	CHL	C1C-CHC-C4B	3.66	129.16	116.07
29	U	317	Q6L	C40-C32-C33	-3.66	114.70	123.36
25	T	301	CLA	C4A-NA-C1A	3.66	108.35	106.68
24	R	308	CHL	C4D-CHA-CBD	-3.66	105.28	108.97
32	6	617	SQD	O47-C7-C8	3.65	119.38	111.48
29	X	317	Q6L	C40-C32-C33	-3.65	114.72	123.36
24	5	605	CHL	C1C-CHC-C4B	3.65	129.14	116.07
38	V	308	KC2	O2D-CGD-O1D	-3.65	116.74	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	V	303	CLA	CMB-C2B-C1B	-3.65	119.86	125.42
25	A	825	CLA	CBA-CAA-C2A	3.65	124.66	113.79
30	B	848	BCR	C15-C16-C17	-3.65	116.05	123.52
30	3	319	BCR	C8-C7-C6	-3.64	117.27	127.00
30	J	101	BCR	C15-C16-C17	-3.64	116.06	123.52
24	U	305	CHL	C1C-CHC-C4B	3.64	129.10	116.07
30	B	846	BCR	C33-C5-C6	-3.64	120.51	124.48
25	A	820	CLA	O2A-CGA-O1A	-3.64	114.52	123.63
25	5	608	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
25	3	302	CLA	C4-C3-C5	3.64	121.54	115.23
30	A	849	BCR	C20-C21-C22	-3.64	122.18	127.28
25	6	611	CLA	CBA-CAA-C2A	3.64	121.56	114.05
25	A	806	CLA	CHB-C4A-NA	3.63	129.65	124.40
29	S	323	Q6L	C38-C36-C35	-3.63	102.63	109.41
25	Q	301	CLA	CBA-CAA-C2A	3.63	124.61	113.79
24	S	306	CHL	C1C-CHC-C4B	3.63	129.07	116.07
25	1	607	CLA	CBD-CHA-C4D	-3.63	110.88	117.29
25	B	815	CLA	CHB-C4A-NA	3.63	129.64	124.40
25	A	805	CLA	CMB-C2B-C1B	-3.63	119.89	125.42
25	P	302	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
26	T	318	IWJ	C01-C02-C03	-3.63	114.78	123.36
27	3	316	XAT	O4-C5-C18	3.63	119.10	115.05
36	A	854	DGD	O2G-C1B-C2B	3.63	119.33	111.48
27	1	612	XAT	C38-C25-C26	-3.63	116.33	122.30
24	R	311	CHL	CHA-C1A-C2A	-3.63	124.80	133.31
24	W	314	CHL	C1C-CHC-C4B	3.62	129.04	116.07
29	S	321	Q6L	C40-C32-C33	-3.62	114.78	123.36
25	B	805	CLA	CHB-C4A-NA	3.62	129.63	124.40
25	B	827	CLA	CHB-C4A-NA	3.62	129.63	124.40
24	5	605	CHL	CMB-C2B-C3B	3.62	131.92	124.68
25	H	301	CLA	CHB-C4A-NA	3.62	129.63	124.40
25	2	613	CLA	C4A-NA-C1A	3.62	108.33	106.68
25	A	819	CLA	C4-C3-C5	3.62	121.51	115.23
25	R	305	CLA	C1D-ND-C4D	-3.62	103.77	106.31
29	R	319	Q6L	C05-C04-C03	3.62	115.40	110.61
25	4	311	CLA	C4B-C3B-C2B	-3.62	102.80	107.30
25	B	829	CLA	CMB-C2B-C1B	-3.62	119.91	125.42
24	T	320	CHL	C1C-CHC-C4B	3.61	129.00	116.07
24	Q	316	CHL	C1C-CHC-C4B	3.61	129.00	116.07
30	F	804	BCR	C19-C18-C17	-3.61	113.33	119.01
30	M	101	BCR	C8-C7-C6	-3.61	117.36	127.00
24	R	302	CHL	C1B-CHB-C4A	3.61	123.64	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	318	IWJ	C01-C02-C03	-3.61	114.82	123.36
25	B	805	CLA	C4A-NA-C1A	3.61	108.32	106.68
25	2	606	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
24	S	306	CHL	C4C-CHD-C1D	3.60	128.96	116.07
25	A	824	CLA	C4A-NA-C1A	3.60	108.32	106.68
25	A	829	CLA	CHB-C4A-NA	3.60	129.60	124.40
25	3	314	CLA	CMB-C2B-C1B	-3.60	119.93	125.42
25	A	806	CLA	C1-O2A-CGA	3.60	125.37	116.65
28	3	323	LHG	O7-C7-C8	3.60	119.27	111.48
25	T	313	CLA	C4A-NA-C1A	3.60	108.32	106.68
30	3	319	BCR	C3-C4-C5	-3.60	107.64	114.06
26	S	322	IWJ	C01-C02-C03	-3.60	114.84	123.36
25	2	608	CLA	O2D-CGD-CBD	3.60	117.52	111.23
30	J	103	BCR	C33-C5-C6	3.60	128.41	124.48
29	R	320	Q6L	C40-C32-C33	-3.60	114.85	123.36
25	Q	306	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
30	K	202	BCR	C15-C16-C17	-3.59	116.16	123.52
30	B	849	BCR	C36-C18-C17	-3.59	116.99	122.82
27	3	316	XAT	O24-C25-C38	3.59	119.06	115.05
26	T	321	IWJ	C01-C02-C03	-3.59	114.86	123.36
25	B	839	CLA	CBA-CAA-C2A	3.59	124.48	113.79
27	1	612	XAT	C38-C25-C24	3.59	118.28	114.24
30	B	848	BCR	C8-C9-C10	-3.59	113.36	119.01
30	A	850	BCR	C36-C18-C17	-3.59	117.00	122.82
25	A	838	CLA	C4-C3-C5	3.59	121.45	115.23
30	3	317	BCR	C3-C4-C5	-3.59	107.66	114.06
30	M	101	BCR	C34-C9-C8	-3.59	112.61	118.09
37	T	317	NEX	C38-C25-C26	-3.58	116.40	122.30
24	W	307	CHL	C1C-CHC-C4B	3.58	128.89	116.07
30	B	845	BCR	C15-C16-C17	-3.58	116.19	123.52
24	U	304	CHL	O2D-CGD-CBD	3.58	114.88	110.95
25	A	822	CLA	C4A-NA-C1A	3.58	108.31	106.68
24	X	307	CHL	C1C-CHC-C4B	3.58	128.88	116.07
25	S	301	CLA	C3B-C4B-NB	-3.58	107.33	110.53
29	2	616	Q6L	C40-C32-C33	-3.58	114.89	123.36
25	A	803	CLA	C4A-NA-C1A	3.58	108.31	106.68
26	Q	320	IWJ	C01-C02-C03	-3.58	114.89	123.36
31	O	2008	LMG	O2-C2-C1	3.58	118.60	110.08
25	X	304	CLA	C4A-NA-C1A	3.57	108.31	106.68
30	L	305	BCR	C3-C4-C5	-3.57	107.68	114.06
30	L	305	BCR	C23-C22-C21	-3.57	113.39	119.01
24	S	314	CHL	C1B-CHB-C4A	3.57	123.62	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	851	BCR	C37-C22-C23	3.57	123.54	118.09
25	P	310	CLA	C4A-NA-C1A	3.57	108.31	106.68
25	4	310	CLA	CMB-C2B-C1B	-3.57	119.99	125.42
27	6	615	XAT	C18-C5-C6	-3.57	116.43	122.30
28	6	616	LHG	O7-C7-C8	3.57	119.20	111.48
38	V	308	KC2	C1D-ND-C4D	3.57	108.81	106.31
25	A	825	CLA	CMB-C2B-C1B	-3.57	119.99	125.42
25	B	836	CLA	C3B-C4B-NB	-3.56	107.35	110.53
26	Q	320	IWJ	C28-C29-C35	-3.56	105.96	111.97
24	P	306	CHL	C1C-CHC-C4B	3.56	128.82	116.07
38	X	309	KC2	O2D-CGD-O1D	-3.56	116.92	123.85
25	B	809	CLA	C6-C5-C3	-3.56	104.80	113.47
29	2	616	Q6L	C31-C30-C29	-3.56	119.04	124.58
25	2	612	CLA	CAA-C2A-C3A	-3.56	103.38	113.00
24	3	306	CHL	C1B-CHB-C4A	3.56	123.61	121.32
30	B	847	BCR	C36-C18-C17	-3.56	117.05	122.82
26	S	319	IWJ	C01-C02-C03	-3.55	114.95	123.36
24	R	302	CHL	C4D-CHA-CBD	-3.55	105.38	108.97
25	A	831	CLA	C4A-NA-C1A	3.55	108.30	106.68
25	H	304	CLA	CBA-CAA-C2A	3.55	124.36	113.79
24	6	606	CHL	C1C-CHC-C4B	3.55	128.78	116.07
30	G	205	BCR	C37-C22-C21	-3.55	117.06	122.82
25	1	607	CLA	CMB-C2B-C1B	-3.55	120.01	125.42
24	U	313	CHL	C1B-CHB-C4A	3.55	123.61	121.32
26	3	315	IWJ	C01-C02-C03	-3.55	114.97	123.36
24	P	314	CHL	C1C-CHC-C4B	3.55	128.75	116.07
30	B	848	BCR	C20-C21-C22	-3.54	122.31	127.28
24	X	307	CHL	O2D-CGD-O1D	-3.54	116.95	123.85
37	T	317	NEX	O24-C25-C38	3.54	119.01	115.05
30	L	306	BCR	C34-C9-C10	3.54	128.55	122.82
24	P	307	CHL	O2D-CGD-CBD	3.54	114.83	110.95
24	X	306	CHL	CMB-C2B-C3B	3.54	131.75	124.68
30	G	201	BCR	C23-C22-C21	-3.54	113.44	119.01
38	V	308	KC2	CBA-CAA-C2A	-3.54	111.26	125.45
24	4	302	CHL	C4-C3-C5	3.54	120.29	116.13
24	R	309	CHL	C1C-CHC-C4B	3.53	128.72	116.07
24	R	309	CHL	O2D-CGD-CBD	3.53	114.83	110.95
25	S	303	CLA	CMB-C2B-C3B	3.53	134.86	126.55
26	R	322	IWJ	C01-C02-C03	-3.53	115.00	123.36
25	4	311	CLA	CMB-C2B-C1B	-3.53	120.04	125.42
30	B	847	BCR	C2-C1-C6	3.53	115.57	110.44
25	B	806	CLA	C4-C3-C2	-3.53	114.57	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	612	XAT	C18-C5-C4	-3.53	110.28	114.24
32	H	303	SQD	O47-C7-C8	3.52	119.10	111.48
25	4	314	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
25	3	307	CLA	C4-C3-C2	-3.52	114.58	123.63
25	5	609	CLA	CHB-C4A-NA	3.52	129.48	124.40
30	K	202	BCR	C8-C9-C10	-3.52	113.47	119.01
25	4	315	CLA	C4A-NA-C1A	3.52	108.28	106.68
25	A	840	CLA	CBA-CAA-C2A	3.52	124.25	113.79
25	3	302	CLA	O2A-CGA-CBA	3.52	122.56	111.83
25	O	2004	CLA	CHB-C4A-NA	3.51	129.47	124.40
30	M	101	BCR	C15-C14-C13	-3.51	122.35	127.28
26	V	320	IWJ	C35-C29-C30	3.51	112.38	108.78
30	G	205	BCR	C15-C16-C17	-3.51	116.33	123.52
30	F	801	BCR	C20-C21-C22	-3.50	122.36	127.28
31	5	613	LMG	O7-C10-C11	3.50	119.06	111.48
31	F	805	LMG	O7-C10-C11	3.50	119.05	111.48
25	B	820	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
24	S	307	CHL	C1C-CHC-C4B	3.50	128.58	116.07
27	1	612	XAT	C15-C14-C13	-3.49	122.38	127.28
31	A	855	LMG	O1-C1-C2	3.49	113.58	108.27
24	P	305	CHL	C4D-CHA-CBD	-3.49	105.45	108.97
29	R	301	Q6L	C12-C11-C03	3.49	120.60	113.64
25	6	613	CLA	C6-C5-C3	-3.49	104.97	113.47
30	2	618	BCR	C36-C18-C17	-3.49	117.17	122.82
30	I	101	BCR	C37-C22-C23	3.49	123.41	118.09
25	B	802	CLA	C4A-NA-C1A	3.49	108.27	106.68
25	B	818	CLA	CHB-C4A-NA	3.48	129.43	124.40
25	N	203	CLA	C2D-C1D-ND	-3.48	106.68	110.13
24	T	304	CHL	C1B-CHB-C4A	3.48	123.56	121.32
30	B	845	BCR	C8-C7-C6	-3.48	117.71	127.00
29	T	316	Q6L	C40-C32-C33	-3.48	115.13	123.36
29	R	319	Q6L	C40-C32-C33	-3.48	115.13	123.36
25	K	204	CLA	CHB-C4A-NA	3.47	129.41	124.40
25	Q	315	CLA	C1-O2A-CGA	3.47	125.06	116.65
38	V	308	KC2	O2D-CGD-CBD	3.47	117.30	111.23
25	B	838	CLA	CMB-C2B-C3B	3.47	134.72	126.55
27	6	615	XAT	C36-C21-C22	-3.47	102.87	108.97
25	W	309	CLA	C4A-NA-C1A	3.47	108.26	106.68
27	1	612	XAT	C6-C7-C8	-3.46	118.67	125.99
24	R	318	CHL	O2D-CGD-CBD	3.46	114.75	110.95
30	2	618	BCR	C28-C27-C26	-3.46	107.88	114.06
30	B	846	BCR	C36-C18-C19	3.46	123.37	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	824	CLA	CMB-C2B-C1B	-3.46	120.16	125.42
25	B	836	CLA	C4A-NA-C1A	3.46	108.26	106.68
30	A	851	BCR	C36-C18-C17	-3.46	117.22	122.82
30	F	801	BCR	C23-C22-C21	-3.45	113.58	119.01
24	W	304	CHL	O2D-CGD-CBD	3.45	114.74	110.95
24	T	304	CHL	C1C-CHC-C4B	3.45	128.43	116.07
24	4	308	CHL	C1C-CHC-C4B	3.45	128.42	116.07
30	G	205	BCR	C11-C10-C9	-3.45	122.45	127.28
30	L	305	BCR	C37-C22-C23	3.45	123.35	118.09
25	B	815	CLA	O2D-CGD-CBD	3.44	117.25	111.23
25	T	311	CLA	CMB-C2B-C1B	-3.44	120.18	125.42
25	A	818	CLA	C4A-NA-C1A	3.44	108.25	106.68
25	4	304	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
25	B	806	CLA	CMC-C2C-C1C	3.44	130.41	125.03
29	X	316	Q6L	C25-C26-C27	3.44	132.10	127.28
30	A	851	BCR	C15-C16-C17	-3.44	116.48	123.52
24	1	601	CHL	C1C-CHC-C4B	3.43	128.35	116.07
25	B	803	CLA	O2D-CGD-CBD	3.43	117.23	111.23
30	F	801	BCR	C36-C18-C17	-3.43	117.25	122.82
25	A	834	CLA	C4A-NA-C1A	3.43	108.24	106.68
30	A	851	BCR	C3-C4-C5	-3.43	107.94	114.06
25	H	301	CLA	C4A-NA-C1A	3.43	108.24	106.68
24	S	305	CHL	C1C-CHC-C4B	3.43	128.33	116.07
30	L	307	BCR	C15-C16-C17	-3.43	116.51	123.52
24	U	304	CHL	C4D-CHA-CBD	-3.43	105.51	108.97
25	A	819	CLA	CHB-C4A-NA	3.42	129.34	124.40
29	T	319	Q6L	C40-C32-C33	-3.42	115.26	123.36
24	Q	316	CHL	OBD-CAD-CBD	-3.42	120.80	125.82
25	4	311	CLA	C3B-C2B-C1B	3.42	111.20	107.17
30	H	305	BCR	C8-C7-C6	-3.42	117.86	127.00
25	A	821	CLA	CMB-C2B-C1B	-3.42	120.21	125.42
30	B	848	BCR	C31-C1-C6	-3.42	104.88	110.24
30	L	305	BCR	C8-C9-C10	-3.42	113.63	119.01
25	B	805	CLA	C4-C3-C5	3.42	121.16	115.23
25	P	309	CLA	CHB-C4A-NA	3.42	129.33	124.40
25	5	608	CLA	O2D-CGD-CBD	3.42	117.20	111.23
24	X	307	CHL	C3C-C4C-NC	-3.42	106.30	114.65
25	V	309	CLA	O2D-CGD-CBD	3.42	117.20	111.23
25	B	842	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
30	J	103	BCR	C3-C4-C5	-3.42	107.97	114.06
25	A	836	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
25	2	612	CLA	C6-C5-C3	3.41	121.78	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	W	314	CHL	C2A-C3A-C4A	-3.41	101.30	103.53
38	S	308	KC2	C1A-C2A-C3A	-3.41	104.15	107.28
24	V	305	CHL	C1C-CHC-C4B	3.41	128.26	116.07
25	X	302	CLA	C4A-NA-C1A	3.41	108.23	106.68
30	4	319	BCR	C36-C18-C17	-3.41	117.30	122.82
37	S	317	NEX	C39-C29-C30	-3.41	117.30	122.82
30	A	848	BCR	C36-C18-C17	-3.41	117.30	122.82
25	K	201	CLA	CED-O2D-CGD	3.41	123.64	115.92
29	W	319	Q6L	C40-C32-C33	-3.40	115.30	123.36
30	G	201	BCR	C3-C4-C5	-3.40	107.99	114.06
30	L	305	BCR	C31-C1-C6	3.40	115.58	110.24
37	W	317	NEX	C28-C29-C30	3.40	124.36	119.01
31	2	620	LMG	O7-C10-C11	3.40	118.83	111.48
24	V	307	CHL	C1C-CHC-C4B	3.40	128.23	116.07
24	6	605	CHL	C1C-CHC-C4B	3.40	128.22	116.07
24	X	307	CHL	CAA-C2A-C3A	3.40	122.17	113.00
30	G	205	BCR	C37-C22-C23	3.39	123.27	118.09
25	1	603	CLA	CHB-C4A-NA	3.39	129.30	124.40
25	X	302	CLA	C3B-C4B-NB	-3.39	107.50	110.53
30	K	207	BCR	C19-C18-C17	-3.39	113.68	119.01
25	6	609	CLA	CMB-C2B-C3B	3.39	134.52	126.55
31	B	801	LMG	O7-C10-C11	3.39	118.81	111.48
25	L	303	CLA	CHB-C4A-NA	3.39	129.29	124.40
30	L	305	BCR	C36-C18-C17	-3.39	117.33	122.82
25	U	311	CLA	CHB-C4A-NA	3.39	129.29	124.40
30	L	306	BCR	C36-C18-C17	-3.39	117.33	122.82
25	W	302	CLA	C4A-NA-C1A	3.38	108.22	106.68
30	B	846	BCR	C8-C7-C6	-3.38	117.96	127.00
28	A	847	LHG	O7-C7-C8	3.38	118.80	111.48
24	Q	307	CHL	O2D-CGD-O1D	-3.38	117.26	123.85
24	4	302	CHL	CMD-C2D-C3D	3.38	131.44	124.68
24	R	309	CHL	CHA-C1A-C2A	-3.38	125.37	133.31
30	A	852	BCR	C30-C25-C26	3.38	127.25	122.64
30	A	850	BCR	C20-C21-C22	-3.38	122.54	127.28
30	L	306	BCR	C11-C10-C9	-3.38	122.54	127.28
24	W	306	CHL	C3C-C4C-NC	-3.38	106.39	114.65
24	T	307	CHL	C1C-CHC-C4B	3.38	128.15	116.07
38	W	308	KC2	O2D-CGD-O1D	-3.38	117.28	123.85
27	3	316	XAT	C36-C21-C22	-3.38	103.03	108.97
24	2	607	CHL	CHA-C1A-C2A	-3.38	125.38	133.31
24	S	314	CHL	C1C-CHC-C4B	3.38	128.15	116.07
24	6	601	CHL	C1C-CHC-C4B	3.37	128.15	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	J	101	BCR	C7-C8-C9	-3.37	121.24	126.23
30	3	318	BCR	C19-C18-C17	-3.37	113.70	119.01
24	Q	309	CHL	C1C-CHC-C4B	3.37	128.14	116.07
26	P	318	IWJ	C01-C02-C03	-3.37	115.38	123.36
29	S	323	Q6L	C12-C11-C03	3.37	120.36	113.64
30	A	850	BCR	C12-C13-C14	-3.37	113.71	119.01
25	A	815	CLA	CMB-C2B-C3B	3.37	134.47	126.55
25	B	836	CLA	C1-C2-C3	3.37	131.72	126.20
27	3	316	XAT	C28-C29-C30	-3.37	113.71	119.01
38	S	308	KC2	CAA-CBA-CGA	-3.37	109.93	127.05
25	B	842	CLA	CHB-C4A-NA	3.37	129.26	124.40
28	A	846	LHG	O7-C7-C8	3.36	118.76	111.48
30	J	101	BCR	C20-C21-C22	-3.36	122.56	127.28
25	H	302	CLA	CHB-C4A-NA	3.36	129.25	124.40
30	J	101	BCR	C3-C4-C5	-3.36	108.06	114.06
25	B	806	CLA	C4-C3-C5	3.36	121.06	115.23
25	Q	314	CLA	C4-C3-C5	3.36	121.06	115.23
24	T	305	CHL	C1C-CHC-C4B	3.36	128.09	116.07
29	W	315	Q6L	C40-C32-C33	-3.36	115.41	123.36
25	A	812	CLA	O2D-CGD-CBD	3.36	117.10	111.23
30	J	103	BCR	C23-C24-C25	-3.36	118.03	127.00
27	6	615	XAT	C37-C21-C36	-3.35	102.50	107.37
25	2	606	CLA	O2D-CGD-CBD	3.35	117.09	111.23
25	5	601	CLA	C2A-C1A-CHA	3.35	129.69	123.87
24	T	314	CHL	CMB-C2B-C3B	3.35	131.38	124.68
29	Q	318	Q6L	C40-C32-C33	-3.35	115.42	123.36
24	X	306	CHL	C1C-CHC-C4B	3.35	128.06	116.07
25	A	803	CLA	CHB-C4A-NA	3.35	129.24	124.40
24	Q	309	CHL	OMC-CMC-C2C	-3.35	119.30	125.12
24	Q	308	CHL	CHA-C1A-C2A	-3.35	125.44	133.31
27	4	318	XAT	C11-C10-C9	3.35	131.98	127.28
29	P	319	Q6L	C20-C21-C22	3.35	131.98	127.28
30	K	207	BCR	C38-C26-C25	-3.35	120.83	124.48
25	X	310	CLA	C4A-NA-C1A	3.35	108.21	106.68
30	3	318	BCR	C36-C18-C17	-3.35	117.39	122.82
25	A	840	CLA	C4-C3-C5	3.35	121.04	115.23
29	R	323	Q6L	C40-C32-C33	-3.35	115.44	123.36
38	P	308	KC2	CBA-CAA-C2A	-3.34	112.03	125.45
30	L	307	BCR	C16-C17-C18	3.34	131.97	127.28
29	R	319	Q6L	C11-C03-C04	-3.34	114.86	116.81
24	4	306	CHL	CMB-C2B-C3B	3.34	131.36	124.68
25	K	203	CLA	CHB-C4A-NA	3.34	129.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	308	CHL	C1C-CHC-C4B	3.34	128.02	116.07
25	B	811	CLA	CMC-C2C-C1C	3.34	130.25	125.03
30	A	851	BCR	C34-C9-C8	-3.34	112.99	118.09
30	2	618	BCR	C37-C22-C21	-3.34	117.41	122.82
30	F	804	BCR	C20-C21-C22	-3.34	122.60	127.28
27	3	316	XAT	C4-C3-C2	-3.34	104.55	110.79
34	A	844	PQN	C14-C13-C12	-3.34	115.06	123.63
25	A	803	CLA	C3B-C4B-NB	-3.34	107.55	110.53
25	A	831	CLA	C6-C5-C3	3.34	121.59	113.47
25	P	303	CLA	C4A-NA-C1A	3.33	108.20	106.68
30	B	845	BCR	C36-C18-C17	-3.33	117.42	122.82
25	A	822	CLA	CMB-C2B-C1B	-3.33	120.34	125.42
25	A	820	CLA	CHB-C4A-NA	3.33	129.21	124.40
24	P	306	CHL	C1B-CHB-C4A	3.33	123.47	121.32
25	L	303	CLA	CBA-CAA-C2A	3.33	123.71	113.79
25	X	310	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
25	6	602	CLA	CMB-C2B-C3B	3.33	134.39	126.55
24	P	304	CHL	C1C-CHC-C4B	3.33	127.99	116.07
25	1	603	CLA	C4-C3-C2	-3.33	115.07	123.63
25	B	820	CLA	CHB-C4A-NA	3.33	129.21	124.40
30	B	846	BCR	C3-C4-C5	-3.33	108.12	114.06
24	P	304	CHL	CBC-CAC-C3C	-3.33	108.11	112.87
25	P	311	CLA	C4-C3-C2	-3.33	115.08	123.63
25	A	830	CLA	C1-O2A-CGA	3.33	124.71	116.65
38	P	308	KC2	O2D-CGD-O1D	-3.33	117.37	123.85
25	6	607	CLA	C4B-C3B-C2B	-3.33	103.17	107.30
30	B	848	BCR	C34-C9-C10	3.32	128.20	122.82
25	B	829	CLA	CHB-C4A-NA	3.32	129.20	124.40
24	4	302	CHL	C4D-ND-C1D	3.32	107.74	105.22
37	T	317	NEX	C15-C35-C34	-3.32	116.73	123.52
24	S	306	CHL	CMB-C2B-C3B	3.32	131.31	124.68
24	P	307	CHL	CHA-C1A-C2A	-3.32	125.51	133.31
27	4	318	XAT	C6-C7-C8	-3.32	118.98	125.99
24	T	314	CHL	C1C-CHC-C4B	3.32	127.94	116.07
28	1	614	LHG	O8-C23-C24	3.32	121.95	111.83
25	A	819	CLA	C4-C3-C2	-3.32	115.11	123.63
25	3	312	CLA	CMB-C2B-C1B	-3.31	120.37	125.42
25	3	308	CLA	CMC-C2C-C1C	3.31	130.21	125.03
24	U	304	CHL	C1C-CHC-C4B	3.31	127.92	116.07
26	4	317	IWJ	C01-C02-C03	-3.31	115.52	123.36
25	T	301	CLA	O1D-CGD-CBD	3.31	131.05	124.52
24	X	315	CHL	C1C-CHC-C4B	3.31	127.91	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	808	CLA	CHB-C4A-NA	3.31	129.18	124.40
25	A	842	CLA	CHD-C1D-ND	-3.31	120.15	124.80
25	B	825	CLA	C4A-NA-C1A	3.31	108.19	106.68
37	T	317	NEX	C39-C29-C30	-3.30	117.47	122.82
24	X	307	CHL	C1B-CHB-C4A	3.30	123.45	121.32
25	4	303	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
30	F	804	BCR	C37-C22-C23	3.30	123.13	118.09
25	3	302	CLA	CMB-C2B-C1B	-3.30	120.39	125.42
33	A	802	CL0	C4D-CHA-CBD	-3.30	105.64	108.97
24	V	314	CHL	C1C-CHC-C4B	3.30	127.87	116.07
24	W	304	CHL	O2D-CGD-O1D	-3.30	117.43	123.85
24	2	615	CHL	CBC-CAC-C3C	3.30	117.59	112.87
30	3	318	BCR	C39-C30-C25	-3.29	105.08	110.24
30	K	202	BCR	C12-C13-C14	-3.29	113.83	119.01
24	U	306	CHL	C1B-CHB-C4A	3.29	123.44	121.32
24	U	305	CHL	C4D-CHA-CBD	-3.29	105.65	108.97
25	U	301	CLA	CHB-C4A-NA	3.29	129.15	124.40
25	P	313	CLA	C4A-NA-C1A	3.29	108.18	106.68
25	A	804	CLA	CMB-C2B-C3B	3.29	134.29	126.55
25	6	611	CLA	C4A-NA-C1A	3.29	108.18	106.68
25	A	839	CLA	CMB-C2B-C3B	3.29	134.28	126.55
30	A	850	BCR	C23-C24-C25	-3.29	118.22	127.00
37	S	317	NEX	C17-C1-C6	3.29	113.41	110.47
24	W	314	CHL	O2D-CGD-CBD	3.28	114.55	110.95
25	P	309	CLA	C4-C3-C5	3.28	120.93	115.23
25	Q	306	CLA	CHD-C1D-ND	-3.28	120.18	124.80
25	O	2002	CLA	C4-C3-C2	-3.28	115.20	123.63
29	X	319	Q6L	C40-C32-C33	-3.28	115.61	123.36
38	U	307	KC2	O2D-CGD-O1D	-3.28	117.47	123.85
25	U	301	CLA	C4A-NA-C1A	3.27	108.17	106.68
25	L	302	CLA	CHD-C1D-ND	-3.27	120.19	124.80
27	3	316	XAT	C38-C25-C26	-3.27	116.92	122.30
25	5	602	CLA	C4A-NA-C1A	3.27	108.17	106.68
25	P	310	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
25	B	825	CLA	O2A-CGA-O1A	-3.27	114.92	123.33
25	B	826	CLA	CMB-C2B-C1B	-3.27	120.44	125.42
30	B	845	BCR	C11-C10-C9	-3.27	122.69	127.28
30	L	305	BCR	C34-C9-C10	3.27	128.11	122.82
25	A	804	CLA	CHA-C1A-NA	-3.27	119.00	126.39
24	Q	316	CHL	O2D-CGD-O1D	-3.27	117.49	123.85
26	P	318	IWJ	C35-C29-C30	3.26	112.13	108.78
25	B	835	CLA	C4A-NA-C1A	3.26	108.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	202	BCR	C34-C9-C10	3.26	128.10	122.82
25	A	808	CLA	C3B-C4B-NB	-3.26	107.62	110.53
24	5	605	CHL	C1B-CHB-C4A	3.26	123.42	121.32
24	V	314	CHL	O2D-CGD-CBD	3.26	114.53	110.95
37	W	317	NEX	C15-C35-C34	-3.26	116.85	123.52
30	F	804	BCR	C34-C9-C8	-3.26	113.11	118.09
29	Q	317	Q6L	C40-C32-C33	-3.26	115.65	123.36
25	V	302	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
30	L	306	BCR	C20-C21-C22	-3.25	122.71	127.28
25	B	842	CLA	C1-C2-C3	-3.25	120.87	126.20
25	T	301	CLA	CMB-C2B-C1B	-3.25	120.47	125.42
27	6	615	XAT	C39-C29-C30	3.25	128.08	122.82
30	4	319	BCR	C28-C27-C26	-3.25	108.26	114.06
38	V	308	KC2	CHB-C4A-C3A	-3.25	119.90	125.03
24	R	318	CHL	CHA-C1A-C2A	-3.25	125.68	133.31
30	2	618	BCR	C31-C1-C6	-3.25	105.15	110.24
29	V	315	Q6L	C40-C32-C33	-3.25	115.68	123.36
25	V	301	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
29	P	319	Q6L	C11-C03-C04	-3.24	114.91	116.81
29	Q	319	Q6L	C40-C32-C33	-3.24	115.69	123.36
25	S	309	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
25	X	311	CLA	C4A-NA-C1A	3.24	108.16	106.68
24	X	306	CHL	O2D-CGD-CBD	3.24	114.50	110.95
25	3	311	CLA	O2A-CGA-O1A	-3.24	115.53	123.63
24	P	304	CHL	C3D-C4D-CHA	3.24	113.46	108.54
29	T	315	Q6L	C40-C32-C33	-3.23	115.70	123.36
25	W	303	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
29	V	319	Q6L	C30-C29-C27	-3.23	119.37	126.32
25	A	815	CLA	CHB-C4A-NA	3.23	129.06	124.40
26	S	318	IWJ	C17-C18-C19	-3.23	122.75	127.28
24	S	306	CHL	C4D-ND-C1D	3.23	107.67	105.22
37	H	306	NEX	O24-C25-C38	3.23	118.66	115.05
24	V	306	CHL	O2D-CGD-O1D	-3.23	117.56	123.85
26	3	315	IWJ	C35-C29-C30	3.23	112.09	108.78
29	R	323	Q6L	C12-C11-C03	3.23	120.07	113.64
25	A	804	CLA	CMB-C2B-C1B	-3.23	120.51	125.42
30	3	319	BCR	C15-C16-C17	-3.23	116.92	123.52
30	3	318	BCR	C28-C27-C26	-3.23	108.30	114.06
24	S	304	CHL	CBC-CAC-C3C	3.23	117.49	112.87
24	T	314	CHL	O2D-CGD-O1D	-3.22	117.57	123.85
25	A	811	CLA	CHB-C4A-NA	3.22	129.05	124.40
24	P	305	CHL	CHA-C1A-C2A	-3.22	125.74	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Q	311	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
25	B	807	CLA	CHB-C4A-NA	3.22	129.05	124.40
25	V	301	CLA	CMB-C2B-C3B	3.22	134.12	126.55
24	W	306	CHL	C1C-CHC-C4B	3.22	127.58	116.07
37	H	306	NEX	C11-C10-C9	-3.22	122.77	127.28
25	A	814	CLA	C4A-NA-C1A	3.22	108.15	106.68
27	1	612	XAT	C32-C33-C34	-3.21	113.95	119.01
25	B	815	CLA	C4-C3-C5	3.21	120.81	115.23
25	B	842	CLA	C2C-C1C-NC	3.21	113.36	109.98
25	W	312	CLA	C1D-ND-C4D	-3.21	104.06	106.31
24	4	302	CHL	C1-O2A-CGA	3.21	124.43	116.65
25	5	607	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
25	4	310	CLA	C4A-NA-C1A	3.21	108.14	106.68
24	2	607	CHL	C1C-CHC-C4B	3.21	127.57	116.07
24	U	306	CHL	CHA-C1A-C2A	-3.21	125.77	133.31
25	B	813	CLA	O2A-CGA-CBA	3.21	121.62	111.83
24	R	309	CHL	O2D-CGD-O1D	-3.21	117.60	123.85
30	B	847	BCR	C28-C27-C26	-3.21	108.33	114.06
30	B	845	BCR	C30-C25-C26	-3.21	118.25	122.64
25	B	814	CLA	CMB-C2B-C1B	-3.21	120.53	125.42
24	6	605	CHL	CHA-C1A-C2A	-3.21	125.78	133.31
25	B	824	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
24	X	305	CHL	C4D-CHA-CBD	-3.20	105.74	108.97
25	5	603	CLA	C4A-NA-C1A	3.20	108.14	106.68
27	1	612	XAT	C35-C15-C14	-3.20	116.97	123.52
24	R	309	CHL	CMB-C2B-C3B	3.20	131.08	124.68
30	3	318	BCR	C16-C15-C14	-3.20	116.97	123.52
24	U	313	CHL	C1C-CHC-C4B	3.20	127.52	116.07
25	W	303	CLA	CMB-C2B-C3B	3.20	134.08	126.55
25	B	837	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
25	B	826	CLA	C4-C3-C5	3.20	120.78	115.23
29	V	319	Q6L	C26-C25-C24	-3.20	113.94	123.20
30	J	101	BCR	C37-C22-C23	3.20	122.97	118.09
24	R	309	CHL	CBC-CAC-C3C	3.19	117.45	112.87
25	1	602	CLA	C4A-NA-C1A	3.19	108.14	106.68
25	R	313	CLA	O2D-CGD-CBD	3.19	116.81	111.23
38	Q	310	KC2	O2D-CGD-O1D	-3.19	117.63	123.85
30	G	201	BCR	C15-C14-C13	-3.19	122.80	127.28
24	2	601	CHL	C4D-CHA-CBD	-3.19	105.75	108.97
25	Q	305	CLA	C4A-NA-C1A	3.19	108.14	106.68
25	A	805	CLA	C1-C2-C3	-3.19	120.97	126.20
30	M	101	BCR	C11-C10-C9	-3.19	122.81	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	207	BCR	C23-C24-C25	-3.18	118.49	127.00
25	B	831	CLA	CMB-C2B-C3B	3.18	134.04	126.55
25	A	810	CLA	CBA-CAA-C2A	3.18	123.26	113.79
27	1	612	XAT	O24-C25-C38	3.18	118.60	115.05
29	R	301	Q6L	C42-C13-C12	3.18	120.75	115.23
27	6	615	XAT	O24-C25-C24	3.18	116.47	113.49
24	R	310	CHL	C1B-CHB-C4A	3.18	123.37	121.32
25	A	841	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	X	307	CHL	C4D-ND-C1D	3.18	107.63	105.22
25	5	602	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
24	Q	309	CHL	CHA-C1A-C2A	-3.18	125.85	133.31
24	W	306	CHL	O2D-CGD-O1D	-3.18	117.67	123.85
38	T	308	KC2	O2D-CGD-O1D	-3.18	117.67	123.85
30	B	847	BCR	C23-C24-C25	-3.17	118.52	127.00
25	V	312	CLA	O2A-CGA-O1A	-3.17	115.69	123.63
34	A	844	PQN	C16-C15-C13	3.17	121.20	113.47
25	B	841	CLA	CHB-C4A-NA	3.17	128.98	124.40
25	V	309	CLA	C3A-C2A-C1A	-3.17	96.59	101.34
25	5	606	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
25	2	609	CLA	CHB-C4A-NA	3.17	128.98	124.40
25	Q	306	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
29	W	315	Q6L	C05-C04-C03	3.17	114.80	110.61
24	V	306	CHL	C1C-CHC-C4B	3.17	127.41	116.07
38	V	308	KC2	C3A-C4A-NA	3.17	114.37	110.45
25	6	609	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
25	5	604	CLA	C4A-NA-C1A	3.17	108.12	106.68
30	3	317	BCR	C19-C18-C17	-3.16	114.03	119.01
29	T	322	Q6L	C19-C18-C17	-3.16	122.84	127.28
25	Q	315	CLA	O2A-CGA-O1A	-3.16	115.72	123.63
30	F	804	BCR	C34-C9-C10	3.16	127.94	122.82
25	T	303	CLA	C4A-NA-C1A	3.16	108.12	106.68
25	A	828	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
25	R	305	CLA	CBA-CAA-C2A	3.16	123.19	113.79
25	A	836	CLA	CHB-C4A-NA	3.16	128.96	124.40
25	1	610	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
25	A	826	CLA	CHB-C4A-NA	3.16	128.96	124.40
31	A	801	LMG	O7-C10-C11	3.15	118.30	111.48
25	1	603	CLA	CBC-CAC-C3C	-3.15	103.87	112.42
38	U	307	KC2	CBA-CAA-C2A	-3.15	112.81	125.45
37	P	317	NEX	C39-C29-C30	-3.15	117.71	122.82
30	G	201	BCR	C31-C1-C6	3.15	115.18	110.24
30	H	305	BCR	C3-C4-C5	-3.15	108.44	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	838	CLA	O2D-CGD-CBD	3.15	116.73	111.23
30	B	849	BCR	C20-C21-C22	-3.15	122.86	127.28
37	S	317	NEX	C15-C35-C34	-3.14	117.08	123.52
24	X	315	CHL	CHA-C1A-C2A	-3.14	125.92	133.31
25	X	302	CLA	C4D-CHA-C1A	3.14	124.99	121.24
38	R	312	KC2	CBA-CAA-C2A	-3.14	112.83	125.45
25	A	821	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
25	G	202	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
30	B	845	BCR	C37-C22-C21	-3.14	117.73	122.82
38	W	308	KC2	C3C-C2C-C1C	3.14	108.77	106.41
24	W	304	CHL	C1B-CHB-C4A	3.14	123.34	121.32
24	T	320	CHL	C3D-C4D-CHA	3.14	113.31	108.54
24	4	306	CHL	C1C-CHC-C4B	3.14	127.29	116.07
25	A	843	CLA	C4-C3-C5	3.14	120.67	115.23
30	G	205	BCR	C36-C18-C17	-3.13	117.74	122.82
25	5	601	CLA	O2D-CGD-CBD	3.13	116.71	111.23
25	1	609	CLA	CHD-C1D-ND	-3.13	120.39	124.80
25	J	102	CLA	C3B-C4B-NB	-3.13	107.73	110.53
25	H	302	CLA	C5-C3-C2	3.13	128.20	121.17
25	B	810	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
25	P	301	CLA	CHB-C4A-NA	3.13	128.92	124.40
28	1	614	LHG	O7-C7-C8	3.13	118.25	111.48
37	W	317	NEX	C39-C29-C30	-3.13	117.75	122.82
25	T	301	CLA	C1-C2-C3	-3.13	121.07	126.20
24	U	313	CHL	CMB-C2B-C3B	3.13	130.93	124.68
25	A	830	CLA	C1-C2-C3	-3.13	121.08	126.20
25	A	808	CLA	C11-C12-C13	-3.13	105.57	115.97
30	A	850	BCR	C16-C15-C14	-3.12	117.12	123.52
29	R	323	Q6L	C35-C34-C33	3.12	115.82	111.18
38	X	309	KC2	CAA-C2A-C1A	-3.12	110.96	124.64
25	B	803	CLA	C1-O2A-CGA	-3.12	109.09	116.65
30	L	306	BCR	C39-C30-C25	3.12	115.14	110.24
30	K	202	BCR	C2-C1-C6	3.12	114.97	110.44
24	X	306	CHL	O2D-CGD-O1D	-3.12	117.78	123.85
24	T	307	CHL	CHA-C1A-C2A	-3.12	125.98	133.31
25	O	2002	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
25	A	808	CLA	CMB-C2B-C3B	3.12	133.88	126.55
25	A	833	CLA	C3B-C4B-NB	-3.12	107.75	110.53
25	F	803	CLA	OBD-CAD-C3D	-3.12	121.13	128.42
26	4	317	IWJ	C29-C30-C31	-3.12	120.38	124.22
38	P	308	KC2	CHB-C4A-NA	3.11	129.06	124.23
29	W	320	Q6L	C11-C03-C04	-3.11	114.99	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	804	CLA	C2A-C1A-CHA	3.11	129.27	123.87
37	R	321	NEX	C39-C29-C30	-3.11	117.78	122.82
27	6	615	XAT	C35-C15-C14	-3.11	117.15	123.52
25	B	803	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
25	B	814	CLA	O2D-CGD-CBD	3.11	116.67	111.23
28	3	321	LHG	O7-C7-C8	3.11	118.21	111.48
25	5	609	CLA	O2D-CGD-O1D	-3.11	117.03	124.08
25	4	304	CLA	O2D-CGD-CBD	3.11	116.67	111.23
30	K	207	BCR	C33-C5-C6	3.11	127.88	124.48
25	A	830	CLA	CHB-C4A-NA	3.11	128.88	124.40
25	6	603	CLA	C2C-C1C-NC	3.11	113.25	109.98
25	1	603	CLA	C2A-C1A-CHA	3.11	129.26	123.87
25	6	613	CLA	CMB-C2B-C1B	-3.11	120.69	125.42
25	1	605	CLA	C4A-NA-C1A	3.10	108.09	106.68
25	B	817	CLA	CHB-C4A-NA	3.10	128.88	124.40
25	A	827	CLA	O2D-CGD-CBD	3.10	116.66	111.23
38	R	312	KC2	O2D-CGD-O1D	-3.10	117.81	123.85
30	A	849	BCR	C8-C7-C6	-3.10	118.72	127.00
30	B	849	BCR	C40-C30-C25	-3.10	105.38	110.24
24	R	308	CHL	C3D-C4D-CHA	3.10	113.25	108.54
24	X	315	CHL	C1B-CHB-C4A	3.10	123.32	121.32
27	6	615	XAT	C8-C9-C10	-3.10	114.14	119.01
25	B	820	CLA	CMB-C2B-C1B	-3.10	120.70	125.42
25	6	613	CLA	C4-C3-C2	-3.09	115.69	123.63
30	K	202	BCR	C38-C26-C25	3.09	127.86	124.48
25	X	312	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
25	A	804	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
30	A	852	BCR	C12-C13-C14	-3.09	114.15	119.01
25	B	802	CLA	CMB-C2B-C3B	3.09	133.81	126.55
25	Q	311	CLA	C1-C2-C3	-3.09	121.14	126.20
25	W	312	CLA	CMB-C2B-C1B	-3.08	120.72	125.42
24	X	307	CHL	O2A-CGA-O1A	-3.08	115.92	123.63
25	H	304	CLA	CHB-C4A-NA	3.08	128.85	124.40
30	K	202	BCR	C35-C13-C12	3.08	122.79	118.09
30	A	848	BCR	C12-C13-C14	-3.08	114.17	119.01
25	B	819	CLA	CHB-C4A-NA	3.08	128.84	124.40
24	Q	309	CHL	CMB-C2B-C3B	3.08	130.84	124.68
26	R	303	IWJ	C35-C29-C30	3.08	111.94	108.78
30	B	847	BCR	C11-C10-C9	-3.08	122.96	127.28
30	M	101	BCR	C38-C26-C25	-3.08	121.13	124.48
24	T	304	CHL	O2D-CGD-O1D	-3.08	117.86	123.85
25	V	303	CLA	O2D-CGD-O1D	-3.08	117.86	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	M	101	BCR	C3-C4-C5	-3.08	108.57	114.06
30	F	804	BCR	C16-C15-C14	-3.08	117.23	123.52
30	J	101	BCR	C38-C26-C27	3.07	120.15	113.60
25	1	608	CLA	CBA-CAA-C2A	3.07	122.94	113.79
24	X	306	CHL	CBC-CAC-C3C	3.07	117.27	112.87
25	A	821	CLA	C4A-NA-C1A	3.07	108.08	106.68
37	T	317	NEX	C31-C30-C29	-3.07	122.97	127.28
24	T	320	CHL	C1B-CHB-C4A	3.07	123.30	121.32
25	B	818	CLA	CBA-CAA-C2A	3.07	122.93	113.79
24	Q	307	CHL	C4D-CHA-CBD	-3.07	105.87	108.97
25	B	808	CLA	CAC-C3C-C4C	3.07	128.78	124.79
25	A	843	CLA	CHB-C4A-NA	3.07	128.83	124.40
24	V	304	CHL	C1C-CHC-C4B	3.07	127.05	116.07
30	G	201	BCR	C12-C13-C14	-3.07	114.18	119.01
25	V	302	CLA	C1-C2-C3	-3.07	121.80	126.76
25	5	608	CLA	CHB-C4A-NA	3.07	128.83	124.40
30	A	851	BCR	C4-C5-C6	-3.07	118.56	122.70
29	O	2007	Q6L	C11-C03-C04	-3.07	115.02	116.81
24	2	605	CHL	CHA-C1A-C2A	-3.07	126.11	133.31
25	B	807	CLA	CBA-CAA-C2A	3.06	122.91	113.79
38	T	308	KC2	CAA-CBA-CGA	-3.06	111.48	127.05
30	F	801	BCR	C33-C5-C6	-3.06	121.14	124.48
25	B	818	CLA	C3B-C4B-NB	-3.06	107.80	110.53
25	P	303	CLA	CHB-C4A-NA	3.06	128.81	124.40
25	A	823	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
24	2	607	CHL	OMC-CMC-C2C	-3.06	119.81	125.12
25	B	828	CLA	CHB-C4A-NA	3.06	128.81	124.40
25	B	802	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
25	X	304	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
30	J	101	BCR	C19-C18-C17	-3.06	114.20	119.01
24	P	306	CHL	O2D-CGD-CBD	3.06	114.30	110.95
25	A	820	CLA	CBA-CAA-C2A	3.06	122.89	113.79
24	P	305	CHL	CMB-C2B-C3B	3.05	130.78	124.68
28	1	614	LHG	C5-O7-C7	-3.05	110.50	117.80
30	L	306	BCR	C23-C22-C21	-3.05	114.21	119.01
30	K	207	BCR	C15-C14-C13	-3.05	123.00	127.28
30	M	101	BCR	C15-C16-C17	-3.05	117.28	123.52
25	3	311	CLA	O2A-CGA-CBA	3.05	121.13	111.83
25	B	818	CLA	C1-O2A-CGA	3.05	124.03	116.65
25	O	2002	CLA	C1-C2-C3	3.05	131.19	126.20
25	T	303	CLA	CMB-C2B-C3B	3.05	133.71	126.55
25	R	314	CLA	O2D-CGD-CBD	3.05	116.55	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	307	CHL	C3C-C4C-NC	-3.04	107.21	114.65
25	B	805	CLA	CHD-C1D-ND	-3.04	120.52	124.80
29	S	320	Q6L	O39-C34-C35	-3.04	104.66	110.06
30	A	849	BCR	C19-C18-C17	-3.04	114.22	119.01
30	F	804	BCR	C35-C13-C12	3.04	122.73	118.09
25	A	856	CLA	CMC-C2C-C1C	3.04	129.78	125.03
25	Q	311	CLA	C4A-NA-C1A	3.04	108.07	106.68
24	2	601	CHL	C3D-C4D-CHA	3.04	113.16	108.54
25	4	311	CLA	C4A-NA-C1A	3.04	108.06	106.68
37	S	317	NEX	C31-C30-C29	-3.04	123.02	127.28
25	A	856	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
25	A	825	CLA	CMC-C2C-C1C	3.03	129.78	125.03
25	G	204	CLA	CMB-C2B-C1B	-3.03	120.80	125.42
30	B	846	BCR	C35-C13-C12	3.03	122.72	118.09
30	A	851	BCR	C7-C6-C5	-3.03	114.57	121.56
25	2	608	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
25	B	833	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	6	610	CLA	CHB-C4A-NA	3.03	128.78	124.40
37	P	317	NEX	C11-C10-C9	-3.03	123.03	127.28
30	J	101	BCR	C27-C26-C25	-3.03	118.61	122.70
25	T	313	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
32	6	617	SQD	O48-C23-C24	3.03	121.07	111.83
24	V	306	CHL	C4D-ND-C1D	3.03	107.52	105.22
37	P	317	NEX	C40-C33-C32	3.03	122.72	118.09
25	G	203	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
25	B	803	CLA	CMB-C2B-C3B	3.03	133.67	126.55
25	3	312	CLA	C4A-NA-C1A	3.03	108.06	106.68
25	A	832	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
25	B	806	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
30	L	305	BCR	C29-C30-C25	-3.03	106.04	110.44
25	P	302	CLA	CHB-C4A-NA	3.03	128.77	124.40
38	S	308	KC2	CHB-C4A-C3A	-3.03	120.25	125.03
25	R	305	CLA	CHB-C4A-NA	3.02	128.76	124.40
25	W	312	CLA	CAC-C3C-C4C	3.02	128.72	124.79
25	B	834	CLA	O2D-CGD-CBD	3.02	116.52	111.23
25	A	803	CLA	C1-O2A-CGA	3.02	123.97	116.65
30	B	849	BCR	C2-C1-C6	3.02	114.83	110.44
30	M	101	BCR	C19-C18-C17	-3.02	114.25	119.01
25	P	311	CLA	O2A-CGA-O1A	-3.02	116.07	123.63
25	4	316	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
25	B	813	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
25	4	313	CLA	CHD-C1D-ND	-3.02	120.55	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	849	BCR	C11-C10-C9	-3.02	123.04	127.28
25	4	314	CLA	O2D-CGD-CBD	3.02	116.50	111.23
25	5	603	CLA	CMB-C2B-C3B	3.02	133.64	126.55
25	V	301	CLA	CAA-C2A-C1A	-3.02	102.09	111.97
24	V	305	CHL	C4D-ND-C1D	3.01	107.51	105.22
24	4	307	CHL	O2D-CGD-O1D	-3.01	117.98	123.85
27	4	318	XAT	C31-C30-C29	-3.01	123.05	127.28
30	3	318	BCR	C32-C1-C6	3.01	114.97	110.24
24	6	605	CHL	C1B-CHB-C4A	3.01	123.26	121.32
30	3	318	BCR	C35-C13-C12	3.01	122.69	118.09
25	W	303	CLA	C1-C2-C3	-3.01	121.89	126.76
25	U	301	CLA	C3B-C4B-NB	-3.01	107.84	110.53
25	A	856	CLA	CHB-C4A-NA	3.01	128.74	124.40
29	X	319	Q6L	C42-C13-C12	3.01	120.45	115.23
30	I	101	BCR	C30-C25-C26	-3.01	118.53	122.64
24	4	307	CHL	CMB-C2B-C3B	3.01	130.98	124.69
30	F	804	BCR	C33-C5-C6	3.01	127.76	124.48
25	B	812	CLA	C3B-C4B-NB	-3.01	107.85	110.53
25	4	313	CLA	CHB-C4A-NA	3.01	128.74	124.40
25	V	302	CLA	C4A-NA-C1A	3.01	108.05	106.68
25	3	311	CLA	CHB-C4A-NA	3.00	128.74	124.40
26	V	318	IWJ	C35-C29-C30	3.00	111.86	108.78
25	R	313	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
30	B	846	BCR	C12-C13-C14	-3.00	114.29	119.01
25	Q	301	CLA	CHB-C4A-NA	3.00	128.73	124.40
30	F	804	BCR	C3-C4-C5	-3.00	108.70	114.06
25	S	313	CLA	C3B-C4B-NB	-3.00	107.85	110.53
25	3	307	CLA	C1-C2-C3	3.00	131.11	126.20
24	T	320	CHL	O2D-CGD-O1D	-3.00	118.01	123.85
25	T	302	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
30	F	804	BCR	C15-C16-C17	-3.00	117.38	123.52
30	B	846	BCR	C39-C30-C25	-3.00	105.54	110.24
25	B	839	CLA	C3B-C4B-NB	-3.00	107.85	110.53
25	R	314	CLA	CHB-C4A-NA	3.00	128.73	124.40
30	J	103	BCR	C8-C7-C6	-3.00	118.99	127.00
25	A	837	CLA	C4-C3-C2	-3.00	115.93	123.63
25	L	303	CLA	CMB-C2B-C3B	3.00	133.60	126.55
25	A	818	CLA	CMB-C2B-C3B	3.00	133.59	126.55
24	Q	307	CHL	CHA-C1A-C2A	-3.00	126.27	133.31
37	H	306	NEX	C12-C13-C14	-3.00	114.30	119.01
25	3	308	CLA	C1C-C2C-C3C	-2.99	103.83	106.98
29	P	315	Q6L	C40-C32-C33	-2.99	116.27	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	835	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
27	1	612	XAT	C12-C13-C14	-2.99	114.30	119.01
27	5	612	XAT	C8-C9-C10	-2.99	114.30	119.01
30	K	202	BCR	C15-C14-C13	-2.99	123.08	127.28
24	3	306	CHL	CHA-C1A-C2A	-2.99	126.28	133.31
38	S	308	KC2	CAA-C2A-C1A	-2.99	111.53	124.64
30	B	845	BCR	C19-C18-C17	-2.99	114.30	119.01
38	Q	310	KC2	CHB-C4A-NA	2.99	128.87	124.23
27	2	617	XAT	C31-C30-C29	-2.99	123.09	127.28
25	S	303	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
25	H	302	CLA	CBA-CAA-C2A	2.99	122.68	113.79
24	P	305	CHL	CBC-CAC-C3C	-2.99	108.60	112.87
25	P	310	CLA	O2A-CGA-O1A	-2.99	116.16	123.63
24	V	307	CHL	CHA-C1A-C2A	-2.99	126.30	133.31
25	B	834	CLA	CHB-C4A-NA	2.98	128.71	124.40
24	2	607	CHL	CMB-C2B-C3B	2.98	130.64	124.68
25	A	843	CLA	C1-C2-C3	2.98	131.08	126.20
24	2	615	CHL	CHA-C1A-C2A	-2.98	126.31	133.31
25	6	608	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	4	311	CLA	O2D-CGD-CBD	2.98	116.44	111.23
25	A	828	CLA	CHB-C4A-NA	2.98	128.70	124.40
25	2	602	CLA	C7-C6-C5	2.98	121.20	113.26
38	T	308	KC2	CHB-C4A-C3A	-2.98	120.33	125.03
30	G	201	BCR	C27-C26-C25	-2.98	118.68	122.70
25	A	819	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	4	303	CLA	CHB-C4A-NA	2.98	128.70	124.40
25	A	805	CLA	O2D-CGD-CBD	2.98	116.44	111.23
30	J	101	BCR	C38-C26-C25	-2.98	121.24	124.48
25	R	306	CLA	CHB-C4A-NA	2.97	128.69	124.40
25	B	821	CLA	C4A-NA-C1A	2.97	108.04	106.68
25	R	316	CLA	CBA-CAA-C2A	2.97	122.64	113.79
25	6	602	CLA	O2A-CGA-O1A	-2.97	116.19	123.63
24	W	305	CHL	C4D-CHA-CBD	-2.97	105.97	108.97
28	2	619	LHG	O7-C7-C8	2.97	117.91	111.48
37	P	317	NEX	C20-C13-C12	2.97	122.63	118.09
31	2	620	LMG	C8-O7-C10	-2.97	110.69	117.80
27	6	615	XAT	C28-C29-C30	-2.97	114.34	119.01
24	S	307	CHL	CBC-CAC-C3C	2.97	117.12	112.87
30	A	851	BCR	C15-C14-C13	-2.97	123.11	127.28
24	4	302	CHL	C4D-CHA-CBD	-2.97	105.97	108.97
24	P	307	CHL	C3C-C4C-NC	-2.97	107.40	114.65
30	B	847	BCR	C20-C21-C22	-2.97	123.12	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	306	CHL	C1B-CHB-C4A	2.97	123.23	121.32
24	6	601	CHL	C4D-ND-C1D	2.97	107.47	105.22
24	R	302	CHL	C3D-C4D-CHA	2.96	113.05	108.54
24	T	306	CHL	C1C-CHC-C4B	2.96	126.68	116.07
25	B	827	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	X	303	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	S	310	CLA	C4-C3-C5	2.96	120.37	115.23
27	6	615	XAT	C32-C33-C34	-2.96	114.35	119.01
30	3	318	BCR	C12-C13-C14	-2.96	114.35	119.01
25	B	836	CLA	CHB-C4A-NA	2.96	128.68	124.40
25	T	311	CLA	CHB-C4A-NA	2.96	128.68	124.40
24	2	601	CHL	C3C-C4C-NC	-2.96	107.41	114.65
30	B	847	BCR	C32-C1-C6	2.96	114.89	110.24
30	L	306	BCR	C27-C26-C25	-2.96	118.70	122.70
30	L	307	BCR	C23-C24-C25	-2.96	119.09	127.00
24	X	305	CHL	C4C-CHD-C1D	2.96	126.66	116.07
30	F	804	BCR	C8-C7-C6	-2.96	119.09	127.00
25	A	825	CLA	CAC-C3C-C4C	2.96	128.64	124.79
31	N	201	LMG	O6-C5-C6	2.96	113.77	106.44
27	2	617	XAT	C17-C1-C16	-2.96	103.07	107.37
37	R	321	NEX	C16-C1-C6	2.96	113.12	110.47
30	A	848	BCR	C16-C15-C14	-2.96	117.47	123.52
29	Q	317	Q6L	C42-C13-C12	2.96	120.36	115.23
25	G	204	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
30	B	847	BCR	C35-C13-C12	2.95	122.60	118.09
25	2	602	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	A	809	CLA	C3A-C2A-C1A	2.95	105.76	101.34
37	R	321	NEX	C38-C25-C26	-2.95	117.45	122.30
25	B	841	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
25	A	803	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
27	1	612	XAT	C39-C29-C30	2.95	127.59	122.82
33	A	802	CL0	CHA-C1A-C2A	-2.95	126.39	133.31
24	V	304	CHL	O2D-CGD-CBD	2.95	114.18	110.95
29	W	320	Q6L	C01-C02-C07	-2.95	109.00	114.42
24	4	302	CHL	C3D-C4D-CHA	2.95	113.02	108.54
29	R	323	Q6L	C42-C13-C12	2.95	120.34	115.23
24	R	302	CHL	C3C-C4C-NC	-2.94	107.45	114.65
26	U	316	IWJ	C29-C30-C31	-2.94	120.59	124.22
30	3	318	BCR	C3-C4-C5	-2.94	108.81	114.06
25	4	312	CLA	CHB-C4A-NA	2.94	128.65	124.40
30	3	319	BCR	C11-C10-C9	-2.94	123.15	127.28
25	V	311	CLA	O2D-CGD-O1D	-2.94	118.12	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	V	304	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
24	R	310	CHL	CHA-C1A-C2A	-2.94	126.40	133.31
25	3	303	CLA	O1D-CGD-CBD	2.94	130.32	124.52
25	R	317	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
31	F	805	LMG	O8-C28-C29	2.94	120.79	111.83
30	4	319	BCR	C3-C4-C5	-2.94	108.82	114.06
33	A	802	CL0	CBC-CAC-C3C	-2.94	108.67	112.87
25	A	814	CLA	CMB-C2B-C1B	-2.94	120.95	125.42
25	A	817	CLA	CHD-C1D-ND	-2.93	120.67	124.80
25	6	604	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
25	L	302	CLA	CHB-C4A-NA	2.93	128.63	124.40
30	F	804	BCR	C36-C18-C17	-2.93	118.06	122.82
24	6	601	CHL	O2D-CGD-CBD	2.93	114.17	110.95
26	Q	320	IWJ	C32-C30-C29	-2.93	110.94	113.96
30	B	846	BCR	C36-C18-C17	-2.93	118.06	122.82
24	Q	316	CHL	C4D-CHA-CBD	-2.93	106.01	108.97
27	5	612	XAT	C32-C33-C34	-2.93	114.40	119.01
24	V	307	CHL	C3C-C4C-NC	-2.93	107.49	114.65
24	R	302	CHL	O2D-CGD-O1D	-2.93	118.14	123.85
25	6	602	CLA	CED-O2D-CGD	2.93	122.56	115.92
30	3	319	BCR	C20-C21-C22	-2.93	123.17	127.28
24	W	307	CHL	C4D-CHA-CBD	-2.93	106.02	108.97
24	S	304	CHL	CAA-C2A-C3A	-2.93	109.52	116.23
30	H	305	BCR	C36-C18-C17	-2.92	118.08	122.82
25	A	830	CLA	O2A-CGA-O1A	-2.92	116.31	123.63
29	P	316	Q6L	C15-C14-C13	-2.92	123.58	127.69
25	Q	305	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	K	201	CLA	CMB-C2B-C3B	2.92	133.43	126.55
25	L	302	CLA	CBA-CAA-C2A	2.92	122.49	113.79
37	W	317	NEX	C16-C1-C6	2.92	113.09	110.47
25	K	206	CLA	CHB-C4A-NA	2.92	128.62	124.40
27	2	617	XAT	C36-C21-C22	-2.92	103.83	108.97
25	V	303	CLA	CMB-C2B-C3B	2.92	133.42	126.55
25	4	303	CLA	CAC-C3C-C4C	2.92	128.59	124.79
29	S	315	Q6L	C35-C34-C33	2.92	115.52	111.18
30	F	801	BCR	C12-C13-C14	-2.92	114.42	119.01
25	A	839	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	R	311	CHL	CMB-C2B-C3B	2.92	130.51	124.68
24	T	307	CHL	C4D-CHA-CBD	-2.92	106.03	108.97
25	Q	301	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
29	X	301	Q6L	C19-C18-C17	-2.92	123.19	127.28
26	S	318	IWJ	C36-C35-C34	-2.92	103.84	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	612	CLA	CHB-C4A-NA	2.92	128.61	124.40
25	B	826	CLA	CHA-C1A-NA	-2.91	119.79	126.39
30	4	319	BCR	C35-C13-C12	2.91	122.54	118.09
24	T	306	CHL	CMB-C2B-C3B	2.91	130.50	124.68
24	Q	309	CHL	C4D-CHA-CBD	-2.91	106.03	108.97
38	W	308	KC2	CAC-C3C-C2C	-2.91	118.96	128.43
24	V	305	CHL	O2D-CGD-O1D	-2.91	118.18	123.85
25	T	303	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
29	W	320	Q6L	C35-C34-C33	2.91	115.51	111.18
25	3	301	CLA	C1D-ND-C4D	-2.91	104.27	106.31
37	H	306	NEX	C15-C35-C34	-2.91	117.56	123.52
30	G	201	BCR	C36-C18-C17	-2.91	118.10	122.82
25	G	202	CLA	C4A-NA-C1A	2.91	108.00	106.68
24	W	304	CHL	C1C-CHC-C4B	2.91	126.47	116.07
25	V	311	CLA	CHB-C4A-NA	2.91	128.59	124.40
30	A	848	BCR	C40-C30-C39	-2.90	100.32	108.63
25	B	806	CLA	C1-C2-C3	2.90	130.95	126.20
38	T	308	KC2	CAA-C2A-C1A	-2.90	111.93	124.64
25	A	845	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
24	U	313	CHL	O2D-CGD-CBD	2.90	114.13	110.95
25	5	602	CLA	CHB-C4A-NA	2.90	128.58	124.40
25	Q	311	CLA	CHB-C4A-NA	2.90	128.58	124.40
29	Q	317	Q6L	C31-C30-C29	-2.90	120.07	124.58
38	R	312	KC2	CMD-C2D-C1D	-2.90	121.01	125.42
25	O	2005	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
24	S	314	CHL	CHA-C1A-C2A	-2.90	126.50	133.31
30	B	845	BCR	C35-C13-C12	2.90	122.51	118.09
30	J	103	BCR	C19-C18-C17	-2.90	114.45	119.01
38	P	308	KC2	CAA-C2A-C1A	-2.89	111.96	124.64
25	A	813	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
34	A	844	PQN	C11-C3-C2	-2.89	119.93	124.89
25	A	834	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	U	313	CHL	C4D-CHA-CBD	-2.89	106.05	108.97
25	B	826	CLA	C6-C5-C3	-2.89	106.43	113.47
25	A	830	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	3	307	CLA	CHB-C4A-NA	2.89	128.57	124.40
25	3	303	CLA	CHB-C4A-NA	2.89	128.57	124.40
24	R	308	CHL	CMB-C2B-C3B	2.89	130.45	124.68
25	A	812	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
25	4	311	CLA	CED-O2D-CGD	2.89	122.46	115.92
30	G	205	BCR	C8-C7-C6	-2.89	119.29	127.00
24	T	305	CHL	O2D-CGD-O1D	-2.88	118.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	311	CLA	CMB-C2B-C3B	2.88	133.33	126.55
24	W	305	CHL	CMB-C2B-C3B	2.88	130.44	124.68
36	B	850	DGD	O1G-C1A-C2A	2.88	120.62	111.83
30	M	101	BCR	C29-C30-C25	-2.88	106.26	110.44
24	U	304	CHL	C3D-C4D-CHA	2.88	112.92	108.54
30	K	202	BCR	C33-C5-C6	2.88	127.62	124.48
25	A	834	CLA	CMB-C2B-C1B	-2.88	121.04	125.42
25	6	611	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
25	A	804	CLA	C2B-C1B-NB	2.88	113.31	110.33
24	W	314	CHL	O2D-CGD-O1D	-2.88	118.25	123.85
29	S	323	Q6L	C11-C03-C04	-2.87	115.13	116.81
25	Q	311	CLA	O2D-CGD-CBD	2.87	116.25	111.23
25	B	803	CLA	C4D-C3D-CAD	-2.87	104.99	108.11
27	6	615	XAT	O24-C25-C38	2.87	118.26	115.05
25	B	821	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
29	R	320	Q6L	C15-C14-C13	-2.87	123.66	127.69
31	B	801	LMG	O1-C1-C2	2.87	112.63	108.27
25	B	831	CLA	O1D-CGD-CBD	2.87	130.17	124.52
30	A	851	BCR	C39-C30-C25	2.87	114.74	110.24
25	O	2001	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
26	T	318	IWJ	C35-C29-C30	2.86	111.72	108.78
25	1	608	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	B	813	CLA	C3C-C4C-NC	-2.86	106.76	110.43
25	A	829	CLA	CMB-C2B-C3B	2.86	133.28	126.55
25	B	820	CLA	C2A-C1A-CHA	2.86	128.83	123.87
24	R	310	CHL	C4D-ND-C1D	2.86	107.39	105.22
25	A	805	CLA	CMB-C2B-C3B	2.86	133.28	126.55
25	P	311	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	R	313	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
25	A	839	CLA	C1-C2-C3	-2.86	121.51	126.20
25	B	813	CLA	CMC-C2C-C1C	2.86	129.50	125.03
24	Q	316	CHL	C3D-C4D-CHA	2.86	112.89	108.54
30	K	205	BCR	C4-C5-C6	-2.86	118.84	122.70
30	A	849	BCR	C1-C6-C5	-2.86	118.73	122.64
27	4	318	XAT	O23-C23-C22	2.86	115.59	109.75
25	2	602	CLA	CMC-C2C-C1C	2.86	129.50	125.03
25	A	817	CLA	CHB-C4A-NA	2.86	128.53	124.40
25	Q	311	CLA	CBA-CAA-C2A	2.86	122.30	113.79
25	R	305	CLA	CAA-CBA-CGA	2.86	121.32	113.21
25	4	310	CLA	CHB-C4A-NA	2.86	128.52	124.40
25	S	311	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
25	1	607	CLA	CMB-C2B-C3B	2.86	133.27	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	V	321	Q6L	C38-C36-C35	-2.86	104.08	109.41
25	V	303	CLA	CAC-C3C-C2C	-2.86	122.31	127.56
37	W	317	NEX	C15-C14-C13	-2.86	123.27	127.28
25	B	820	CLA	O2D-CGD-CBD	2.86	116.22	111.23
25	B	806	CLA	CHC-C4B-NB	2.85	128.33	124.05
25	S	301	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	U	312	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
38	U	307	KC2	C2A-C3A-C4A	-2.85	104.27	106.41
24	V	314	CHL	CHA-C1A-C2A	-2.85	126.61	133.31
25	A	818	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	A	805	CLA	CHB-C4A-NA	2.85	128.52	124.40
38	Q	310	KC2	O2A-CGA-O1A	-2.85	116.89	122.70
27	5	612	XAT	C35-C15-C14	-2.85	117.68	123.52
25	3	314	CLA	CMB-C2B-C3B	2.85	133.26	126.55
26	R	322	IWJ	C35-C29-C30	2.85	111.70	108.78
24	S	304	CHL	C1B-CHB-C4A	2.85	123.16	121.32
25	5	610	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	5	603	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	B	836	CLA	CHD-C1D-ND	-2.85	120.79	124.80
25	B	817	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	B	833	CLA	CHB-C4A-NA	2.85	128.51	124.40
30	M	101	BCR	C23-C22-C21	-2.85	114.53	119.01
24	X	307	CHL	O2A-CGA-CBA	2.85	120.51	111.83
25	B	807	CLA	CMB-C2B-C3B	2.84	133.24	126.55
25	5	602	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
24	P	314	CHL	CHA-C1A-C2A	-2.84	126.63	133.31
29	U	315	Q6L	C19-C20-C21	-2.84	117.70	123.52
25	P	302	CLA	O2D-CGD-CBD	2.84	116.20	111.23
27	4	318	XAT	C8-C9-C10	-2.84	114.54	119.01
24	2	615	CHL	O2D-CGD-CBD	2.84	114.07	110.95
24	3	306	CHL	C3C-C4C-NC	-2.84	107.71	114.65
25	1	603	CLA	C5-C3-C2	2.84	127.54	121.17
24	S	314	CHL	O2D-CGD-O1D	-2.84	118.32	123.85
24	W	307	CHL	C1-C2-C3	-2.84	121.54	126.20
30	L	306	BCR	C33-C5-C6	-2.84	121.39	124.48
25	A	806	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
24	W	305	CHL	CBC-CAC-C3C	-2.84	108.81	112.87
24	X	308	CHL	O2D-CGD-O1D	-2.83	118.33	123.85
37	R	321	NEX	C40-C33-C32	2.83	122.42	118.09
25	3	302	CLA	CHB-C4A-NA	2.83	128.49	124.40
27	5	612	XAT	O24-C25-C38	2.83	118.22	115.05
25	V	302	CLA	O2D-CGD-CBD	2.83	116.18	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	605	CHL	C1C-CHC-C4B	2.83	126.21	116.07
29	S	323	Q6L	C20-C21-C22	2.83	131.25	127.28
37	R	321	NEX	C11-C10-C9	-2.83	123.30	127.28
25	B	804	CLA	CAC-C3C-C4C	2.83	128.48	124.79
24	T	306	CHL	C3D-C4D-CHA	2.83	112.84	108.54
30	3	318	BCR	C23-C22-C21	-2.83	114.56	119.01
25	B	815	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	V	304	CHL	O2A-CGA-O1A	-2.83	116.06	123.33
25	4	303	CLA	CBA-CAA-C2A	2.83	122.21	113.79
24	V	314	CHL	C4D-CHA-CBD	-2.83	106.12	108.97
30	3	317	BCR	C8-C7-C6	-2.83	119.44	127.00
25	A	820	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	2	607	CHL	C3C-C4C-NC	-2.83	107.74	114.65
30	B	847	BCR	C37-C22-C23	2.83	122.41	118.09
25	2	604	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
30	L	305	BCR	C20-C21-C22	-2.83	123.32	127.28
25	A	820	CLA	CHA-C1A-NA	-2.82	119.99	126.39
24	S	314	CHL	O2D-CGD-CBD	2.82	114.05	110.95
30	B	847	BCR	C38-C26-C27	2.82	119.62	113.60
25	6	610	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
25	5	601	CLA	CBA-CAA-C2A	2.82	122.19	113.79
37	T	317	NEX	C19-C9-C10	2.82	127.39	122.82
24	W	306	CHL	C1B-CHB-C4A	2.82	123.14	121.32
24	P	314	CHL	C4C-CHD-C1D	2.82	126.17	116.07
25	T	301	CLA	CHB-C4A-NA	2.82	128.47	124.40
25	G	203	CLA	CHB-C4A-NA	2.82	128.47	124.40
24	P	306	CHL	C3C-C4C-NC	-2.82	107.75	114.65
29	V	319	Q6L	C29-C27-C26	-2.82	114.57	119.01
25	S	313	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
25	A	804	CLA	O2D-CGD-CBD	2.82	116.16	111.23
25	B	811	CLA	CHB-C4A-NA	2.82	128.47	124.40
24	2	601	CHL	CHA-C1A-C2A	-2.82	126.69	133.31
25	K	206	CLA	C6-C5-C3	2.82	120.33	113.47
25	A	832	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
24	U	313	CHL	O2D-CGD-O1D	-2.82	118.36	123.85
25	V	312	CLA	CHB-C4A-NA	2.82	128.46	124.40
24	U	306	CHL	C4D-CHA-CBD	-2.81	106.13	108.97
25	A	839	CLA	CMB-C2B-C1B	-2.81	121.13	125.42
25	P	301	CLA	CMC-C2C-C1C	2.81	129.43	125.03
34	B	844	PQN	O1-C1-C2	-2.81	116.75	120.45
29	X	301	Q6L	C19-C20-C21	-2.81	117.76	123.52
25	L	303	CLA	O2D-CGD-O1D	-2.81	118.37	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	W	306	CHL	C1-C2-C3	-2.81	121.59	126.20
25	S	310	CLA	C1-C2-C3	-2.81	121.59	126.20
25	6	603	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
25	B	826	CLA	C2A-C1A-CHA	2.81	128.75	123.87
25	3	304	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
38	W	308	KC2	CMC-C2C-C1C	2.81	129.43	125.03
25	A	831	CLA	C3B-C4B-NB	-2.81	108.02	110.53
24	3	306	CHL	CMB-C2B-C3B	2.81	130.29	124.68
25	B	806	CLA	CAC-C3C-C4C	2.81	128.44	124.79
24	6	605	CHL	OMC-CMC-C2C	-2.81	120.25	125.12
25	A	856	CLA	O2D-CGD-CBD	2.81	116.14	111.23
25	U	303	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
24	1	601	CHL	O2D-CGD-O1D	-2.81	117.72	124.08
29	X	317	Q6L	C19-C20-C21	-2.80	117.78	123.52
24	Q	308	CHL	C3C-C4C-NC	-2.80	107.80	114.65
37	S	317	NEX	C8-C7-C6	-2.80	174.35	177.66
25	B	816	CLA	CHB-C4A-NA	2.80	128.45	124.40
24	U	313	CHL	CHA-C1A-C2A	-2.80	126.72	133.31
25	A	807	CLA	CBC-CAC-C3C	2.80	120.02	112.42
25	Q	301	CLA	C2A-C1A-CHA	2.80	128.73	123.87
25	W	310	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
29	W	316	Q6L	C19-C20-C21	-2.80	117.78	123.52
25	K	206	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
24	4	307	CHL	CHA-C1A-C2A	-2.80	126.73	133.31
25	A	814	CLA	CBA-CAA-C2A	2.80	122.13	113.79
24	P	306	CHL	C4D-CHA-CBD	-2.80	106.14	108.97
30	K	202	BCR	C20-C19-C18	-2.80	118.69	126.36
26	U	316	IWJ	C36-C35-C34	-2.80	104.05	108.97
24	V	305	CHL	C4D-CHA-CBD	-2.80	106.15	108.97
24	6	605	CHL	O2D-CGD-O1D	-2.80	118.40	123.85
25	U	308	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	A	824	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
26	4	317	IWJ	C28-C29-C35	-2.80	107.25	111.97
25	P	302	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	3	307	CLA	C2A-C1A-CHA	2.80	128.72	123.87
25	T	310	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
25	A	830	CLA	C6-C5-C3	-2.80	106.66	113.47
25	B	804	CLA	C3B-C4B-NB	-2.79	108.04	110.53
25	4	315	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
29	V	319	Q6L	C19-C20-C21	-2.79	117.80	123.52
29	Q	317	Q6L	C05-C04-C03	2.79	114.31	110.61
24	2	601	CHL	CMB-C2B-C3B	2.79	130.26	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	H	302	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
38	W	308	KC2	CBA-CAA-C2A	-2.79	114.25	125.45
25	A	809	CLA	C1-C2-C3	-2.79	122.25	126.76
24	V	305	CHL	CHA-C1A-C2A	-2.79	126.75	133.31
25	Q	301	CLA	C6-C5-C3	2.79	120.26	113.47
25	L	304	CLA	CHB-C4A-NA	2.79	128.42	124.40
25	1	609	CLA	CMA-C3A-C2A	-2.79	109.84	116.23
24	V	314	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
27	2	617	XAT	C32-C33-C34	-2.79	114.63	119.01
25	S	310	CLA	O2D-CGD-CBD	2.79	116.10	111.23
30	4	319	BCR	C39-C30-C25	-2.79	105.88	110.24
25	R	316	CLA	CHB-C4A-NA	2.78	128.42	124.40
30	L	307	BCR	C3-C4-C5	-2.78	109.09	114.06
25	P	302	CLA	C4-C3-C5	2.78	120.06	115.23
33	A	802	CL0	C4D-ND-C1D	2.78	107.33	105.22
29	P	321	Q6L	C19-C18-C17	-2.78	123.38	127.28
30	G	205	BCR	C35-C13-C12	2.78	122.33	118.09
25	U	309	CLA	CHB-C4A-NA	2.78	128.41	124.40
38	V	308	KC2	CAC-C3C-C2C	-2.78	119.40	128.43
24	R	318	CHL	CMB-C2B-C3B	2.78	130.24	124.68
24	X	305	CHL	C3D-C4D-CHA	2.78	112.76	108.54
25	V	310	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
24	W	305	CHL	CMA-C3A-C2A	-2.77	109.87	116.23
25	O	2001	CLA	C3A-C2A-C1A	2.77	105.50	101.34
24	V	306	CHL	C3C-C4C-NC	-2.77	107.87	114.65
25	B	834	CLA	CHD-C1D-ND	-2.77	120.90	124.80
25	B	840	CLA	C3B-C4B-NB	-2.77	108.05	110.53
24	X	305	CHL	C1B-CHB-C4A	2.77	123.11	121.32
24	S	306	CHL	C4-C3-C5	2.77	119.39	116.13
24	S	304	CHL	C4D-CHA-CBD	-2.77	106.17	108.97
25	1	606	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
25	6	611	CLA	CHB-C4A-NA	2.77	128.40	124.40
30	I	101	BCR	C34-C9-C10	2.77	127.31	122.82
25	B	830	CLA	CHC-C4B-NB	2.77	128.21	124.05
25	P	310	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	R	310	CHL	C4D-CHA-CBD	-2.77	106.17	108.97
25	B	816	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
30	L	306	BCR	C3-C4-C5	-2.77	109.12	114.06
27	4	318	XAT	C38-C25-C26	-2.77	117.75	122.30
25	U	308	CLA	C2C-C1C-NC	2.77	112.89	109.98
25	B	843	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	X	308	CHL	CMD-C2D-C3D	2.77	130.21	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	820	CLA	C2A-C1A-CHA	2.77	128.67	123.87
25	F	803	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
25	R	305	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
25	B	837	CLA	CHD-C1D-ND	-2.77	120.91	124.80
25	R	315	CLA	O2D-CGD-CBD	2.76	116.06	111.23
25	R	315	CLA	O2A-CGA-O1A	-2.76	116.71	123.63
25	B	813	CLA	C7-C6-C5	-2.76	105.90	113.26
25	V	313	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
33	A	802	CL0	C1C-CHC-C4B	2.76	125.95	116.07
25	B	809	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	3	314	CLA	O2D-CGD-O1D	-2.76	117.81	124.08
25	3	311	CLA	CHD-C1D-ND	-2.76	120.92	124.80
25	6	602	CLA	CHB-C4A-NA	2.76	128.39	124.40
25	1	613	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
25	T	301	CLA	CMB-C2B-C3B	2.76	133.04	126.55
25	S	309	CLA	CHB-C4A-NA	2.76	128.38	124.40
30	L	307	BCR	C28-C27-C26	-2.76	109.13	114.06
25	U	301	CLA	C2A-C1A-CHA	2.76	128.66	123.87
25	B	802	CLA	CMC-C2C-C1C	2.76	129.35	125.03
25	A	845	CLA	CHB-C4A-NA	2.76	128.38	124.40
30	M	101	BCR	C28-C27-C26	-2.76	109.14	114.06
25	H	302	CLA	C4-C3-C2	-2.76	116.54	123.63
25	1	608	CLA	C2D-C1D-ND	-2.76	107.40	110.13
30	3	317	BCR	C12-C13-C14	-2.76	114.67	119.01
24	Q	309	CHL	O2D-CGD-O1D	-2.76	118.48	123.85
38	U	307	KC2	CHB-C4A-C3A	-2.76	120.68	125.03
24	T	306	CHL	C1B-CHB-C4A	2.75	123.09	121.32
27	1	612	XAT	C37-C21-C36	-2.75	103.37	107.37
30	3	317	BCR	C20-C21-C22	-2.75	123.42	127.28
25	6	612	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
24	S	304	CHL	CMD-C2D-C3D	2.75	130.18	124.68
34	B	844	PQN	C11-C3-C2	-2.75	120.17	124.89
37	T	317	NEX	C11-C10-C9	-2.75	123.42	127.28
25	3	311	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
25	T	301	CLA	C3B-C4B-NB	-2.75	108.08	110.53
30	J	101	BCR	C34-C9-C8	-2.75	113.89	118.09
25	P	313	CLA	CAA-C2A-C3A	-2.75	105.57	113.00
24	S	306	CHL	CHA-C1A-C2A	-2.75	126.85	133.31
24	6	601	CHL	C4D-CHA-CBD	-2.75	106.19	108.97
38	V	308	KC2	O2A-CGA-O1A	-2.75	117.10	122.70
24	X	308	CHL	C4D-CHA-CBD	-2.75	106.20	108.97
24	S	304	CHL	CMA-C3A-C4A	2.75	120.53	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	609	CLA	CHB-C4A-NA	2.75	128.36	124.40
24	U	305	CHL	CHA-C1A-C2A	-2.75	126.86	133.31
25	Q	304	CLA	C2B-C1B-NB	2.75	113.17	110.33
25	1	602	CLA	CAC-C3C-C4C	2.75	128.36	124.79
25	A	816	CLA	CHD-C1D-ND	-2.75	120.94	124.80
25	U	301	CLA	CMB-C2B-C3B	2.75	133.01	126.55
29	T	316	Q6L	C29-C27-C26	-2.75	114.69	119.01
24	4	306	CHL	O2D-CGD-O1D	-2.74	117.85	124.08
25	X	311	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
28	3	322	LHG	O7-C7-C8	2.74	117.42	111.48
25	L	303	CLA	C4A-NA-C1A	2.74	107.93	106.68
38	R	312	KC2	CAA-C2A-C1A	-2.74	112.62	124.64
30	K	205	BCR	C16-C15-C14	-2.74	117.90	123.52
30	I	101	BCR	C15-C16-C17	-2.74	117.91	123.52
25	B	832	CLA	C2D-C1D-ND	-2.74	107.41	110.13
25	B	803	CLA	OBD-CAD-C3D	2.74	134.82	128.42
24	W	304	CHL	C3D-C4D-CHA	2.74	112.70	108.54
25	B	826	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
29	U	317	Q6L	C42-C13-C12	2.74	119.98	115.23
25	B	818	CLA	C6-C5-C3	2.74	120.14	113.47
25	Q	306	CLA	CBA-CAA-C2A	2.74	121.94	113.79
25	A	842	CLA	CHB-C4A-NA	2.74	128.35	124.40
24	W	314	CHL	C2A-C1A-CHA	2.74	126.38	121.84
38	W	308	KC2	CMC-C2C-C3C	-2.74	121.80	128.43
25	N	202	CLA	O2D-CGD-O1D	-2.74	117.87	124.08
24	2	615	CHL	O2D-CGD-O1D	-2.74	118.52	123.85
25	O	2004	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
25	2	608	CLA	C4A-NA-C1A	2.74	107.93	106.68
31	2	620	LMG	O8-C28-C29	2.73	120.17	111.83
25	1	606	CLA	CAB-C3B-C2B	2.73	130.80	123.53
25	W	311	CLA	CHB-C4A-NA	2.73	128.35	124.40
25	S	309	CLA	CBA-CAA-C2A	2.73	121.93	113.79
25	L	303	CLA	CAA-CBA-CGA	2.73	119.78	112.49
25	V	303	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	6	601	CHL	C3D-C4D-CHA	2.73	112.69	108.54
24	2	615	CHL	C4D-CHA-CBD	-2.73	106.21	108.97
25	X	313	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	U	308	CLA	CMC-C2C-C1C	2.73	129.30	125.03
25	3	301	CLA	CHB-C4A-NA	2.73	128.34	124.40
30	A	849	BCR	C15-C16-C17	-2.73	117.93	123.52
25	A	835	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
26	V	318	IWJ	O27-C26-C28	-2.73	116.17	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	812	CLA	CHB-C4A-NA	2.73	128.34	124.40
25	B	826	CLA	C4D-CHA-C1A	2.73	124.50	121.24
24	V	304	CHL	O2D-CGD-O1D	-2.73	118.54	123.85
27	5	612	XAT	C37-C21-C36	-2.73	103.41	107.37
25	A	817	CLA	C1-C2-C3	-2.73	121.73	126.20
27	2	617	XAT	C28-C29-C30	-2.73	114.72	119.01
30	F	801	BCR	C16-C15-C14	-2.73	117.94	123.52
30	G	205	BCR	C10-C11-C12	2.73	131.10	123.20
25	B	807	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
30	K	207	BCR	C20-C21-C22	-2.73	123.46	127.28
30	4	319	BCR	C16-C15-C14	-2.72	117.94	123.52
25	A	843	CLA	CMC-C2C-C1C	2.72	129.29	125.03
24	P	304	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
24	V	306	CHL	C3D-C4D-CHA	2.72	112.68	108.54
24	P	314	CHL	O2D-CGD-O1D	-2.72	118.55	123.85
25	1	608	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	1	609	CLA	CHB-C4A-NA	2.72	128.33	124.40
25	3	307	CLA	CBA-CAA-C2A	2.72	121.89	113.79
25	A	821	CLA	O2D-CGD-CBD	2.72	115.99	111.23
30	H	305	BCR	C36-C18-C19	2.72	122.25	118.09
25	O	2004	CLA	CMA-C3A-C2A	-2.72	109.99	116.23
24	3	306	CHL	O1D-CGD-CBD	2.72	128.85	124.72
25	X	313	CLA	CHB-C4A-NA	2.72	128.33	124.40
30	A	850	BCR	C19-C18-C17	-2.72	114.73	119.01
30	M	101	BCR	C36-C18-C17	-2.72	118.41	122.82
25	W	311	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	B	829	CLA	CMB-C2B-C3B	2.72	132.95	126.55
25	R	307	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
25	B	831	CLA	CMC-C2C-C1C	2.72	129.28	125.03
25	1	603	CLA	CHA-C1A-NA	-2.72	120.23	126.39
25	H	301	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
29	T	316	Q6L	C26-C25-C24	-2.72	115.32	123.20
25	A	823	CLA	O2A-C1-C2	-2.72	97.65	108.11
25	A	807	CLA	CHB-C4A-NA	2.72	128.32	124.40
38	X	309	KC2	CAA-CBA-CGA	-2.72	113.23	127.05
30	B	848	BCR	C3-C4-C5	-2.72	109.21	114.06
27	5	612	XAT	C38-C25-C24	2.72	117.29	114.24
30	B	847	BCR	C21-C20-C19	2.72	131.07	123.20
24	W	306	CHL	C4D-CHA-CBD	-2.72	106.23	108.97
24	4	307	CHL	C1C-CHC-C4B	2.72	125.78	116.07
29	V	319	Q6L	C28-C27-C26	2.71	127.21	122.82
25	S	311	CLA	O2D-CGD-O1D	-2.71	118.56	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	U	304	CHL	O2D-CGD-O1D	-2.71	118.56	123.85
24	2	615	CHL	C3C-C4C-NC	-2.71	108.02	114.65
25	R	313	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
30	K	205	BCR	C35-C13-C12	2.71	122.23	118.09
25	6	603	CLA	C4A-NA-C1A	2.71	107.92	106.68
25	B	820	CLA	C4A-NA-C1A	2.71	107.92	106.68
25	A	824	CLA	CHD-C1D-ND	-2.71	120.99	124.80
30	4	319	BCR	C16-C17-C18	-2.71	123.48	127.28
26	S	318	IWJ	C17-C16-C15	-2.71	117.97	123.52
31	F	805	LMG	O1-C1-C2	2.71	112.39	108.27
25	B	804	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
30	H	305	BCR	C37-C22-C21	-2.71	118.43	122.82
25	2	606	CLA	CHD-C1D-ND	-2.71	120.99	124.80
29	2	616	Q6L	C29-C27-C26	-2.71	114.75	119.01
32	6	617	SQD	O7-S-C6	2.71	110.80	106.76
25	W	311	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
25	A	837	CLA	CHB-C4A-NA	2.71	128.31	124.40
30	A	851	BCR	C32-C1-C6	2.71	114.48	110.24
30	2	618	BCR	C27-C26-C25	-2.70	119.05	122.70
37	P	317	NEX	C12-C13-C14	-2.70	114.76	119.01
25	S	311	CLA	CED-O2D-CGD	2.70	122.05	115.92
25	A	837	CLA	C4-C3-C5	2.70	119.92	115.23
29	P	316	Q6L	C01-C02-C07	-2.70	109.45	114.42
25	B	805	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
26	V	318	IWJ	C22-C21-C19	2.70	133.77	126.36
25	V	310	CLA	C4A-NA-C1A	2.70	107.91	106.68
24	R	310	CHL	CMD-C2D-C3D	2.70	130.08	124.68
30	L	306	BCR	C15-C16-C17	-2.70	117.99	123.52
24	R	309	CHL	O2A-CGA-O1A	-2.70	116.87	123.63
24	V	307	CHL	C4D-CHA-CBD	-2.70	106.24	108.97
38	T	308	KC2	O1A-CGA-CBA	2.70	129.34	121.06
24	R	308	CHL	C1B-CHB-C4A	2.70	123.06	121.32
26	W	318	IWJ	C35-C29-C30	2.70	111.55	108.78
24	P	306	CHL	CHA-C1A-C2A	-2.70	126.97	133.31
25	A	834	CLA	CMB-C2B-C3B	2.70	132.90	126.55
38	X	309	KC2	CBA-CAA-C2A	-2.70	114.62	125.45
24	P	305	CHL	CMD-C2D-C3D	2.70	130.08	124.68
25	W	312	CLA	CBC-CAC-C3C	2.70	119.74	112.42
29	V	319	Q6L	C42-C13-C12	2.70	119.91	115.23
24	W	304	CHL	C4D-CHA-CBD	-2.70	106.25	108.97
25	A	856	CLA	C3A-C2A-C1A	2.70	105.38	101.34
30	B	849	BCR	C30-C25-C26	-2.70	118.95	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	805	CLA	O2D-CGD-CBD	2.70	115.94	111.23
38	W	308	KC2	CAA-CBA-CGA	-2.70	113.34	127.05
25	B	827	CLA	C2A-C1A-CHA	2.70	128.55	123.87
24	P	306	CHL	O2D-CGD-O1D	-2.70	118.60	123.85
30	3	317	BCR	C16-C15-C14	-2.70	118.00	123.52
30	L	307	BCR	C12-C13-C14	-2.69	114.77	119.01
25	1	607	CLA	CHD-C1D-ND	-2.69	121.01	124.80
24	X	306	CHL	CAA-C2A-C3A	-2.69	110.05	116.23
24	6	605	CHL	O2D-CGD-CBD	2.69	113.91	110.95
24	P	305	CHL	C3D-C4D-CHA	2.69	112.63	108.54
30	A	848	BCR	C11-C10-C9	-2.69	123.50	127.28
36	A	854	DGD	O5E-C6E-C5E	-2.69	102.17	111.33
25	L	302	CLA	C4-C3-C5	2.69	119.90	115.23
24	X	307	CHL	CMB-C2B-C3B	2.69	130.06	124.68
25	Q	314	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	S	301	CLA	CMD-C2D-C3D	2.69	133.86	127.69
24	S	304	CHL	C3D-C4D-CHA	2.69	112.63	108.54
24	X	315	CHL	O2D-CGD-O1D	-2.69	118.61	123.85
25	B	829	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
30	B	849	BCR	C4-C5-C6	-2.69	119.07	122.70
25	A	806	CLA	CMB-C2B-C3B	2.69	132.87	126.55
25	3	307	CLA	C4-C3-C5	2.69	119.89	115.23
25	3	313	CLA	CED-O2D-CGD	2.69	122.01	115.92
38	R	312	KC2	O1A-CGA-CBA	2.69	129.29	121.06
29	T	316	Q6L	C01-C02-C07	-2.69	109.48	114.42
25	R	316	CLA	C5-C3-C2	-2.69	115.14	121.17
24	V	304	CHL	CMB-C2B-C3B	2.68	130.05	124.68
25	A	835	CLA	O2D-CGD-CBD	2.68	115.92	111.23
25	5	606	CLA	CHB-C4A-NA	2.68	128.27	124.40
29	Q	318	Q6L	C23-C22-C21	2.68	127.16	122.82
25	W	302	CLA	CHB-C4A-NA	2.68	128.27	124.40
29	P	319	Q6L	C05-C04-C03	2.68	114.16	110.61
25	R	307	CLA	CHB-C4A-NA	2.68	128.27	124.40
25	A	837	CLA	C6-C5-C3	2.68	120.00	113.47
25	3	308	CLA	C2C-C1C-NC	2.68	112.80	109.98
25	3	310	CLA	CHB-C4A-NA	2.68	128.27	124.40
25	2	608	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
26	1	611	IWJ	C32-C30-C31	2.68	126.44	121.19
30	J	103	BCR	C8-C9-C10	-2.68	114.80	119.01
25	A	818	CLA	CHB-C4A-NA	2.68	128.26	124.40
24	W	306	CHL	CBC-CAC-C3C	2.68	116.71	112.87
25	Q	312	CLA	C4A-NA-C1A	2.68	107.90	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	W	303	CLA	CED-O2D-CGD	-2.68	109.84	115.92
30	J	103	BCR	C37-C22-C21	-2.68	118.48	122.82
24	X	308	CHL	C3D-C4D-CHA	2.67	112.61	108.54
29	S	323	Q6L	C04-C05-C06	-2.67	107.73	113.59
25	4	310	CLA	C1-C2-C3	2.67	130.58	126.20
25	B	831	CLA	CHB-C4A-NA	2.67	128.26	124.40
24	S	305	CHL	C3D-C4D-CHA	2.67	112.60	108.54
25	X	304	CLA	CMB-C2B-C3B	2.67	132.83	126.55
30	4	319	BCR	C20-C21-C22	-2.67	123.53	127.28
24	1	601	CHL	C3D-C4D-CHA	2.67	112.60	108.54
25	3	311	CLA	C5-C3-C2	2.67	127.16	121.17
26	Q	320	IWJ	O27-C26-C28	-2.67	116.29	121.76
25	T	303	CLA	C3B-C4B-NB	-2.67	108.15	110.53
37	R	321	NEX	C20-C13-C12	2.67	122.17	118.09
26	6	614	IWJ	C35-C29-C30	2.67	111.52	108.78
25	B	826	CLA	CHB-C4A-NA	2.67	128.25	124.40
32	H	303	SQD	O48-C23-C24	2.67	119.97	111.83
25	A	837	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
25	5	604	CLA	O2D-CGD-O1D	-2.67	118.03	124.08
25	2	602	CLA	CHB-C4A-NA	2.67	128.25	124.40
30	K	205	BCR	C20-C21-C22	-2.67	123.54	127.28
25	2	604	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
25	2	612	CLA	C4-C3-C5	2.67	119.85	115.23
25	A	805	CLA	O2A-CGA-O1A	-2.66	116.96	123.63
24	T	305	CHL	O2D-CGD-CBD	2.66	113.87	110.95
26	P	320	IWJ	C25-C24-C26	2.66	120.32	116.00
37	H	306	NEX	C39-C29-C30	-2.66	118.50	122.82
24	P	314	CHL	O2D-CGD-CBD	2.66	113.87	110.95
25	2	606	CLA	CHB-C4A-NA	2.66	128.24	124.40
25	4	310	CLA	CMB-C2B-C3B	2.66	132.81	126.55
24	W	306	CHL	CHA-C1A-C2A	-2.66	127.06	133.31
30	J	103	BCR	C40-C30-C25	2.66	114.42	110.24
27	4	318	XAT	C15-C35-C34	-2.66	118.07	123.52
30	A	848	BCR	C27-C26-C25	-2.66	119.11	122.70
25	4	305	CLA	CAB-C3B-C2B	2.66	130.61	123.53
24	T	304	CHL	O2D-CGD-CBD	2.66	113.87	110.95
25	R	317	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
24	V	305	CHL	CBC-CAC-C3C	2.66	116.68	112.87
24	5	605	CHL	C4D-CHA-CBD	-2.66	106.29	108.97
25	F	802	CLA	CBC-CAC-C3C	2.66	119.62	112.42
29	S	320	Q6L	C37-C36-C35	-2.66	104.45	109.41
30	M	101	BCR	C37-C22-C23	2.66	122.15	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	839	CLA	C3B-C4B-NB	-2.66	108.16	110.53
30	B	846	BCR	C16-C15-C14	-2.65	118.09	123.52
24	Q	316	CHL	CHA-C1A-C2A	-2.65	127.08	133.31
25	O	2002	CLA	CHB-C4A-NA	2.65	128.23	124.40
25	3	312	CLA	CAA-C2A-C3A	-2.65	110.15	116.23
25	W	310	CLA	CHB-C4A-NA	2.65	128.22	124.40
25	P	313	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
30	4	319	BCR	C4-C5-C6	-2.65	119.12	122.70
25	V	309	CLA	C3B-C4B-NB	-2.65	108.17	110.53
25	A	835	CLA	CHC-C4B-NB	2.65	128.02	124.05
25	B	843	CLA	CMB-C2B-C3B	2.65	132.78	126.55
30	F	801	BCR	C35-C13-C12	2.65	122.13	118.09
27	1	612	XAT	C35-C34-C33	-2.65	123.56	127.28
24	5	605	CHL	O2D-CGD-O1D	-2.65	118.07	124.08
25	A	817	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
25	6	609	CLA	O2A-CGA-O1A	-2.65	116.52	123.33
24	P	307	CHL	O2D-CGD-O1D	-2.65	118.70	123.85
30	L	306	BCR	C8-C7-C6	-2.65	119.93	127.00
24	R	309	CHL	C3D-C4D-CHA	2.65	112.56	108.54
27	6	615	XAT	C36-C21-C26	2.64	117.19	110.05
25	W	312	CLA	C4-C3-C5	2.64	119.82	115.23
25	B	805	CLA	C4D-C3D-CAD	-2.64	105.23	108.11
25	5	602	CLA	CBC-CAC-C3C	2.64	119.59	112.42
25	6	602	CLA	CHD-C1D-ND	-2.64	121.08	124.80
29	R	320	Q6L	C35-C34-C33	2.64	115.11	111.18
25	L	303	CLA	CHA-C1A-NA	-2.64	120.41	126.39
27	6	615	XAT	C31-C30-C29	-2.64	123.58	127.28
24	1	601	CHL	C3C-C4C-NC	-2.64	108.20	114.65
25	A	809	CLA	CHB-C4A-NA	2.64	128.21	124.40
30	I	101	BCR	C29-C30-C25	-2.64	106.61	110.44
25	6	607	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
25	X	303	CLA	C4A-NA-C1A	2.64	107.88	106.68
24	S	305	CHL	O2D-CGD-O1D	-2.64	118.72	123.85
25	A	826	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
27	3	316	XAT	C15-C14-C13	-2.63	123.58	127.28
25	R	316	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
25	A	825	CLA	C5-C3-C2	2.63	127.08	121.17
24	U	304	CHL	C3C-C4C-NC	-2.63	108.22	114.65
24	W	306	CHL	C3D-C4D-CHA	2.63	112.54	108.54
25	A	842	CLA	C1-C2-C3	-2.63	121.89	126.20
24	V	304	CHL	C3D-C4D-CHA	2.63	112.54	108.54
25	B	823	CLA	O1D-CGD-CBD	2.63	129.71	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	205	BCR	C34-C9-C10	2.63	127.08	122.82
24	R	310	CHL	CMB-C2B-C3B	2.63	129.94	124.68
29	2	616	Q6L	C05-C04-C03	2.63	114.09	110.61
24	R	318	CHL	C1B-CHB-C4A	2.63	123.01	121.32
26	W	318	IWJ	C21-C19-C18	-2.63	114.88	119.01
38	X	309	KC2	CAC-C3C-C2C	-2.63	119.89	128.43
24	V	305	CHL	C3D-C4D-CHA	2.63	112.53	108.54
25	O	2002	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
25	A	856	CLA	C3B-C4B-NB	-2.63	108.18	110.53
29	V	321	Q6L	C01-C02-C07	-2.63	109.59	114.42
29	W	319	Q6L	C42-C13-C12	2.63	119.79	115.23
29	X	319	Q6L	C01-C02-C07	-2.63	109.59	114.42
24	X	306	CHL	C3D-C4D-CHA	2.62	112.53	108.54
24	X	305	CHL	O2D-CGD-O1D	-2.62	118.74	123.85
25	A	804	CLA	C4D-C3D-CAD	-2.62	105.26	108.11
24	P	305	CHL	C3C-C4C-NC	-2.62	108.24	114.65
25	5	606	CLA	CAB-C3B-C2B	2.62	130.50	123.53
25	R	305	CLA	CMC-C2C-C1C	2.62	129.13	125.03
26	T	318	IWJ	C16-C17-C18	-2.62	118.16	123.52
24	T	304	CHL	CHA-C1A-C2A	-2.62	127.15	133.31
25	A	808	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
30	J	103	BCR	C15-C16-C17	-2.62	118.16	123.52
24	R	309	CHL	CMD-C2D-C3D	2.62	129.92	124.68
38	R	312	KC2	C3C-C2C-C1C	2.62	108.38	106.41
25	R	314	CLA	C1-C2-C3	-2.62	121.91	126.20
24	V	314	CHL	C3D-C4D-CHA	2.62	112.52	108.54
38	X	309	KC2	O1A-CGA-CBA	2.62	129.08	121.06
30	K	205	BCR	C1-C6-C5	2.62	126.21	122.64
30	L	305	BCR	C24-C23-C22	-2.62	122.36	126.23
25	X	310	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	O	2002	CLA	C1-O2A-CGA	2.62	122.98	116.65
29	2	616	Q6L	C25-C26-C27	2.61	130.94	127.28
25	B	829	CLA	O2D-CGD-CBD	2.61	115.80	111.23
29	V	315	Q6L	C24-C22-C21	-2.61	114.90	119.01
24	P	314	CHL	CMB-C2B-C3B	2.61	129.91	124.68
25	W	303	CLA	C4A-NA-C1A	2.61	107.87	106.68
38	U	307	KC2	CAA-C2A-C1A	-2.61	113.19	124.64
25	T	313	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	Q	306	CLA	CGD-CBD-CAD	-2.61	102.39	110.85
25	1	613	CLA	C5-C3-C2	2.61	127.03	121.17
29	V	316	Q6L	C15-C14-C13	-2.61	124.02	127.69
25	A	824	CLA	C1C-C2C-C3C	-2.61	104.23	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	W	307	CHL	C4-C3-C2	-2.61	116.92	123.63
25	A	827	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
24	X	307	CHL	C3D-C4D-CHA	2.61	112.50	108.54
25	2	612	CLA	C2A-C1A-CHA	2.61	128.39	123.87
24	1	601	CHL	CMD-C2D-C3D	2.61	129.89	124.68
25	2	611	CLA	O2D-CGD-O1D	-2.61	118.17	124.08
25	A	807	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
27	3	316	XAT	C12-C13-C14	-2.61	114.91	119.01
26	4	317	IWJ	C32-C30-C31	2.61	126.29	121.19
25	R	317	CLA	CHB-C4A-NA	2.60	128.16	124.40
25	Q	314	CLA	CBA-CAA-C2A	2.60	121.54	113.79
30	B	849	BCR	C12-C13-C14	-2.60	114.91	119.01
24	4	306	CHL	CHA-C1A-C2A	-2.60	127.19	133.31
25	1	609	CLA	CAB-C3B-C2B	2.60	130.45	123.53
24	S	306	CHL	CAC-C3C-C4C	2.60	130.72	124.03
24	1	601	CHL	CBA-CAA-C2A	2.60	121.44	113.78
24	X	315	CHL	O2D-CGD-CBD	2.60	113.81	110.95
24	S	305	CHL	C4D-CHA-CBD	-2.60	106.34	108.97
25	4	303	CLA	O1D-CGD-CBD	2.60	129.65	124.52
25	W	312	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	4	302	CHL	C3C-C4C-NC	-2.60	108.29	114.65
26	P	320	IWJ	C23-C22-C21	-2.60	115.67	123.20
25	B	828	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
25	P	312	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	A	828	CLA	C6-C5-C3	-2.60	107.14	113.47
37	S	317	NEX	C15-C14-C13	-2.60	123.63	127.28
25	2	613	CLA	O2D-CGD-O1D	-2.60	118.19	124.08
24	T	307	CHL	CMD-C2D-C3D	2.60	129.87	124.68
25	W	301	CLA	C4-C3-C5	2.60	119.73	115.23
30	A	850	BCR	C2-C1-C6	-2.60	106.67	110.44
25	V	309	CLA	CHB-C4A-NA	2.60	128.15	124.40
25	B	809	CLA	C6-C7-C8	2.60	124.59	115.97
28	6	616	LHG	O8-C23-C24	2.60	119.75	111.83
25	F	803	CLA	CMA-C3A-C2A	-2.60	110.28	116.23
25	S	309	CLA	O2D-CGD-CBD	2.59	115.77	111.23
25	U	301	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
24	Q	316	CHL	CMB-C2B-C3B	2.59	129.87	124.68
25	B	817	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
25	1	603	CLA	C6-C5-C3	2.59	119.79	113.47
24	4	306	CHL	OMC-CMC-C2C	-2.59	120.62	125.12
29	S	316	Q6L	C19-C20-C21	-2.59	118.21	123.52
25	S	311	CLA	CMB-C2B-C3B	2.59	132.65	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	314	CLA	C1-O2A-CGA	2.59	122.92	116.65
25	T	312	CLA	CHB-C4A-NA	2.59	128.14	124.40
30	F	804	BCR	C12-C13-C14	2.59	123.08	119.01
30	B	847	BCR	C8-C9-C10	-2.59	114.94	119.01
25	P	311	CLA	C4-C3-C5	2.59	119.72	115.23
27	4	318	XAT	O4-C5-C18	2.59	117.94	115.05
29	W	315	Q6L	C42-C13-C12	2.59	119.72	115.23
25	B	839	CLA	CHD-C1D-ND	-2.59	121.16	124.80
24	R	308	CHL	CMD-C2D-C3D	2.59	129.85	124.68
25	H	301	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	B	834	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
25	B	837	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
30	B	845	BCR	C8-C9-C10	-2.59	114.94	119.01
24	W	305	CHL	C3C-C4C-NC	-2.59	108.33	114.65
25	B	832	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	B	839	CLA	CHB-C4A-NA	2.59	128.13	124.40
25	6	608	CLA	CMB-C2B-C3B	2.59	132.63	126.55
25	B	816	CLA	CMB-C2B-C3B	2.59	132.63	126.55
25	A	833	CLA	CHC-C4B-NB	2.59	127.93	124.05
25	A	825	CLA	CMB-C2B-C3B	2.59	132.63	126.55
24	W	314	CHL	C4D-ND-C1D	2.59	107.18	105.22
25	3	304	CLA	O2D-CGD-O1D	-2.59	118.22	124.08
27	2	617	XAT	C35-C15-C14	-2.58	118.23	123.52
25	2	602	CLA	CMB-C2B-C3B	2.58	132.63	126.55
25	A	806	CLA	O2A-CGA-CBA	-2.58	103.95	111.83
30	B	849	BCR	C23-C24-C25	-2.58	120.09	127.00
24	U	305	CHL	C3D-C4D-CHA	2.58	112.47	108.54
29	P	316	Q6L	C10-C04-C03	2.58	113.81	109.78
25	4	311	CLA	CHB-C1B-NB	2.58	127.92	124.05
25	U	302	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
25	R	314	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
31	A	855	LMG	O6-C5-C4	2.58	114.35	109.70
30	H	305	BCR	C12-C13-C14	-2.58	114.95	119.01
24	P	306	CHL	C4-C3-C5	2.58	119.17	116.13
25	1	605	CLA	O2D-CGD-O1D	-2.58	118.22	124.08
25	3	304	CLA	CHD-C1D-ND	-2.58	121.17	124.80
25	4	304	CLA	CAB-C3B-C2B	2.58	130.39	123.53
25	R	313	CLA	C1D-ND-C4D	-2.58	104.50	106.31
25	A	824	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
24	6	606	CHL	O1D-CGD-CBD	2.58	128.64	124.72
38	W	308	KC2	O1A-CGA-CBA	2.58	128.97	121.06
26	T	321	IWJ	C25-C24-C26	2.58	120.18	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	X	302	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
30	3	319	BCR	C15-C14-C13	-2.58	123.66	127.28
29	T	322	Q6L	C15-C14-C13	-2.58	124.06	127.69
38	P	308	KC2	CHB-C4A-C3A	-2.58	120.96	125.03
37	W	317	NEX	C31-C30-C29	-2.58	123.66	127.28
24	5	605	CHL	C3D-C4D-CHA	2.58	112.46	108.54
25	W	309	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	V	304	CHL	CHA-C1A-C2A	-2.58	127.26	133.31
25	A	836	CLA	O2D-CGD-CBD	2.58	115.73	111.23
25	2	613	CLA	CHD-C1D-ND	-2.58	121.18	124.80
25	R	316	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
25	A	803	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
25	2	611	CLA	O2A-CGA-O1A	-2.57	116.71	123.33
24	R	309	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
24	V	306	CHL	C4D-CHA-CBD	-2.57	106.37	108.97
25	T	309	CLA	CHB-C4A-NA	2.57	128.11	124.40
29	S	323	Q6L	C19-C18-C17	-2.57	123.67	127.28
25	3	314	CLA	CHD-C1D-ND	-2.57	121.18	124.80
25	U	311	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
25	J	102	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
25	Q	315	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	1	601	CHL	C4D-ND-C1D	2.57	107.17	105.22
30	K	205	BCR	C11-C10-C9	-2.57	123.67	127.28
25	A	827	CLA	C6-C5-C3	-2.57	107.20	113.47
24	T	304	CHL	C3C-C4C-NC	-2.57	108.37	114.65
24	X	307	CHL	CHA-C1A-C2A	-2.57	127.27	133.31
29	X	317	Q6L	C31-C30-C29	-2.57	120.58	124.58
25	B	832	CLA	CHB-C1B-NB	2.57	127.90	124.05
25	Q	306	CLA	CMB-C2B-C3B	2.57	132.59	126.55
25	1	610	CLA	CAB-C3B-C2B	2.57	130.35	123.53
25	6	613	CLA	C5-C3-C2	2.57	126.93	121.17
29	2	616	Q6L	C28-C27-C26	2.57	126.97	122.82
30	A	851	BCR	C20-C21-C22	-2.57	123.68	127.28
24	1	601	CHL	C4D-CHA-CBD	-2.57	106.38	108.97
24	T	307	CHL	C3D-C4D-CHA	2.56	112.44	108.54
38	X	309	KC2	O2D-CGD-CBD	2.56	115.71	111.23
38	R	312	KC2	CAA-CBA-CGA	-2.56	114.01	127.05
38	U	307	KC2	CAA-CBA-CGA	-2.56	114.01	127.05
30	I	101	BCR	C16-C15-C14	-2.56	118.27	123.52
24	X	315	CHL	C3D-C4D-CHA	2.56	112.44	108.54
30	3	317	BCR	C2-C3-C4	-2.56	105.64	111.28
25	X	302	CLA	CHB-C4A-NA	2.56	128.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	307	CHL	O1D-CGD-CBD	2.56	128.61	124.72
25	B	840	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	A	827	CLA	C2A-C1A-CHA	2.56	128.31	123.87
25	U	308	CLA	CMA-C3A-C2A	-2.56	110.35	116.23
25	N	202	CLA	CHB-C4A-NA	2.56	128.10	124.40
25	B	832	CLA	CAC-C3C-C4C	2.56	128.12	124.79
36	B	850	DGD	O2G-C1B-C2B	2.56	117.02	111.48
24	P	304	CHL	CBA-CAA-C2A	2.56	121.32	113.78
25	X	302	CLA	O1D-CGD-CBD	2.56	129.57	124.52
24	V	314	CHL	C4D-ND-C1D	2.56	107.16	105.22
25	U	302	CLA	CHB-C4A-NA	2.56	128.09	124.40
31	O	2008	LMG	O8-C28-C29	2.56	119.64	111.83
25	V	309	CLA	CMC-C2C-C3C	-2.56	119.23	126.15
29	V	316	Q6L	C01-C02-C07	-2.56	109.72	114.42
25	P	311	CLA	CHB-C4A-NA	2.56	128.09	124.40
25	A	834	CLA	CHB-C4A-NA	2.56	128.09	124.40
24	W	307	CHL	CHA-C1A-C2A	-2.56	127.30	133.31
30	G	201	BCR	C38-C26-C27	2.56	119.05	113.60
25	B	820	CLA	CMB-C2B-C3B	2.56	132.56	126.55
24	4	308	CHL	C3C-C4C-NC	-2.56	108.40	114.65
25	B	810	CLA	C1-C2-C3	2.56	130.38	126.20
25	U	311	CLA	O2A-CGA-O1A	-2.56	117.24	123.63
33	A	802	CL0	C4C-CHD-C1D	2.56	125.21	116.07
25	2	602	CLA	C4B-C3B-C2B	-2.55	104.12	107.30
25	1	609	CLA	O2D-CGD-O1D	-2.55	118.28	124.08
24	R	318	CHL	O1D-CGD-CBD	2.55	128.60	124.72
25	B	802	CLA	CAC-C3C-C4C	2.55	128.11	124.79
30	A	850	BCR	C8-C7-C6	-2.55	120.18	127.00
25	2	602	CLA	C5-C3-C2	-2.55	115.44	121.17
25	K	206	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
38	W	308	KC2	CAC-C3C-C4C	2.55	135.66	124.39
25	B	832	CLA	CHA-C1A-NA	-2.55	120.61	126.39
25	3	302	CLA	CMC-C2C-C1C	2.55	129.02	125.03
24	6	601	CHL	O2D-CGD-O1D	-2.55	118.88	123.85
24	T	306	CHL	C3C-C4C-NC	-2.55	108.42	114.65
25	O	2005	CLA	CHD-C1D-ND	-2.55	121.21	124.80
30	A	848	BCR	C16-C17-C18	-2.55	123.70	127.28
25	B	838	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
25	R	315	CLA	CHB-C4A-NA	2.55	128.08	124.40
30	4	319	BCR	C19-C18-C17	-2.55	115.00	119.01
25	A	810	CLA	C4-C3-C5	2.55	119.65	115.23
25	6	608	CLA	CMB-C2B-C1B	-2.55	121.54	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	605	CHL	C4D-CHA-CBD	-2.55	106.40	108.97
25	A	814	CLA	C4B-C3B-C2B	-2.55	104.14	107.30
27	5	612	XAT	C28-C29-C30	-2.55	115.00	119.01
30	I	101	BCR	C23-C22-C21	-2.55	115.00	119.01
24	X	308	CHL	O1D-CGD-CBD	2.55	128.59	124.72
24	S	307	CHL	O2D-CGD-O1D	-2.55	118.89	123.85
25	A	834	CLA	C3B-C4B-NB	-2.55	108.26	110.53
37	W	317	NEX	C19-C9-C10	2.55	126.94	122.82
24	T	320	CHL	CMD-C2D-C3D	2.55	129.77	124.68
25	2	603	CLA	O2D-CGD-O1D	-2.55	118.31	124.08
30	A	852	BCR	C40-C30-C25	2.54	114.23	110.24
30	K	207	BCR	C10-C11-C12	2.54	130.57	123.20
25	B	833	CLA	CHD-C1D-ND	-2.54	121.22	124.80
25	B	843	CLA	CMB-C2B-C1B	-2.54	121.54	125.42
25	T	309	CLA	C4A-NA-C1A	2.54	107.84	106.68
25	6	613	CLA	O1D-CGD-CBD	2.54	129.54	124.52
24	P	304	CHL	C4D-ND-C1D	2.54	107.15	105.22
29	P	319	Q6L	C23-C22-C21	2.54	126.94	122.82
24	R	311	CHL	C3C-C4C-NC	-2.54	108.43	114.65
38	P	308	KC2	CAA-CBA-CGA	-2.54	114.11	127.05
25	4	310	CLA	C6-C5-C3	2.54	119.66	113.47
25	A	809	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
25	1	608	CLA	CAC-C3C-C4C	2.54	128.10	124.79
30	A	849	BCR	C24-C23-C22	-2.54	122.47	126.23
25	R	307	CLA	CHD-C1D-ND	-2.54	121.22	124.80
25	B	836	CLA	CHD-C1D-C2D	2.54	130.77	125.49
25	A	825	CLA	CAC-C3C-C2C	-2.54	122.89	127.56
30	K	205	BCR	C38-C26-C25	-2.54	121.71	124.48
25	B	818	CLA	CMB-C2B-C3B	2.54	132.53	126.55
24	T	306	CHL	O2D-CGD-O1D	-2.54	118.90	123.85
25	F	802	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
25	A	811	CLA	CAA-CBA-CGA	-2.54	106.00	113.21
29	Q	319	Q6L	C01-C02-C07	-2.54	109.75	114.42
25	B	832	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
25	4	309	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
25	Q	315	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
27	2	617	XAT	C6-C7-C8	-2.54	120.62	125.99
26	W	318	IWJ	C17-C18-C19	2.54	130.84	127.28
24	W	305	CHL	O2D-CGD-O1D	-2.54	118.91	123.85
30	B	848	BCR	C15-C14-C13	-2.54	123.72	127.28
30	B	845	BCR	C31-C1-C6	2.54	114.22	110.24
25	R	305	CLA	O2A-CGA-O1A	-2.54	117.28	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	607	CLA	O2D-CGD-CBD	2.54	115.66	111.23
37	R	321	NEX	C15-C35-C34	-2.54	118.33	123.52
25	A	806	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
29	V	319	Q6L	C40-C32-C33	-2.53	117.36	123.36
30	A	848	BCR	C30-C25-C26	2.53	126.10	122.64
25	L	301	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	5	610	CLA	C4A-NA-C1A	2.53	107.83	106.68
31	A	855	LMG	O8-C28-C29	2.53	119.56	111.83
24	1	604	CHL	CMB-C2B-C3B	2.53	129.75	124.68
25	B	819	CLA	CHA-C1A-NA	-2.53	120.66	126.39
25	A	806	CLA	C3B-C4B-NB	-2.53	108.27	110.53
37	H	306	NEX	C15-C14-C13	-2.53	123.73	127.28
29	S	320	Q6L	C35-C34-C33	2.53	114.94	111.18
25	V	309	CLA	CMB-C2B-C3B	2.53	132.50	126.55
25	S	312	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	X	313	CLA	CAA-C2A-C3A	-2.53	110.43	116.23
25	B	822	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	S	312	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
29	V	315	Q6L	C19-C20-C21	-2.53	118.35	123.52
25	5	607	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	P	312	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
30	H	305	BCR	C23-C22-C21	-2.53	115.03	119.01
24	6	601	CHL	CHA-C1A-C2A	-2.53	127.38	133.31
30	B	845	BCR	C40-C30-C39	2.53	115.86	108.63
25	X	313	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
26	P	320	IWJ	C21-C19-C18	-2.52	115.04	119.01
25	3	312	CLA	O2D-CGD-O1D	-2.52	118.36	124.08
25	B	826	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
25	A	827	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
25	A	828	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	P	312	CLA	O2A-C1-C2	2.52	117.81	108.11
25	A	840	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	R	307	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
30	K	207	BCR	C37-C22-C23	2.52	121.94	118.09
25	A	825	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	T	303	CLA	CHB-C4A-NA	2.52	128.03	124.40
25	B	812	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
25	2	613	CLA	CHB-C4A-NA	2.52	128.03	124.40
25	3	308	CLA	C1D-ND-C4D	-2.52	104.55	106.31
30	I	101	BCR	C16-C17-C18	-2.52	123.75	127.28
30	K	207	BCR	C15-C16-C17	-2.52	118.37	123.52
25	2	602	CLA	O2A-C1-C2	2.52	117.79	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	813	CLA	C14-C13-C15	2.52	120.24	111.27
38	P	308	KC2	O2A-CGA-O1A	-2.52	117.58	122.70
24	P	304	CHL	CMD-C2D-C3D	2.52	129.71	124.68
25	6	603	CLA	CHB-C1B-NB	2.52	127.82	124.05
37	R	321	NEX	C12-C13-C14	-2.51	115.05	119.01
30	G	201	BCR	C34-C9-C8	2.51	121.93	118.09
25	S	303	CLA	CHB-C4A-NA	2.51	128.03	124.40
25	N	203	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
29	X	319	Q6L	C35-C34-C33	2.51	114.92	111.18
25	S	310	CLA	CHB-C4A-NA	2.51	128.03	124.40
25	2	608	CLA	CMB-C2B-C3B	2.51	132.46	126.55
25	H	304	CLA	C3A-C2A-C1A	2.51	105.10	101.34
25	B	825	CLA	C3B-C4B-NB	-2.51	108.29	110.53
31	J	104	LMG	O1-C1-C2	2.51	112.09	108.27
25	B	819	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
25	A	805	CLA	CAC-C3C-C4C	2.51	128.06	124.79
25	4	312	CLA	O2D-CGD-O1D	-2.51	118.38	124.08
25	5	609	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
29	R	320	Q6L	C19-C20-C21	-2.51	118.38	123.52
24	T	305	CHL	OMC-CMC-C2C	-2.51	120.76	125.12
36	A	854	DGD	O1G-C1A-C2A	2.51	119.49	111.83
25	J	102	CLA	CMC-C2C-C1C	2.51	128.96	125.03
24	S	306	CHL	C1B-CHB-C4A	2.51	122.94	121.32
25	B	821	CLA	C4-C3-C5	2.51	119.58	115.23
25	N	203	CLA	C3B-C4B-NB	-2.51	108.29	110.53
25	U	301	CLA	CAA-C2A-C1A	-2.51	103.76	111.97
25	B	821	CLA	C1-O2A-CGA	-2.51	110.58	116.65
25	B	813	CLA	C11-C10-C8	2.51	124.30	115.97
25	P	312	CLA	CHD-C1D-ND	-2.51	121.27	124.80
25	W	312	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
25	2	610	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	4	308	CHL	O2D-CGD-O1D	-2.51	118.97	123.85
24	S	304	CHL	O2D-CGD-O1D	-2.51	118.97	123.85
25	3	312	CLA	CMA-C3A-C2A	-2.51	110.48	116.23
25	V	310	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	W	305	CHL	CMD-C2D-C3D	2.51	129.69	124.68
30	A	850	BCR	C11-C10-C9	-2.51	123.76	127.28
30	3	317	BCR	C11-C10-C9	-2.50	123.77	127.28
25	4	310	CLA	CBA-CAA-C2A	2.50	121.24	113.79
25	2	611	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	V	317	IWJ	C35-C29-C30	2.50	111.34	108.78
30	3	317	BCR	C39-C30-C25	2.50	114.17	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	828	CLA	O2D-CGD-CBD	2.50	115.60	111.23
25	A	819	CLA	CHD-C1D-ND	-2.50	121.28	124.80
25	4	309	CLA	CED-O2D-CGD	2.50	121.58	115.92
28	3	322	LHG	O8-C23-C24	2.50	119.45	111.83
25	Q	305	CLA	C2D-C1D-ND	-2.50	107.65	110.13
24	6	606	CHL	CMD-C2D-C3D	2.50	129.68	124.68
30	3	317	BCR	C36-C18-C17	-2.50	118.77	122.82
25	W	302	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
25	4	303	CLA	CHA-C1A-NA	-2.50	120.74	126.39
30	2	618	BCR	C11-C10-C9	-2.50	123.78	127.28
25	B	827	CLA	O2D-CGD-CBD	2.50	115.59	111.23
38	V	308	KC2	CAA-CBA-CGA	-2.50	114.36	127.05
25	H	304	CLA	CHD-C1D-ND	-2.50	121.29	124.80
25	R	313	CLA	CMB-C2B-C3B	2.50	132.42	126.55
24	W	307	CHL	C3D-C4D-CHA	2.49	112.33	108.54
25	6	610	CLA	CBA-CAA-C2A	2.49	121.21	113.79
25	6	604	CLA	CHB-C4A-NA	2.49	128.00	124.40
25	6	603	CLA	CHA-C1A-NA	-2.49	120.74	126.39
29	V	316	Q6L	C37-C36-C31	2.49	113.32	109.55
29	T	316	Q6L	C24-C22-C21	-2.49	115.09	119.01
25	U	311	CLA	O1D-CGD-CBD	2.49	129.43	124.52
25	A	838	CLA	CHD-C1D-ND	-2.49	121.30	124.80
24	X	306	CHL	CMD-C2D-C3D	2.49	129.66	124.68
24	P	314	CHL	C4D-CHA-CBD	-2.49	106.45	108.97
24	6	601	CHL	CAA-C2A-C1A	-2.49	108.42	113.35
27	5	612	XAT	C17-C1-C16	-2.49	103.75	107.37
25	A	830	CLA	CMB-C2B-C3B	2.49	132.41	126.55
25	B	806	CLA	CHB-C4A-NA	2.49	127.99	124.40
34	B	844	PQN	C2M-C2-C3	2.49	128.55	124.45
31	L	308	LMG	O8-C28-C29	2.49	119.42	111.83
25	V	301	CLA	CHB-C4A-NA	2.49	127.99	124.40
27	3	316	XAT	C15-C35-C34	-2.49	118.43	123.52
25	P	309	CLA	CHD-C1D-ND	-2.49	121.30	124.80
25	B	820	CLA	CHA-C1A-NA	-2.48	120.77	126.39
24	T	306	CHL	CHA-C1A-C2A	-2.48	127.47	133.31
25	P	303	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
25	P	303	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
25	5	602	CLA	CAC-C3C-C4C	2.48	128.02	124.79
25	A	856	CLA	CAC-C3C-C4C	2.48	128.02	124.79
25	X	314	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
25	A	816	CLA	C3B-C4B-NB	-2.48	108.31	110.53
37	P	317	NEX	C15-C35-C34	-2.48	118.44	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	841	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
25	L	301	CLA	CHB-C4A-NA	2.48	127.98	124.40
25	A	841	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
24	V	307	CHL	O2D-CGD-O1D	-2.48	119.02	123.85
25	1	602	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
30	4	319	BCR	C33-C5-C6	2.48	127.19	124.48
25	U	301	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
26	4	301	IWJ	C35-C29-C30	2.48	111.32	108.78
30	J	101	BCR	C20-C19-C18	-2.48	119.57	126.36
25	B	811	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
25	K	201	CLA	CAC-C3C-C4C	2.48	128.01	124.79
25	A	842	CLA	CHD-C1D-C2D	2.48	130.64	125.49
27	3	316	XAT	C20-C13-C12	2.48	121.87	118.09
25	A	837	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
38	V	308	KC2	CMD-C2D-C1D	-2.47	121.65	125.42
29	W	316	Q6L	C41-C17-C18	2.47	126.83	122.82
25	A	821	CLA	CMB-C2B-C3B	2.47	132.37	126.55
24	X	308	CHL	OMC-CMC-C2C	-2.47	120.82	125.12
29	S	320	Q6L	C01-C02-C07	-2.47	109.87	114.42
24	S	307	CHL	C4C-CHD-C1D	2.47	124.92	116.07
29	S	320	Q6L	C42-C13-C12	2.47	119.52	115.23
25	G	204	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	X	312	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	B	827	CLA	C1-C2-C3	-2.47	122.76	126.76
29	S	323	Q6L	C09-C04-C03	2.47	113.63	109.78
25	1	602	CLA	O1D-CGD-CBD	2.47	129.39	124.52
25	K	206	CLA	CMB-C2B-C3B	2.47	132.36	126.55
30	3	319	BCR	C19-C18-C17	-2.47	115.12	119.01
25	A	812	CLA	C3A-C2A-C1A	2.47	105.04	101.34
30	L	305	BCR	C15-C16-C17	-2.47	118.47	123.52
37	P	317	NEX	C31-C30-C29	-2.47	123.81	127.28
24	V	307	CHL	C3D-C4D-CHA	2.47	112.29	108.54
27	1	612	XAT	O24-C25-C26	-2.47	56.97	58.93
25	B	814	CLA	CHB-C4A-NA	2.47	127.96	124.40
25	Q	314	CLA	C3B-C4B-NB	-2.47	108.33	110.53
25	B	816	CLA	CHD-C1D-ND	-2.47	121.33	124.80
30	3	318	BCR	C20-C21-C22	-2.47	123.82	127.28
24	5	605	CHL	CMD-C2D-C3D	2.47	129.61	124.68
25	O	2002	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
29	U	314	Q6L	C42-C13-C12	2.47	119.51	115.23
25	P	309	CLA	CBA-CAA-C2A	2.47	121.13	113.79
24	V	306	CHL	CHA-C1A-C2A	-2.47	127.51	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	O	2002	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
25	A	856	CLA	C2A-C1A-CHA	2.47	128.15	123.87
25	1	613	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
25	G	202	CLA	O2A-CGA-O1A	-2.46	116.99	123.33
29	P	321	Q6L	C05-C04-C03	2.46	113.87	110.61
28	A	846	LHG	O8-C23-C24	2.46	119.35	111.83
24	4	307	CHL	C3D-C4D-CHA	2.46	112.28	108.54
27	6	615	XAT	C12-C13-C14	-2.46	115.13	119.01
24	R	302	CHL	CMB-C2B-C3B	2.46	129.61	124.68
24	W	307	CHL	O2D-CGD-O1D	-2.46	119.05	123.85
30	B	846	BCR	C15-C16-C17	-2.46	118.48	123.52
29	T	322	Q6L	C38-C36-C35	-2.46	104.81	109.41
25	A	823	CLA	CHD-C1D-ND	-2.46	121.34	124.80
38	R	312	KC2	C2A-C3A-C4A	-2.46	104.56	106.41
25	B	818	CLA	CED-O2D-CGD	2.46	121.50	115.92
30	B	848	BCR	C19-C18-C17	-2.46	115.14	119.01
24	S	305	CHL	CMA-C3A-C4A	-2.46	109.31	114.61
24	X	305	CHL	CMD-C2D-C3D	2.46	129.60	124.68
25	4	303	CLA	C4A-NA-C1A	2.46	107.80	106.68
25	B	815	CLA	CGD-CBD-CAD	-2.46	102.89	110.85
25	V	311	CLA	C2A-C1A-CHA	2.46	128.13	123.87
38	R	312	KC2	C4C-C3C-C2C	-2.46	105.02	107.28
25	Q	314	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
24	X	305	CHL	C1C-CHC-C4B	2.46	124.86	116.07
24	1	604	CHL	C4D-ND-C1D	2.46	107.08	105.22
25	6	613	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
25	4	304	CLA	CHB-C4A-NA	2.46	127.94	124.40
25	6	607	CLA	C3B-C2B-C1B	2.46	110.06	107.17
25	A	823	CLA	CAC-C3C-C4C	2.46	127.98	124.79
27	4	318	XAT	C19-C9-C8	2.45	121.84	118.09
30	J	103	BCR	C35-C13-C12	2.45	121.84	118.09
26	1	611	IWJ	C35-C29-C30	-2.45	106.26	108.78
25	B	810	CLA	CBA-CAA-C2A	2.45	121.09	113.79
24	X	307	CHL	C4D-CHA-CBD	-2.45	106.49	108.97
24	X	315	CHL	C4D-CHA-CBD	-2.45	106.49	108.97
25	U	302	CLA	C4-C3-C5	2.45	119.49	115.23
38	Q	310	KC2	C3A-C4A-NA	2.45	113.49	110.45
24	R	308	CHL	C4D-ND-C1D	2.45	107.08	105.22
25	4	309	CLA	CHA-C1A-NA	-2.45	120.84	126.39
25	O	2001	CLA	CHB-C4A-NA	2.45	127.94	124.40
26	Q	320	IWJ	C25-C24-C26	2.45	119.98	116.00
24	R	310	CHL	C3C-C4C-NC	-2.45	108.66	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	303	CLA	O2D-CGD-CBD	2.45	115.52	111.23
25	P	309	CLA	CAA-C2A-C3A	2.45	119.62	113.00
38	V	308	KC2	CAA-C2A-C1A	-2.45	113.90	124.64
25	A	827	CLA	CMB-C2B-C3B	2.45	132.31	126.55
29	U	314	Q6L	C16-C17-C18	-2.45	115.16	119.01
29	R	304	Q6L	C19-C18-C17	-2.45	123.84	127.28
38	R	312	KC2	CMD-C2D-C3D	2.45	133.40	125.67
34	B	844	PQN	C21-C22-C23	-2.45	107.83	115.97
30	F	804	BCR	C1-C6-C5	-2.45	119.29	122.64
29	S	320	Q6L	C40-C32-C33	-2.45	117.57	123.36
25	A	817	CLA	C14-C13-C12	-2.45	102.55	111.27
25	O	2002	CLA	C3C-C4C-NC	-2.45	107.30	110.43
24	1	601	CHL	CHA-C1A-C2A	-2.45	127.56	133.31
25	A	810	CLA	C11-C12-C13	-2.45	107.83	115.97
37	W	317	NEX	C11-C10-C9	-2.45	123.85	127.28
29	X	316	Q6L	C31-C30-C29	-2.45	120.77	124.58
25	A	836	CLA	CHD-C1D-ND	-2.45	121.36	124.80
25	B	823	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
25	1	610	CLA	O1D-CGD-CBD	2.45	129.34	124.52
38	W	308	KC2	O2D-CGD-CBD	2.44	115.50	111.23
25	U	303	CLA	CHB-C4A-NA	2.44	127.93	124.40
25	A	837	CLA	C6-C7-C8	2.44	124.09	115.97
25	1	605	CLA	CHD-C1D-ND	-2.44	121.36	124.80
24	T	314	CHL	C3C-C4C-NC	-2.44	108.68	114.65
25	5	602	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
30	G	205	BCR	C27-C26-C25	-2.44	119.40	122.70
25	B	819	CLA	C5-C3-C2	2.44	126.65	121.17
25	V	312	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
25	4	313	CLA	CBA-CAA-C2A	2.44	121.06	113.79
30	K	205	BCR	C12-C13-C14	-2.44	115.17	119.01
29	O	2007	Q6L	C15-C14-C13	-2.44	124.26	127.69
27	5	612	XAT	C35-C34-C33	-2.44	123.85	127.28
24	U	313	CHL	C3D-C4D-CHA	2.44	112.25	108.54
25	A	811	CLA	CHD-C1D-ND	-2.44	121.37	124.80
31	N	201	LMG	O6-C1-C2	-2.44	105.36	110.37
24	4	302	CHL	O2D-CGD-O1D	-2.44	119.10	123.85
37	P	317	NEX	C32-C33-C34	-2.44	115.17	119.01
30	B	846	BCR	C16-C17-C18	-2.44	123.86	127.28
25	3	309	CLA	O2D-CGD-CBD	2.44	115.49	111.23
25	B	826	CLA	O2D-CGD-CBD	2.44	115.49	111.23
25	B	805	CLA	C3B-C4B-NB	-2.44	108.35	110.53
25	B	830	CLA	C2D-C1D-ND	-2.44	107.71	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	317	IWJ	C36-C35-C34	-2.44	104.69	108.97
30	A	848	BCR	C33-C5-C4	-2.44	108.40	113.60
30	4	319	BCR	C2-C1-C6	2.44	113.98	110.44
25	B	826	CLA	CMB-C2B-C3B	2.44	132.28	126.55
30	K	205	BCR	C24-C25-C26	-2.44	115.94	121.56
25	A	833	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	S	306	CHL	C3C-C4C-NC	-2.44	108.70	114.65
25	B	824	CLA	CAC-C3C-C4C	2.44	127.96	124.79
25	A	813	CLA	CHD-C1D-ND	-2.43	121.38	124.80
25	4	309	CLA	CBC-CAC-C3C	-2.43	105.82	112.42
24	R	308	CHL	CHA-C1A-C2A	-2.43	127.59	133.31
25	B	838	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	Q	309	CHL	C3D-C4D-CHA	2.43	112.24	108.54
25	6	603	CLA	O2D-CGD-O1D	-2.43	118.56	124.08
25	2	609	CLA	CMC-C2C-C1C	2.43	128.84	125.03
25	4	313	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
30	A	851	BCR	C1-C6-C7	2.43	122.24	115.65
25	P	312	CLA	O2D-CGD-CBD	2.43	115.48	111.23
25	B	813	CLA	C5-C3-C2	2.43	126.62	121.17
25	O	2001	CLA	C5-C3-C2	2.43	126.62	121.17
25	P	303	CLA	CMB-C2B-C3B	2.43	132.26	126.55
25	A	842	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
24	P	314	CHL	C3D-C4D-CHA	2.43	112.23	108.54
38	T	308	KC2	CHB-C4A-NA	2.43	128.00	124.23
27	2	617	XAT	O24-C25-C26	-2.43	57.00	58.93
24	U	306	CHL	CMB-C2B-C3B	2.43	129.53	124.68
25	A	829	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
25	Q	315	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
31	A	857	LMG	O7-C10-C11	2.43	116.73	111.48
25	O	2002	CLA	CHD-C1D-ND	-2.43	121.39	124.80
25	V	309	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
29	T	315	Q6L	C01-C02-C07	-2.43	109.96	114.42
25	A	823	CLA	C5-C3-C2	2.43	126.61	121.17
25	B	842	CLA	C1-O2A-CGA	-2.43	110.78	116.65
29	V	319	Q6L	C24-C22-C21	-2.43	115.19	119.01
25	U	311	CLA	CMB-C2B-C3B	2.43	132.25	126.55
25	6	607	CLA	CHB-C4A-NA	2.42	127.90	124.40
25	B	832	CLA	CHB-C4A-NA	2.42	127.90	124.40
38	T	308	KC2	CAC-C3C-C2C	-2.42	120.55	128.43
30	J	103	BCR	C11-C10-C9	-2.42	123.88	127.28
25	X	314	CLA	CAA-C2A-C3A	-2.42	110.67	116.23
25	A	804	CLA	O2A-CGA-CBA	-2.42	104.44	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	610	CLA	CMB-C2B-C3B	2.42	129.97	123.53
25	B	822	CLA	CBA-CAA-C2A	2.42	121.00	113.79
25	A	829	CLA	CBA-CAA-C2A	2.42	121.00	113.79
25	B	826	CLA	CHD-C1D-ND	-2.42	121.39	124.80
24	V	305	CHL	O2D-CGD-CBD	2.42	113.61	110.95
25	A	814	CLA	CAC-C3C-C4C	2.42	127.94	124.79
25	A	822	CLA	CMB-C2B-C3B	2.42	132.25	126.55
24	6	606	CHL	C3D-C4D-CHA	2.42	112.22	108.54
25	J	102	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	B	804	CLA	CHC-C4B-NB	2.42	127.68	124.05
25	B	811	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
25	B	813	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
25	5	602	CLA	O2D-CGD-CBD	2.42	115.46	111.23
25	A	823	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
26	W	318	IWJ	C25-C24-C26	2.42	119.92	116.00
37	R	321	NEX	O24-C25-C38	2.42	117.75	115.05
25	4	313	CLA	CMC-C2C-C1C	2.42	128.81	125.03
30	3	318	BCR	C8-C7-C6	-2.42	120.55	127.00
25	P	303	CLA	CHD-C1D-ND	-2.41	121.40	124.80
30	3	318	BCR	C33-C5-C4	-2.41	108.45	113.60
27	1	612	XAT	C15-C35-C34	-2.41	118.58	123.52
30	G	205	BCR	C12-C13-C14	-2.41	115.21	119.01
25	A	827	CLA	CBC-CAC-C3C	2.41	118.96	112.42
27	4	318	XAT	C20-C13-C14	2.41	126.72	122.82
25	H	302	CLA	CHD-C1D-ND	-2.41	121.41	124.80
24	S	307	CHL	CMD-C2D-C3D	2.41	129.50	124.68
28	6	616	LHG	O8-C6-C5	2.41	115.35	108.40
30	M	101	BCR	C32-C1-C6	2.41	114.03	110.24
25	6	603	CLA	CMC-C2C-C1C	2.41	128.80	125.03
25	B	813	CLA	O2D-CGD-CBD	2.41	115.44	111.23
25	T	312	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
24	X	315	CHL	OBD-CAD-CBD	-2.41	122.29	125.82
38	X	309	KC2	C2D-C1D-ND	-2.41	107.83	110.33
25	W	311	CLA	CMB-C2B-C3B	2.41	132.22	126.55
24	T	320	CHL	CHA-C1A-C2A	-2.41	127.65	133.31
25	P	311	CLA	CAC-C3C-C4C	2.41	127.93	124.79
28	A	847	LHG	O8-C23-C24	2.41	119.18	111.83
25	3	305	CLA	CHB-C4A-NA	2.41	127.88	124.40
25	5	609	CLA	CBA-CAA-C2A	2.41	120.96	113.79
30	G	201	BCR	C38-C26-C25	-2.41	121.86	124.48
37	H	306	NEX	C20-C13-C12	2.41	121.77	118.09
24	T	307	CHL	C3C-C4C-NC	-2.41	108.77	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	301	CLA	C5-C3-C2	-2.41	115.77	121.17
25	3	304	CLA	CMC-C2C-C1C	2.41	128.79	125.03
25	A	843	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
24	S	307	CHL	CMA-C3A-C2A	-2.41	110.71	116.23
24	6	606	CHL	C3C-C4C-NC	-2.40	108.78	114.65
25	T	309	CLA	CBA-CAA-C2A	2.40	120.94	113.79
24	R	310	CHL	O1D-CGD-CBD	2.40	128.37	124.72
25	A	821	CLA	CBA-CAA-C2A	2.40	120.94	113.79
29	O	2006	Q6L	C35-C34-C33	2.40	114.75	111.18
25	N	203	CLA	C2C-C1C-NC	2.40	112.51	109.98
24	Q	307	CHL	C3C-C4C-NC	-2.40	108.78	114.65
37	H	306	NEX	C38-C25-C26	-2.40	118.35	122.30
25	X	302	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
38	X	309	KC2	CAC-C3C-C4C	2.40	135.01	124.39
30	A	852	BCR	C8-C7-C6	-2.40	120.58	127.00
25	3	303	CLA	CAB-C3B-C2B	2.40	129.92	123.53
30	A	851	BCR	C7-C8-C9	-2.40	122.68	126.23
24	W	314	CHL	OMC-CMC-C2C	-2.40	120.95	125.12
38	U	307	KC2	O2A-CGA-O1A	-2.40	117.81	122.70
29	P	319	Q6L	C19-C20-C21	-2.40	118.61	123.52
25	T	301	CLA	C6-C5-C3	2.40	119.32	113.47
25	5	610	CLA	O2D-CGD-CBD	2.40	115.43	111.23
25	2	602	CLA	CBA-CAA-C2A	2.40	120.94	113.79
25	S	301	CLA	CMD-C2D-C1D	-2.40	120.50	124.73
26	4	301	IWJ	C36-C35-C34	-2.40	104.75	108.97
25	P	302	CLA	C14-C13-C15	2.40	119.83	111.27
25	U	309	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
26	V	318	IWJ	C36-C35-C34	-2.40	104.75	108.97
24	S	304	CHL	CAA-C2A-C1A	-2.40	109.04	114.49
25	W	309	CLA	C6-C5-C3	2.40	119.31	113.47
25	A	810	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
26	S	319	IWJ	C25-C24-C26	2.40	119.89	116.00
25	B	824	CLA	CMB-C2B-C3B	2.40	132.19	126.55
25	1	606	CLA	CHD-C1D-ND	-2.40	121.43	124.80
29	R	323	Q6L	C10-C04-C03	-2.40	106.05	109.78
25	K	201	CLA	CHB-C4A-NA	2.40	127.86	124.40
29	P	316	Q6L	C19-C20-C21	-2.40	118.62	123.52
25	A	833	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
25	Q	301	CLA	CAA-CBA-CGA	-2.39	106.41	113.21
25	H	302	CLA	C1-C2-C3	2.39	130.12	126.20
25	3	308	CLA	C2B-C1B-NB	2.39	112.81	110.33
24	1	604	CHL	O2D-CGD-O1D	-2.39	118.65	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	841	CLA	O2D-CGD-CBD	2.39	115.42	111.23
37	T	317	NEX	C15-C14-C13	-2.39	123.92	127.28
25	5	606	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	2	614	CLA	CHC-C4B-NB	2.39	127.64	124.05
25	B	831	CLA	CAA-CBA-CGA	-2.39	106.42	113.21
25	P	302	CLA	C11-C12-C13	2.39	123.91	115.97
24	W	307	CHL	CMD-C2D-C3D	2.39	129.46	124.68
30	K	202	BCR	C16-C17-C18	-2.39	123.92	127.28
25	T	312	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
25	B	813	CLA	C14-C13-C12	-2.39	102.75	111.27
25	B	806	CLA	C1-O2A-CGA	-2.39	110.86	116.65
38	X	309	KC2	C4C-C3C-C2C	-2.39	105.08	107.28
24	S	304	CHL	C4C-CHD-C1D	2.39	124.62	116.07
25	U	310	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
29	O	2006	Q6L	C01-C02-C07	-2.39	110.03	114.42
25	A	816	CLA	O2A-CGA-O1A	-2.39	117.19	123.33
30	A	848	BCR	C20-C21-C22	-2.39	123.93	127.28
24	R	311	CHL	C4C-CHD-C1D	2.39	124.61	116.07
25	A	856	CLA	CMB-C2B-C3B	2.39	132.16	126.55
24	Q	307	CHL	C3D-C4D-CHA	2.39	112.17	108.54
24	W	314	CHL	C4D-CHA-CBD	-2.39	106.56	108.97
30	H	305	BCR	C11-C10-C9	-2.39	123.93	127.28
38	V	308	KC2	O1A-CGA-CBA	2.39	128.37	121.06
24	X	315	CHL	CMD-C2D-C3D	2.39	129.45	124.68
25	V	311	CLA	C1-C2-C3	-2.38	122.29	126.20
25	U	302	CLA	C3B-C4B-NB	-2.38	108.40	110.53
24	U	306	CHL	C3D-C4D-CHA	2.38	112.16	108.54
24	S	314	CHL	C4D-CHA-CBD	-2.38	106.56	108.97
38	S	308	KC2	O1A-CGA-CBA	2.38	128.36	121.06
24	S	305	CHL	C4D-ND-C1D	2.38	107.03	105.22
24	4	307	CHL	C4D-CHA-CBD	-2.38	106.56	108.97
25	3	303	CLA	O2A-CGA-O1A	-2.38	117.21	123.33
25	X	310	CLA	O2D-CGD-CBD	2.38	115.39	111.23
25	K	204	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
25	N	203	CLA	O2D-CGD-CBD	2.38	115.39	111.23
24	T	306	CHL	CMD-C2D-C3D	2.38	129.44	124.68
25	B	813	CLA	CHD-C4C-C3C	2.38	128.25	124.77
25	A	838	CLA	CHB-C4A-NA	2.38	127.83	124.40
30	J	103	BCR	C20-C21-C22	-2.38	123.94	127.28
25	X	312	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
25	B	819	CLA	C2A-C1A-CHA	2.38	128.00	123.87
37	W	317	NEX	C32-C33-C34	-2.38	115.27	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	302	CLA	CMB-C2B-C3B	2.38	132.15	126.55
24	2	615	CHL	C3D-C4D-CHA	2.38	112.16	108.54
27	2	617	XAT	C12-C13-C14	-2.38	115.27	119.01
25	1	610	CLA	C4D-C3D-CAD	-2.38	105.52	108.11
25	B	821	CLA	C6-C5-C3	2.38	119.26	113.47
25	U	308	CLA	CHD-C4C-C3C	-2.38	121.31	124.77
24	U	304	CHL	C4D-ND-C1D	2.38	107.02	105.22
24	S	307	CHL	O1D-CGD-CBD	2.38	128.33	124.72
25	1	606	CLA	CMB-C2B-C3B	2.38	129.84	123.53
30	K	202	BCR	C16-C15-C14	-2.38	118.66	123.52
32	6	617	SQD	O9-S-C6	2.37	110.30	106.76
25	3	302	CLA	C3B-C4B-NB	-2.37	108.41	110.53
25	4	316	CLA	CED-O2D-CGD	2.37	121.30	115.92
29	W	319	Q6L	C19-C20-C21	-2.37	118.66	123.52
25	B	825	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
25	2	608	CLA	CMC-C2C-C1C	2.37	128.74	125.03
38	S	308	KC2	CAC-C3C-C2C	-2.37	120.72	128.43
30	F	804	BCR	C11-C12-C13	-2.37	119.86	126.36
26	Q	320	IWJ	C16-C17-C18	-2.37	118.67	123.52
24	W	305	CHL	C3D-C4D-CHA	2.37	112.14	108.54
25	1	608	CLA	C4-C3-C5	2.37	119.34	115.23
25	B	810	CLA	C6-C7-C8	2.37	123.85	115.97
27	6	615	XAT	C35-C34-C33	-2.37	123.95	127.28
25	T	309	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
27	5	612	XAT	C12-C13-C14	-2.37	115.28	119.01
30	I	101	BCR	C12-C13-C14	-2.37	115.28	119.01
25	B	841	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	1	606	CLA	CHB-C4A-NA	2.37	127.82	124.40
25	2	606	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
37	T	317	NEX	C32-C33-C34	-2.37	115.28	119.01
25	5	602	CLA	CMB-C2B-C3B	2.37	132.12	126.55
38	S	308	KC2	O2D-CGD-CBD	2.37	115.37	111.23
25	A	829	CLA	CED-O2D-CGD	2.37	121.29	115.92
24	1	604	CHL	C4D-CHA-CBD	-2.37	106.58	108.97
25	B	829	CLA	C2D-C1D-ND	-2.37	107.78	110.13
24	3	306	CHL	C1C-CHC-C4B	2.37	124.54	116.07
25	S	303	CLA	C4A-NA-C1A	2.37	107.76	106.68
37	H	306	NEX	C24-C23-C22	-2.37	106.36	110.79
28	Q	302	LHG	O8-C23-C24	2.37	119.05	111.83
25	K	203	CLA	C2A-C1A-CHA	2.37	127.97	123.87
25	P	301	CLA	C6-C5-C3	2.36	119.23	113.47
25	B	818	CLA	O2D-CGD-O1D	-2.36	119.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	607	CLA	CAC-C3C-C4C	2.36	127.86	124.79
26	V	318	IWJ	C23-C22-C21	-2.36	116.35	123.20
25	A	805	CLA	CMC-C2C-C1C	2.36	128.73	125.03
30	3	319	BCR	C23-C22-C21	-2.36	115.29	119.01
25	B	827	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	B	831	CLA	CBA-CAA-C2A	2.36	120.82	113.79
25	B	809	CLA	CAA-C2A-C1A	2.36	119.71	111.97
25	A	834	CLA	C6-C5-C3	2.36	119.22	113.47
25	3	312	CLA	CMB-C2B-C3B	2.36	132.10	126.55
38	U	307	KC2	CHB-C4A-NA	2.36	127.89	124.23
25	B	828	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
26	3	315	IWJ	C29-C30-C31	2.36	127.13	124.22
25	U	310	CLA	CHA-C1A-NA	-2.36	121.05	126.39
25	T	309	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	4	307	CHL	CMD-C2D-C3D	2.36	129.39	124.68
26	X	318	IWJ	C23-C22-C21	-2.36	116.37	123.20
29	W	315	Q6L	C01-C02-C07	-2.36	110.09	114.42
30	F	801	BCR	C8-C7-C6	-2.36	120.70	127.00
30	H	305	BCR	C24-C23-C22	-2.36	122.75	126.23
25	P	313	CLA	CBA-CAA-C2A	2.35	120.80	113.79
24	R	302	CHL	C1C-C2C-CMC	2.35	131.04	126.80
30	3	317	BCR	C37-C22-C23	2.35	121.68	118.09
25	4	309	CLA	CHB-C4A-NA	2.35	127.80	124.40
24	V	307	CHL	O2D-CGD-CBD	2.35	113.53	110.95
25	P	309	CLA	C1-C2-C3	-2.35	122.34	126.20
31	A	855	LMG	O7-C10-C11	2.35	119.57	110.93
25	B	814	CLA	CMB-C2B-C3B	2.35	132.08	126.55
25	T	312	CLA	CBA-CAA-C2A	2.35	120.79	113.79
25	U	302	CLA	CMB-C2B-C3B	2.35	132.08	126.55
30	K	205	BCR	C28-C27-C26	-2.35	109.86	114.06
25	A	817	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
37	S	317	NEX	C32-C33-C34	-2.35	115.31	119.01
24	4	302	CHL	CHA-C1A-C2A	-2.35	127.79	133.31
25	3	305	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
30	B	849	BCR	C33-C5-C6	2.35	127.05	124.48
30	3	318	BCR	C21-C20-C19	2.35	130.01	123.20
25	S	301	CLA	CAC-C3C-C4C	2.35	127.85	124.79
25	A	820	CLA	CHB-C1B-C2B	-2.35	120.61	127.43
25	S	301	CLA	CHA-C1A-NA	-2.35	121.07	126.39
26	S	322	IWJ	C25-C24-C26	2.35	119.81	116.00
24	T	314	CHL	CBC-CAC-C3C	-2.35	109.51	112.87
25	A	841	CLA	CHB-C4A-NA	2.35	127.79	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	307	CHL	C4C-CHD-C1D	2.35	124.47	116.07
25	A	829	CLA	C3B-C4B-NB	-2.35	108.44	110.53
25	4	304	CLA	CMB-C2B-C3B	2.35	129.77	123.53
27	1	612	XAT	C17-C1-C16	-2.35	103.96	107.37
30	M	101	BCR	C38-C26-C27	2.35	118.60	113.60
25	G	203	CLA	C2A-C1A-CHA	2.35	127.94	123.87
25	A	803	CLA	C11-C10-C8	-2.35	108.17	115.97
25	A	833	CLA	CMC-C2C-C1C	2.35	128.70	125.03
29	Q	318	Q6L	C06-C07-C02	2.35	118.02	112.18
36	A	854	DGD	O3G-C1D-C2D	-2.34	104.71	108.27
25	A	814	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
30	B	848	BCR	C40-C30-C25	2.34	113.92	110.24
25	S	310	CLA	CED-O2D-CGD	2.34	121.23	115.92
25	6	613	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	B	843	CLA	C3B-C4B-NB	-2.34	108.44	110.53
30	A	850	BCR	C29-C30-C25	-2.34	107.04	110.44
25	3	310	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	U	304	CHL	CED-O2D-CGD	2.34	121.23	115.92
25	S	312	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	V	313	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	B	830	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
38	T	308	KC2	O2D-CGD-CBD	2.34	115.32	111.23
25	A	810	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	A	806	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	H	301	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	B	828	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
25	W	309	CLA	C1-C2-C3	-2.34	122.36	126.20
25	U	309	CLA	CED-O2D-CGD	2.34	121.22	115.92
25	B	828	CLA	C2A-C1A-CHA	2.34	127.93	123.87
25	4	314	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	B	821	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	S	301	CLA	CMB-C2B-C3B	2.34	132.05	126.55
25	T	301	CLA	CHA-C1A-NA	-2.34	121.09	126.39
25	R	317	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
25	A	829	CLA	C2A-C1A-CHA	2.34	127.92	123.87
24	T	304	CHL	O1D-CGD-CBD	2.34	128.27	124.72
25	A	827	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
30	A	850	BCR	C15-C16-C17	-2.34	118.74	123.52
27	5	612	XAT	C36-C21-C26	2.34	116.35	110.05
24	W	314	CHL	C3D-C4D-CHA	2.34	112.09	108.54
30	J	101	BCR	C8-C9-C10	-2.34	115.33	119.01
24	Q	316	CHL	C4D-ND-C1D	2.34	106.99	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	839	CLA	CHB-C4A-NA	2.34	127.77	124.40
25	O	2005	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	5	612	XAT	C16-C1-C2	-2.34	104.86	108.97
25	O	2003	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
25	1	613	CLA	CHB-C4A-NA	2.34	127.77	124.40
24	V	304	CHL	C3C-C4C-NC	-2.34	108.94	114.65
25	A	815	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
31	2	620	LMG	O6-C1-C2	-2.33	105.57	110.37
29	V	319	Q6L	C16-C17-C18	-2.33	115.34	119.01
25	3	311	CLA	CBA-CAA-C2A	2.33	120.73	113.79
24	P	304	CHL	CMA-C3A-C4A	2.33	119.64	114.61
25	O	2001	CLA	C4-C3-C5	2.33	119.28	115.23
25	S	302	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
25	Q	314	CLA	CAC-C3C-C4C	2.33	127.82	124.79
24	2	607	CHL	C3D-C4D-CHA	2.33	112.08	108.54
24	U	306	CHL	C3C-C4C-NC	-2.33	108.96	114.65
30	B	847	BCR	C34-C9-C10	2.33	126.59	122.82
25	B	837	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
25	3	305	CLA	CAB-C3B-C2B	2.33	129.72	123.53
27	2	617	XAT	C4-C3-C2	-2.33	106.43	110.79
26	S	319	IWJ	C21-C19-C18	-2.33	115.35	119.01
25	S	313	CLA	CMA-C3A-C2A	-2.33	110.89	116.23
24	W	304	CHL	CMB-C2B-C3B	2.33	129.34	124.68
25	B	808	CLA	CHD-C4C-C3C	2.33	128.17	124.77
27	3	316	XAT	C24-C23-C22	-2.33	106.44	110.79
25	B	830	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	A	839	CLA	CAA-CBA-CGA	-2.33	106.60	113.21
30	L	305	BCR	C19-C18-C17	-2.33	115.35	119.01
24	P	306	CHL	C4C-CHD-C1D	2.33	124.39	116.07
24	R	302	CHL	CHA-C1A-C2A	-2.33	127.85	133.31
26	5	611	IWJ	C35-C29-C30	2.32	111.16	108.78
25	W	310	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
25	A	842	CLA	CBA-CAA-C2A	2.32	120.71	113.79
29	U	314	Q6L	C01-C02-C03	2.32	127.34	124.45
29	R	320	Q6L	C24-C22-C21	-2.32	115.35	119.01
25	2	604	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	W	316	Q6L	C30-C29-C27	2.32	131.32	126.32
25	U	302	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
25	A	814	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	3	317	BCR	C15-C16-C17	-2.32	118.77	123.52
26	6	614	IWJ	C36-C35-C34	-2.32	104.89	108.97
25	5	606	CLA	CMB-C2B-C3B	2.32	129.70	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	804	CLA	CAC-C3C-C4C	2.32	127.81	124.79
26	V	318	IWJ	C21-C19-C18	-2.32	115.36	119.01
38	R	312	KC2	O2A-CGA-O1A	-2.32	117.98	122.70
25	B	803	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
25	R	313	CLA	CAA-C2A-C1A	-2.32	104.37	111.97
25	X	314	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	I	101	BCR	C2-C3-C4	-2.32	106.18	111.28
24	V	305	CHL	CMD-C2D-C3D	2.32	129.31	124.68
24	S	304	CHL	O2D-CGD-CBD	2.32	113.49	110.95
24	6	606	CHL	C4D-CHA-CBD	-2.32	106.63	108.97
25	3	302	CLA	O2A-C1-C2	2.32	117.03	108.11
25	A	822	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
30	L	305	BCR	C38-C26-C27	2.32	118.54	113.60
26	Q	303	IWJ	C12-C11-C10	2.32	130.53	127.28
25	A	823	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
24	R	310	CHL	C4C-CHD-C1D	2.32	124.36	116.07
24	2	601	CHL	O2D-CGD-O1D	-2.32	119.34	123.85
37	H	306	NEX	C31-C30-C29	-2.32	124.03	127.28
37	H	306	NEX	C32-C33-C34	-2.32	115.36	119.01
25	S	301	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	A	808	CLA	CMC-C2C-C1C	2.31	128.65	125.03
24	R	309	CHL	OBD-CAD-CBD	-2.31	122.43	125.82
30	3	317	BCR	C38-C26-C25	-2.31	121.96	124.48
25	L	303	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	V	309	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	Q	306	CLA	O2D-CGD-CBD	2.31	115.28	111.23
25	X	310	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
29	V	315	Q6L	C35-C34-C33	2.31	114.62	111.18
25	A	811	CLA	C2A-C1A-CHA	2.31	127.88	123.87
38	T	308	KC2	O2A-CGA-O1A	-2.31	117.99	122.70
25	4	316	CLA	CHD-C1D-ND	-2.31	121.55	124.80
37	R	321	NEX	C38-C25-C24	-2.31	111.64	114.24
25	3	307	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
30	B	847	BCR	C15-C16-C17	-2.31	118.79	123.52
24	2	615	CHL	OMC-CMC-C2C	2.31	129.13	125.12
24	6	605	CHL	C4D-ND-C1D	2.31	106.97	105.22
25	3	307	CLA	CAC-C3C-C4C	2.31	127.80	124.79
25	K	204	CLA	C2A-C1A-CHA	2.31	127.88	123.87
25	B	807	CLA	C2A-C1A-CHA	2.31	127.87	123.87
25	X	303	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	1	602	CLA	CMB-C2B-C3B	2.31	131.98	126.55
38	U	307	KC2	O1A-CGA-CBA	2.31	128.13	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	825	CLA	CED-O2D-CGD	2.31	121.15	115.92
25	B	820	CLA	CBA-CAA-C2A	2.31	120.66	113.79
25	B	841	CLA	CAA-C2A-C3A	-2.31	106.77	113.00
24	1	604	CHL	C3D-C4D-CHA	2.31	112.05	108.54
25	3	301	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
25	S	301	CLA	C4A-NA-C1A	2.31	107.73	106.68
25	W	312	CLA	CMB-C2B-C3B	2.31	131.97	126.55
30	I	101	BCR	C35-C13-C12	2.31	121.61	118.09
25	O	2003	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	B	821	CLA	CHB-C4A-NA	2.30	127.73	124.40
25	5	601	CLA	C3B-C4B-NB	-2.30	108.47	110.53
24	R	318	CHL	C3D-C4D-CHA	2.30	112.04	108.54
25	T	311	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
25	W	312	CLA	O2D-CGD-CBD	2.30	115.25	111.23
24	W	306	CHL	CAA-C2A-C3A	2.30	119.22	113.00
25	2	603	CLA	O1A-CGA-CBA	2.30	130.39	123.09
30	K	202	BCR	C40-C30-C25	2.30	113.85	110.24
25	B	830	CLA	CMB-C2B-C3B	2.30	131.96	126.55
24	V	305	CHL	O1D-CGD-CBD	2.30	128.21	124.72
25	4	304	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	O	2002	CLA	CMB-C2B-C3B	2.30	131.96	126.55
24	W	306	CHL	C1C-C2C-CMC	2.30	130.94	126.80
29	S	321	Q6L	C19-C18-C17	-2.30	124.06	127.28
25	6	612	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
25	3	313	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	A	850	BCR	C24-C23-C22	-2.30	122.84	126.23
25	A	830	CLA	C2A-C1A-CHA	2.30	127.85	123.87
25	A	825	CLA	C6-C5-C3	2.30	119.06	113.47
24	U	313	CHL	C3C-C4C-NC	-2.30	109.04	114.65
25	A	809	CLA	CHD-C1D-ND	-2.30	121.57	124.80
29	S	321	Q6L	C15-C14-C13	-2.30	124.46	127.69
25	O	2005	CLA	CMA-C3A-C2A	-2.30	110.97	116.23
25	Q	315	CLA	O2A-CGA-CBA	2.30	118.83	111.83
25	B	832	CLA	C2A-C1A-CHA	2.30	127.85	123.87
25	R	317	CLA	CMB-C2B-C3B	2.30	131.95	126.55
29	U	315	Q6L	C29-C27-C26	-2.30	115.40	119.01
38	P	308	KC2	CAC-C3C-C2C	-2.29	120.97	128.43
25	6	609	CLA	CMC-C2C-C1C	2.29	128.62	125.03
34	B	844	PQN	C14-C13-C12	-2.29	117.73	123.63
30	B	849	BCR	C31-C1-C6	-2.29	106.64	110.24
30	F	801	BCR	C20-C19-C18	-2.29	120.07	126.36
25	L	304	CLA	CHD-C1D-ND	-2.29	121.58	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	306	CHL	C3D-C4D-CHA	2.29	112.03	108.54
30	4	319	BCR	C7-C6-C5	-2.29	116.27	121.56
38	R	312	KC2	CAC-C3C-C2C	-2.29	120.98	128.43
25	B	824	CLA	C4A-NA-C1A	2.29	107.72	106.68
24	P	306	CHL	CMB-C2B-C3B	2.29	129.26	124.68
25	A	825	CLA	CHD-C1D-ND	-2.29	121.58	124.80
25	1	607	CLA	CHB-C4A-NA	2.29	127.71	124.40
25	A	807	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
30	F	801	BCR	C37-C22-C23	2.29	121.59	118.09
24	X	308	CHL	C3C-C4C-NC	-2.29	109.05	114.65
24	1	601	CHL	CMB-C2B-C3B	2.29	129.26	124.68
24	T	305	CHL	C3D-C4D-CHA	2.29	112.02	108.54
25	Q	304	CLA	O2A-CGA-CBA	2.29	118.81	111.83
25	4	309	CLA	C4D-CHA-C1A	2.29	123.97	121.24
25	K	206	CLA	CHD-C1D-ND	-2.29	121.58	124.80
25	3	302	CLA	C5-C3-C2	2.29	126.30	121.17
29	S	315	Q6L	O39-C34-C35	-2.29	106.00	110.06
25	1	606	CLA	CAC-C3C-C4C	2.29	127.76	124.79
25	K	203	CLA	C1-O2A-CGA	2.29	122.18	116.65
25	Q	306	CLA	C3B-C4B-NB	-2.29	108.49	110.53
25	6	602	CLA	CMC-C2C-C1C	2.29	128.60	125.03
25	B	840	CLA	O1D-CGD-CBD	2.29	129.03	124.52
25	A	810	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	4	313	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
27	1	612	XAT	C40-C33-C32	2.28	121.58	118.09
36	A	854	DGD	O2E-C2E-C1E	-2.28	104.63	110.08
25	B	808	CLA	CBA-CAA-C2A	2.28	120.59	113.79
25	5	610	CLA	CHD-C1D-ND	-2.28	121.59	124.80
29	S	316	Q6L	C15-C14-C13	-2.28	124.48	127.69
24	P	314	CHL	CMD-C2D-C3D	2.28	129.24	124.68
27	2	617	XAT	C36-C21-C26	2.28	116.20	110.05
25	G	202	CLA	CBA-CAA-C2A	2.28	120.58	113.79
24	2	615	CHL	CMD-C2D-C3D	2.28	129.24	124.68
25	V	302	CLA	CAC-C3C-C4C	2.28	127.76	124.79
25	A	823	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	B	802	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	B	831	CLA	C1-O2A-CGA	2.28	122.17	116.65
30	A	850	BCR	C37-C22-C23	2.28	121.57	118.09
30	3	317	BCR	C35-C13-C12	2.28	121.57	118.09
25	A	835	CLA	CHB-C4A-NA	2.28	127.69	124.40
24	W	307	CHL	C4C-CHD-C1D	2.28	124.22	116.07
25	A	829	CLA	C3B-C2B-C1B	-2.28	104.48	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	856	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
25	B	840	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
24	4	306	CHL	C4C-CHD-C1D	2.28	124.22	116.07
38	U	307	KC2	CAC-C3C-C2C	-2.28	121.03	128.43
37	P	317	NEX	C35-C15-C14	-2.28	118.86	123.52
25	V	301	CLA	C4-C3-C2	-2.28	117.78	123.63
30	3	317	BCR	C24-C23-C22	-2.28	122.87	126.23
25	3	302	CLA	O1D-CGD-CBD	2.28	129.01	124.52
25	5	601	CLA	C2B-C1B-NB	2.28	112.69	110.33
25	U	310	CLA	CHB-C4A-NA	2.28	127.68	124.40
25	3	309	CLA	CHD-C1D-ND	-2.28	121.60	124.80
27	1	612	XAT	O4-C5-C6	-2.27	57.13	58.93
25	P	309	CLA	C11-C12-C13	-2.27	108.41	115.97
24	W	304	CHL	CMD-C2D-C3D	2.27	129.23	124.68
25	Q	312	CLA	O1D-CGD-CBD	2.27	129.00	124.52
25	6	609	CLA	C4B-C3B-C2B	-2.27	104.47	107.30
25	2	609	CLA	C3B-C4B-NB	-2.27	108.50	110.53
25	B	810	CLA	O2D-CGD-CBD	2.27	115.20	111.23
25	A	819	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
24	R	310	CHL	O2D-CGD-O1D	-2.27	119.42	123.85
26	4	317	IWJ	C35-C29-C30	2.27	111.11	108.78
30	A	851	BCR	C20-C19-C18	-2.27	120.14	126.36
24	S	314	CHL	C3D-C4D-CHA	2.27	111.99	108.54
25	B	843	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
29	X	316	Q6L	C29-C27-C26	-2.27	115.44	119.01
30	H	305	BCR	C16-C17-C18	-2.27	124.10	127.28
29	S	316	Q6L	C24-C22-C21	-2.27	115.44	119.01
25	B	824	CLA	CMC-C2C-C1C	2.27	128.58	125.03
25	5	603	CLA	CHA-C1A-NA	-2.27	121.26	126.39
24	1	604	CHL	C1B-CHB-C4A	2.27	122.78	121.32
25	O	2002	CLA	CAA-CBA-CGA	2.27	119.64	113.21
25	H	304	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
25	A	826	CLA	CHD-C1D-ND	-2.27	121.61	124.80
25	T	301	CLA	CBA-CAA-C2A	2.27	120.53	113.79
27	6	615	XAT	C6-C7-C8	-2.27	121.20	125.99
25	3	311	CLA	C6-C5-C3	-2.27	107.95	113.47
25	B	802	CLA	C15-C13-C12	2.26	123.54	112.07
25	A	809	CLA	CMB-C2B-C3B	2.26	131.88	126.55
25	1	603	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
32	H	303	SQD	O7-S-C6	2.26	110.14	106.76
24	2	607	CHL	C4D-CHA-CBD	-2.26	106.68	108.97
38	V	308	KC2	C2A-C1A-NA	2.26	112.97	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	812	CLA	CHB-C4A-NA	2.26	127.67	124.40
24	R	318	CHL	C4D-CHA-CBD	-2.26	106.69	108.97
25	W	312	CLA	C2C-C1C-NC	2.26	112.36	109.98
24	R	310	CHL	O2A-CGA-O1A	-2.26	117.97	123.63
25	P	303	CLA	CBA-CAA-C2A	2.26	120.52	113.79
29	P	321	Q6L	C01-C02-C03	2.26	127.27	124.45
30	H	305	BCR	C16-C15-C14	-2.26	118.89	123.52
25	A	830	CLA	O2A-CGA-CBA	2.26	118.73	111.83
25	3	310	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
25	U	310	CLA	C4D-CHA-C1A	2.26	123.94	121.24
25	5	604	CLA	CMB-C2B-C3B	2.26	129.54	123.53
25	L	302	CLA	CAC-C3C-C4C	2.26	127.73	124.79
24	U	306	CHL	O1D-CGD-CBD	2.26	128.15	124.72
30	L	307	BCR	C30-C25-C26	2.26	125.72	122.64
25	B	808	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
25	4	312	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
29	P	316	Q6L	C24-C22-C21	-2.26	115.46	119.01
25	U	311	CLA	C1-C2-C3	-2.26	122.50	126.20
25	B	841	CLA	C6-C5-C3	2.26	118.97	113.47
24	Q	307	CHL	CMD-C2D-C3D	2.26	129.19	124.68
30	4	319	BCR	C38-C26-C27	2.26	118.41	113.60
25	T	312	CLA	O2D-CGD-CBD	2.26	115.17	111.23
25	4	309	CLA	CMB-C2B-C3B	2.26	131.85	126.55
25	3	307	CLA	CMC-C2C-C1C	2.26	128.56	125.03
29	V	319	Q6L	C01-C02-C07	-2.25	110.28	114.42
38	V	308	KC2	CAC-C3C-C4C	2.25	134.35	124.39
25	3	305	CLA	CBA-CAA-C2A	2.25	118.19	113.41
25	B	837	CLA	C4B-C3B-C2B	-2.25	104.50	107.30
27	3	316	XAT	O3-C3-C4	2.25	114.36	109.75
25	S	302	CLA	CHB-C4A-NA	2.25	127.65	124.40
30	A	848	BCR	C32-C1-C6	2.25	113.78	110.24
24	V	305	CHL	C3C-C4C-NC	-2.25	109.15	114.65
24	X	305	CHL	C3C-C4C-NC	-2.25	109.15	114.65
38	W	308	KC2	C4C-C3C-C2C	-2.25	105.21	107.28
24	T	304	CHL	C4D-ND-C1D	2.25	106.93	105.22
25	N	203	CLA	C3D-C2D-C1D	2.25	108.90	105.83
37	R	321	NEX	C31-C30-C29	-2.25	124.12	127.28
25	Q	301	CLA	C4-C3-C2	-2.25	117.84	123.63
25	S	309	CLA	C3A-C2A-C1A	-2.25	97.97	101.34
25	A	833	CLA	CHB-C1B-NB	2.25	127.43	124.05
30	G	201	BCR	C20-C21-C22	-2.25	124.12	127.28
25	U	310	CLA	C2A-C1A-CHA	2.25	127.77	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	304	CHL	C3D-C4D-CHA	2.25	111.96	108.54
30	A	849	BCR	C16-C15-C14	-2.25	118.92	123.52
25	B	815	CLA	CMA-C3A-C4A	2.25	117.82	111.77
31	N	201	LMG	O8-C28-C29	2.25	118.69	111.83
38	Q	310	KC2	CAA-CBA-CGA	-2.25	115.62	127.05
24	4	306	CHL	C3D-C4D-CHA	2.25	111.95	108.54
25	5	601	CLA	CMA-C3A-C4A	2.25	117.81	111.77
29	U	315	Q6L	C20-C19-C18	2.25	128.12	123.52
25	2	613	CLA	OBD-CAD-C3D	2.25	133.67	128.42
25	P	310	CLA	C11-C10-C8	2.25	123.43	115.97
30	B	847	BCR	C19-C18-C17	-2.25	115.47	119.01
25	A	845	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
25	B	804	CLA	C1-C2-C3	-2.25	122.52	126.20
30	F	801	BCR	C16-C17-C18	-2.25	124.13	127.28
25	A	829	CLA	O1D-CGD-CBD	2.25	128.95	124.52
24	R	310	CHL	C3D-C4D-CHA	2.25	111.95	108.54
25	L	303	CLA	C2A-C1A-CHA	2.25	127.76	123.87
26	S	322	IWJ	C36-C35-C34	-2.25	105.02	108.97
25	A	822	CLA	O1D-CGD-CBD	2.24	128.94	124.52
25	A	818	CLA	CHD-C1D-ND	-2.24	121.64	124.80
25	P	301	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
24	S	307	CHL	C3C-C4C-NC	-2.24	109.17	114.65
25	V	310	CLA	CAC-C3C-C4C	2.24	127.71	124.79
30	B	846	BCR	C23-C22-C21	2.24	122.54	119.01
25	P	302	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
25	V	309	CLA	C3D-C4D-ND	2.24	113.63	109.99
25	B	811	CLA	CHD-C1D-ND	-2.24	121.65	124.80
24	T	314	CHL	C4D-CHA-CBD	-2.24	106.71	108.97
25	R	314	CLA	CMA-C3A-C4A	2.24	117.80	111.77
30	4	319	BCR	C11-C10-C9	-2.24	124.14	127.28
25	T	311	CLA	CAA-C2A-C3A	-2.24	106.94	113.00
25	P	309	CLA	C6-C5-C3	2.24	118.93	113.47
26	T	318	IWJ	C05-C04-C03	2.24	114.51	111.18
29	T	316	Q6L	C31-C30-C29	-2.24	121.09	124.58
25	2	602	CLA	O2A-CGA-CBA	2.24	118.66	111.83
25	V	309	CLA	C4A-NA-C1A	2.24	107.70	106.68
38	P	308	KC2	C3C-C2C-C1C	2.24	108.09	106.41
38	W	308	KC2	CAA-C2A-C1A	-2.24	114.84	124.64
25	B	841	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
25	A	806	CLA	O2D-CGD-CBD	2.24	115.14	111.23
24	P	304	CHL	CED-O2D-CGD	2.24	120.99	115.92
24	T	320	CHL	C4-C3-C5	-2.24	113.50	116.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	P	313	CLA	CHD-C1D-ND	-2.24	121.66	124.80
30	F	801	BCR	C40-C30-C39	-2.23	102.23	108.63
25	P	313	CLA	CHB-C4A-NA	2.23	127.62	124.40
25	A	804	CLA	C1D-ND-C4D	2.23	107.88	106.31
24	5	605	CHL	C3C-C4C-NC	-2.23	109.19	114.65
30	A	851	BCR	C2-C3-C4	-2.23	106.36	111.28
25	B	809	CLA	CBA-CAA-C2A	2.23	120.44	113.79
25	1	609	CLA	CMC-C2C-C1C	2.23	128.52	125.03
25	T	309	CLA	C1D-ND-C4D	-2.23	104.75	106.31
25	P	311	CLA	CBA-CAA-C2A	2.23	120.44	113.79
25	L	303	CLA	C4B-C3B-C2B	-2.23	104.53	107.30
30	A	849	BCR	C35-C13-C12	2.23	121.50	118.09
38	X	309	KC2	C3C-C2C-C1C	2.23	108.09	106.41
24	3	306	CHL	C3D-C4D-CHA	2.23	111.93	108.54
25	B	808	CLA	CMA-C3A-C2A	-2.23	105.36	113.98
24	X	305	CHL	O2D-CGD-CBD	2.23	113.40	110.95
27	6	615	XAT	C19-C9-C8	2.23	121.50	118.09
25	P	301	CLA	CAC-C3C-C4C	2.23	127.69	124.79
25	O	2002	CLA	C2B-C1B-NB	2.23	112.64	110.33
25	A	822	CLA	CHB-C4A-NA	2.23	127.62	124.40
25	4	315	CLA	CMA-C3A-C2A	-2.23	111.12	116.23
25	6	611	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
25	6	607	CLA	O2A-CGA-O1A	-2.23	117.60	123.33
25	L	304	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
25	U	312	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	X	305	CHL	CAA-C2A-C3A	-2.23	111.12	116.23
25	5	604	CLA	CHB-C4A-NA	2.23	127.61	124.40
25	6	602	CLA	CAC-C3C-C4C	2.23	127.69	124.79
33	A	802	CL0	O2A-CGA-O1A	-2.23	118.06	123.63
30	L	306	BCR	C35-C13-C12	2.23	121.49	118.09
25	2	610	CLA	O1D-CGD-CBD	2.23	128.91	124.52
25	W	311	CLA	CHA-C1A-NA	-2.23	121.35	126.39
25	B	835	CLA	O2A-CGA-O1A	-2.23	117.61	123.33
25	R	317	CLA	CHD-C1D-ND	-2.23	121.67	124.80
38	W	308	KC2	O2A-CGA-O1A	-2.23	118.17	122.70
24	4	307	CHL	O2D-CGD-CBD	2.23	113.39	110.95
24	W	305	CHL	O1D-CGD-CBD	2.22	128.10	124.72
24	6	601	CHL	CMD-C2D-C3D	2.22	129.13	124.68
26	S	319	IWJ	C23-C22-C21	-2.22	116.75	123.20
27	2	617	XAT	C35-C34-C33	-2.22	124.16	127.28
25	V	303	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
25	B	819	CLA	CHB-C1B-NB	2.22	127.39	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	830	CLA	CAC-C3C-C4C	2.22	127.68	124.79
26	R	303	IWJ	C21-C19-C18	-2.22	115.51	119.01
25	B	827	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
25	A	809	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
25	A	825	CLA	CHB-C4A-NA	2.22	127.61	124.40
36	A	854	DGD	C4D-C3D-C2D	-2.22	106.93	110.83
25	A	842	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
26	V	318	IWJ	C37-C35-C34	-2.22	105.06	108.97
25	O	2004	CLA	CHD-C1D-ND	-2.22	121.68	124.80
25	B	826	CLA	C1-O2A-CGA	2.22	122.03	116.65
24	X	315	CHL	C3C-C4C-NC	-2.22	109.22	114.65
25	B	821	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
29	S	315	Q6L	C42-C13-C12	2.22	119.08	115.23
29	2	616	Q6L	C01-C02-C07	-2.22	110.34	114.42
25	B	818	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
25	2	614	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	B	816	CLA	C3B-C4B-NB	-2.22	108.55	110.53
24	1	604	CHL	C1C-C2C-CMC	2.22	130.80	126.80
24	T	307	CHL	O1D-CGD-CBD	2.22	128.09	124.72
25	Q	306	CLA	CHA-C1A-NA	-2.22	121.37	126.39
25	T	301	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
25	1	610	CLA	CBA-CAA-C2A	2.22	118.12	113.41
25	U	303	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
29	S	315	Q6L	C06-C07-C02	2.22	117.70	112.18
24	T	306	CHL	O2A-CGA-O1A	-2.22	118.08	123.63
25	B	808	CLA	O1D-CGD-CBD	2.22	128.89	124.52
29	S	321	Q6L	C19-C20-C21	-2.22	118.98	123.52
25	2	603	CLA	CMC-C2C-C1C	2.22	128.50	125.03
25	3	310	CLA	CED-O2D-CGD	2.22	120.94	115.92
25	6	607	CLA	CMB-C2B-C3B	2.22	131.76	126.55
30	A	851	BCR	C27-C26-C25	-2.22	119.71	122.70
25	A	833	CLA	CBA-CAA-C2A	2.22	120.39	113.79
25	V	302	CLA	CHB-C4A-NA	2.22	127.60	124.40
30	L	305	BCR	C2-C1-C6	-2.22	107.22	110.44
25	B	802	CLA	CBA-CAA-C2A	2.22	120.38	113.79
37	T	317	NEX	C16-C1-C6	2.21	112.45	110.47
25	P	301	CLA	C5-C3-C2	-2.21	116.20	121.17
25	3	304	CLA	CHB-C4A-NA	2.21	127.59	124.40
25	X	303	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	P	310	CLA	C1-C2-C3	-2.21	122.57	126.20
37	S	317	NEX	C19-C9-C10	2.21	126.40	122.82
30	H	305	BCR	C34-C9-C8	-2.21	114.71	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	W	313	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
25	3	312	CLA	CHD-C1D-ND	-2.21	121.69	124.80
24	6	606	CHL	C4C-CHD-C1D	2.21	123.98	116.07
33	A	802	CL0	CMA-C3A-C4A	-2.21	109.85	114.61
25	U	312	CLA	CMA-C3A-C2A	-2.21	111.16	116.23
25	B	806	CLA	CAC-C3C-C2C	-2.21	123.50	127.56
25	B	828	CLA	CHA-C1A-NA	-2.21	121.39	126.39
25	N	202	CLA	C3A-C2A-C1A	2.21	104.65	101.34
25	X	302	CLA	CHC-C4B-NB	2.21	127.36	124.05
24	U	304	CHL	CMB-C2B-C3B	2.21	129.10	124.68
24	V	304	CHL	C4D-ND-C1D	2.21	106.89	105.22
25	3	311	CLA	O2D-CGD-O1D	-2.21	119.07	124.08
25	K	203	CLA	C1C-C2C-C3C	-2.21	104.66	106.98
30	3	319	BCR	C27-C26-C25	-2.21	119.72	122.70
30	B	847	BCR	C33-C5-C6	-2.21	122.08	124.48
30	M	101	BCR	C11-C12-C13	-2.21	120.31	126.36
25	3	311	CLA	C3A-C2A-C1A	2.21	104.64	101.34
24	S	304	CHL	C3C-C4C-NC	-2.21	109.26	114.65
24	P	307	CHL	C4D-CHA-CBD	-2.21	106.74	108.97
27	1	612	XAT	O23-C23-C22	-2.21	105.24	109.75
27	4	318	XAT	C12-C13-C14	-2.20	115.54	119.01
25	G	204	CLA	C3B-C4B-NB	-2.20	108.56	110.53
30	B	845	BCR	C24-C23-C22	-2.20	122.97	126.23
25	A	827	CLA	CMA-C3A-C4A	2.20	117.70	111.77
30	L	307	BCR	C7-C6-C5	-2.20	116.48	121.56
25	A	821	CLA	C2A-C1A-CHA	2.20	127.69	123.87
24	P	304	CHL	C3C-C4C-NC	-2.20	109.27	114.65
25	1	607	CLA	CMD-C2D-C1D	2.20	129.24	125.46
38	P	308	KC2	O1A-CGA-CBA	2.20	127.81	121.06
25	6	613	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
25	A	829	CLA	CBC-CAC-C3C	2.20	118.39	112.42
37	S	317	NEX	C35-C34-C33	-2.20	124.19	127.28
24	4	308	CHL	CMB-C2B-C3B	2.20	129.08	124.68
29	R	319	Q6L	C01-C02-C07	-2.20	110.38	114.42
30	F	804	BCR	C29-C30-C25	-2.20	107.24	110.44
24	X	315	CHL	CMB-C2B-C3B	2.20	129.08	124.68
25	1	602	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	B	822	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	2	603	CLA	O2A-CGA-O1A	-2.20	117.68	123.33
25	4	310	CLA	C4-C3-C2	-2.20	117.98	123.63
25	3	308	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
25	6	604	CLA	CMB-C2B-C1B	-2.20	122.07	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	804	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
26	V	320	IWJ	C22-C21-C19	2.20	132.39	126.36
30	H	305	BCR	C35-C13-C12	2.20	121.44	118.09
25	B	822	CLA	O1D-CGD-CBD	2.20	128.85	124.52
25	L	302	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
30	A	848	BCR	C21-C20-C19	2.20	129.56	123.20
25	A	821	CLA	C16-C15-C13	-2.20	108.67	115.97
25	B	809	CLA	C4-C3-C2	-2.19	117.99	123.63
24	4	308	CHL	O2D-CGD-CBD	2.19	113.36	110.95
24	T	320	CHL	CBC-CAC-C3C	2.19	116.01	112.87
24	P	304	CHL	CHA-C1A-C2A	-2.19	128.16	133.31
25	F	803	CLA	CAA-C2A-C3A	-2.19	111.20	116.23
25	S	313	CLA	CAA-C2A-C3A	-2.19	111.20	116.23
25	A	843	CLA	CBA-CAA-C2A	2.19	120.31	113.79
25	P	303	CLA	C1-C2-C3	-2.19	123.22	126.76
25	A	838	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
26	Q	303	IWJ	C21-C19-C18	-2.19	115.56	119.01
25	A	839	CLA	C3B-C2B-C1B	-2.19	104.59	107.17
25	B	828	CLA	C1-C2-C3	-2.19	122.61	126.20
25	V	311	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
25	1	613	CLA	CMB-C2B-C3B	2.19	131.70	126.55
25	A	817	CLA	CHA-C1A-NA	-2.19	121.43	126.39
25	W	302	CLA	CAC-C3C-C4C	2.19	127.64	124.79
25	F	802	CLA	CHB-C4A-NA	2.19	127.56	124.40
37	S	317	NEX	O24-C26-C27	2.19	123.15	116.88
25	A	821	CLA	CHD-C1D-ND	-2.19	121.72	124.80
25	T	301	CLA	C2A-C1A-CHA	2.19	127.67	123.87
26	X	318	IWJ	C25-C24-C26	2.19	119.55	116.00
25	B	832	CLA	CHD-C1D-C2D	2.19	130.04	125.49
24	6	601	CHL	C1C-C2C-CMC	2.19	130.75	126.80
25	2	603	CLA	CHB-C4A-NA	2.19	127.56	124.40
25	1	603	CLA	CBA-CAA-C2A	2.19	120.30	113.79
25	B	803	CLA	CHD-C1D-ND	-2.19	121.72	124.80
25	3	302	CLA	CHA-C1A-NA	-2.19	121.44	126.39
25	T	311	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
24	S	304	CHL	C1C-CHC-C4B	2.19	123.90	116.07
29	S	323	Q6L	C01-C02-C07	-2.19	110.40	114.42
25	3	309	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	W	318	IWJ	C32-C30-C31	2.19	125.47	121.19
30	K	202	BCR	C8-C7-C6	-2.19	121.16	127.00
25	X	313	CLA	CMA-C3A-C2A	-2.19	111.22	116.23
26	4	317	IWJ	C06-C07-C08	-2.19	110.31	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	309	CHL	C3C-C4C-NC	-2.18	109.31	114.65
25	A	828	CLA	CHD-C1D-C2D	2.18	130.03	125.49
24	T	320	CHL	C3C-C4C-NC	-2.18	109.31	114.65
25	R	307	CLA	CMB-C2B-C3B	2.18	131.69	126.55
25	F	802	CLA	CHD-C1D-ND	-2.18	121.73	124.80
25	B	824	CLA	C6-C5-C3	-2.18	108.15	113.47
27	1	612	XAT	C11-C12-C13	-2.18	120.38	126.36
25	A	818	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
25	A	807	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
31	A	857	LMG	O8-C28-C29	2.18	118.49	111.83
25	V	312	CLA	O1D-CGD-CBD	2.18	128.82	124.52
25	A	816	CLA	C3B-C2B-C1B	-2.18	104.60	107.17
29	T	316	Q6L	C25-C26-C27	2.18	130.34	127.28
29	T	319	Q6L	C42-C13-C12	2.18	119.02	115.23
24	4	308	CHL	C3D-C4D-CHA	2.18	111.86	108.54
24	S	305	CHL	CMD-C2D-C3D	2.18	129.04	124.68
25	Q	313	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
24	2	605	CHL	CMB-C2B-C3B	2.18	129.04	124.68
29	S	323	Q6L	C24-C22-C21	-2.18	115.58	119.01
25	4	315	CLA	CHD-C1D-ND	-2.18	121.73	124.80
25	4	312	CLA	CAC-C3C-C4C	2.18	127.63	124.79
24	T	314	CHL	C3D-C4D-CHA	2.18	111.85	108.54
25	L	303	CLA	O2A-CGA-O1A	-2.18	117.73	123.33
25	K	204	CLA	CAC-C3C-C4C	2.18	127.62	124.79
25	U	310	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
25	2	612	CLA	CHA-C1A-NA	-2.18	121.46	126.39
28	3	323	LHG	O8-C23-C24	2.18	118.48	111.83
25	A	832	CLA	CMB-C2B-C3B	2.18	131.67	126.55
28	3	322	LHG	C25-C24-C23	-2.18	105.71	113.69
25	U	311	CLA	O2A-CGA-CBA	2.18	118.47	111.83
25	H	301	CLA	CHA-C1A-NA	-2.18	121.46	126.39
25	A	804	CLA	CHD-C1D-C2D	2.18	130.02	125.49
26	Q	303	IWJ	C36-C35-C34	-2.18	105.14	108.97
24	W	307	CHL	CBA-CAA-C2A	2.18	120.19	113.78
29	U	315	Q6L	C20-C21-C22	2.18	130.33	127.28
30	L	307	BCR	C27-C26-C25	-2.18	119.76	122.70
25	4	311	CLA	CHA-C1A-NA	-2.18	121.46	126.39
24	P	306	CHL	C4D-ND-C1D	2.18	106.87	105.22
25	3	313	CLA	CHD-C1D-ND	-2.18	121.74	124.80
25	4	309	CLA	CHD-C1D-ND	-2.18	121.74	124.80
25	A	830	CLA	O1D-CGD-CBD	2.18	128.81	124.52
25	A	837	CLA	CHD-C1D-ND	-2.17	121.74	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	W	318	IWJ	C36-C35-C34	-2.17	105.15	108.97
25	L	303	CLA	CMC-C2C-C1C	2.17	128.43	125.03
30	A	848	BCR	C37-C22-C23	2.17	121.41	118.09
25	N	203	CLA	CHA-C4D-ND	2.17	137.03	132.55
25	R	314	CLA	CHA-C1A-NA	-2.17	121.47	126.39
25	F	802	CLA	C1C-C2C-C3C	-2.17	104.69	106.98
25	B	813	CLA	CAC-C3C-C2C	-2.17	123.56	127.56
25	1	602	CLA	CMC-C2C-C1C	2.17	128.43	125.03
24	U	305	CHL	CMD-C2D-C3D	2.17	129.02	124.68
25	4	309	CLA	C4A-NA-C1A	2.17	107.67	106.68
25	A	803	CLA	CMB-C2B-C3B	2.17	131.66	126.55
25	R	316	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
29	S	315	Q6L	C05-C04-C03	2.17	113.48	110.61
24	Q	316	CHL	C1A-CHA-C4D	2.17	122.61	118.98
25	6	604	CLA	CMB-C2B-C3B	2.17	131.66	126.55
25	W	309	CLA	C1-O2A-CGA	-2.17	111.39	116.65
25	Q	305	CLA	CHB-C4A-NA	2.17	127.53	124.40
25	B	824	CLA	C3B-C2B-C1B	2.17	109.73	107.17
25	A	808	CLA	CHA-C4D-ND	2.17	137.03	132.55
24	S	305	CHL	O1D-CGD-CBD	2.17	128.01	124.72
25	B	814	CLA	CMC-C2C-C1C	2.17	128.43	125.03
25	A	821	CLA	CAC-C3C-C4C	2.17	127.61	124.79
25	S	309	CLA	C3B-C4B-NB	-2.17	108.59	110.53
25	5	610	CLA	CHB-C4A-NA	2.17	127.53	124.40
24	S	305	CHL	C4C-CHD-C1D	2.17	123.83	116.07
24	T	306	CHL	C4C-CHD-C1D	2.17	123.83	116.07
25	2	614	CLA	CHB-C4A-NA	2.17	127.53	124.40
24	5	605	CHL	CBC-CAC-C3C	-2.17	109.77	112.87
25	A	829	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	U	308	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
25	6	611	CLA	CHD-C1D-ND	-2.17	121.75	124.80
25	4	303	CLA	CMC-C2C-C1C	2.17	128.42	125.03
25	A	838	CLA	CHA-C1A-NA	-2.17	121.48	126.39
30	F	804	BCR	C2-C1-C6	2.17	113.59	110.44
25	V	303	CLA	CHD-C1D-ND	-2.17	121.75	124.80
24	2	601	CHL	C1A-CHA-C4D	2.17	122.60	118.98
25	A	820	CLA	CHB-C1B-NB	2.16	127.30	124.05
25	B	812	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
24	V	307	CHL	C4C-CHD-C1D	2.16	123.81	116.07
30	A	849	BCR	C20-C19-C18	-2.16	120.43	126.36
38	Q	310	KC2	CAC-C3C-C2C	-2.16	121.40	128.43
25	S	301	CLA	CMB-C2B-C1B	-2.16	122.13	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	306	CHL	C4D-CHA-CBD	-2.16	106.79	108.97
25	3	305	CLA	CMC-C2C-C1C	2.16	128.41	125.03
25	V	301	CLA	C4D-CHA-C1A	2.16	123.82	121.24
26	X	318	IWJ	C33-C32-C30	2.16	115.53	112.06
26	U	316	IWJ	C17-C16-C15	-2.16	119.10	123.52
25	1	610	CLA	CHB-C4A-NA	2.16	127.52	124.40
25	A	842	CLA	CED-O2D-CGD	2.16	120.81	115.92
25	B	818	CLA	CAC-C3C-C4C	2.16	127.60	124.79
25	6	608	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	A	804	CLA	CHD-C1D-ND	-2.16	121.76	124.80
29	S	315	Q6L	C01-C02-C07	-2.16	110.45	114.42
27	5	612	XAT	C15-C35-C34	-2.16	119.10	123.52
25	1	610	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	1	613	CLA	CHD-C1D-ND	-2.16	121.76	124.80
26	S	319	IWJ	C33-C32-C30	2.16	115.52	112.06
24	Q	309	CHL	CMD-C2D-C3D	2.16	129.00	124.68
25	A	842	CLA	O1D-CGD-CBD	2.16	128.78	124.52
25	K	201	CLA	C4B-C3B-C2B	-2.16	104.62	107.30
24	W	314	CHL	C3C-C4C-NC	-2.16	109.38	114.65
24	2	615	CHL	CMB-C2B-C3B	2.16	129.00	124.68
25	T	309	CLA	C6-C5-C3	2.16	118.72	113.47
37	R	321	NEX	C35-C15-C14	-2.16	119.11	123.52
25	3	314	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
25	B	843	CLA	CHD-C1D-ND	-2.16	121.77	124.80
27	2	617	XAT	C24-C23-C22	-2.16	106.76	110.79
24	S	305	CHL	C3C-C4C-NC	-2.16	109.38	114.65
30	L	305	BCR	C12-C13-C14	-2.16	115.62	119.01
24	T	306	CHL	C4-C3-C2	-2.16	118.09	123.63
28	2	619	LHG	O8-C23-C24	2.16	118.41	111.83
25	O	2004	CLA	C2A-C3A-C4A	2.15	104.12	101.59
25	2	604	CLA	CMB-C2B-C3B	2.15	131.62	126.55
24	U	313	CHL	C4D-ND-C1D	2.15	106.85	105.22
25	U	302	CLA	C2D-C1D-ND	-2.15	107.99	110.13
24	4	308	CHL	CMD-C2D-C3D	2.15	128.99	124.68
25	A	843	CLA	C7-C6-C5	-2.15	107.52	113.26
25	B	822	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
25	B	842	CLA	CMC-C2C-C1C	2.15	128.40	125.03
24	3	306	CHL	C4C-CHD-C1D	2.15	123.77	116.07
30	B	848	BCR	C33-C5-C6	-2.15	122.14	124.48
25	V	302	CLA	C4D-C3D-CAD	-2.15	105.77	108.11
25	U	303	CLA	C1-C2-C3	-2.15	123.28	126.76
25	B	812	CLA	C1-C2-C3	-2.15	122.67	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	813	CLA	O2D-CGD-CBD	2.15	114.99	111.23
25	5	603	CLA	CMC-C2C-C1C	2.15	128.39	125.03
25	V	310	CLA	CMC-C2C-C1C	2.15	128.39	125.03
26	Q	303	IWJ	C33-C32-C30	2.15	115.51	112.06
38	R	312	KC2	CAC-C3C-C4C	2.15	133.89	124.39
25	W	312	CLA	C3A-C2A-C1A	2.15	104.56	101.34
25	F	803	CLA	O2D-CGD-CBD	2.15	114.99	111.23
25	A	827	CLA	CHA-C1A-NA	-2.15	121.53	126.39
25	S	301	CLA	O1D-CGD-CBD	2.15	128.76	124.52
25	P	310	CLA	CHD-C1D-ND	-2.15	121.78	124.80
25	X	304	CLA	CAC-C3C-C4C	2.15	127.58	124.79
25	S	311	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
38	X	309	KC2	C1B-CHB-C4A	2.15	130.58	126.02
30	A	849	BCR	C11-C12-C13	-2.15	120.48	126.36
25	5	601	CLA	C3A-C2A-C1A	2.15	104.55	101.34
25	3	308	CLA	CED-O2D-CGD	2.15	120.78	115.92
28	3	323	LHG	C5-O7-C7	-2.15	112.66	117.80
25	3	302	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
25	A	810	CLA	CMB-C2B-C3B	2.14	131.59	126.55
25	S	310	CLA	CHA-C1A-NA	-2.14	121.53	126.39
25	3	303	CLA	C4C-C3C-C2C	-2.14	105.09	107.09
25	B	812	CLA	O1D-CGD-CBD	2.14	128.75	124.52
25	2	608	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	G	204	CLA	CHB-C1B-NB	2.14	127.27	124.05
25	A	835	CLA	CAA-CBA-CGA	-2.14	107.12	113.21
25	B	828	CLA	CMB-C2B-C3B	2.14	131.59	126.55
25	G	203	CLA	O2D-CGD-CBD	2.14	114.98	111.23
25	B	808	CLA	CHA-C1A-NA	-2.14	121.54	126.39
24	R	308	CHL	C4C-CHD-C1D	2.14	123.73	116.07
25	B	840	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	B	816	CLA	CBA-CAA-C2A	2.14	120.17	113.79
25	A	816	CLA	CAA-CBA-CGA	2.14	118.20	112.49
25	4	313	CLA	C5-C3-C2	2.14	125.97	121.17
25	Q	301	CLA	C3A-C2A-C1A	2.14	104.55	101.34
38	X	309	KC2	CHB-C4A-C3A	-2.14	121.65	125.03
24	T	307	CHL	O2D-CGD-O1D	-2.14	119.68	123.85
24	U	305	CHL	C3C-C4C-NC	-2.14	109.42	114.65
25	B	820	CLA	C1C-C2C-C3C	-2.14	104.73	106.98
24	T	320	CHL	CMB-C2B-C3B	2.14	128.96	124.68
25	A	815	CLA	O1A-CGA-CBA	2.14	132.16	123.78
25	1	613	CLA	C4-C3-C2	-2.14	118.13	123.63
24	X	307	CHL	C4C-CHD-C1D	2.14	123.73	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	317	IWJ	C33-C32-C30	2.14	115.49	112.06
25	A	814	CLA	C2D-C1D-ND	-2.14	108.01	110.13
25	L	301	CLA	CHD-C1D-ND	-2.14	121.79	124.80
30	L	306	BCR	C16-C17-C18	-2.14	124.28	127.28
24	U	304	CHL	OMC-CMC-C2C	-2.14	121.41	125.12
25	Q	301	CLA	CHA-C1A-NA	-2.14	121.55	126.39
25	4	311	CLA	CAC-C3C-C4C	2.14	127.57	124.79
24	W	306	CHL	C4C-CHD-C1D	2.14	123.72	116.07
24	Q	309	CHL	C3C-C4C-NC	-2.14	109.42	114.65
26	Q	303	IWJ	C25-C24-C26	2.14	119.47	116.00
25	A	812	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	Q	304	CLA	C1D-ND-C4D	-2.14	104.81	106.31
25	F	803	CLA	CHB-C4A-NA	2.14	127.48	124.40
25	X	302	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	P	306	CHL	CMD-C2D-C3D	2.14	128.96	124.68
25	W	303	CLA	C3A-C2A-C1A	2.14	104.54	101.34
29	R	301	Q6L	C14-C15-C16	-2.14	117.01	123.20
29	O	2007	Q6L	C01-C02-C07	-2.14	110.49	114.42
25	S	303	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	S	307	CHL	C3D-C4D-CHA	2.14	111.79	108.54
28	2	619	LHG	O8-C6-C5	-2.14	102.24	108.40
25	B	830	CLA	CHB-C1B-NB	2.14	127.25	124.05
30	F	801	BCR	C27-C26-C25	-2.13	119.82	122.70
25	2	608	CLA	CBA-CAA-C2A	2.13	120.14	113.79
25	X	304	CLA	CMA-C3A-C4A	-2.13	106.04	111.77
25	4	314	CLA	CHB-C4A-NA	2.13	127.48	124.40
24	T	305	CHL	C4C-CHD-C1D	2.13	123.70	116.07
24	S	306	CHL	C4D-CHA-CBD	-2.13	106.81	108.97
25	W	311	CLA	C2A-C1A-CHA	2.13	127.57	123.87
27	1	612	XAT	C4-C3-C2	-2.13	106.80	110.79
29	T	316	Q6L	C19-C20-C21	-2.13	119.16	123.52
29	V	321	Q6L	C05-C04-C03	2.13	113.43	110.61
25	A	832	CLA	CHB-C4A-NA	2.13	127.48	124.40
25	G	204	CLA	CAC-C3C-C4C	2.13	127.56	124.79
25	1	603	CLA	CHD-C1D-ND	-2.13	121.80	124.80
30	L	306	BCR	C10-C11-C12	2.13	129.38	123.20
25	B	812	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
25	1	606	CLA	CAA-C2A-C3A	-2.13	111.34	116.23
25	U	308	CLA	CHB-C4A-NA	2.13	127.47	124.40
25	B	819	CLA	C4A-NA-C1A	2.13	107.65	106.68
25	T	302	CLA	CAC-C3C-C4C	2.13	127.56	124.79
25	N	203	CLA	CMB-C2B-C1B	-2.13	122.18	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	301	CLA	C5-C3-C2	2.13	125.95	121.17
25	A	842	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
26	5	611	IWJ	C12-C11-C10	-2.13	124.29	127.28
25	B	841	CLA	CHB-C1B-NB	2.13	127.24	124.05
25	A	839	CLA	C3A-C2A-C1A	2.13	104.53	101.34
24	S	314	CHL	C3C-C4C-NC	-2.13	109.45	114.65
25	B	831	CLA	C4B-C3B-C2B	-2.13	104.66	107.30
25	X	304	CLA	C4B-C3B-C2B	-2.13	104.66	107.30
25	W	309	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
38	R	312	KC2	O1D-CGD-CBD	2.13	128.72	124.52
24	S	306	CHL	C3D-C4D-CHA	2.13	111.77	108.54
24	T	320	CHL	C4D-ND-C1D	2.13	106.83	105.22
25	B	810	CLA	CHB-C4A-NA	2.13	127.47	124.40
30	J	101	BCR	C11-C12-C13	-2.13	120.53	126.36
24	U	305	CHL	C4C-CHD-C1D	2.13	123.68	116.07
25	B	837	CLA	CHB-C4A-NA	2.13	127.47	124.40
25	A	845	CLA	O1D-CGD-CBD	2.13	128.71	124.52
30	A	850	BCR	C31-C1-C2	2.13	117.11	108.95
25	4	311	CLA	C2C-C1C-NC	2.13	112.22	109.98
29	U	315	Q6L	C31-C30-C29	-2.13	121.27	124.58
29	U	315	Q6L	C35-C34-C33	2.13	114.34	111.18
25	V	313	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
29	U	317	Q6L	C01-C02-C07	-2.12	110.51	114.42
26	3	315	IWJ	C21-C19-C18	-2.12	115.67	119.01
25	B	809	CLA	C11-C10-C8	-2.12	108.90	115.97
25	A	825	CLA	C4B-C3B-C2B	-2.12	104.66	107.30
38	S	308	KC2	O2A-CGA-O1A	-2.12	118.38	122.70
29	2	616	Q6L	C06-C07-C02	2.12	117.46	112.18
29	Q	319	Q6L	C25-C26-C27	-2.12	124.30	127.28
24	W	307	CHL	CBC-CAC-C3C	2.12	115.91	112.87
25	O	2002	CLA	C11-C12-C13	-2.12	108.91	115.97
25	O	2003	CLA	CHD-C1D-ND	-2.12	121.82	124.80
25	4	314	CLA	CMC-C2C-C1C	2.12	128.35	125.03
25	4	310	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	B	835	CLA	O1A-CGA-CBA	2.12	129.82	123.09
25	2	610	CLA	CHD-C1D-ND	-2.12	121.82	124.80
25	T	310	CLA	CHB-C4A-NA	2.12	127.46	124.40
24	P	307	CHL	C3D-C4D-CHA	2.12	111.76	108.54
25	A	840	CLA	CHD-C1D-ND	-2.12	121.82	124.80
25	Q	313	CLA	C2A-C1A-CHA	2.12	127.55	123.87
25	1	609	CLA	CMB-C2B-C3B	2.12	129.17	123.53
25	A	809	CLA	CBA-CAA-C2A	2.12	120.10	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	S	317	NEX	C40-C33-C32	2.12	121.33	118.09
25	5	604	CLA	C3B-C4B-NB	-2.12	108.13	110.33
25	2	612	CLA	O2D-CGD-CBD	2.12	114.94	111.23
25	B	829	CLA	CBA-CAA-C2A	2.12	120.10	113.79
37	W	317	NEX	C40-C33-C32	2.12	121.33	118.09
25	B	813	CLA	CHD-C1D-ND	-2.12	121.82	124.80
30	G	201	BCR	C35-C13-C14	2.12	126.25	122.82
24	R	311	CHL	O2D-CGD-O1D	-2.12	119.73	123.85
25	B	825	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
25	1	610	CLA	CMC-C2C-C1C	2.12	128.34	125.03
25	W	301	CLA	CAA-C2A-C1A	-2.12	105.04	111.97
38	Q	310	KC2	O1A-CGA-CBA	2.12	127.55	121.06
30	H	305	BCR	C39-C30-C25	2.12	113.56	110.24
25	6	609	CLA	O2D-CGD-CBD	2.12	114.93	111.23
24	R	309	CHL	C4C-CHD-C1D	2.12	123.64	116.07
24	T	306	CHL	O1D-CGD-CBD	2.12	127.93	124.72
25	B	824	CLA	CHD-C1D-ND	-2.12	121.82	124.80
25	Q	313	CLA	CHD-C1D-ND	-2.12	121.82	124.80
24	R	308	CHL	O2A-CGA-O1A	-2.12	117.89	123.33
25	A	814	CLA	CHD-C1D-C2D	2.12	129.89	125.49
25	1	610	CLA	CHC-C4B-NB	2.12	127.22	124.05
26	T	318	IWJ	C36-C35-C34	-2.12	105.25	108.97
25	B	807	CLA	CHD-C1D-ND	-2.12	121.83	124.80
25	B	827	CLA	CMC-C2C-C1C	2.11	128.34	125.03
25	R	313	CLA	CHD-C1D-ND	-2.11	121.83	124.80
26	X	318	IWJ	C22-C23-C24	2.11	132.61	126.64
25	F	802	CLA	CHD-C1D-C2D	2.11	129.88	125.49
29	W	316	Q6L	C26-C25-C24	-2.11	117.08	123.20
25	K	206	CLA	C14-C13-C15	-2.11	103.74	111.27
24	S	305	CHL	O2D-CGD-CBD	2.11	113.27	110.95
25	A	807	CLA	C1-C2-C3	2.11	129.66	126.20
25	B	832	CLA	CHC-C4B-NB	2.11	127.22	124.05
25	4	315	CLA	CHB-C4A-NA	2.11	127.45	124.40
30	A	849	BCR	C12-C13-C14	-2.11	115.69	119.01
25	F	803	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
37	T	317	NEX	C36-C21-C22	-2.11	105.26	108.97
25	A	808	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
29	V	319	Q6L	C14-C15-C16	-2.11	117.08	123.20
25	B	834	CLA	CHD-C1D-C2D	2.11	129.87	125.49
25	W	303	CLA	CHB-C4A-NA	2.11	127.44	124.40
25	A	833	CLA	CHD-C1D-ND	-2.11	121.83	124.80
25	6	603	CLA	C4B-C3B-C2B	-2.11	104.68	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	801	LMG	C3-C4-C5	2.11	114.06	110.23
24	V	314	CHL	C3C-C4C-NC	-2.11	109.50	114.65
25	S	302	CLA	C3A-C2A-C1A	2.11	104.50	101.34
25	1	602	CLA	C1D-ND-C4D	-2.11	104.83	106.31
25	4	315	CLA	CAA-C2A-C3A	-2.11	111.40	116.23
25	W	313	CLA	CHB-C4A-NA	2.11	127.44	124.40
25	X	312	CLA	C2A-C1A-CHA	2.11	127.52	123.87
24	4	302	CHL	O2A-CGA-O1A	-2.11	118.36	123.63
24	Q	309	CHL	C4C-CHD-C1D	2.11	123.61	116.07
29	W	315	Q6L	C19-C20-C21	-2.11	119.21	123.52
30	3	318	BCR	C11-C10-C9	-2.11	124.32	127.28
26	R	303	IWJ	C36-C35-C34	-2.11	105.27	108.97
25	S	311	CLA	C2A-C3A-C4A	2.11	105.27	101.87
29	Q	318	Q6L	C10-C04-C03	2.10	113.06	109.78
25	2	604	CLA	CMC-C2C-C1C	2.10	128.32	125.03
25	V	311	CLA	CHA-C1A-NA	-2.10	121.63	126.39
25	6	603	CLA	C2A-C1A-CHA	2.10	127.52	123.87
26	Q	320	IWJ	C21-C19-C18	-2.10	115.70	119.01
25	B	803	CLA	CMD-C2D-C3D	2.10	132.51	127.69
24	U	306	CHL	OMC-CMC-C2C	-2.10	121.47	125.12
25	A	826	CLA	C1-O2A-CGA	-2.10	111.56	116.65
25	A	838	CLA	O1A-CGA-CBA	2.10	132.01	123.78
25	H	301	CLA	C2A-C1A-CHA	2.10	127.52	123.87
29	P	315	Q6L	C01-C02-C07	-2.10	110.56	114.42
25	B	842	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
24	P	306	CHL	CAA-C2A-C3A	2.10	118.68	113.00
25	U	303	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
25	B	810	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
30	B	845	BCR	C23-C22-C21	-2.10	115.71	119.01
25	L	304	CLA	O1D-CGD-CBD	2.10	128.66	124.52
24	T	320	CHL	CAA-CBA-CGA	-2.10	107.25	113.21
25	B	833	CLA	C1C-C2C-C3C	-2.10	104.77	106.98
30	A	850	BCR	C38-C26-C27	2.10	118.07	113.60
25	X	310	CLA	C3B-C4B-NB	-2.10	108.66	110.53
27	4	318	XAT	O23-C23-C24	-2.10	105.45	109.75
29	2	616	Q6L	C19-C20-C21	-2.10	119.22	123.52
26	T	321	IWJ	C36-C35-C34	-2.10	105.28	108.97
24	T	305	CHL	C3C-C4C-NC	-2.10	109.52	114.65
29	X	301	Q6L	C15-C14-C13	-2.10	124.74	127.69
25	6	603	CLA	C2D-C1D-ND	-2.10	108.05	110.13
33	A	802	CL0	CMB-C2B-C3B	2.10	128.87	124.68
25	R	315	CLA	C5-C3-C2	2.10	125.88	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	816	CLA	CHD-C1D-C2D	2.10	129.85	125.49
27	2	617	XAT	C15-C35-C34	-2.10	119.23	123.52
25	G	204	CLA	CHD-C1D-ND	-2.10	121.85	124.80
25	A	829	CLA	C2C-C1C-NC	2.10	112.18	109.98
25	A	803	CLA	C4-C3-C5	2.10	118.87	115.23
25	2	612	CLA	CMC-C2C-C1C	2.10	128.31	125.03
30	J	103	BCR	C12-C13-C14	-2.10	115.71	119.01
26	1	611	IWJ	C36-C35-C34	-2.10	105.29	108.97
25	4	316	CLA	CGD-CBD-CAD	2.09	117.63	110.85
34	A	844	PQN	C19-C18-C17	-2.09	103.81	111.27
29	W	316	Q6L	C41-C17-C16	-2.09	114.89	118.09
25	5	607	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	4	315	CLA	C3B-C4B-NB	-2.09	108.66	110.53
29	R	320	Q6L	C11-C03-C04	-2.09	115.59	116.81
30	A	852	BCR	C32-C1-C6	2.09	113.53	110.24
25	A	822	CLA	CHA-C1A-NA	-2.09	121.65	126.39
25	A	803	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	4	308	CHL	OMC-CMC-C2C	-2.09	121.49	125.12
29	Q	319	Q6L	C38-C36-C35	-2.09	105.50	109.41
25	K	201	CLA	O1A-CGA-CBA	2.09	129.73	123.09
25	A	828	CLA	C2D-C1D-ND	-2.09	108.06	110.13
25	3	301	CLA	O1D-CGD-CBD	2.09	128.64	124.52
25	5	601	CLA	CHA-C1A-NA	-2.09	121.65	126.39
25	V	313	CLA	CHD-C1D-ND	-2.09	121.86	124.80
25	U	312	CLA	CAA-C2A-C3A	-2.09	111.43	116.23
25	A	829	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
25	3	302	CLA	CHA-C4D-ND	2.09	136.86	132.55
25	A	831	CLA	O1D-CGD-CBD	2.09	128.64	124.52
25	U	310	CLA	C3B-C4B-NB	-2.09	108.66	110.53
25	2	609	CLA	CBA-CAA-C2A	2.09	120.01	113.79
29	P	315	Q6L	C19-C20-C21	-2.09	119.24	123.52
25	4	316	CLA	CHC-C4B-NB	2.09	127.18	124.05
25	B	802	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
29	U	315	Q6L	C41-C17-C16	-2.09	114.90	118.09
25	B	832	CLA	C1D-ND-C4D	2.09	107.78	106.31
38	P	308	KC2	CAC-C3C-C4C	2.09	133.62	124.39
25	B	829	CLA	CHA-C4D-ND	2.09	136.86	132.55
24	T	305	CHL	O1D-CGD-CBD	2.09	127.89	124.72
25	U	301	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	Q	306	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	J	104	LMG	O7-C10-C11	2.09	116.00	111.48
25	5	601	CLA	C3B-C2B-C1B	-2.09	104.71	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	603	CLA	CHC-C4B-NB	2.09	127.18	124.05
30	K	202	BCR	C11-C12-C13	-2.09	120.64	126.36
25	A	842	CLA	C3D-C4D-ND	2.09	113.38	109.99
29	V	319	Q6L	C23-C22-C21	2.09	126.20	122.82
25	V	310	CLA	C2C-C1C-NC	2.09	112.17	109.98
24	2	605	CHL	C3D-C4D-CHA	2.09	111.71	108.54
25	X	304	CLA	O2D-CGD-CBD	2.09	114.88	111.23
25	2	608	CLA	C2A-C1A-CHA	2.08	127.48	123.87
25	A	810	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
24	P	304	CHL	OMC-CMC-C2C	-2.08	121.50	125.12
24	4	302	CHL	O2D-CGD-CBD	2.08	113.23	110.95
30	A	849	BCR	C38-C26-C27	2.08	118.04	113.60
25	N	203	CLA	C4A-NA-C1A	2.08	107.63	106.68
30	H	305	BCR	C7-C8-C9	-2.08	123.16	126.23
25	6	611	CLA	CMB-C2B-C3B	2.08	131.45	126.55
24	R	318	CHL	C3C-C4C-NC	-2.08	109.56	114.65
25	B	813	CLA	CHD-C1D-C2D	2.08	129.82	125.49
25	X	302	CLA	CMC-C2C-C1C	2.08	128.29	125.03
26	S	319	IWJ	C36-C35-C34	-2.08	105.31	108.97
27	4	318	XAT	C4-C3-C2	-2.08	106.90	110.79
38	R	312	KC2	CHB-C4A-NA	2.08	127.46	124.23
25	U	308	CLA	CBC-CAC-C3C	2.08	118.06	112.42
36	B	850	DGD	O4D-C4D-C3D	2.08	115.28	110.38
25	R	315	CLA	CAC-C3C-C4C	2.08	127.50	124.79
37	S	317	NEX	C36-C21-C22	-2.08	105.31	108.97
25	R	315	CLA	CBA-CAA-C2A	2.08	119.98	113.79
30	K	202	BCR	C21-C20-C19	2.08	129.23	123.20
25	B	842	CLA	CHD-C1D-C2D	2.08	129.81	125.49
25	4	312	CLA	CMB-C2B-C3B	2.08	131.44	126.55
25	3	312	CLA	CMC-C2C-C1C	2.08	128.28	125.03
25	P	311	CLA	CMC-C2C-C1C	2.08	128.28	125.03
25	P	310	CLA	CHA-C1A-NA	-2.08	121.68	126.39
25	B	803	CLA	CMD-C2D-C1D	-2.08	121.07	124.73
25	A	815	CLA	CHD-C1D-ND	-2.08	121.88	124.80
27	2	617	XAT	C37-C21-C36	-2.08	104.35	107.37
25	1	603	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	B	830	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
25	B	805	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
25	B	815	CLA	C1-O2A-CGA	-2.08	111.62	116.65
26	6	614	IWJ	C17-C16-C15	-2.08	119.27	123.52
26	P	318	IWJ	C33-C32-C30	2.08	115.39	112.06
25	2	614	CLA	C4D-C3D-CAD	-2.08	105.85	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	322	IWJ	C36-C35-C34	-2.08	105.32	108.97
36	B	850	DGD	C2G-O2G-C1B	-2.08	112.83	117.80
25	S	302	CLA	C3B-C4B-NB	-2.08	108.68	110.53
25	P	312	CLA	CBA-CAA-C2A	2.08	119.97	113.79
37	R	321	NEX	C15-C14-C13	-2.08	124.37	127.28
29	R	323	Q6L	C14-C15-C16	-2.08	117.19	123.20
25	B	809	CLA	C1C-C2C-C3C	-2.08	104.80	106.98
25	6	603	CLA	CHA-C4D-ND	2.08	136.83	132.55
24	Q	316	CHL	CMD-C2D-C3D	2.07	128.83	124.68
25	B	807	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
25	B	825	CLA	CHD-C1D-ND	-2.07	121.89	124.80
29	O	2007	Q6L	C42-C13-C12	2.07	118.83	115.23
25	A	831	CLA	C1D-ND-C4D	2.07	107.77	106.31
30	B	846	BCR	C29-C30-C25	2.07	113.45	110.44
25	4	305	CLA	CHB-C4A-NA	2.07	127.39	124.40
25	G	202	CLA	CHD-C1D-ND	-2.07	121.89	124.80
25	A	826	CLA	O2D-CGD-CBD	2.07	114.85	111.23
25	B	841	CLA	C3A-C2A-C1A	2.07	104.44	101.34
29	P	319	Q6L	C01-C02-C07	-2.07	110.61	114.42
25	A	819	CLA	C2B-C1B-NB	2.07	112.47	110.33
25	B	808	CLA	C2B-C1B-NB	2.07	112.47	110.33
25	Q	301	CLA	C7-C6-C5	2.07	118.78	113.26
26	U	316	IWJ	C05-C04-C03	2.07	114.26	111.18
29	S	321	Q6L	C01-C02-C07	-2.07	110.62	114.42
24	S	305	CHL	CAA-C2A-C3A	-2.07	111.48	116.23
25	5	608	CLA	CHD-C1D-ND	-2.07	121.89	124.80
27	1	612	XAT	C26-C27-C28	-2.07	121.62	125.99
24	X	305	CHL	O1D-CGD-CBD	2.07	127.86	124.72
25	B	821	CLA	C1-C2-C3	-2.07	122.81	126.20
25	2	602	CLA	CAC-C3C-C4C	2.07	127.48	124.79
25	4	310	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
25	A	823	CLA	O1D-CGD-CBD	2.07	128.59	124.52
25	Q	311	CLA	CHD-C1D-ND	-2.07	121.89	124.80
24	R	302	CHL	CMD-C2D-C3D	2.07	128.81	124.68
25	K	201	CLA	CAA-C2A-C3A	-2.07	107.42	113.00
25	X	311	CLA	CHB-C4A-NA	2.07	127.38	124.40
25	S	312	CLA	C4-C3-C5	2.06	118.81	115.23
29	Q	318	Q6L	C23-C22-C24	-2.06	114.94	118.09
37	S	317	NEX	C11-C12-C13	-2.06	120.70	126.36
29	T	319	Q6L	C19-C20-C21	-2.06	119.30	123.52
25	K	204	CLA	CHA-C4D-ND	2.06	136.81	132.55
29	P	321	Q6L	C19-C20-C21	-2.06	119.30	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	802	CLA	C11-C10-C8	-2.06	109.11	115.97
33	A	802	CL0	C3C-C4C-NC	-2.06	109.61	114.65
38	X	309	KC2	O2A-CGA-O1A	-2.06	118.50	122.70
25	G	204	CLA	O1A-CGA-CBA	2.06	129.63	123.09
25	6	610	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
25	2	612	CLA	CHD-C1D-ND	-2.06	121.90	124.80
27	2	617	XAT	C8-C9-C10	-2.06	115.77	119.01
25	1	610	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	K	206	CLA	CAA-C2A-C3A	2.06	118.56	113.00
30	B	846	BCR	C11-C10-C9	-2.06	124.39	127.28
25	X	311	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
30	B	845	BCR	C12-C13-C14	-2.06	115.77	119.01
25	Q	306	CLA	CHB-C1B-NB	2.06	127.14	124.05
29	S	316	Q6L	C26-C25-C24	-2.06	117.23	123.20
24	W	307	CHL	O1D-CGD-CBD	2.06	127.84	124.72
24	V	314	CHL	C1B-CHB-C4A	2.06	122.65	121.32
25	5	602	CLA	CBA-CAA-C2A	2.06	119.92	113.79
25	5	606	CLA	CAA-C2A-C3A	-2.06	111.51	116.23
30	L	306	BCR	C16-C15-C14	-2.06	119.31	123.52
25	T	302	CLA	C3B-C4B-NB	-2.06	108.69	110.53
24	1	604	CHL	C3C-C4C-NC	-2.06	109.62	114.65
25	B	808	CLA	CAC-C3C-C2C	-2.06	123.78	127.56
24	V	306	CHL	CMD-C2D-C3D	2.06	128.79	124.68
25	A	838	CLA	CHB-C1B-NB	2.06	127.13	124.05
25	H	304	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
37	H	306	NEX	C40-C33-C32	2.06	121.23	118.09
25	A	831	CLA	CHA-C1A-NA	-2.06	121.73	126.39
27	2	617	XAT	O23-C23-C24	2.06	113.95	109.75
25	2	612	CLA	O2D-CGD-O1D	-2.06	119.85	123.85
30	4	319	BCR	C20-C19-C18	-2.06	120.73	126.36
25	A	828	CLA	CHD-C1D-ND	-2.06	121.91	124.80
24	4	302	CHL	CMB-C2B-C3B	2.06	128.79	124.68
25	X	312	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
30	B	848	BCR	C24-C23-C22	-2.05	123.19	126.23
30	B	849	BCR	C15-C16-C17	-2.05	119.31	123.52
25	2	606	CLA	CMB-C2B-C3B	2.05	131.38	126.55
25	U	311	CLA	O2D-CGD-CBD	2.05	114.82	111.23
30	J	103	BCR	C16-C15-C14	-2.05	119.32	123.52
25	O	2002	CLA	CHD-C1D-C2D	2.05	129.76	125.49
29	X	319	Q6L	C14-C15-C16	-2.05	117.25	123.20
25	6	609	CLA	C2A-C1A-CHA	2.05	127.43	123.87
30	4	319	BCR	C15-C16-C17	-2.05	119.32	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	617	XAT	C19-C9-C8	2.05	121.22	118.09
25	6	612	CLA	CHC-C4B-NB	2.05	127.13	124.05
25	A	820	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
27	4	318	XAT	C10-C11-C12	-2.05	117.25	123.20
24	P	305	CHL	O1A-CGA-CBA	2.05	129.60	123.09
25	A	820	CLA	CHA-C4D-ND	2.05	136.78	132.55
29	R	301	Q6L	C19-C20-C21	-2.05	119.32	123.52
24	T	305	CHL	CHA-C1A-C2A	-2.05	128.49	133.31
25	H	304	CLA	O2D-CGD-CBD	2.05	114.82	111.23
25	B	841	CLA	C5-C3-C2	2.05	125.77	121.17
29	S	320	Q6L	C16-C17-C18	-2.05	115.78	119.01
29	S	321	Q6L	C38-C36-C35	-2.05	105.58	109.41
25	H	302	CLA	C1C-C2C-C3C	-2.05	104.82	106.98
25	2	610	CLA	O2D-CGD-CBD	2.05	114.81	111.23
25	A	845	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	A	804	CLA	C2D-C1D-ND	-2.05	108.10	110.13
29	Q	317	Q6L	C14-C15-C16	-2.05	117.26	123.20
30	L	307	BCR	C37-C22-C21	-2.05	119.50	122.82
30	B	848	BCR	C29-C28-C27	-2.05	106.77	111.28
25	B	820	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
25	V	302	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
29	W	316	Q6L	C31-C30-C29	-2.05	121.39	124.58
29	Q	319	Q6L	C16-C17-C18	-2.05	115.79	119.01
25	2	604	CLA	C3B-C4B-NB	-2.05	108.70	110.53
25	A	839	CLA	O2D-CGD-CBD	2.05	114.81	111.23
38	S	308	KC2	CAC-C3C-C4C	2.05	133.44	124.39
25	X	313	CLA	CMB-C2B-C3B	2.05	131.37	126.55
29	S	323	Q6L	C35-C34-C33	2.05	114.22	111.18
38	P	308	KC2	C4C-C3C-C2C	-2.05	105.40	107.28
24	T	306	CHL	CAA-C2A-C3A	-2.05	107.47	113.00
25	T	311	CLA	CHA-C1A-NA	-2.05	121.76	126.39
25	B	819	CLA	CHD-C1D-ND	-2.05	121.92	124.80
25	B	823	CLA	CHD-C1D-ND	-2.05	121.92	124.80
24	W	304	CHL	O1D-CGD-CBD	2.05	127.83	124.72
24	S	307	CHL	C4D-CHA-CBD	-2.05	106.90	108.97
29	W	316	Q6L	C01-C02-C07	-2.05	110.66	114.42
29	R	323	Q6L	C19-C20-C21	-2.05	119.33	123.52
25	3	304	CLA	CHD-C1D-C2D	2.04	129.74	125.49
25	X	312	CLA	C4-C3-C2	-2.04	118.38	123.63
30	3	319	BCR	C12-C13-C14	-2.04	115.79	119.01
25	4	303	CLA	C2A-C1A-CHA	2.04	127.41	123.87
28	2	619	LHG	O7-C7-O9	-2.04	118.93	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	X	309	KC2	CMD-C2D-C3D	2.04	132.11	125.67
26	4	317	IWJ	C17-C16-C15	-2.04	119.34	123.52
29	Q	319	Q6L	C42-C13-C12	2.04	118.77	115.23
30	L	306	BCR	C12-C13-C14	-2.04	115.80	119.01
25	2	602	CLA	C1C-C2C-C3C	-2.04	104.83	106.98
25	A	804	CLA	CHB-C4A-NA	2.04	127.35	124.40
25	A	823	CLA	C3B-C4B-NB	-2.04	108.71	110.53
25	B	814	CLA	CAC-C3C-C4C	2.04	127.45	124.79
26	5	611	IWJ	C37-C35-C36	2.04	110.34	107.37
25	A	829	CLA	CHA-C1A-NA	-2.04	121.77	126.39
25	A	827	CLA	CHA-C4D-ND	2.04	136.76	132.55
25	1	608	CLA	CMC-C2C-C1C	2.04	128.22	125.03
29	R	320	Q6L	C26-C25-C24	-2.04	117.29	123.20
29	R	304	Q6L	C01-C02-C07	-2.04	110.67	114.42
29	X	316	Q6L	C40-C32-C33	-2.04	115.51	122.37
24	Q	307	CHL	O2A-CGA-O1A	-2.04	118.08	123.33
25	6	612	CLA	CHB-C4A-NA	2.04	127.34	124.40
25	O	2003	CLA	CAA-C2A-C3A	-2.04	111.55	116.23
27	6	615	XAT	C37-C21-C22	2.04	112.55	108.97
30	B	845	BCR	C38-C26-C27	2.04	117.94	113.60
25	P	312	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
30	4	319	BCR	C12-C13-C14	-2.04	115.80	119.01
25	A	838	CLA	CAA-C2A-C3A	2.04	118.51	113.00
37	H	306	NEX	C35-C15-C14	-2.04	119.35	123.52
25	R	316	CLA	C1-O2A-CGA	-2.04	111.71	116.65
38	W	308	KC2	C1B-CHB-C4A	2.04	130.35	126.02
25	3	309	CLA	CAC-C3C-C4C	2.04	127.44	124.79
29	S	315	Q6L	C19-C20-C21	-2.04	119.35	123.52
24	4	302	CHL	C4C-CHD-C1D	2.04	123.36	116.07
25	V	312	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
25	A	813	CLA	C6-C5-C3	-2.04	108.50	113.47
25	2	613	CLA	CHD-C1D-C2D	2.04	129.72	125.49
30	3	318	BCR	C20-C19-C18	-2.04	120.78	126.36
24	X	308	CHL	C4D-ND-C1D	2.04	106.77	105.22
30	3	319	BCR	C10-C11-C12	2.04	129.10	123.20
25	3	313	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
38	P	308	KC2	O1D-CGD-CBD	2.04	128.53	124.52
25	4	312	CLA	CBA-CAA-C2A	-2.04	109.09	113.41
30	K	202	BCR	C4-C5-C6	-2.04	119.95	122.70
25	W	303	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
30	A	850	BCR	C8-C9-C10	-2.04	115.81	119.01
30	B	845	BCR	C28-C27-C26	-2.04	110.43	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	849	BCR	C28-C27-C26	-2.04	110.43	114.06
24	P	305	CHL	C1A-CHA-C4D	2.04	122.38	118.98
34	B	844	PQN	C10-C5-C4	-2.04	118.53	120.71
38	T	308	KC2	CAC-C3C-C4C	2.03	133.38	124.39
24	R	302	CHL	C4C-CHD-C1D	2.03	123.35	116.07
25	W	303	CLA	CHD-C1D-ND	-2.03	121.94	124.80
25	P	311	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
25	B	820	CLA	C2D-C1D-ND	-2.03	108.11	110.13
25	B	805	CLA	C6-C5-C3	2.03	118.42	113.47
25	3	310	CLA	CHA-C1A-NA	-2.03	121.79	126.39
25	S	301	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
25	1	607	CLA	CMC-C2C-C1C	2.03	128.21	125.03
25	3	310	CLA	CMB-C2B-C3B	2.03	131.33	126.55
25	X	311	CLA	CBC-CAC-C3C	2.03	117.93	112.42
25	A	814	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
25	B	820	CLA	CHD-C1D-C2D	2.03	129.72	125.49
25	2	614	CLA	CMB-C2B-C3B	2.03	131.33	126.55
25	F	803	CLA	CHD-C1D-ND	-2.03	121.94	124.80
25	N	203	CLA	CHA-C1A-NA	-2.03	121.79	126.39
24	P	304	CHL	O1A-CGA-CBA	2.03	129.54	123.09
25	Q	315	CLA	CMB-C2B-C3B	2.03	131.33	126.55
30	F	801	BCR	C21-C20-C19	2.03	129.08	123.20
25	6	602	CLA	CHA-C1A-NA	-2.03	121.79	126.39
30	B	847	BCR	C16-C17-C18	-2.03	124.43	127.28
25	5	604	CLA	CHD-C1D-ND	-2.03	121.95	124.80
29	X	301	Q6L	C24-C22-C21	-2.03	115.82	119.01
25	X	314	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	A	803	CLA	C4D-C3D-CAD	-2.03	105.90	108.11
29	2	616	Q6L	C26-C25-C24	-2.03	117.32	123.20
25	X	302	CLA	C4-C3-C2	-2.03	118.42	123.63
25	P	302	CLA	CHD-C1D-ND	-2.03	121.95	124.80
25	R	306	CLA	CHD-C1D-ND	-2.03	121.95	124.80
24	P	306	CHL	C1C-C2C-CMC	2.03	130.46	126.80
24	T	304	CHL	C4D-CHA-CBD	-2.03	106.92	108.97
25	3	314	CLA	CHB-C4A-NA	2.03	127.33	124.40
25	G	204	CLA	C2B-C1B-NB	-2.03	108.22	110.33
25	R	313	CLA	CAA-C2A-C3A	2.03	118.48	113.00
24	P	307	CHL	CMD-C2D-C3D	2.03	128.73	124.68
26	P	320	IWJ	C36-C35-C34	-2.03	105.41	108.97
24	W	307	CHL	C3C-C4C-NC	-2.03	109.70	114.65
25	S	302	CLA	C1-O2A-CGA	2.03	121.56	116.65
25	N	202	CLA	C3B-C4B-NB	-2.03	108.72	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	601	CHL	C4C-CHD-C1D	2.03	123.32	116.07
25	A	834	CLA	C3A-C2A-C1A	2.03	104.37	101.34
30	L	307	BCR	C1-C6-C5	2.03	125.40	122.64
25	P	301	CLA	C1D-ND-C4D	-2.03	104.89	106.31
25	B	843	CLA	O2D-CGD-O1D	-2.03	119.91	123.85
25	S	312	CLA	C1-C2-C3	-2.03	122.88	126.20
25	T	302	CLA	CHB-C4A-NA	2.02	127.32	124.40
25	B	825	CLA	CHA-C1A-NA	-2.02	121.81	126.39
25	U	301	CLA	C4D-CHA-C1A	2.02	123.66	121.24
25	V	312	CLA	CBA-CAA-C2A	2.02	119.82	113.79
25	X	310	CLA	CMB-C2B-C3B	2.02	131.31	126.55
29	T	315	Q6L	C42-C13-C12	2.02	118.74	115.23
24	2	605	CHL	C4C-CHD-C1D	2.02	123.31	116.07
25	Q	312	CLA	O2D-CGD-CBD	2.02	114.77	111.23
25	R	313	CLA	CMC-C2C-C1C	2.02	128.20	125.03
24	T	320	CHL	C4C-CHD-C1D	2.02	123.31	116.07
25	A	825	CLA	C3C-C4C-NC	-2.02	107.84	110.43
25	V	312	CLA	C1-C2-C3	-2.02	122.88	126.20
25	S	312	CLA	CBA-CAA-C2A	2.02	119.81	113.79
30	2	618	BCR	C34-C9-C10	2.02	126.09	122.82
29	S	320	Q6L	C14-C15-C16	-2.02	117.34	123.20
25	2	604	CLA	CHD-C1D-ND	-2.02	121.96	124.80
25	B	812	CLA	C3A-C2A-C1A	2.02	104.37	101.34
25	W	302	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
25	6	611	CLA	C1C-C2C-C3C	-2.02	104.86	106.98
30	H	305	BCR	C15-C16-C17	-2.02	119.39	123.52
25	3	308	CLA	CHA-C4D-ND	2.02	136.72	132.55
37	T	317	NEX	C11-C12-C13	-2.02	120.82	126.36
25	A	821	CLA	CHA-C1A-NA	-2.02	121.82	126.39
25	A	815	CLA	C4B-C3B-C2B	-2.02	104.79	107.30
37	P	317	NEX	C36-C21-C22	-2.02	105.42	108.97
24	R	308	CHL	OMC-CMC-C2C	-2.02	121.61	125.12
25	A	816	CLA	CHB-C4A-NA	2.02	127.31	124.40
25	B	842	CLA	CHD-C1D-ND	-2.02	121.96	124.80
24	T	306	CHL	O2D-CGD-CBD	2.02	113.16	110.95
29	Q	319	Q6L	C35-C34-C33	2.02	114.18	111.18
29	Q	319	Q6L	C20-C19-C18	-2.02	119.39	123.52
25	R	317	CLA	CAC-C3C-C4C	2.02	127.42	124.79
25	1	606	CLA	CMC-C2C-C1C	2.02	128.19	125.03
25	W	313	CLA	O1D-CGD-CBD	2.02	128.50	124.52
29	X	316	Q6L	C26-C25-C24	-2.02	117.36	123.20
25	B	803	CLA	C5-C3-C2	2.02	125.69	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X	318	IWJ	C36-C35-C34	-2.02	105.42	108.97
30	B	849	BCR	C16-C15-C14	-2.02	119.39	123.52
25	4	305	CLA	CMB-C2B-C3B	2.02	128.89	123.53
25	4	303	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
24	Q	316	CHL	C3C-C4C-NC	-2.02	109.72	114.65
25	Q	313	CLA	CMC-C2C-C1C	2.02	128.18	125.03
25	6	604	CLA	CHD-C1D-ND	-2.02	121.97	124.80
30	B	848	BCR	C35-C13-C12	2.02	121.17	118.09
24	2	605	CHL	OMC-CMC-C2C	-2.02	121.62	125.12
30	I	101	BCR	C36-C18-C17	-2.02	119.55	122.82
25	B	803	CLA	CHB-C4A-NA	2.02	127.31	124.40
30	A	849	BCR	C1-C6-C7	2.02	121.12	115.65
25	2	609	CLA	C2A-C1A-CHA	2.02	127.36	123.87
26	Q	320	IWJ	C36-C35-C34	-2.01	105.43	108.97
29	Q	317	Q6L	C16-C17-C18	-2.01	115.84	119.01
25	4	304	CLA	CHD-C4C-NC	2.01	127.36	124.23
24	4	308	CHL	C4D-CHA-CBD	-2.01	106.94	108.97
25	4	303	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
34	A	844	PQN	C10-C1-C2	2.01	121.77	118.97
29	R	304	Q6L	C19-C20-C21	-2.01	119.40	123.52
25	4	305	CLA	CHD-C1D-ND	-2.01	121.97	124.80
25	A	827	CLA	C1-O2A-CGA	2.01	121.52	116.65
25	B	809	CLA	CMC-C2C-C1C	2.01	128.18	125.03
25	4	316	CLA	CHB-C4A-NA	2.01	127.31	124.40
24	2	607	CHL	O2D-CGD-O1D	-2.01	119.93	123.85
25	A	814	CLA	CHA-C1A-NA	-2.01	121.83	126.39
25	V	301	CLA	O2D-CGD-CBD	2.01	114.75	111.23
25	2	612	CLA	C11-C10-C8	2.01	122.65	115.97
27	6	615	XAT	C10-C11-C12	-2.01	117.37	123.20
24	R	308	CHL	O2D-CGD-O1D	-2.01	119.93	123.85
25	2	613	CLA	C3D-C4D-ND	2.01	113.26	109.99
25	3	314	CLA	CMC-C2C-C1C	2.01	128.18	125.03
25	G	202	CLA	CAC-C3C-C4C	2.01	127.41	124.79
24	W	306	CHL	C1-O2A-CGA	2.01	121.52	116.65
24	S	314	CHL	C4D-ND-C1D	2.01	106.75	105.22
26	R	303	IWJ	C25-C24-C26	2.01	119.26	116.00
25	B	808	CLA	C4A-NA-C1A	2.01	107.60	106.68
25	A	815	CLA	CMA-C3A-C2A	-2.01	106.21	113.98
24	R	309	CHL	C1C-C2C-CMC	2.01	130.42	126.80
25	Q	311	CLA	C3B-C4B-NB	-2.01	108.74	110.53
25	P	303	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
30	F	804	BCR	C15-C14-C13	-2.01	124.46	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	V	310	CLA	O2D-CGD-CBD	2.01	114.74	111.23
25	K	204	CLA	CHA-C1A-NA	-2.01	121.85	126.39
25	3	305	CLA	CMB-C2B-C3B	2.01	128.86	123.53
25	B	818	CLA	CHA-C4D-ND	2.01	136.69	132.55
25	V	310	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
25	5	607	CLA	C4-C3-C2	-2.01	118.48	123.63
25	B	819	CLA	C1-O2A-CGA	2.01	121.50	116.65
24	T	305	CHL	O2A-CGA-O1A	-2.00	118.61	123.63
25	P	301	CLA	C9-C8-C10	-2.00	104.13	111.27
25	S	303	CLA	C3B-C4B-NB	-2.00	108.74	110.53
24	1	604	CHL	CMD-C2D-C3D	2.00	128.69	124.68
25	4	304	CLA	C3A-C2A-C1A	2.00	104.34	101.34
25	A	807	CLA	CAC-C3C-C4C	2.00	127.40	124.79
25	B	834	CLA	C6-C5-C3	-2.00	108.59	113.47
26	R	303	IWJ	C23-C22-C21	-2.00	117.40	123.20
25	P	311	CLA	CMB-C2B-C3B	2.00	131.26	126.55
29	U	317	Q6L	C19-C20-C21	-2.00	119.42	123.52
30	M	101	BCR	C27-C26-C25	-2.00	120.00	122.70
25	1	603	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
25	K	201	CLA	CHA-C1A-NA	-2.00	121.86	126.39
25	P	311	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	R	308	CHL	C3C-C4C-NC	-2.00	109.76	114.65
25	4	310	CLA	CHD-C1D-ND	-2.00	121.99	124.80
26	Q	303	IWJ	C23-C22-C21	-2.00	117.40	123.20
25	L	301	CLA	CAC-C3C-C4C	2.00	127.39	124.79
25	B	825	CLA	O1D-CGD-CBD	2.00	128.46	124.52

All (413) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	601	CHL	ND
24	1	601	CHL	NC
24	1	601	CHL	NA
24	1	604	CHL	ND
24	1	604	CHL	NC
24	1	604	CHL	NA
24	2	601	CHL	ND
24	2	601	CHL	NC
24	2	601	CHL	NA
24	2	605	CHL	ND
24	2	605	CHL	NC
24	2	605	CHL	NA

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Mol	Chain	Res	Type	Atom
24	2	607	CHL	ND
24	2	607	CHL	NC
24	2	607	CHL	NA
24	2	615	CHL	ND
24	2	615	CHL	NC
24	2	615	CHL	NA
24	3	306	CHL	ND
24	3	306	CHL	NC
24	3	306	CHL	NA
24	4	302	CHL	ND
24	4	302	CHL	NC
24	4	302	CHL	NA
24	4	306	CHL	ND
24	4	306	CHL	NC
24	4	306	CHL	NA
24	4	307	CHL	ND
24	4	307	CHL	NC
24	4	307	CHL	NA
24	4	308	CHL	ND
24	4	308	CHL	NC
24	4	308	CHL	NA
24	5	605	CHL	ND
24	5	605	CHL	NC
24	5	605	CHL	NA
24	6	601	CHL	ND
24	6	601	CHL	NC
24	6	601	CHL	NA
24	6	605	CHL	ND
24	6	605	CHL	NC
24	6	605	CHL	NA
24	6	606	CHL	ND
24	6	606	CHL	NC
24	6	606	CHL	NA
24	P	304	CHL	ND
24	P	304	CHL	NC
24	P	304	CHL	NA
24	P	305	CHL	ND
24	P	305	CHL	NC
24	P	305	CHL	NA
24	P	306	CHL	ND
24	P	306	CHL	NC
24	P	306	CHL	NA

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Mol	Chain	Res	Type	Atom
24	P	307	CHL	ND
24	P	307	CHL	NC
24	P	307	CHL	NA
24	P	314	CHL	ND
24	P	314	CHL	NC
24	P	314	CHL	NA
24	Q	307	CHL	ND
24	Q	307	CHL	NC
24	Q	307	CHL	NA
24	Q	308	CHL	ND
24	Q	308	CHL	NC
24	Q	308	CHL	NA
24	Q	309	CHL	ND
24	Q	309	CHL	NC
24	Q	309	CHL	NA
24	Q	316	CHL	ND
24	Q	316	CHL	NC
24	Q	316	CHL	NA
24	R	302	CHL	ND
24	R	302	CHL	NC
24	R	302	CHL	NA
24	R	308	CHL	ND
24	R	308	CHL	NC
24	R	308	CHL	NA
24	R	309	CHL	ND
24	R	309	CHL	NC
24	R	309	CHL	NA
24	R	310	CHL	ND
24	R	310	CHL	NC
24	R	310	CHL	NA
24	R	311	CHL	ND
24	R	311	CHL	NC
24	R	311	CHL	NA
24	R	318	CHL	ND
24	R	318	CHL	NC
24	R	318	CHL	NA
24	S	304	CHL	ND
24	S	304	CHL	NC
24	S	304	CHL	NA
24	S	305	CHL	ND
24	S	305	CHL	NC
24	S	305	CHL	NA

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Mol	Chain	Res	Type	Atom
24	S	306	CHL	ND
24	S	306	CHL	NC
24	S	306	CHL	NA
24	S	307	CHL	ND
24	S	307	CHL	NC
24	S	307	CHL	NA
24	S	314	CHL	ND
24	S	314	CHL	NC
24	S	314	CHL	NA
24	T	304	CHL	ND
24	T	304	CHL	NC
24	T	304	CHL	NA
24	T	305	CHL	ND
24	T	305	CHL	NC
24	T	305	CHL	NA
24	T	306	CHL	ND
24	T	306	CHL	NC
24	T	306	CHL	NA
24	T	307	CHL	ND
24	T	307	CHL	NC
24	T	307	CHL	NA
24	T	314	CHL	ND
24	T	314	CHL	NC
24	T	314	CHL	NA
24	T	320	CHL	ND
24	T	320	CHL	NC
24	T	320	CHL	NA
24	U	304	CHL	ND
24	U	304	CHL	NC
24	U	304	CHL	NA
24	U	305	CHL	ND
24	U	305	CHL	NC
24	U	305	CHL	NA
24	U	306	CHL	ND
24	U	306	CHL	NC
24	U	306	CHL	NA
24	U	313	CHL	ND
24	U	313	CHL	NC
24	U	313	CHL	NA
24	V	304	CHL	ND
24	V	304	CHL	NC
24	V	304	CHL	NA

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Mol	Chain	Res	Type	Atom
24	V	305	CHL	ND
24	V	305	CHL	NC
24	V	305	CHL	NA
24	V	306	CHL	ND
24	V	306	CHL	NC
24	V	306	CHL	NA
24	V	307	CHL	ND
24	V	307	CHL	NC
24	V	307	CHL	NA
24	V	314	CHL	ND
24	V	314	CHL	NC
24	V	314	CHL	NA
24	W	304	CHL	ND
24	W	304	CHL	NC
24	W	304	CHL	NA
24	W	305	CHL	ND
24	W	305	CHL	NC
24	W	305	CHL	NA
24	W	306	CHL	ND
24	W	306	CHL	NC
24	W	306	CHL	NA
24	W	307	CHL	ND
24	W	307	CHL	NC
24	W	307	CHL	NA
24	W	314	CHL	ND
24	W	314	CHL	NC
24	W	314	CHL	NA
24	X	305	CHL	ND
24	X	305	CHL	NC
24	X	305	CHL	NA
24	X	306	CHL	ND
24	X	306	CHL	NC
24	X	306	CHL	NA
24	X	307	CHL	ND
24	X	307	CHL	NC
24	X	307	CHL	NA
24	X	308	CHL	ND
24	X	308	CHL	NC
24	X	308	CHL	NA
24	X	315	CHL	ND
24	X	315	CHL	NC
24	X	315	CHL	NA

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Mol	Chain	Res	Type	Atom
25	1	602	CLA	ND
25	1	603	CLA	ND
25	1	605	CLA	ND
25	1	606	CLA	ND
25	1	607	CLA	ND
25	1	608	CLA	ND
25	1	609	CLA	ND
25	1	613	CLA	ND
25	2	602	CLA	ND
25	2	603	CLA	ND
25	2	604	CLA	ND
25	2	606	CLA	ND
25	2	608	CLA	ND
25	2	609	CLA	ND
25	2	610	CLA	ND
25	2	611	CLA	ND
25	2	612	CLA	ND
25	2	613	CLA	ND
25	2	614	CLA	ND
25	3	301	CLA	ND
25	3	302	CLA	ND
25	3	303	CLA	ND
25	3	304	CLA	ND
25	3	305	CLA	ND
25	3	307	CLA	ND
25	3	308	CLA	ND
25	3	309	CLA	ND
25	3	310	CLA	ND
25	3	311	CLA	ND
25	3	312	CLA	ND
25	3	313	CLA	ND
25	4	303	CLA	ND
25	4	304	CLA	ND
25	4	305	CLA	ND
25	4	309	CLA	ND
25	4	310	CLA	ND
25	4	311	CLA	ND
25	4	312	CLA	ND
25	4	314	CLA	ND
25	4	315	CLA	ND
25	4	316	CLA	ND
25	5	601	CLA	ND

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Mol	Chain	Res	Type	Atom
25	5	602	CLA	ND
25	5	603	CLA	ND
25	5	604	CLA	ND
25	5	606	CLA	ND
25	5	607	CLA	ND
25	5	608	CLA	ND
25	5	609	CLA	ND
25	5	610	CLA	ND
25	6	602	CLA	ND
25	6	603	CLA	ND
25	6	604	CLA	ND
25	6	607	CLA	ND
25	6	608	CLA	ND
25	6	609	CLA	ND
25	6	610	CLA	ND
25	6	611	CLA	ND
25	6	612	CLA	ND
25	A	803	CLA	ND
25	A	804	CLA	ND
25	A	805	CLA	ND
25	A	806	CLA	ND
25	A	807	CLA	ND
25	A	808	CLA	ND
25	A	809	CLA	ND
25	A	810	CLA	ND
25	A	811	CLA	ND
25	A	812	CLA	ND
25	A	813	CLA	ND
25	A	814	CLA	ND
25	A	815	CLA	ND
25	A	816	CLA	ND
25	A	818	CLA	ND
25	A	819	CLA	ND
25	A	820	CLA	ND
25	A	821	CLA	ND
25	A	822	CLA	ND
25	A	823	CLA	ND
25	A	824	CLA	ND
25	A	825	CLA	ND
25	A	826	CLA	ND
25	A	827	CLA	ND
25	A	829	CLA	ND

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Mol	Chain	Res	Type	Atom
25	A	830	CLA	ND
25	A	831	CLA	ND
25	A	832	CLA	ND
25	A	834	CLA	ND
25	A	835	CLA	ND
25	A	836	CLA	ND
25	A	837	CLA	ND
25	A	839	CLA	ND
25	A	841	CLA	ND
25	A	842	CLA	ND
25	A	843	CLA	ND
25	A	845	CLA	ND
25	A	856	CLA	ND
25	B	802	CLA	ND
25	B	803	CLA	ND
25	B	804	CLA	ND
25	B	805	CLA	ND
25	B	806	CLA	ND
25	B	807	CLA	ND
25	B	808	CLA	ND
25	B	809	CLA	ND
25	B	810	CLA	ND
25	B	811	CLA	ND
25	B	812	CLA	ND
25	B	813	CLA	ND
25	B	814	CLA	ND
25	B	815	CLA	ND
25	B	816	CLA	ND
25	B	817	CLA	ND
25	B	818	CLA	ND
25	B	819	CLA	ND
25	B	820	CLA	ND
25	B	821	CLA	ND
25	B	822	CLA	ND
25	B	823	CLA	ND
25	B	824	CLA	ND
25	B	825	CLA	ND
25	B	826	CLA	ND
25	B	827	CLA	ND
25	B	828	CLA	ND
25	B	829	CLA	ND
25	B	830	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	831	CLA	ND
25	B	832	CLA	ND
25	B	833	CLA	ND
25	B	834	CLA	ND
25	B	835	CLA	ND
25	B	837	CLA	ND
25	B	838	CLA	ND
25	B	839	CLA	ND
25	B	841	CLA	ND
25	B	842	CLA	ND
25	B	843	CLA	ND
25	F	802	CLA	ND
25	F	803	CLA	ND
25	G	202	CLA	ND
25	G	203	CLA	ND
25	G	204	CLA	ND
25	H	301	CLA	ND
25	H	302	CLA	ND
25	H	304	CLA	ND
25	J	102	CLA	ND
25	K	201	CLA	ND
25	K	203	CLA	ND
25	K	204	CLA	ND
25	K	206	CLA	ND
25	L	301	CLA	ND
25	L	303	CLA	ND
25	L	304	CLA	ND
25	N	202	CLA	ND
25	N	203	CLA	ND
25	O	2001	CLA	ND
25	O	2002	CLA	ND
25	O	2003	CLA	ND
25	O	2004	CLA	ND
25	O	2005	CLA	ND
25	P	301	CLA	ND
25	P	302	CLA	ND
25	P	303	CLA	ND
25	P	309	CLA	ND
25	P	310	CLA	ND
25	P	311	CLA	ND
25	P	312	CLA	ND
25	Q	301	CLA	ND

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Mol	Chain	Res	Type	Atom
25	Q	304	CLA	ND
25	Q	305	CLA	ND
25	Q	306	CLA	ND
25	Q	311	CLA	ND
25	Q	312	CLA	ND
25	Q	313	CLA	ND
25	Q	314	CLA	ND
25	Q	315	CLA	ND
25	R	305	CLA	ND
25	R	306	CLA	ND
25	R	307	CLA	ND
25	R	313	CLA	ND
25	R	314	CLA	ND
25	R	315	CLA	ND
25	R	316	CLA	ND
25	S	301	CLA	ND
25	S	302	CLA	ND
25	S	303	CLA	ND
25	S	309	CLA	ND
25	S	310	CLA	ND
25	S	311	CLA	ND
25	S	312	CLA	ND
25	S	313	CLA	ND
25	T	301	CLA	ND
25	T	302	CLA	ND
25	T	303	CLA	ND
25	T	309	CLA	ND
25	T	310	CLA	ND
25	T	311	CLA	ND
25	T	312	CLA	ND
25	T	313	CLA	ND
25	U	301	CLA	ND
25	U	302	CLA	ND
25	U	303	CLA	ND
25	U	308	CLA	ND
25	U	309	CLA	ND
25	U	310	CLA	ND
25	U	311	CLA	ND
25	U	312	CLA	ND
25	V	301	CLA	ND
25	V	302	CLA	ND
25	V	303	CLA	ND

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Mol	Chain	Res	Type	Atom
25	V	309	CLA	ND
25	V	310	CLA	ND
25	V	311	CLA	ND
25	V	313	CLA	ND
25	W	301	CLA	ND
25	W	302	CLA	ND
25	W	303	CLA	ND
25	W	309	CLA	ND
25	W	310	CLA	ND
25	W	311	CLA	ND
25	W	312	CLA	ND
25	W	313	CLA	ND
25	X	302	CLA	ND
25	X	303	CLA	ND
25	X	304	CLA	ND
25	X	310	CLA	ND
25	X	311	CLA	ND
25	X	312	CLA	ND
25	X	313	CLA	ND
25	X	314	CLA	ND
33	A	802	CL0	ND
33	A	802	CL0	NC
33	A	802	CL0	NA

All (2891) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	2	601	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	CAD-CBD-CGD-O1D
24	2	605	CHL	CAD-CBD-CGD-O2D
24	2	605	CHL	CBD-CGD-O2D-CED
24	2	607	CHL	CAA-CBA-CGA-O1A
24	2	607	CHL	C1C-C2C-CMC-OMC
24	2	607	CHL	C3C-C2C-CMC-OMC
24	4	307	CHL	C1A-C2A-CAA-CBA
24	4	307	CHL	C1C-C2C-CMC-OMC
24	4	307	CHL	C3C-C2C-CMC-OMC
24	4	307	CHL	CBD-CGD-O2D-CED
24	6	606	CHL	C1A-C2A-CAA-CBA
24	6	606	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	6	606	CHL	CAD-CBD-CGD-O1D
24	6	606	CHL	CAD-CBD-CGD-O2D
24	6	606	CHL	CBD-CGD-O2D-CED
24	P	304	CHL	C3A-C2A-CAA-CBA
24	P	304	CHL	C1C-C2C-CMC-OMC
24	P	304	CHL	C3C-C2C-CMC-OMC
24	P	304	CHL	CBD-CGD-O2D-CED
24	P	305	CHL	C1A-C2A-CAA-CBA
24	P	307	CHL	C1A-C2A-CAA-CBA
24	P	314	CHL	C1A-C2A-CAA-CBA
24	Q	307	CHL	C1A-C2A-CAA-CBA
24	Q	316	CHL	CAA-CBA-CGA-O1A
24	R	302	CHL	CBA-CGA-O2A-C1
24	R	309	CHL	CBD-CGD-O2D-CED
24	R	310	CHL	C2-C3-C5-C6
24	R	310	CHL	C4-C3-C5-C6
24	R	311	CHL	CBD-CGD-O2D-CED
24	R	318	CHL	CBD-CGD-O2D-CED
24	S	304	CHL	C1C-C2C-CMC-OMC
24	S	304	CHL	C3C-C2C-CMC-OMC
24	S	306	CHL	CAD-CBD-CGD-O1D
24	S	306	CHL	CAD-CBD-CGD-O2D
24	S	307	CHL	CBD-CGD-O2D-CED
24	T	304	CHL	CBD-CGD-O2D-CED
24	U	304	CHL	CBD-CGD-O2D-CED
24	V	304	CHL	CBD-CGD-O2D-CED
24	V	305	CHL	C3C-C2C-CMC-OMC
24	V	305	CHL	CHA-CBD-CGD-O1D
24	V	305	CHL	CHA-CBD-CGD-O2D
24	V	307	CHL	C4C-C3C-CAC-CBC
24	V	314	CHL	C1A-C2A-CAA-CBA
24	W	307	CHL	C1A-C2A-CAA-CBA
24	W	314	CHL	C3C-C2C-CMC-OMC
24	X	307	CHL	C1A-C2A-CAA-CBA
24	X	307	CHL	C3A-C2A-CAA-CBA
24	X	307	CHL	CBA-CGA-O2A-C1
24	X	307	CHL	O1A-CGA-O2A-C1
24	X	307	CHL	C1C-C2C-CMC-OMC
24	X	307	CHL	C3C-C2C-CMC-OMC
24	X	308	CHL	CAD-CBD-CGD-O1D
24	X	308	CHL	CAD-CBD-CGD-O2D
24	X	308	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	X	315	CHL	CAA-CBA-CGA-O1A
24	X	315	CHL	CBD-CGD-O2D-CED
25	1	602	CLA	CAD-CBD-CGD-O1D
25	1	605	CLA	C1A-C2A-CAA-CBA
25	1	605	CLA	C3A-C2A-CAA-CBA
25	1	606	CLA	CBD-CGD-O2D-CED
25	1	608	CLA	C1A-C2A-CAA-CBA
25	1	608	CLA	C3A-C2A-CAA-CBA
25	1	608	CLA	CBD-CGD-O2D-CED
25	1	610	CLA	C1A-C2A-CAA-CBA
25	1	610	CLA	C3A-C2A-CAA-CBA
25	1	610	CLA	CBD-CGD-O2D-CED
25	2	602	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C3A-C2A-CAA-CBA
25	2	603	CLA	C1A-C2A-CAA-CBA
25	2	606	CLA	C1A-C2A-CAA-CBA
25	2	606	CLA	C3A-C2A-CAA-CBA
25	2	608	CLA	C1A-C2A-CAA-CBA
25	2	608	CLA	C3A-C2A-CAA-CBA
25	2	608	CLA	CBD-CGD-O2D-CED
25	2	610	CLA	CBD-CGD-O2D-CED
25	2	611	CLA	C1A-C2A-CAA-CBA
25	2	611	CLA	C3A-C2A-CAA-CBA
25	2	611	CLA	CHA-CBD-CGD-O2D
25	2	612	CLA	C2B-C3B-CAB-CBB
25	2	612	CLA	C4B-C3B-CAB-CBB
25	2	614	CLA	C1A-C2A-CAA-CBA
25	2	614	CLA	CHA-CBD-CGD-O2D
25	3	302	CLA	CBA-CGA-O2A-C1
25	3	304	CLA	C1A-C2A-CAA-CBA
25	3	304	CLA	C3A-C2A-CAA-CBA
25	3	307	CLA	C1A-C2A-CAA-CBA
25	3	307	CLA	C3A-C2A-CAA-CBA
25	3	310	CLA	CBD-CGD-O2D-CED
25	3	311	CLA	CBA-CGA-O2A-C1
25	3	311	CLA	O1A-CGA-O2A-C1
25	3	311	CLA	CAD-CBD-CGD-O2D
25	4	303	CLA	C3A-C2A-CAA-CBA
25	4	303	CLA	CBD-CGD-O2D-CED
25	4	304	CLA	CBD-CGD-O2D-CED
25	4	304	CLA	O1D-CGD-O2D-CED
25	4	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	4	311	CLA	C1A-C2A-CAA-CBA
25	4	311	CLA	C3A-C2A-CAA-CBA
25	4	311	CLA	CBD-CGD-O2D-CED
25	4	312	CLA	C1A-C2A-CAA-CBA
25	4	312	CLA	C3A-C2A-CAA-CBA
25	4	314	CLA	CAD-CBD-CGD-O2D
25	4	315	CLA	CBD-CGD-O2D-CED
25	4	316	CLA	C1A-C2A-CAA-CBA
25	4	316	CLA	C3A-C2A-CAA-CBA
25	5	601	CLA	C3A-C2A-CAA-CBA
25	5	601	CLA	CBA-CGA-O2A-C1
25	5	601	CLA	C2B-C3B-CAB-CBB
25	5	601	CLA	C4B-C3B-CAB-CBB
25	5	602	CLA	C1A-C2A-CAA-CBA
25	5	602	CLA	C3A-C2A-CAA-CBA
25	5	608	CLA	CHA-CBD-CGD-O1D
25	5	608	CLA	CHA-CBD-CGD-O2D
25	5	609	CLA	C1A-C2A-CAA-CBA
25	5	609	CLA	C3A-C2A-CAA-CBA
25	6	602	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C3A-C2A-CAA-CBA
25	6	602	CLA	CHA-CBD-CGD-O2D
25	6	607	CLA	C1A-C2A-CAA-CBA
25	6	608	CLA	C1A-C2A-CAA-CBA
25	6	608	CLA	C3A-C2A-CAA-CBA
25	6	608	CLA	CBD-CGD-O2D-CED
25	6	609	CLA	CHA-CBD-CGD-O1D
25	6	609	CLA	CHA-CBD-CGD-O2D
25	6	610	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	CAD-CBD-CGD-O2D
25	6	611	CLA	C1A-C2A-CAA-CBA
25	6	611	CLA	C3A-C2A-CAA-CBA
25	6	611	CLA	CHA-CBD-CGD-O1D
25	6	611	CLA	CHA-CBD-CGD-O2D
25	A	804	CLA	CBD-CGD-O2D-CED
25	A	806	CLA	C1A-C2A-CAA-CBA
25	A	810	CLA	CHA-CBD-CGD-O1D
25	A	810	CLA	CHA-CBD-CGD-O2D
25	A	813	CLA	CHA-CBD-CGD-O1D
25	A	813	CLA	CHA-CBD-CGD-O2D
25	A	814	CLA	C1A-C2A-CAA-CBA
25	A	814	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	A	817	CLA	C3A-C2A-CAA-CBA
25	A	819	CLA	CBD-CGD-O2D-CED
25	A	820	CLA	C3A-C2A-CAA-CBA
25	A	821	CLA	C3A-C2A-CAA-CBA
25	A	821	CLA	CAD-CBD-CGD-O1D
25	A	821	CLA	CAD-CBD-CGD-O2D
25	A	824	CLA	C1A-C2A-CAA-CBA
25	A	824	CLA	CBD-CGD-O2D-CED
25	A	825	CLA	C1A-C2A-CAA-CBA
25	A	826	CLA	C2B-C3B-CAB-CBB
25	A	826	CLA	C4B-C3B-CAB-CBB
25	A	830	CLA	C1A-C2A-CAA-CBA
25	A	830	CLA	C3A-C2A-CAA-CBA
25	A	832	CLA	CHA-CBD-CGD-O1D
25	A	832	CLA	CHA-CBD-CGD-O2D
25	A	835	CLA	C2B-C3B-CAB-CBB
25	A	835	CLA	C4B-C3B-CAB-CBB
25	A	835	CLA	CBD-CGD-O2D-CED
25	A	836	CLA	C4B-C3B-CAB-CBB
25	A	836	CLA	CBD-CGD-O2D-CED
25	A	839	CLA	CHA-CBD-CGD-O1D
25	A	839	CLA	CHA-CBD-CGD-O2D
25	A	840	CLA	C1A-C2A-CAA-CBA
25	A	842	CLA	C1A-C2A-CAA-CBA
25	A	842	CLA	C2B-C3B-CAB-CBB
25	A	842	CLA	C4B-C3B-CAB-CBB
25	A	843	CLA	C1A-C2A-CAA-CBA
25	A	843	CLA	C3A-C2A-CAA-CBA
25	A	856	CLA	CAD-CBD-CGD-O1D
25	A	856	CLA	CAD-CBD-CGD-O2D
25	B	803	CLA	CBD-CGD-O2D-CED
25	B	804	CLA	C2B-C3B-CAB-CBB
25	B	804	CLA	C4B-C3B-CAB-CBB
25	B	805	CLA	CBD-CGD-O2D-CED
25	B	807	CLA	C1A-C2A-CAA-CBA
25	B	807	CLA	C3A-C2A-CAA-CBA
25	B	809	CLA	C1A-C2A-CAA-CBA
25	B	809	CLA	C6-C7-C8-C9
25	B	810	CLA	C1A-C2A-CAA-CBA
25	B	810	CLA	CHA-CBD-CGD-O1D
25	B	810	CLA	CHA-CBD-CGD-O2D
25	B	812	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	814	CLA	CAD-CBD-CGD-O1D
25	B	814	CLA	CAD-CBD-CGD-O2D
25	B	816	CLA	C2-C3-C5-C6
25	B	817	CLA	CBD-CGD-O2D-CED
25	B	818	CLA	C1A-C2A-CAA-CBA
25	B	820	CLA	C3A-C2A-CAA-CBA
25	B	821	CLA	C1A-C2A-CAA-CBA
25	B	821	CLA	C2B-C3B-CAB-CBB
25	B	821	CLA	C4B-C3B-CAB-CBB
25	B	823	CLA	CBD-CGD-O2D-CED
25	B	827	CLA	CHA-CBD-CGD-O1D
25	B	827	CLA	CHA-CBD-CGD-O2D
25	B	829	CLA	C1A-C2A-CAA-CBA
25	B	829	CLA	C3A-C2A-CAA-CBA
25	B	829	CLA	CBD-CGD-O2D-CED
25	B	830	CLA	C1A-C2A-CAA-CBA
25	B	831	CLA	CHA-CBD-CGD-O2D
25	B	832	CLA	C1A-C2A-CAA-CBA
25	B	832	CLA	C3A-C2A-CAA-CBA
25	B	834	CLA	CAD-CBD-CGD-O1D
25	B	834	CLA	CAD-CBD-CGD-O2D
25	B	838	CLA	CHA-CBD-CGD-O2D
25	B	839	CLA	C1A-C2A-CAA-CBA
25	B	840	CLA	CHA-CBD-CGD-O2D
25	B	842	CLA	C1A-C2A-CAA-CBA
25	B	842	CLA	C3A-C2A-CAA-CBA
25	B	842	CLA	CAD-CBD-CGD-O1D
25	B	842	CLA	CAD-CBD-CGD-O2D
25	G	202	CLA	CAD-CBD-CGD-O2D
25	G	204	CLA	C1A-C2A-CAA-CBA
25	G	204	CLA	C3A-C2A-CAA-CBA
25	G	204	CLA	CAD-CBD-CGD-O1D
25	G	204	CLA	CAD-CBD-CGD-O2D
25	H	301	CLA	C1A-C2A-CAA-CBA
25	H	301	CLA	C3A-C2A-CAA-CBA
25	H	301	CLA	CAA-CBA-CGA-O1A
25	H	302	CLA	C1A-C2A-CAA-CBA
25	J	102	CLA	C1A-C2A-CAA-CBA
25	J	102	CLA	C3A-C2A-CAA-CBA
25	K	201	CLA	CBD-CGD-O2D-CED
25	K	203	CLA	C1A-C2A-CAA-CBA
25	K	204	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	K	204	CLA	CBD-CGD-O2D-CED
25	K	206	CLA	C1A-C2A-CAA-CBA
25	K	206	CLA	C3A-C2A-CAA-CBA
25	K	206	CLA	CBD-CGD-O2D-CED
25	L	302	CLA	C1A-C2A-CAA-CBA
25	L	302	CLA	C3A-C2A-CAA-CBA
25	L	303	CLA	C1A-C2A-CAA-CBA
25	L	303	CLA	C3A-C2A-CAA-CBA
25	L	304	CLA	C1A-C2A-CAA-CBA
25	L	304	CLA	C3A-C2A-CAA-CBA
25	N	202	CLA	C1A-C2A-CAA-CBA
25	N	202	CLA	C3A-C2A-CAA-CBA
25	N	203	CLA	CHA-CBD-CGD-O1D
25	N	203	CLA	CHA-CBD-CGD-O2D
25	O	2002	CLA	C1A-C2A-CAA-CBA
25	O	2002	CLA	C3A-C2A-CAA-CBA
25	P	301	CLA	C3A-C2A-CAA-CBA
25	P	302	CLA	CAD-CBD-CGD-O1D
25	P	302	CLA	CAD-CBD-CGD-O2D
25	P	303	CLA	C1A-C2A-CAA-CBA
25	P	303	CLA	C3A-C2A-CAA-CBA
25	P	303	CLA	CBD-CGD-O2D-CED
25	P	309	CLA	C3A-C2A-CAA-CBA
25	Q	301	CLA	C1A-C2A-CAA-CBA
25	Q	301	CLA	C3A-C2A-CAA-CBA
25	Q	306	CLA	C1A-C2A-CAA-CBA
25	Q	311	CLA	C1A-C2A-CAA-CBA
25	Q	312	CLA	C1A-C2A-CAA-CBA
25	Q	313	CLA	CBA-CGA-O2A-C1
25	R	305	CLA	C1A-C2A-CAA-CBA
25	R	307	CLA	CHA-CBD-CGD-O2D
25	R	313	CLA	C1A-C2A-CAA-CBA
25	R	313	CLA	C3A-C2A-CAA-CBA
25	R	314	CLA	C3A-C2A-CAA-CBA
25	R	315	CLA	CAD-CBD-CGD-O1D
25	R	315	CLA	CAD-CBD-CGD-O2D
25	R	316	CLA	C1A-C2A-CAA-CBA
25	R	316	CLA	C3A-C2A-CAA-CBA
25	R	317	CLA	O1A-CGA-O2A-C1
25	S	301	CLA	C3A-C2A-CAA-CBA
25	S	302	CLA	C2B-C3B-CAB-CBB
25	S	302	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	S	302	CLA	C6-C7-C8-C9
25	S	309	CLA	C1A-C2A-CAA-CBA
25	S	309	CLA	C3A-C2A-CAA-CBA
25	S	310	CLA	C1A-C2A-CAA-CBA
25	S	311	CLA	CBD-CGD-O2D-CED
25	T	301	CLA	C3A-C2A-CAA-CBA
25	T	302	CLA	C1A-C2A-CAA-CBA
25	T	302	CLA	C3A-C2A-CAA-CBA
25	T	303	CLA	CBD-CGD-O2D-CED
25	T	309	CLA	C1A-C2A-CAA-CBA
25	T	309	CLA	C3A-C2A-CAA-CBA
25	T	309	CLA	C4B-C3B-CAB-CBB
25	T	309	CLA	C4-C3-C5-C6
25	T	310	CLA	C1A-C2A-CAA-CBA
25	T	311	CLA	CBD-CGD-O2D-CED
25	T	312	CLA	C1A-C2A-CAA-CBA
25	T	313	CLA	C1A-C2A-CAA-CBA
25	U	301	CLA	C1A-C2A-CAA-CBA
25	U	301	CLA	C3A-C2A-CAA-CBA
25	U	301	CLA	CBD-CGD-O2D-CED
25	U	310	CLA	CAA-CBA-CGA-O1A
25	U	311	CLA	CBD-CGD-O2D-CED
25	V	302	CLA	C4B-C3B-CAB-CBB
25	V	302	CLA	CAD-CBD-CGD-O2D
25	V	303	CLA	CHA-CBD-CGD-O2D
25	V	303	CLA	CBD-CGD-O2D-CED
25	V	311	CLA	C2B-C3B-CAB-CBB
25	V	311	CLA	C4B-C3B-CAB-CBB
25	V	312	CLA	C1A-C2A-CAA-CBA
25	V	312	CLA	C3A-C2A-CAA-CBA
25	W	301	CLA	C1A-C2A-CAA-CBA
25	W	309	CLA	C2B-C3B-CAB-CBB
25	W	309	CLA	C4B-C3B-CAB-CBB
25	X	302	CLA	C2B-C3B-CAB-CBB
25	X	302	CLA	C4B-C3B-CAB-CBB
25	X	303	CLA	C1A-C2A-CAA-CBA
25	X	303	CLA	C3A-C2A-CAA-CBA
25	X	311	CLA	C1A-C2A-CAA-CBA
25	X	311	CLA	C3A-C2A-CAA-CBA
25	X	311	CLA	CBD-CGD-O2D-CED
25	X	312	CLA	CBD-CGD-O2D-CED
25	X	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	X	314	CLA	CAD-CBD-CGD-O1D
25	X	314	CLA	CAD-CBD-CGD-O2D
25	X	314	CLA	CBD-CGD-O2D-CED
26	1	611	IWJ	C18-C19-C21-C22
26	3	315	IWJ	C26-C28-C29-C35
26	4	301	IWJ	C02-C07-C08-C09
26	4	301	IWJ	C06-C07-C08-C09
26	4	301	IWJ	C26-C28-C29-C30
26	4	301	IWJ	C26-C28-C29-C35
26	4	301	IWJ	C26-C28-C29-O39
26	5	611	IWJ	C02-C07-C08-C09
26	5	611	IWJ	C26-C28-C29-C30
26	5	611	IWJ	C26-C28-C29-C35
26	5	611	IWJ	C26-C28-C29-O39
26	6	614	IWJ	C26-C28-C29-C30
26	6	614	IWJ	C26-C28-C29-C35
26	6	614	IWJ	C26-C28-C29-O39
26	P	318	IWJ	C18-C19-C21-C22
26	P	318	IWJ	C20-C19-C21-C22
26	P	320	IWJ	C26-C28-C29-C30
26	P	320	IWJ	C26-C28-C29-O39
26	Q	303	IWJ	C26-C28-C29-C30
26	Q	303	IWJ	C26-C28-C29-O39
26	Q	320	IWJ	C18-C19-C21-C22
26	Q	320	IWJ	O27-C26-C28-C29
26	Q	320	IWJ	C26-C28-C29-C30
26	Q	320	IWJ	C26-C28-C29-O39
26	R	303	IWJ	C26-C28-C29-C30
26	R	303	IWJ	C26-C28-C29-C35
26	R	303	IWJ	C26-C28-C29-O39
26	R	322	IWJ	C18-C19-C21-C22
26	R	322	IWJ	O27-C26-C28-C29
26	R	322	IWJ	C26-C28-C29-C30
26	R	322	IWJ	C26-C28-C29-C35
26	R	322	IWJ	C26-C28-C29-O39
26	S	319	IWJ	C18-C19-C21-C22
26	S	319	IWJ	C26-C28-C29-C30
26	S	319	IWJ	C26-C28-C29-C35
26	S	319	IWJ	C26-C28-C29-O39
26	S	322	IWJ	C26-C28-C29-C30
26	S	322	IWJ	C26-C28-C29-C35
26	S	322	IWJ	C26-C28-C29-O39

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Mol	Chain	Res	Type	Atoms
26	T	318	IWJ	C18-C19-C21-C22
26	T	318	IWJ	C26-C28-C29-C30
26	T	318	IWJ	C26-C28-C29-C35
26	T	318	IWJ	C26-C28-C29-O39
26	T	321	IWJ	C26-C28-C29-C30
26	T	321	IWJ	C26-C28-C29-C35
26	T	321	IWJ	C26-C28-C29-O39
26	V	317	IWJ	C18-C19-C21-C22
26	V	317	IWJ	C26-C28-C29-C30
26	V	317	IWJ	C26-C28-C29-O39
26	V	318	IWJ	C26-C28-C29-C30
26	V	318	IWJ	C26-C28-C29-O39
26	V	320	IWJ	C26-C28-C29-C30
26	V	320	IWJ	C26-C28-C29-C35
26	V	320	IWJ	C26-C28-C29-O39
26	W	318	IWJ	C18-C19-C21-C22
26	W	318	IWJ	C20-C19-C21-C22
26	W	318	IWJ	C26-C28-C29-C30
26	W	318	IWJ	C26-C28-C29-O39
26	X	318	IWJ	C18-C19-C21-C22
26	X	318	IWJ	C20-C19-C21-C22
26	X	318	IWJ	O27-C26-C28-C29
26	X	318	IWJ	C26-C28-C29-C30
26	X	318	IWJ	C26-C28-C29-O39
27	1	612	XAT	O4-C6-C7-C8
27	1	612	XAT	C11-C12-C13-C14
27	1	612	XAT	O24-C26-C27-C28
27	3	316	XAT	O4-C6-C7-C8
27	3	316	XAT	C7-C8-C9-C19
27	4	318	XAT	O4-C6-C7-C8
27	4	318	XAT	C27-C28-C29-C39
28	1	614	LHG	C3-O3-P-O5
28	1	614	LHG	C4-O6-P-O3
28	1	614	LHG	C4-O6-P-O4
28	2	619	LHG	C4-O6-P-O3
28	3	320	LHG	C4-O6-P-O3
28	3	320	LHG	C4-O6-P-O5
28	3	321	LHG	C3-O3-P-O5
28	3	321	LHG	C3-O3-P-O6
28	3	321	LHG	C4-O6-P-O3
28	3	322	LHG	C3-O3-P-O5
28	3	322	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
28	3	323	LHG	C1-C2-C3-O3
28	6	616	LHG	C3-O3-P-O4
28	6	616	LHG	C3-O3-P-O6
28	6	616	LHG	C4-O6-P-O3
28	6	616	LHG	C4-O6-P-O5
28	A	846	LHG	C3-O3-P-O5
28	Q	302	LHG	C4-O6-P-O3
28	Q	302	LHG	C4-O6-P-O4
29	2	616	Q6L	C02-C03-C11-C12
29	2	616	Q6L	C29-C30-C31-C32
29	O	2006	Q6L	C21-C22-C24-C25
29	O	2006	Q6L	C23-C22-C24-C25
29	O	2006	Q6L	C29-C30-C31-C36
29	O	2006	Q6L	C29-C30-C31-C32
29	O	2007	Q6L	C29-C30-C31-C32
29	O	2007	Q6L	C27-C29-C30-C31
29	P	315	Q6L	C26-C27-C29-C30
29	P	315	Q6L	C15-C16-C17-C18
29	P	319	Q6L	C29-C30-C31-C32
29	P	321	Q6L	C29-C30-C31-C32
29	Q	317	Q6L	C11-C12-C13-C14
29	Q	317	Q6L	C11-C12-C13-C42
29	Q	317	Q6L	C28-C27-C29-C30
29	Q	317	Q6L	C26-C27-C29-C30
29	Q	317	Q6L	C29-C30-C31-C32
29	Q	317	Q6L	C27-C29-C30-C31
29	Q	318	Q6L	C26-C27-C29-C30
29	R	301	Q6L	C21-C22-C24-C25
29	R	301	Q6L	C23-C22-C24-C25
29	R	301	Q6L	C28-C27-C29-C30
29	R	301	Q6L	C26-C27-C29-C30
29	R	301	Q6L	C29-C30-C31-C32
29	R	301	Q6L	C27-C29-C30-C31
29	R	304	Q6L	C29-C30-C31-C32
29	R	319	Q6L	C11-C12-C13-C14
29	R	319	Q6L	C11-C12-C13-C42
29	R	319	Q6L	C21-C22-C24-C25
29	R	319	Q6L	C29-C30-C31-C36
29	R	319	Q6L	C29-C30-C31-C32
29	R	323	Q6L	C28-C27-C29-C30
29	R	323	Q6L	C29-C30-C31-C32
29	R	323	Q6L	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	S	315	Q6L	C04-C03-C11-C12
29	S	315	Q6L	C26-C27-C29-C30
29	S	320	Q6L	C11-C12-C13-C42
29	S	320	Q6L	C21-C22-C24-C25
29	S	320	Q6L	C29-C30-C31-C32
29	S	320	Q6L	C27-C29-C30-C31
29	S	321	Q6L	C29-C30-C31-C36
29	S	321	Q6L	C29-C30-C31-C32
29	S	321	Q6L	C15-C16-C17-C18
29	S	323	Q6L	C02-C03-C11-C12
29	S	323	Q6L	C29-C30-C31-C36
29	S	323	Q6L	C29-C30-C31-C32
29	T	315	Q6L	C15-C16-C17-C18
29	T	315	Q6L	C15-C16-C17-C41
29	T	316	Q6L	C13-C14-C15-C16
29	T	319	Q6L	C29-C30-C31-C32
29	T	319	Q6L	C27-C29-C30-C31
29	T	322	Q6L	C02-C03-C11-C12
29	T	322	Q6L	C28-C27-C29-C30
29	T	322	Q6L	C29-C30-C31-C36
29	T	322	Q6L	C29-C30-C31-C32
29	U	314	Q6L	C28-C27-C29-C30
29	U	314	Q6L	C26-C27-C29-C30
29	U	317	Q6L	C29-C30-C31-C36
29	U	317	Q6L	C29-C30-C31-C32
29	V	315	Q6L	C02-C03-C11-C12
29	V	315	Q6L	C21-C22-C24-C25
29	V	315	Q6L	C23-C22-C24-C25
29	V	315	Q6L	C29-C30-C31-C32
29	V	315	Q6L	C27-C29-C30-C31
29	V	315	Q6L	C15-C16-C17-C18
29	V	316	Q6L	C29-C30-C31-C36
29	V	316	Q6L	C29-C30-C31-C32
29	V	316	Q6L	C27-C29-C30-C31
29	V	316	Q6L	C19-C20-C21-C22
29	V	319	Q6L	C02-C03-C11-C12
29	V	319	Q6L	C28-C27-C29-C30
29	V	319	Q6L	C26-C27-C29-C30
29	V	319	Q6L	C29-C30-C31-C36
29	V	319	Q6L	C29-C30-C31-C32
29	V	321	Q6L	C29-C30-C31-C32
29	W	315	Q6L	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	W	315	Q6L	C15-C16-C17-C41
29	W	316	Q6L	C04-C03-C11-C12
29	W	319	Q6L	C28-C27-C29-C30
29	W	319	Q6L	C26-C27-C29-C30
29	W	319	Q6L	C29-C30-C31-C32
29	W	320	Q6L	C02-C03-C11-C12
29	W	320	Q6L	C28-C27-C29-C30
29	W	320	Q6L	C29-C30-C31-C36
29	W	320	Q6L	C29-C30-C31-C32
29	X	301	Q6L	C29-C30-C31-C32
29	X	301	Q6L	C27-C29-C30-C31
29	X	319	Q6L	C21-C22-C24-C25
29	X	319	Q6L	C23-C22-C24-C25
29	X	319	Q6L	C28-C27-C29-C30
29	X	319	Q6L	C26-C27-C29-C30
29	X	319	Q6L	C29-C30-C31-C36
29	X	319	Q6L	C29-C30-C31-C32
29	X	319	Q6L	C27-C29-C30-C31
29	X	319	Q6L	C24-C25-C26-C27
30	3	317	BCR	C21-C22-C23-C24
30	4	319	BCR	C21-C22-C23-C24
30	A	851	BCR	C37-C22-C23-C24
30	B	848	BCR	C21-C22-C23-C24
30	B	849	BCR	C21-C22-C23-C24
30	B	849	BCR	C37-C22-C23-C24
30	F	804	BCR	C7-C8-C9-C10
30	F	804	BCR	C11-C12-C13-C14
30	G	201	BCR	C17-C18-C19-C20
30	G	201	BCR	C36-C18-C19-C20
30	H	305	BCR	C7-C8-C9-C10
30	H	305	BCR	C11-C12-C13-C14
30	I	101	BCR	C7-C8-C9-C34
30	I	101	BCR	C21-C22-C23-C24
30	K	205	BCR	C21-C22-C23-C24
30	L	305	BCR	C21-C22-C23-C24
30	L	305	BCR	C37-C22-C23-C24
30	L	306	BCR	C21-C22-C23-C24
30	L	306	BCR	C37-C22-C23-C24
30	M	101	BCR	C21-C22-C23-C24
32	6	617	SQD	O5-C5-C6-S
36	B	850	DGD	O6D-C1D-O3G-C3G
37	H	306	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
38	P	308	KC2	C1A-C2A-CAA-CBA
38	P	308	KC2	C2A-CAA-CBA-CGA
38	Q	310	KC2	C1A-C2A-CAA-CBA
38	Q	310	KC2	C3A-C2A-CAA-CBA
38	Q	310	KC2	C2A-CAA-CBA-CGA
38	R	312	KC2	C1A-C2A-CAA-CBA
38	R	312	KC2	C2A-CAA-CBA-CGA
38	S	308	KC2	C3A-C2A-CAA-CBA
38	S	308	KC2	C2A-CAA-CBA-CGA
38	S	308	KC2	CHA-CBD-CGD-O1D
38	S	308	KC2	CHA-CBD-CGD-O2D
38	T	308	KC2	C3A-C2A-CAA-CBA
38	T	308	KC2	C2A-CAA-CBA-CGA
38	U	307	KC2	C3A-C2A-CAA-CBA
38	U	307	KC2	C2A-CAA-CBA-CGA
38	V	308	KC2	C3A-C2A-CAA-CBA
38	V	308	KC2	C2A-CAA-CBA-CGA
38	V	308	KC2	CHA-CBD-CGD-O1D
38	V	308	KC2	CHA-CBD-CGD-O2D
38	W	308	KC2	C3A-C2A-CAA-CBA
38	W	308	KC2	C2A-CAA-CBA-CGA
38	X	309	KC2	C3A-C2A-CAA-CBA
38	X	309	KC2	C2A-CAA-CBA-CGA
24	P	304	CHL	O1D-CGD-O2D-CED
24	S	307	CHL	O1D-CGD-O2D-CED
24	U	304	CHL	O1D-CGD-O2D-CED
24	V	307	CHL	O1D-CGD-O2D-CED
24	X	308	CHL	O1D-CGD-O2D-CED
24	X	315	CHL	O1D-CGD-O2D-CED
25	4	311	CLA	O1D-CGD-O2D-CED
25	6	609	CLA	O1D-CGD-O2D-CED
25	A	830	CLA	O1D-CGD-O2D-CED
25	B	804	CLA	O1D-CGD-O2D-CED
25	B	805	CLA	O1D-CGD-O2D-CED
25	K	201	CLA	O1D-CGD-O2D-CED
25	U	311	CLA	O1D-CGD-O2D-CED
25	V	310	CLA	O1D-CGD-O2D-CED
25	W	303	CLA	O1D-CGD-O2D-CED
25	1	608	CLA	O1D-CGD-O2D-CED
25	5	603	CLA	O1D-CGD-O2D-CED
25	O	2005	CLA	O1D-CGD-O2D-CED
25	S	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	W	311	CLA	O1D-CGD-O2D-CED
25	X	312	CLA	O1D-CGD-O2D-CED
24	3	306	CHL	CBD-CGD-O2D-CED
24	S	305	CHL	CBD-CGD-O2D-CED
24	T	305	CHL	CBD-CGD-O2D-CED
24	V	307	CHL	CBD-CGD-O2D-CED
24	W	307	CHL	CBD-CGD-O2D-CED
25	1	602	CLA	CBD-CGD-O2D-CED
25	3	301	CLA	CBD-CGD-O2D-CED
25	4	314	CLA	CBD-CGD-O2D-CED
25	5	601	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	609	CLA	CBD-CGD-O2D-CED
25	A	830	CLA	CBD-CGD-O2D-CED
25	A	838	CLA	CBD-CGD-O2D-CED
25	B	804	CLA	CBD-CGD-O2D-CED
25	B	808	CLA	CBD-CGD-O2D-CED
25	B	834	CLA	CBD-CGD-O2D-CED
25	B	840	CLA	CBD-CGD-O2D-CED
25	G	204	CLA	CBD-CGD-O2D-CED
25	O	2004	CLA	CBD-CGD-O2D-CED
25	O	2005	CLA	CBD-CGD-O2D-CED
25	P	311	CLA	CBD-CGD-O2D-CED
25	Q	314	CLA	CBD-CGD-O2D-CED
25	R	306	CLA	CBD-CGD-O2D-CED
25	S	309	CLA	CBD-CGD-O2D-CED
25	T	302	CLA	CBD-CGD-O2D-CED
25	T	312	CLA	CBD-CGD-O2D-CED
25	T	313	CLA	CBD-CGD-O2D-CED
25	U	302	CLA	CBD-CGD-O2D-CED
25	U	310	CLA	CBD-CGD-O2D-CED
25	V	301	CLA	CBD-CGD-O2D-CED
25	V	310	CLA	CBD-CGD-O2D-CED
25	W	301	CLA	CBD-CGD-O2D-CED
25	W	303	CLA	CBD-CGD-O2D-CED
25	W	311	CLA	CBD-CGD-O2D-CED
25	W	313	CLA	CBD-CGD-O2D-CED
25	X	303	CLA	CBD-CGD-O2D-CED
38	U	307	KC2	CBD-CGD-O2D-CED
38	X	309	KC2	CBD-CGD-O2D-CED
25	1	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	1	613	CLA	O1A-CGA-O2A-C1
25	3	302	CLA	O1A-CGA-O2A-C1
25	A	830	CLA	O1A-CGA-O2A-C1
25	A	856	CLA	O1A-CGA-O2A-C1
25	B	813	CLA	O1A-CGA-O2A-C1
25	O	2002	CLA	O1A-CGA-O2A-C1
25	Q	315	CLA	O1A-CGA-O2A-C1
25	R	314	CLA	O1A-CGA-O2A-C1
25	U	311	CLA	O1A-CGA-O2A-C1
25	V	302	CLA	O1A-CGA-O2A-C1
25	5	601	CLA	O1A-CGA-O2A-C1
25	Q	313	CLA	O1A-CGA-O2A-C1
24	V	304	CHL	O1D-CGD-O2D-CED
25	1	610	CLA	O1D-CGD-O2D-CED
25	X	313	CLA	O1D-CGD-O2D-CED
25	X	314	CLA	O1D-CGD-O2D-CED
24	W	307	CHL	O1D-CGD-O2D-CED
25	4	309	CLA	O1D-CGD-O2D-CED
25	5	601	CLA	O1D-CGD-O2D-CED
25	T	302	CLA	O1D-CGD-O2D-CED
25	W	313	CLA	O1D-CGD-O2D-CED
25	A	827	CLA	CBA-CGA-O2A-C1
25	A	830	CLA	CBA-CGA-O2A-C1
25	B	813	CLA	CBA-CGA-O2A-C1
25	O	2002	CLA	CBA-CGA-O2A-C1
25	Q	315	CLA	CBA-CGA-O2A-C1
25	R	317	CLA	CBA-CGA-O2A-C1
25	U	311	CLA	CBA-CGA-O2A-C1
25	V	302	CLA	CBA-CGA-O2A-C1
25	L	304	CLA	CBD-CGD-O2D-CED
24	P	306	CHL	O1A-CGA-O2A-C1
24	R	310	CHL	O1A-CGA-O2A-C1
24	S	306	CHL	O1A-CGA-O2A-C1
24	W	306	CHL	O1A-CGA-O2A-C1
24	W	307	CHL	O1A-CGA-O2A-C1
25	2	602	CLA	O1A-CGA-O2A-C1
25	A	805	CLA	O1A-CGA-O2A-C1
25	A	807	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	O1A-CGA-O2A-C1
25	A	814	CLA	O1A-CGA-O2A-C1
25	A	819	CLA	O1A-CGA-O2A-C1
25	A	827	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	829	CLA	O1A-CGA-O2A-C1
25	A	835	CLA	O1A-CGA-O2A-C1
25	A	837	CLA	O1A-CGA-O2A-C1
25	A	845	CLA	O1A-CGA-O2A-C1
25	B	812	CLA	O1A-CGA-O2A-C1
25	B	819	CLA	O1A-CGA-O2A-C1
25	B	831	CLA	O1A-CGA-O2A-C1
25	B	839	CLA	O1A-CGA-O2A-C1
25	P	302	CLA	O1A-CGA-O2A-C1
25	P	311	CLA	O1A-CGA-O2A-C1
25	Q	304	CLA	O1A-CGA-O2A-C1
25	R	305	CLA	O1A-CGA-O2A-C1
25	R	315	CLA	O1A-CGA-O2A-C1
25	S	311	CLA	O1A-CGA-O2A-C1
25	T	309	CLA	O1A-CGA-O2A-C1
25	V	313	CLA	O1A-CGA-O2A-C1
25	X	302	CLA	O1A-CGA-O2A-C1
25	X	311	CLA	O1A-CGA-O2A-C1
25	X	312	CLA	O1A-CGA-O2A-C1
24	R	302	CHL	O1A-CGA-O2A-C1
24	R	309	CHL	O1D-CGD-O2D-CED
25	3	310	CLA	O1D-CGD-O2D-CED
25	4	303	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	B	817	CLA	O1D-CGD-O2D-CED
25	K	204	CLA	O1D-CGD-O2D-CED
25	P	303	CLA	O1D-CGD-O2D-CED
25	R	306	CLA	O1D-CGD-O2D-CED
25	T	303	CLA	O1D-CGD-O2D-CED
25	V	303	CLA	O1D-CGD-O2D-CED
25	X	303	CLA	O1D-CGD-O2D-CED
38	U	307	KC2	CAA-CBA-CGA-O1A
38	U	307	KC2	CAA-CBA-CGA-O2A
24	2	605	CHL	O1D-CGD-O2D-CED
24	4	307	CHL	O1D-CGD-O2D-CED
24	R	311	CHL	O1D-CGD-O2D-CED
24	R	318	CHL	O1D-CGD-O2D-CED
24	T	304	CHL	O1D-CGD-O2D-CED
25	1	602	CLA	O1D-CGD-O2D-CED
25	2	608	CLA	O1D-CGD-O2D-CED
25	2	610	CLA	O1D-CGD-O2D-CED
25	4	315	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	A	819	CLA	O1D-CGD-O2D-CED
25	A	824	CLA	O1D-CGD-O2D-CED
25	A	835	CLA	O1D-CGD-O2D-CED
25	B	823	CLA	O1D-CGD-O2D-CED
25	T	311	CLA	O1D-CGD-O2D-CED
25	U	301	CLA	O1D-CGD-O2D-CED
24	4	302	CHL	CBD-CGD-O2D-CED
25	B	812	CLA	CBD-CGD-O2D-CED
25	R	316	CLA	CBD-CGD-O2D-CED
25	X	304	CLA	CBD-CGD-O2D-CED
25	A	823	CLA	C3-C5-C6-C7
25	A	830	CLA	C3-C5-C6-C7
25	A	839	CLA	C3-C5-C6-C7
25	B	808	CLA	C3-C5-C6-C7
25	B	813	CLA	C3-C5-C6-C7
25	B	814	CLA	C3-C5-C6-C7
25	B	815	CLA	C3-C5-C6-C7
25	B	836	CLA	C3-C5-C6-C7
25	K	206	CLA	C3-C5-C6-C7
25	R	315	CLA	C3-C5-C6-C7
25	S	301	CLA	C3-C5-C6-C7
25	T	309	CLA	C3-C5-C6-C7
25	V	312	CLA	C3-C5-C6-C7
25	W	302	CLA	C3-C5-C6-C7
25	W	312	CLA	C3-C5-C6-C7
24	6	606	CHL	O1D-CGD-O2D-CED
24	P	306	CHL	CBA-CGA-O2A-C1
24	S	306	CHL	CBA-CGA-O2A-C1
24	W	307	CHL	CBA-CGA-O2A-C1
25	1	603	CLA	CBA-CGA-O2A-C1
25	1	613	CLA	CBA-CGA-O2A-C1
25	A	807	CLA	CBA-CGA-O2A-C1
25	A	820	CLA	CBA-CGA-O2A-C1
25	A	845	CLA	CBA-CGA-O2A-C1
25	A	856	CLA	CBA-CGA-O2A-C1
25	B	818	CLA	CBA-CGA-O2A-C1
25	B	819	CLA	CBA-CGA-O2A-C1
25	B	831	CLA	CBA-CGA-O2A-C1
25	B	839	CLA	CBA-CGA-O2A-C1
25	P	302	CLA	CBA-CGA-O2A-C1
25	Q	304	CLA	CBA-CGA-O2A-C1
25	R	305	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	R	314	CLA	CBA-CGA-O2A-C1
25	R	316	CLA	CBA-CGA-O2A-C1
25	S	311	CLA	CBA-CGA-O2A-C1
25	X	302	CLA	CBA-CGA-O2A-C1
25	X	311	CLA	CBA-CGA-O2A-C1
24	2	615	CHL	CBD-CGD-O2D-CED
24	Q	307	CHL	CBD-CGD-O2D-CED
24	U	306	CHL	CBD-CGD-O2D-CED
24	X	306	CHL	CBD-CGD-O2D-CED
25	2	609	CLA	CBD-CGD-O2D-CED
25	5	607	CLA	CBD-CGD-O2D-CED
25	5	608	CLA	CBD-CGD-O2D-CED
25	6	612	CLA	CBD-CGD-O2D-CED
25	A	812	CLA	CBD-CGD-O2D-CED
25	A	815	CLA	CBD-CGD-O2D-CED
25	A	825	CLA	CBD-CGD-O2D-CED
25	A	839	CLA	CBD-CGD-O2D-CED
25	B	811	CLA	CBD-CGD-O2D-CED
25	B	818	CLA	CBD-CGD-O2D-CED
25	B	820	CLA	CBD-CGD-O2D-CED
25	B	835	CLA	CBD-CGD-O2D-CED
25	O	2002	CLA	CBD-CGD-O2D-CED
25	Q	311	CLA	CBD-CGD-O2D-CED
25	V	302	CLA	CBD-CGD-O2D-CED
25	V	309	CLA	CBD-CGD-O2D-CED
38	P	308	KC2	CBD-CGD-O2D-CED
38	W	308	KC2	CBD-CGD-O2D-CED
24	3	306	CHL	O1D-CGD-O2D-CED
24	T	305	CHL	O1D-CGD-O2D-CED
25	1	606	CLA	O1D-CGD-O2D-CED
25	6	608	CLA	O1D-CGD-O2D-CED
25	A	804	CLA	O1D-CGD-O2D-CED
25	A	836	CLA	O1D-CGD-O2D-CED
25	B	803	CLA	O1D-CGD-O2D-CED
25	B	829	CLA	O1D-CGD-O2D-CED
25	B	840	CLA	O1D-CGD-O2D-CED
25	K	206	CLA	O1D-CGD-O2D-CED
25	P	311	CLA	O1D-CGD-O2D-CED
25	U	302	CLA	O1D-CGD-O2D-CED
25	X	311	CLA	O1D-CGD-O2D-CED
25	B	808	CLA	O1D-CGD-O2D-CED
25	2	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	819	CLA	C4-C3-C5-C6
25	A	831	CLA	C4-C3-C5-C6
25	K	206	CLA	C4-C3-C5-C6
25	P	301	CLA	C4-C3-C5-C6
25	R	316	CLA	C4-C3-C5-C6
25	T	301	CLA	C4-C3-C5-C6
29	2	616	Q6L	C11-C12-C13-C42
29	P	319	Q6L	C11-C12-C13-C42
29	R	301	Q6L	C11-C12-C13-C42
29	R	323	Q6L	C11-C12-C13-C42
29	T	319	Q6L	C11-C12-C13-C42
29	T	322	Q6L	C11-C12-C13-C42
29	U	314	Q6L	C11-C12-C13-C42
29	W	320	Q6L	C11-C12-C13-C42
29	X	319	Q6L	C11-C12-C13-C42
25	K	206	CLA	C2-C3-C5-C6
25	P	301	CLA	C2-C3-C5-C6
25	T	309	CLA	C2-C3-C5-C6
29	2	616	Q6L	C11-C12-C13-C14
29	P	319	Q6L	C11-C12-C13-C14
29	S	320	Q6L	C11-C12-C13-C14
29	T	322	Q6L	C11-C12-C13-C14
29	U	314	Q6L	C11-C12-C13-C14
29	W	320	Q6L	C11-C12-C13-C14
29	X	319	Q6L	C11-C12-C13-C14
25	1	613	CLA	CBD-CGD-O2D-CED
25	6	610	CLA	CBD-CGD-O2D-CED
25	O	2004	CLA	O1D-CGD-O2D-CED
25	1	613	CLA	C3-C5-C6-C7
25	5	607	CLA	C3-C5-C6-C7
25	6	613	CLA	C3-C5-C6-C7
25	A	820	CLA	C3-C5-C6-C7
25	A	837	CLA	C3-C5-C6-C7
25	B	824	CLA	C3-C5-C6-C7
25	B	842	CLA	C3-C5-C6-C7
25	T	301	CLA	C3-C5-C6-C7
25	W	301	CLA	C3-C5-C6-C7
25	B	808	CLA	C2C-C3C-CAC-CBC
24	R	310	CHL	CBA-CGA-O2A-C1
24	W	306	CHL	CBA-CGA-O2A-C1
25	1	608	CLA	CBA-CGA-O2A-C1
25	2	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	4	303	CLA	CBA-CGA-O2A-C1
25	A	805	CLA	CBA-CGA-O2A-C1
25	A	808	CLA	CBA-CGA-O2A-C1
25	A	809	CLA	CBA-CGA-O2A-C1
25	A	812	CLA	CBA-CGA-O2A-C1
25	A	814	CLA	CBA-CGA-O2A-C1
25	A	819	CLA	CBA-CGA-O2A-C1
25	A	823	CLA	CBA-CGA-O2A-C1
25	A	829	CLA	CBA-CGA-O2A-C1
25	A	835	CLA	CBA-CGA-O2A-C1
25	A	837	CLA	CBA-CGA-O2A-C1
25	B	802	CLA	CBA-CGA-O2A-C1
25	B	812	CLA	CBA-CGA-O2A-C1
25	B	821	CLA	CBA-CGA-O2A-C1
25	B	823	CLA	CBA-CGA-O2A-C1
25	B	829	CLA	CBA-CGA-O2A-C1
25	P	311	CLA	CBA-CGA-O2A-C1
25	Q	314	CLA	CBA-CGA-O2A-C1
25	R	315	CLA	CBA-CGA-O2A-C1
25	T	309	CLA	CBA-CGA-O2A-C1
25	V	313	CLA	CBA-CGA-O2A-C1
25	X	312	CLA	CBA-CGA-O2A-C1
34	A	844	PQN	C11-C12-C13-C14
34	B	844	PQN	C11-C12-C13-C14
26	V	320	IWJ	C10-C11-C12-C13
29	P	321	Q6L	C13-C14-C15-C16
29	R	323	Q6L	C24-C25-C26-C27
29	S	320	Q6L	C24-C25-C26-C27
29	U	315	Q6L	C13-C14-C15-C16
29	V	315	Q6L	C17-C18-C19-C20
25	6	602	CLA	O1A-CGA-O2A-C1
25	A	809	CLA	O1A-CGA-O2A-C1
25	A	820	CLA	O1A-CGA-O2A-C1
25	A	823	CLA	O1A-CGA-O2A-C1
25	B	802	CLA	O1A-CGA-O2A-C1
25	B	804	CLA	O1A-CGA-O2A-C1
25	B	805	CLA	O1A-CGA-O2A-C1
25	B	823	CLA	O1A-CGA-O2A-C1
25	B	829	CLA	O1A-CGA-O2A-C1
25	Q	314	CLA	O1A-CGA-O2A-C1
33	A	802	CL0	O1A-CGA-O2A-C1
25	W	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	A	838	CLA	O1D-CGD-O2D-CED
25	B	834	CLA	O1D-CGD-O2D-CED
25	A	817	CLA	C3-C5-C6-C7
25	B	834	CLA	C3-C5-C6-C7
25	Q	304	CLA	C3-C5-C6-C7
24	U	305	CHL	CBD-CGD-O2D-CED
25	A	814	CLA	CBD-CGD-O2D-CED
25	A	816	CLA	CBD-CGD-O2D-CED
25	A	821	CLA	CBD-CGD-O2D-CED
25	B	815	CLA	CBD-CGD-O2D-CED
25	P	309	CLA	CBD-CGD-O2D-CED
25	S	312	CLA	CBD-CGD-O2D-CED
28	3	323	LHG	O2-C2-C3-O3
24	S	305	CHL	O1D-CGD-O2D-CED
25	3	301	CLA	O1D-CGD-O2D-CED
25	4	314	CLA	O1D-CGD-O2D-CED
25	T	313	CLA	O1D-CGD-O2D-CED
25	U	310	CLA	O1D-CGD-O2D-CED
25	V	301	CLA	O1D-CGD-O2D-CED
25	5	607	CLA	CBA-CGA-O2A-C1
25	A	843	CLA	CBA-CGA-O2A-C1
25	B	805	CLA	CBA-CGA-O2A-C1
25	W	303	CLA	CBA-CGA-O2A-C1
25	W	310	CLA	CBA-CGA-O2A-C1
25	X	303	CLA	CBA-CGA-O2A-C1
33	A	802	CL0	CBA-CGA-O2A-C1
25	4	303	CLA	O1A-CGA-O2A-C1
25	5	602	CLA	O1A-CGA-O2A-C1
25	B	818	CLA	O1A-CGA-O2A-C1
25	O	2001	CLA	O1A-CGA-O2A-C1
28	6	616	LHG	O10-C23-O8-C6
24	T	307	CHL	CBD-CGD-O2D-CED
25	A	818	CLA	CBD-CGD-O2D-CED
25	A	833	CLA	CBD-CGD-O2D-CED
25	A	841	CLA	CBD-CGD-O2D-CED
25	N	203	CLA	CBD-CGD-O2D-CED
28	3	322	LHG	C8-C7-O7-C5
25	T	312	CLA	O1D-CGD-O2D-CED
25	G	204	CLA	O1D-CGD-O2D-CED
38	X	309	KC2	O1D-CGD-O2D-CED
25	B	820	CLA	C3-C5-C6-C7
25	V	311	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	W	309	CLA	C3-C5-C6-C7
25	X	302	CLA	C3-C5-C6-C7
25	Q	304	CLA	CBD-CGD-O2D-CED
25	T	301	CLA	CBD-CGD-O2D-CED
25	V	311	CLA	CBD-CGD-O2D-CED
25	Q	314	CLA	O1D-CGD-O2D-CED
38	U	307	KC2	O1D-CGD-O2D-CED
25	5	602	CLA	CBA-CGA-O2A-C1
25	6	602	CLA	CBA-CGA-O2A-C1
25	B	804	CLA	CBA-CGA-O2A-C1
25	B	820	CLA	CBA-CGA-O2A-C1
25	O	2001	CLA	CBA-CGA-O2A-C1
28	6	616	LHG	C24-C23-O8-C6
38	S	308	KC2	CAA-CBA-CGA-O2A
25	V	301	CLA	C4-C3-C5-C6
29	O	2006	Q6L	C11-C12-C13-C42
29	Q	319	Q6L	C11-C12-C13-C42
29	S	323	Q6L	C11-C12-C13-C42
29	U	317	Q6L	C11-C12-C13-C42
29	V	315	Q6L	C11-C12-C13-C42
25	2	612	CLA	C2-C3-C5-C6
25	A	819	CLA	C2-C3-C5-C6
25	R	316	CLA	C2-C3-C5-C6
25	T	301	CLA	C2-C3-C5-C6
25	V	301	CLA	C2-C3-C5-C6
29	O	2006	Q6L	C11-C12-C13-C14
29	Q	319	Q6L	C11-C12-C13-C14
29	R	301	Q6L	C11-C12-C13-C14
29	R	323	Q6L	C11-C12-C13-C14
29	S	321	Q6L	C11-C12-C13-C14
29	S	323	Q6L	C11-C12-C13-C14
29	T	319	Q6L	C11-C12-C13-C14
29	V	315	Q6L	C11-C12-C13-C14
25	1	608	CLA	O1A-CGA-O2A-C1
25	A	843	CLA	O1A-CGA-O2A-C1
25	B	820	CLA	O1A-CGA-O2A-C1
25	B	821	CLA	O1A-CGA-O2A-C1
25	R	316	CLA	O1A-CGA-O2A-C1
25	B	842	CLA	CBD-CGD-O2D-CED
24	Q	308	CHL	C2A-CAA-CBA-CGA
25	V	313	CLA	C2A-CAA-CBA-CGA
25	L	304	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	5	607	CLA	O1A-CGA-O2A-C1
25	A	812	CLA	O1A-CGA-O2A-C1
25	A	821	CLA	O1A-CGA-O2A-C1
25	W	303	CLA	O1A-CGA-O2A-C1
25	W	310	CLA	O1A-CGA-O2A-C1
25	X	303	CLA	O1A-CGA-O2A-C1
32	6	617	SQD	O5-C1-O6-C44
32	H	303	SQD	O5-C1-O6-C44
25	S	309	CLA	O1D-CGD-O2D-CED
25	A	826	CLA	CBA-CGA-O2A-C1
25	T	312	CLA	CBA-CGA-O2A-C1
25	V	311	CLA	CBA-CGA-O2A-C1
24	2	607	CHL	CBD-CGD-O2D-CED
24	P	306	CHL	CBD-CGD-O2D-CED
24	X	307	CHL	CBD-CGD-O2D-CED
25	2	606	CLA	CBD-CGD-O2D-CED
25	2	614	CLA	CBD-CGD-O2D-CED
25	3	308	CLA	CBD-CGD-O2D-CED
25	6	611	CLA	CBD-CGD-O2D-CED
25	A	805	CLA	CBD-CGD-O2D-CED
25	A	823	CLA	CBD-CGD-O2D-CED
25	F	802	CLA	CBD-CGD-O2D-CED
25	F	803	CLA	CBD-CGD-O2D-CED
25	J	102	CLA	CBD-CGD-O2D-CED
25	L	301	CLA	CBD-CGD-O2D-CED
25	L	302	CLA	CBD-CGD-O2D-CED
25	Q	301	CLA	CBD-CGD-O2D-CED
25	Q	306	CLA	CBD-CGD-O2D-CED
25	R	307	CLA	CBD-CGD-O2D-CED
25	W	310	CLA	CBD-CGD-O2D-CED
38	R	312	KC2	CAA-CBA-CGA-O1A
24	4	302	CHL	O1D-CGD-O2D-CED
24	T	314	CHL	CBD-CGD-O2D-CED
34	A	844	PQN	C13-C15-C16-C17
29	P	319	Q6L	C13-C14-C15-C16
25	A	826	CLA	O1A-CGA-O2A-C1
25	B	842	CLA	O1A-CGA-O2A-C1
25	V	311	CLA	O1A-CGA-O2A-C1
24	T	306	CHL	CBA-CGA-O2A-C1
25	4	310	CLA	CBA-CGA-O2A-C1
25	6	610	CLA	CBA-CGA-O2A-C1
25	A	813	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	821	CLA	CBA-CGA-O2A-C1
25	A	831	CLA	CBA-CGA-O2A-C1
25	B	806	CLA	CBA-CGA-O2A-C1
25	B	827	CLA	CBA-CGA-O2A-C1
25	B	830	CLA	CBA-CGA-O2A-C1
25	B	842	CLA	CBA-CGA-O2A-C1
25	P	301	CLA	CBA-CGA-O2A-C1
25	W	301	CLA	CBA-CGA-O2A-C1
25	W	302	CLA	CBA-CGA-O2A-C1
25	5	602	CLA	CBD-CGD-O2D-CED
25	B	843	CLA	CBD-CGD-O2D-CED
25	S	303	CLA	CBD-CGD-O2D-CED
25	U	309	CLA	CBD-CGD-O2D-CED
24	Q	307	CHL	O1D-CGD-O2D-CED
25	2	609	CLA	O1D-CGD-O2D-CED
25	A	839	CLA	O1D-CGD-O2D-CED
25	B	811	CLA	O1D-CGD-O2D-CED
25	B	812	CLA	O1D-CGD-O2D-CED
25	R	316	CLA	O1D-CGD-O2D-CED
25	X	304	CLA	O1D-CGD-O2D-CED
38	V	308	KC2	CAA-CBA-CGA-O2A
38	W	308	KC2	CAA-CBA-CGA-O1A
25	3	302	CLA	C4-C3-C5-C6
29	S	321	Q6L	C11-C12-C13-C42
29	V	319	Q6L	C11-C12-C13-C42
25	3	302	CLA	C2-C3-C5-C6
25	A	831	CLA	C2-C3-C5-C6
25	Q	314	CLA	C2-C3-C5-C6
29	U	317	Q6L	C11-C12-C13-C14
29	V	319	Q6L	C11-C12-C13-C14
24	W	314	CHL	CBD-CGD-O2D-CED
24	W	307	CHL	C6-C7-C8-C9
25	2	612	CLA	C11-C10-C8-C9
25	A	819	CLA	C11-C10-C8-C9
25	A	828	CLA	C11-C10-C8-C9
25	B	813	CLA	C14-C13-C15-C16
25	B	815	CLA	C6-C7-C8-C9
25	B	834	CLA	C11-C12-C13-C14
25	L	302	CLA	C11-C10-C8-C9
25	P	310	CLA	C11-C10-C8-C9
25	R	315	CLA	C11-C10-C8-C9
25	V	301	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
34	A	844	PQN	C24-C23-C25-C26
24	X	306	CHL	O1D-CGD-O2D-CED
25	V	309	CLA	O1D-CGD-O2D-CED
38	W	308	KC2	O1D-CGD-O2D-CED
32	6	617	SQD	C2-C1-O6-C44
32	H	303	SQD	C2-C1-O6-C44
25	T	312	CLA	O1A-CGA-O2A-C1
25	6	612	CLA	O1D-CGD-O2D-CED
25	B	818	CLA	O1D-CGD-O2D-CED
25	B	835	CLA	O1D-CGD-O2D-CED
26	1	611	IWJ	C20-C19-C21-C22
26	Q	320	IWJ	C20-C19-C21-C22
26	R	322	IWJ	C20-C19-C21-C22
26	S	319	IWJ	C20-C19-C21-C22
26	T	318	IWJ	C20-C19-C21-C22
26	V	317	IWJ	C20-C19-C21-C22
27	1	612	XAT	C7-C8-C9-C19
27	1	612	XAT	C11-C12-C13-C20
29	2	616	Q6L	C28-C27-C29-C30
29	O	2006	Q6L	C28-C27-C29-C30
29	P	315	Q6L	C28-C27-C29-C30
29	P	315	Q6L	C15-C16-C17-C41
29	P	321	Q6L	C28-C27-C29-C30
29	Q	318	Q6L	C28-C27-C29-C30
29	Q	319	Q6L	C28-C27-C29-C30
29	R	304	Q6L	C28-C27-C29-C30
29	R	319	Q6L	C23-C22-C24-C25
29	R	323	Q6L	C23-C22-C24-C25
29	S	315	Q6L	C28-C27-C29-C30
29	S	320	Q6L	C23-C22-C24-C25
29	S	321	Q6L	C28-C27-C29-C30
29	S	321	Q6L	C15-C16-C17-C41
29	S	323	Q6L	C28-C27-C29-C30
29	T	315	Q6L	C28-C27-C29-C30
29	T	319	Q6L	C28-C27-C29-C30
29	U	314	Q6L	C15-C16-C17-C41
29	V	315	Q6L	C15-C16-C17-C41
29	V	321	Q6L	C28-C27-C29-C30
29	W	319	Q6L	C23-C22-C24-C25
30	3	317	BCR	C37-C22-C23-C24
30	4	319	BCR	C37-C22-C23-C24
30	A	848	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
30	A	849	BCR	C11-C12-C13-C35
30	B	848	BCR	C37-C22-C23-C24
30	F	801	BCR	C37-C22-C23-C24
30	F	804	BCR	C7-C8-C9-C34
30	F	804	BCR	C11-C12-C13-C35
30	H	305	BCR	C7-C8-C9-C34
30	H	305	BCR	C36-C18-C19-C20
30	I	101	BCR	C37-C22-C23-C24
30	K	205	BCR	C37-C22-C23-C24
30	M	101	BCR	C37-C22-C23-C24
29	2	616	Q6L	C26-C27-C29-C30
29	O	2006	Q6L	C26-C27-C29-C30
29	P	319	Q6L	C26-C27-C29-C30
29	P	321	Q6L	C26-C27-C29-C30
29	Q	319	Q6L	C26-C27-C29-C30
29	R	304	Q6L	C26-C27-C29-C30
29	R	323	Q6L	C26-C27-C29-C30
29	S	321	Q6L	C26-C27-C29-C30
29	S	323	Q6L	C26-C27-C29-C30
29	T	319	Q6L	C26-C27-C29-C30
29	T	322	Q6L	C26-C27-C29-C30
29	V	321	Q6L	C26-C27-C29-C30
29	W	319	Q6L	C21-C22-C24-C25
29	W	320	Q6L	C26-C27-C29-C30
30	B	845	BCR	C7-C8-C9-C10
30	F	801	BCR	C21-C22-C23-C24
25	B	811	CLA	C2A-CAA-CBA-CGA
25	B	841	CLA	C2A-CAA-CBA-CGA
25	Q	301	CLA	C2A-CAA-CBA-CGA
25	Q	314	CLA	C2A-CAA-CBA-CGA
25	4	310	CLA	O1A-CGA-O2A-C1
25	A	831	CLA	O1A-CGA-O2A-C1
25	B	827	CLA	O1A-CGA-O2A-C1
25	B	830	CLA	O1A-CGA-O2A-C1
25	H	301	CLA	CBD-CGD-O2D-CED
38	R	312	KC2	CAA-CBA-CGA-O2A
38	S	308	KC2	CAA-CBA-CGA-O1A
38	T	308	KC2	CAA-CBA-CGA-O1A
38	V	308	KC2	CAA-CBA-CGA-O1A
38	W	308	KC2	CAA-CBA-CGA-O2A
25	K	204	CLA	CBA-CGA-O2A-C1
25	U	309	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	832	CLA	CBA-CGA-O2A-C1
25	A	838	CLA	CBA-CGA-O2A-C1
25	S	309	CLA	CBA-CGA-O2A-C1
25	W	310	CLA	C8-C10-C11-C12
25	A	830	CLA	C2-C1-O2A-CGA
25	B	805	CLA	C2-C1-O2A-CGA
33	A	802	CL0	C2-C1-O2A-CGA
25	5	607	CLA	O1D-CGD-O2D-CED
25	V	302	CLA	O1D-CGD-O2D-CED
38	P	308	KC2	O1D-CGD-O2D-CED
24	W	307	CHL	C5-C6-C7-C8
25	A	830	CLA	C10-C11-C12-C13
25	B	807	CLA	C13-C15-C16-C17
25	B	813	CLA	C8-C10-C11-C12
25	B	834	CLA	C10-C11-C12-C13
25	T	311	CLA	C5-C6-C7-C8
24	U	306	CHL	O1D-CGD-O2D-CED
25	5	608	CLA	O1D-CGD-O2D-CED
25	A	825	CLA	O1D-CGD-O2D-CED
25	O	2002	CLA	C15-C16-C17-C18
25	2	604	CLA	CBD-CGD-O2D-CED
25	A	830	CLA	C11-C10-C8-C7
25	B	810	CLA	C6-C7-C8-C10
25	B	813	CLA	C11-C10-C8-C7
25	T	302	CLA	C6-C7-C8-C10
25	A	839	CLA	CBA-CGA-O2A-C1
25	W	312	CLA	CBA-CGA-O2A-C1
38	T	308	KC2	CAA-CBA-CGA-O2A
25	B	820	CLA	O1D-CGD-O2D-CED
25	O	2002	CLA	O1D-CGD-O2D-CED
26	V	318	IWJ	C10-C11-C12-C13
29	S	316	Q6L	C13-C14-C15-C16
29	W	319	Q6L	C24-C25-C26-C27
25	Q	311	CLA	O1D-CGD-O2D-CED
25	A	842	CLA	C3-C5-C6-C7
25	B	804	CLA	C3-C5-C6-C7
25	A	821	CLA	C15-C16-C17-C18
25	A	838	CLA	C13-C15-C16-C17
28	A	846	LHG	C23-C24-C25-C26
25	6	610	CLA	O1A-CGA-O2A-C1
25	A	813	CLA	O1A-CGA-O2A-C1
25	A	838	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	W	301	CLA	O1A-CGA-O2A-C1
24	P	314	CHL	CBD-CGD-O2D-CED
25	Q	304	CLA	O1D-CGD-O2D-CED
25	A	835	CLA	C5-C6-C7-C8
25	B	826	CLA	C10-C11-C12-C13
25	H	302	CLA	C15-C16-C17-C18
25	R	305	CLA	C13-C15-C16-C17
24	V	304	CHL	C2A-CAA-CBA-CGA
25	5	601	CLA	C2A-CAA-CBA-CGA
25	A	810	CLA	C2A-CAA-CBA-CGA
25	A	833	CLA	C2A-CAA-CBA-CGA
25	B	806	CLA	C2A-CAA-CBA-CGA
25	B	816	CLA	C2A-CAA-CBA-CGA
25	B	843	CLA	C2A-CAA-CBA-CGA
25	K	204	CLA	C2A-CAA-CBA-CGA
25	O	2001	CLA	C2A-CAA-CBA-CGA
25	U	309	CLA	C2A-CAA-CBA-CGA
25	W	301	CLA	C2A-CAA-CBA-CGA
25	A	812	CLA	O1D-CGD-O2D-CED
25	A	815	CLA	O1D-CGD-O2D-CED
25	A	804	CLA	C15-C16-C17-C18
25	A	842	CLA	C5-C6-C7-C8
25	B	807	CLA	C15-C16-C17-C18
25	B	809	CLA	C5-C6-C7-C8
25	B	814	CLA	C10-C11-C12-C13
25	B	829	CLA	C15-C16-C17-C18
25	B	834	CLA	C8-C10-C11-C12
25	S	301	CLA	C8-C10-C11-C12
25	S	302	CLA	C5-C6-C7-C8
25	T	301	CLA	C8-C10-C11-C12
34	A	844	PQN	C18-C20-C21-C22
28	2	619	LHG	C7-C8-C9-C10
28	2	619	LHG	C23-C24-C25-C26
36	B	850	DGD	C1B-C2B-C3B-C4B
24	T	306	CHL	O1A-CGA-O2A-C1
25	W	302	CLA	O1A-CGA-O2A-C1
25	1	613	CLA	O1D-CGD-O2D-CED
25	2	612	CLA	C5-C6-C7-C8
25	A	815	CLA	C8-C10-C11-C12
25	A	825	CLA	C15-C16-C17-C18
25	A	837	CLA	C5-C6-C7-C8
25	B	805	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	B	809	CLA	C15-C16-C17-C18
25	P	301	CLA	C10-C11-C12-C13
25	R	306	CLA	C10-C11-C12-C13
25	W	310	CLA	C5-C6-C7-C8
25	P	301	CLA	O1A-CGA-O2A-C1
25	B	810	CLA	C8-C10-C11-C12
28	3	322	LHG	O9-C7-O7-C5
24	2	615	CHL	O1D-CGD-O2D-CED
25	A	814	CLA	O1D-CGD-O2D-CED
25	4	313	CLA	C5-C6-C7-C8
25	A	817	CLA	C13-C15-C16-C17
25	B	824	CLA	C10-C11-C12-C13
25	R	306	CLA	C15-C16-C17-C18
25	U	303	CLA	CBD-CGD-O2D-CED
25	B	806	CLA	O1A-CGA-O2A-C1
25	S	309	CLA	O1A-CGA-O2A-C1
25	W	312	CLA	O1A-CGA-O2A-C1
25	A	825	CLA	C2-C3-C5-C6
25	6	610	CLA	O1D-CGD-O2D-CED
25	A	833	CLA	O1D-CGD-O2D-CED
25	3	307	CLA	C5-C6-C7-C8
25	A	831	CLA	C15-C16-C17-C18
24	T	305	CHL	CBA-CGA-O2A-C1
25	6	613	CLA	CBA-CGA-O2A-C1
25	P	310	CLA	CBA-CGA-O2A-C1
25	X	310	CLA	CBD-CGD-O2D-CED
31	2	620	LMG	C11-C10-O7-C8
25	A	832	CLA	O1A-CGA-O2A-C1
25	A	839	CLA	O1A-CGA-O2A-C1
25	N	203	CLA	O1D-CGD-O2D-CED
25	R	314	CLA	C3-C5-C6-C7
25	S	312	CLA	O1D-CGD-O2D-CED
25	B	813	CLA	C10-C11-C12-C13
31	2	620	LMG	O9-C10-O7-C8
25	1	603	CLA	C2A-CAA-CBA-CGA
25	3	311	CLA	C2A-CAA-CBA-CGA
25	A	819	CLA	C2A-CAA-CBA-CGA
25	A	829	CLA	C2A-CAA-CBA-CGA
25	A	845	CLA	C2A-CAA-CBA-CGA
25	A	856	CLA	C2A-CAA-CBA-CGA
25	B	830	CLA	C2A-CAA-CBA-CGA
25	H	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	L	303	CLA	C2A-CAA-CBA-CGA
25	V	311	CLA	C2A-CAA-CBA-CGA
25	P	309	CLA	O1D-CGD-O2D-CED
24	Q	308	CHL	CBA-CGA-O2A-C1
24	R	309	CHL	CBA-CGA-O2A-C1
25	A	817	CLA	CBA-CGA-O2A-C1
25	B	803	CLA	CBA-CGA-O2A-C1
25	1	603	CLA	C5-C6-C7-C8
25	B	802	CLA	C15-C16-C17-C18
25	B	810	CLA	C5-C6-C7-C8
25	P	310	CLA	C8-C10-C11-C12
25	P	311	CLA	C8-C10-C11-C12
25	R	314	CLA	C5-C6-C7-C8
25	V	301	CLA	C10-C11-C12-C13
25	B	806	CLA	CBD-CGD-O2D-CED
24	T	307	CHL	O1D-CGD-O2D-CED
24	U	305	CHL	O1D-CGD-O2D-CED
25	A	818	CLA	O1D-CGD-O2D-CED
25	T	301	CLA	O1D-CGD-O2D-CED
25	A	807	CLA	C13-C15-C16-C17
25	A	819	CLA	C10-C11-C12-C13
25	A	827	CLA	C5-C6-C7-C8
25	A	839	CLA	C13-C15-C16-C17
25	A	842	CLA	C13-C15-C16-C17
25	B	802	CLA	C13-C15-C16-C17
25	B	804	CLA	C10-C11-C12-C13
25	B	819	CLA	C5-C6-C7-C8
25	B	839	CLA	C5-C6-C7-C8
25	P	309	CLA	C13-C15-C16-C17
25	R	313	CLA	C8-C10-C11-C12
34	A	844	PQN	C25-C26-C27-C28
25	A	841	CLA	O1D-CGD-O2D-CED
25	Q	306	CLA	O1D-CGD-O2D-CED
25	A	804	CLA	CBA-CGA-O2A-C1
25	Q	301	CLA	CBA-CGA-O2A-C1
25	2	613	CLA	C2A-CAA-CBA-CGA
25	K	203	CLA	C13-C15-C16-C17
29	P	315	Q6L	C11-C12-C13-C42
29	W	315	Q6L	C11-C12-C13-C42
25	A	816	CLA	O1D-CGD-O2D-CED
25	U	302	CLA	C5-C6-C7-C8
25	2	609	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B	815	CLA	O1D-CGD-O2D-CED
25	B	814	CLA	C15-C16-C17-C18
25	R	314	CLA	CBD-CGD-O2D-CED
25	V	311	CLA	O1D-CGD-O2D-CED
25	A	803	CLA	C16-C17-C18-C20
25	A	819	CLA	C11-C12-C13-C14
25	B	839	CLA	C15-C16-C17-C18
25	B	843	CLA	C15-C16-C17-C18
26	S	318	IWJ	C20-C19-C21-C22
29	2	616	Q6L	C23-C22-C24-C25
29	P	319	Q6L	C28-C27-C29-C30
29	R	319	Q6L	C28-C27-C29-C30
29	X	301	Q6L	C28-C27-C29-C30
30	3	318	BCR	C11-C12-C13-C35
30	B	845	BCR	C7-C8-C9-C34
30	H	305	BCR	C11-C12-C13-C35
30	M	101	BCR	C7-C8-C9-C34
25	B	832	CLA	C2A-CAA-CBA-CGA
26	S	318	IWJ	C18-C19-C21-C22
27	1	612	XAT	C7-C8-C9-C10
27	4	318	XAT	C27-C28-C29-C30
29	R	319	Q6L	C26-C27-C29-C30
29	R	323	Q6L	C21-C22-C24-C25
29	T	315	Q6L	C26-C27-C29-C30
29	U	314	Q6L	C15-C16-C17-C18
29	X	301	Q6L	C26-C27-C29-C30
30	A	851	BCR	C21-C22-C23-C24
30	I	101	BCR	C7-C8-C9-C10
36	A	854	DGD	O6D-C5D-C6D-O5D
25	P	310	CLA	O1A-CGA-O2A-C1
24	3	306	CHL	C2A-CAA-CBA-CGA
24	T	306	CHL	C2A-CAA-CBA-CGA
25	2	606	CLA	C2A-CAA-CBA-CGA
25	B	840	CLA	C2A-CAA-CBA-CGA
25	A	832	CLA	C16-C17-C18-C19
25	T	312	CLA	C6-C7-C8-C9
34	A	844	PQN	C26-C27-C28-C30
24	R	309	CHL	O1A-CGA-O2A-C1
25	A	819	CLA	C3-C5-C6-C7
36	A	854	DGD	C4D-C5D-C6D-O5D
25	3	308	CLA	O1D-CGD-O2D-CED
25	A	805	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	A	821	CLA	O1D-CGD-O2D-CED
25	V	312	CLA	CBA-CGA-O2A-C1
24	P	306	CHL	C2-C1-O2A-CGA
24	S	306	CHL	C2-C1-O2A-CGA
25	A	827	CLA	C2-C1-O2A-CGA
25	B	819	CLA	C2-C1-O2A-CGA
25	B	831	CLA	C2-C1-O2A-CGA
25	2	609	CLA	C6-C7-C8-C10
25	3	311	CLA	C6-C7-C8-C9
25	B	811	CLA	C16-C17-C18-C19
25	B	818	CLA	C6-C7-C8-C9
25	T	312	CLA	C6-C7-C8-C10
34	A	844	PQN	C26-C27-C28-C29
25	6	613	CLA	O1A-CGA-O2A-C1
25	B	803	CLA	O1A-CGA-O2A-C1
25	A	830	CLA	C15-C16-C17-C18
25	A	838	CLA	C15-C16-C17-C18
25	K	206	CLA	C15-C16-C17-C18
25	2	606	CLA	O1D-CGD-O2D-CED
25	B	842	CLA	O1D-CGD-O2D-CED
25	W	310	CLA	O1D-CGD-O2D-CED
25	B	810	CLA	C15-C16-C17-C18
25	B	828	CLA	C13-C15-C16-C17
25	A	817	CLA	O1A-CGA-O2A-C1
25	B	807	CLA	CBA-CGA-O2A-C1
25	Q	306	CLA	CBA-CGA-O2A-C1
25	H	301	CLA	C2A-CAA-CBA-CGA
25	F	802	CLA	O1D-CGD-O2D-CED
25	2	613	CLA	C4B-C3B-CAB-CBB
25	2	614	CLA	C4B-C3B-CAB-CBB
25	4	303	CLA	C4B-C3B-CAB-CBB
25	4	315	CLA	C4B-C3B-CAB-CBB
25	5	610	CLA	C4B-C3B-CAB-CBB
25	6	612	CLA	C4B-C3B-CAB-CBB
25	A	833	CLA	C4B-C3B-CAB-CBB
25	B	819	CLA	C4B-C3B-CAB-CBB
25	B	823	CLA	C4B-C3B-CAB-CBB
25	B	832	CLA	C4B-C3B-CAB-CBB
25	B	835	CLA	C4B-C3B-CAB-CBB
25	G	202	CLA	C4B-C3B-CAB-CBB
25	G	203	CLA	C4B-C3B-CAB-CBB
25	H	301	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	J	102	CLA	C4B-C3B-CAB-CBB
25	K	203	CLA	C4B-C3B-CAB-CBB
25	P	313	CLA	C4B-C3B-CAB-CBB
25	Q	312	CLA	C4B-C3B-CAB-CBB
25	R	305	CLA	C4B-C3B-CAB-CBB
25	R	315	CLA	C4B-C3B-CAB-CBB
25	S	313	CLA	C4B-C3B-CAB-CBB
25	T	313	CLA	C4B-C3B-CAB-CBB
25	U	309	CLA	C4B-C3B-CAB-CBB
25	W	302	CLA	C4B-C3B-CAB-CBB
25	3	301	CLA	C11-C12-C13-C14
25	3	301	CLA	C11-C12-C13-C15
25	3	311	CLA	C6-C7-C8-C10
25	B	811	CLA	C16-C17-C18-C20
25	Q	311	CLA	C6-C7-C8-C10
25	W	312	CLA	C6-C7-C8-C9
25	2	612	CLA	C2A-CAA-CBA-CGA
25	X	302	CLA	C5-C6-C7-C8
28	1	614	LHG	C8-C7-O7-C5
25	A	821	CLA	C11-C10-C8-C7
25	A	839	CLA	C12-C13-C15-C16
25	B	814	CLA	C11-C10-C8-C7
25	R	306	CLA	C11-C12-C13-C15
33	A	802	CL0	C12-C13-C15-C16
25	B	813	CLA	C13-C15-C16-C17
25	4	313	CLA	C3-C5-C6-C7
24	2	601	CHL	C3A-C2A-CAA-CBA
24	P	305	CHL	C3A-C2A-CAA-CBA
24	P	314	CHL	C3A-C2A-CAA-CBA
24	Q	307	CHL	C3A-C2A-CAA-CBA
24	R	302	CHL	C3A-C2A-CAA-CBA
24	V	314	CHL	C3A-C2A-CAA-CBA
24	W	307	CHL	C3A-C2A-CAA-CBA
25	2	603	CLA	C3A-C2A-CAA-CBA
25	2	614	CLA	C3A-C2A-CAA-CBA
25	3	302	CLA	C3A-C2A-CAA-CBA
25	3	310	CLA	C3A-C2A-CAA-CBA
25	6	610	CLA	C3A-C2A-CAA-CBA
25	6	613	CLA	C3A-C2A-CAA-CBA
25	A	805	CLA	C3A-C2A-CAA-CBA
25	A	811	CLA	C3A-C2A-CAA-CBA
25	A	840	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	A	842	CLA	C3A-C2A-CAA-CBA
25	B	809	CLA	C3A-C2A-CAA-CBA
25	B	818	CLA	C3A-C2A-CAA-CBA
25	B	821	CLA	C3A-C2A-CAA-CBA
25	B	839	CLA	C3A-C2A-CAA-CBA
25	H	302	CLA	C3A-C2A-CAA-CBA
25	Q	306	CLA	C3A-C2A-CAA-CBA
25	Q	311	CLA	C3A-C2A-CAA-CBA
25	Q	313	CLA	C3A-C2A-CAA-CBA
25	R	305	CLA	C3A-C2A-CAA-CBA
25	S	310	CLA	C3A-C2A-CAA-CBA
25	S	311	CLA	C3A-C2A-CAA-CBA
25	T	312	CLA	C3A-C2A-CAA-CBA
25	F	803	CLA	O1D-CGD-O2D-CED
25	L	301	CLA	O1D-CGD-O2D-CED
25	R	307	CLA	O1D-CGD-O2D-CED
25	Q	301	CLA	C5-C6-C7-C8
24	P	306	CHL	O1D-CGD-O2D-CED
26	1	611	IWJ	C10-C11-C12-C13
29	V	319	Q6L	C24-C25-C26-C27
29	X	301	Q6L	C24-C25-C26-C27
25	A	803	CLA	C16-C17-C18-C19
25	B	810	CLA	C16-C17-C18-C20
25	Q	311	CLA	C6-C7-C8-C9
25	W	312	CLA	C6-C7-C8-C10
24	T	305	CHL	O1A-CGA-O2A-C1
25	A	826	CLA	CBD-CGD-O2D-CED
25	A	815	CLA	CBA-CGA-O2A-C1
25	P	313	CLA	CBA-CGA-O2A-C1
25	6	611	CLA	O1D-CGD-O2D-CED
25	A	823	CLA	O1D-CGD-O2D-CED
25	Q	301	CLA	O1D-CGD-O2D-CED
25	3	307	CLA	O1A-CGA-O2A-C1
25	A	804	CLA	O1A-CGA-O2A-C1
25	Q	301	CLA	O1A-CGA-O2A-C1
32	6	617	SQD	C31-C32-C33-C34
25	2	602	CLA	C8-C10-C11-C12
24	2	607	CHL	O1D-CGD-O2D-CED
25	B	810	CLA	C16-C17-C18-C19
31	A	857	LMG	C28-C29-C30-C31
25	V	312	CLA	O1A-CGA-O2A-C1
25	2	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	2	614	CLA	C2B-C3B-CAB-CBB
25	4	315	CLA	C2B-C3B-CAB-CBB
25	5	610	CLA	C2B-C3B-CAB-CBB
25	A	836	CLA	C2B-C3B-CAB-CBB
25	A	838	CLA	C2B-C3B-CAB-CBB
25	B	819	CLA	C2B-C3B-CAB-CBB
25	B	823	CLA	C2B-C3B-CAB-CBB
25	B	832	CLA	C2B-C3B-CAB-CBB
25	G	202	CLA	C2B-C3B-CAB-CBB
25	G	203	CLA	C2B-C3B-CAB-CBB
25	J	102	CLA	C2B-C3B-CAB-CBB
25	K	203	CLA	C2B-C3B-CAB-CBB
25	O	2004	CLA	C2B-C3B-CAB-CBB
25	Q	313	CLA	C2B-C3B-CAB-CBB
25	R	315	CLA	C2B-C3B-CAB-CBB
25	S	310	CLA	C2B-C3B-CAB-CBB
25	S	313	CLA	C2B-C3B-CAB-CBB
25	T	309	CLA	C2B-C3B-CAB-CBB
25	T	313	CLA	C2B-C3B-CAB-CBB
25	U	310	CLA	C2B-C3B-CAB-CBB
25	V	302	CLA	C2B-C3B-CAB-CBB
25	W	302	CLA	C2B-C3B-CAB-CBB
25	X	312	CLA	C2B-C3B-CAB-CBB
25	X	314	CLA	C2B-C3B-CAB-CBB
30	I	101	BCR	C23-C24-C25-C26
30	I	101	BCR	C23-C24-C25-C30
30	J	101	BCR	C23-C24-C25-C26
30	J	101	BCR	C23-C24-C25-C30
30	K	207	BCR	C1-C6-C7-C8
30	L	305	BCR	C5-C6-C7-C8
30	L	307	BCR	C1-C6-C7-C8
30	M	101	BCR	C23-C24-C25-C26
30	M	101	BCR	C23-C24-C25-C30
25	B	837	CLA	CBD-CGD-O2D-CED
25	J	102	CLA	O1D-CGD-O2D-CED
25	3	307	CLA	CBA-CGA-O2A-C1
25	A	842	CLA	CBA-CGA-O2A-C1
25	P	312	CLA	CBA-CGA-O2A-C1
25	B	806	CLA	C5-C6-C7-C8
25	2	611	CLA	C2A-CAA-CBA-CGA
25	4	313	CLA	C2A-CAA-CBA-CGA
25	B	821	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	Q	314	CLA	C4-C3-C5-C6
25	W	309	CLA	C4-C3-C5-C6
29	P	315	Q6L	C11-C12-C13-C14
29	W	315	Q6L	C11-C12-C13-C14
28	3	321	LHG	C34-C35-C36-C37
31	5	613	LMG	C16-C17-C18-C19
25	4	313	CLA	CBA-CGA-O2A-C1
25	B	809	CLA	CBA-CGA-O2A-C1
25	R	313	CLA	CBA-CGA-O2A-C1
25	R	306	CLA	C3-C5-C6-C7
25	B	842	CLA	C6-C7-C8-C9
25	P	311	CLA	C5-C6-C7-C8
24	Q	308	CHL	O1A-CGA-O2A-C1
32	6	617	SQD	C29-C30-C31-C32
25	K	204	CLA	O1A-CGA-O2A-C1
25	A	834	CLA	CBA-CGA-O2A-C1
29	O	2007	Q6L	C24-C25-C26-C27
29	X	316	Q6L	C17-C18-C19-C20
25	A	825	CLA	C16-C17-C18-C19
25	B	843	CLA	C16-C17-C18-C19
28	6	616	LHG	C8-C7-O7-C5
28	1	614	LHG	C28-C29-C30-C31
28	1	614	LHG	O9-C7-O7-C5
31	B	801	LMG	C12-C13-C14-C15
25	A	837	CLA	C15-C16-C17-C18
25	T	302	CLA	C8-C10-C11-C12
29	R	319	Q6L	C15-C16-C17-C41
29	X	316	Q6L	C15-C16-C17-C41
30	A	849	BCR	C37-C22-C23-C24
28	1	614	LHG	C30-C31-C32-C33
25	B	830	CLA	C3-C5-C6-C7
25	L	302	CLA	C2C-C3C-CAC-CBC
25	2	603	CLA	C2A-CAA-CBA-CGA
25	3	307	CLA	C2A-CAA-CBA-CGA
25	T	311	CLA	C2A-CAA-CBA-CGA
25	6	610	CLA	C14-C13-C15-C16
25	2	609	CLA	C6-C7-C8-C9
25	A	813	CLA	C16-C17-C18-C20
25	A	821	CLA	C16-C17-C18-C19
25	B	818	CLA	C6-C7-C8-C10
25	B	839	CLA	C16-C17-C18-C19
25	L	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	S	303	CLA	O1D-CGD-O2D-CED
25	A	835	CLA	C13-C15-C16-C17
25	A	842	CLA	O1A-CGA-O2A-C1
25	Q	306	CLA	O1A-CGA-O2A-C1
25	R	313	CLA	O1A-CGA-O2A-C1
25	3	301	CLA	C3-C5-C6-C7
31	F	805	LMG	O6-C5-C6-O5
25	A	805	CLA	C15-C16-C17-C18
25	A	813	CLA	C15-C16-C17-C18
25	B	810	CLA	C10-C11-C12-C13
25	H	302	CLA	C8-C10-C11-C12
25	S	310	CLA	C10-C11-C12-C13
28	3	323	LHG	C15-C16-C17-C18
24	W	314	CHL	O1D-CGD-O2D-CED
28	A	847	LHG	C8-C7-O7-C5
31	L	308	LMG	C11-C10-O7-C8
38	P	308	KC2	C4C-C3C-CAC-CBC
38	Q	310	KC2	C4C-C3C-CAC-CBC
38	T	308	KC2	C4C-C3C-CAC-CBC
38	U	307	KC2	C4C-C3C-CAC-CBC
38	X	309	KC2	C4C-C3C-CAC-CBC
25	A	813	CLA	C16-C17-C18-C19
25	A	819	CLA	C11-C12-C13-C15
25	A	825	CLA	C16-C17-C18-C20
25	A	815	CLA	O1A-CGA-O2A-C1
25	B	807	CLA	O1A-CGA-O2A-C1
25	B	809	CLA	O1A-CGA-O2A-C1
24	X	307	CHL	O1D-CGD-O2D-CED
31	J	104	LMG	C10-C11-C12-C13
25	A	819	CLA	C8-C10-C11-C12
25	A	843	CLA	C13-C15-C16-C17
25	Q	304	CLA	C10-C11-C12-C13
25	R	306	CLA	C8-C10-C11-C12
24	T	314	CHL	O1D-CGD-O2D-CED
31	A	855	LMG	O6-C5-C6-O5
31	O	2008	LMG	O6-C5-C6-O5
25	B	819	CLA	C3-C5-C6-C7
25	A	832	CLA	CBD-CGD-O2D-CED
36	B	850	DGD	O2G-C2G-C3G-O3G
32	6	617	SQD	C24-C23-O48-C46
25	P	312	CLA	O1A-CGA-O2A-C1
36	A	854	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
25	A	834	CLA	C5-C6-C7-C8
25	B	808	CLA	C4C-C3C-CAC-CBC
24	4	307	CHL	C3A-C2A-CAA-CBA
25	Q	315	CLA	C2-C1-O2A-CGA
25	B	843	CLA	C16-C17-C18-C20
25	A	825	CLA	C4-C3-C5-C6
25	A	807	CLA	C15-C16-C17-C18
25	4	303	CLA	C2A-CAA-CBA-CGA
25	A	808	CLA	C2A-CAA-CBA-CGA
25	B	813	CLA	C2A-CAA-CBA-CGA
25	B	814	CLA	C2A-CAA-CBA-CGA
25	B	815	CLA	C2A-CAA-CBA-CGA
25	R	315	CLA	C2A-CAA-CBA-CGA
25	S	302	CLA	CBD-CGD-O2D-CED
25	H	301	CLA	O1D-CGD-O2D-CED
25	U	309	CLA	O1D-CGD-O2D-CED
25	O	2002	CLA	C8-C10-C11-C12
25	5	602	CLA	O1D-CGD-O2D-CED
25	B	843	CLA	O1D-CGD-O2D-CED
25	P	313	CLA	O1A-CGA-O2A-C1
25	3	302	CLA	C1A-C2A-CAA-CBA
25	3	310	CLA	C1A-C2A-CAA-CBA
25	4	303	CLA	C1A-C2A-CAA-CBA
25	4	310	CLA	C1A-C2A-CAA-CBA
25	5	601	CLA	C1A-C2A-CAA-CBA
25	A	805	CLA	C1A-C2A-CAA-CBA
25	A	811	CLA	C1A-C2A-CAA-CBA
25	A	813	CLA	C1A-C2A-CAA-CBA
25	A	817	CLA	C1A-C2A-CAA-CBA
25	A	820	CLA	C1A-C2A-CAA-CBA
25	A	821	CLA	C1A-C2A-CAA-CBA
25	A	834	CLA	C1A-C2A-CAA-CBA
25	B	811	CLA	C1A-C2A-CAA-CBA
25	B	813	CLA	C1A-C2A-CAA-CBA
25	B	820	CLA	C1A-C2A-CAA-CBA
25	P	301	CLA	C1A-C2A-CAA-CBA
25	P	309	CLA	C1A-C2A-CAA-CBA
25	Q	313	CLA	C1A-C2A-CAA-CBA
25	R	306	CLA	C1A-C2A-CAA-CBA
25	R	314	CLA	C1A-C2A-CAA-CBA
25	S	301	CLA	C1A-C2A-CAA-CBA
25	S	311	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	T	301	CLA	C1A-C2A-CAA-CBA
25	2	614	CLA	O1D-CGD-O2D-CED
25	B	811	CLA	C5-C6-C7-C8
25	4	310	CLA	C5-C6-C7-C8
25	4	313	CLA	O1A-CGA-O2A-C1
25	T	301	CLA	O1A-CGA-O2A-C1
24	W	307	CHL	C15-C16-C17-C18
25	R	314	CLA	O1D-CGD-O2D-CED
24	W	307	CHL	C11-C12-C13-C15
25	2	612	CLA	C11-C10-C8-C7
25	5	607	CLA	C6-C7-C8-C10
25	A	812	CLA	C6-C7-C8-C10
25	A	812	CLA	C12-C13-C15-C16
25	A	815	CLA	C12-C13-C15-C16
25	A	821	CLA	C12-C13-C15-C16
25	A	823	CLA	C12-C13-C15-C16
25	A	825	CLA	C11-C12-C13-C15
25	A	827	CLA	C11-C10-C8-C7
25	A	828	CLA	C11-C10-C8-C7
25	A	830	CLA	C6-C7-C8-C10
25	A	830	CLA	C12-C13-C15-C16
25	A	831	CLA	C12-C13-C15-C16
25	B	803	CLA	C12-C13-C15-C16
25	B	804	CLA	C11-C10-C8-C7
25	B	842	CLA	C12-C13-C15-C16
25	R	305	CLA	C11-C12-C13-C15
25	S	302	CLA	C11-C12-C13-C15
34	A	844	PQN	C16-C17-C18-C20
25	A	831	CLA	C16-C17-C18-C19
25	B	839	CLA	C16-C17-C18-C20
25	A	803	CLA	C15-C16-C17-C18
25	U	309	CLA	O1A-CGA-O2A-C1
32	6	617	SQD	O10-C23-O48-C46
25	3	305	CLA	C3A-C2A-CAA-CBA
25	B	831	CLA	C10-C11-C12-C13
25	K	203	CLA	C10-C11-C12-C13
29	S	315	Q6L	C11-C12-C13-C14
29	V	316	Q6L	C11-C12-C13-C14
25	B	803	CLA	C2A-CAA-CBA-CGA
25	P	312	CLA	C2A-CAA-CBA-CGA
25	R	313	CLA	C2A-CAA-CBA-CGA
25	W	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	5	602	CLA	C11-C10-C8-C9
25	A	812	CLA	C6-C7-C8-C9
25	A	812	CLA	C14-C13-C15-C16
25	A	813	CLA	C11-C10-C8-C9
25	A	825	CLA	C11-C12-C13-C14
25	A	830	CLA	C11-C10-C8-C9
25	A	830	CLA	C14-C13-C15-C16
25	B	803	CLA	C14-C13-C15-C16
25	B	807	CLA	C6-C7-C8-C9
25	B	807	CLA	C14-C13-C15-C16
25	B	811	CLA	C11-C12-C13-C14
25	B	813	CLA	C11-C10-C8-C9
25	B	814	CLA	C11-C10-C8-C9
25	B	826	CLA	C11-C10-C8-C9
25	S	302	CLA	C11-C12-C13-C14
25	S	309	CLA	C11-C10-C8-C9
29	U	314	Q6L	C24-C25-C26-C27
25	A	832	CLA	C16-C17-C18-C20
24	T	320	CHL	CBA-CGA-O2A-C1
25	B	840	CLA	CBA-CGA-O2A-C1
25	P	309	CLA	CBA-CGA-O2A-C1
25	S	310	CLA	CBA-CGA-O2A-C1
25	T	301	CLA	CBA-CGA-O2A-C1
24	P	314	CHL	O1D-CGD-O2D-CED
25	2	604	CLA	O1D-CGD-O2D-CED
28	6	616	LHG	O9-C7-O7-C5
25	B	808	CLA	C8-C10-C11-C12
28	Q	302	LHG	C4-C5-C6-O8
31	L	308	LMG	O6-C5-C6-O5
25	5	609	CLA	CBA-CGA-O2A-C1
25	B	810	CLA	CBA-CGA-O2A-C1
25	V	310	CLA	CBA-CGA-O2A-C1
28	3	322	LHG	C24-C23-O8-C6
25	A	821	CLA	C16-C17-C18-C20
25	P	311	CLA	C11-C12-C13-C14
25	X	310	CLA	O1D-CGD-O2D-CED
24	3	306	CHL	CHA-CBD-CGD-O2D
24	Q	307	CHL	CHA-CBD-CGD-O1D
24	R	302	CHL	CHA-CBD-CGD-O1D
24	R	302	CHL	CHA-CBD-CGD-O2D
24	T	320	CHL	CHA-CBD-CGD-O1D
24	T	320	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	U	305	CHL	CHA-CBD-CGD-O1D
29	S	315	Q6L	C11-C12-C13-C42
34	B	844	PQN	C14-C13-C15-C16
29	P	321	Q6L	C11-C12-C13-C14
29	W	319	Q6L	C11-C12-C13-C14
25	A	808	CLA	C13-C15-C16-C17
29	W	316	Q6L	C28-C27-C29-C30
30	A	851	BCR	C7-C8-C9-C34
30	J	101	BCR	C7-C8-C9-C34
28	A	847	LHG	O9-C7-O7-C5
25	X	311	CLA	C4C-C3C-CAC-CBC
36	B	850	DGD	O6E-C5E-C6E-O5E
27	3	316	XAT	C7-C8-C9-C10
29	2	616	Q6L	C21-C22-C24-C25
25	2	612	CLA	C8-C10-C11-C12
31	J	104	LMG	C11-C12-C13-C14
25	B	842	CLA	C5-C6-C7-C8
25	P	309	CLA	O1A-CGA-O2A-C1
25	U	303	CLA	O1D-CGD-O2D-CED
25	P	313	CLA	O2A-C1-C2-C3
24	X	307	CHL	O2A-C1-C2-C3
24	R	302	CHL	C3C-C2C-CMC-OMC
24	V	304	CHL	C3C-C2C-CMC-OMC
26	X	318	IWJ	C21-C22-C23-C24
25	B	826	CLA	C3-C5-C6-C7
24	U	313	CHL	CBD-CGD-O2D-CED
28	3	323	LHG	O6-C4-C5-O7
25	K	206	CLA	CBA-CGA-O2A-C1
25	P	303	CLA	CBA-CGA-O2A-C1
25	S	301	CLA	CBA-CGA-O2A-C1
28	Q	302	LHG	C29-C30-C31-C32
25	A	838	CLA	C4-C3-C5-C6
29	V	316	Q6L	C11-C12-C13-C42
25	W	309	CLA	C2-C3-C5-C6
29	R	304	Q6L	C11-C12-C13-C14
25	A	831	CLA	C16-C17-C18-C20
25	R	305	CLA	CBD-CGD-O2D-CED
28	A	846	LHG	C27-C28-C29-C30
28	Q	302	LHG	O7-C5-C6-O8
32	6	617	SQD	O6-C44-C45-O47
25	H	302	CLA	CBA-CGA-O2A-C1
25	U	301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	W	312	CLA	C2A-CAA-CBA-CGA
25	P	302	CLA	C2-C1-O2A-CGA
25	B	840	CLA	O1A-CGA-O2A-C1
31	B	801	LMG	C4-C5-C6-O5
25	A	825	CLA	CBA-CGA-O2A-C1
25	B	808	CLA	CBA-CGA-O2A-C1
24	4	308	CHL	C1C-C2C-CMC-OMC
24	6	605	CHL	C1C-C2C-CMC-OMC
24	Q	309	CHL	C1C-C2C-CMC-OMC
24	V	305	CHL	C1C-C2C-CMC-OMC
24	X	308	CHL	C1C-C2C-CMC-OMC
25	A	856	CLA	CBD-CGD-O2D-CED
25	P	312	CLA	C3-C5-C6-C7
25	U	302	CLA	C11-C10-C8-C9
25	P	311	CLA	C11-C12-C13-C15
34	B	844	PQN	C26-C27-C28-C29
25	A	806	CLA	C4-C3-C5-C6
29	W	319	Q6L	C11-C12-C13-C42
25	B	802	CLA	C10-C11-C12-C13
31	F	805	LMG	C10-C11-C12-C13
24	W	307	CHL	C11-C12-C13-C14
25	2	612	CLA	C11-C12-C13-C14
25	A	810	CLA	C11-C12-C13-C14
25	A	815	CLA	C14-C13-C15-C16
25	A	821	CLA	C14-C13-C15-C16
25	A	823	CLA	C14-C13-C15-C16
25	A	827	CLA	C11-C10-C8-C9
25	A	830	CLA	C6-C7-C8-C9
25	A	831	CLA	C6-C7-C8-C9
25	A	831	CLA	C14-C13-C15-C16
25	B	814	CLA	C6-C7-C8-C9
25	B	830	CLA	C6-C7-C8-C9
25	B	831	CLA	C11-C12-C13-C14
25	O	2001	CLA	C6-C7-C8-C9
25	Q	304	CLA	C6-C7-C8-C9
25	R	305	CLA	C11-C12-C13-C14
25	R	306	CLA	C11-C12-C13-C14
25	S	301	CLA	C6-C7-C8-C9
25	S	310	CLA	C11-C10-C8-C9
25	T	302	CLA	C6-C7-C8-C9
34	A	844	PQN	C16-C17-C18-C19
25	A	813	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	A	834	CLA	O1A-CGA-O2A-C1
25	V	310	CLA	O1A-CGA-O2A-C1
25	1	608	CLA	C4B-C3B-CAB-CBB
25	A	816	CLA	C4B-C3B-CAB-CBB
25	A	838	CLA	C4B-C3B-CAB-CBB
25	O	2004	CLA	C4B-C3B-CAB-CBB
25	Q	304	CLA	C4B-C3B-CAB-CBB
25	Q	313	CLA	C4B-C3B-CAB-CBB
25	R	314	CLA	C4B-C3B-CAB-CBB
25	S	310	CLA	C4B-C3B-CAB-CBB
25	S	312	CLA	C4B-C3B-CAB-CBB
25	T	310	CLA	C4B-C3B-CAB-CBB
25	U	310	CLA	C4B-C3B-CAB-CBB
25	V	310	CLA	C4B-C3B-CAB-CBB
25	V	313	CLA	C4B-C3B-CAB-CBB
25	X	312	CLA	C4B-C3B-CAB-CBB
25	X	314	CLA	C4B-C3B-CAB-CBB
25	2	612	CLA	C13-C15-C16-C17
25	A	810	CLA	C13-C15-C16-C17
25	B	808	CLA	C2A-CAA-CBA-CGA
24	V	314	CHL	C2A-CAA-CBA-CGA
25	2	612	CLA	C6-C7-C8-C10
25	5	602	CLA	C11-C10-C8-C7
25	A	804	CLA	C11-C12-C13-C15
25	A	805	CLA	C11-C12-C13-C15
25	A	807	CLA	C11-C10-C8-C7
25	A	807	CLA	C12-C13-C15-C16
25	A	810	CLA	C11-C12-C13-C15
25	A	813	CLA	C11-C10-C8-C7
25	A	831	CLA	C6-C7-C8-C10
25	A	832	CLA	C11-C12-C13-C15
25	A	832	CLA	C12-C13-C15-C16
25	A	838	CLA	C12-C13-C15-C16
25	B	803	CLA	C11-C10-C8-C7
25	B	807	CLA	C6-C7-C8-C10
25	B	807	CLA	C12-C13-C15-C16
25	B	809	CLA	C6-C7-C8-C10
25	B	811	CLA	C11-C12-C13-C15
25	B	813	CLA	C12-C13-C15-C16
25	B	814	CLA	C6-C7-C8-C10
25	B	830	CLA	C6-C7-C8-C10
25	B	834	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	B	836	CLA	C11-C10-C8-C7
25	O	2001	CLA	C6-C7-C8-C10
25	P	310	CLA	C11-C10-C8-C7
25	S	302	CLA	C6-C7-C8-C10
25	S	309	CLA	C11-C10-C8-C7
25	S	310	CLA	C11-C10-C8-C7
25	W	309	CLA	C11-C10-C8-C7
25	A	825	CLA	O1A-CGA-O2A-C1
25	S	310	CLA	O1A-CGA-O2A-C1
25	P	309	CLA	C15-C16-C17-C18
25	B	808	CLA	C15-C16-C17-C18
34	A	844	PQN	C23-C25-C26-C27
25	X	302	CLA	C6-C7-C8-C10
24	T	320	CHL	O1A-CGA-O2A-C1
24	1	601	CHL	C3A-C2A-CAA-CBA
25	4	309	CLA	C3A-C2A-CAA-CBA
25	6	607	CLA	C3A-C2A-CAA-CBA
25	A	806	CLA	C3A-C2A-CAA-CBA
25	A	813	CLA	C3A-C2A-CAA-CBA
25	A	825	CLA	C3A-C2A-CAA-CBA
25	A	826	CLA	C3A-C2A-CAA-CBA
25	B	810	CLA	C3A-C2A-CAA-CBA
25	B	811	CLA	C3A-C2A-CAA-CBA
25	B	830	CLA	C3A-C2A-CAA-CBA
25	K	204	CLA	C3A-C2A-CAA-CBA
25	W	301	CLA	C3A-C2A-CAA-CBA
29	R	304	Q6L	C11-C12-C13-C42
25	2	602	CLA	C10-C11-C12-C13
25	A	817	CLA	C8-C10-C11-C12
25	A	839	CLA	C5-C6-C7-C8
25	B	836	CLA	C10-C11-C12-C13
29	Q	318	Q6L	C11-C12-C13-C14
25	A	812	CLA	C5-C6-C7-C8
26	S	318	IWJ	C14-C15-C16-C17
29	2	616	Q6L	C13-C14-C15-C16
29	S	321	Q6L	C17-C18-C19-C20
29	T	319	Q6L	C24-C25-C26-C27
29	V	316	Q6L	C24-C25-C26-C27
29	W	316	Q6L	C13-C14-C15-C16
29	X	317	Q6L	C13-C14-C15-C16
25	U	302	CLA	C3-C5-C6-C7
26	4	317	IWJ	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
25	B	816	CLA	C4-C3-C5-C6
25	B	808	CLA	O1A-CGA-O2A-C1
25	H	302	CLA	O1A-CGA-O2A-C1
31	L	308	LMG	O9-C10-O7-C8
25	R	317	CLA	O2A-C1-C2-C3
25	P	311	CLA	C2A-CAA-CBA-CGA
31	5	613	LMG	C35-C36-C37-C38
26	Q	320	IWJ	C25-C24-C26-O27
26	W	318	IWJ	C25-C24-C26-O27
28	A	847	LHG	C4-C5-C6-O8
31	A	857	LMG	O1-C7-C8-C9
32	6	617	SQD	C44-C45-C46-O48
24	R	302	CHL	C1A-C2A-CAA-CBA
25	3	307	CLA	C10-C11-C12-C13
25	4	303	CLA	C4-C3-C5-C6
25	A	829	CLA	C4-C3-C5-C6
29	P	321	Q6L	C11-C12-C13-C42
29	Q	318	Q6L	C11-C12-C13-C42
25	B	815	CLA	CBA-CGA-O2A-C1
25	A	806	CLA	C2-C3-C5-C6
25	A	837	CLA	C2-C3-C5-C6
25	T	311	CLA	C3-C5-C6-C7
26	Q	320	IWJ	C23-C24-C26-O27
26	W	318	IWJ	C23-C24-C26-O27
25	A	838	CLA	C16-C17-C18-C19
25	A	839	CLA	C16-C17-C18-C19
25	X	302	CLA	C6-C7-C8-C9
25	A	804	CLA	C8-C10-C11-C12
25	B	810	CLA	O1A-CGA-O2A-C1
25	Q	312	CLA	C2B-C3B-CAB-CBB
25	T	310	CLA	C2B-C3B-CAB-CBB
30	2	618	BCR	C23-C24-C25-C30
30	A	851	BCR	C1-C6-C7-C8
30	I	101	BCR	C1-C6-C7-C8
25	2	602	CLA	C14-C13-C15-C16
25	Q	301	CLA	C3-C5-C6-C7
25	H	302	CLA	C10-C11-C12-C13
24	S	314	CHL	CBD-CGD-O2D-CED
25	A	829	CLA	CBD-CGD-O2D-CED
25	B	806	CLA	O1D-CGD-O2D-CED
25	B	837	CLA	O1D-CGD-O2D-CED
25	B	805	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	A	847	LHG	O7-C5-C6-O8
32	6	617	SQD	O47-C45-C46-O48
25	A	826	CLA	O1D-CGD-O2D-CED
25	S	301	CLA	O1A-CGA-O2A-C1
28	3	322	LHG	O10-C23-O8-C6
25	B	808	CLA	C4-C3-C5-C6
25	A	829	CLA	C2-C3-C5-C6
25	B	808	CLA	C2-C3-C5-C6
25	5	607	CLA	C6-C7-C8-C9
25	A	804	CLA	C6-C7-C8-C9
25	A	807	CLA	C11-C10-C8-C9
25	A	807	CLA	C14-C13-C15-C16
25	A	817	CLA	C11-C12-C13-C14
25	A	832	CLA	C11-C12-C13-C14
25	A	832	CLA	C14-C13-C15-C16
25	A	838	CLA	C14-C13-C15-C16
25	B	803	CLA	C11-C10-C8-C9
25	B	836	CLA	C11-C10-C8-C9
25	B	842	CLA	C11-C12-C13-C14
25	B	843	CLA	C14-C13-C15-C16
25	A	838	CLA	C16-C17-C18-C20
24	Q	308	CHL	O2A-C1-C2-C3
25	V	313	CLA	O2A-C1-C2-C3
31	N	201	LMG	C18-C19-C20-C21
25	2	610	CLA	C1A-C2A-CAA-CBA
25	V	309	CLA	C1A-C2A-CAA-CBA
25	X	304	CLA	C1A-C2A-CAA-CBA
25	A	832	CLA	O1D-CGD-O2D-CED
25	B	812	CLA	C2A-CAA-CBA-CGA
25	Q	313	CLA	C2A-CAA-CBA-CGA
25	T	302	CLA	C5-C6-C7-C8
34	A	844	PQN	C15-C16-C17-C18
28	A	847	LHG	C7-C8-C9-C10
24	4	302	CHL	CAA-CBA-CGA-O2A
25	5	609	CLA	O1A-CGA-O2A-C1
25	P	312	CLA	O1D-CGD-O2D-CED
25	B	803	CLA	C3-C5-C6-C7
28	3	321	LHG	O6-C4-C5-C6
30	2	618	BCR	C7-C8-C9-C34
30	G	205	BCR	C36-C18-C19-C20
25	2	612	CLA	C11-C12-C13-C15
25	6	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	A	803	CLA	C11-C10-C8-C7
25	A	804	CLA	C6-C7-C8-C10
25	A	805	CLA	C12-C13-C15-C16
25	A	817	CLA	C11-C12-C13-C15
25	A	825	CLA	C11-C10-C8-C7
25	A	842	CLA	C11-C12-C13-C15
25	B	805	CLA	C11-C12-C13-C15
25	B	810	CLA	C11-C12-C13-C15
25	B	813	CLA	C11-C12-C13-C15
25	B	828	CLA	C12-C13-C15-C16
25	B	829	CLA	C11-C10-C8-C7
25	B	843	CLA	C12-C13-C15-C16
25	R	313	CLA	C12-C13-C15-C16
25	R	314	CLA	C6-C7-C8-C10
25	S	310	CLA	C6-C7-C8-C10
28	3	323	LHG	C9-C10-C11-C12
25	A	805	CLA	C13-C15-C16-C17
25	B	820	CLA	C8-C10-C11-C12
29	X	316	Q6L	C15-C16-C17-C18
30	A	848	BCR	C7-C8-C9-C10
30	A	849	BCR	C21-C22-C23-C24
30	A	851	BCR	C7-C8-C9-C10
30	G	205	BCR	C17-C18-C19-C20
30	H	305	BCR	C17-C18-C19-C20
30	I	101	BCR	C17-C18-C19-C20
30	J	101	BCR	C7-C8-C9-C10
30	J	103	BCR	C17-C18-C19-C20
30	M	101	BCR	C7-C8-C9-C10
25	L	302	CLA	CBA-CGA-O2A-C1
31	J	104	LMG	C29-C28-O8-C9
25	P	303	CLA	O1A-CGA-O2A-C1
32	H	303	SQD	C45-C44-O6-C1
25	B	839	CLA	C13-C15-C16-C17
25	T	311	CLA	C8-C10-C11-C12
25	U	311	CLA	C2A-CAA-CBA-CGA
25	A	837	CLA	C4-C3-C5-C6
25	B	815	CLA	C4-C3-C5-C6
29	X	316	Q6L	C11-C12-C13-C42
25	K	206	CLA	O1A-CGA-O2A-C1
38	T	308	KC2	C2B-C3B-CAB-CBB
38	V	308	KC2	C2B-C3B-CAB-CBB
38	X	309	KC2	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	B	830	CLA	C8-C10-C11-C12
25	B	805	CLA	O2A-C1-C2-C3
25	B	814	CLA	O2A-C1-C2-C3
25	3	309	CLA	O1D-CGD-O2D-CED
25	L	302	CLA	O1A-CGA-O2A-C1
31	J	104	LMG	O10-C28-O8-C9
25	A	828	CLA	C3-C5-C6-C7
29	Q	317	Q6L	C02-C03-C11-C12
29	S	321	Q6L	C02-C03-C11-C12
25	S	302	CLA	C10-C11-C12-C13
31	J	104	LMG	C7-C8-C9-O8
36	B	850	DGD	C1G-C2G-C3G-O3G
38	R	312	KC2	C4C-C3C-CAC-CBC
38	S	308	KC2	C4C-C3C-CAC-CBC
38	V	308	KC2	C4C-C3C-CAC-CBC
38	W	308	KC2	C4C-C3C-CAC-CBC
25	3	302	CLA	C3-C5-C6-C7
29	X	301	Q6L	C11-C12-C13-C42
24	T	320	CHL	C2A-CAA-CBA-CGA
25	A	823	CLA	C2A-CAA-CBA-CGA
25	4	303	CLA	C2-C3-C5-C6
29	X	316	Q6L	C11-C12-C13-C14
34	A	844	PQN	C12-C13-C15-C16
28	A	846	LHG	C15-C16-C17-C18
32	6	617	SQD	C14-C15-C16-C17
31	A	857	LMG	O1-C7-C8-O7
31	J	104	LMG	O7-C8-C9-O8
25	A	805	CLA	C14-C13-C15-C16
25	S	310	CLA	C6-C7-C8-C9
25	T	301	CLA	C11-C12-C13-C14
25	W	309	CLA	C11-C10-C8-C9
25	R	316	CLA	C5-C6-C7-C8
29	2	616	Q6L	C27-C29-C30-C31
29	W	319	Q6L	C27-C29-C30-C31
25	R	315	CLA	C10-C11-C12-C13
24	S	314	CHL	O1D-CGD-O2D-CED
31	A	801	LMG	O7-C10-C11-C12
24	6	601	CHL	C3A-C2A-CAA-CBA
25	A	807	CLA	C2-C1-O2A-CGA
26	3	315	IWJ	C16-C17-C18-C19
25	B	824	CLA	C11-C12-C13-C14
25	B	826	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	T	311	CLA	C10-C11-C12-C13
36	B	850	DGD	O1B-C1B-O2G-C2G
25	B	836	CLA	C5-C6-C7-C8
25	A	842	CLA	C10-C11-C12-C13
25	X	311	CLA	C2C-C3C-CAC-CBC
25	A	805	CLA	C3-C5-C6-C7
24	R	310	CHL	C4C-C3C-CAC-CBC
24	S	305	CHL	C4C-C3C-CAC-CBC
24	X	307	CHL	C4C-C3C-CAC-CBC
25	G	202	CLA	CBD-CGD-O2D-CED
25	5	607	CLA	C16-C17-C18-C20
25	B	808	CLA	C16-C17-C18-C19
25	2	602	CLA	C3-C5-C6-C7
25	T	312	CLA	C3-C5-C6-C7
25	3	307	CLA	C4B-C3B-CAB-CBB
25	3	309	CLA	C4B-C3B-CAB-CBB
25	4	309	CLA	C1A-C2A-CAA-CBA
25	6	603	CLA	C4B-C3B-CAB-CBB
25	6	613	CLA	C1A-C2A-CAA-CBA
25	A	845	CLA	C1A-C2A-CAA-CBA
25	A	856	CLA	C1A-C2A-CAA-CBA
25	B	810	CLA	C4B-C3B-CAB-CBB
25	B	834	CLA	C1A-C2A-CAA-CBA
25	B	836	CLA	C4B-C3B-CAB-CBB
25	B	841	CLA	C4B-C3B-CAB-CBB
25	B	843	CLA	C1A-C2A-CAA-CBA
25	P	302	CLA	C4B-C3B-CAB-CBB
25	R	306	CLA	C4B-C3B-CAB-CBB
26	5	611	IWJ	O27-C26-C28-C29
26	Q	303	IWJ	O27-C26-C28-C29
26	R	303	IWJ	O27-C26-C28-C29
26	S	318	IWJ	O27-C26-C28-C29
26	S	319	IWJ	O27-C26-C28-C29
26	S	322	IWJ	O27-C26-C28-C29
26	T	321	IWJ	O27-C26-C28-C29
26	U	316	IWJ	O27-C26-C28-C29
26	V	317	IWJ	O27-C26-C28-C29
26	V	320	IWJ	O27-C26-C28-C29
25	R	305	CLA	O1D-CGD-O2D-CED
25	T	312	CLA	C4-C3-C5-C6
29	R	319	Q6L	C15-C16-C17-C18
30	3	318	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	A	835	CLA	C16-C17-C18-C20
25	A	825	CLA	C2A-CAA-CBA-CGA
25	L	302	CLA	C2A-CAA-CBA-CGA
25	Q	306	CLA	C2A-CAA-CBA-CGA
28	3	323	LHG	O6-C4-C5-C6
25	O	2001	CLA	CBD-CGD-O2D-CED
25	P	312	CLA	CBD-CGD-O2D-CED
24	S	306	CHL	C2-C3-C5-C6
24	T	306	CHL	C2-C3-C5-C6
25	X	303	CLA	C2-C3-C5-C6
26	4	317	IWJ	C26-C28-C29-C30
25	A	810	CLA	C15-C16-C17-C18
24	W	307	CHL	C6-C7-C8-C10
25	1	608	CLA	C6-C7-C8-C10
25	2	602	CLA	C6-C7-C8-C10
25	B	808	CLA	C12-C13-C15-C16
25	B	826	CLA	C11-C10-C8-C7
25	B	830	CLA	C11-C12-C13-C15
25	B	831	CLA	C6-C7-C8-C10
25	L	302	CLA	C11-C10-C8-C7
25	P	309	CLA	C6-C7-C8-C10
25	P	309	CLA	C11-C12-C13-C15
25	A	839	CLA	C16-C17-C18-C20
25	A	829	CLA	O1D-CGD-O2D-CED
28	A	847	LHG	O2-C2-C3-O3
25	S	312	CLA	CBA-CGA-O2A-C1
25	T	311	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	C4-C3-C5-C6
25	K	203	CLA	C3A-C2A-CAA-CBA
25	B	843	CLA	C13-C15-C16-C17
24	U	305	CHL	C2C-C3C-CAC-CBC
28	3	321	LHG	O6-C4-C5-O7
25	2	612	CLA	C6-C7-C8-C9
25	A	803	CLA	C11-C10-C8-C9
25	A	804	CLA	C11-C12-C13-C14
25	A	805	CLA	C11-C12-C13-C14
25	A	825	CLA	C11-C10-C8-C9
25	A	842	CLA	C11-C12-C13-C14
25	B	810	CLA	C11-C12-C13-C14
25	B	829	CLA	C11-C10-C8-C9
25	R	313	CLA	C14-C13-C15-C16
25	R	314	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	830	CLA	C10-C11-C12-C13
27	4	318	XAT	C33-C34-C35-C15
29	S	323	Q6L	C17-C18-C19-C20
25	5	607	CLA	C10-C11-C12-C13
25	B	804	CLA	C8-C10-C11-C12
24	1	601	CHL	CAD-CBD-CGD-O1D
24	5	605	CHL	CAD-CBD-CGD-O1D
25	1	609	CLA	CAD-CBD-CGD-O1D
26	3	315	IWJ	C26-C28-C29-O39
26	4	317	IWJ	C26-C28-C29-O39
29	2	616	Q6L	C29-C30-C31-C36
29	O	2007	Q6L	C29-C30-C31-C36
38	U	307	KC2	C1A-C2A-CAA-CBA
38	X	309	KC2	C1A-C2A-CAA-CBA
25	A	825	CLA	C10-C11-C12-C13
25	3	313	CLA	CBD-CGD-O2D-CED
25	S	312	CLA	O1A-CGA-O2A-C1
28	1	614	LHG	O7-C5-C6-O8
25	6	602	CLA	O1D-CGD-O2D-CED
25	5	609	CLA	C6-C7-C8-C9
25	3	309	CLA	CBD-CGD-O2D-CED
32	6	617	SQD	O6-C44-C45-C46
36	B	850	DGD	O1G-C1G-C2G-C3G
25	B	829	CLA	C2C-C3C-CAC-CBC
24	2	615	CHL	CAD-CBD-CGD-O2D
24	R	308	CHL	CAD-CBD-CGD-O2D
24	T	304	CHL	CAD-CBD-CGD-O2D
25	1	602	CLA	CAD-CBD-CGD-O2D
25	1	610	CLA	CAD-CBD-CGD-O2D
25	A	807	CLA	CAD-CBD-CGD-O2D
25	A	815	CLA	CAD-CBD-CGD-O2D
25	A	816	CLA	CAD-CBD-CGD-O2D
25	A	824	CLA	CAD-CBD-CGD-O2D
25	B	839	CLA	CAD-CBD-CGD-O2D
25	H	302	CLA	CAD-CBD-CGD-O2D
25	O	2004	CLA	CAD-CBD-CGD-O2D
25	U	310	CLA	CAD-CBD-CGD-O2D
25	3	313	CLA	O1D-CGD-O2D-CED
25	T	311	CLA	CBA-CGA-O2A-C1
25	A	839	CLA	C8-C10-C11-C12
34	B	844	PQN	C26-C27-C28-C30
24	U	305	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	A	826	CLA	C2A-CAA-CBA-CGA
25	A	828	CLA	C11-C12-C13-C14
25	A	820	CLA	C5-C6-C7-C8
25	A	831	CLA	C5-C6-C7-C8
24	V	307	CHL	C2C-C3C-CAC-CBC
25	S	302	CLA	O1D-CGD-O2D-CED
24	2	615	CHL	CAD-CBD-CGD-O1D
24	3	306	CHL	CHA-CBD-CGD-O1D
24	6	605	CHL	CHA-CBD-CGD-O1D
24	6	605	CHL	CHA-CBD-CGD-O2D
24	P	306	CHL	CHA-CBD-CGD-O1D
24	P	306	CHL	CHA-CBD-CGD-O2D
24	Q	307	CHL	CHA-CBD-CGD-O2D
24	Q	308	CHL	CHA-CBD-CGD-O1D
24	Q	308	CHL	CHA-CBD-CGD-O2D
24	Q	316	CHL	CHA-CBD-CGD-O1D
24	Q	316	CHL	CHA-CBD-CGD-O2D
24	R	308	CHL	CAD-CBD-CGD-O1D
24	R	310	CHL	CHA-CBD-CGD-O1D
24	R	310	CHL	CHA-CBD-CGD-O2D
24	T	304	CHL	CAD-CBD-CGD-O1D
24	T	306	CHL	CHA-CBD-CGD-O1D
24	T	306	CHL	CHA-CBD-CGD-O2D
24	U	305	CHL	CHA-CBD-CGD-O2D
25	1	605	CLA	CHA-CBD-CGD-O2D
25	1	605	CLA	CAD-CBD-CGD-O2D
25	1	608	CLA	CAD-CBD-CGD-O1D
25	1	610	CLA	CAD-CBD-CGD-O1D
25	1	613	CLA	CHA-CBD-CGD-O1D
25	1	613	CLA	CHA-CBD-CGD-O2D
25	2	602	CLA	CHA-CBD-CGD-O1D
25	2	602	CLA	CHA-CBD-CGD-O2D
25	2	604	CLA	CHA-CBD-CGD-O1D
25	2	604	CLA	CHA-CBD-CGD-O2D
25	2	613	CLA	CHA-CBD-CGD-O2D
25	2	613	CLA	CAD-CBD-CGD-O2D
25	2	614	CLA	CHA-CBD-CGD-O1D
25	3	311	CLA	CHA-CBD-CGD-O2D
25	4	314	CLA	CAD-CBD-CGD-O1D
25	6	602	CLA	CHA-CBD-CGD-O1D
25	6	610	CLA	CAD-CBD-CGD-O1D
25	A	807	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	A	815	CLA	CAD-CBD-CGD-O1D
25	A	816	CLA	CAD-CBD-CGD-O1D
25	A	824	CLA	CAD-CBD-CGD-O1D
25	A	827	CLA	CHA-CBD-CGD-O1D
25	A	827	CLA	CHA-CBD-CGD-O2D
25	B	812	CLA	CHA-CBD-CGD-O1D
25	B	818	CLA	CHA-CBD-CGD-O1D
25	B	818	CLA	CHA-CBD-CGD-O2D
25	B	831	CLA	CHA-CBD-CGD-O1D
25	B	838	CLA	CHA-CBD-CGD-O1D
25	B	839	CLA	CAD-CBD-CGD-O1D
25	B	840	CLA	CHA-CBD-CGD-O1D
25	G	202	CLA	CAD-CBD-CGD-O1D
25	G	203	CLA	CAD-CBD-CGD-O1D
25	H	302	CLA	CAD-CBD-CGD-O1D
25	J	102	CLA	CHA-CBD-CGD-O1D
25	O	2004	CLA	CAD-CBD-CGD-O1D
25	Q	313	CLA	CHA-CBD-CGD-O1D
25	Q	313	CLA	CHA-CBD-CGD-O2D
25	R	307	CLA	CHA-CBD-CGD-O1D
25	U	310	CLA	CAD-CBD-CGD-O1D
25	V	302	CLA	CAD-CBD-CGD-O1D
25	V	303	CLA	CHA-CBD-CGD-O1D
25	V	311	CLA	CAD-CBD-CGD-O1D
25	W	313	CLA	CHA-CBD-CGD-O1D
26	4	317	IWJ	C23-C24-C26-C28
26	P	320	IWJ	C26-C28-C29-C35
26	Q	303	IWJ	C26-C28-C29-C35
26	Q	320	IWJ	C23-C24-C26-C28
26	T	318	IWJ	C16-C17-C18-C19
26	U	316	IWJ	C02-C07-C08-C09
26	V	318	IWJ	C26-C28-C29-C35
26	W	318	IWJ	C16-C17-C18-C19
26	W	318	IWJ	C23-C24-C26-C28
26	X	318	IWJ	C26-C28-C29-C35
28	2	619	LHG	C4-O6-P-O5
28	3	321	LHG	C4-O6-P-O5
28	3	323	LHG	C3-O3-P-O5
28	6	616	LHG	C4-O6-P-O4
28	A	846	LHG	C4-O6-P-O5
28	A	847	LHG	C4-O6-P-O5
29	Q	318	Q6L	C04-C03-C11-C12

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Mol	Chain	Res	Type	Atoms
29	Q	318	Q6L	C24-C25-C26-C27
29	Q	319	Q6L	C24-C25-C26-C27
29	S	316	Q6L	C29-C30-C31-C32
29	S	321	Q6L	C13-C14-C15-C16
29	S	323	Q6L	C04-C03-C11-C12
29	V	321	Q6L	C04-C03-C11-C12
29	X	301	Q6L	C04-C03-C11-C12
29	X	317	Q6L	C04-C03-C11-C12
33	A	802	CL0	CHA-CBD-CGD-O1D
33	A	802	CL0	CHA-CBD-CGD-O2D
25	B	825	CLA	CBD-CGD-O2D-CED
25	A	830	CLA	C5-C6-C7-C8
25	B	805	CLA	C4-C3-C5-C6
25	3	307	CLA	C2B-C3B-CAB-CBB
25	4	303	CLA	C2B-C3B-CAB-CBB
25	6	612	CLA	C2B-C3B-CAB-CBB
25	A	816	CLA	C2B-C3B-CAB-CBB
25	A	833	CLA	C2B-C3B-CAB-CBB
25	B	835	CLA	C2B-C3B-CAB-CBB
25	H	301	CLA	C2B-C3B-CAB-CBB
25	P	302	CLA	C2B-C3B-CAB-CBB
25	P	313	CLA	C2B-C3B-CAB-CBB
25	R	305	CLA	C2B-C3B-CAB-CBB
25	R	306	CLA	C2B-C3B-CAB-CBB
25	S	312	CLA	C2B-C3B-CAB-CBB
25	U	309	CLA	C2B-C3B-CAB-CBB
25	V	310	CLA	C2B-C3B-CAB-CBB
25	V	313	CLA	C2B-C3B-CAB-CBB
30	A	849	BCR	C23-C24-C25-C26
36	A	854	DGD	C2A-C3A-C4A-C5A
25	6	602	CLA	CBD-CGD-O2D-CED
25	P	310	CLA	CAA-CBA-CGA-O2A
25	B	815	CLA	C2-C3-C5-C6
25	T	312	CLA	C2-C3-C5-C6
29	X	301	Q6L	C11-C12-C13-C14
26	Q	320	IWJ	C08-C09-C10-C41
29	X	316	Q6L	C23-C22-C24-C25
30	F	801	BCR	C36-C18-C19-C20
25	B	805	CLA	C5-C6-C7-C8
26	4	317	IWJ	C25-C24-C26-C28
26	Q	320	IWJ	C25-C24-C26-C28
26	W	318	IWJ	C25-C24-C26-C28

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Mol	Chain	Res	Type	Atoms
25	A	807	CLA	C16-C17-C18-C19
25	A	815	CLA	C13-C15-C16-C17
25	2	602	CLA	C12-C13-C15-C16
24	S	307	CHL	C2C-C3C-CAC-CBC
25	B	822	CLA	O2A-C1-C2-C3
28	3	322	LHG	C4-C5-O7-C7
24	U	313	CHL	O1D-CGD-O2D-CED
25	W	310	CLA	CAA-CBA-CGA-O2A
25	T	309	CLA	C11-C12-C13-C14
24	Q	309	CHL	C3C-C2C-CMC-OMC
29	V	321	Q6L	C24-C25-C26-C27
25	5	609	CLA	C6-C7-C8-C10
28	A	846	LHG	C12-C13-C14-C15
36	B	850	DGD	C2A-C3A-C4A-C5A
25	A	807	CLA	C10-C11-C12-C13
25	3	301	CLA	C11-C10-C8-C9
25	6	613	CLA	C11-C12-C13-C14
25	A	839	CLA	C14-C13-C15-C16
25	B	839	CLA	C11-C10-C8-C9
25	3	301	CLA	C11-C10-C8-C7
25	A	808	CLA	C12-C13-C15-C16
25	B	815	CLA	C6-C7-C8-C10
28	A	846	LHG	O6-C4-C5-O7
25	B	808	CLA	C16-C17-C18-C20
25	A	807	CLA	C2C-C3C-CAC-CBC
25	A	838	CLA	C2-C3-C5-C6
28	3	321	LHG	C25-C26-C27-C28
29	R	301	Q6L	C17-C18-C19-C20
29	X	301	Q6L	C19-C20-C21-C22
25	1	608	CLA	C5-C6-C7-C8
25	A	815	CLA	C2A-CAA-CBA-CGA
25	B	812	CLA	C10-C11-C12-C13
25	A	807	CLA	C4C-C3C-CAC-CBC
25	A	804	CLA	C2-C1-O2A-CGA
25	T	311	CLA	C2-C1-O2A-CGA
25	R	313	CLA	C4-C3-C5-C6
29	T	315	Q6L	C11-C12-C13-C42
24	R	309	CHL	O2A-C1-C2-C3
25	2	612	CLA	CAA-CBA-CGA-O2A
30	I	101	BCR	C36-C18-C19-C20
26	4	317	IWJ	C18-C19-C21-C22
26	Q	320	IWJ	C08-C09-C10-C11

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Mol	Chain	Res	Type	Atoms
30	2	618	BCR	C7-C8-C9-C10
31	L	308	LMG	O7-C10-C11-C12
31	L	308	LMG	C8-C7-O1-C1
25	R	306	CLA	C5-C6-C7-C8
25	S	312	CLA	C2A-CAA-CBA-CGA
26	4	301	IWJ	C10-C11-C12-C13
25	B	834	CLA	CAA-CBA-CGA-O2A
25	A	808	CLA	C2-C3-C5-C6
28	3	323	LHG	C24-C23-O8-C6
28	2	619	LHG	O9-C7-O7-C5
25	T	311	CLA	C11-C12-C13-C15
25	B	843	CLA	CAA-CBA-CGA-O2A
25	2	602	CLA	C6-C7-C8-C9
25	A	837	CLA	C11-C12-C13-C14
25	B	808	CLA	C14-C13-C15-C16
25	B	842	CLA	C14-C13-C15-C16
25	P	309	CLA	C11-C12-C13-C14
33	A	802	CL0	C14-C13-C15-C16
24	W	305	CHL	O1D-CGD-O2D-CED
25	B	809	CLA	C4B-C3B-CAB-CBB
25	B	842	CLA	C4B-C3B-CAB-CBB
25	F	803	CLA	C4B-C3B-CAB-CBB
25	P	301	CLA	C4B-C3B-CAB-CBB
25	V	312	CLA	C4B-C3B-CAB-CBB
25	A	843	CLA	C16-C17-C18-C19
25	P	302	CLA	C13-C15-C16-C17
25	Q	315	CLA	O2A-C1-C2-C3
25	P	301	CLA	C8-C10-C11-C12
25	1	607	CLA	CHA-CBD-CGD-O1D
25	O	2001	CLA	O1D-CGD-O2D-CED
38	T	308	KC2	C4B-C3B-CAB-CBB
38	V	308	KC2	C4B-C3B-CAB-CBB
38	X	309	KC2	C4B-C3B-CAB-CBB
25	6	602	CLA	C11-C10-C8-C7
25	A	835	CLA	C11-C12-C13-C15
25	B	808	CLA	C11-C12-C13-C15
25	P	302	CLA	C11-C12-C13-C15
25	A	820	CLA	C10-C11-C12-C13
25	G	202	CLA	O1D-CGD-O2D-CED
25	A	843	CLA	C16-C17-C18-C20
25	B	826	CLA	C16-C17-C18-C19
25	B	808	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	W	312	CLA	C5-C6-C7-C8
24	Q	316	CHL	C3A-C2A-CAA-CBA
25	5	607	CLA	C3A-C2A-CAA-CBA
25	A	804	CLA	C3A-C2A-CAA-CBA
25	G	202	CLA	C3A-C2A-CAA-CBA
25	P	312	CLA	C3A-C2A-CAA-CBA
25	P	313	CLA	C3A-C2A-CAA-CBA
25	Q	314	CLA	C3A-C2A-CAA-CBA
25	U	309	CLA	C3A-C2A-CAA-CBA
36	B	850	DGD	C6B-C7B-C8B-C9B
31	N	201	LMG	C37-C38-C39-C40
30	A	852	BCR	C11-C10-C9-C34
30	A	852	BCR	C16-C17-C18-C36
30	B	846	BCR	C11-C10-C9-C34
30	B	846	BCR	C20-C21-C22-C37
30	F	804	BCR	C35-C13-C14-C15
30	L	307	BCR	C11-C10-C9-C34
31	2	620	LMG	O6-C1-O1-C7
37	H	306	NEX	C39-C29-C30-C31
37	P	317	NEX	C39-C29-C30-C31
37	R	321	NEX	C39-C29-C30-C31
37	S	317	NEX	C39-C29-C30-C31
37	T	317	NEX	C39-C29-C30-C31
37	W	317	NEX	C39-C29-C30-C31
25	B	828	CLA	C2C-C3C-CAC-CBC
24	R	310	CHL	C2-C1-O2A-CGA
25	A	806	CLA	C2-C1-O2A-CGA
25	A	838	CLA	C2-C1-O2A-CGA
25	K	206	CLA	C2-C1-O2A-CGA
25	S	302	CLA	C2-C1-O2A-CGA
26	S	319	IWJ	C21-C22-C23-C24
29	P	316	Q6L	C24-C25-C26-C27
29	P	321	Q6L	C24-C25-C26-C27
25	5	602	CLA	C8-C10-C11-C12
25	H	302	CLA	C5-C6-C7-C8
30	3	319	BCR	C7-C8-C9-C34
24	S	306	CHL	C4-C3-C5-C6
24	T	306	CHL	C4-C3-C5-C6
25	B	815	CLA	O1A-CGA-O2A-C1
25	3	310	CLA	C2A-CAA-CBA-CGA
30	F	801	BCR	C17-C18-C19-C20
25	B	829	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	T	306	CHL	CAA-CBA-CGA-O2A
26	4	317	IWJ	C25-C24-C26-O27
25	4	303	CLA	C6-C7-C8-C9
25	4	303	CLA	C11-C10-C8-C9
25	A	807	CLA	C6-C7-C8-C9
25	A	808	CLA	C6-C7-C8-C9
25	A	808	CLA	C14-C13-C15-C16
25	A	828	CLA	C6-C7-C8-C9
25	A	837	CLA	C6-C7-C8-C9
25	A	856	CLA	C6-C7-C8-C9
25	B	805	CLA	C11-C10-C8-C9
25	B	806	CLA	C11-C12-C13-C14
25	B	808	CLA	C11-C12-C13-C14
25	B	828	CLA	C14-C13-C15-C16
25	B	839	CLA	C11-C12-C13-C14
25	P	302	CLA	C11-C12-C13-C14
34	B	844	PQN	C16-C17-C18-C19
24	4	308	CHL	C1A-C2A-CAA-CBA
24	R	318	CHL	C1A-C2A-CAA-CBA
24	T	306	CHL	C1A-C2A-CAA-CBA
24	T	307	CHL	C1A-C2A-CAA-CBA
24	U	306	CHL	C1A-C2A-CAA-CBA
24	X	315	CHL	C1A-C2A-CAA-CBA
25	2	606	CLA	CAA-CBA-CGA-O2A
25	A	803	CLA	C2A-CAA-CBA-CGA
25	A	807	CLA	C2A-CAA-CBA-CGA
25	B	805	CLA	C2A-CAA-CBA-CGA
25	4	304	CLA	C1A-C2A-CAA-CBA
25	5	607	CLA	C1A-C2A-CAA-CBA
25	6	612	CLA	C1A-C2A-CAA-CBA
25	A	804	CLA	C1A-C2A-CAA-CBA
25	A	826	CLA	C1A-C2A-CAA-CBA
25	A	829	CLA	C1A-C2A-CAA-CBA
25	A	839	CLA	C1A-C2A-CAA-CBA
25	B	804	CLA	C1A-C2A-CAA-CBA
25	G	202	CLA	C1A-C2A-CAA-CBA
25	H	304	CLA	C1A-C2A-CAA-CBA
25	P	312	CLA	C1A-C2A-CAA-CBA
25	Q	314	CLA	C1A-C2A-CAA-CBA
25	U	310	CLA	C1A-C2A-CAA-CBA
26	4	317	IWJ	C23-C24-C26-O27
30	A	852	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	A	852	BCR	C16-C17-C18-C19
30	B	846	BCR	C11-C10-C9-C8
30	B	846	BCR	C20-C21-C22-C23
30	F	804	BCR	C12-C13-C14-C15
30	L	307	BCR	C11-C10-C9-C8
37	H	306	NEX	C28-C29-C30-C31
37	P	317	NEX	C28-C29-C30-C31
37	R	321	NEX	C28-C29-C30-C31
37	S	317	NEX	C28-C29-C30-C31
37	T	317	NEX	C28-C29-C30-C31
37	W	317	NEX	C28-C29-C30-C31
25	1	608	CLA	C2B-C3B-CAB-CBB
25	2	610	CLA	C2B-C3B-CAB-CBB
25	3	309	CLA	C2B-C3B-CAB-CBB
25	5	609	CLA	C2B-C3B-CAB-CBB
25	A	820	CLA	C2B-C3B-CAB-CBB
25	A	823	CLA	C2B-C3B-CAB-CBB
25	B	809	CLA	C2B-C3B-CAB-CBB
25	B	810	CLA	C2B-C3B-CAB-CBB
25	B	836	CLA	C2B-C3B-CAB-CBB
25	B	841	CLA	C2B-C3B-CAB-CBB
25	F	803	CLA	C2B-C3B-CAB-CBB
25	L	302	CLA	C2B-C3B-CAB-CBB
25	U	312	CLA	C2B-C3B-CAB-CBB
25	X	311	CLA	C2B-C3B-CAB-CBB
30	L	307	BCR	C5-C6-C7-C8
36	B	850	DGD	C2B-C1B-O2G-C2G
25	2	606	CLA	CAA-CBA-CGA-O1A
25	5	603	CLA	CAA-CBA-CGA-O2A
25	A	840	CLA	C4-C3-C5-C6
29	V	321	Q6L	C11-C12-C13-C42
24	U	305	CHL	CAA-CBA-CGA-O1A
28	2	619	LHG	C10-C11-C12-C13
25	2	602	CLA	C11-C12-C13-C15
25	6	602	CLA	C6-C7-C8-C10
25	A	838	CLA	C6-C7-C8-C10
25	A	842	CLA	C11-C10-C8-C7
25	A	856	CLA	C11-C10-C8-C7
25	B	802	CLA	C6-C7-C8-C10
25	B	831	CLA	C12-C13-C15-C16
25	B	841	CLA	C11-C12-C13-C15
25	Q	304	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	V	311	CLA	C6-C7-C8-C10
34	A	844	PQN	C22-C23-C25-C26
31	A	855	LMG	O7-C8-C9-O8
32	H	303	SQD	O47-C45-C46-O48
32	H	303	SQD	C28-C29-C30-C31
25	F	802	CLA	C3A-C2A-CAA-CBA
28	3	322	LHG	C14-C15-C16-C17
25	B	843	CLA	C3-C5-C6-C7
31	5	613	LMG	C41-C42-C43-C44
25	6	610	CLA	C12-C13-C15-C16
25	U	302	CLA	C11-C10-C8-C7
30	B	849	BCR	C7-C8-C9-C34
25	6	603	CLA	CAA-CBA-CGA-O2A
25	W	311	CLA	CAA-CBA-CGA-O2A
25	A	830	CLA	C4-C3-C5-C6
31	O	2008	LMG	O7-C10-C11-C12
25	B	805	CLA	C2-C3-C5-C6
25	B	826	CLA	C2-C3-C5-C6
25	B	829	CLA	C2-C3-C5-C6
30	A	849	BCR	C11-C12-C13-C14
28	A	846	LHG	C14-C15-C16-C17
25	Q	314	CLA	C5-C6-C7-C8
24	1	601	CHL	C3-C5-C6-C7
25	R	317	CLA	C2A-CAA-CBA-CGA
25	S	309	CLA	C6-C7-C8-C9
25	B	821	CLA	CBD-CGD-O2D-CED
25	V	301	CLA	C5-C6-C7-C8
33	A	802	CL0	C8-C10-C11-C12
28	3	320	LHG	C9-C10-C11-C12
24	U	305	CHL	CAA-CBA-CGA-O2A
25	K	201	CLA	CAA-CBA-CGA-O2A
38	Q	310	KC2	O1D-CGD-O2D-CED
25	B	826	CLA	C4-C3-C5-C6
29	O	2007	Q6L	C11-C12-C13-C42
25	A	823	CLA	C15-C16-C17-C18
25	4	309	CLA	CAA-CBA-CGA-O2A
25	A	827	CLA	C13-C15-C16-C17
25	B	806	CLA	C8-C10-C11-C12
25	B	820	CLA	C5-C6-C7-C8
25	6	603	CLA	CAA-CBA-CGA-O1A
25	A	818	CLA	CAA-CBA-CGA-O2A
25	W	311	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	5	607	CLA	C5-C6-C7-C8
28	1	614	LHG	C4-C5-C6-O8
24	P	305	CHL	CAA-CBA-CGA-O2A
25	5	603	CLA	CAA-CBA-CGA-O1A
25	B	804	CLA	C2A-CAA-CBA-CGA
25	Q	304	CLA	C2A-CAA-CBA-CGA
25	A	835	CLA	C16-C17-C18-C19
32	H	303	SQD	O49-C7-O47-C45
25	B	807	CLA	C10-C11-C12-C13
25	2	602	CLA	C4-C3-C5-C6
25	P	302	CLA	C5-C6-C7-C8
25	3	312	CLA	C4B-C3B-CAB-CBB
25	4	311	CLA	C4B-C3B-CAB-CBB
25	5	607	CLA	C4B-C3B-CAB-CBB
25	A	813	CLA	C4B-C3B-CAB-CBB
25	L	302	CLA	C4B-C3B-CAB-CBB
25	O	2003	CLA	C4B-C3B-CAB-CBB
25	P	309	CLA	C4B-C3B-CAB-CBB
25	S	309	CLA	C4B-C3B-CAB-CBB
25	U	303	CLA	C4B-C3B-CAB-CBB
25	W	301	CLA	C4B-C3B-CAB-CBB
25	W	310	CLA	C4B-C3B-CAB-CBB
25	X	311	CLA	C4B-C3B-CAB-CBB
24	3	306	CHL	CAA-CBA-CGA-O2A
25	4	309	CLA	CAA-CBA-CGA-O1A
25	A	836	CLA	C16-C17-C18-C19
25	A	840	CLA	C6-C7-C8-C9
24	S	306	CHL	CHA-CBD-CGD-O1D
24	S	306	CHL	CHA-CBD-CGD-O2D
24	S	307	CHL	CHA-CBD-CGD-O1D
24	S	307	CHL	CHA-CBD-CGD-O2D
24	X	315	CHL	CHA-CBD-CGD-O1D
24	X	315	CHL	CHA-CBD-CGD-O2D
25	B	825	CLA	CAA-CBA-CGA-O2A
31	5	613	LMG	C14-C15-C16-C17
25	S	302	CLA	C13-C15-C16-C17
25	4	316	CLA	O1D-CGD-O2D-CED
25	B	829	CLA	C16-C17-C18-C19
28	3	323	LHG	C11-C10-C9-C8
25	A	830	CLA	C2-C3-C5-C6
25	B	815	CLA	C13-C15-C16-C17
30	K	207	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
25	R	313	CLA	C6-C7-C8-C10
28	6	616	LHG	C34-C35-C36-C37
25	5	610	CLA	O1D-CGD-O2D-CED
24	Q	307	CHL	CAA-CBA-CGA-O2A
31	A	857	LMG	C22-C23-C24-C25
32	6	617	SQD	C9-C10-C11-C12
38	P	308	KC2	CAA-CBA-CGA-O2A
26	S	322	IWJ	C16-C17-C18-C19
24	V	304	CHL	CAA-CBA-CGA-O2A
24	1	601	CHL	CBA-CGA-O2A-C1
25	3	307	CLA	C11-C10-C8-C9
25	6	602	CLA	C11-C12-C13-C14
25	A	804	CLA	C11-C10-C8-C9
25	B	810	CLA	C6-C7-C8-C9
25	B	812	CLA	C14-C13-C15-C16
25	B	830	CLA	C11-C12-C13-C14
25	B	831	CLA	C6-C7-C8-C9
25	P	309	CLA	C6-C7-C8-C9
25	U	302	CLA	C6-C7-C8-C9
25	A	822	CLA	CAA-CBA-CGA-O2A
25	B	802	CLA	C2A-CAA-CBA-CGA
25	A	840	CLA	C6-C7-C8-C10
25	T	311	CLA	C11-C12-C13-C14
33	A	802	CL0	C13-C15-C16-C17
24	W	306	CHL	C3A-C2A-CAA-CBA
25	1	603	CLA	C3A-C2A-CAA-CBA
25	A	829	CLA	C3A-C2A-CAA-CBA
25	A	837	CLA	C3A-C2A-CAA-CBA
25	A	845	CLA	C3A-C2A-CAA-CBA
25	B	804	CLA	C3A-C2A-CAA-CBA
25	T	303	CLA	C3A-C2A-CAA-CBA
25	K	201	CLA	CAA-CBA-CGA-O1A
38	U	307	KC2	C2B-C3B-CAB-CBB
31	N	201	LMG	C19-C20-C21-C22
25	6	610	CLA	C3-C5-C6-C7
24	P	305	CHL	CAA-CBA-CGA-O1A
25	B	802	CLA	O2A-C1-C2-C3
25	B	819	CLA	O2A-C1-C2-C3
24	Q	316	CHL	C3C-C2C-CMC-OMC
24	U	304	CHL	C3C-C2C-CMC-OMC
24	U	306	CHL	C3C-C2C-CMC-OMC
25	A	829	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	B	825	CLA	CAA-CBA-CGA-O1A
36	B	850	DGD	C3A-C4A-C5A-C6A
24	Q	307	CHL	CAA-CBA-CGA-O1A
25	A	840	CLA	C2-C3-C5-C6
25	B	841	CLA	C2-C3-C5-C6
25	P	302	CLA	C8-C10-C11-C12
25	A	829	CLA	C16-C17-C18-C19
27	4	318	XAT	O24-C26-C27-C28
29	O	2006	Q6L	C02-C03-C11-C12
29	R	301	Q6L	C02-C03-C11-C12
29	T	319	Q6L	C02-C03-C11-C12
29	U	317	Q6L	C02-C03-C11-C12
37	R	321	NEX	O24-C26-C27-C28
37	S	317	NEX	O24-C26-C27-C28
37	T	317	NEX	O24-C26-C27-C28
25	A	835	CLA	C15-C16-C17-C18
25	1	607	CLA	CHA-CBD-CGD-O2D
25	5	602	CLA	C10-C11-C12-C13
38	R	312	KC2	C4B-C3B-CAB-CBB
38	U	307	KC2	C4B-C3B-CAB-CBB
38	W	308	KC2	C4B-C3B-CAB-CBB
25	5	607	CLA	C16-C17-C18-C19
25	U	301	CLA	CAA-CBA-CGA-O2A
38	P	308	KC2	CAA-CBA-CGA-O1A
25	U	303	CLA	O1A-CGA-O2A-C1
25	U	302	CLA	C4-C3-C5-C6
25	P	302	CLA	CAA-CBA-CGA-O2A
24	3	306	CHL	CAA-CBA-CGA-O1A
25	A	822	CLA	CAA-CBA-CGA-O1A
26	R	322	IWJ	C14-C15-C16-C17
28	3	323	LHG	C11-C12-C13-C14
25	U	301	CLA	CAA-CBA-CGA-O1A
28	A	846	LHG	O8-C23-C24-C25
25	B	831	CLA	C3-C5-C6-C7
32	H	303	SQD	O6-C44-C45-O47
25	1	608	CLA	C6-C7-C8-C9
25	B	841	CLA	C6-C7-C8-C9
25	B	839	CLA	CAA-CBA-CGA-O2A
25	B	840	CLA	CAA-CBA-CGA-O2A
24	4	302	CHL	CAA-CBA-CGA-O1A
25	B	821	CLA	O1D-CGD-O2D-CED
24	V	304	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	B	801	LMG	O6-C5-C6-O5
29	W	316	Q6L	C26-C27-C29-C30
25	3	311	CLA	C3-C5-C6-C7
25	A	813	CLA	C13-C15-C16-C17
25	A	831	CLA	C13-C15-C16-C17
25	A	856	CLA	O1D-CGD-O2D-CED
29	O	2007	Q6L	C11-C12-C13-C14
25	A	818	CLA	CAA-CBA-CGA-O1A
24	V	314	CHL	O1D-CGD-O2D-CED
38	V	308	KC2	CBD-CGD-O2D-CED
25	4	303	CLA	C11-C10-C8-C7
25	6	610	CLA	C11-C10-C8-C7
25	B	804	CLA	C6-C7-C8-C10
25	B	842	CLA	C11-C12-C13-C15
25	R	306	CLA	C12-C13-C15-C16
25	S	309	CLA	C6-C7-C8-C10
25	U	302	CLA	C6-C7-C8-C10
25	B	839	CLA	C3-C5-C6-C7
25	2	609	CLA	C2B-C3B-CAB-CBB
25	3	312	CLA	C2B-C3B-CAB-CBB
25	4	311	CLA	C2B-C3B-CAB-CBB
25	A	813	CLA	C2B-C3B-CAB-CBB
25	B	806	CLA	C2B-C3B-CAB-CBB
25	O	2003	CLA	C2B-C3B-CAB-CBB
25	P	301	CLA	C2B-C3B-CAB-CBB
25	P	309	CLA	C2B-C3B-CAB-CBB
25	P	310	CLA	C2B-C3B-CAB-CBB
25	Q	304	CLA	C2B-C3B-CAB-CBB
25	R	314	CLA	C2B-C3B-CAB-CBB
25	V	312	CLA	C2B-C3B-CAB-CBB
25	W	310	CLA	C2B-C3B-CAB-CBB
30	2	618	BCR	C23-C24-C25-C26
30	K	207	BCR	C5-C6-C7-C8
31	A	855	LMG	O7-C10-C11-C12
32	H	303	SQD	C24-C25-C26-C27
25	3	311	CLA	CAA-CBA-CGA-O2A
25	A	829	CLA	CAA-CBA-CGA-O2A
25	V	301	CLA	CAA-CBA-CGA-O2A
25	V	311	CLA	C2-C1-O2A-CGA
29	W	316	Q6L	C19-C20-C21-C22
28	3	321	LHG	C9-C10-C11-C12
25	4	313	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	819	CLA	C2-C3-C5-C6
29	T	315	Q6L	C11-C12-C13-C14
25	A	829	CLA	C2C-C3C-CAC-CBC
25	5	609	CLA	C5-C6-C7-C8
31	A	857	LMG	O10-C28-O8-C9
25	R	313	CLA	C15-C16-C17-C18
24	R	308	CHL	C1C-C2C-CMC-OMC
24	W	304	CHL	C1C-C2C-CMC-OMC
25	P	303	CLA	C2A-CAA-CBA-CGA
25	X	302	CLA	C2A-CAA-CBA-CGA
24	W	305	CHL	CBD-CGD-O2D-CED
28	2	619	LHG	C8-C7-O7-C5
32	H	303	SQD	O48-C23-C24-C25
25	G	204	CLA	CAA-CBA-CGA-O2A
25	A	821	CLA	C5-C6-C7-C8
25	A	838	CLA	C8-C10-C11-C12
25	B	816	CLA	CBA-CGA-O2A-C1
25	A	831	CLA	CAA-CBA-CGA-O2A
25	P	303	CLA	CAA-CBA-CGA-O2A
25	Q	313	CLA	CAA-CBA-CGA-O2A
25	R	313	CLA	CAA-CBA-CGA-O2A
29	U	315	Q6L	C17-C18-C19-C20
28	1	614	LHG	C29-C30-C31-C32
25	L	303	CLA	CAA-CBA-CGA-O2A
25	B	819	CLA	C4-C3-C5-C6
25	B	806	CLA	CAA-CBA-CGA-O2A
25	V	310	CLA	CAA-CBA-CGA-O2A
38	Q	310	KC2	CBD-CGD-O2D-CED
25	H	304	CLA	CAA-CBA-CGA-O1A
32	H	303	SQD	C8-C7-O47-C45
25	Q	311	CLA	C5-C6-C7-C8
25	4	303	CLA	C8-C10-C11-C12
25	B	842	CLA	C10-C11-C12-C13
25	A	835	CLA	C11-C12-C13-C14
25	A	842	CLA	C11-C10-C8-C9
25	B	813	CLA	C11-C12-C13-C14
25	A	809	CLA	CAA-CBA-CGA-O2A
25	B	812	CLA	CAA-CBA-CGA-O2A
25	K	206	CLA	CAA-CBA-CGA-O2A
25	Q	301	CLA	CAA-CBA-CGA-O2A
25	1	603	CLA	C1A-C2A-CAA-CBA
25	2	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	2	609	CLA	C4B-C3B-CAB-CBB
25	3	308	CLA	C4B-C3B-CAB-CBB
25	5	609	CLA	C4B-C3B-CAB-CBB
25	6	604	CLA	C4B-C3B-CAB-CBB
25	A	823	CLA	C4B-C3B-CAB-CBB
25	A	837	CLA	C4B-C3B-CAB-CBB
25	B	806	CLA	C4B-C3B-CAB-CBB
25	B	808	CLA	C1A-C2A-CAA-CBA
25	B	812	CLA	C4B-C3B-CAB-CBB
25	B	831	CLA	C1A-C2A-CAA-CBA
25	L	304	CLA	C4B-C3B-CAB-CBB
25	P	310	CLA	C4B-C3B-CAB-CBB
25	T	303	CLA	C1A-C2A-CAA-CBA
25	U	312	CLA	C4B-C3B-CAB-CBB
26	1	611	IWJ	O27-C26-C28-C29
25	L	303	CLA	CAA-CBA-CGA-O1A
25	4	313	CLA	C4-C3-C5-C6
25	P	309	CLA	C4-C3-C5-C6
25	A	817	CLA	CAA-CBA-CGA-O2A
25	B	811	CLA	CAA-CBA-CGA-O2A
31	A	857	LMG	O7-C10-C11-C12
25	R	313	CLA	C2-C3-C5-C6
29	X	316	Q6L	C21-C22-C24-C25
30	A	850	BCR	C21-C22-C23-C24
29	V	319	Q6L	C19-C20-C21-C22
33	A	802	CL0	C16-C17-C18-C19
25	B	808	CLA	CAA-CBA-CGA-O2A
25	P	312	CLA	CAA-CBA-CGA-O2A
28	3	323	LHG	O8-C23-C24-C25
25	A	809	CLA	C2A-CAA-CBA-CGA
25	A	820	CLA	C2A-CAA-CBA-CGA
25	T	302	CLA	C16-C17-C18-C19
24	P	306	CHL	C2-C3-C5-C6
25	H	302	CLA	C13-C15-C16-C17
25	4	303	CLA	C2-C1-O2A-CGA
25	A	820	CLA	C2-C1-O2A-CGA
25	R	317	CLA	C2-C1-O2A-CGA
25	B	829	CLA	C6-C7-C8-C10
25	V	301	CLA	C11-C10-C8-C7
34	B	844	PQN	C16-C17-C18-C20
25	U	303	CLA	CBA-CGA-O2A-C1
31	A	857	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	R	313	CLA	C16-C17-C18-C19
25	B	820	CLA	C11-C12-C13-C14
25	H	304	CLA	CAA-CBA-CGA-O2A
25	A	820	CLA	CAA-CBA-CGA-O2A
25	B	824	CLA	C11-C12-C13-C15
28	3	323	LHG	C25-C26-C27-C28
25	2	608	CLA	CAA-CBA-CGA-O1A
25	B	829	CLA	C3-C5-C6-C7
25	P	302	CLA	C10-C11-C12-C13
24	P	307	CHL	C3A-C2A-CAA-CBA
24	S	314	CHL	C3A-C2A-CAA-CBA
24	X	308	CHL	C3A-C2A-CAA-CBA
25	2	611	CLA	CHA-CBD-CGD-O1D
25	4	304	CLA	C3A-C2A-CAA-CBA
25	A	839	CLA	C3A-C2A-CAA-CBA
25	A	856	CLA	C3A-C2A-CAA-CBA
25	U	310	CLA	C3A-C2A-CAA-CBA
25	B	808	CLA	C10-C11-C12-C13
25	G	204	CLA	CAA-CBA-CGA-O1A
25	3	311	CLA	CAA-CBA-CGA-O1A
25	P	312	CLA	CAA-CBA-CGA-O1A
31	5	613	LMG	C32-C33-C34-C35
25	6	613	CLA	CAA-CBA-CGA-O2A
25	B	811	CLA	CAA-CBA-CGA-O1A
25	B	840	CLA	CAA-CBA-CGA-O1A
25	P	303	CLA	CAA-CBA-CGA-O1A
31	A	857	LMG	C11-C10-O7-C8
31	L	308	LMG	C10-C11-C12-C13
25	B	815	CLA	C8-C10-C11-C12
25	B	822	CLA	C2A-CAA-CBA-CGA
25	T	301	CLA	C2A-CAA-CBA-CGA
25	A	838	CLA	C6-C7-C8-C9
25	A	856	CLA	C11-C10-C8-C9
25	B	802	CLA	C6-C7-C8-C9
25	B	805	CLA	C11-C12-C13-C14
25	B	829	CLA	C6-C7-C8-C9
25	R	313	CLA	C6-C7-C8-C9
25	A	831	CLA	CAA-CBA-CGA-O1A
25	B	808	CLA	CAA-CBA-CGA-O1A
25	Q	313	CLA	CAA-CBA-CGA-O1A
25	W	309	CLA	C16-C17-C18-C19
38	X	309	KC2	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	S	318	IWJ	C10-C11-C12-C13
24	1	601	CHL	O1A-CGA-O2A-C1
28	3	323	LHG	O10-C23-O8-C6
29	W	316	Q6L	C11-C12-C13-C42
25	A	829	CLA	CAA-CBA-CGA-O1A
25	K	206	CLA	CAA-CBA-CGA-O1A
29	P	316	Q6L	C29-C30-C31-C36
29	V	315	Q6L	C29-C30-C31-C36
38	P	308	KC2	C3A-C2A-CAA-CBA
38	V	308	KC2	C1A-C2A-CAA-CBA
25	B	806	CLA	CAA-CBA-CGA-O1A
31	B	801	LMG	C33-C34-C35-C36
25	4	303	CLA	CAA-CBA-CGA-O2A
25	5	601	CLA	CAA-CBA-CGA-O2A
25	A	841	CLA	CAA-CBA-CGA-O2A
25	O	2001	CLA	CAA-CBA-CGA-O2A
25	P	302	CLA	CAA-CBA-CGA-O1A
25	V	301	CLA	CAA-CBA-CGA-O1A
28	A	846	LHG	O10-C23-C24-C25
25	B	831	CLA	C13-C15-C16-C17
36	B	850	DGD	C4A-C5A-C6A-C7A
24	T	320	CHL	CAA-CBA-CGA-O2A
25	B	825	CLA	O1D-CGD-O2D-CED
31	5	613	LMG	O1-C7-C8-C9
31	L	308	LMG	O1-C7-C8-C9
25	A	817	CLA	CAA-CBA-CGA-O1A
25	B	839	CLA	CAA-CBA-CGA-O1A
25	R	313	CLA	CAA-CBA-CGA-O1A
31	A	857	LMG	O9-C10-C11-C12
38	R	312	KC2	C2B-C3B-CAB-CBB
38	W	308	KC2	C2B-C3B-CAB-CBB
24	U	306	CHL	CAD-CBD-CGD-O2D
25	3	309	CLA	CAD-CBD-CGD-O2D
25	6	612	CLA	CAD-CBD-CGD-O2D
25	A	822	CLA	CAD-CBD-CGD-O2D
25	B	817	CLA	CAD-CBD-CGD-O2D
25	G	203	CLA	CAD-CBD-CGD-O2D
25	H	304	CLA	CAD-CBD-CGD-O2D
25	T	312	CLA	CAD-CBD-CGD-O2D
25	V	311	CLA	CAD-CBD-CGD-O2D
25	A	816	CLA	CAA-CBA-CGA-O2A
24	R	309	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	T	302	CLA	C2-C1-O2A-CGA
25	A	809	CLA	CAA-CBA-CGA-O1A
25	B	812	CLA	CAA-CBA-CGA-O1A
25	Q	301	CLA	CAA-CBA-CGA-O1A
25	V	310	CLA	CAA-CBA-CGA-O1A
25	V	302	CLA	CAA-CBA-CGA-O2A
25	X	303	CLA	CAA-CBA-CGA-O2A
24	W	307	CHL	C3-C5-C6-C7
25	5	603	CLA	C2A-CAA-CBA-CGA
24	4	308	CHL	CAA-CBA-CGA-O2A
25	A	841	CLA	CAA-CBA-CGA-O1A
25	W	309	CLA	O1A-CGA-O2A-C1
28	1	614	LHG	O8-C23-C24-C25
25	5	601	CLA	CAA-CBA-CGA-O1A
25	5	610	CLA	CBD-CGD-O2D-CED
24	T	305	CHL	CAA-CBA-CGA-O2A
25	3	307	CLA	CAA-CBA-CGA-O2A
25	B	819	CLA	CAA-CBA-CGA-O2A
25	S	309	CLA	CAA-CBA-CGA-O2A
25	2	608	CLA	CAA-CBA-CGA-O2A

All (7) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	3	315	IWJ	C29-C30-C32-C33-C34-C35
26	X	318	IWJ	C29-C30-C32-C33-C34-C35
26	T	321	IWJ	C29-C30-C32-C33-C34-C35
26	S	319	IWJ	C29-C30-C32-C33-C34-C35
26	V	320	IWJ	C29-C30-C32-C33-C34-C35
26	R	322	IWJ	C29-C30-C32-C33-C34-C35
26	5	611	IWJ	C29-C30-C32-C33-C34-C35

159 monomers are involved in 236 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	803	CLA	1	0
24	1	601	CHL	1	0
25	B	843	CLA	1	0
25	J	102	CLA	1	0
38	R	312	KC2	2	0
25	A	832	CLA	1	0
38	S	308	KC2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	822	CLA	1	0
24	P	305	CHL	1	0
25	X	311	CLA	3	0
25	T	312	CLA	1	0
24	R	308	CHL	7	0
24	S	307	CHL	5	0
27	4	318	XAT	1	0
25	V	309	CLA	4	0
26	P	320	IWJ	1	0
25	6	607	CLA	1	0
25	S	301	CLA	7	0
25	6	612	CLA	1	0
25	A	827	CLA	1	0
27	3	316	XAT	1	0
25	U	301	CLA	1	0
24	V	305	CHL	1	0
25	A	803	CLA	1	0
25	B	829	CLA	2	0
25	F	802	CLA	1	0
25	T	310	CLA	1	0
25	B	815	CLA	3	0
25	P	301	CLA	3	0
32	H	303	SQD	1	0
25	P	309	CLA	2	0
30	K	207	BCR	2	0
25	Q	304	CLA	6	0
25	V	311	CLA	3	0
24	R	311	CHL	2	0
25	B	818	CLA	2	0
24	4	308	CHL	1	0
25	T	311	CLA	1	0
24	V	307	CHL	1	0
26	Q	320	IWJ	1	0
25	B	813	CLA	1	0
26	4	301	IWJ	1	0
24	3	306	CHL	2	0
25	W	303	CLA	1	0
25	B	825	CLA	1	0
25	R	306	CLA	1	0
25	A	830	CLA	1	0
25	G	204	CLA	1	0
30	M	101	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	R	322	IWJ	1	0
25	A	825	CLA	1	0
25	6	610	CLA	1	0
26	T	321	IWJ	1	0
25	1	607	CLA	3	0
30	F	801	BCR	1	0
25	A	815	CLA	2	0
29	X	319	Q6L	1	0
24	S	304	CHL	2	0
36	B	850	DGD	1	0
28	2	619	LHG	1	0
25	5	602	CLA	1	0
30	J	101	BCR	2	0
28	1	614	LHG	1	0
29	V	321	Q6L	1	0
25	2	608	CLA	1	0
29	U	314	Q6L	2	0
25	O	2001	CLA	1	0
25	B	835	CLA	1	0
25	S	309	CLA	4	0
25	A	820	CLA	1	0
25	5	607	CLA	1	0
38	P	308	KC2	1	0
30	4	319	BCR	2	0
25	2	609	CLA	4	0
37	P	317	NEX	1	0
38	V	308	KC2	1	0
25	A	856	CLA	1	0
25	4	309	CLA	1	0
29	S	315	Q6L	1	0
26	T	318	IWJ	1	0
25	W	309	CLA	5	0
30	B	848	BCR	1	0
25	B	832	CLA	1	0
25	B	806	CLA	1	0
25	S	310	CLA	2	0
30	A	850	BCR	1	0
30	L	305	BCR	2	0
30	A	852	BCR	2	0
25	X	310	CLA	1	0
25	A	816	CLA	1	0
29	P	316	Q6L	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	2	613	CLA	1	0
26	V	317	IWJ	1	0
24	V	314	CHL	1	0
25	A	813	CLA	1	0
25	R	305	CLA	3	0
24	X	306	CHL	1	0
25	X	313	CLA	1	0
26	S	322	IWJ	1	0
25	A	812	CLA	1	0
25	3	307	CLA	3	0
25	A	808	CLA	1	0
26	S	319	IWJ	1	0
25	Q	314	CLA	1	0
25	X	302	CLA	3	0
29	O	2006	Q6L	1	0
25	R	316	CLA	1	0
28	6	616	LHG	1	0
29	T	316	Q6L	1	0
29	2	616	Q6L	1	0
30	B	845	BCR	1	0
24	X	308	CHL	1	0
29	Q	319	Q6L	1	0
29	W	315	Q6L	2	0
27	6	615	XAT	1	0
25	B	810	CLA	1	0
24	Q	307	CHL	1	0
38	T	308	KC2	1	0
25	6	602	CLA	2	0
30	3	319	BCR	1	0
25	V	302	CLA	1	0
25	K	206	CLA	3	0
25	O	2002	CLA	1	0
25	Q	312	CLA	1	0
24	T	307	CHL	1	0
25	G	203	CLA	1	0
25	A	836	CLA	1	0
25	A	817	CLA	1	0
24	U	304	CHL	1	0
26	V	320	IWJ	1	0
25	4	311	CLA	1	0
24	T	304	CHL	1	0
30	G	201	BCR	4	0

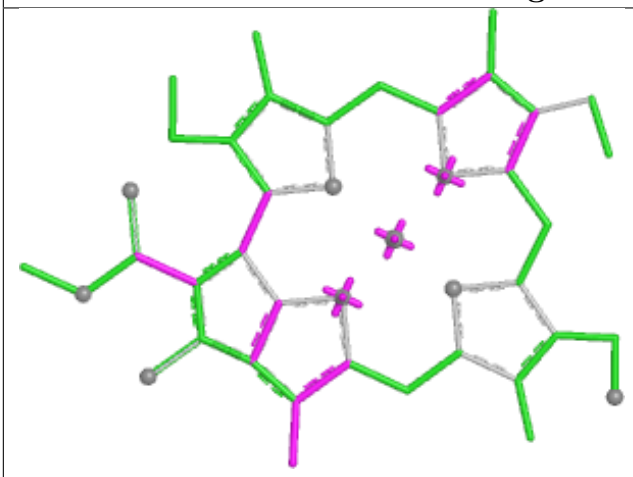
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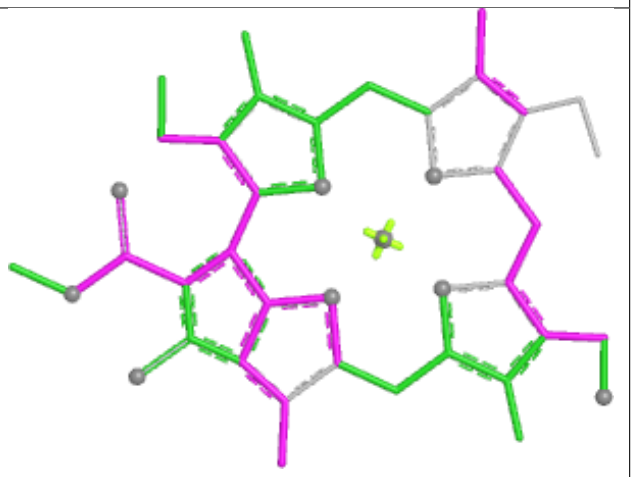
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	1	605	CLA	1	0
24	4	306	CHL	3	0
26	4	317	IWJ	1	0
36	A	854	DGD	1	0
25	B	842	CLA	4	0
25	V	301	CLA	4	0
25	X	304	CLA	1	0
24	W	314	CHL	1	0
26	W	318	IWJ	2	0
25	4	303	CLA	2	0
25	1	610	CLA	1	0
25	W	312	CLA	2	0
25	V	312	CLA	2	0
26	6	614	IWJ	2	0
26	3	315	IWJ	1	0
26	P	318	IWJ	1	0
25	B	808	CLA	2	0
25	B	819	CLA	2	0
30	B	847	BCR	1	0
34	A	844	PQN	1	0
25	B	824	CLA	3	0
25	G	202	CLA	1	0
25	3	301	CLA	2	0
25	W	301	CLA	3	0
31	F	805	LMG	1	0
25	A	824	CLA	1	0

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

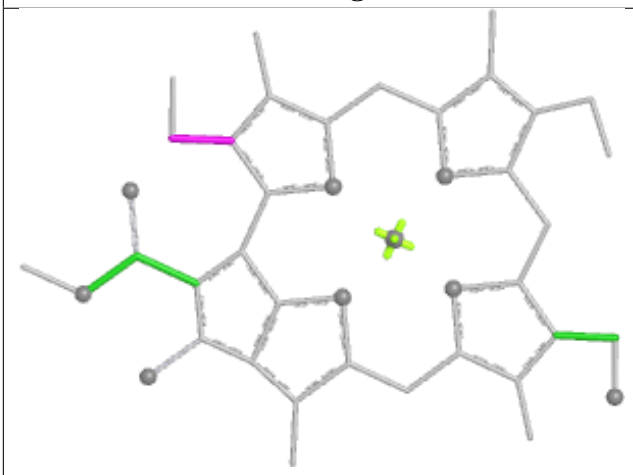
Ligand CHL 6 601



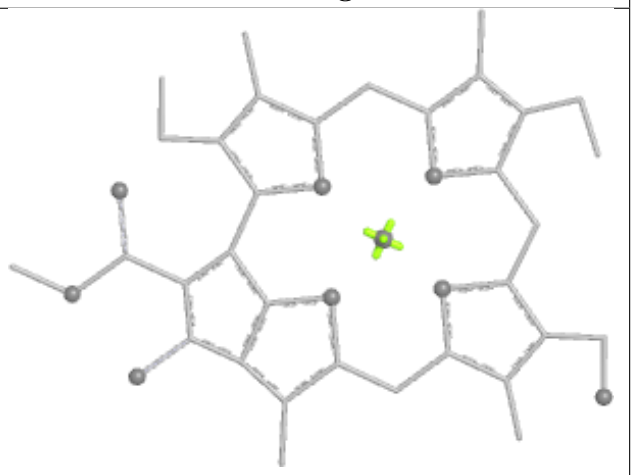
Bond lengths



Bond angles

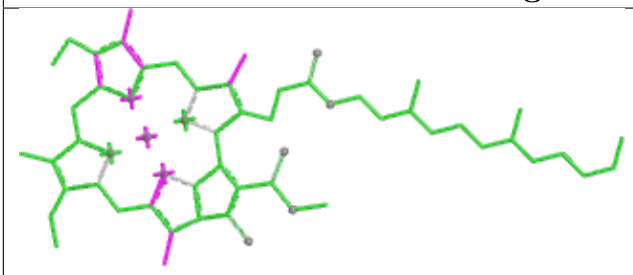


Torsions

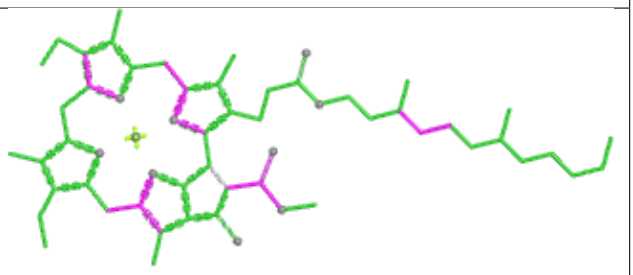


Rings

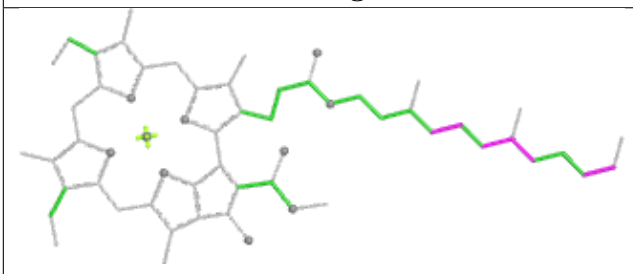
Ligand CLA A 828



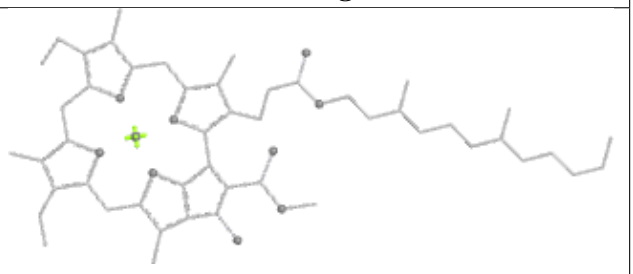
Bond lengths



Bond angles

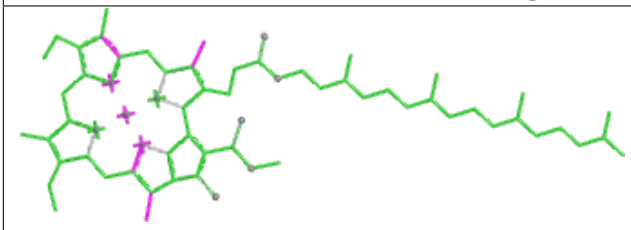


Torsions

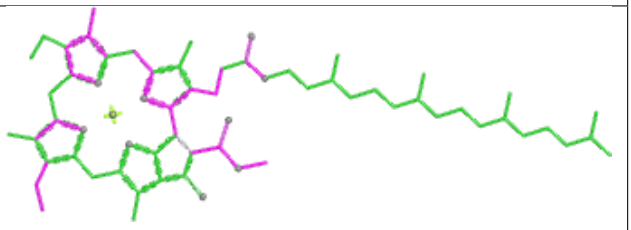


Rings

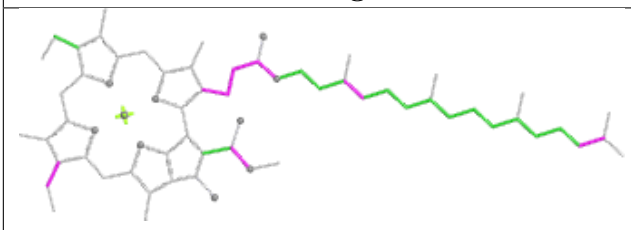
Ligand CLA A 829



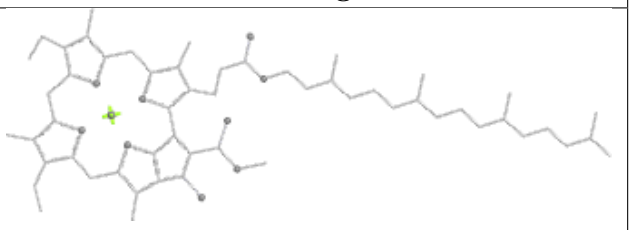
Bond lengths



Bond angles

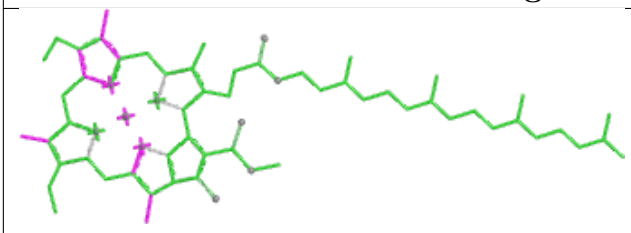


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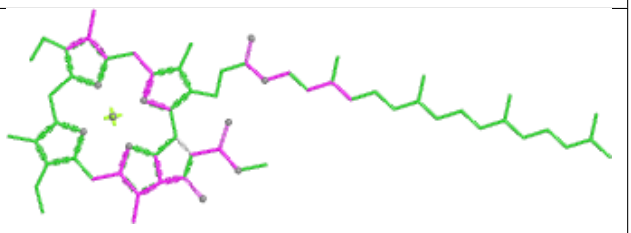


Rings

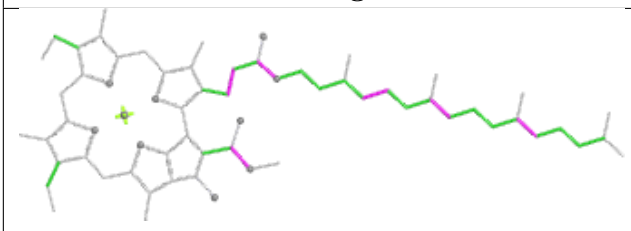
Ligand CLA B 803



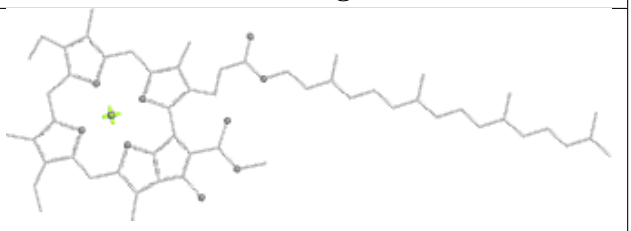
Bond lengths



Bond angles

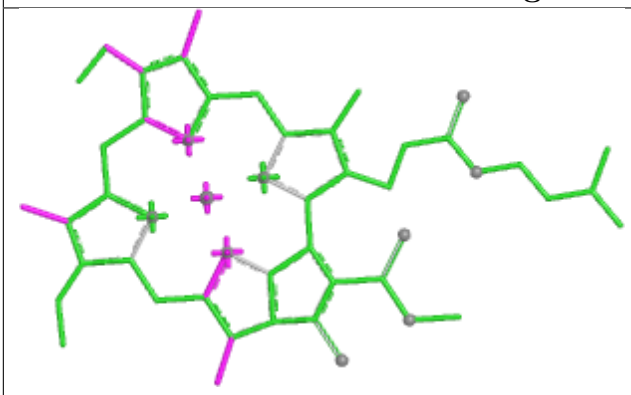


Torsions

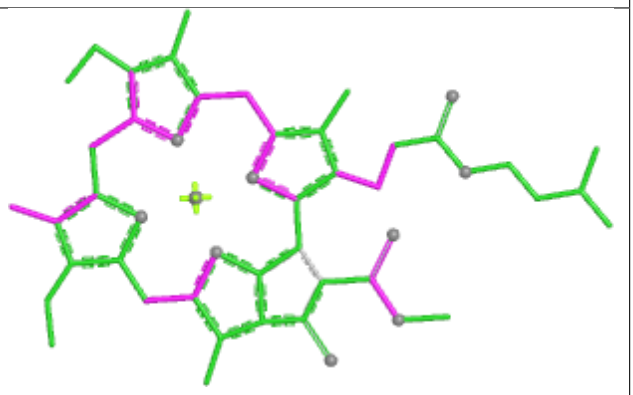


Rings

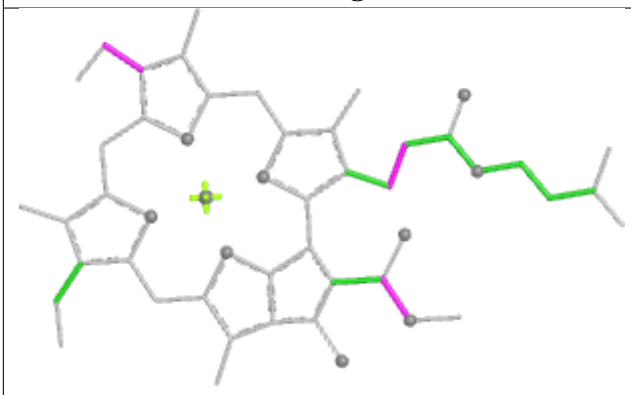
Ligand CLA A 833



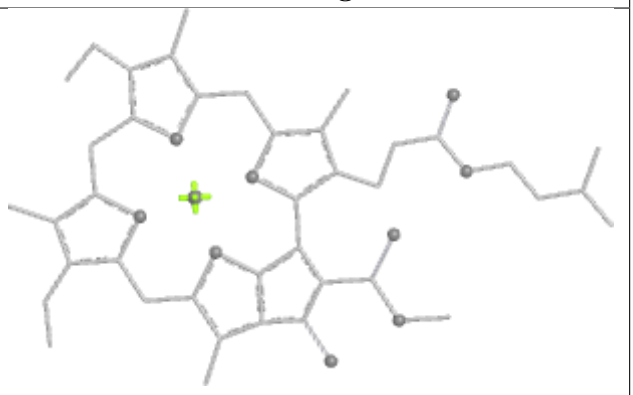
Bond lengths



Bond angles

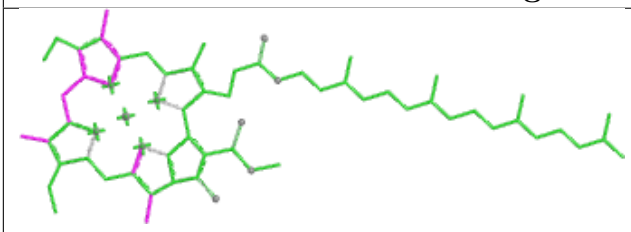


Torsions

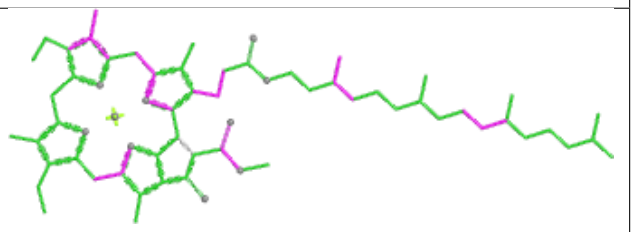


Rings

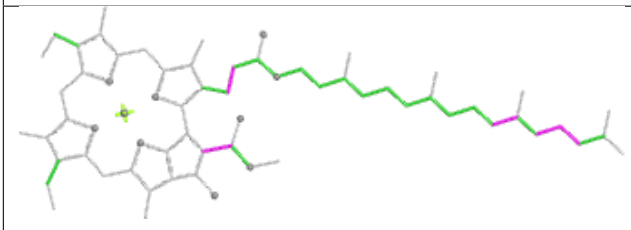
Ligand CLA A 810



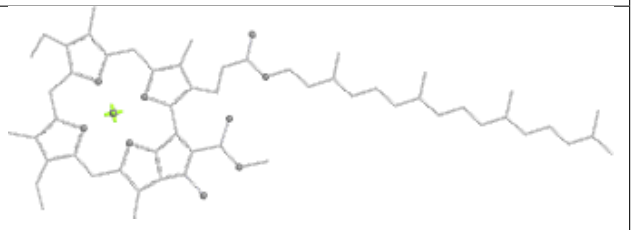
Bond lengths



Bond angles

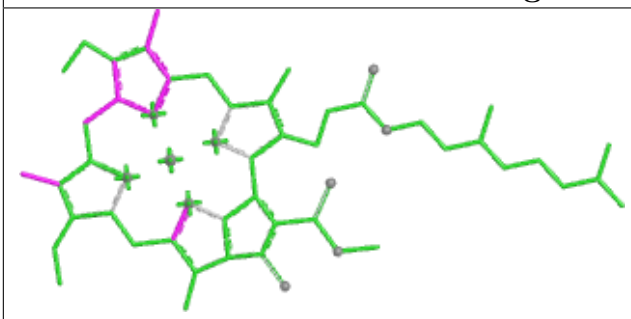


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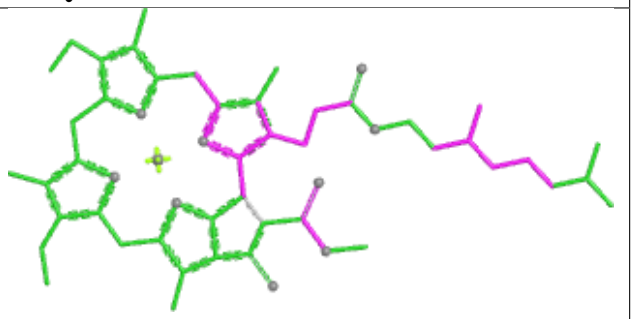


Rings

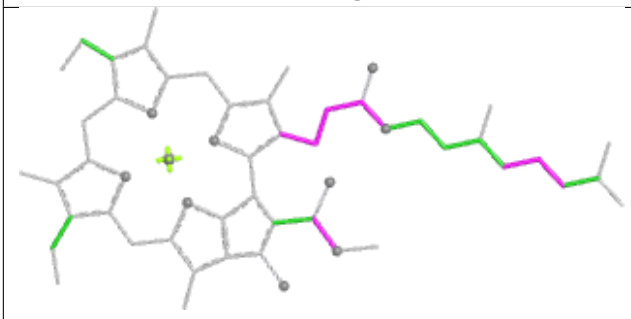
Ligand CLA Q 301



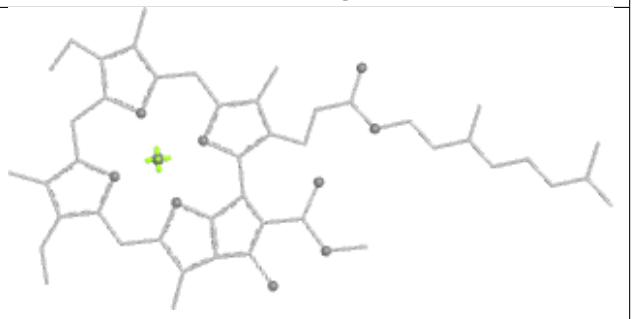
Bond lengths



Bond angles

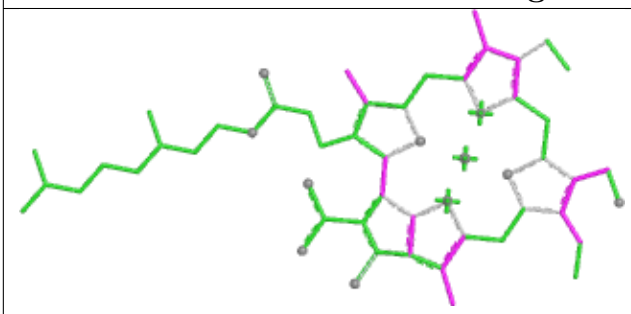


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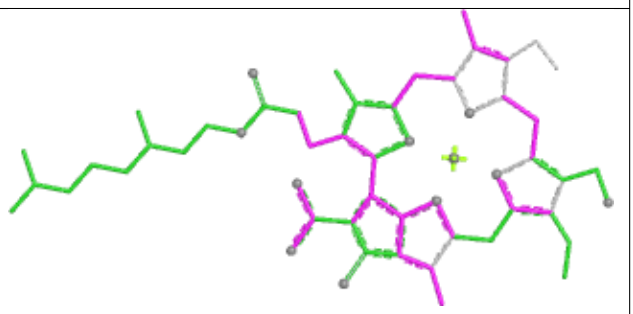


Rings

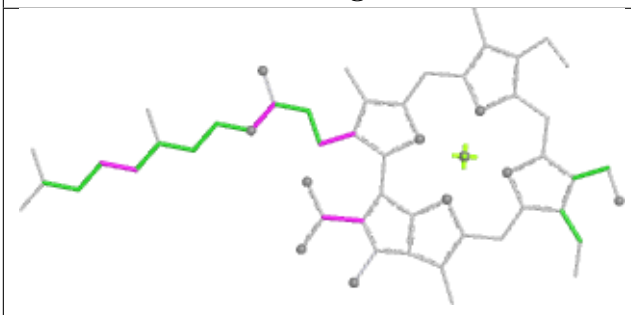
Ligand CHL 1 601



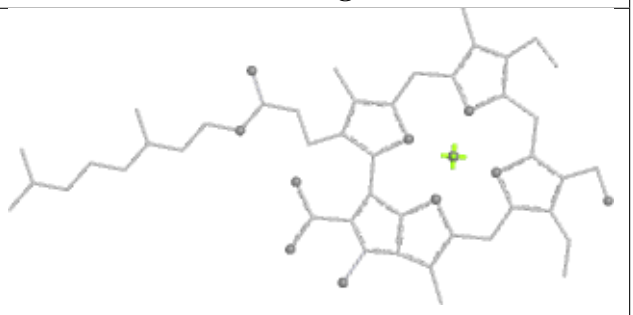
Bond lengths



Bond angles

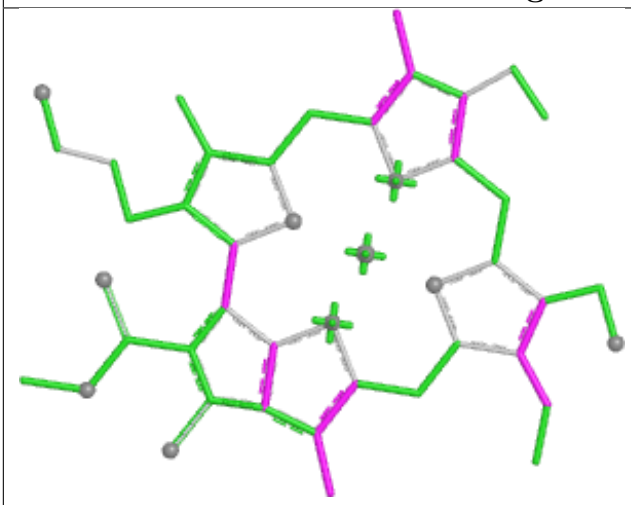


Torsions

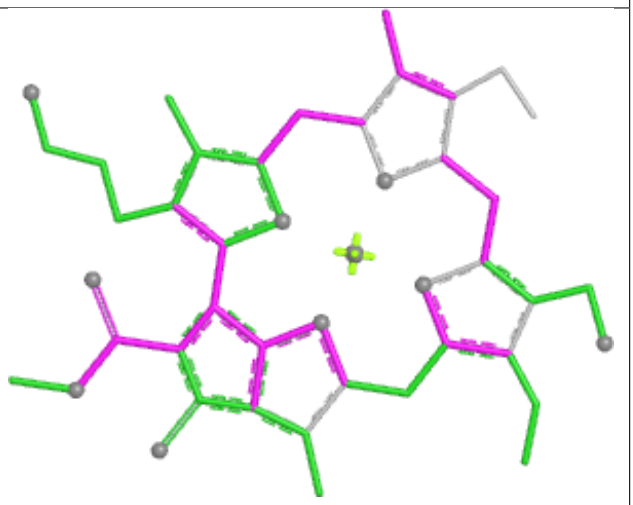


Rings

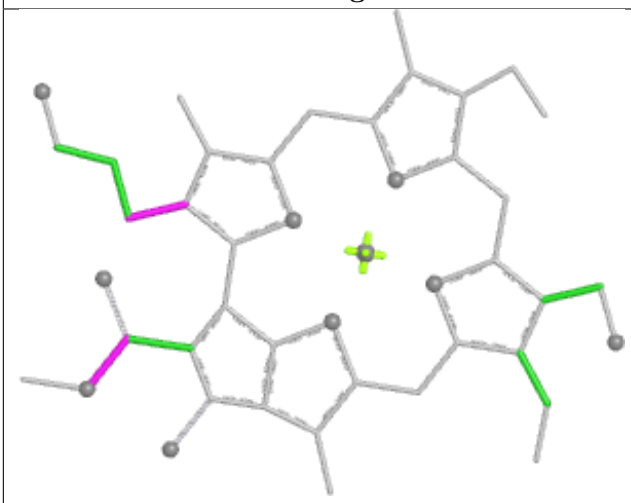
Ligand CHL S 314



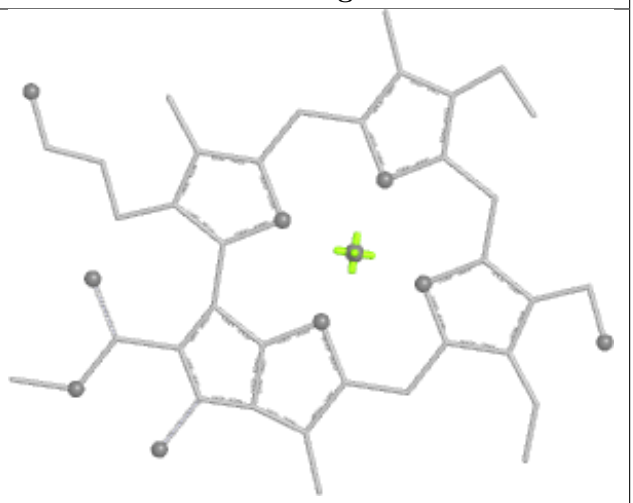
Bond lengths



Bond angles

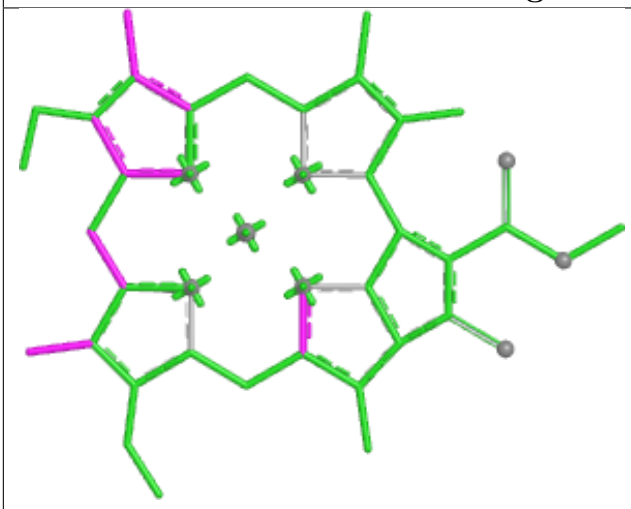


Torsions

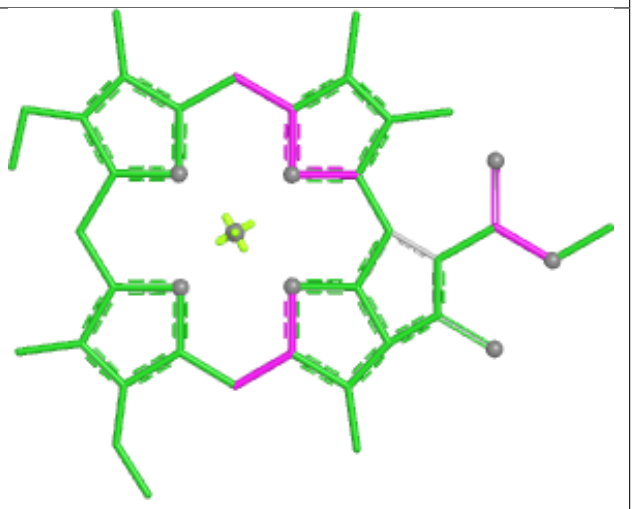


Rings

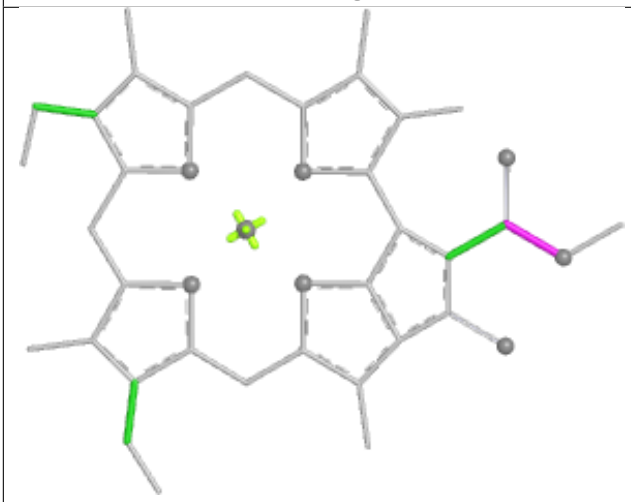
Ligand CLA L 301



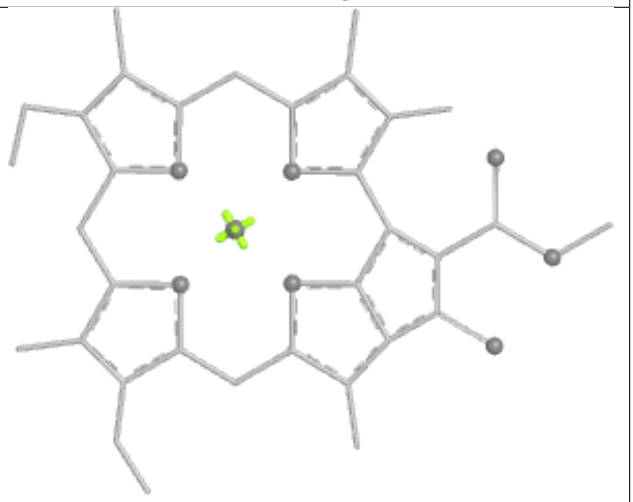
Bond lengths



Bond angles

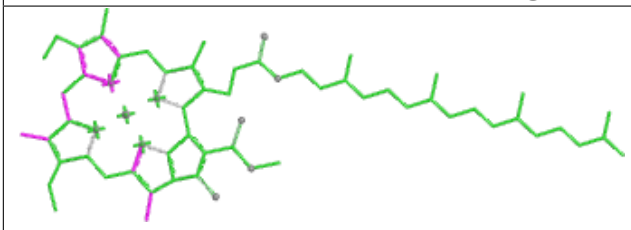


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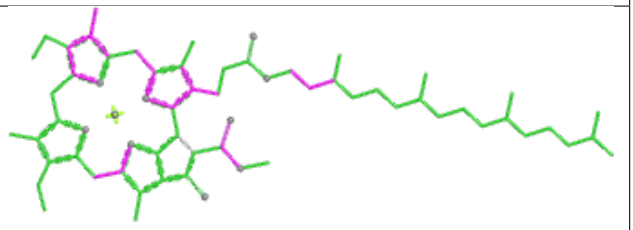


Rings

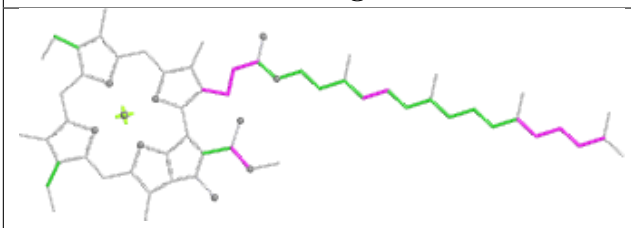
Ligand CLA B 843



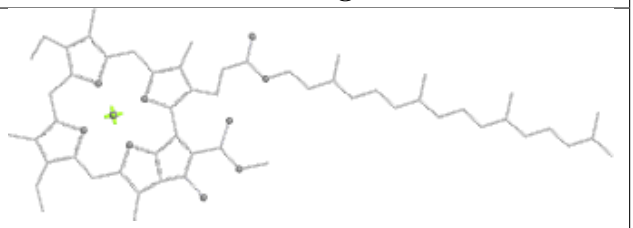
Bond lengths



Bond angles

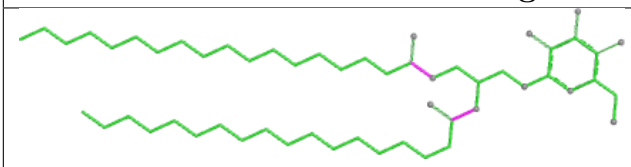


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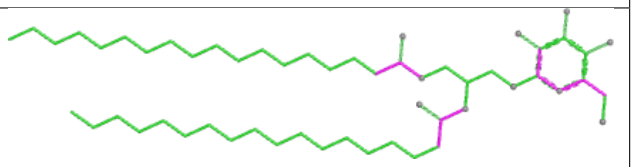


Rings

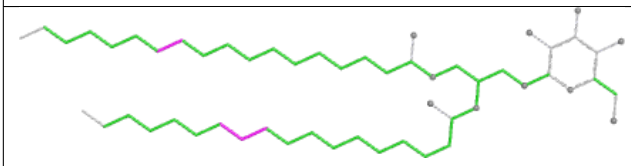
Ligand LMG N 201



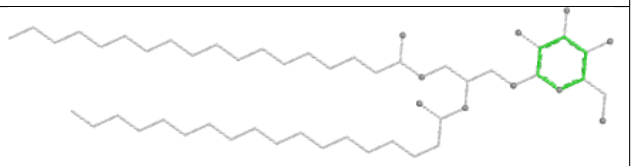
Bond lengths



Bond angles

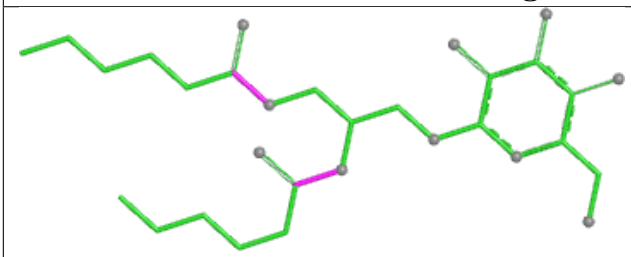


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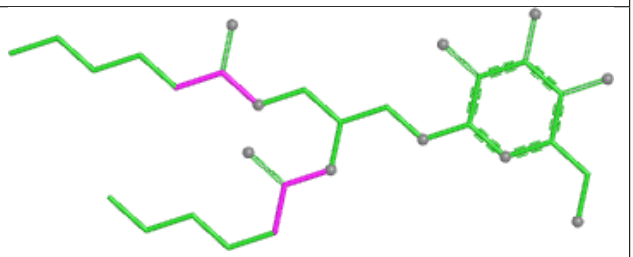


Rings

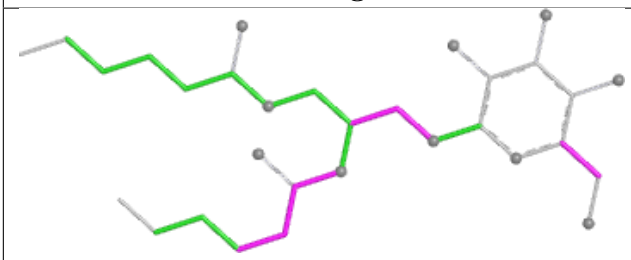
Ligand LMG L 308



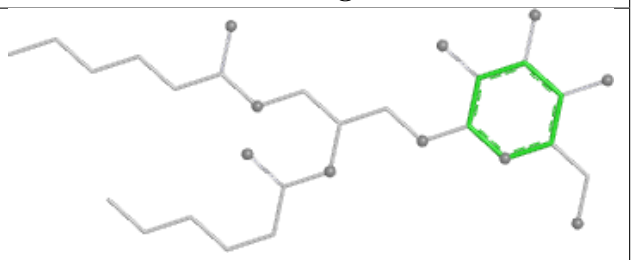
Bond lengths



Bond angles

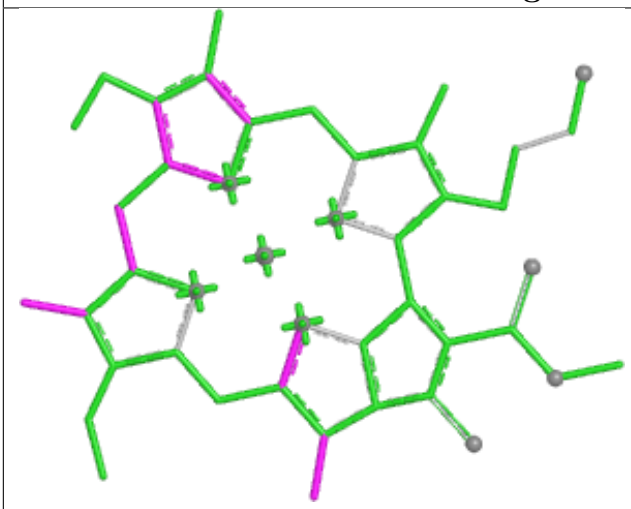


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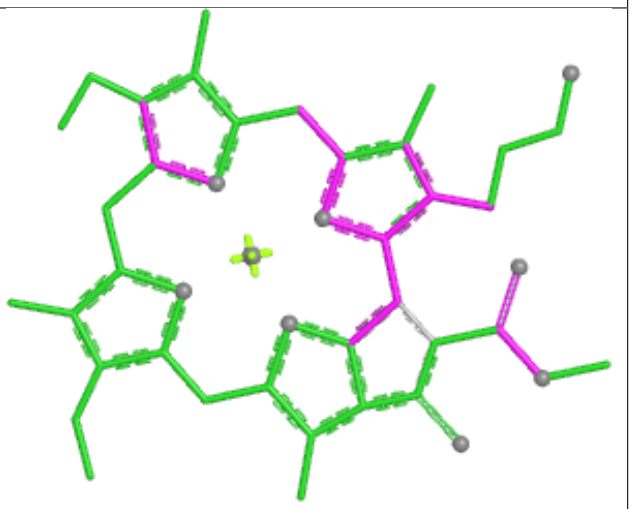


Rings

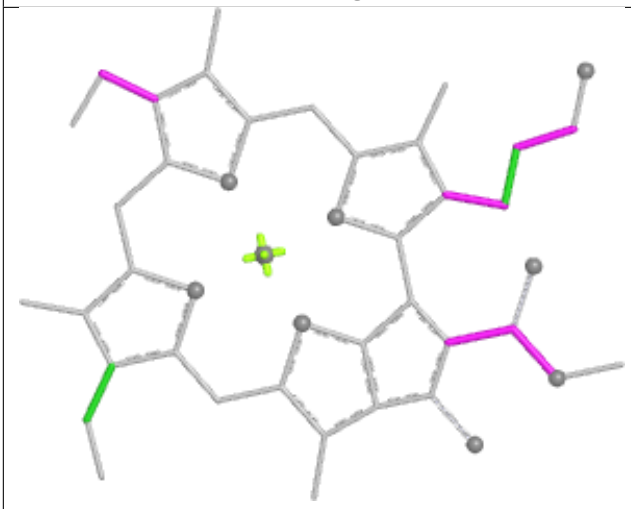
Ligand CLA U 310



Bond lengths



Bond angles

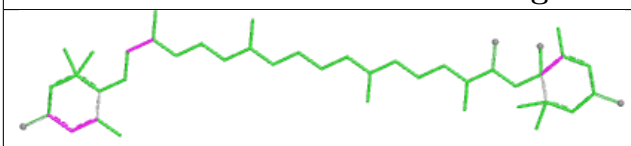


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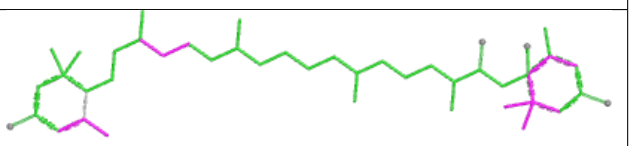


Rings

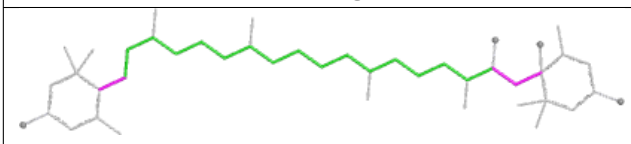
Ligand IWJ 5 611



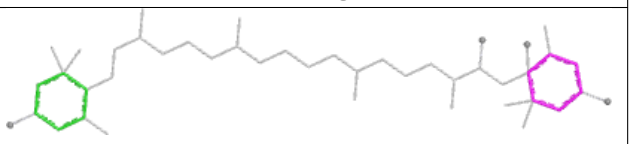
Bond lengths



Bond angles

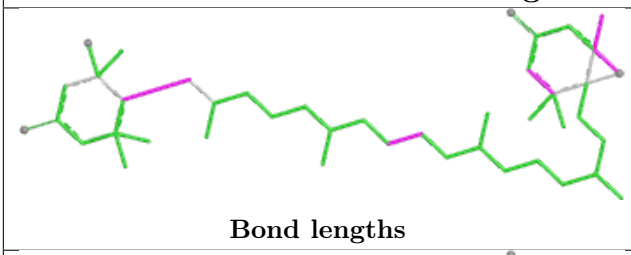


Torsions

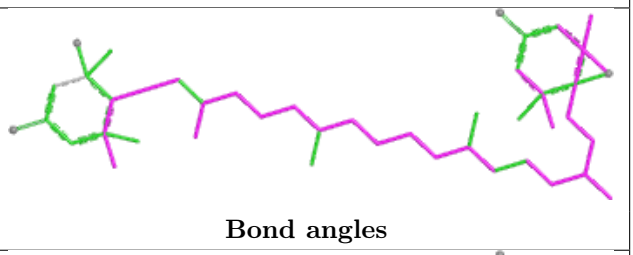


Rings

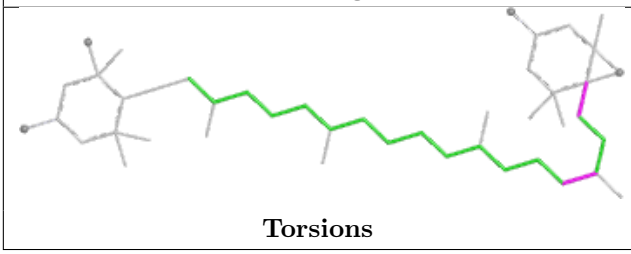
Ligand NEX T 317



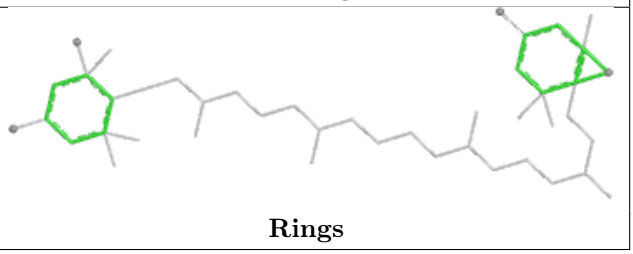
Bond lengths



Bond angles

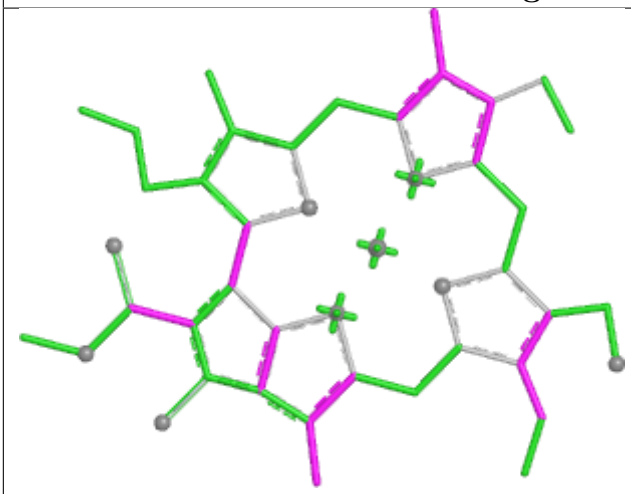


Torsions

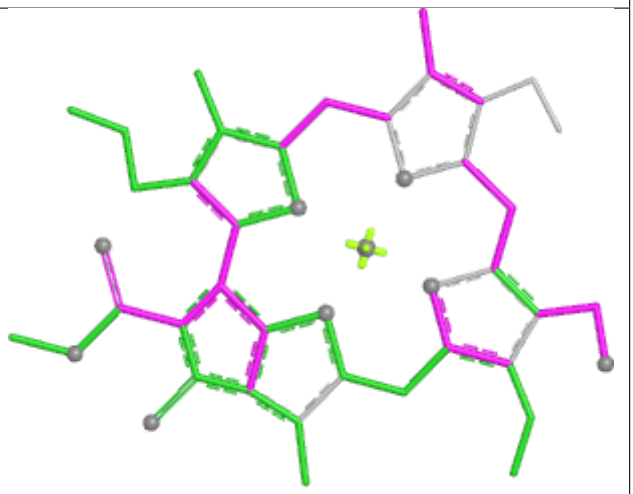


Rings

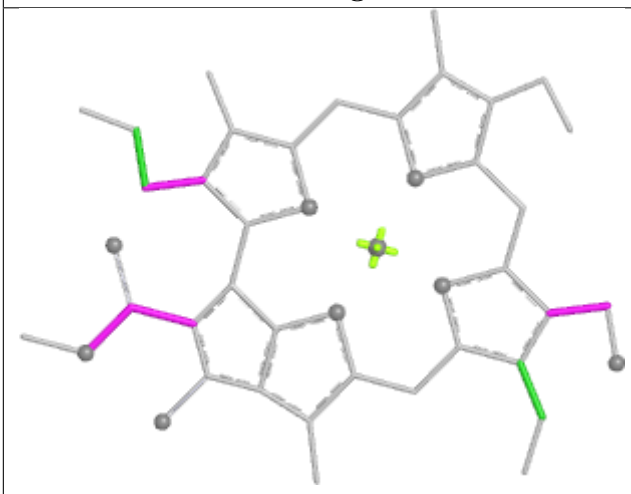
Ligand CHL U 306



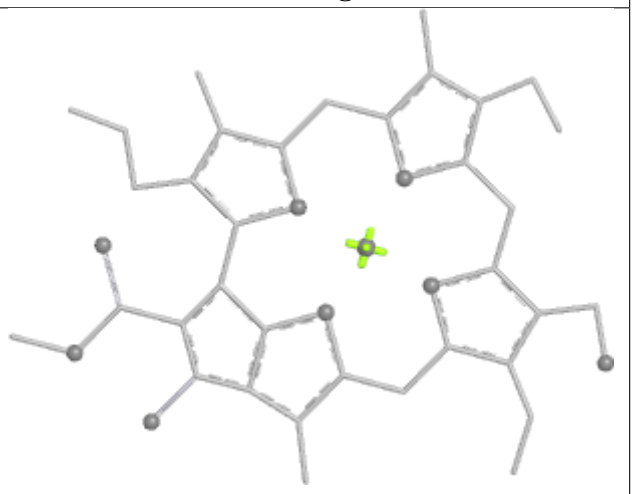
Bond lengths



Bond angles



Torsions

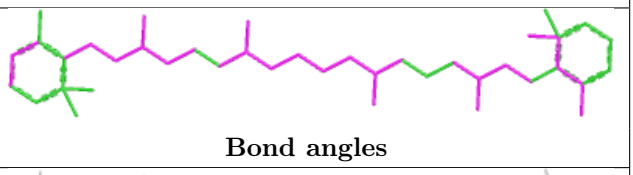


Rings

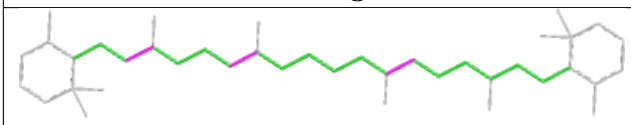
Ligand BCR H 305



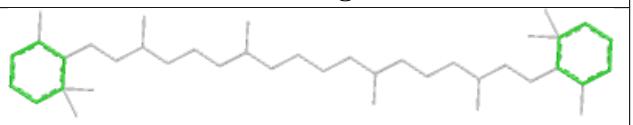
Bond lengths



Bond angles

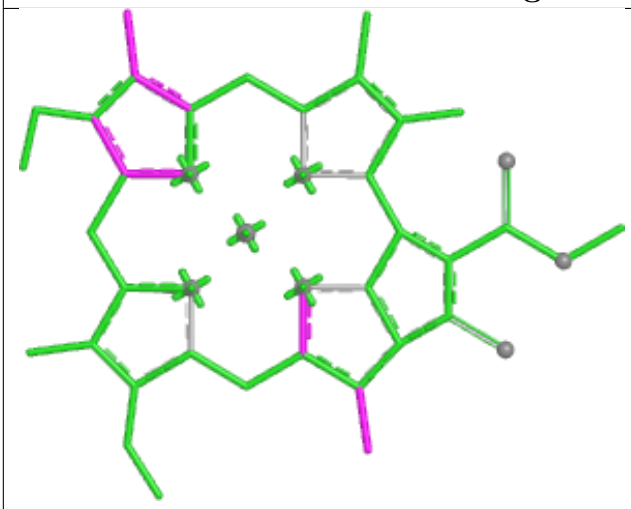


Torsions

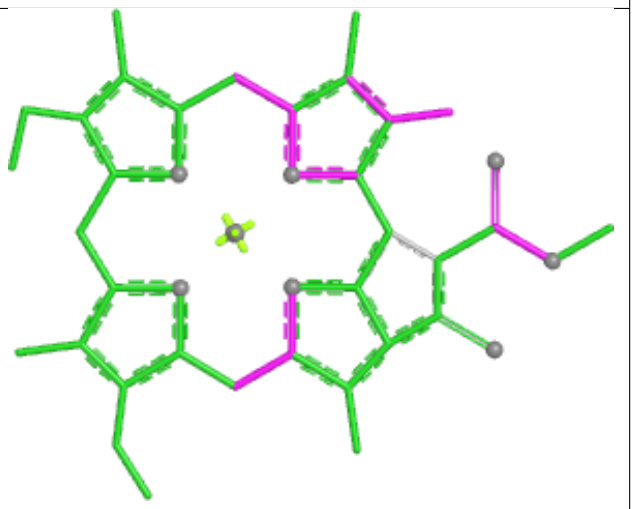


Rings

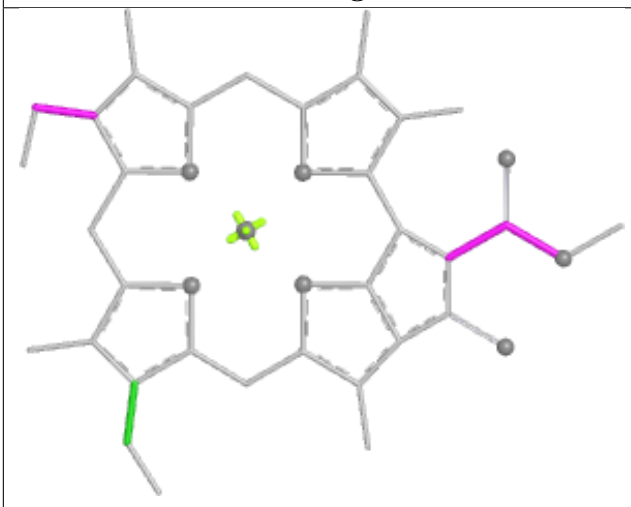
Ligand CLA X 314



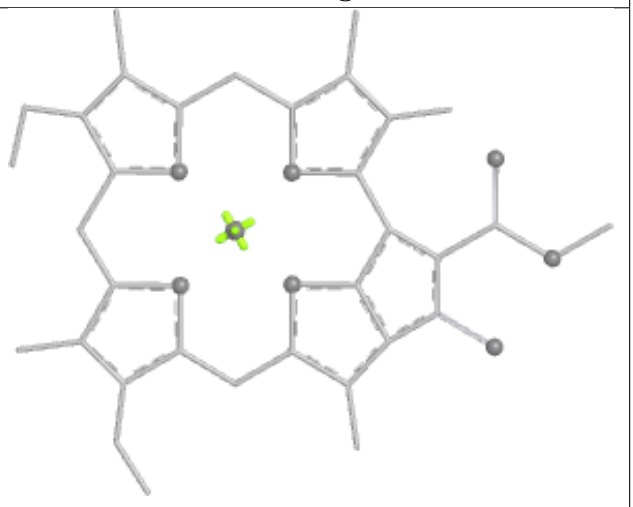
Bond lengths



Bond angles

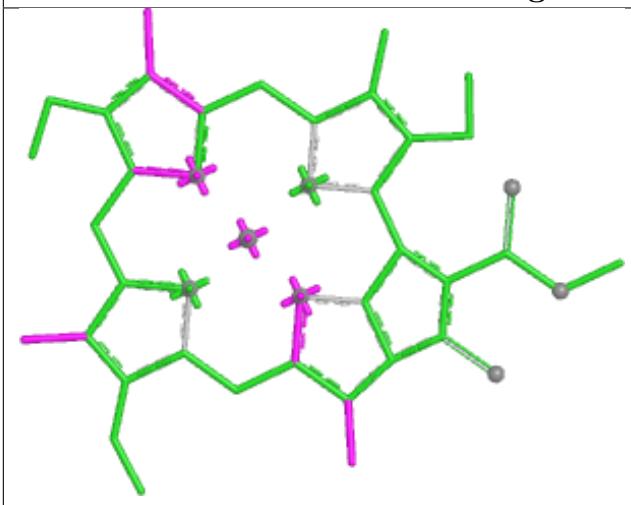


Torsions

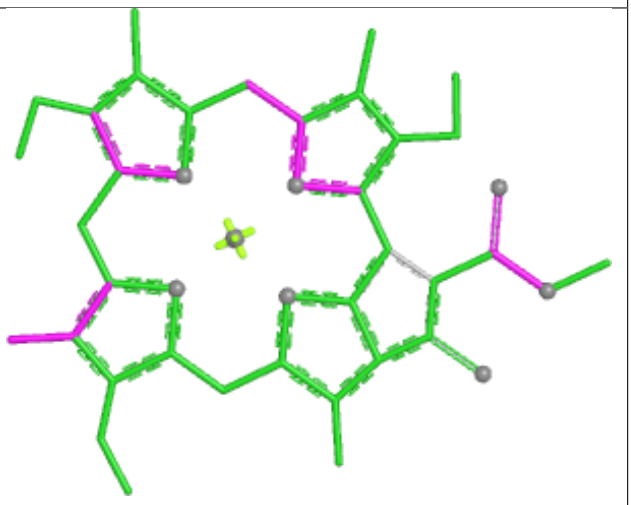


Rings

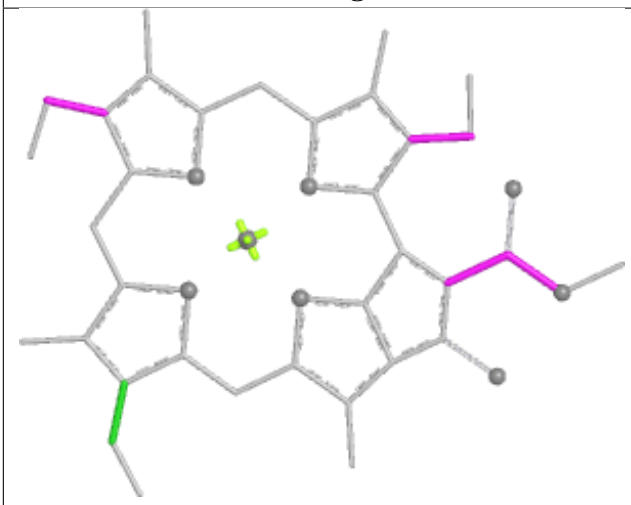
Ligand CLA J 102



Bond lengths



Bond angles

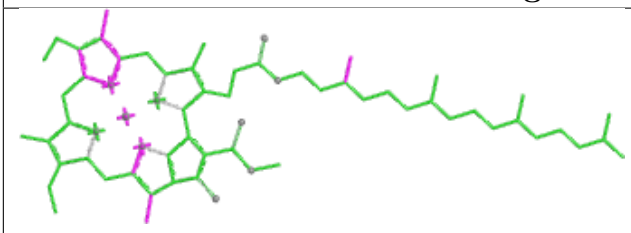


Torsions

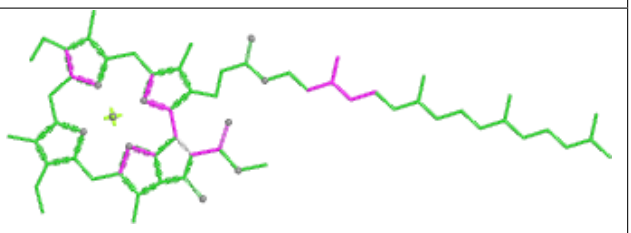


Rings

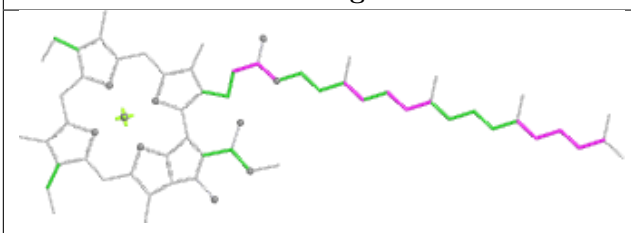
Ligand CLA A 831



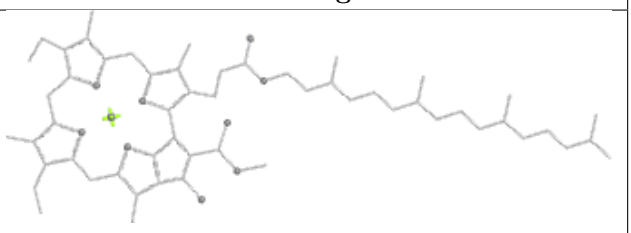
Bond lengths



Bond angles

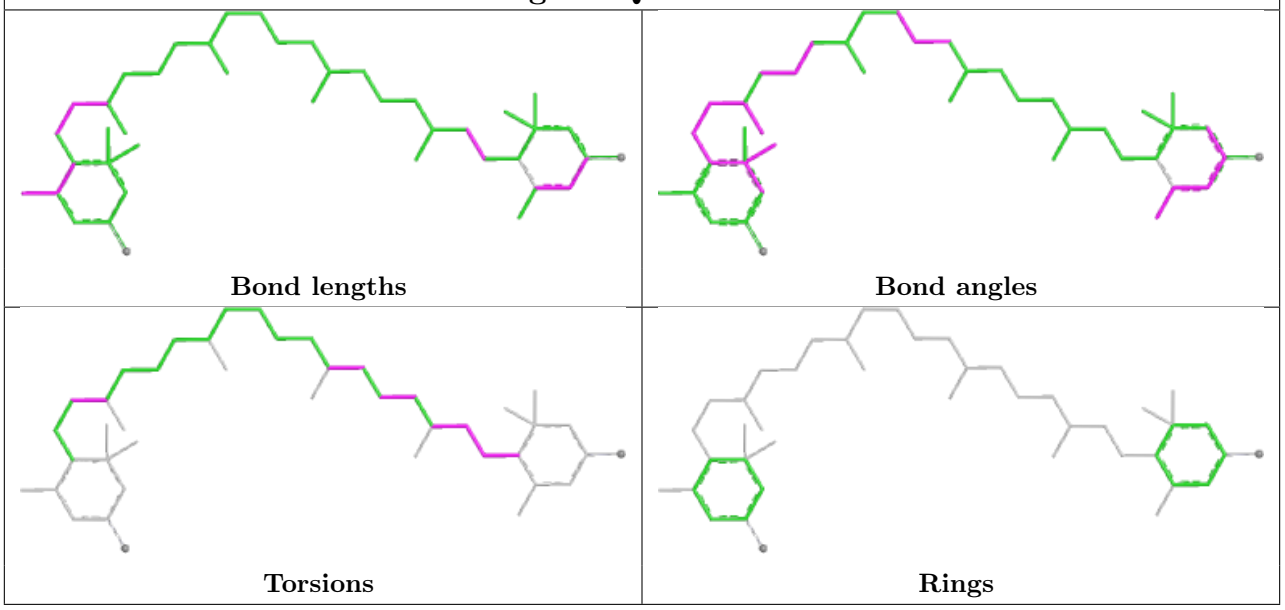


Torsions

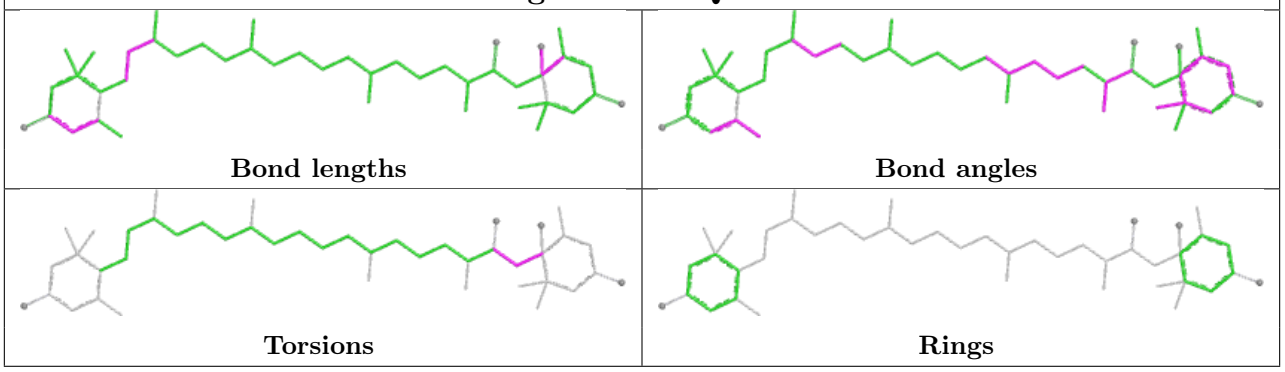


Rings

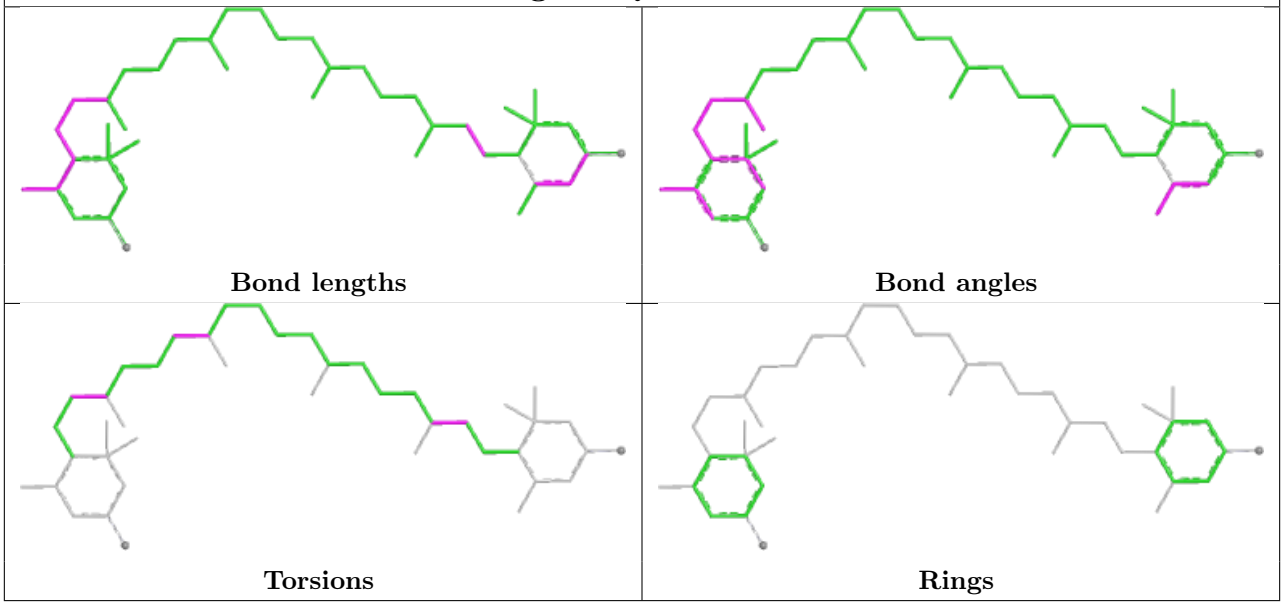
Ligand Q6L R 323



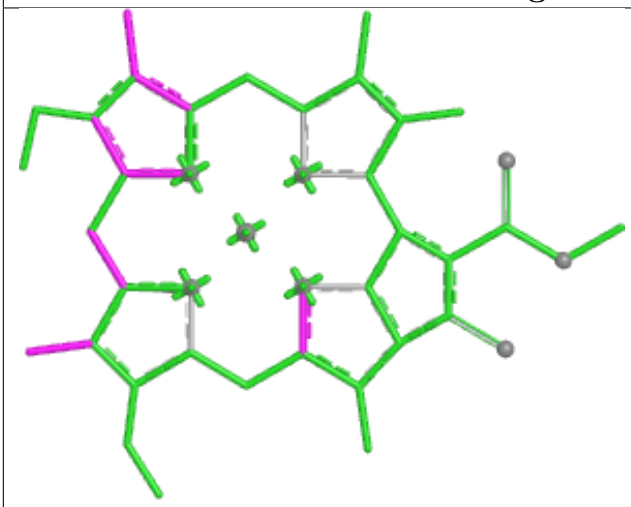
Ligand IWJ Q 303



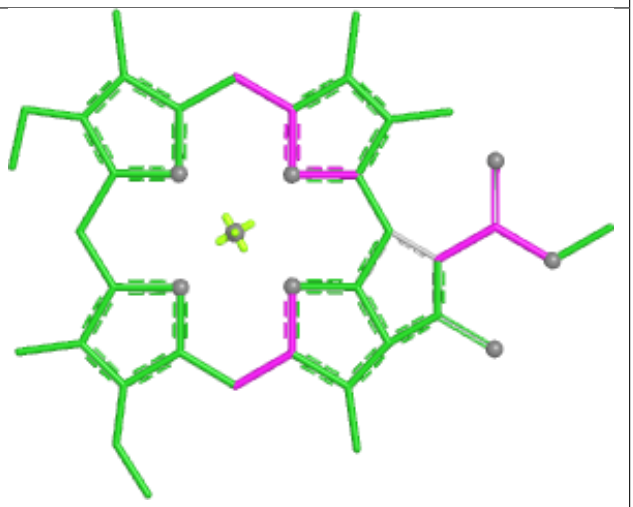
Ligand Q6L T 315



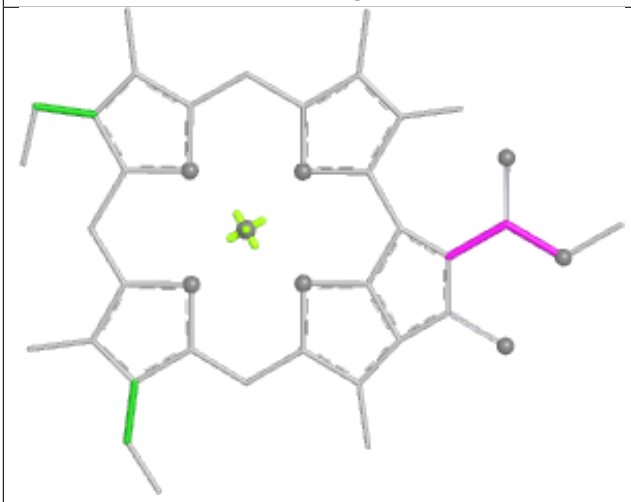
Ligand CLA 5 608



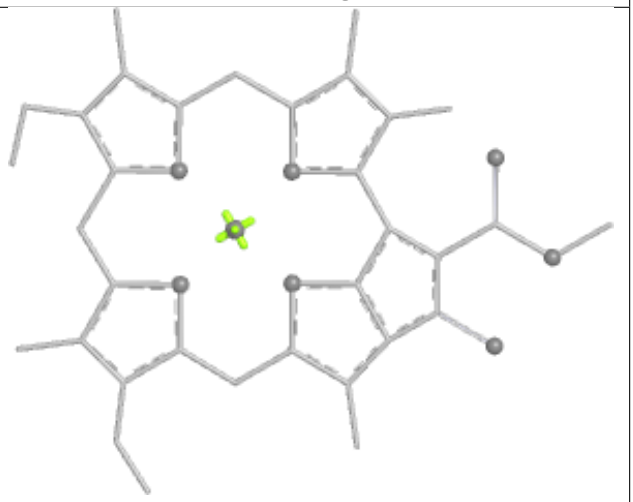
Bond lengths



Bond angles

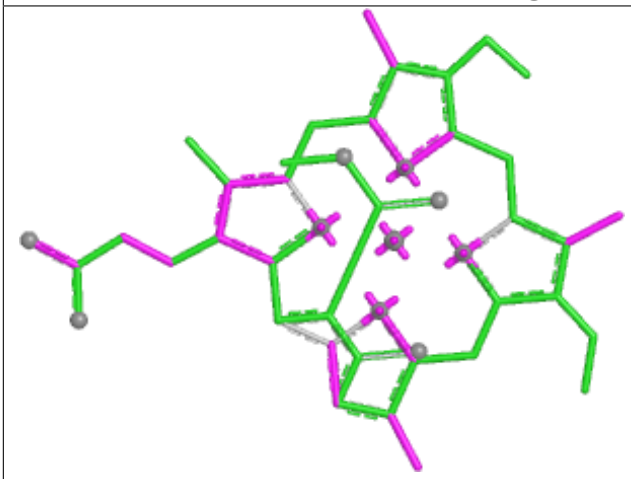


Torsions

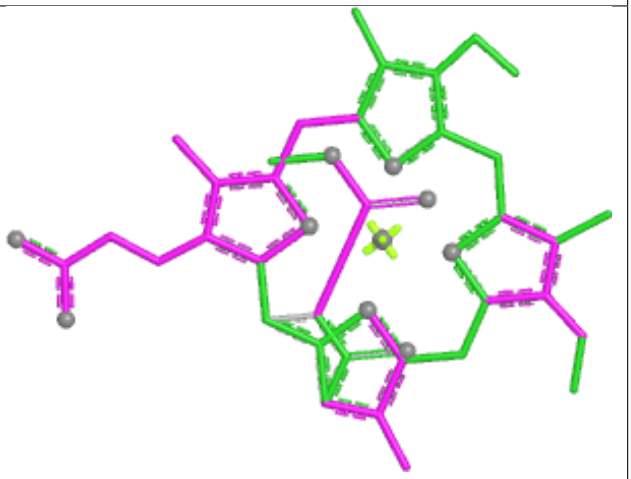


Rings

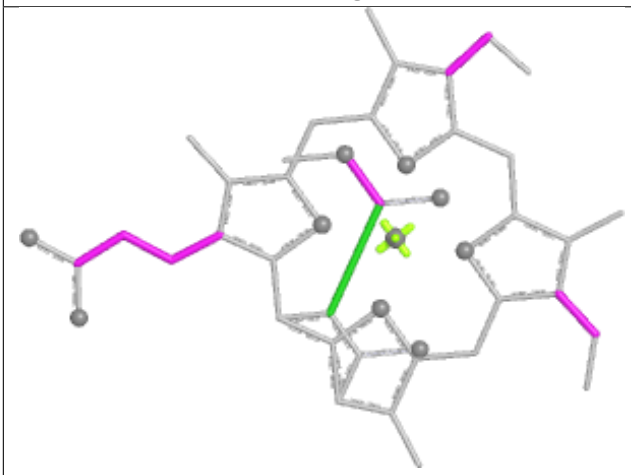
Ligand KC2 X 309



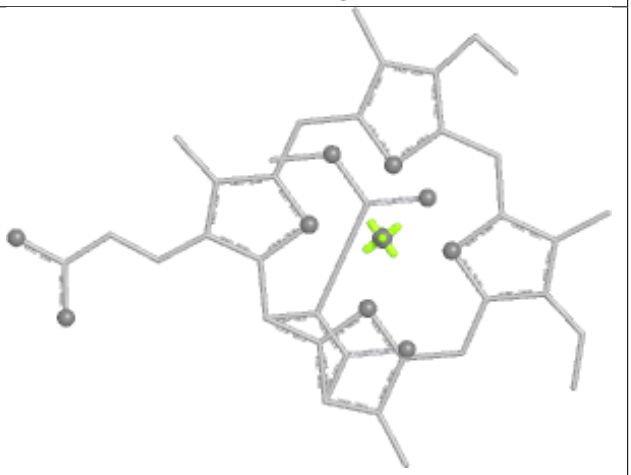
Bond lengths



Bond angles

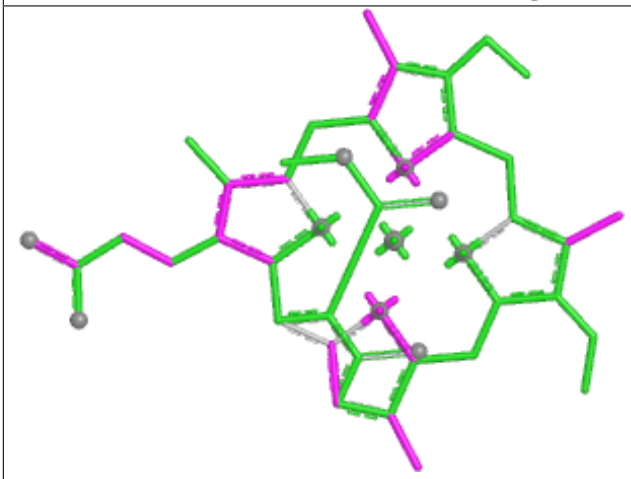


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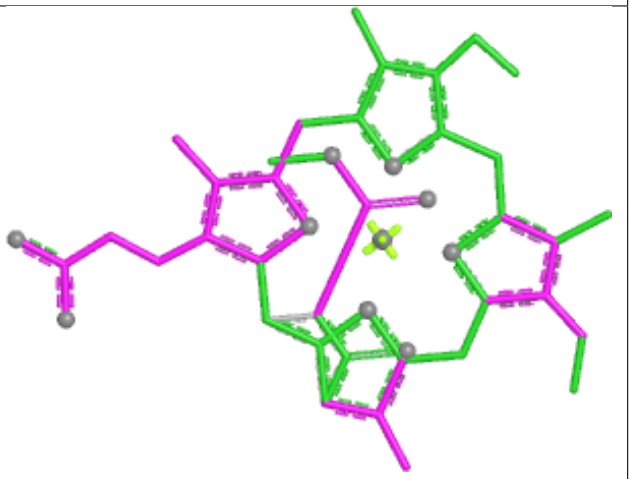


Rings

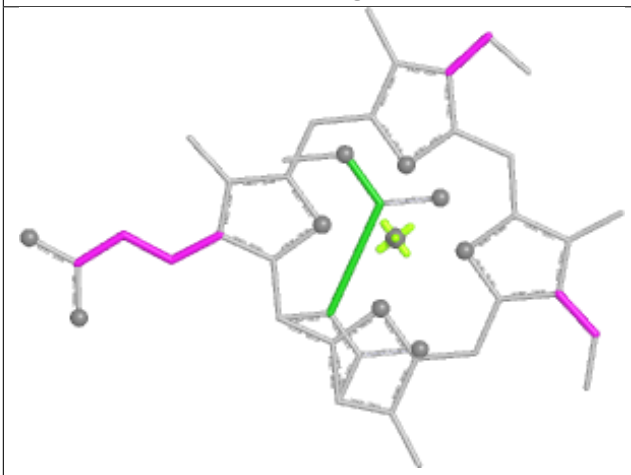
Ligand KC2 R 312



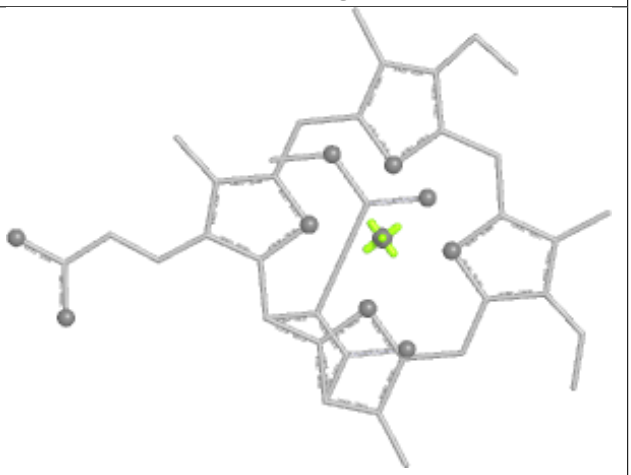
Bond lengths



Bond angles

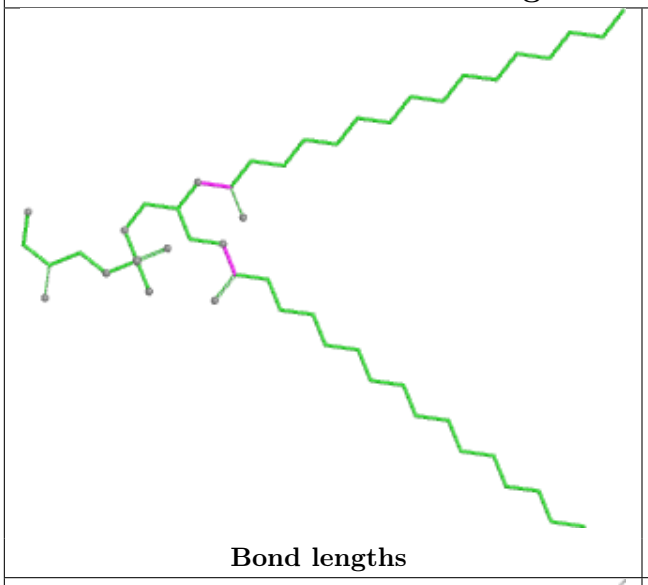


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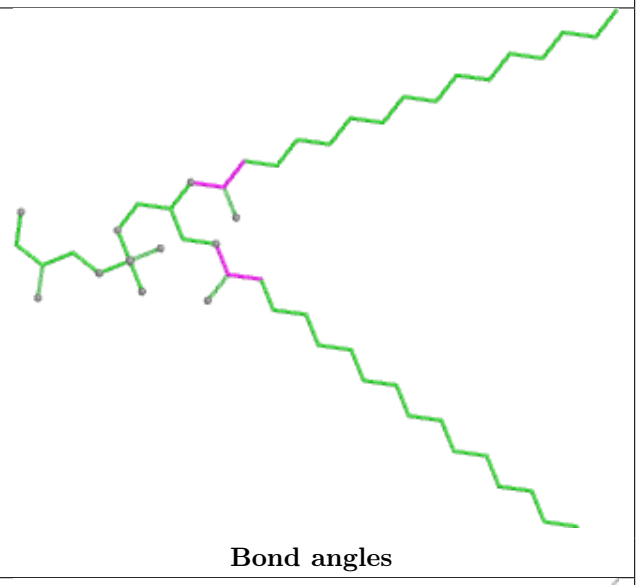


Rings

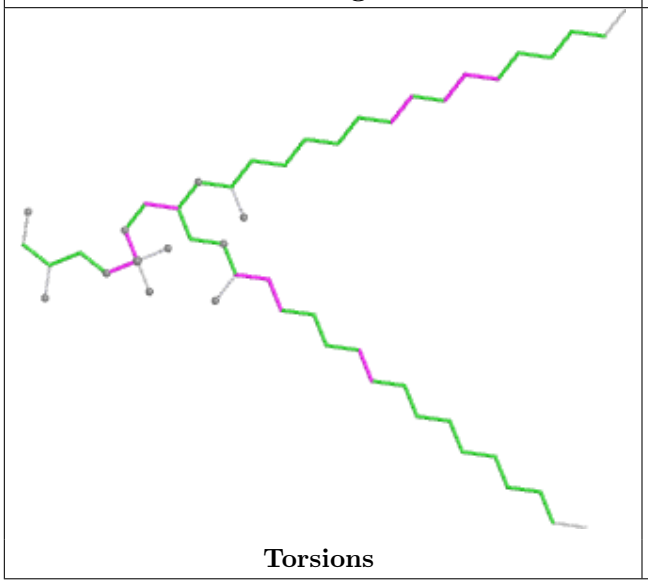
Ligand LHG A 846



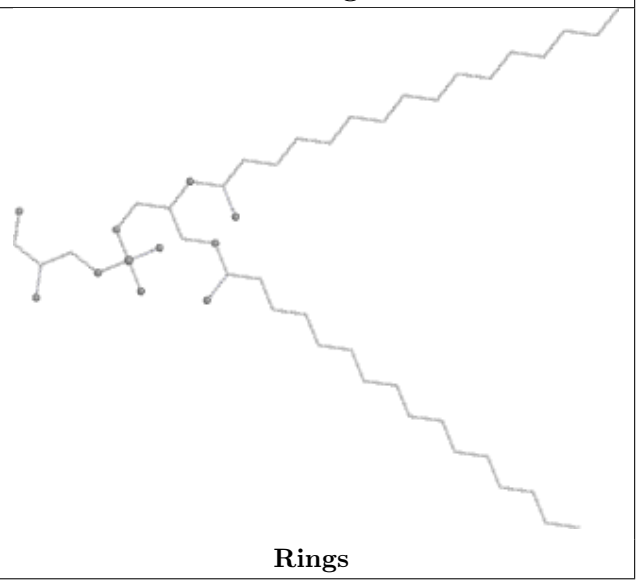
Bond lengths



Bond angles

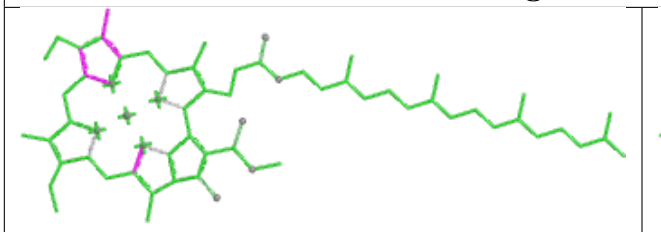


Torsions

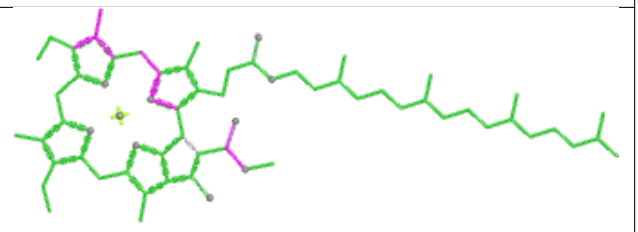


Rings

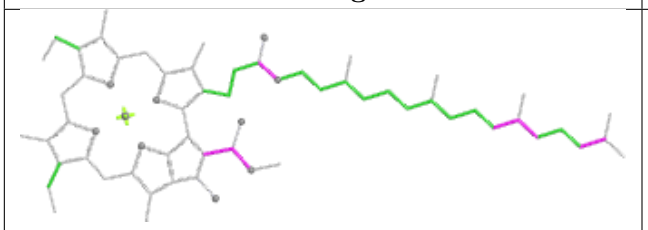
Ligand CLA A 832



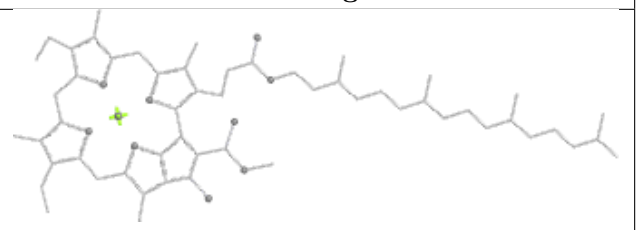
Bond lengths



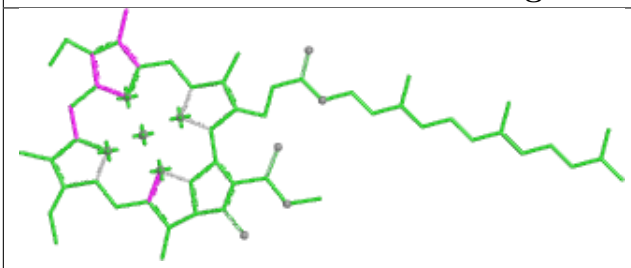
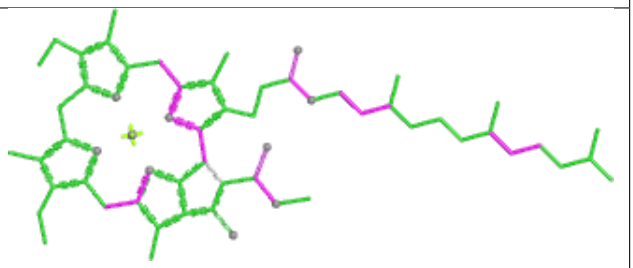
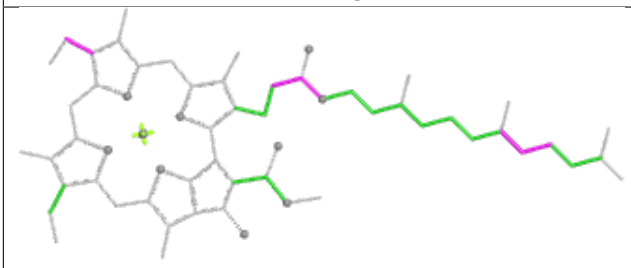
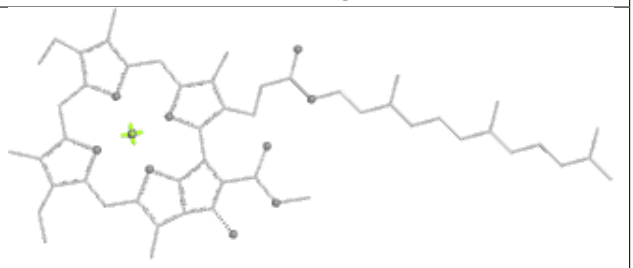
Bond angles

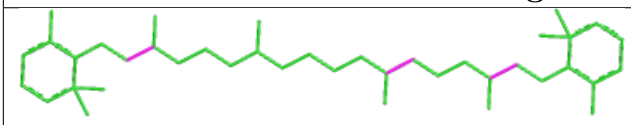
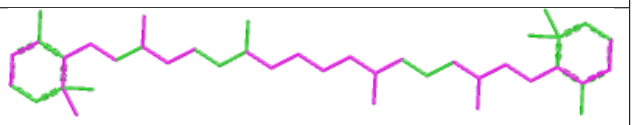
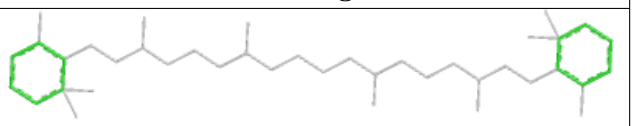


Torsions

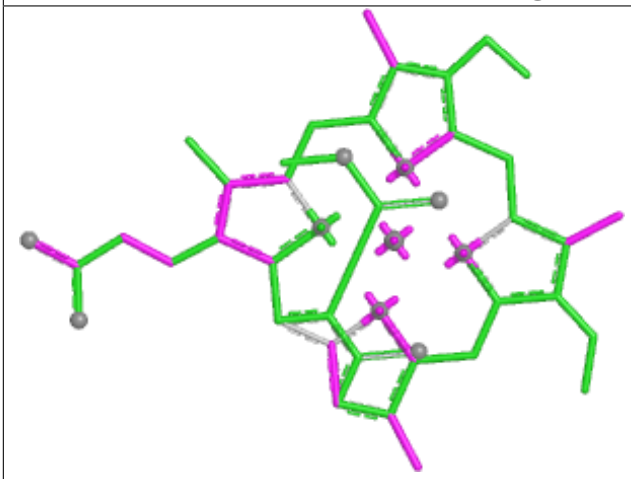


Rings

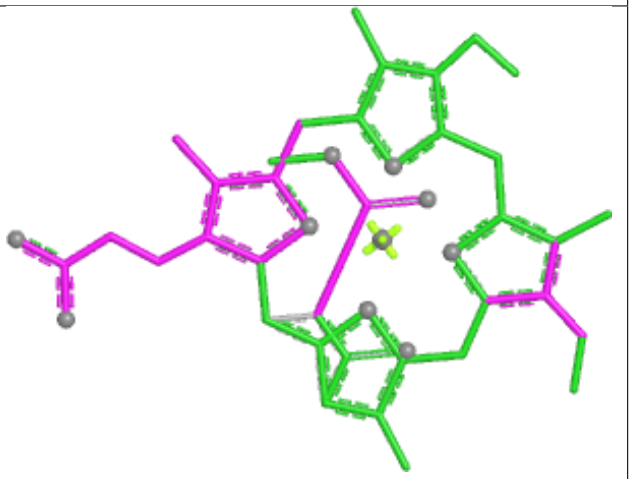
Ligand CLA P 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 2 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

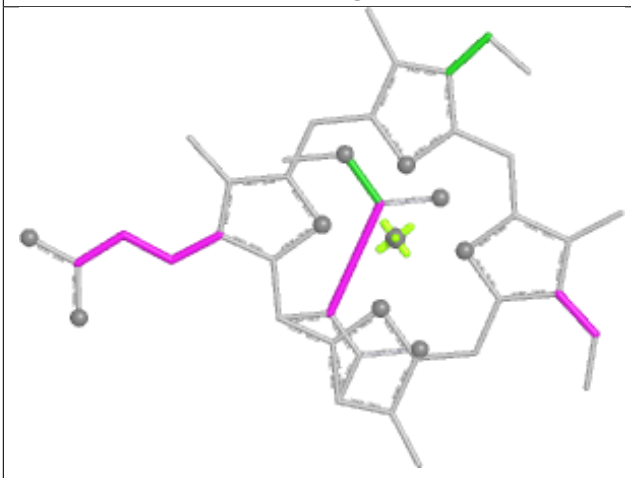
Ligand KC2 S 308



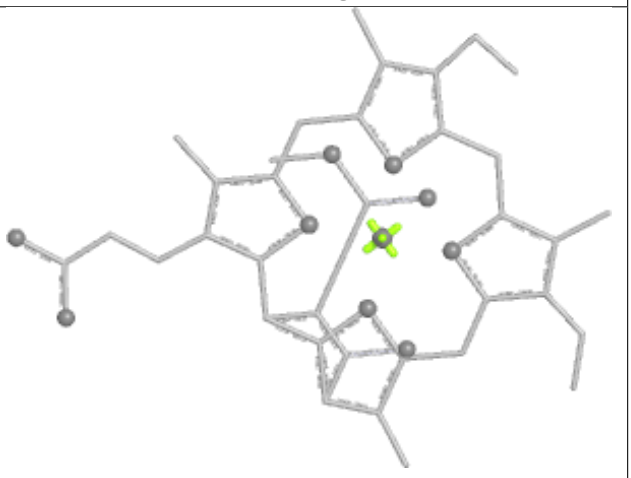
Bond lengths



Bond angles

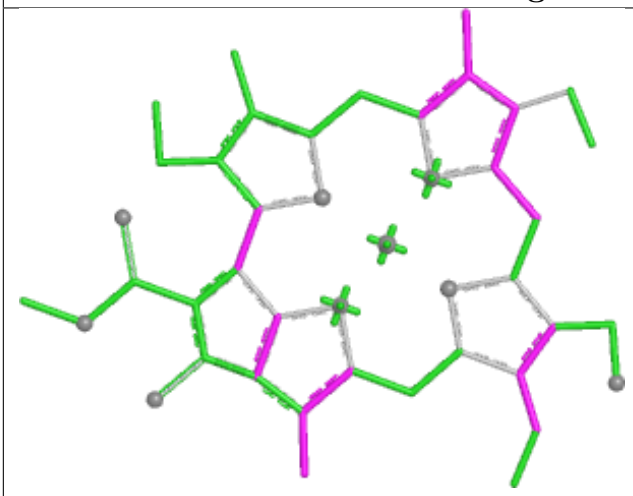


Torsions

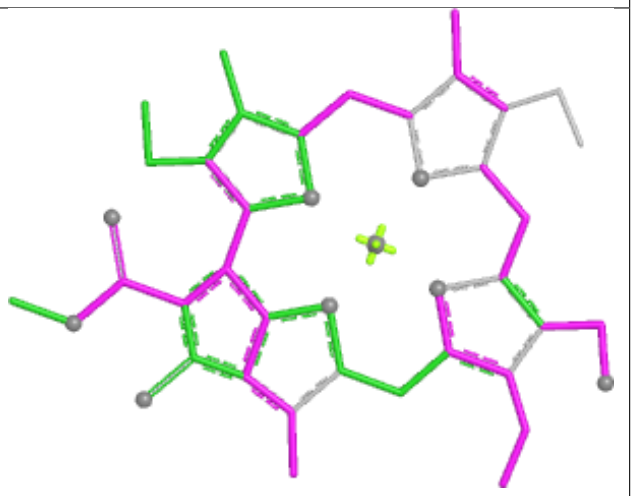


Rings

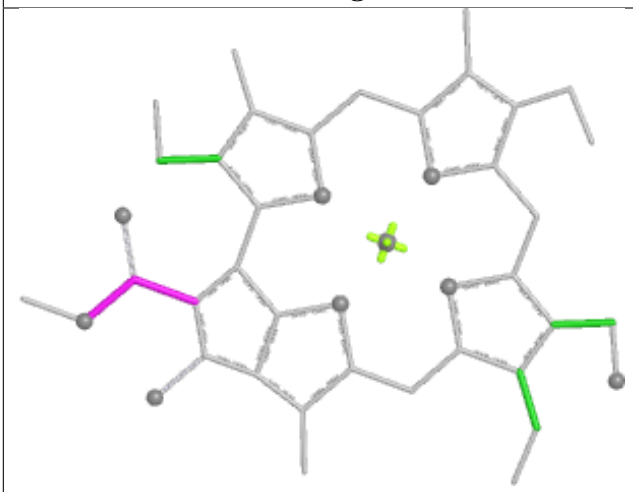
Ligand CHL 2 615



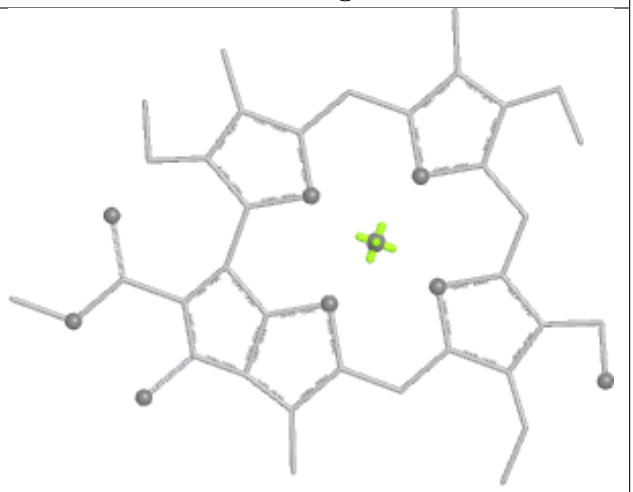
Bond lengths



Bond angles

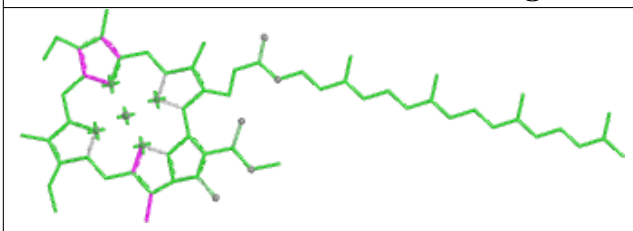


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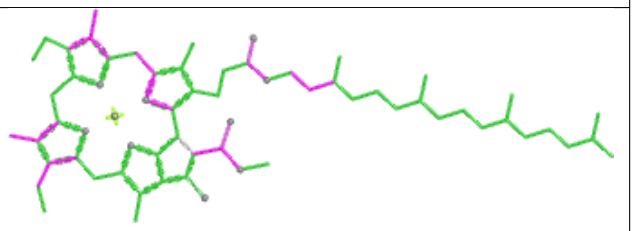


Rings

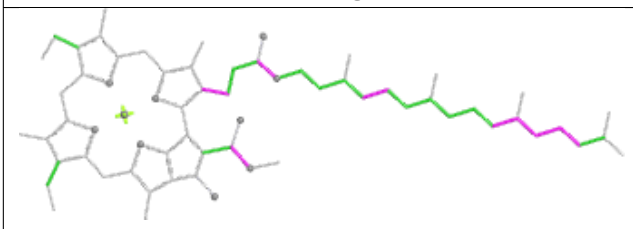
Ligand CLA A 805



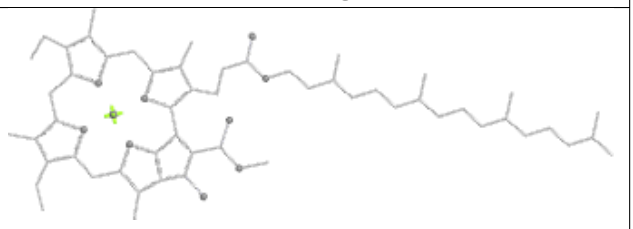
Bond lengths



Bond angles

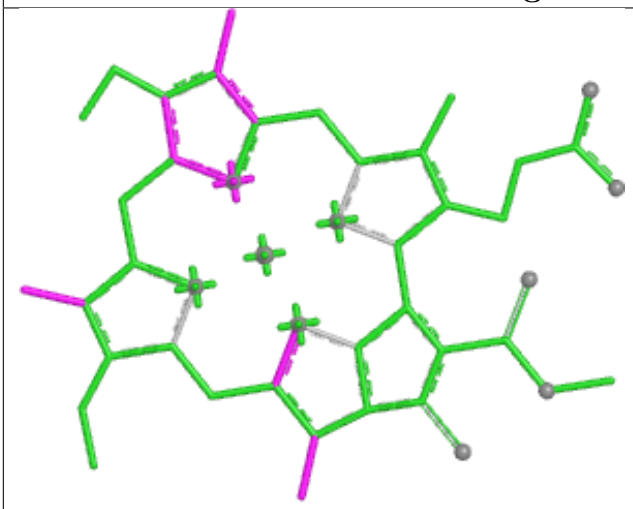


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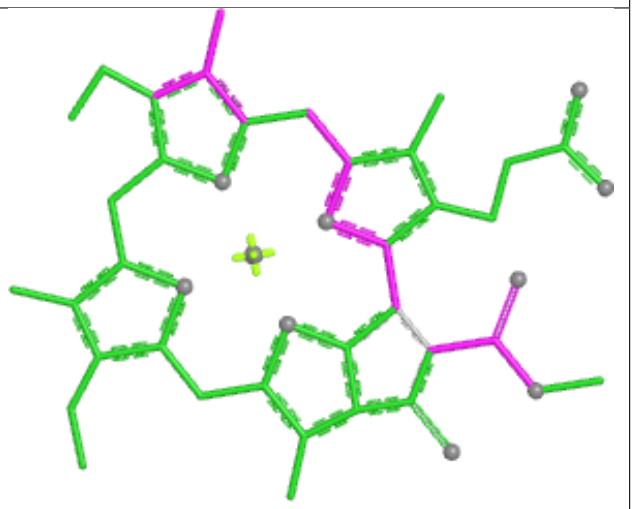


Rings

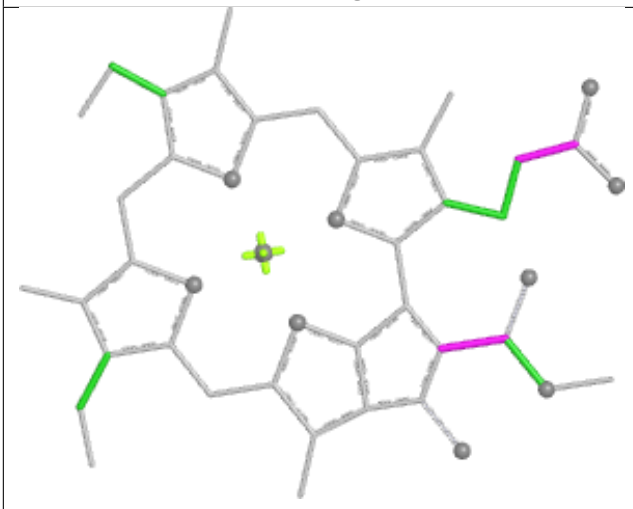
Ligand CLA A 822



Bond lengths



Bond angles

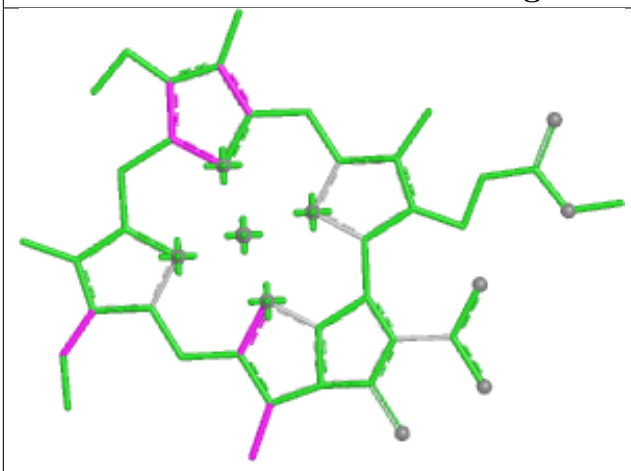


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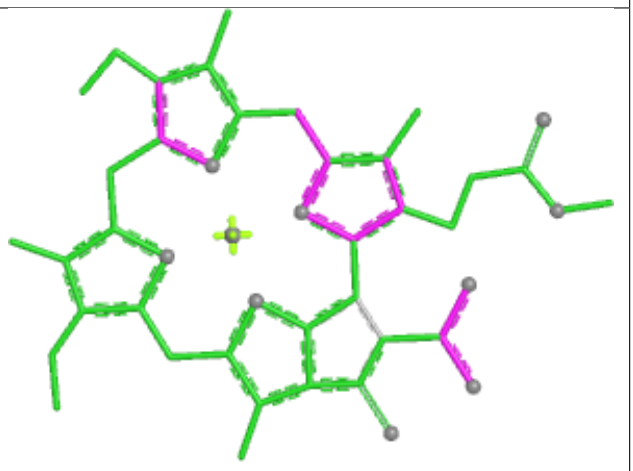


Rings

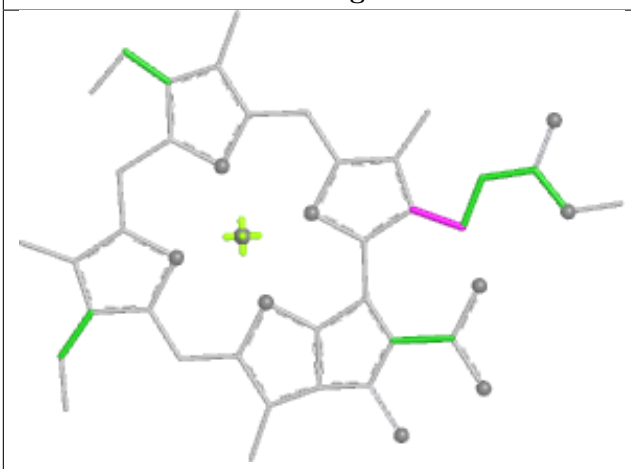
Ligand CLA N 202



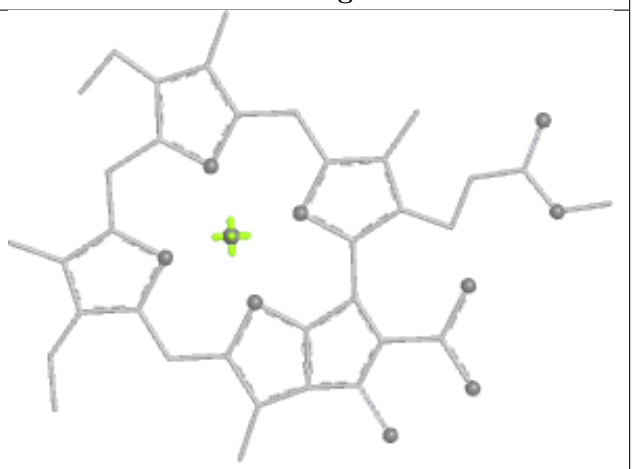
Bond lengths



Bond angles

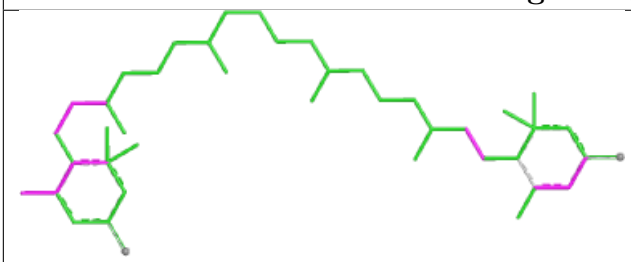


Torsions

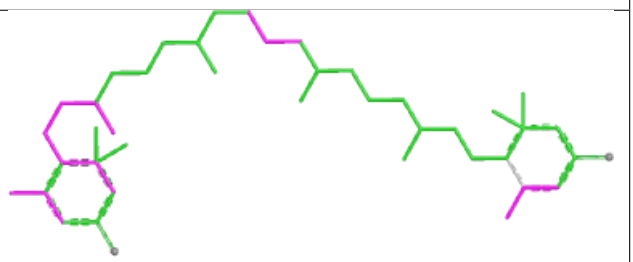


Rings

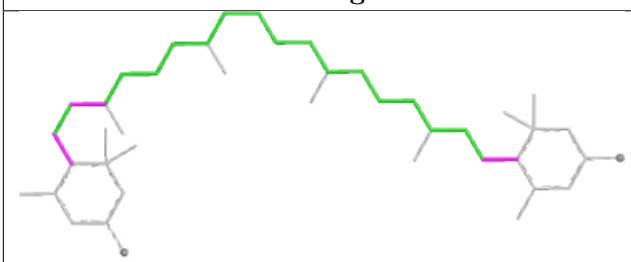
Ligand Q6L U 317



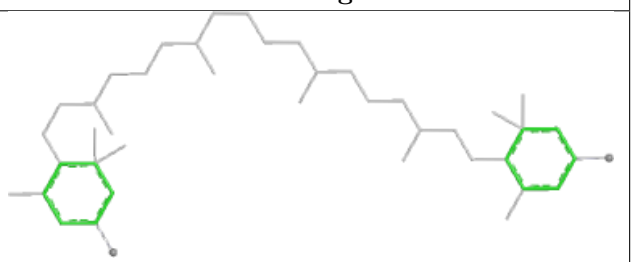
Bond lengths



Bond angles

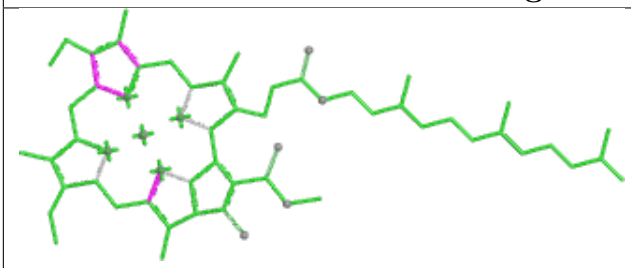


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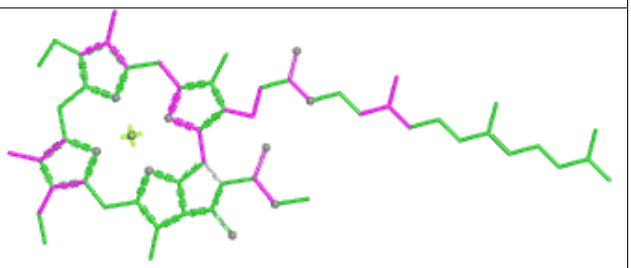


Rings

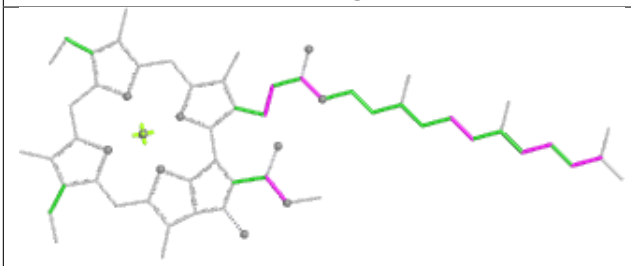
Ligand CLA P 311



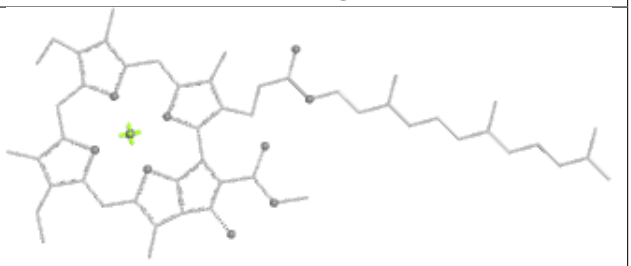
Bond lengths



Bond angles

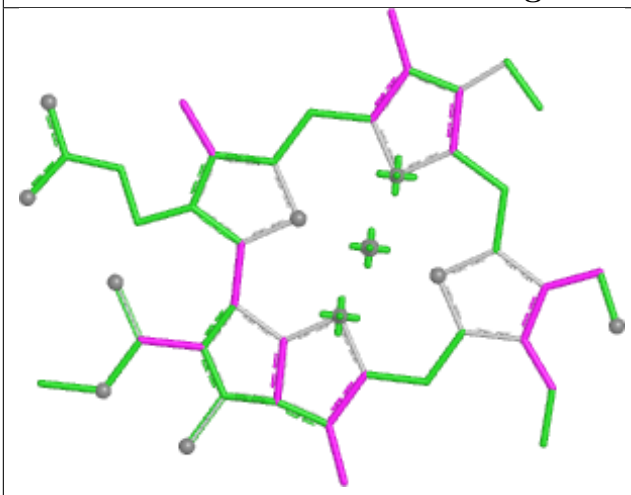


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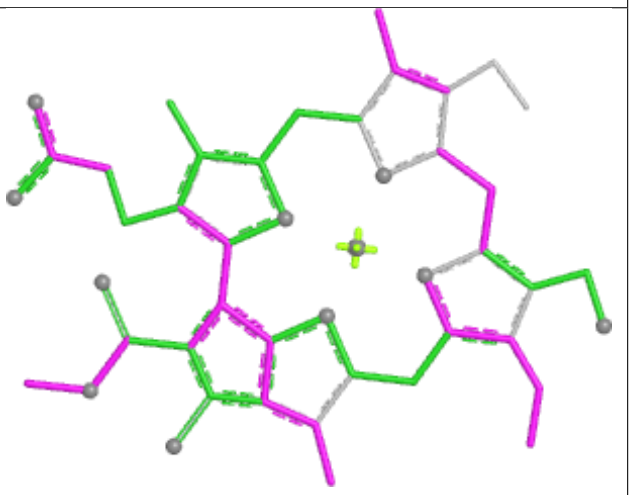


Rings

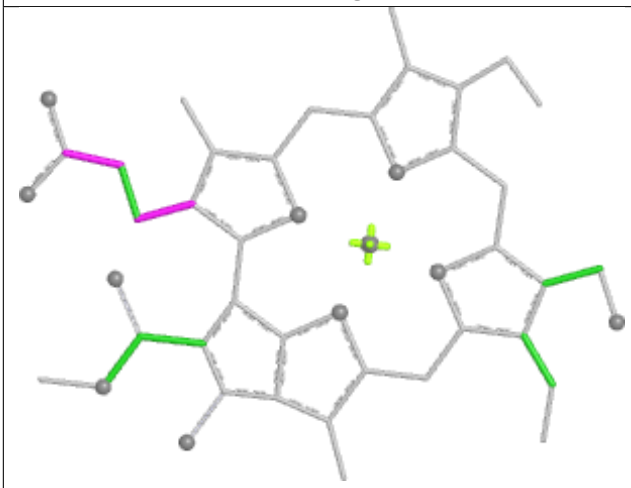
Ligand CHL P 305



Bond lengths



Bond angles

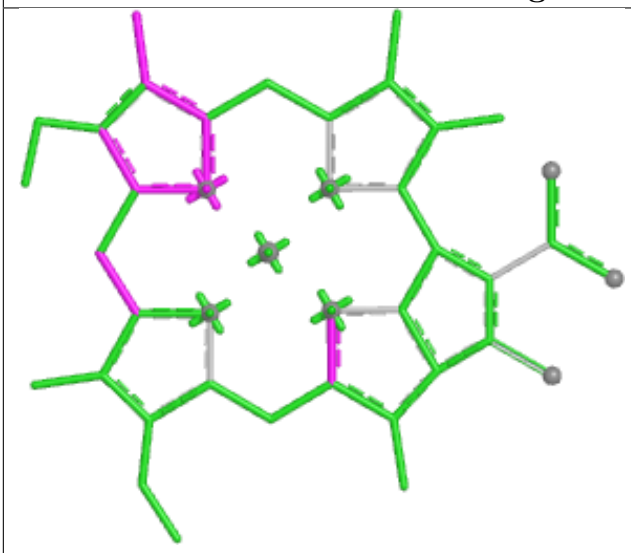


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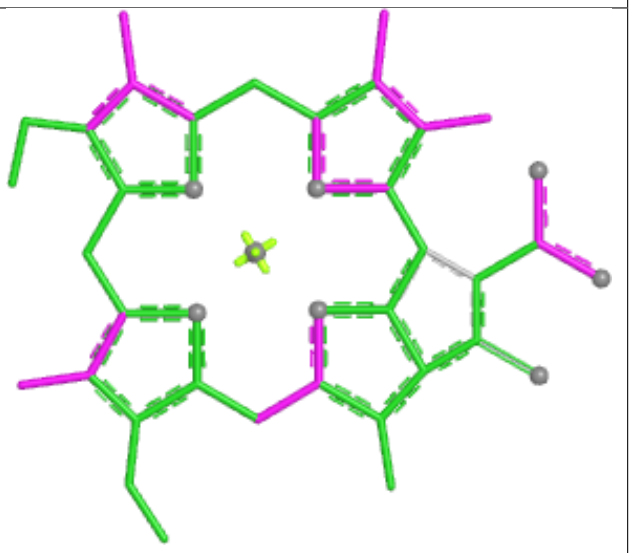


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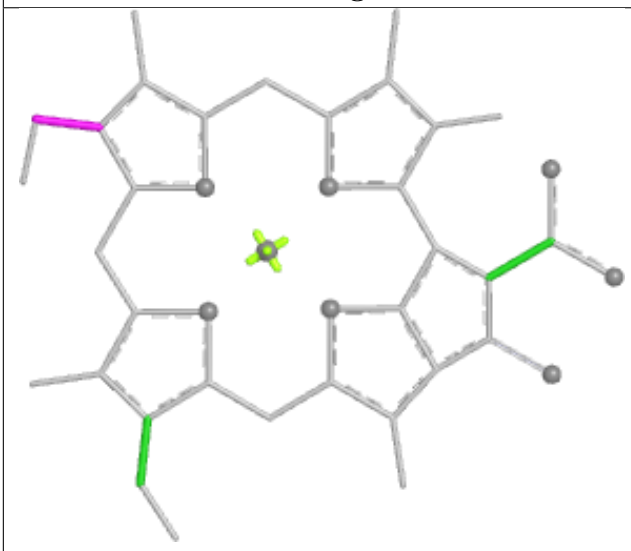
Ligand CLA 3 312



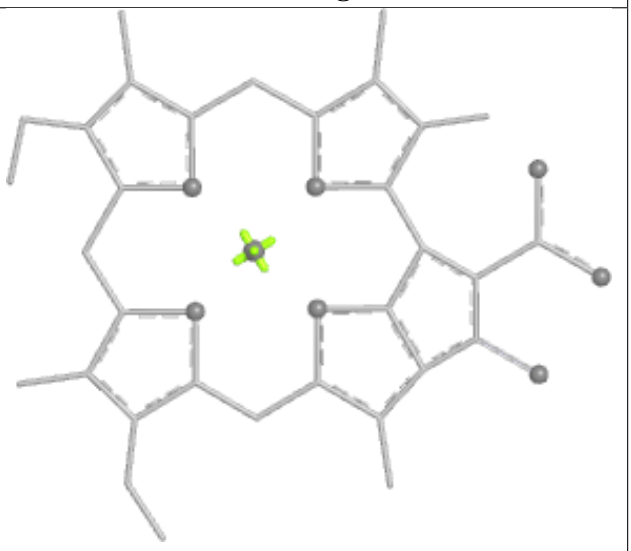
Bond lengths



Bond angles

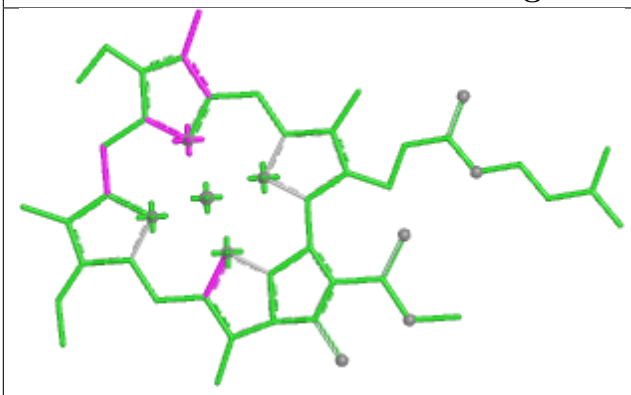


Torsions

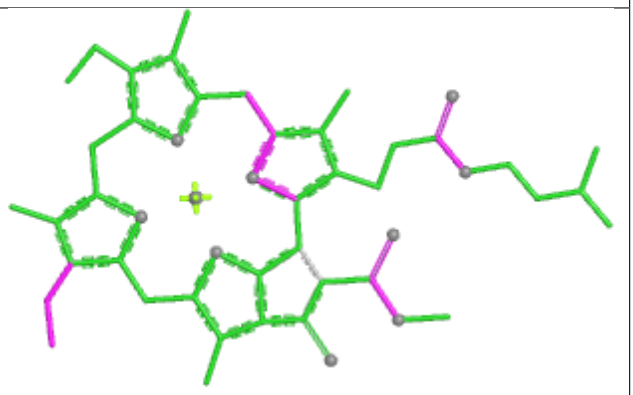


Rings

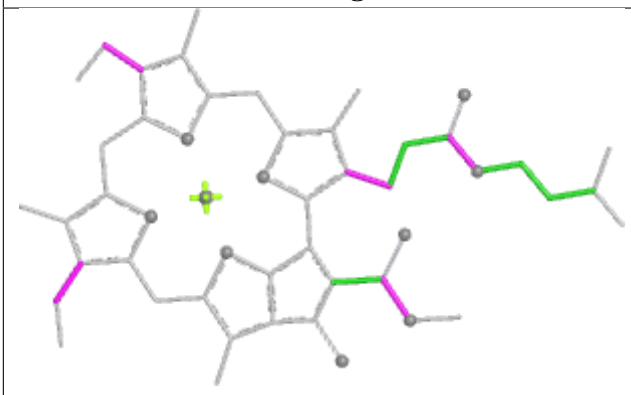
Ligand CLA X 311



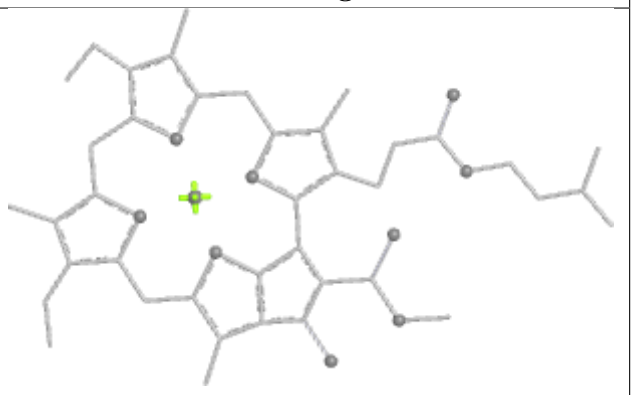
Bond lengths



Bond angles

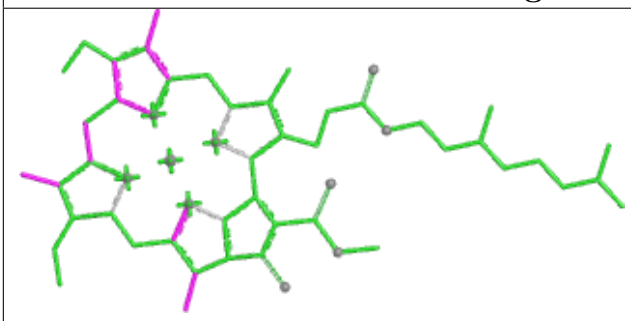


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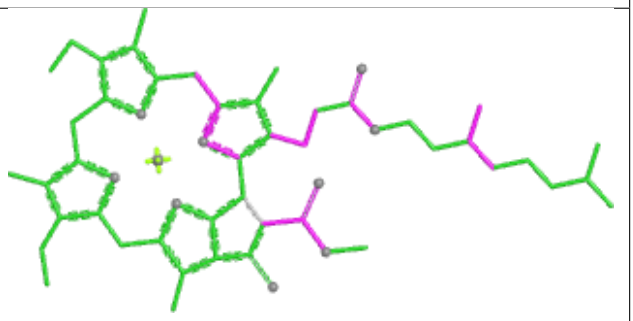


Rings

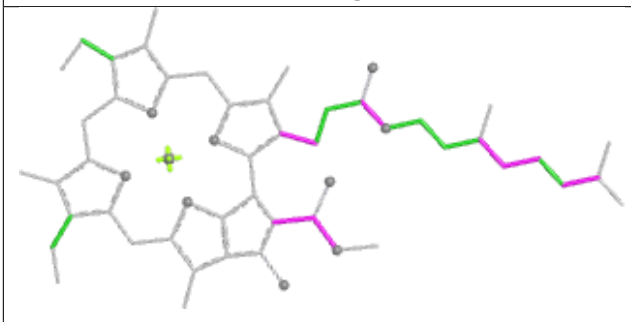
Ligand CLA T 312



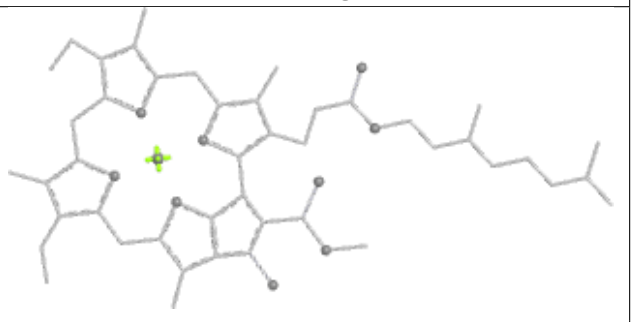
Bond lengths



Bond angles

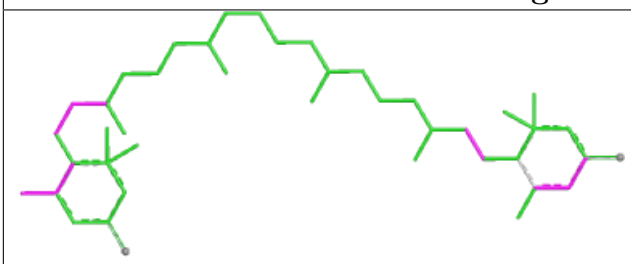


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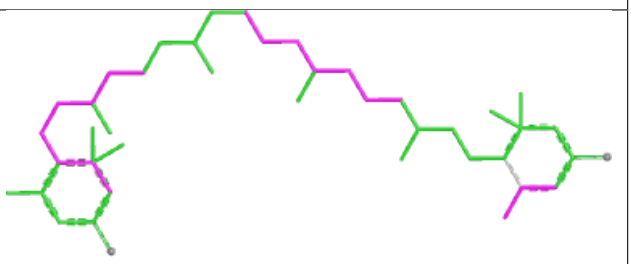


Rings

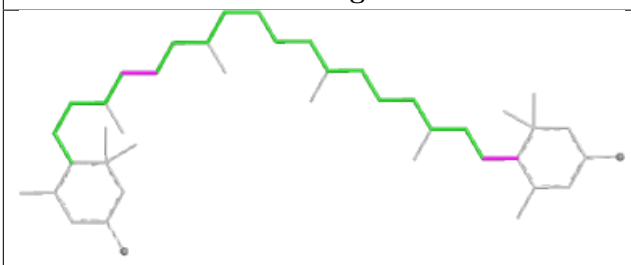
Ligand Q6L S 316



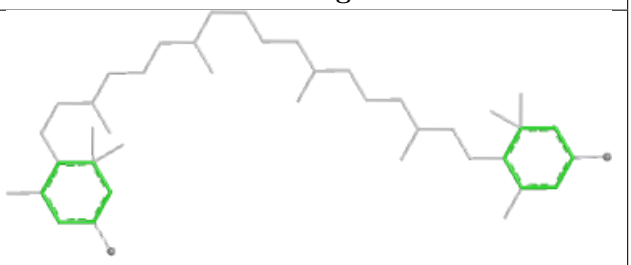
Bond lengths



Bond angles

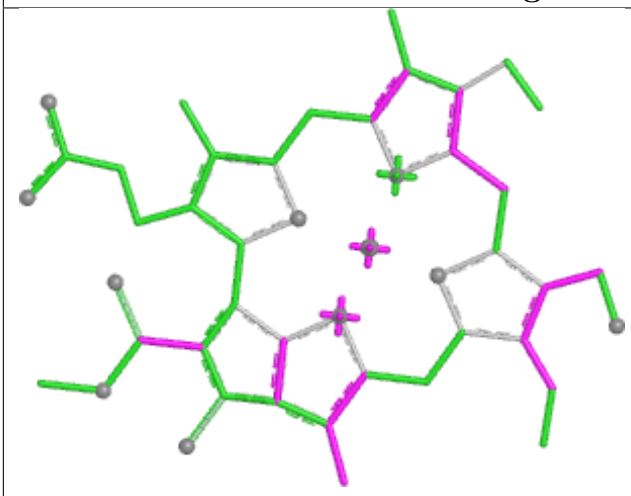


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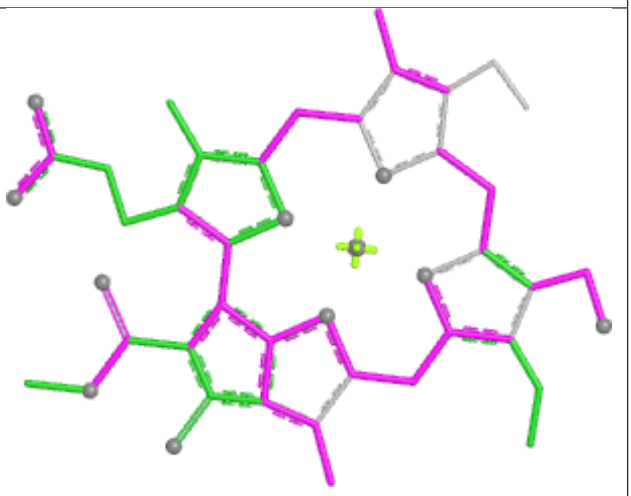


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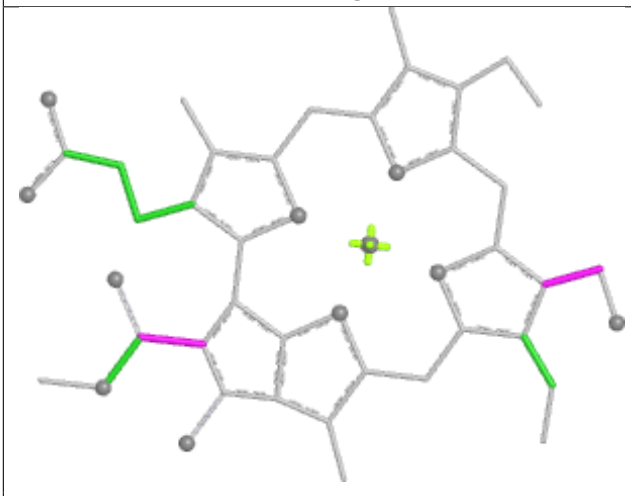
Ligand CHL R 308



Bond lengths



Bond angles

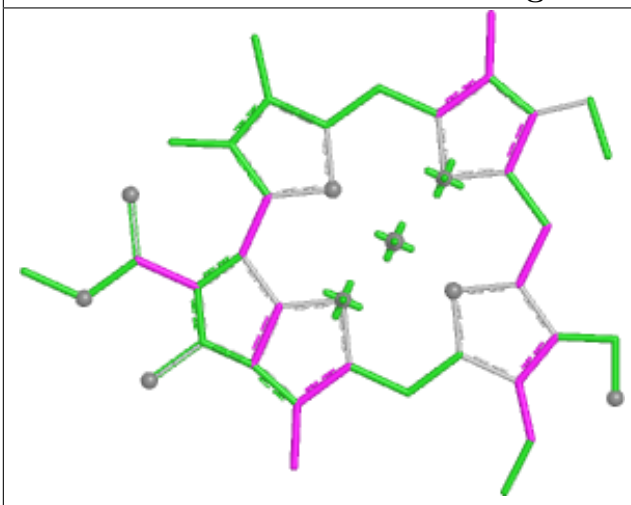


Torsions

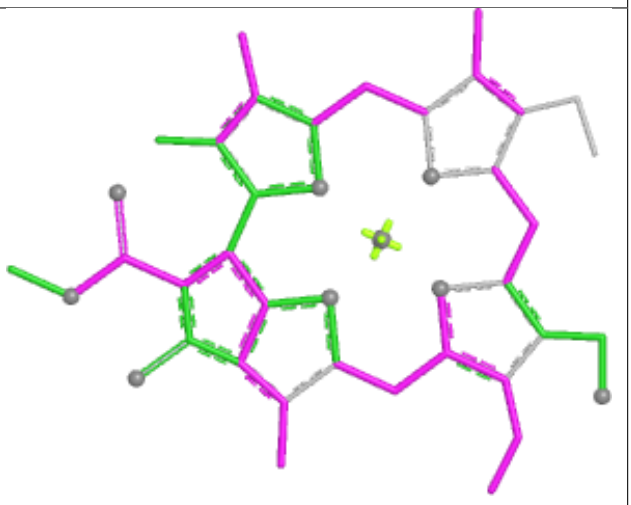


Rings

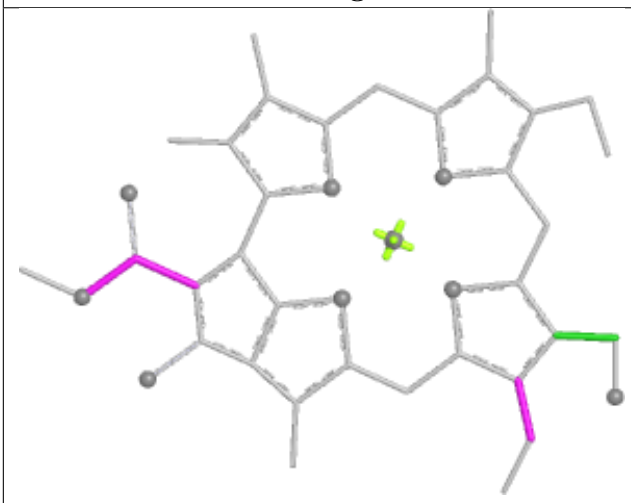
Ligand CHL S 307



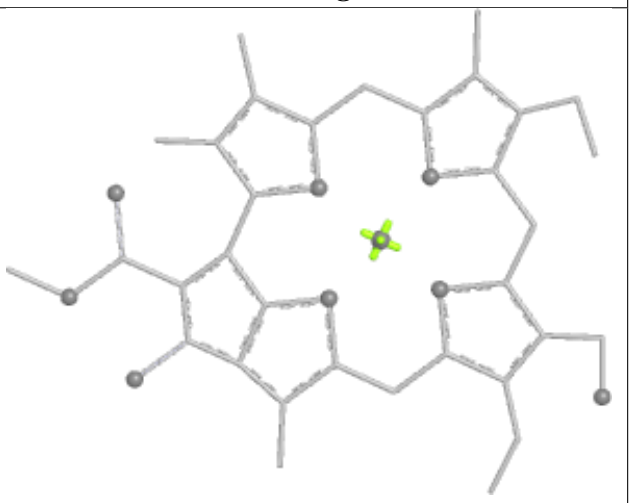
Bond lengths



Bond angles

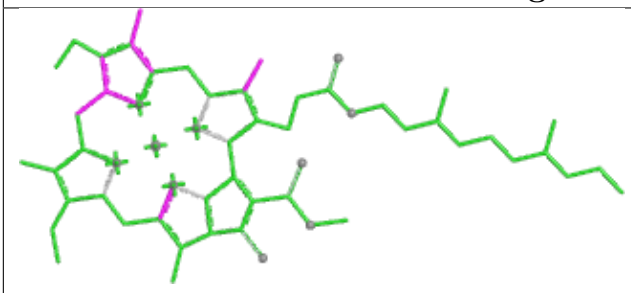


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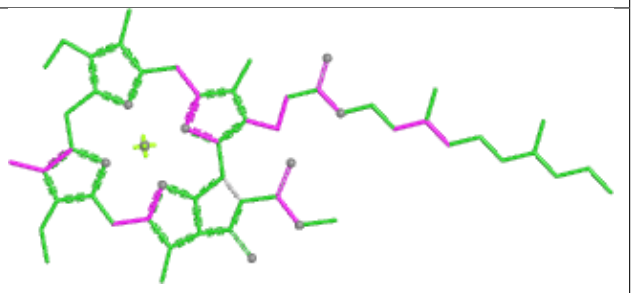


Rings

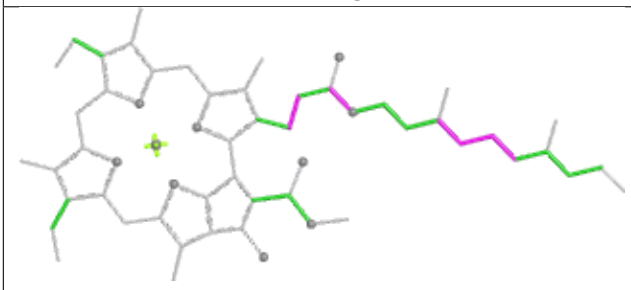
Ligand CLA 4 313



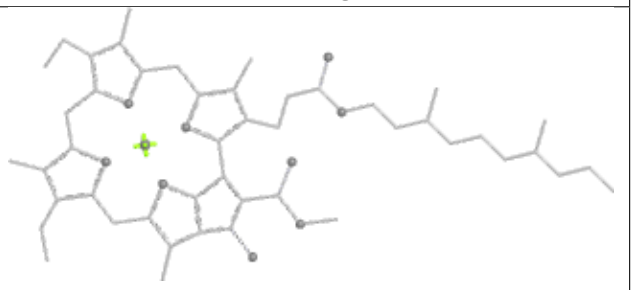
Bond lengths



Bond angles

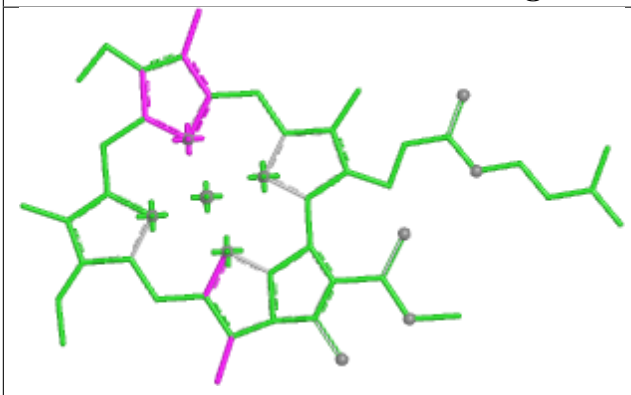


Torsions

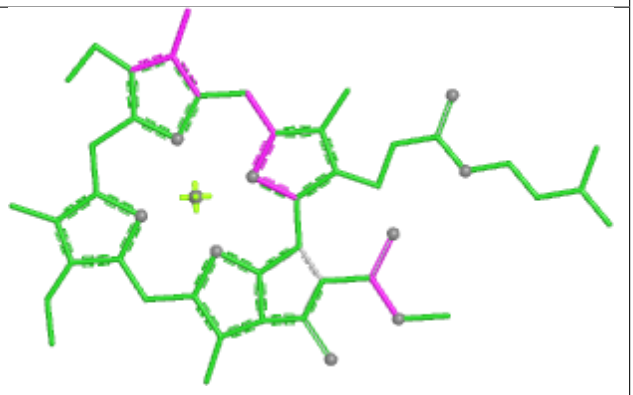


Rings

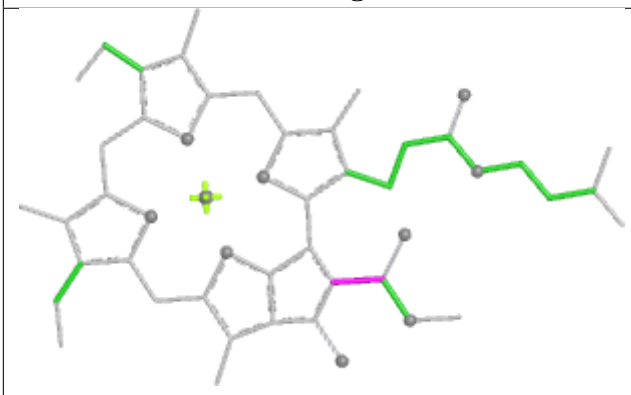
Ligand CLA B 838



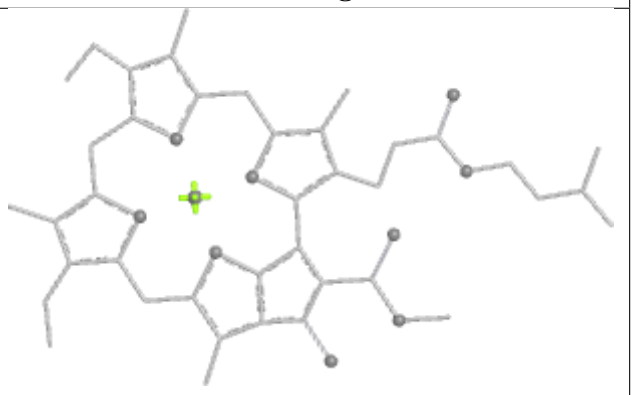
Bond lengths



Bond angles

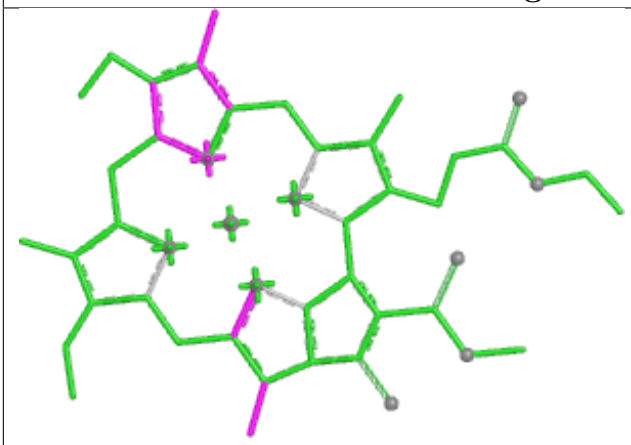


Torsions

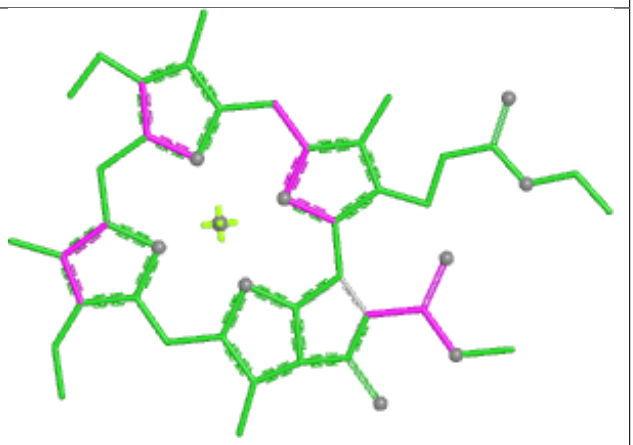


Rings

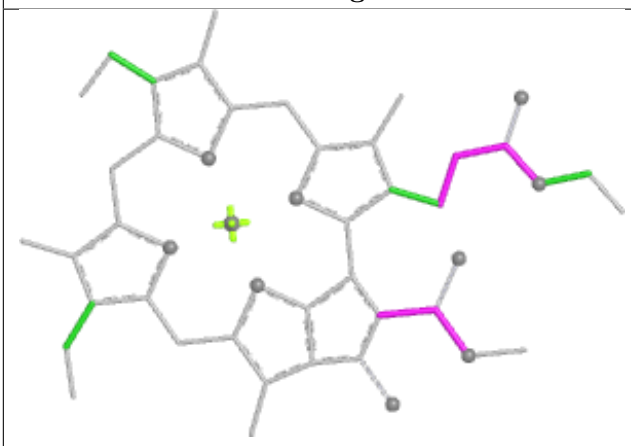
Ligand CLA B 840



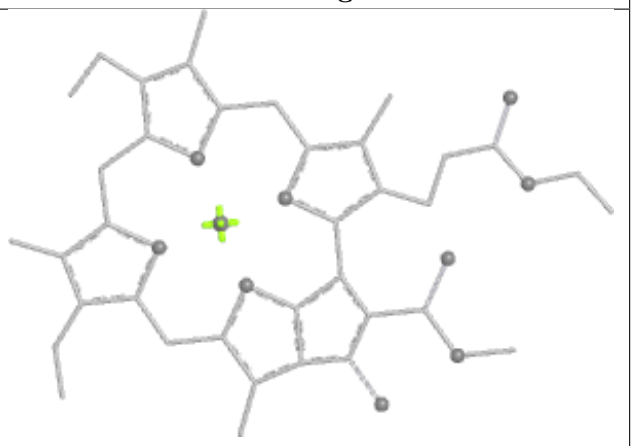
Bond lengths



Bond angles

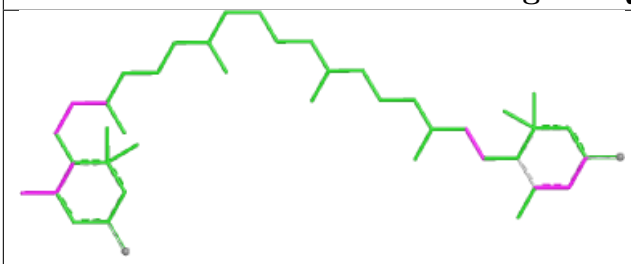


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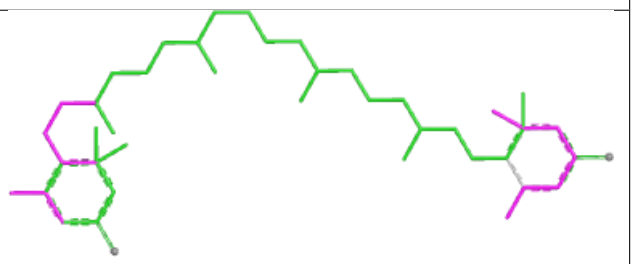


Rings

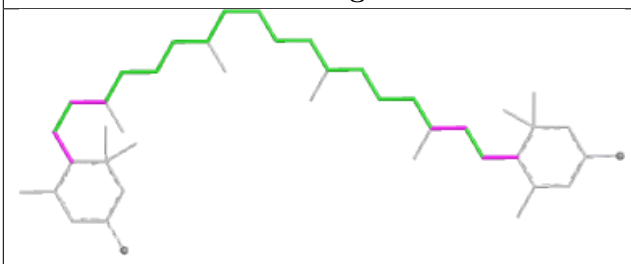
Ligand Q6L W 320



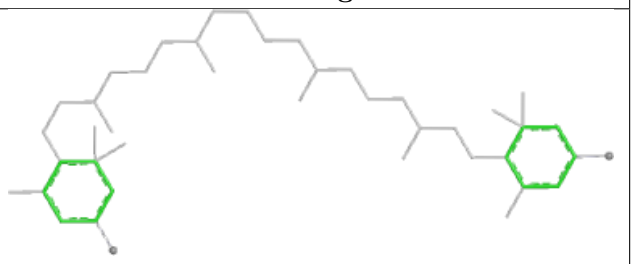
Bond lengths



Bond angles

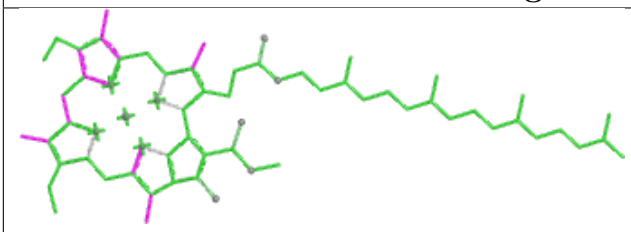


Torsions

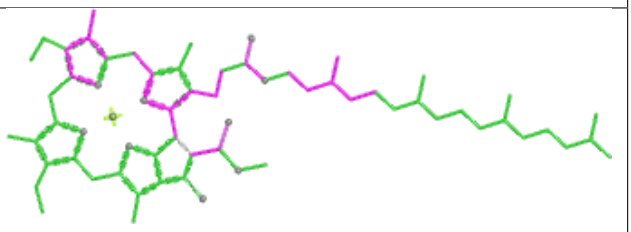


Rings

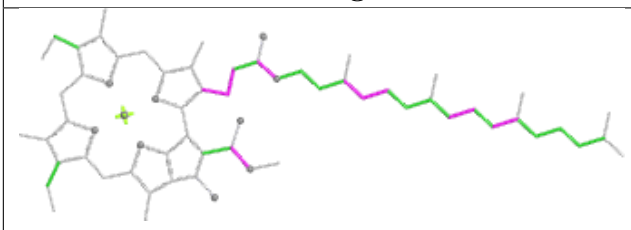
Ligand CLA T 301



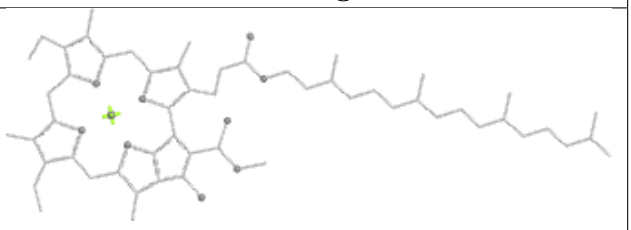
Bond lengths



Bond angles

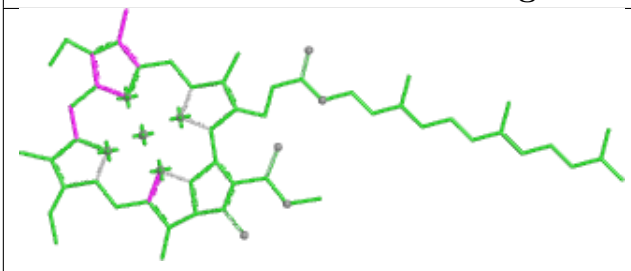


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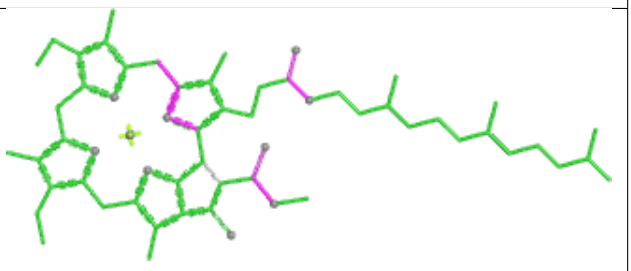


Rings

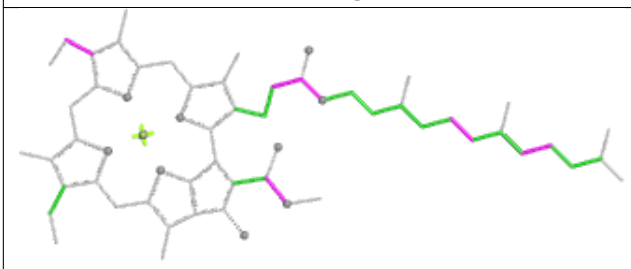
Ligand CLA W 310



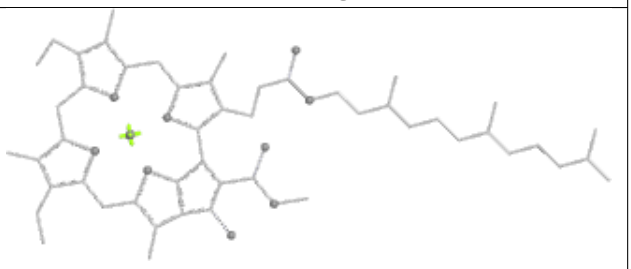
Bond lengths



Bond angles

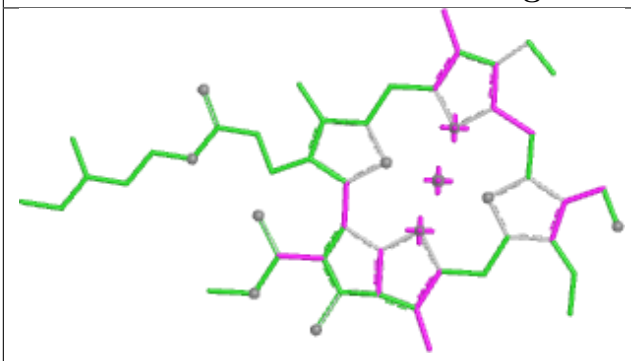


Torsions

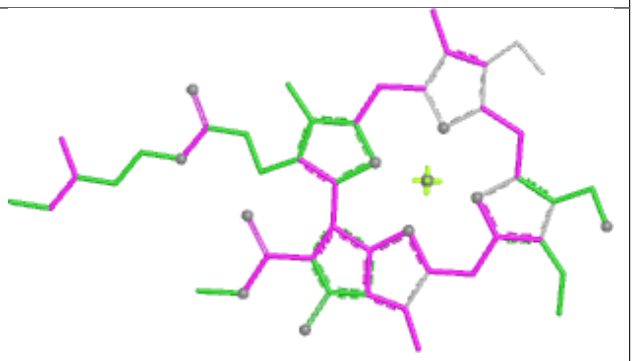


Rings

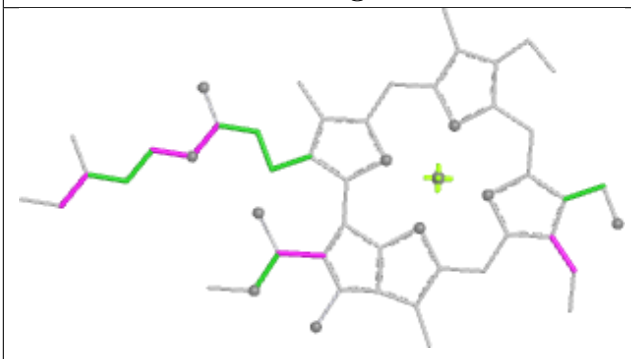
Ligand CHL R 310



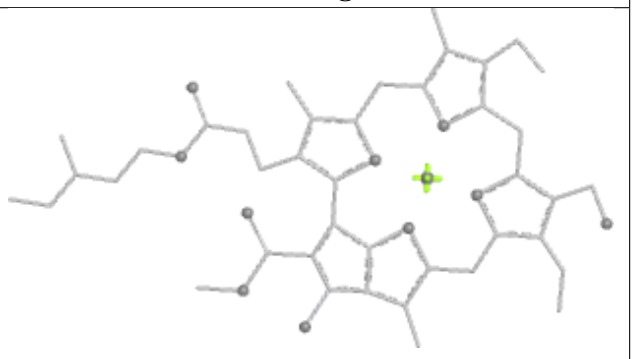
Bond lengths



Bond angles

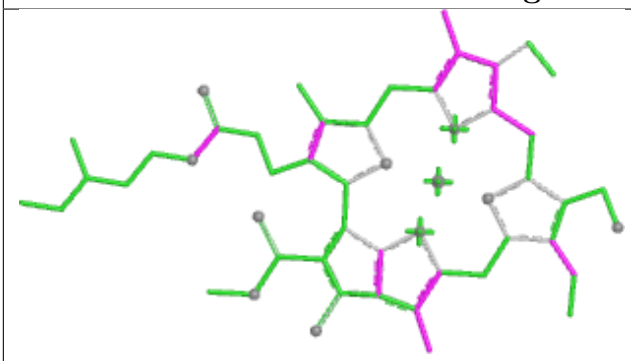


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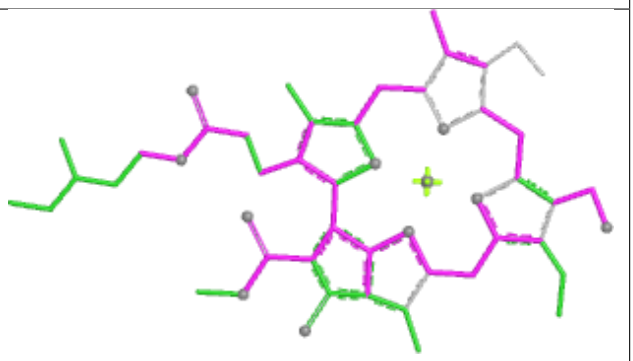


Rings

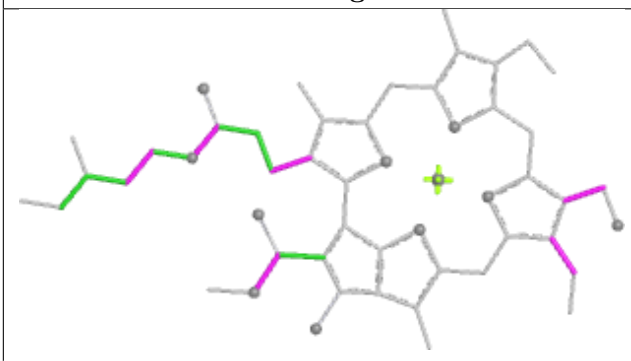
Ligand CHL X 307



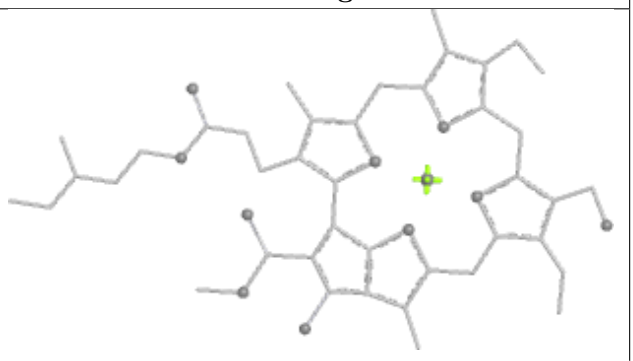
Bond lengths



Bond angles

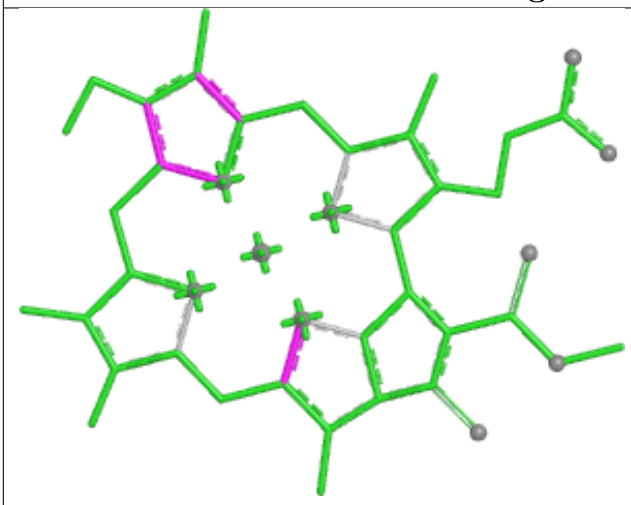


Torsions

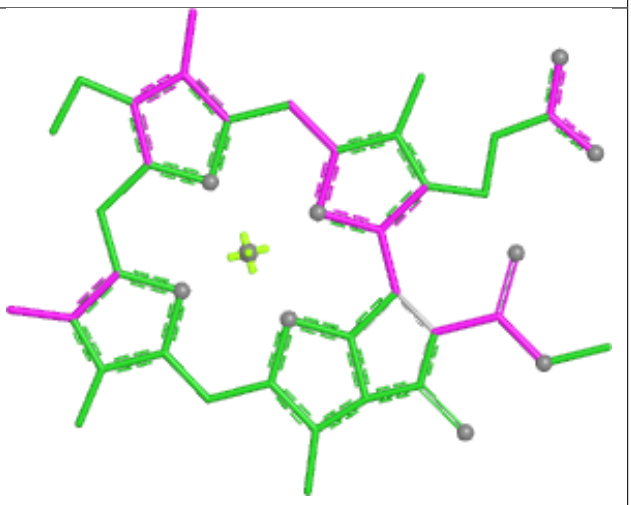


Rings

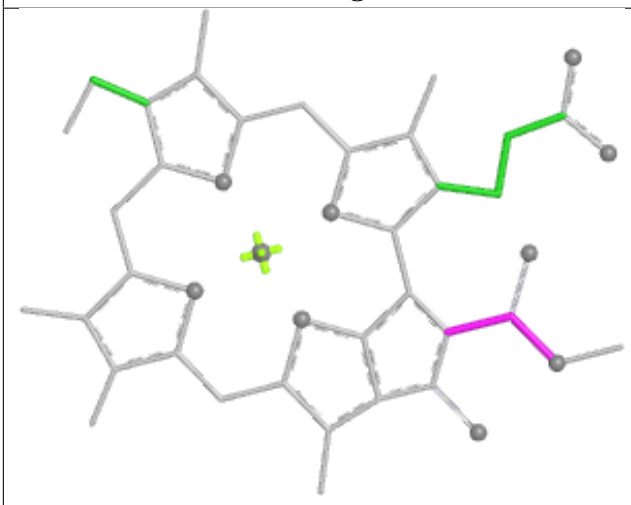
Ligand CLA 6 609



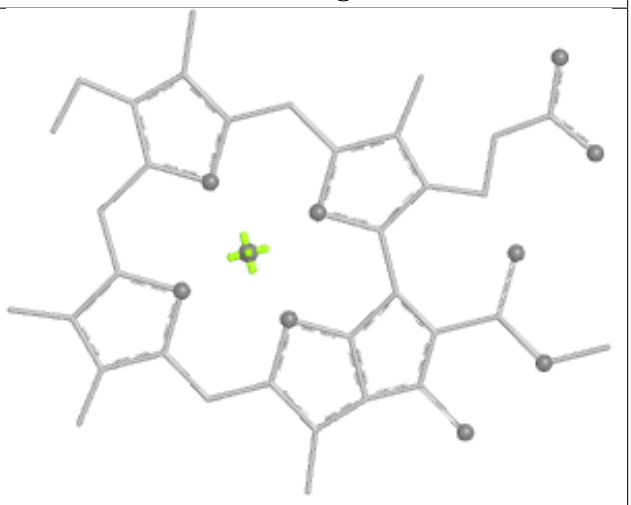
Bond lengths



Bond angles

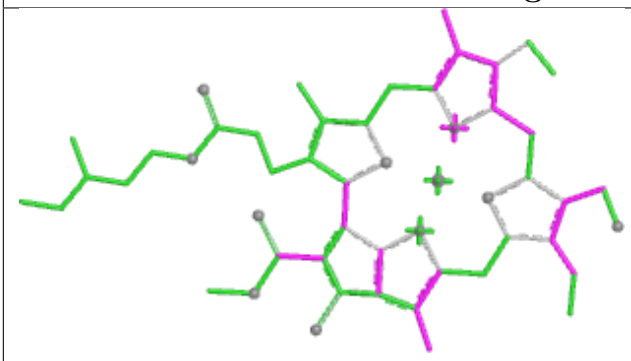


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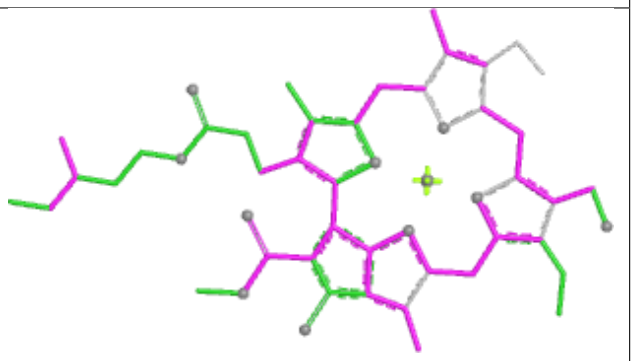


Rings

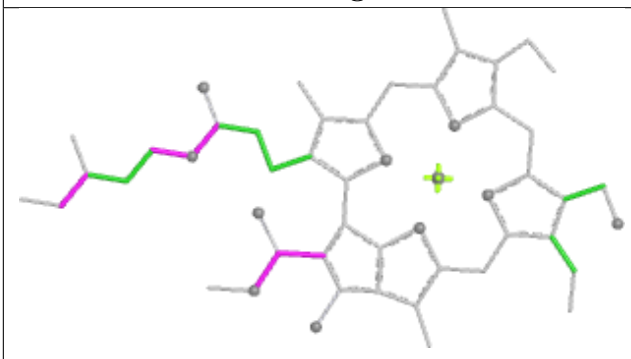
Ligand CHL P 306



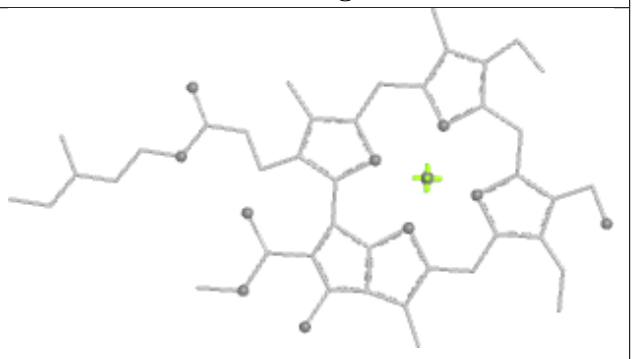
Bond lengths



Bond angles

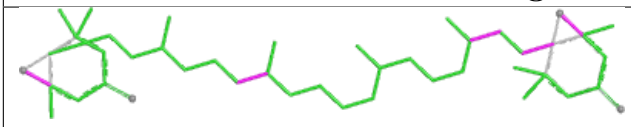


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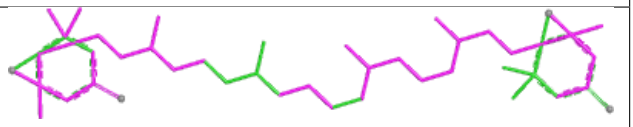


Rings

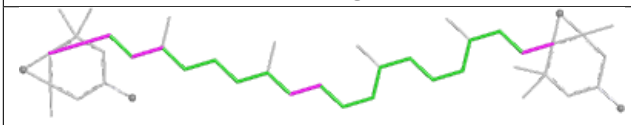
Ligand XAT 4 318



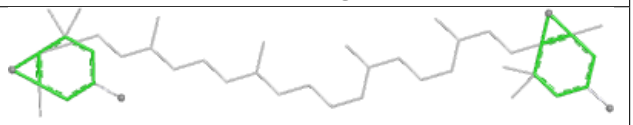
Bond lengths



Bond angles

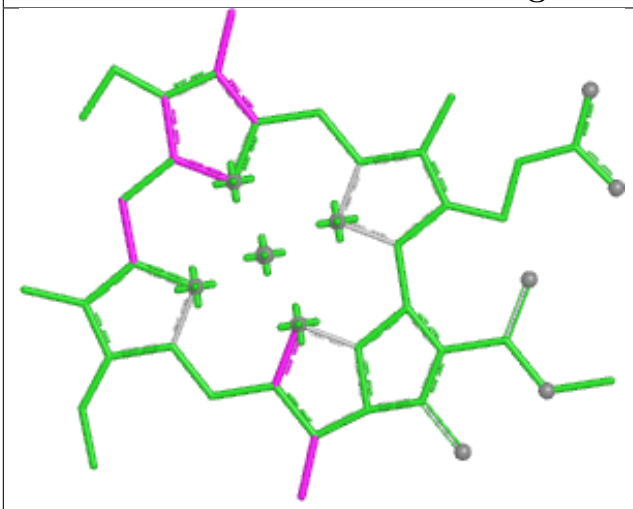


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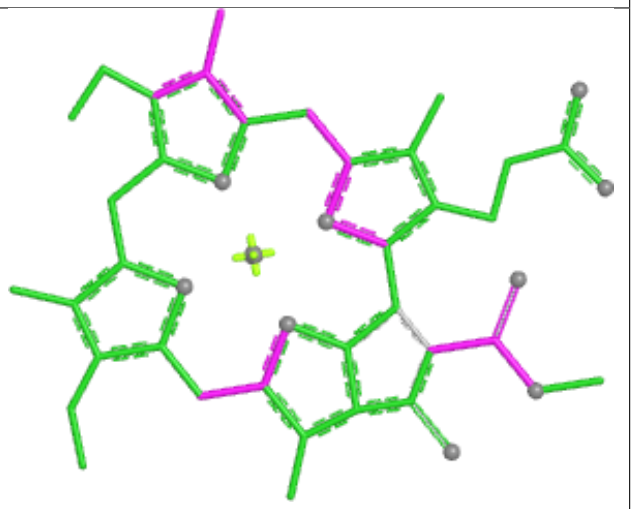


Rings

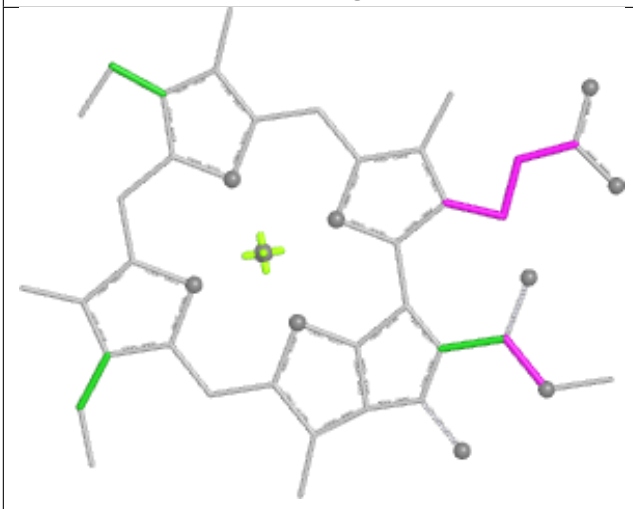
Ligand CLA 2 606



Bond lengths



Bond angles

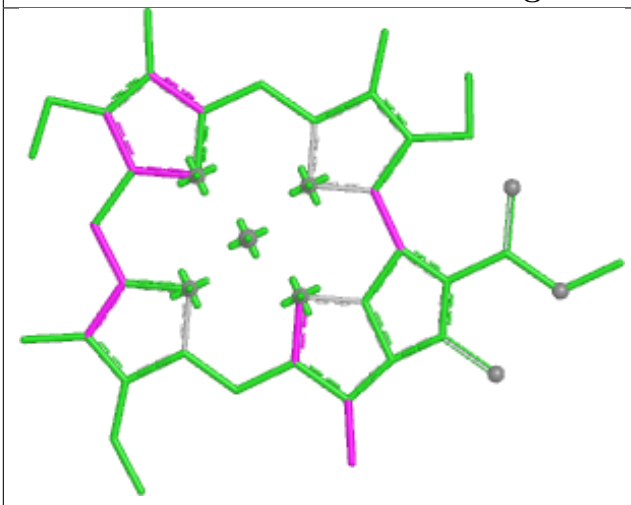


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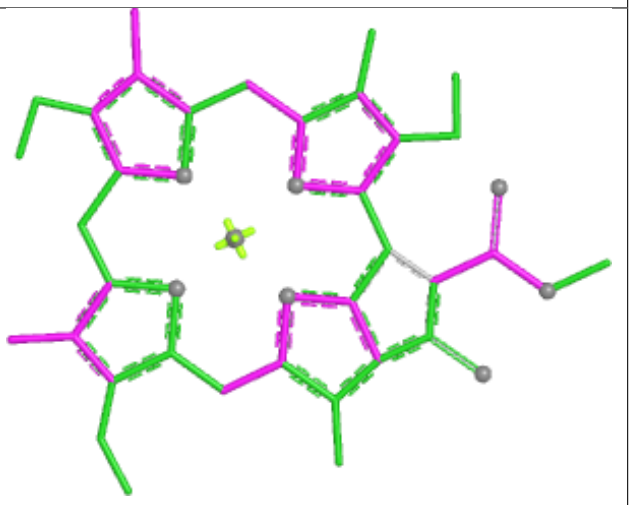


Rings

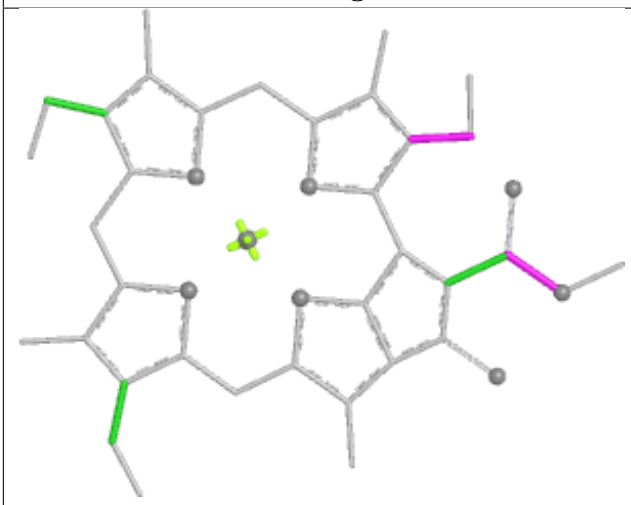
Ligand CLA V 309



Bond lengths



Bond angles

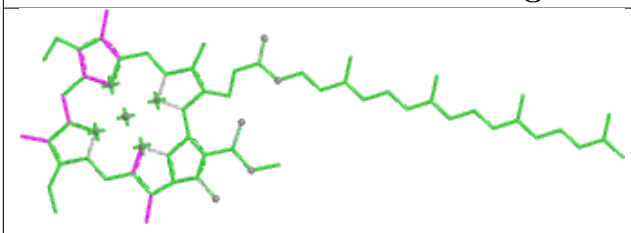


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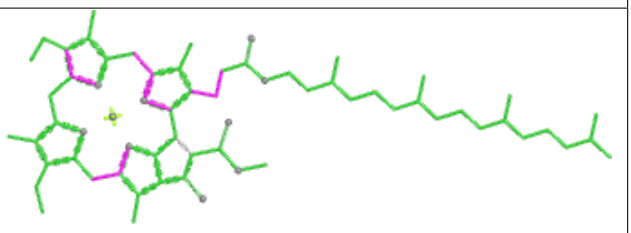


Rings

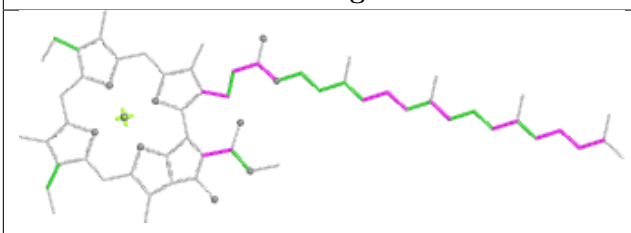
Ligand CLA B 839



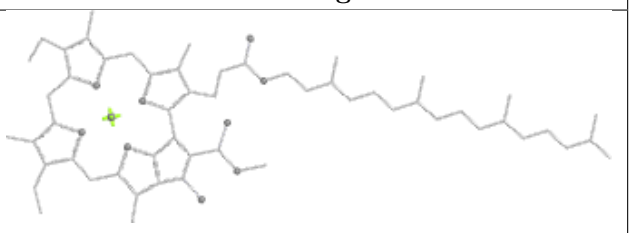
Bond lengths



Bond angles

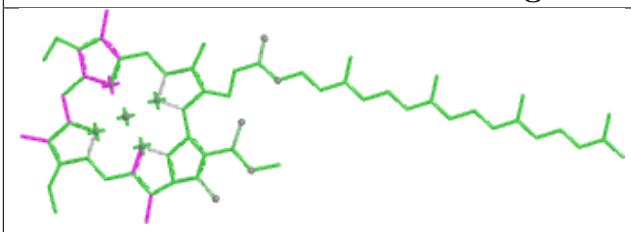


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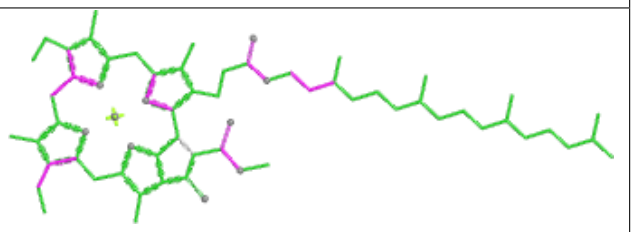


Rings

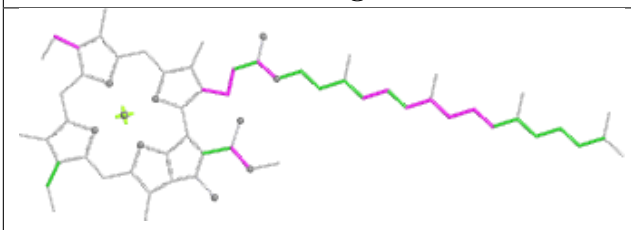
Ligand CLA B 804



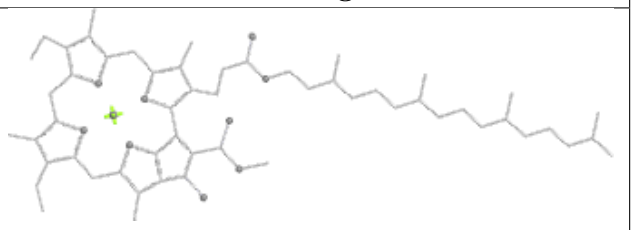
Bond lengths



Bond angles

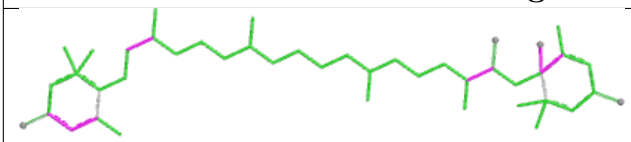


Torsions



Rings

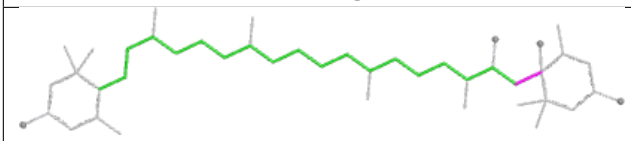
Ligand IWJ P 320



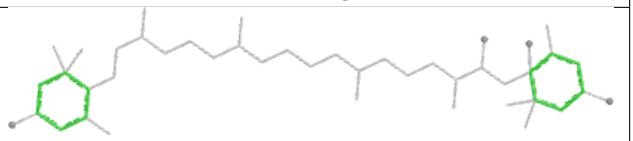
Bond lengths



Bond angles

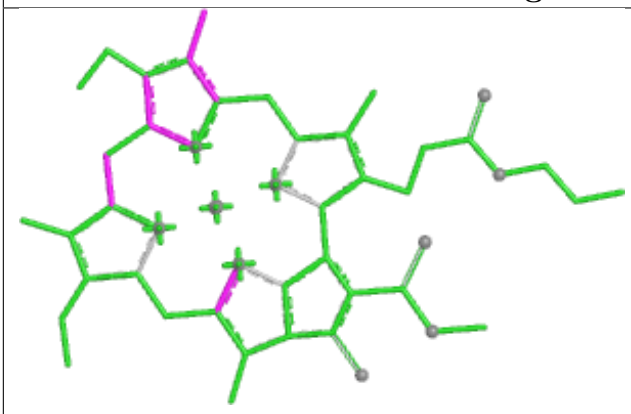


Torsions

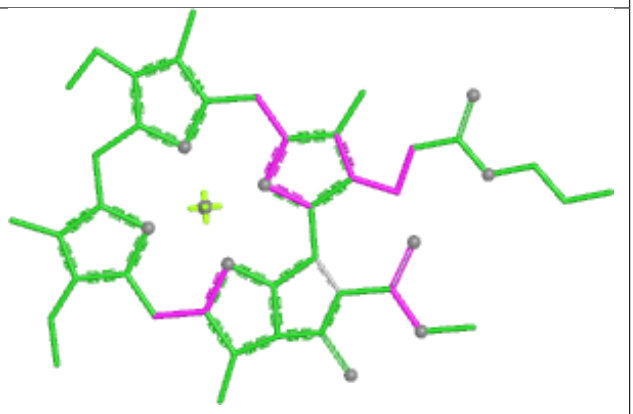


Rings

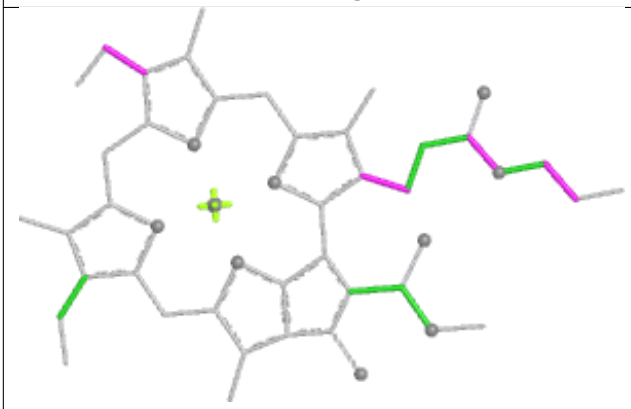
Ligand CLA P 313



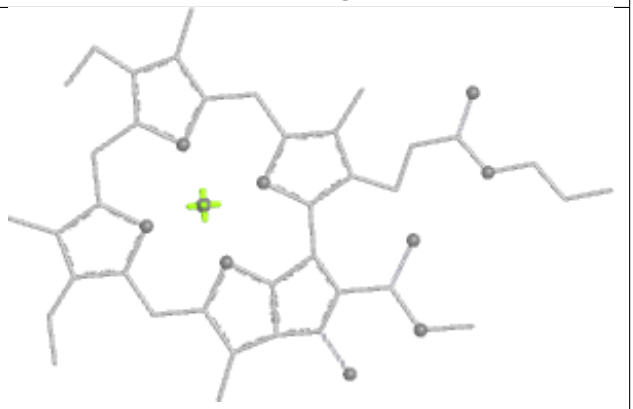
Bond lengths



Bond angles

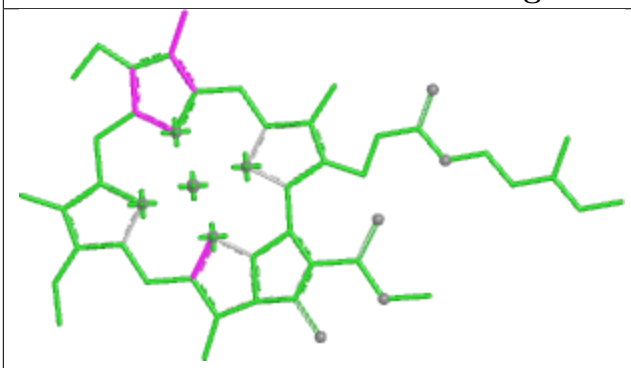


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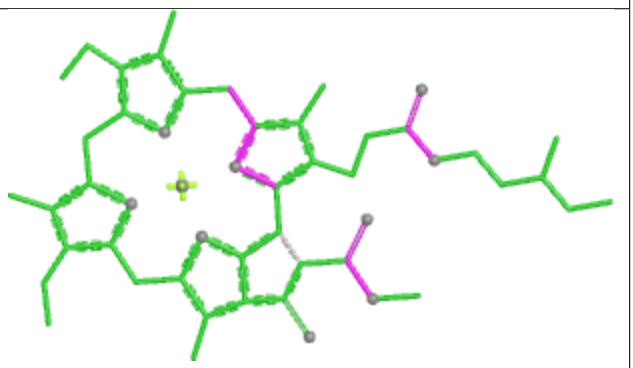


Rings

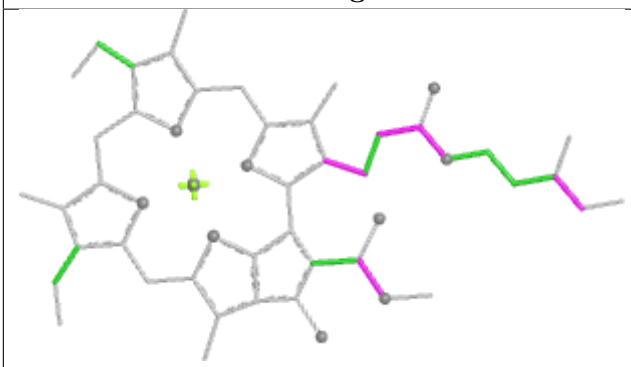
Ligand CLA X 303



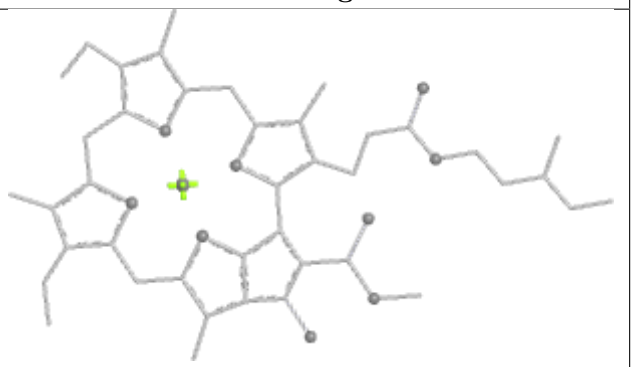
Bond lengths



Bond angles

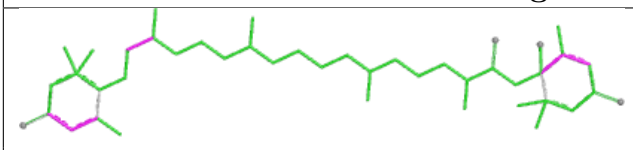


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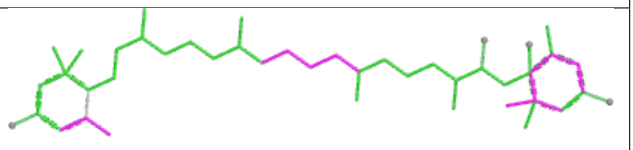


Rings

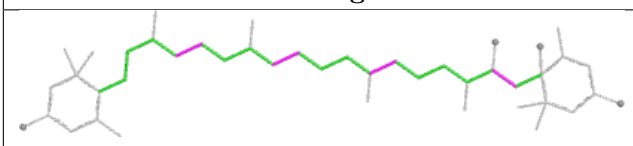
Ligand IWJ S 318



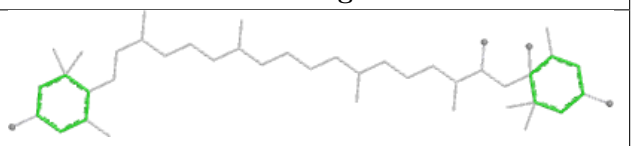
Bond lengths



Bond angles

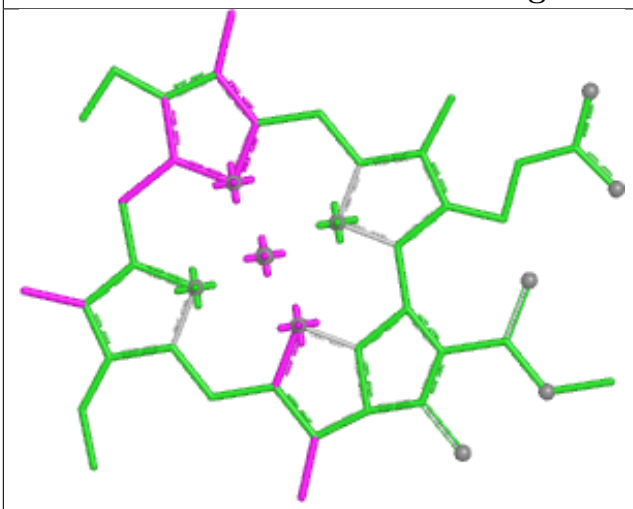


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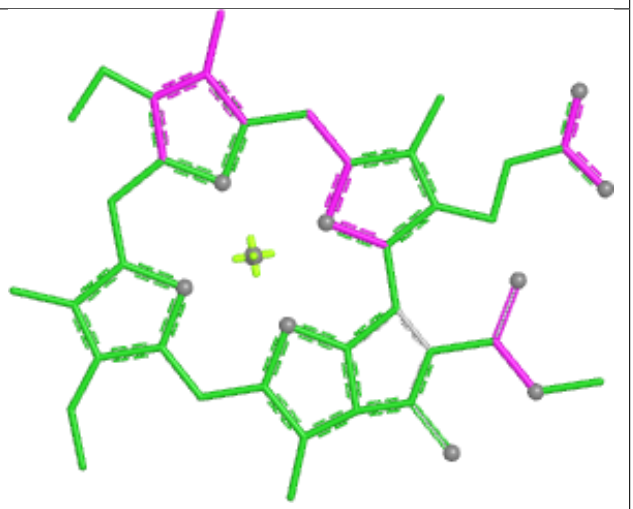


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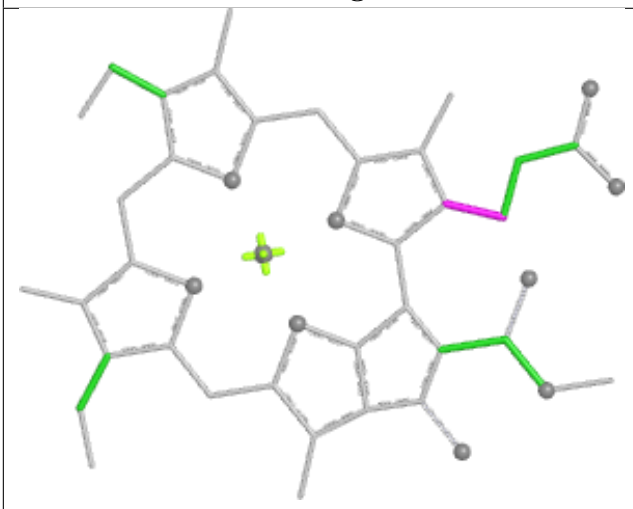
Ligand CLA 6 607



Bond lengths



Bond angles

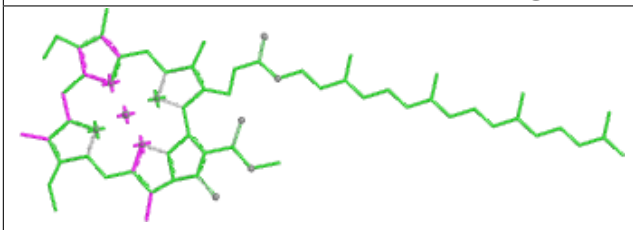


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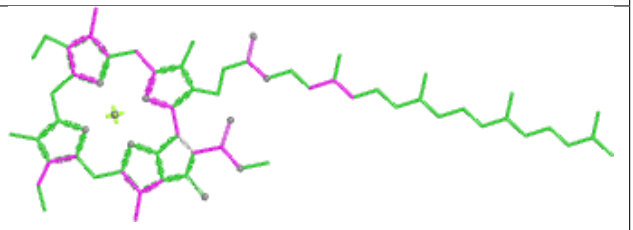


Rings

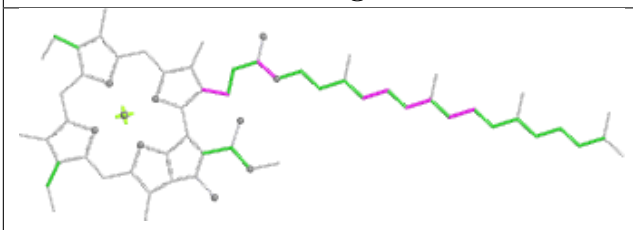
Ligand CLA S 301



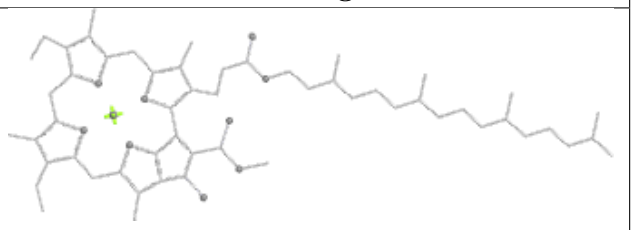
Bond lengths



Bond angles

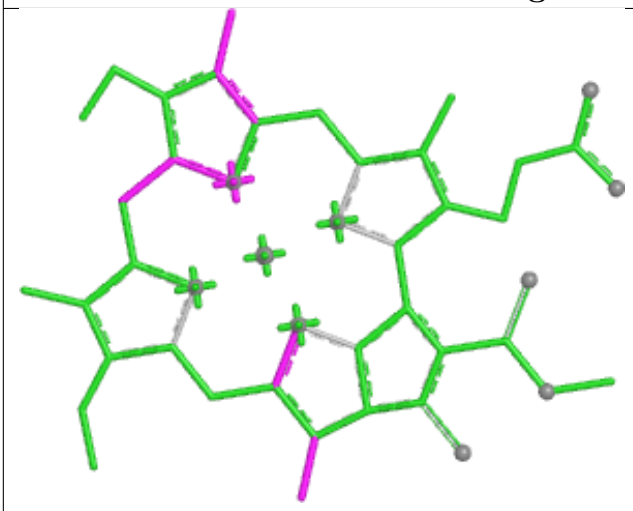


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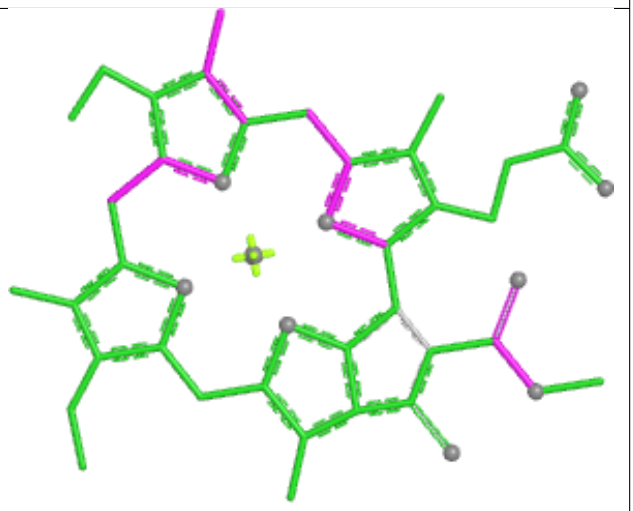


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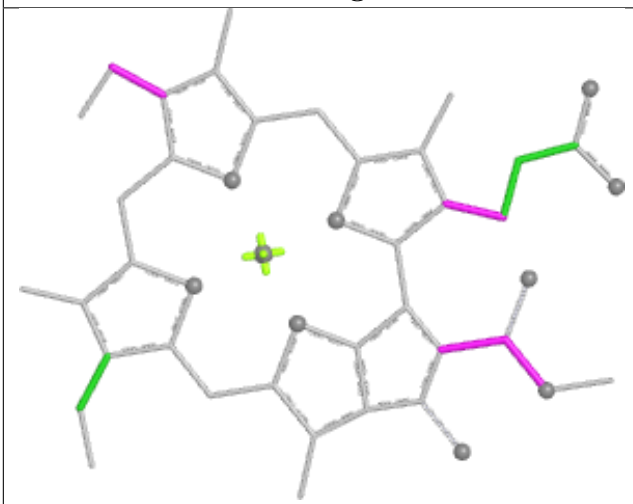
Ligand CLA 6 612



Bond lengths



Bond angles

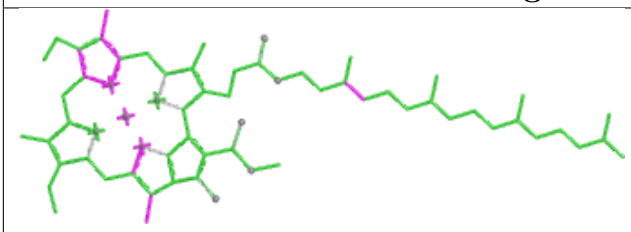


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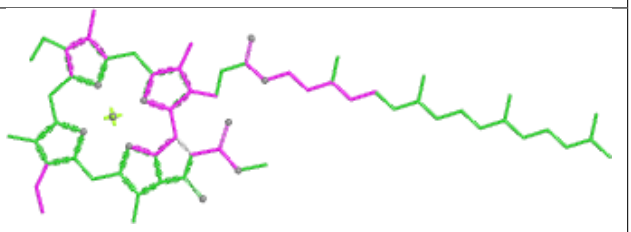


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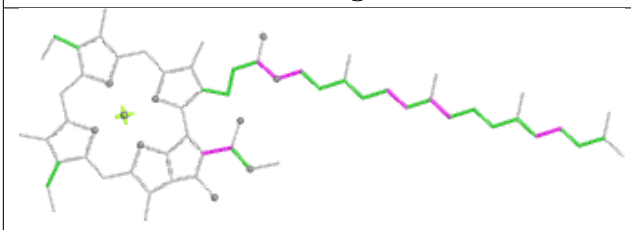
Ligand CLA A 827



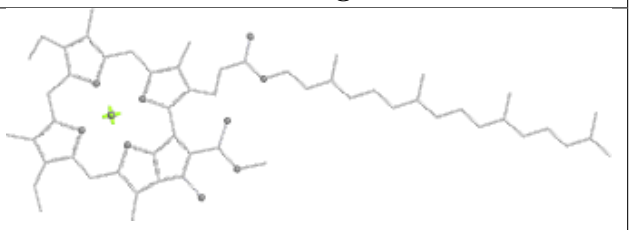
Bond lengths



Bond angles

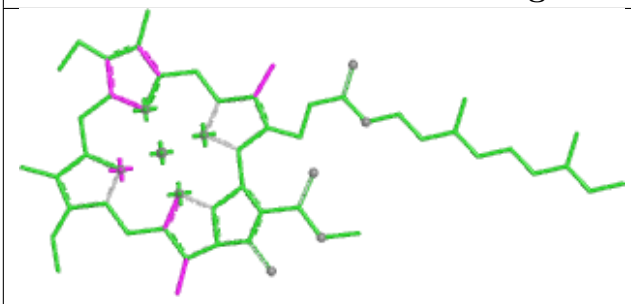


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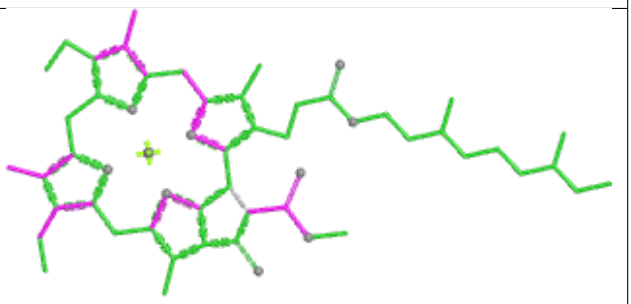


Rings

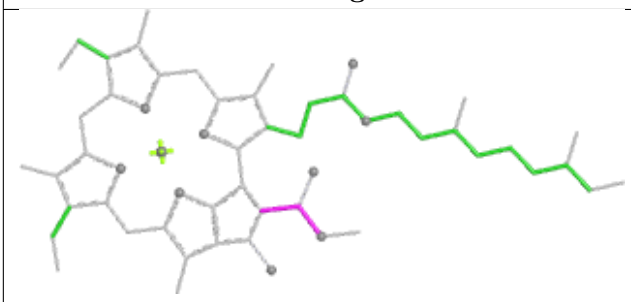
Ligand CLA 1 602



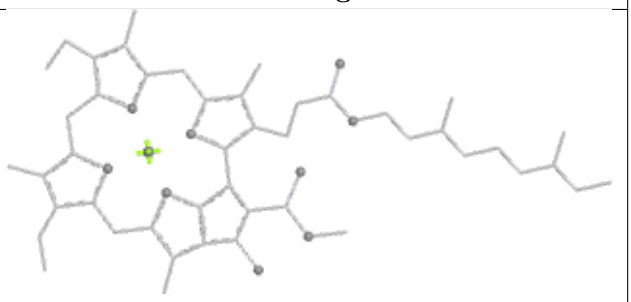
Bond lengths



Bond angles

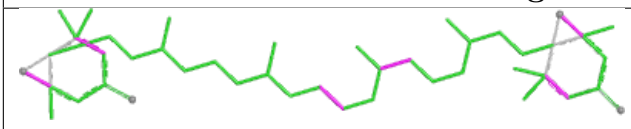


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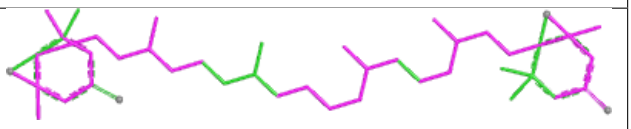


Rings

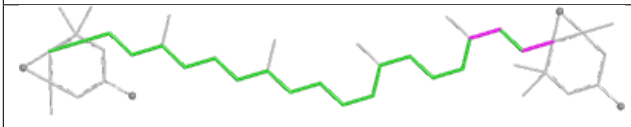
Ligand XAT 3 316



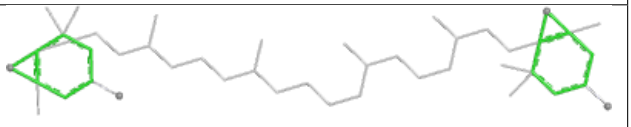
Bond lengths



Bond angles

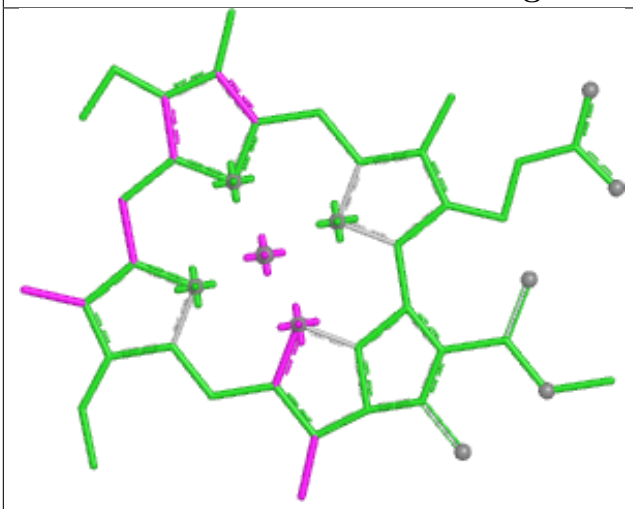


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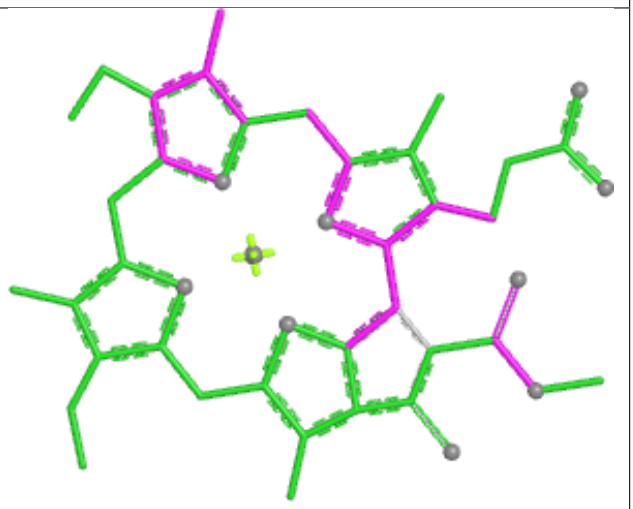


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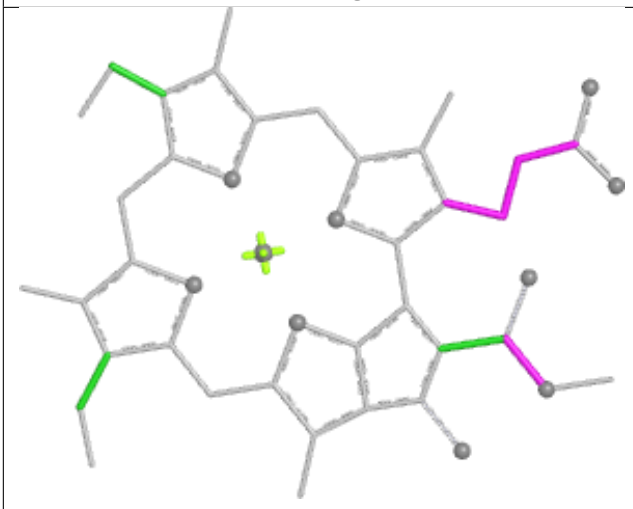
Ligand CLA U 301



Bond lengths



Bond angles

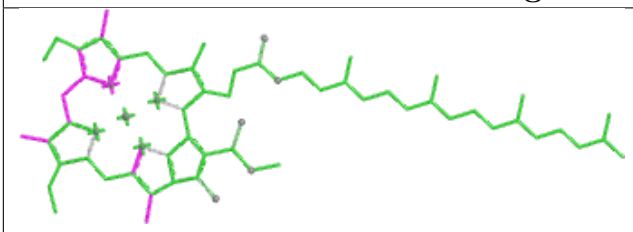


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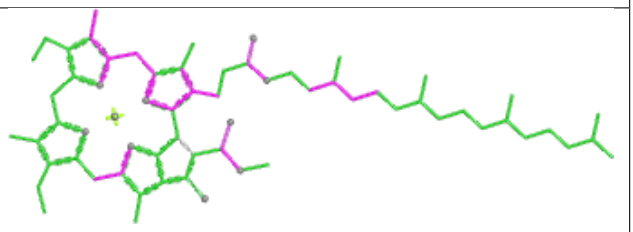


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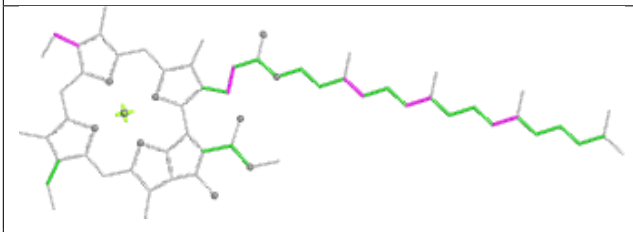
Ligand CLA B 841



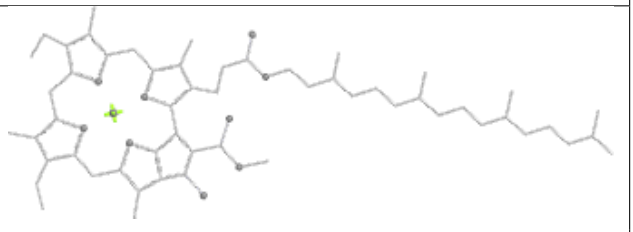
Bond lengths



Bond angles

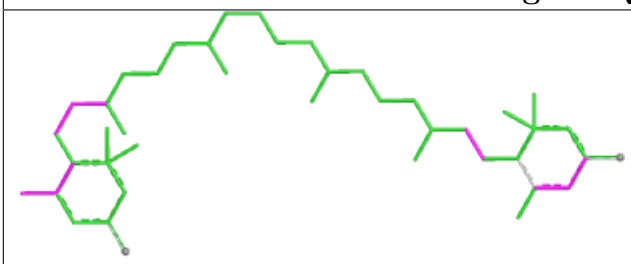


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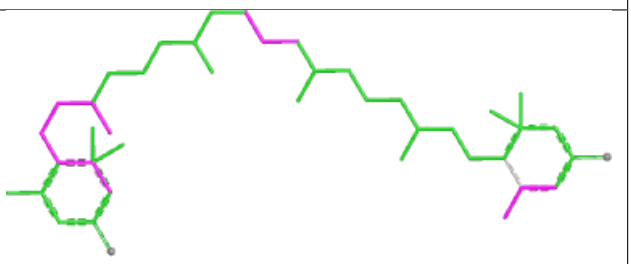


Rings

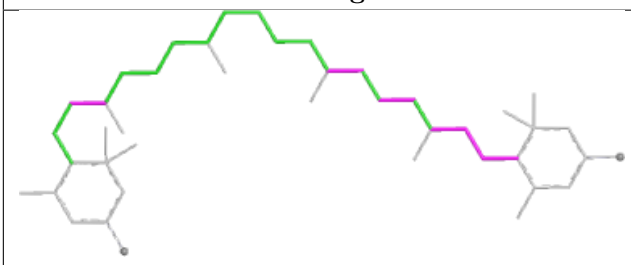
Ligand Q6L W 319



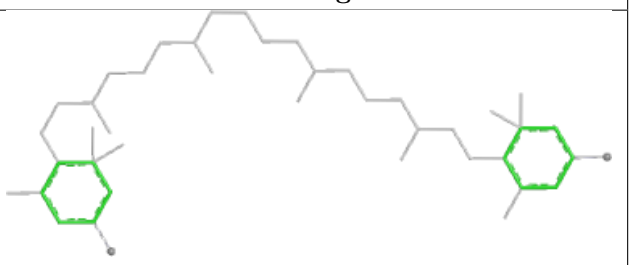
Bond lengths



Bond angles

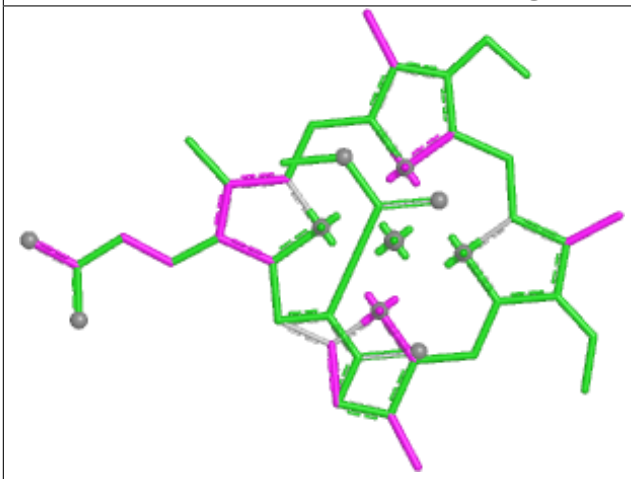


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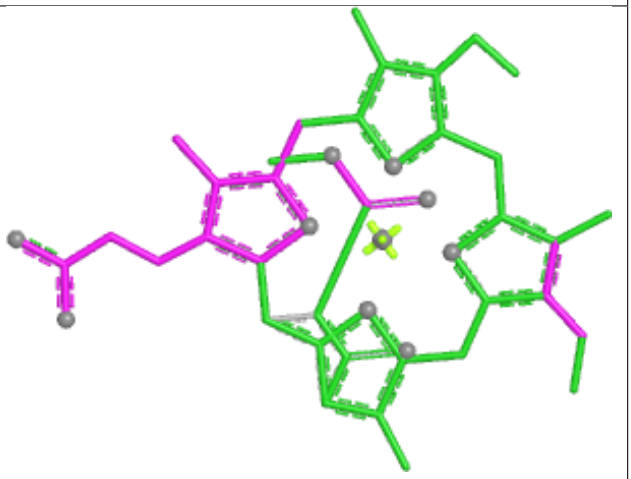


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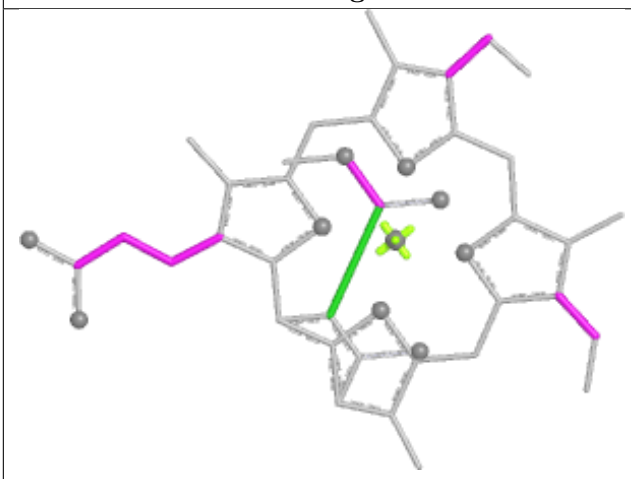
Ligand KC2 U 307



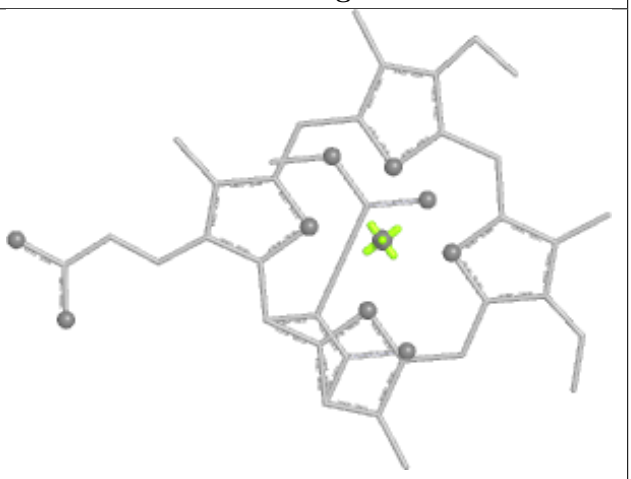
Bond lengths



Bond angles



Torsions

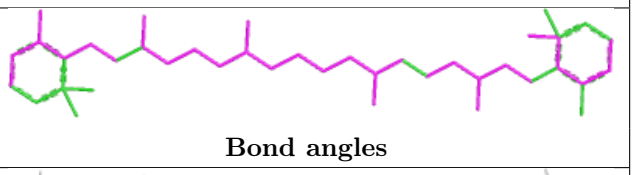


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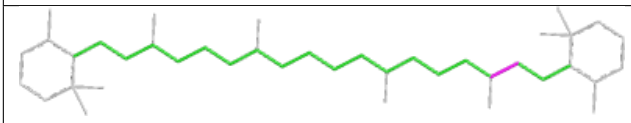
Ligand BCR L 306



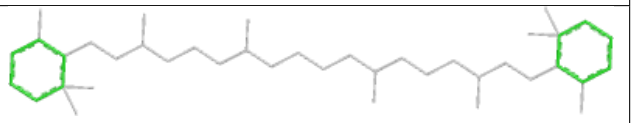
Bond lengths



Bond angles

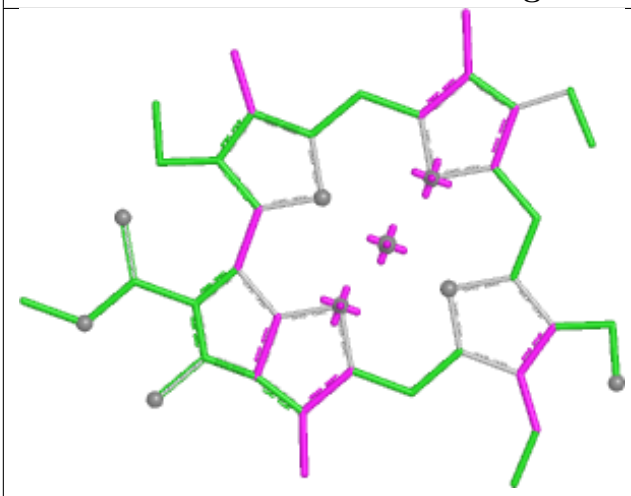


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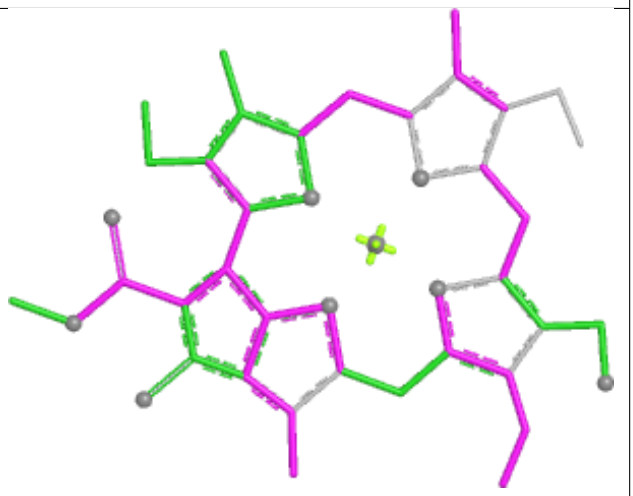


Rings

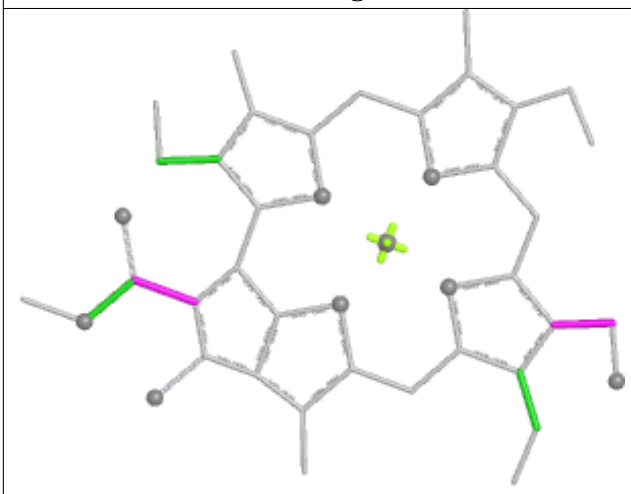
Ligand CHL V 305



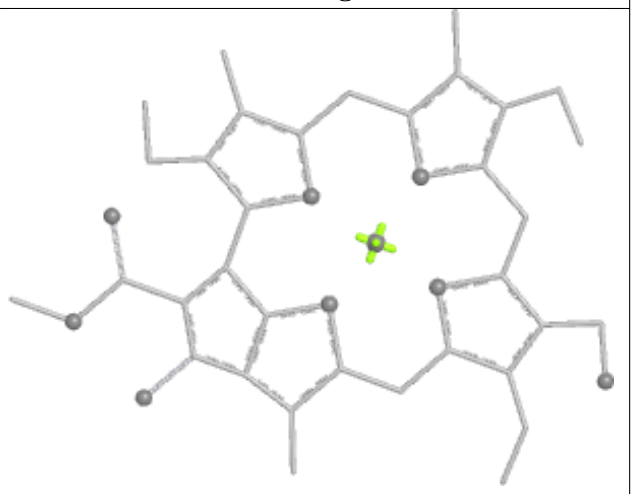
Bond lengths



Bond angles

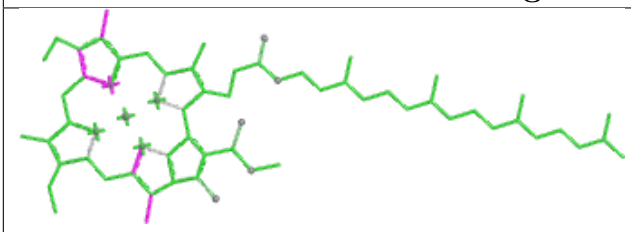


Torsions

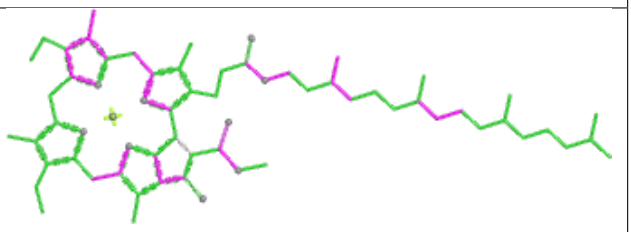


Rings

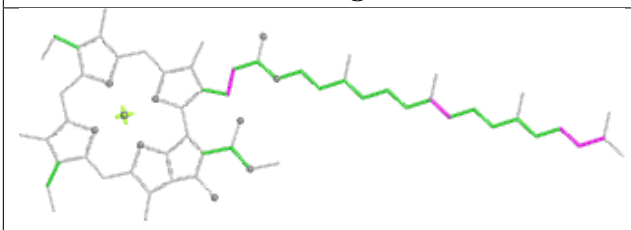
Ligand CLA A 803



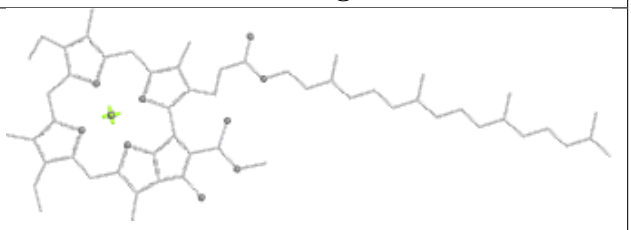
Bond lengths



Bond angles

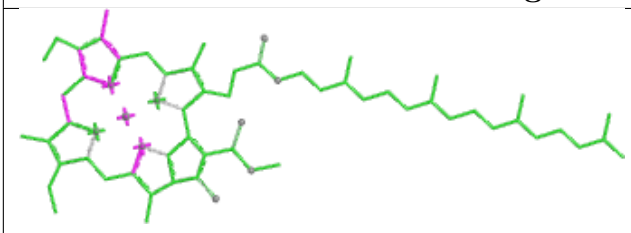


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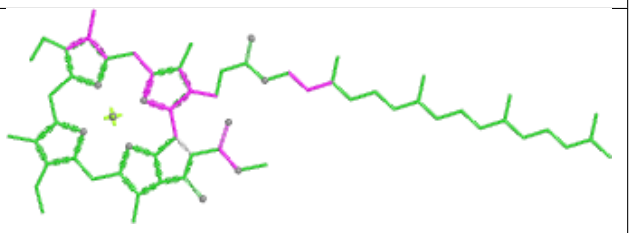


Rings

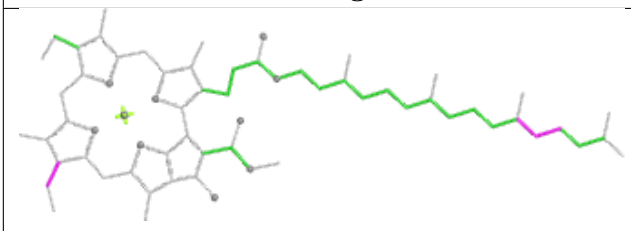
Ligand CLA B 828



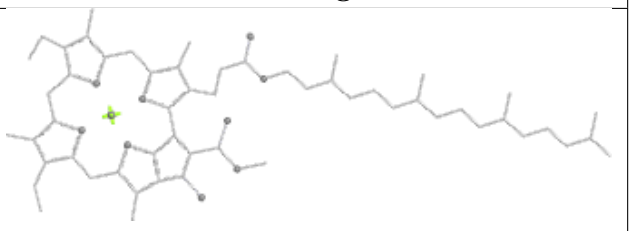
Bond lengths



Bond angles

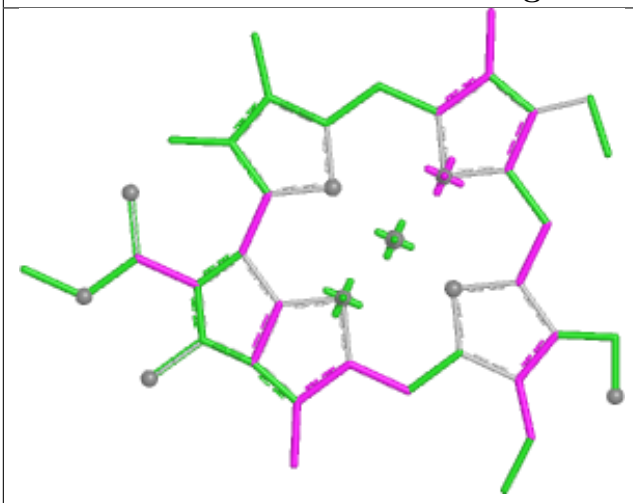


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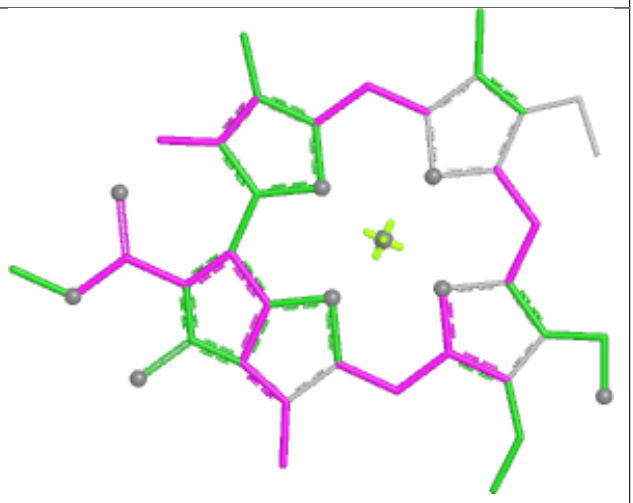


Rings

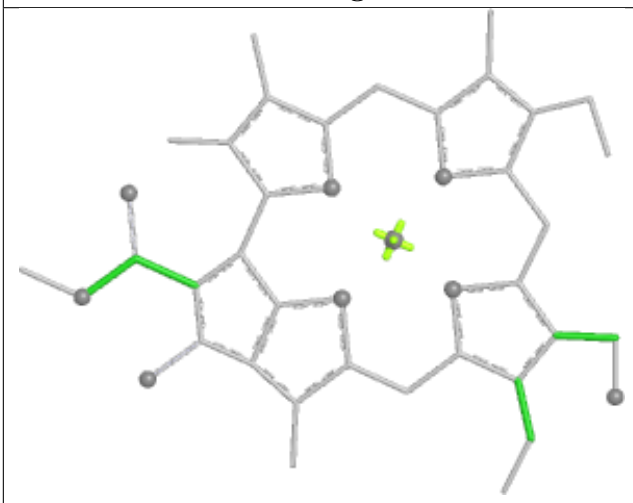
Ligand CHL X 305



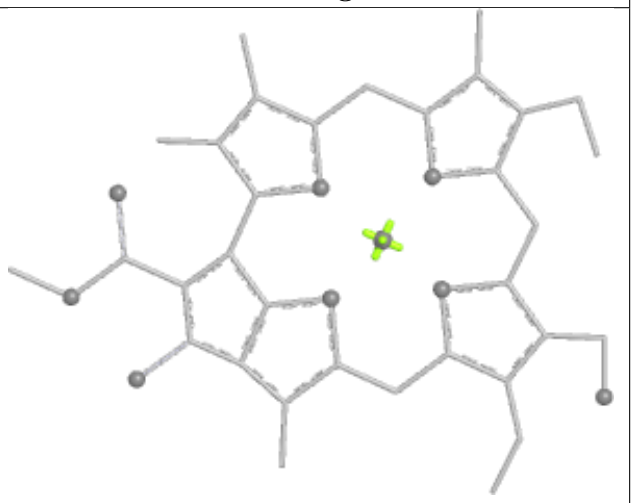
Bond lengths



Bond angles

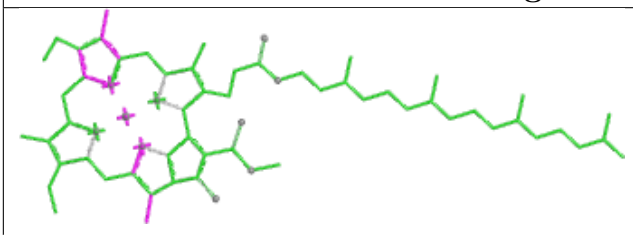


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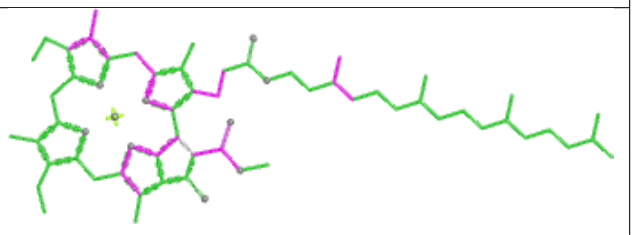


Rings

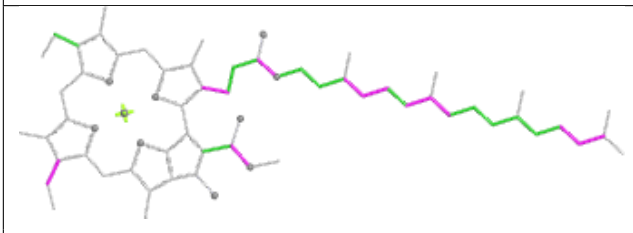
Ligand CLA B 829



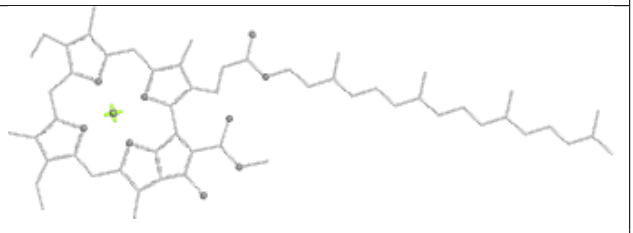
Bond lengths



Bond angles

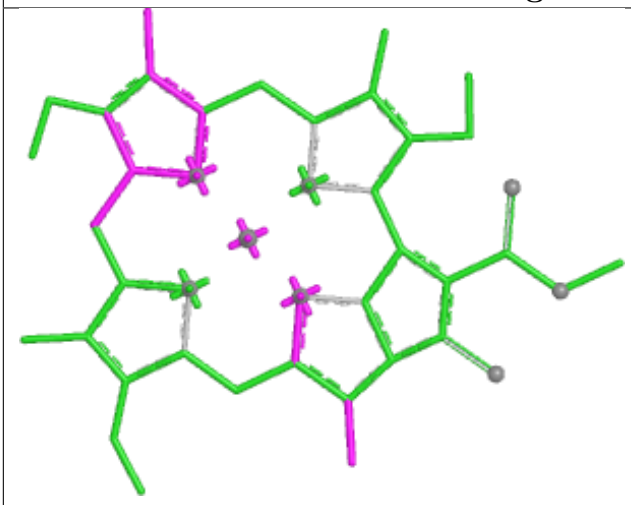


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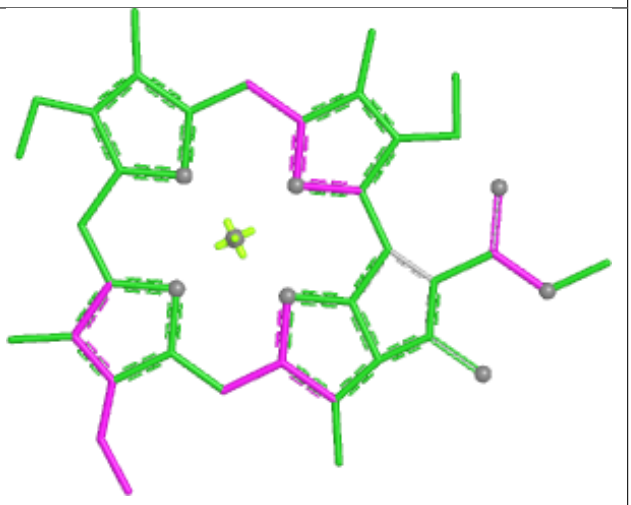


Rings

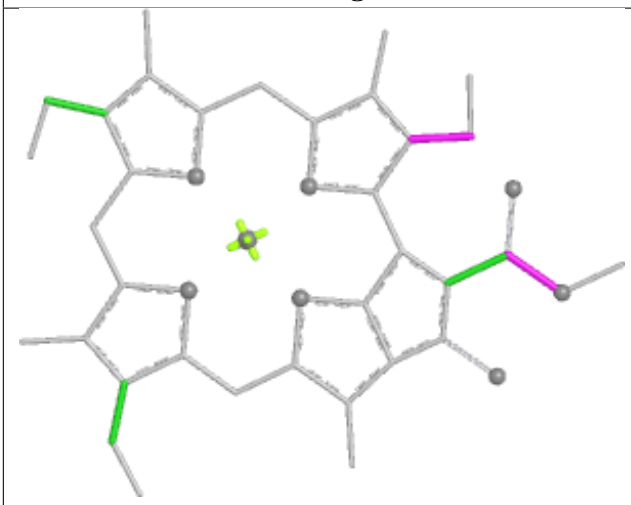
Ligand CLA F 802



Bond lengths



Bond angles

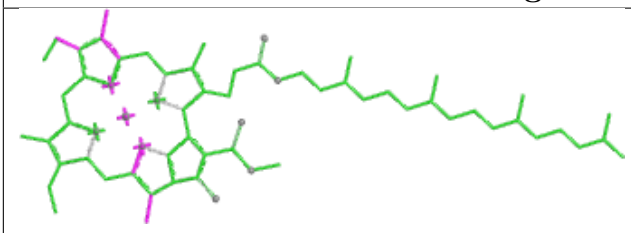


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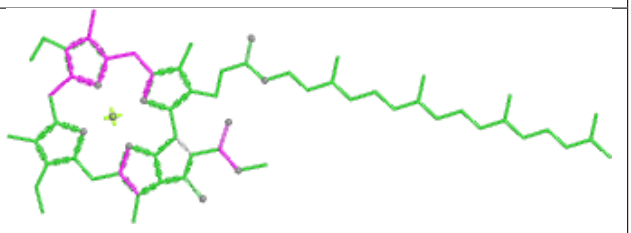


Rings

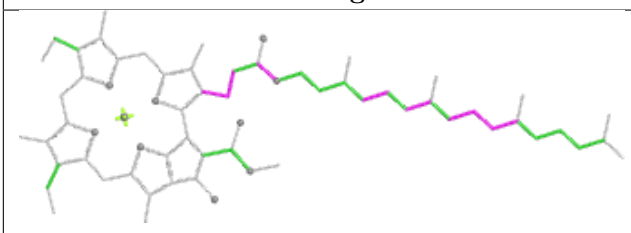
Ligand CLA B 830



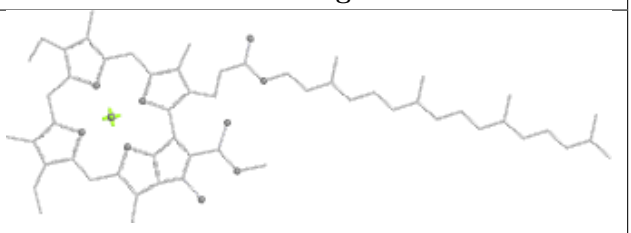
Bond lengths



Bond angles



Torsions

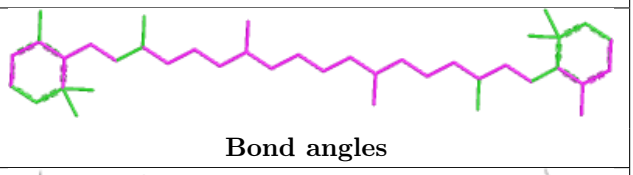


Rings

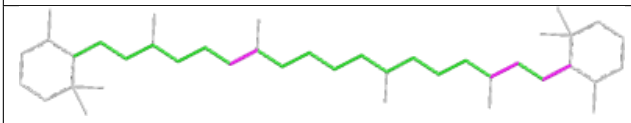
Ligand BCR A 849



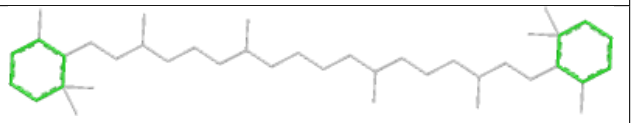
Bond lengths



Bond angles

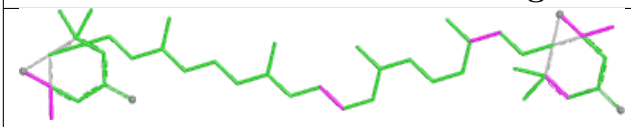


Torsions

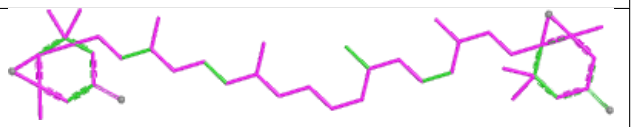


Rings

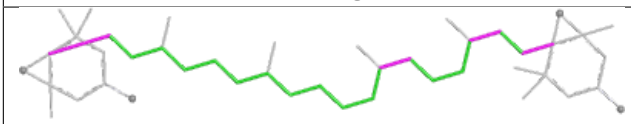
Ligand XAT 1 612



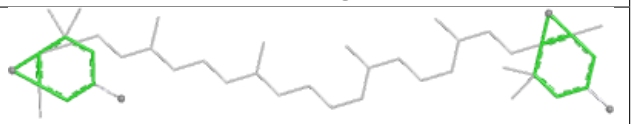
Bond lengths



Bond angles

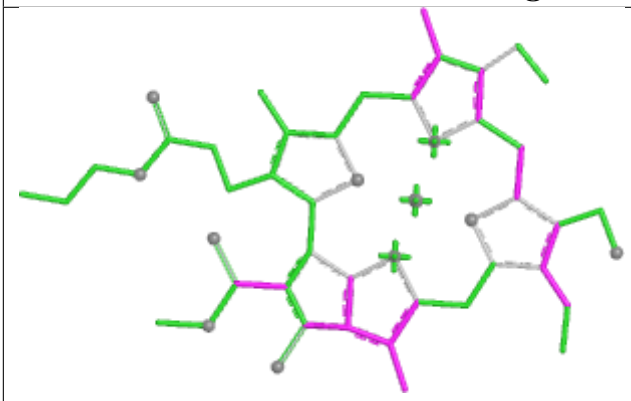


Torsions

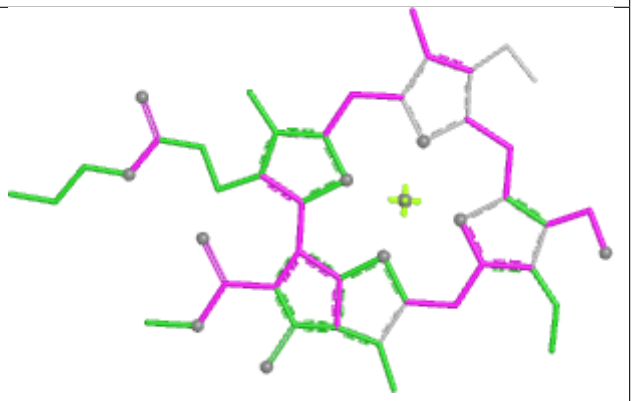


Rings

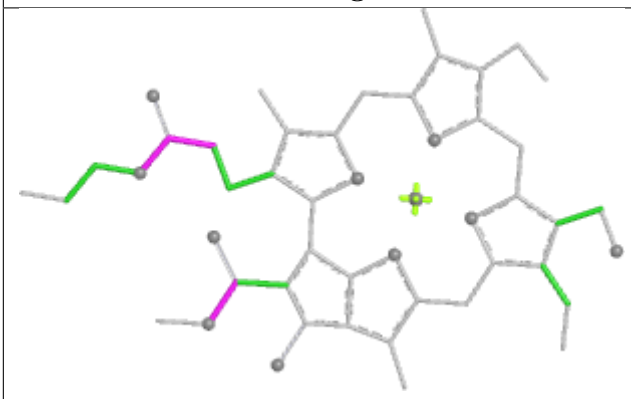
Ligand CHL T 305



Bond lengths



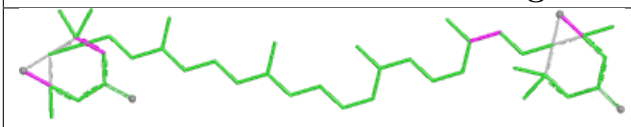
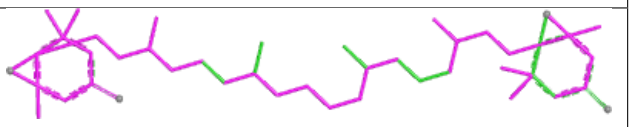
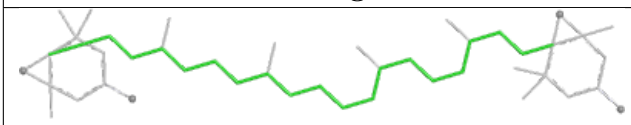
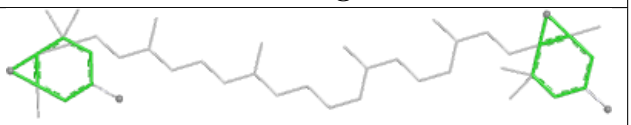
Bond angles

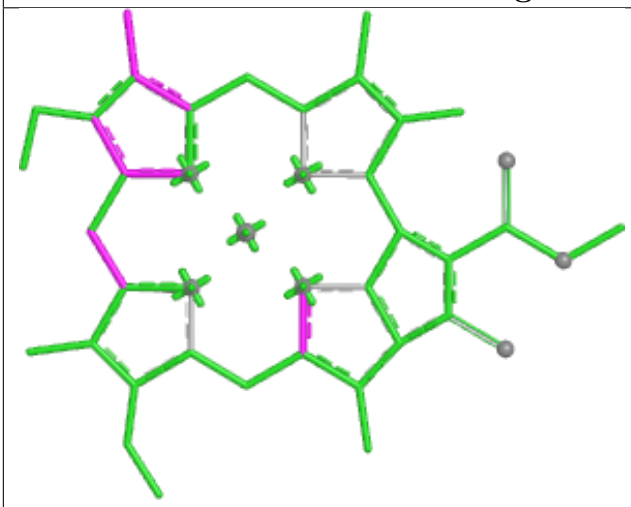
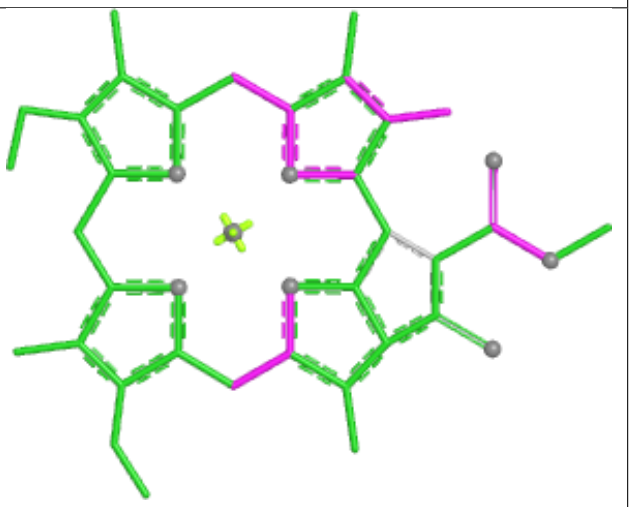
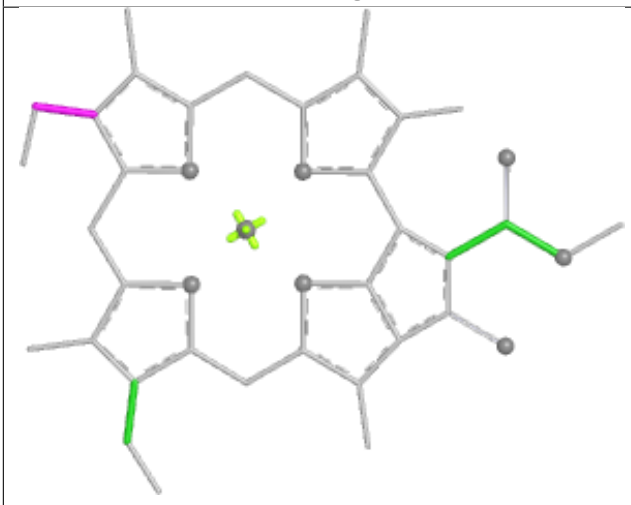
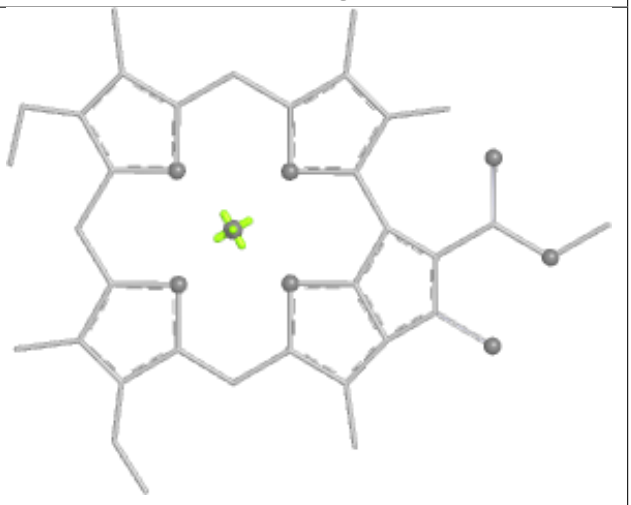


Torsions

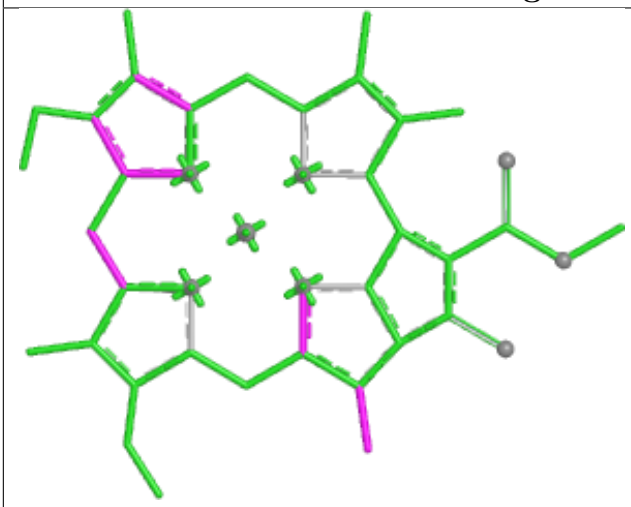


Rings

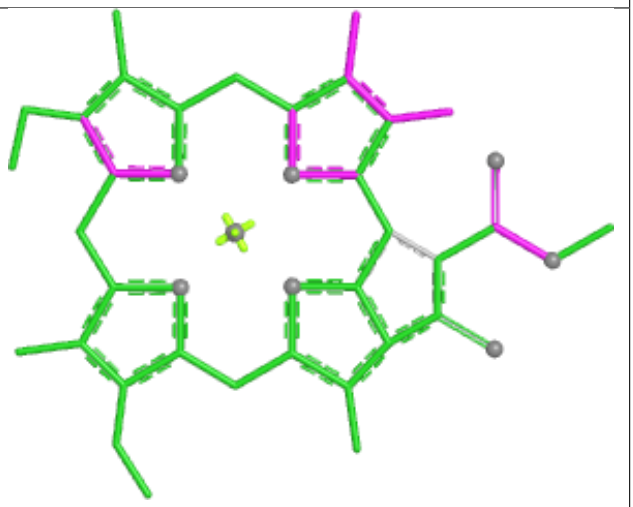
Ligand XAT 2 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 2003	
 Bond lengths	 Bond angles
 Torsions	 Rings

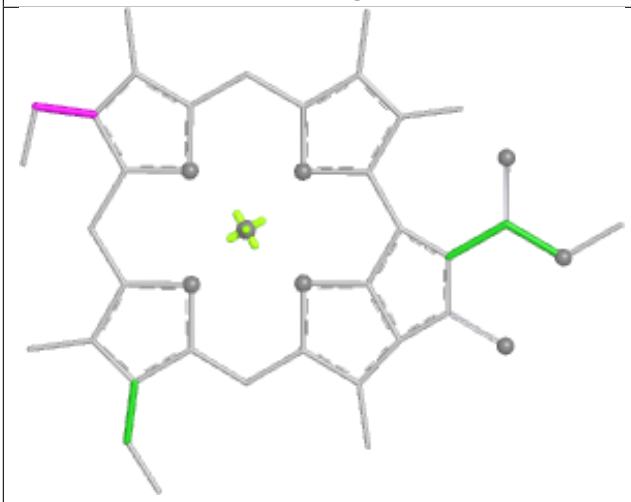
Ligand CLA U 312



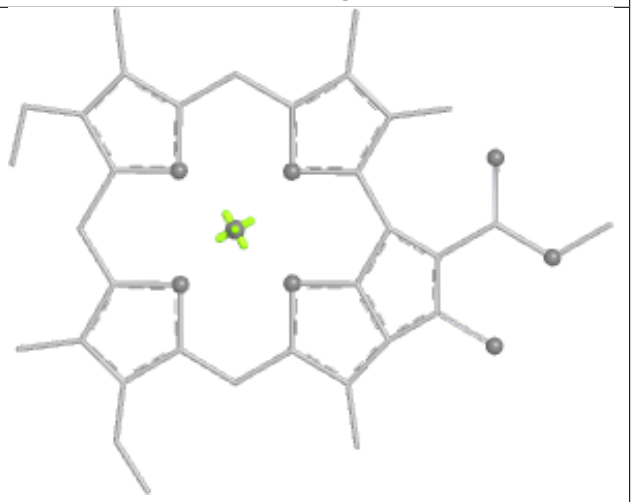
Bond lengths



Bond angles

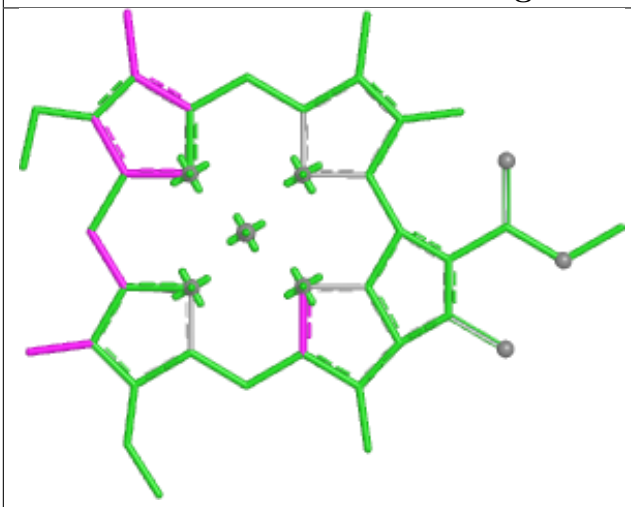


Torsions

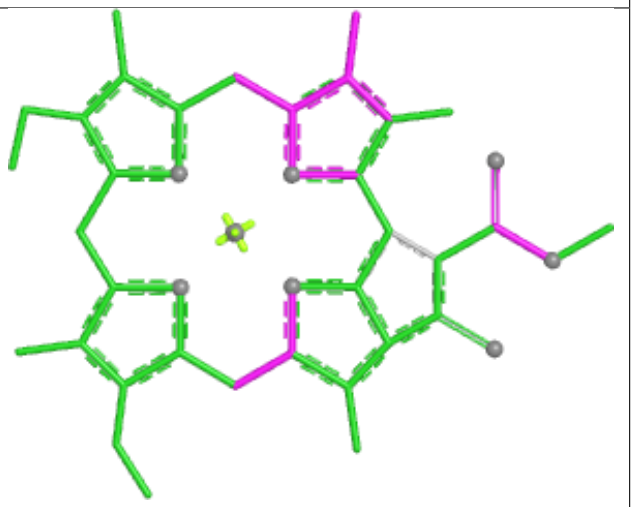


Rings

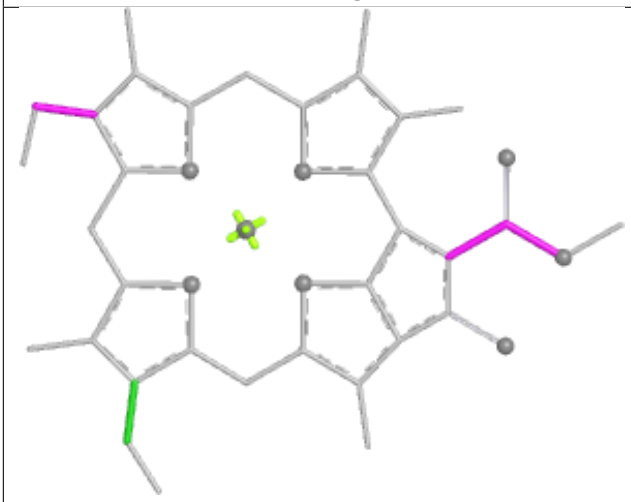
Ligand CLA O 2004



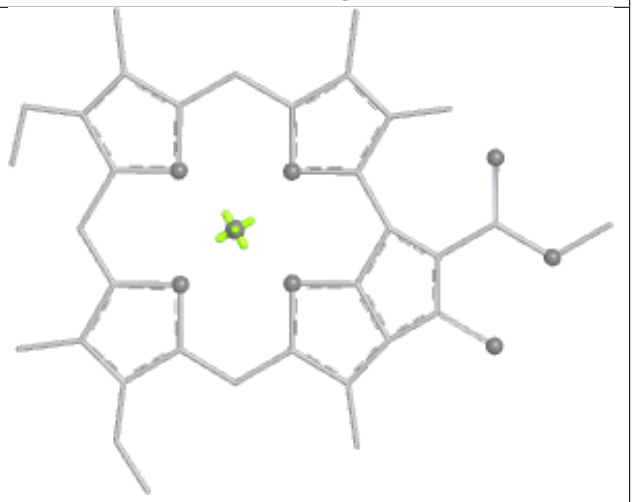
Bond lengths



Bond angles

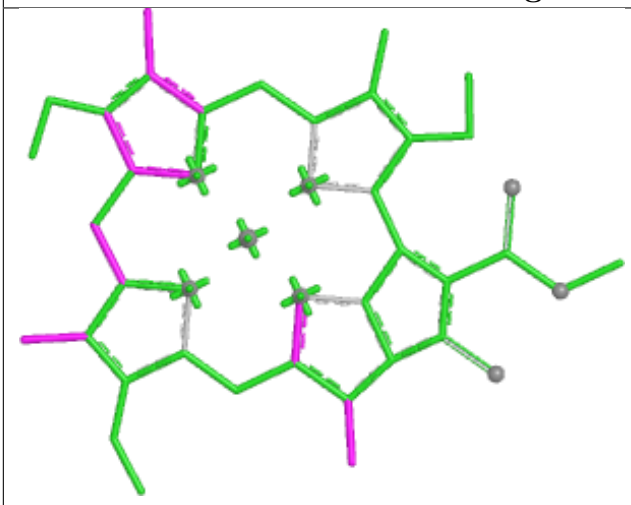


Torsions

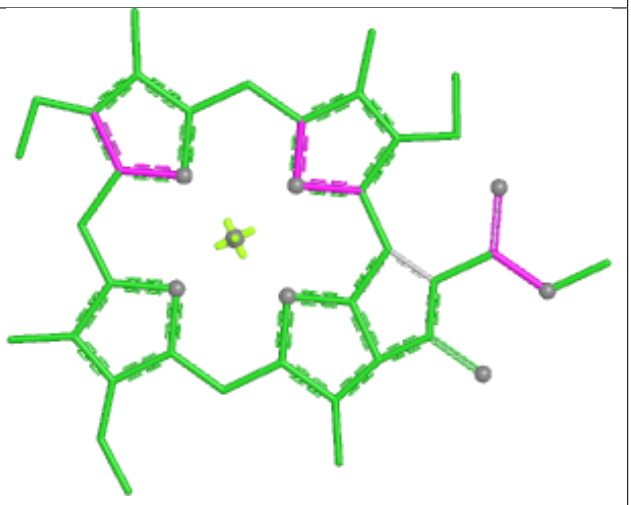


Rings

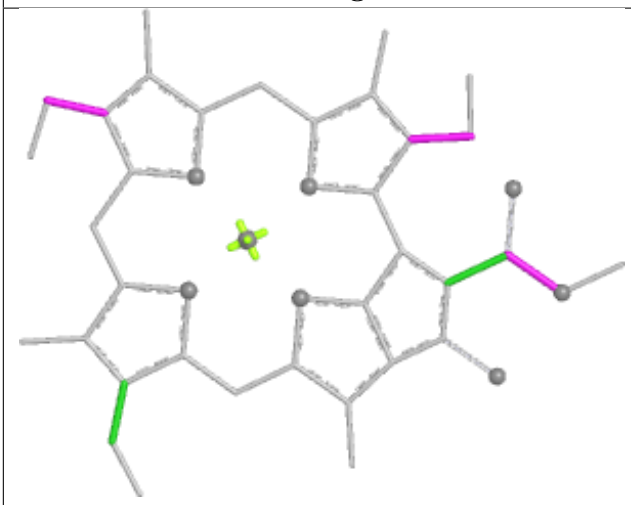
Ligand CLA T 313



Bond lengths



Bond angles

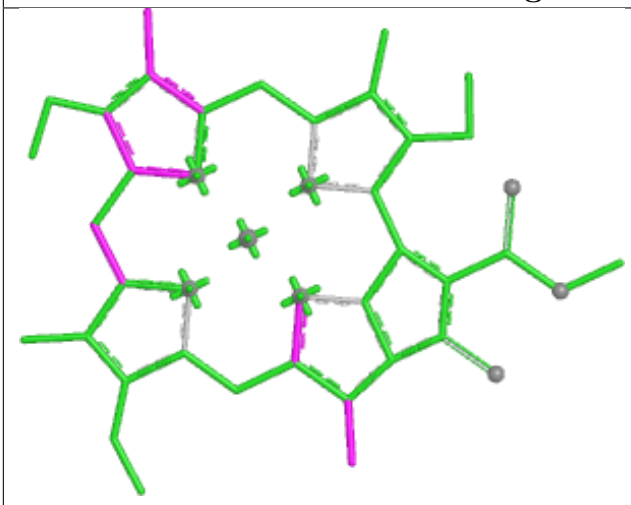


Torsions

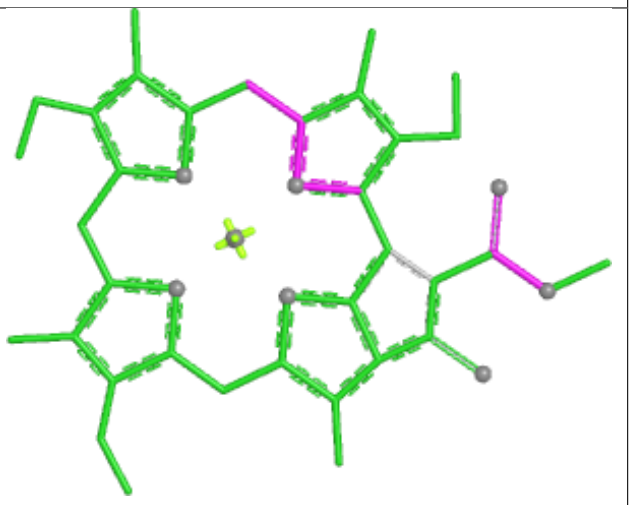


Rings

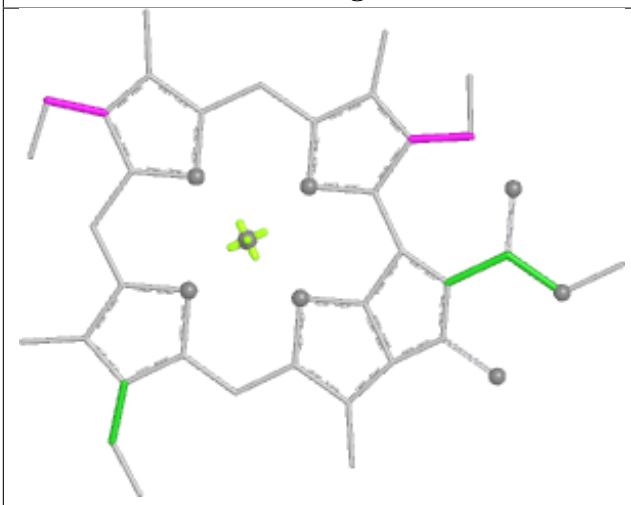
Ligand CLA T 310



Bond lengths



Bond angles

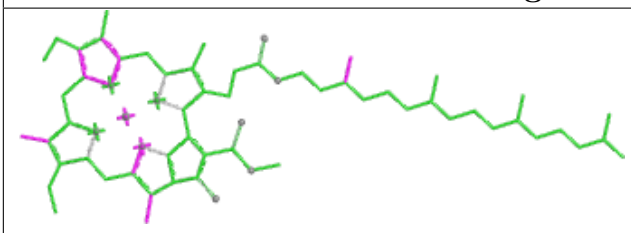


Torsions

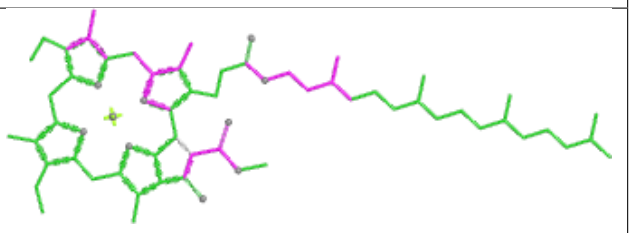


Rings

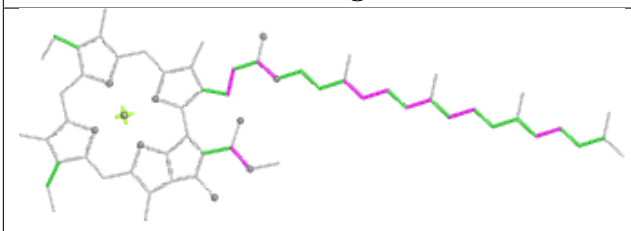
Ligand CLA B 815



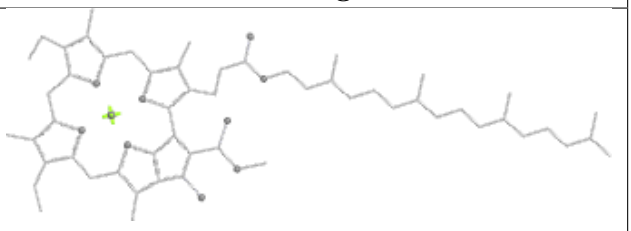
Bond lengths



Bond angles

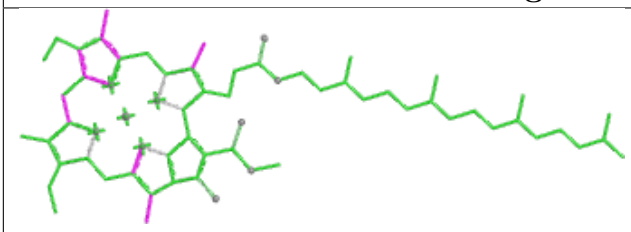


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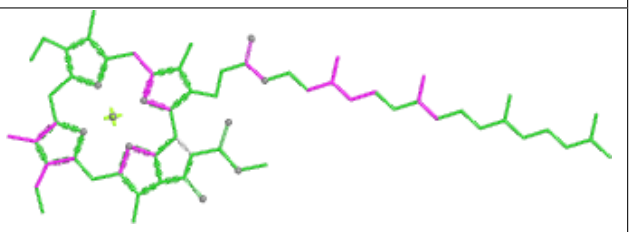


Rings

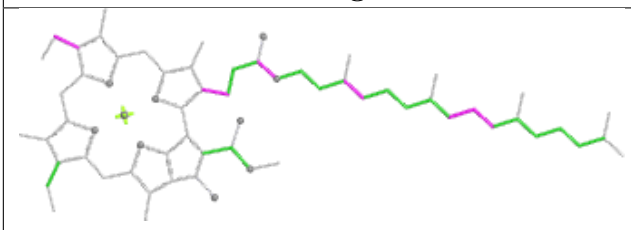
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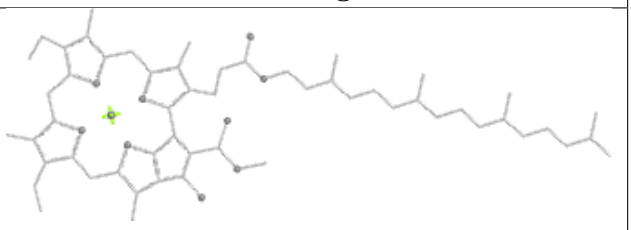
Bond lengths



Bond angles

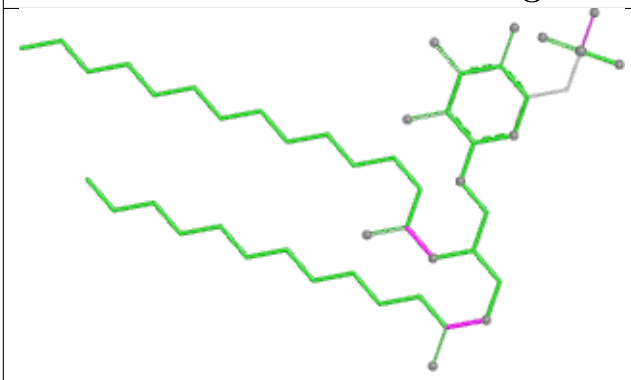


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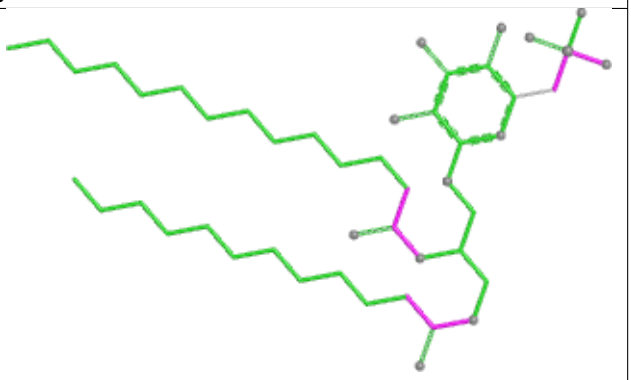


Rings

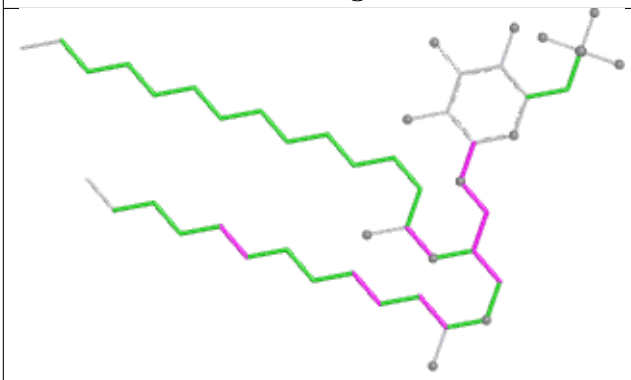
Ligand SQD H 303



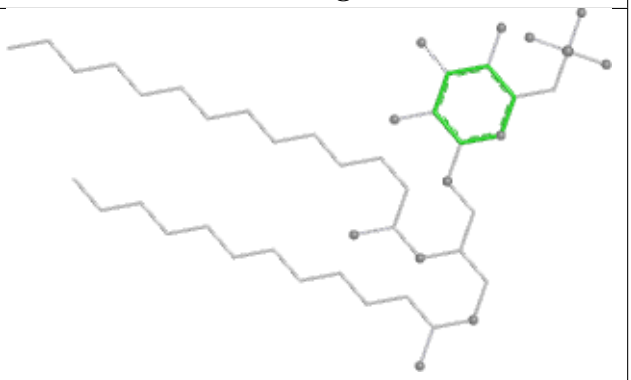
Bond lengths



Bond angles

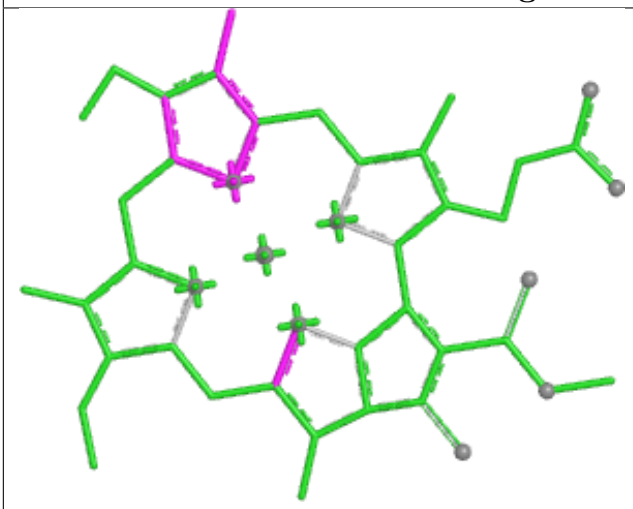


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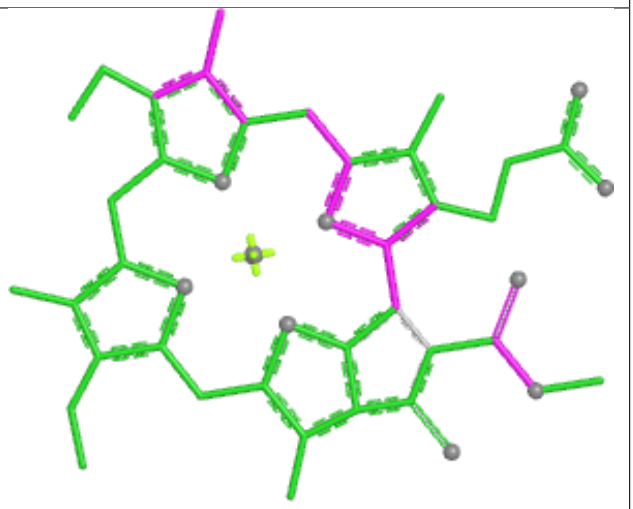


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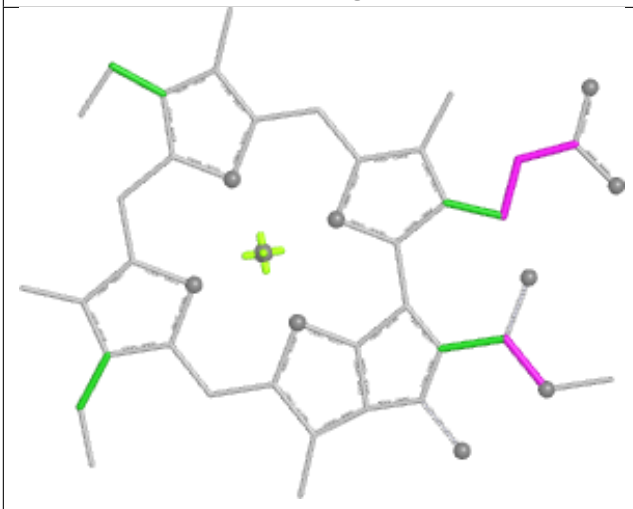
Ligand CLA W 311



Bond lengths



Bond angles

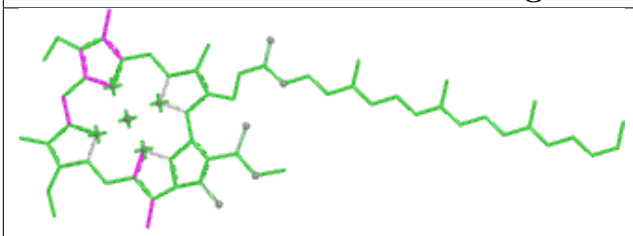


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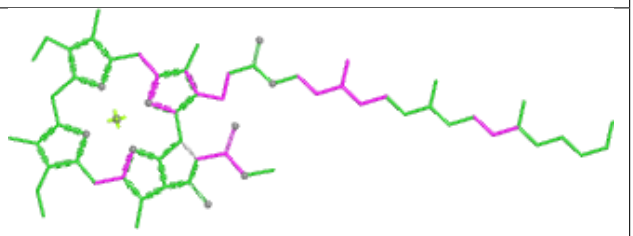


Rings

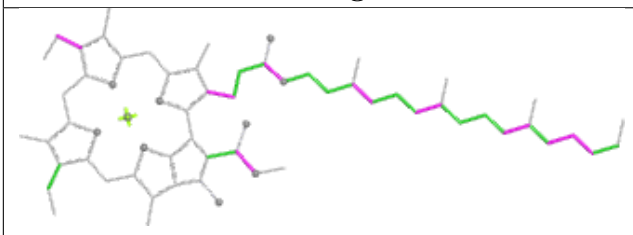
Ligand CLA P 309



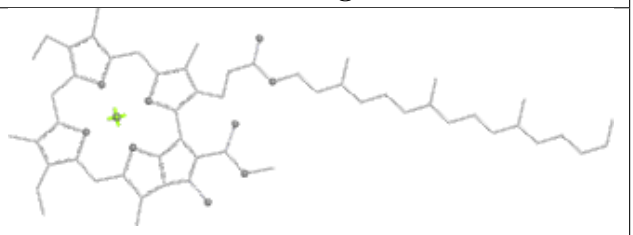
Bond lengths



Bond angles

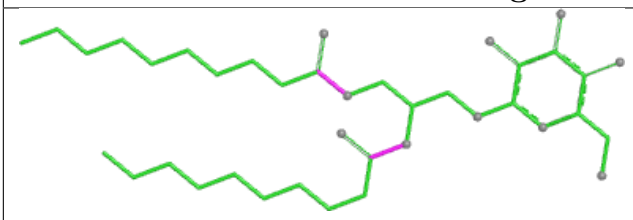


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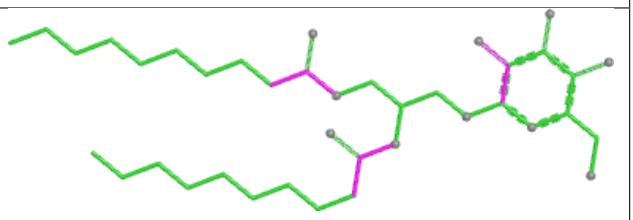


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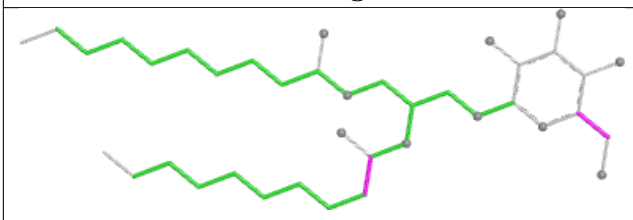
Ligand LMG O 2008



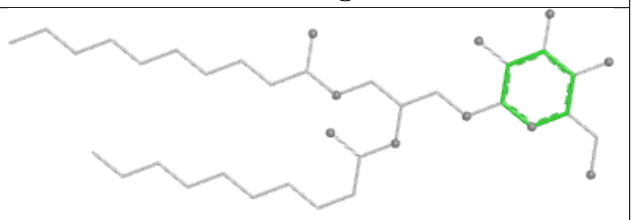
Bond lengths



Bond angles

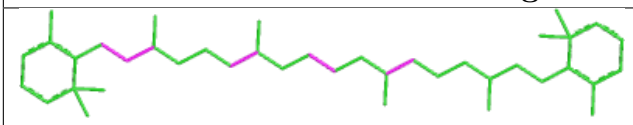


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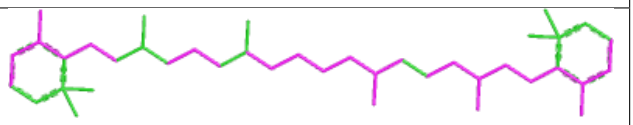


Rings

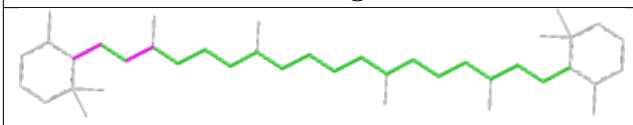
Ligand BCR K 207



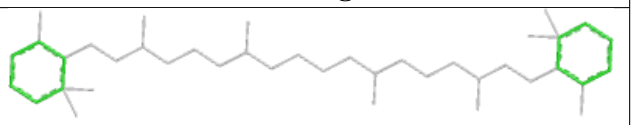
Bond lengths



Bond angles

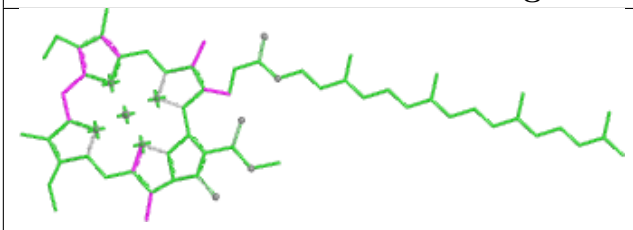


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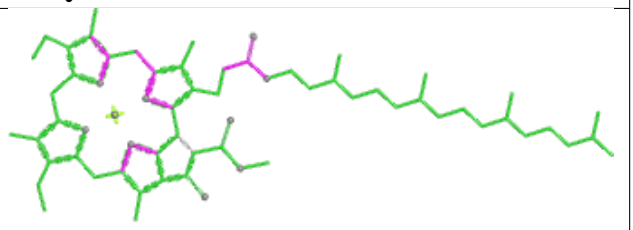


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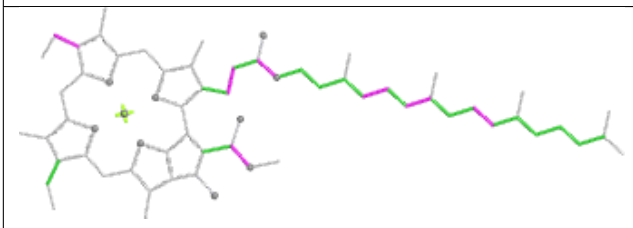
Ligand CLA Q 304



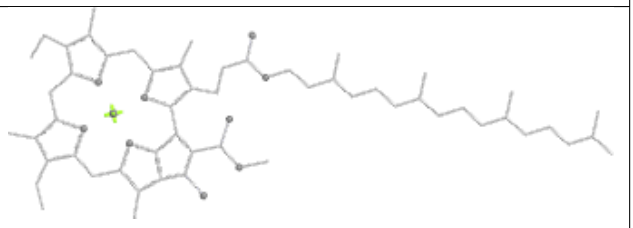
Bond lengths



Bond angles

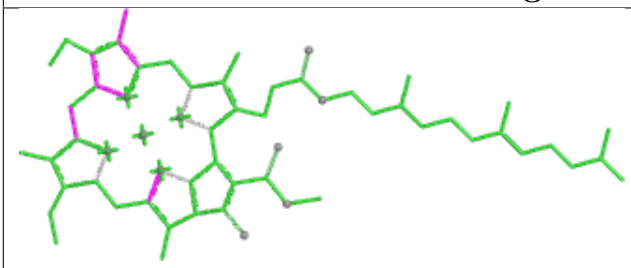


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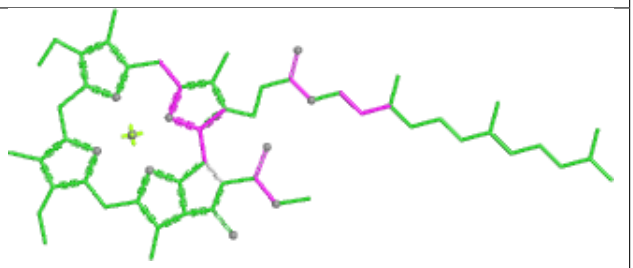


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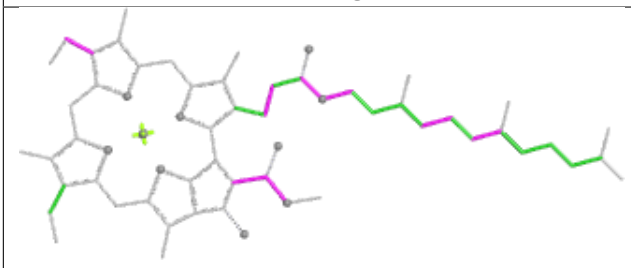
Ligand CLA V 311



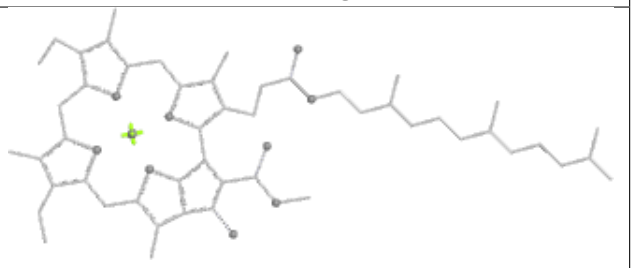
Bond lengths



Bond angles

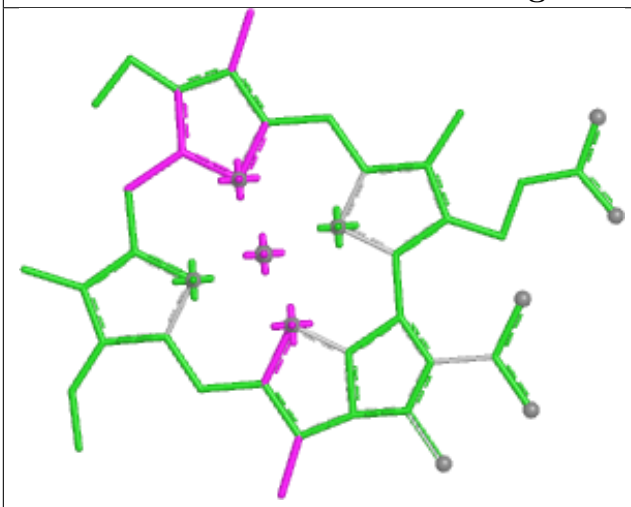


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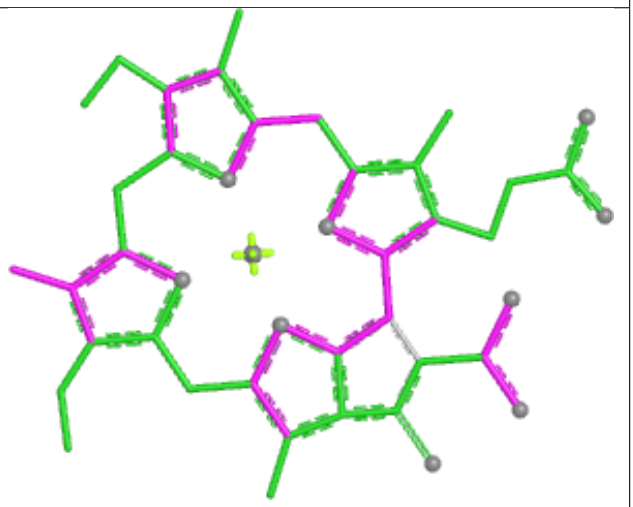


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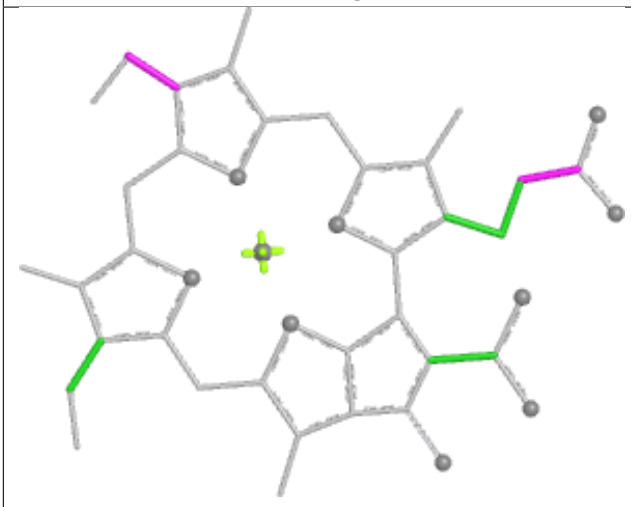
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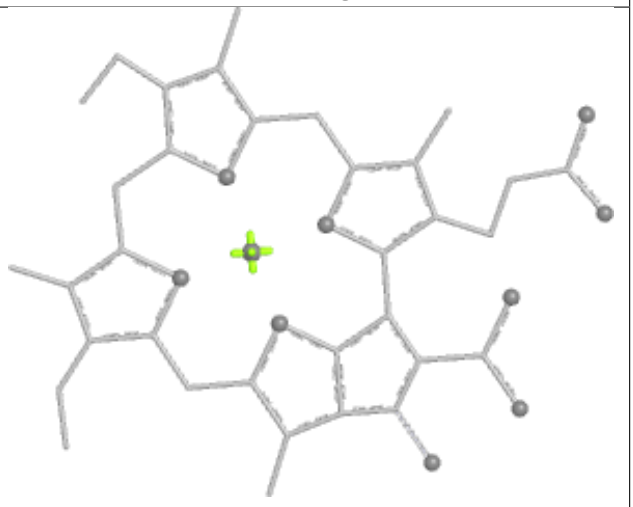
Bond lengths



Bond angles

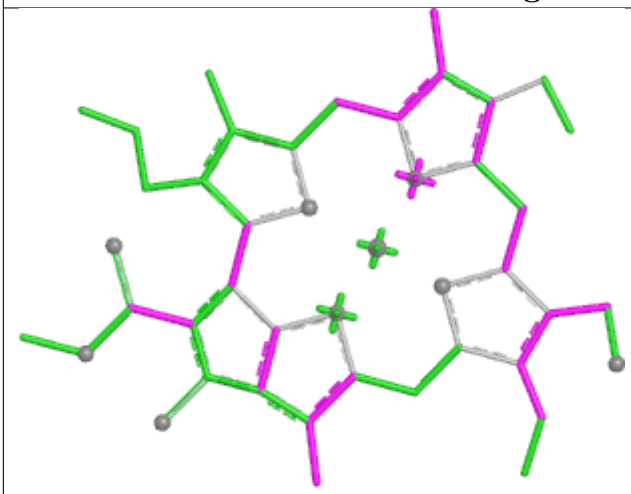


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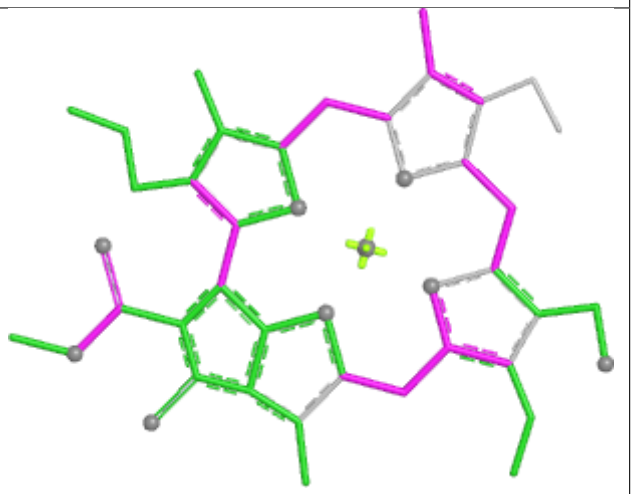


Rings

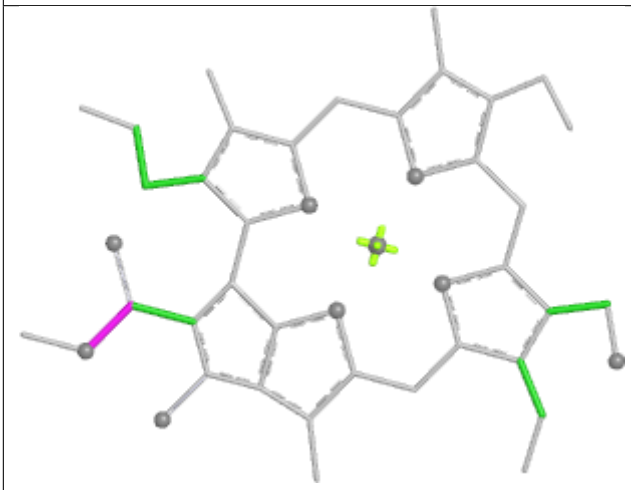
Ligand CHL R 311



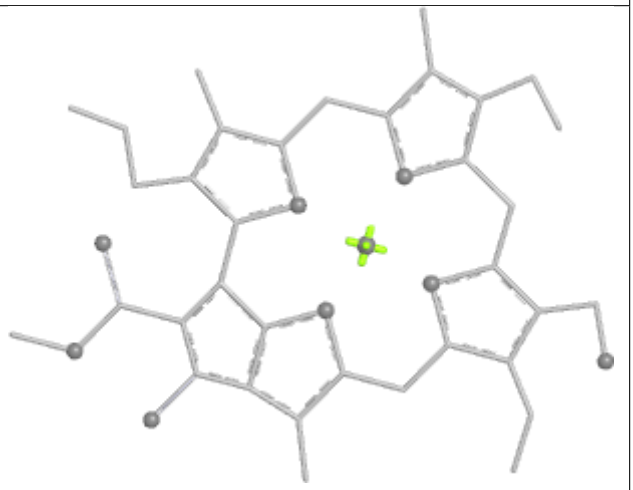
Bond lengths



Bond angles

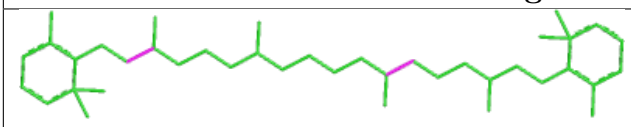


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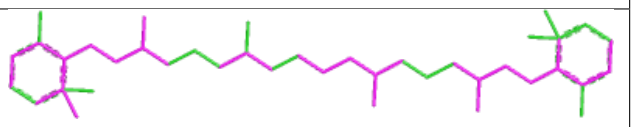


Rings

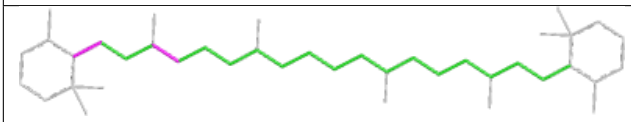
Ligand BCR L 307



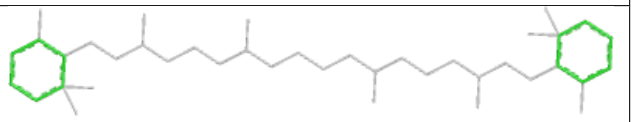
Bond lengths



Bond angles

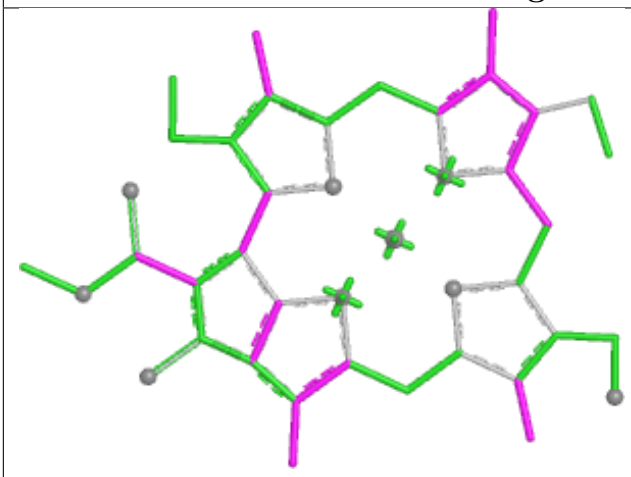


Torsions

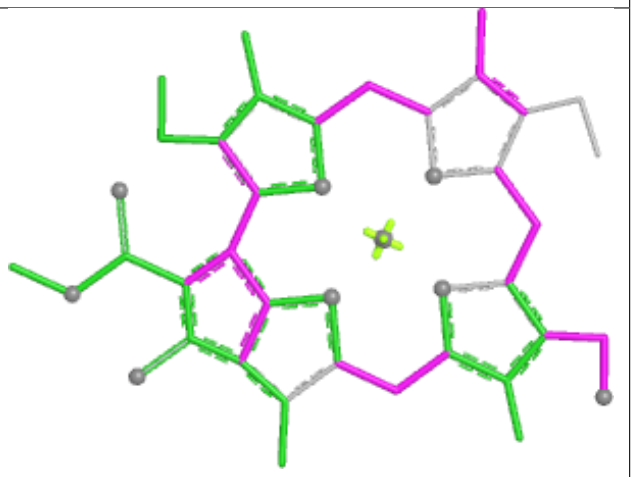


Rings

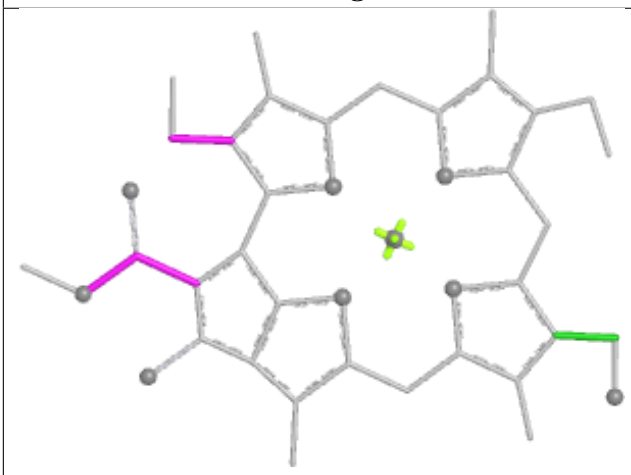
Ligand CHL 2 605



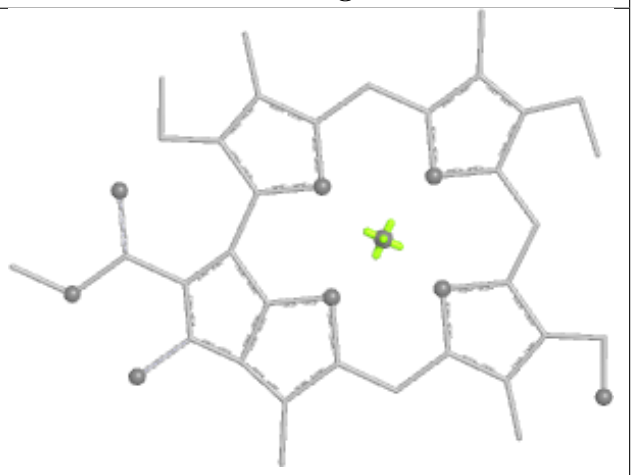
Bond lengths



Bond angles

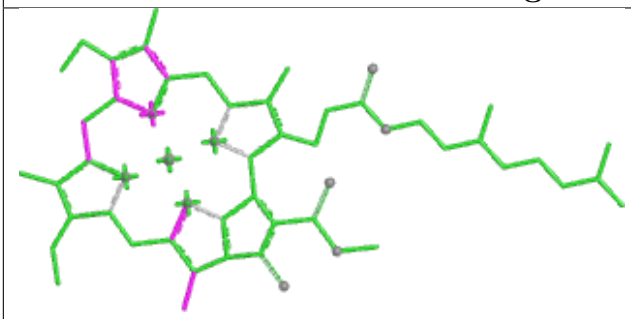


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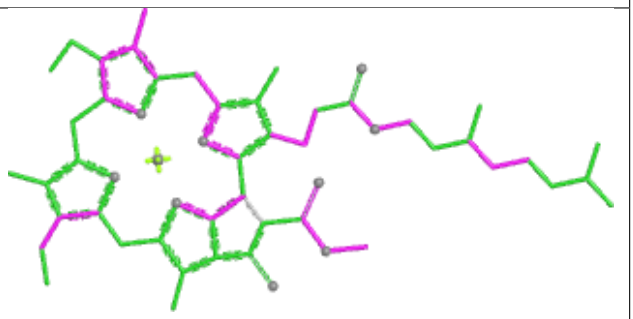


Rings

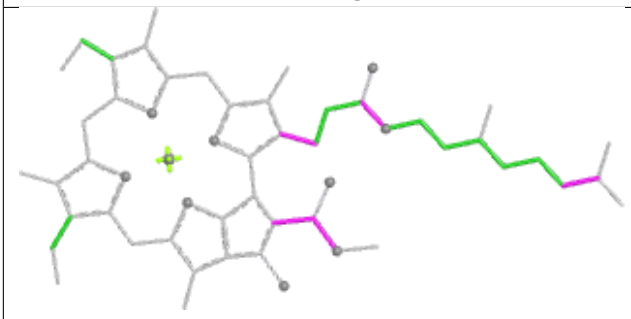
Ligand CLA B 818



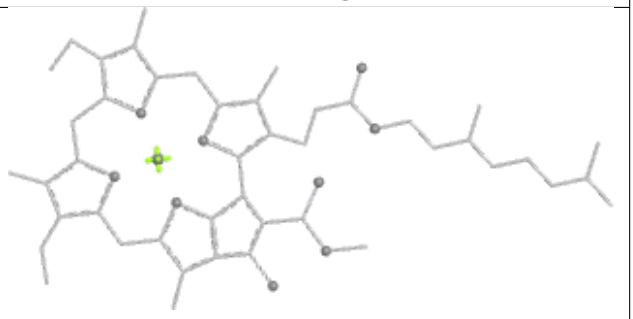
Bond lengths



Bond angles

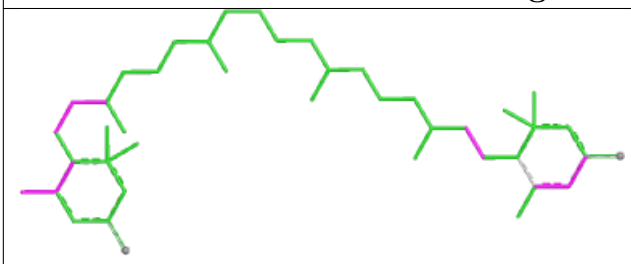


Torsions

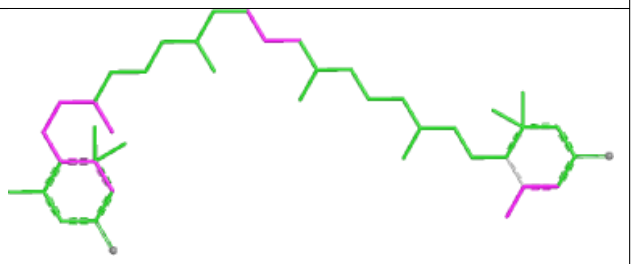


Rings

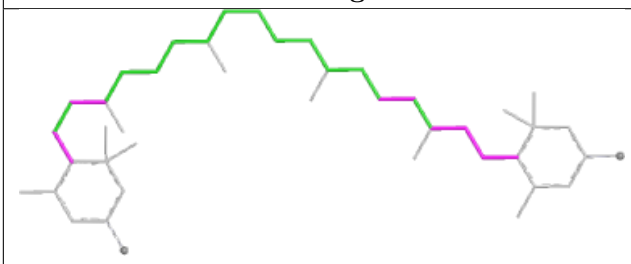
Ligand Q6L T 319



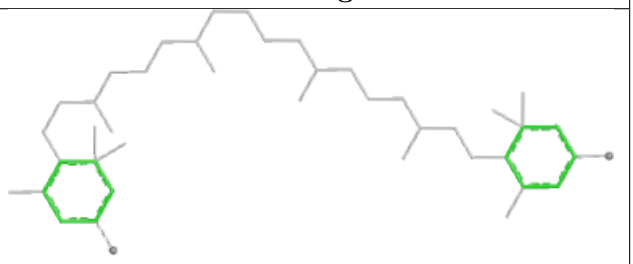
Bond lengths



Bond angles

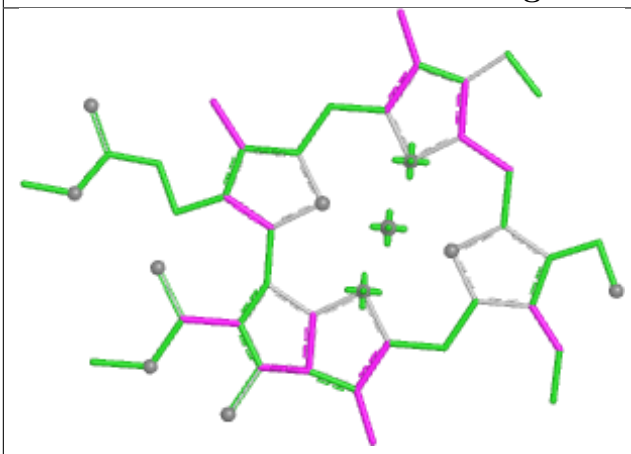


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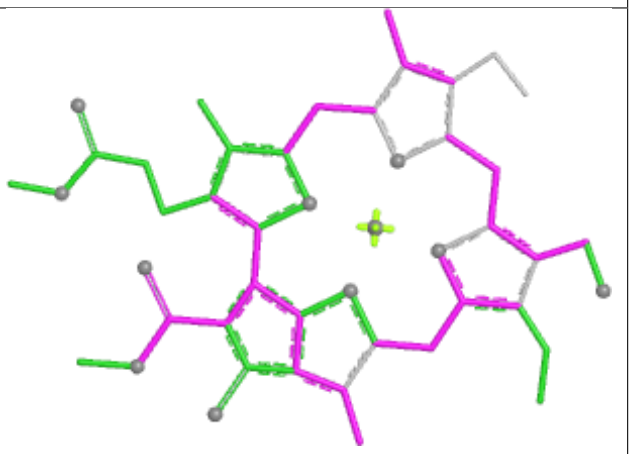


Rings

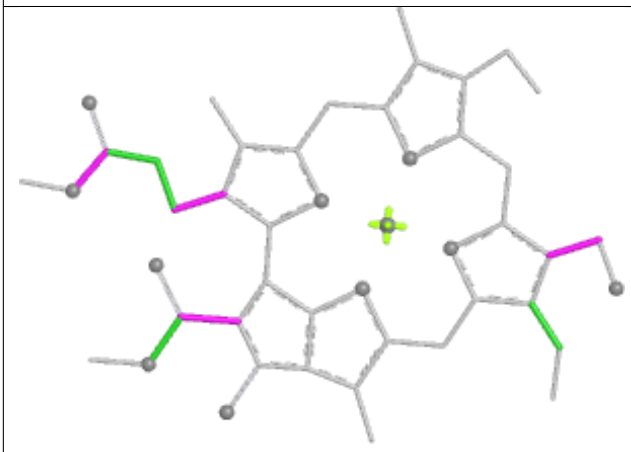
Ligand CHL R 302



Bond lengths



Bond angles

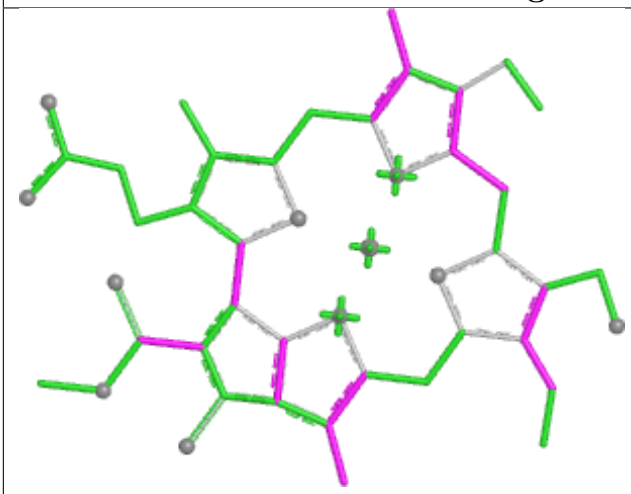


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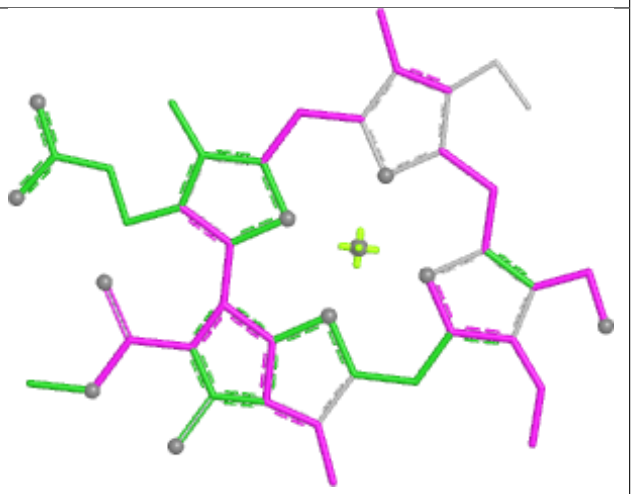


Rings

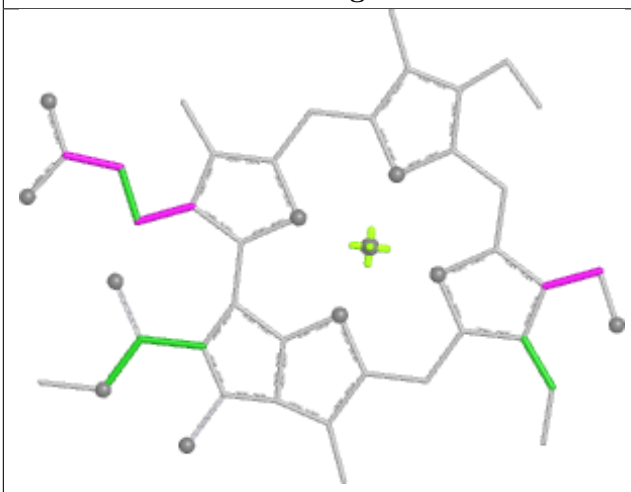
Ligand CHL 4 308



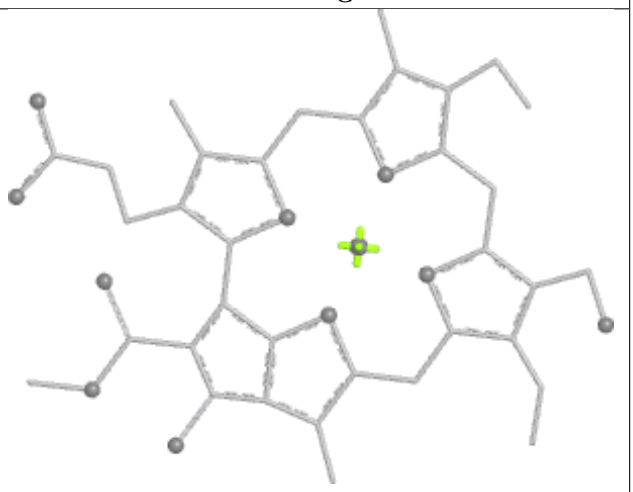
Bond lengths



Bond angles

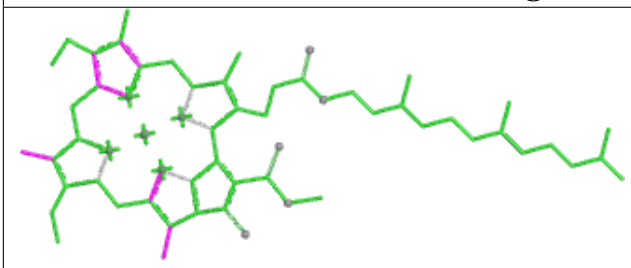


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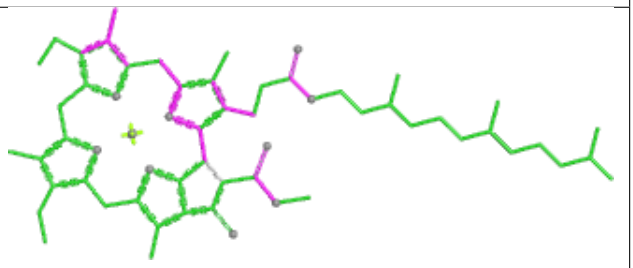


Rings

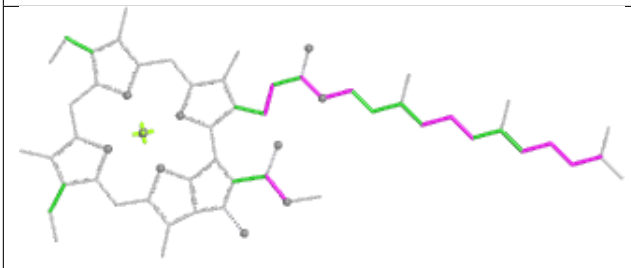
Ligand CLA T 311



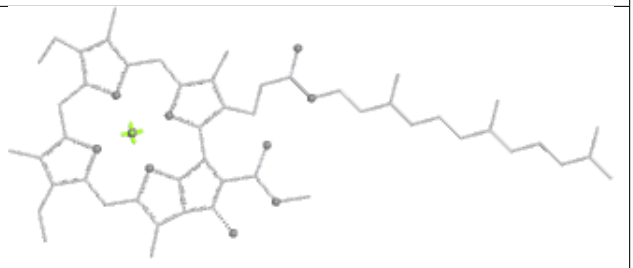
Bond lengths



Bond angles

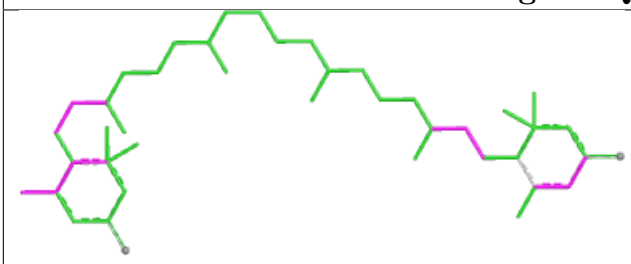


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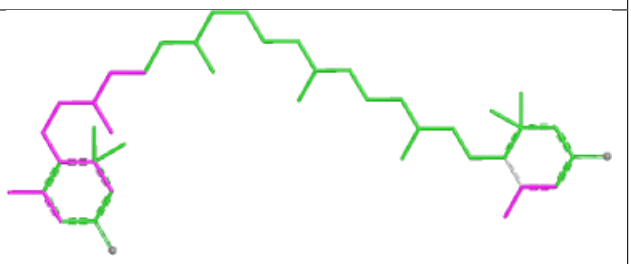


Rings

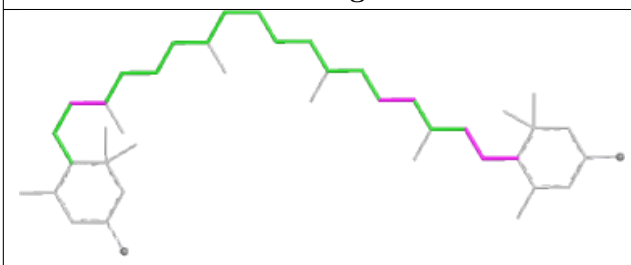
Ligand Q6L O 2007



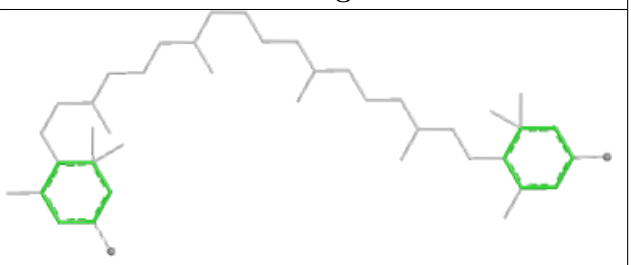
Bond lengths



Bond angles

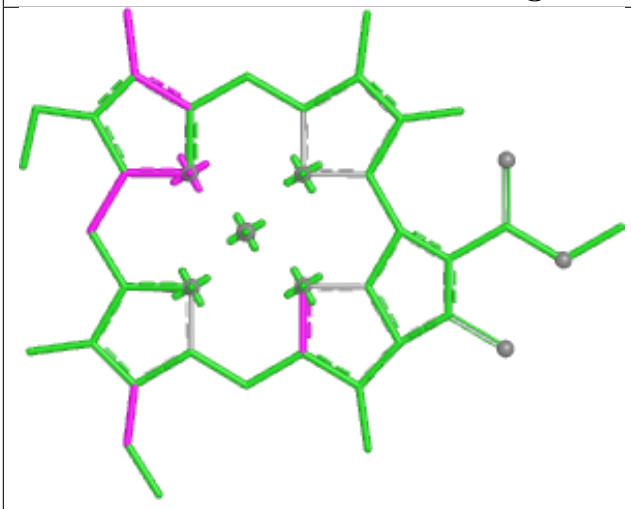


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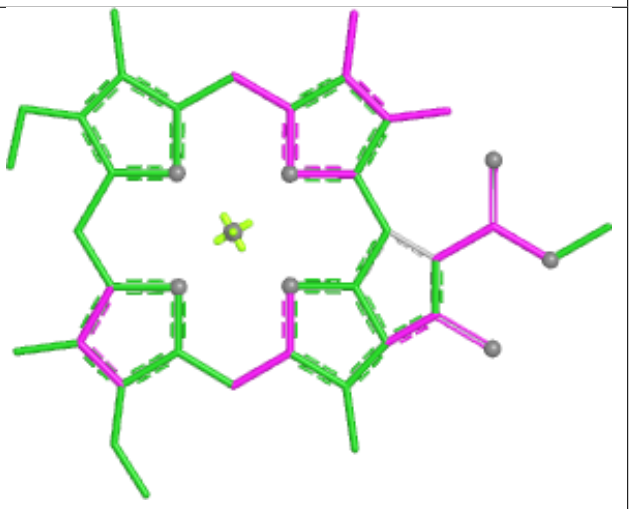


Rings

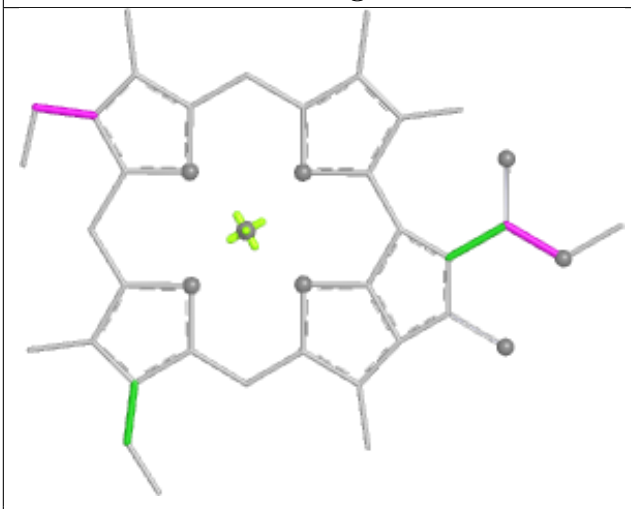
Ligand CLA F 803



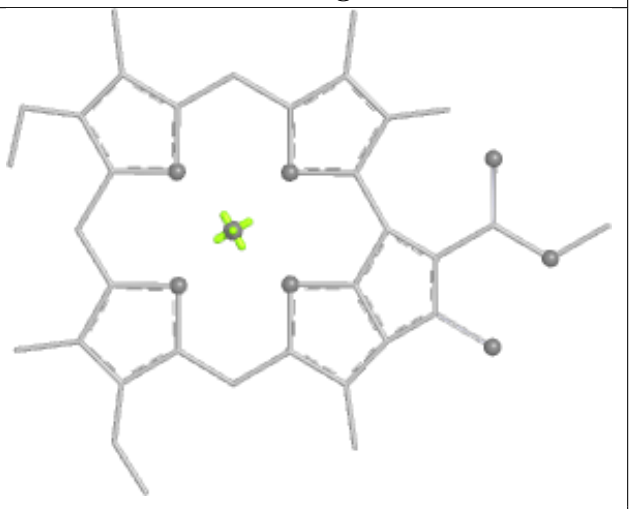
Bond lengths



Bond angles

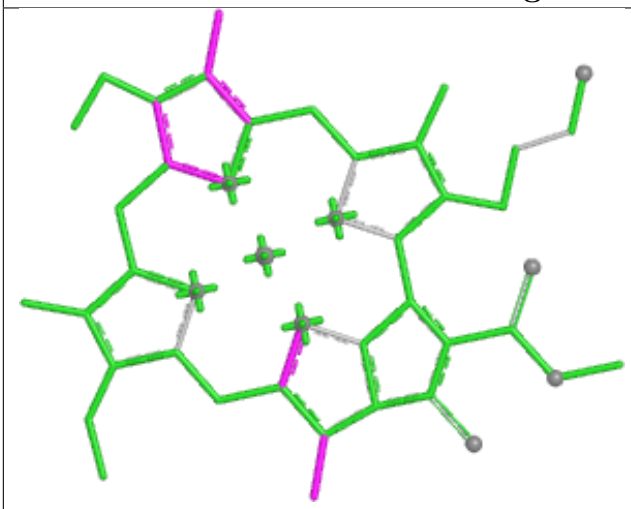


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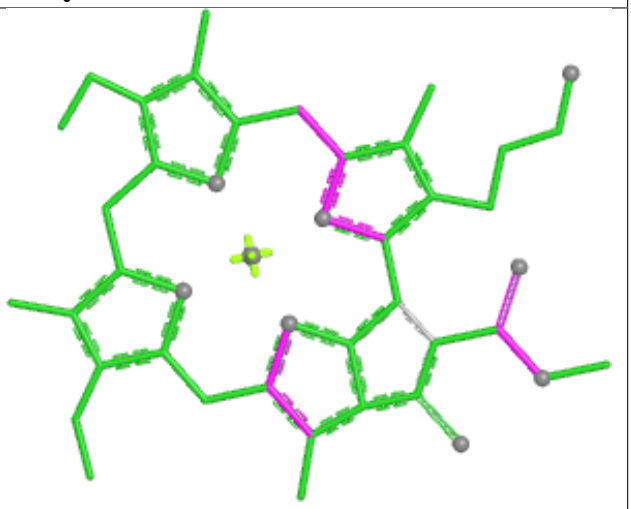


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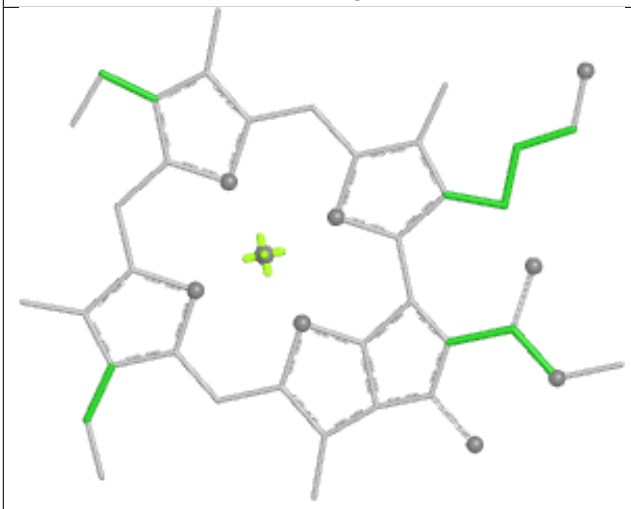
Ligand CLA Q 305



Bond lengths



Bond angles

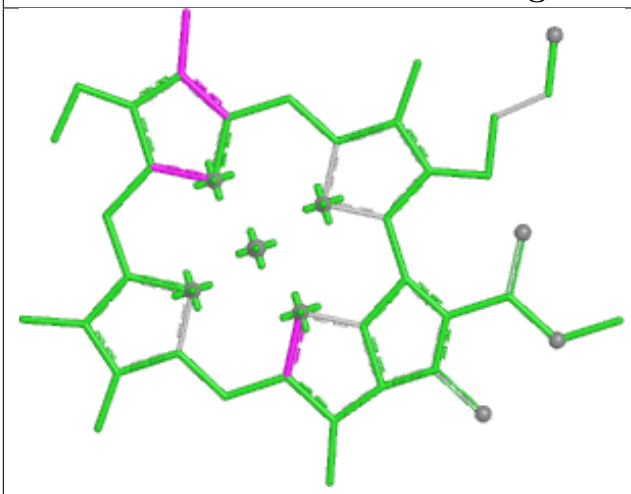


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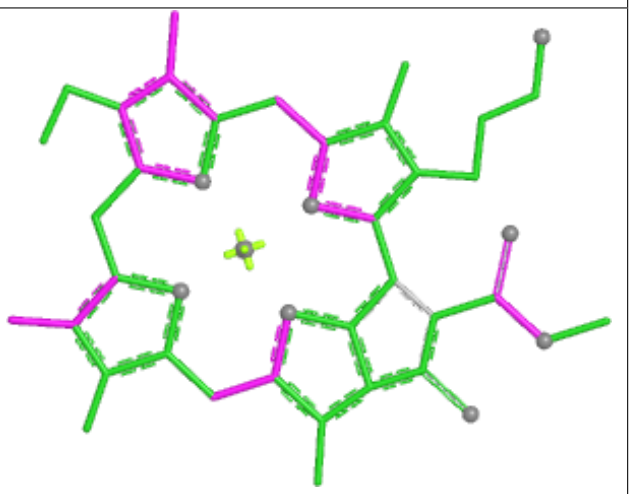


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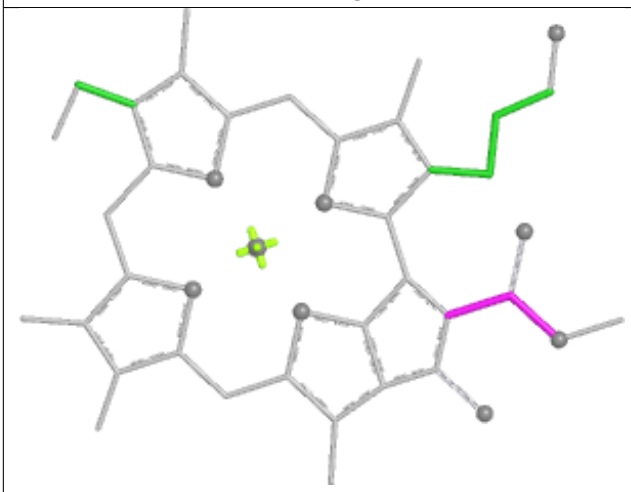
Ligand CLA 2 604



Bond lengths



Bond angles

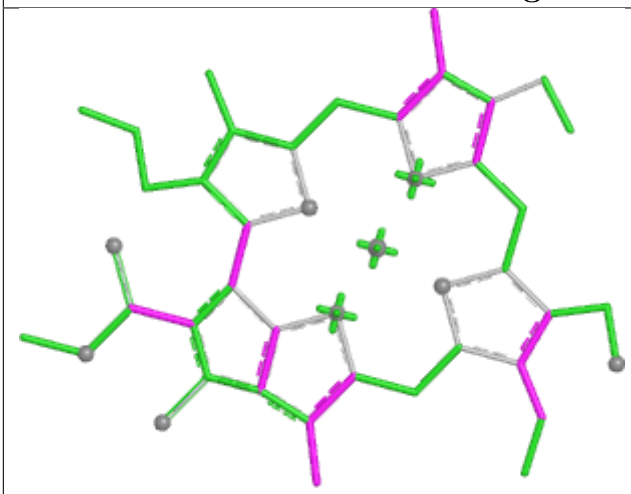


Torsions

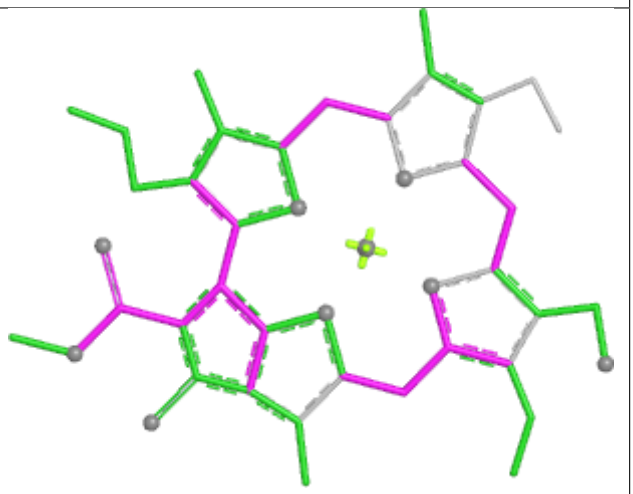


Rings

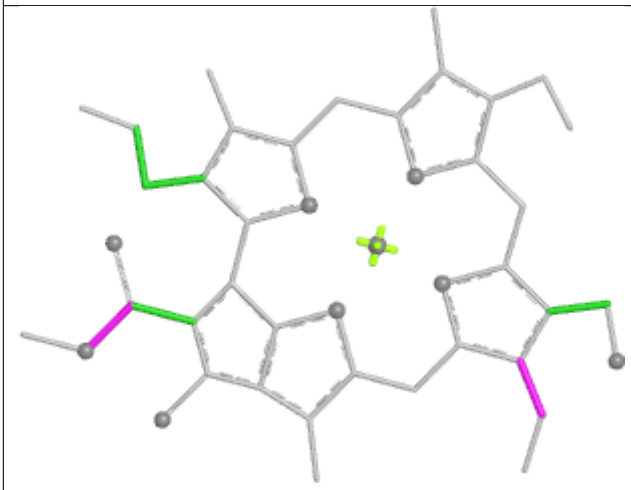
Ligand CHL V 307



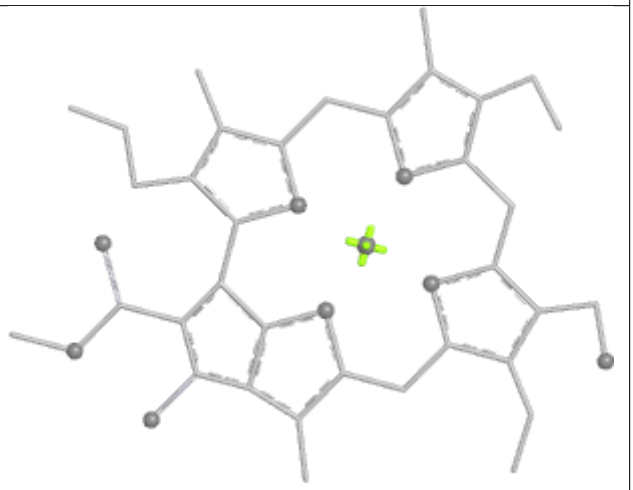
Bond lengths



Bond angles

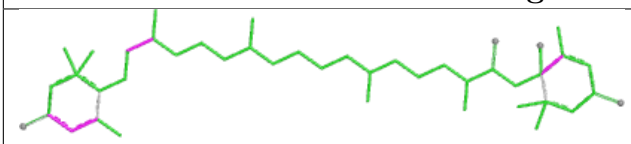


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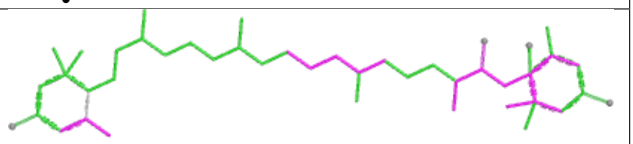


Rings

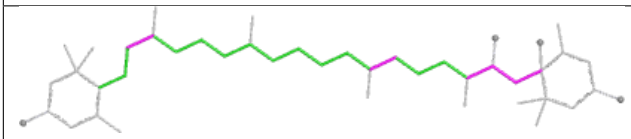
Ligand IWJ Q 320



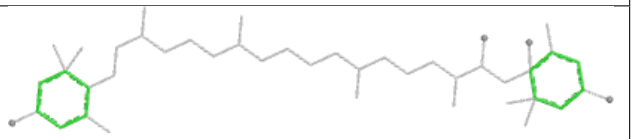
Bond lengths



Bond angles

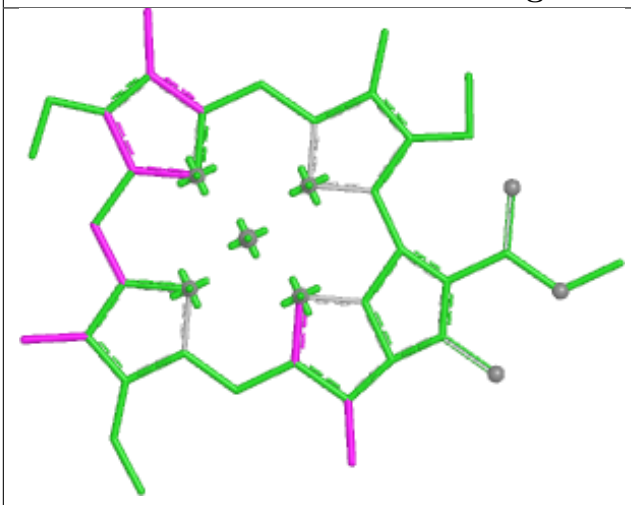


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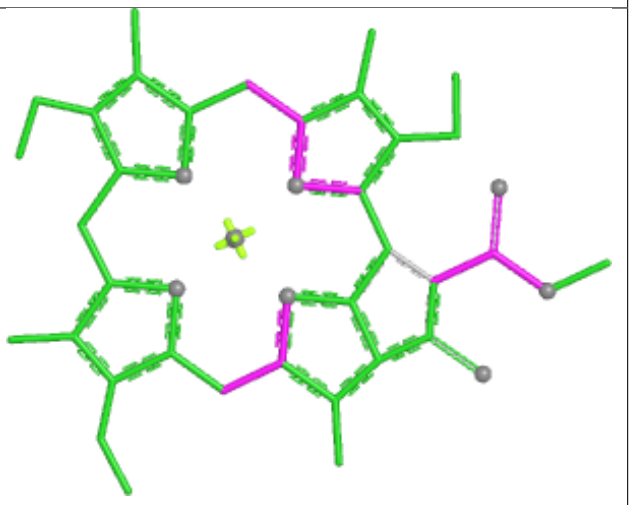


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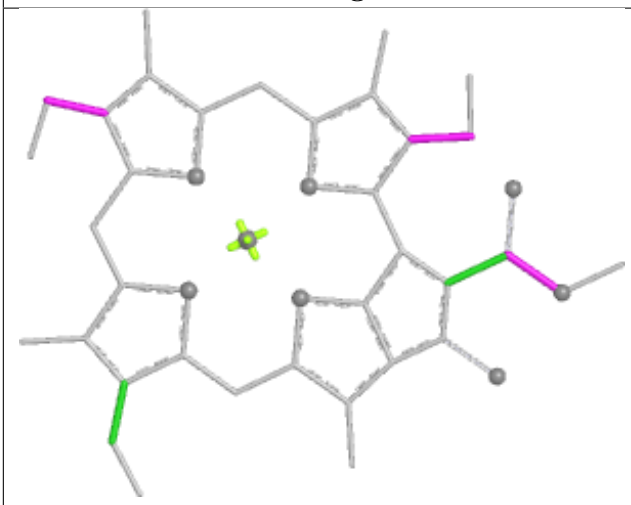
Ligand CLA L 304



Bond lengths



Bond angles

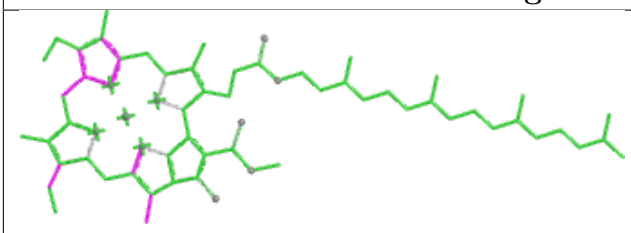


Torsions

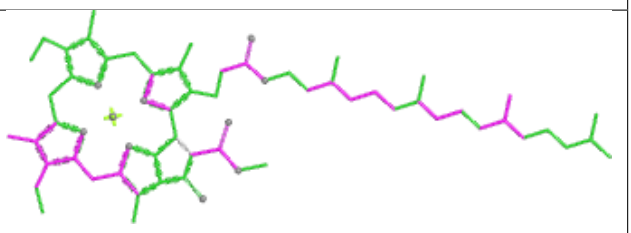


Rings

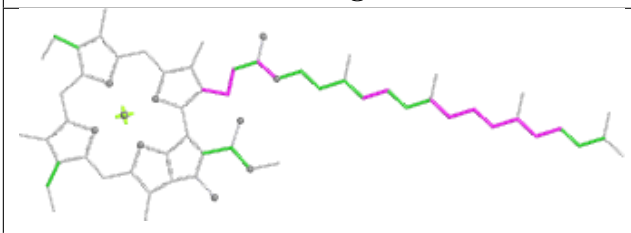
Ligand CLA B 813



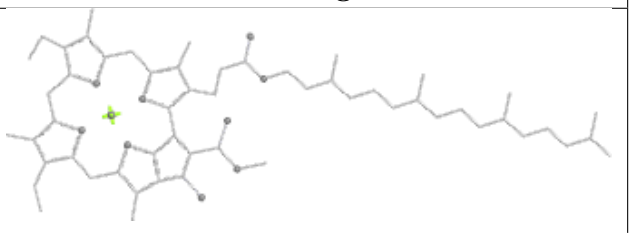
Bond lengths



Bond angles

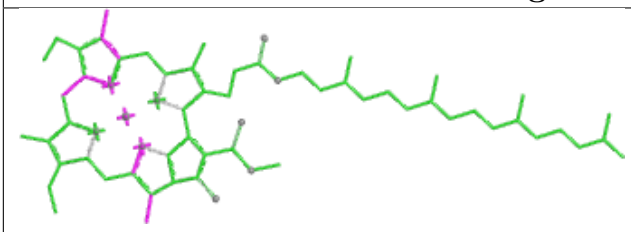


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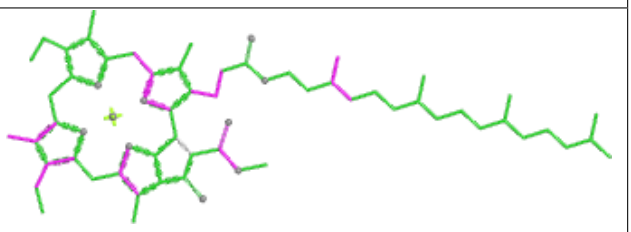


Rings

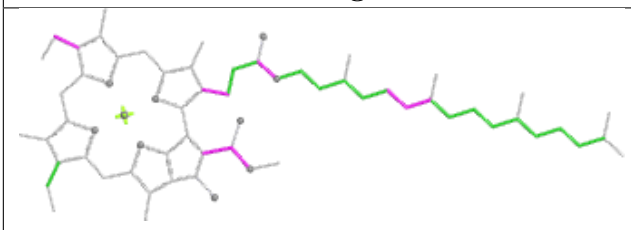
Ligand CLA 1 608



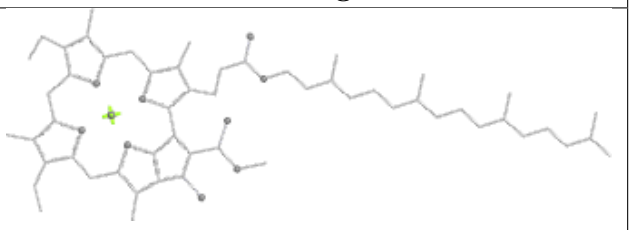
Bond lengths



Bond angles

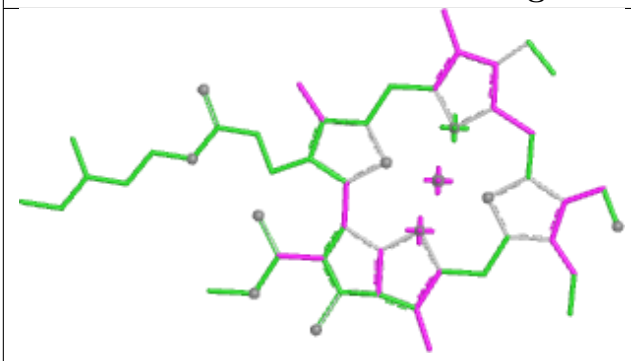


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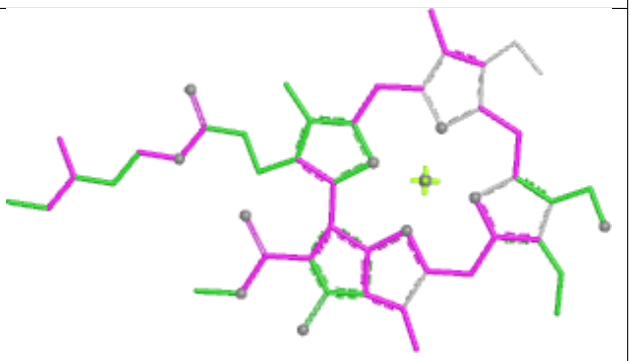


Rings

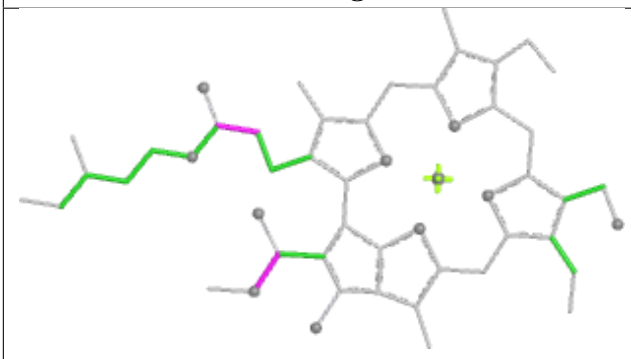
Ligand CHL 4 302



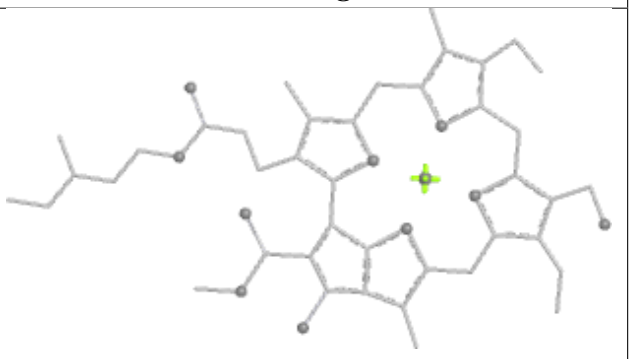
Bond lengths



Bond angles

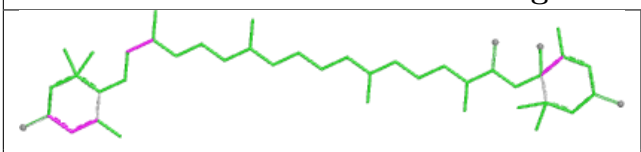


Torsions

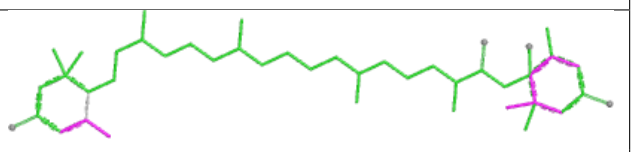


Rings

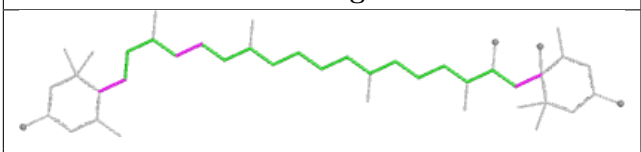
Ligand IWJ 4 301



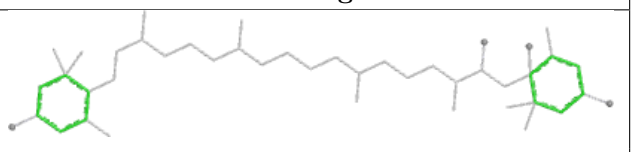
Bond lengths



Bond angles

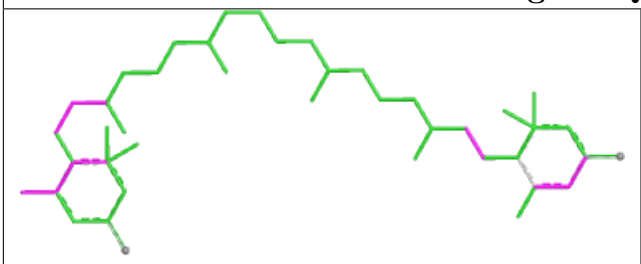


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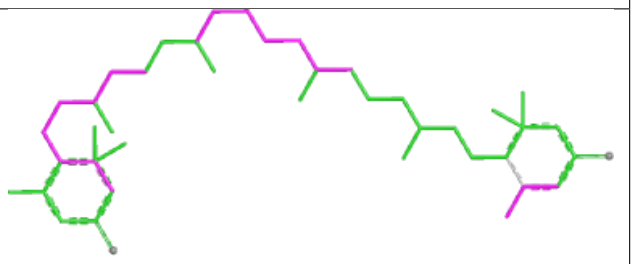


Rings

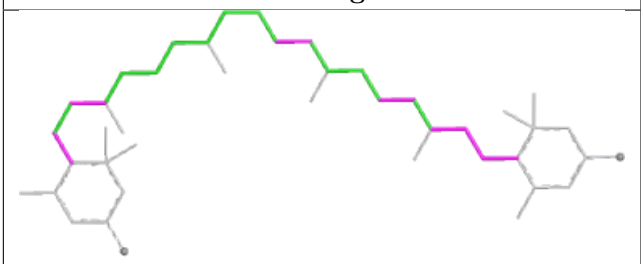
Ligand Q6L X 301



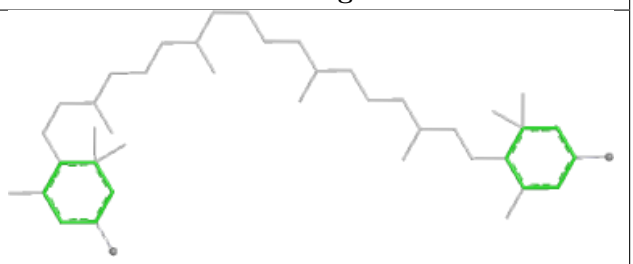
Bond lengths



Bond angles

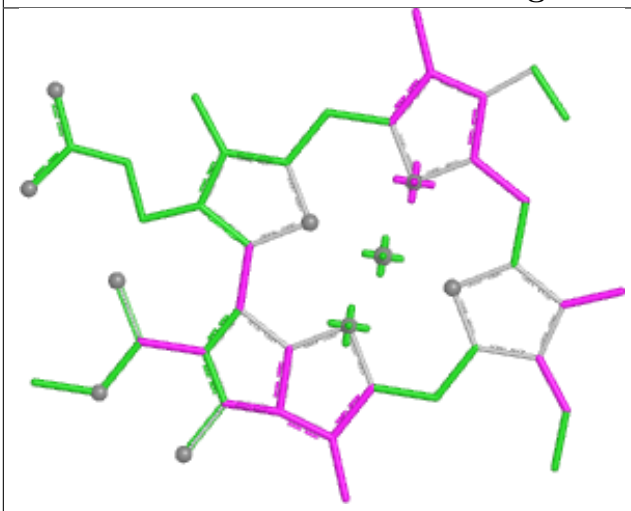


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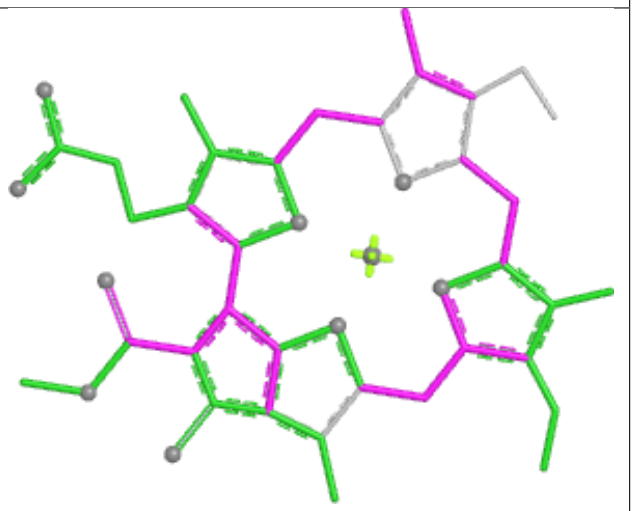


Rings

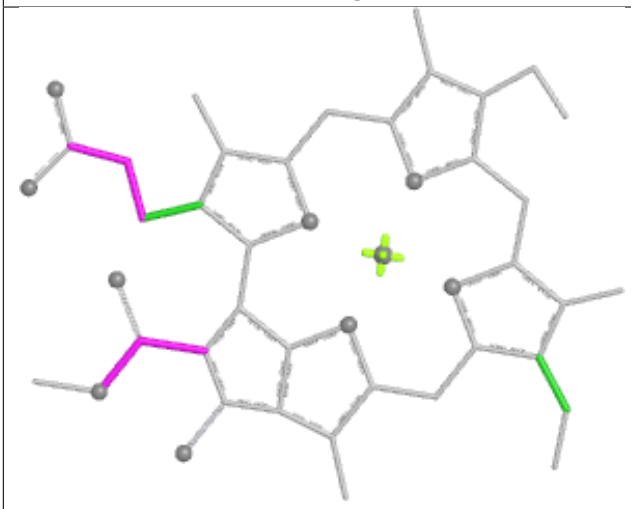
Ligand CHL 3 306



Bond lengths



Bond angles

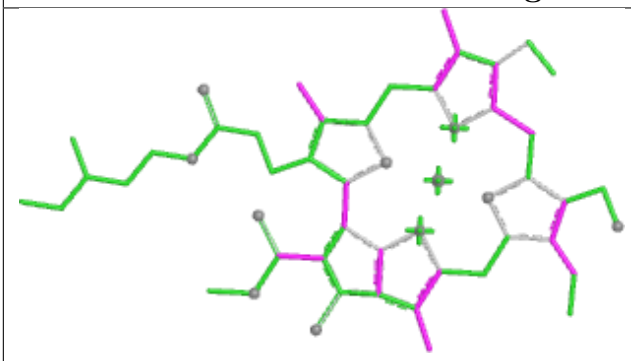


Torsions

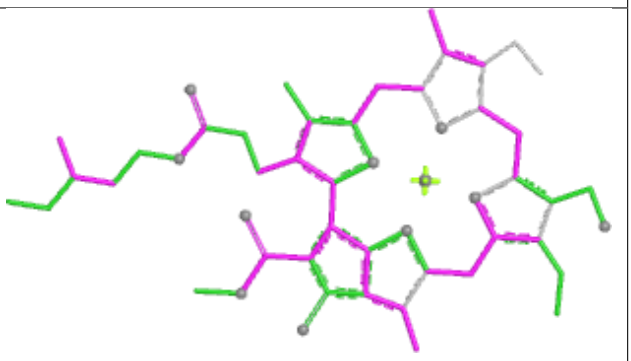


Rings

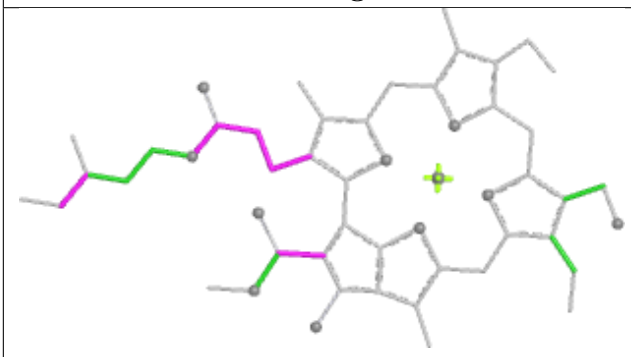
Ligand CHL T 306



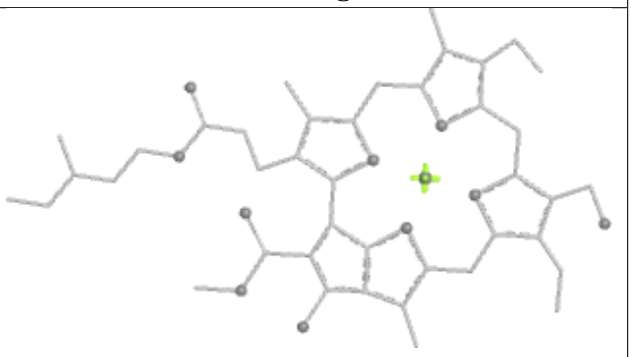
Bond lengths



Bond angles

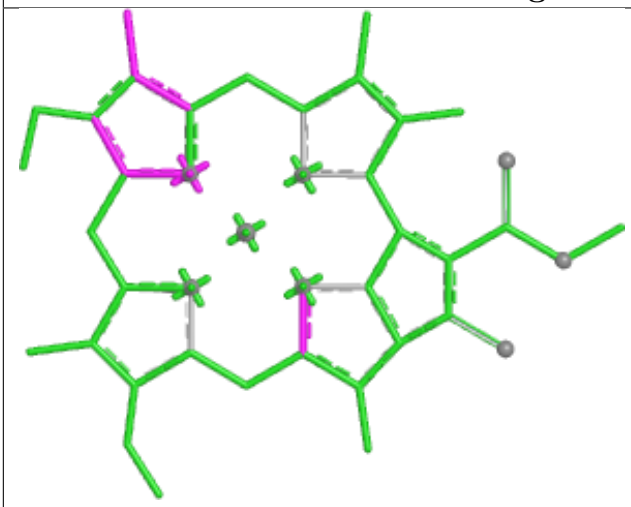


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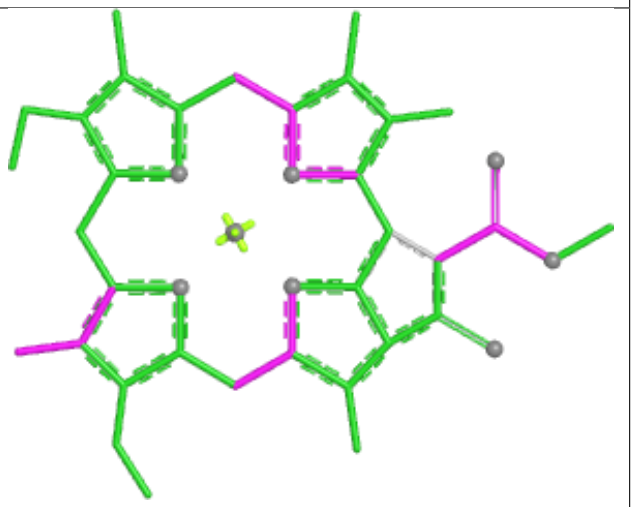


Rings

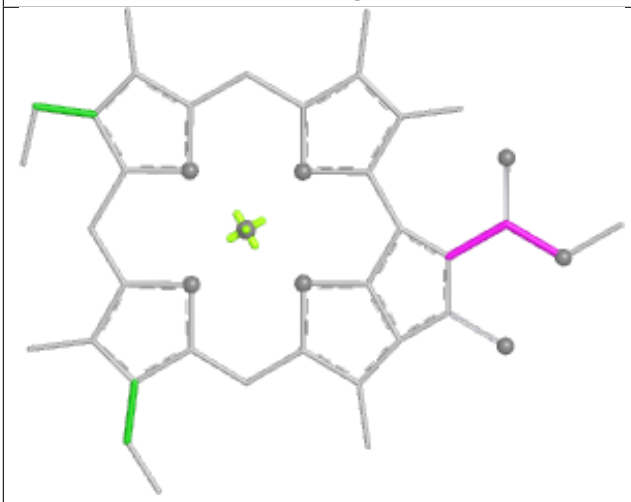
Ligand CLA 4 314



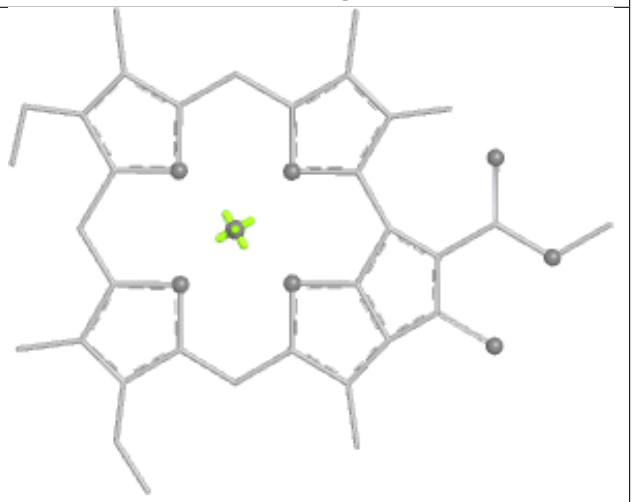
Bond lengths



Bond angles

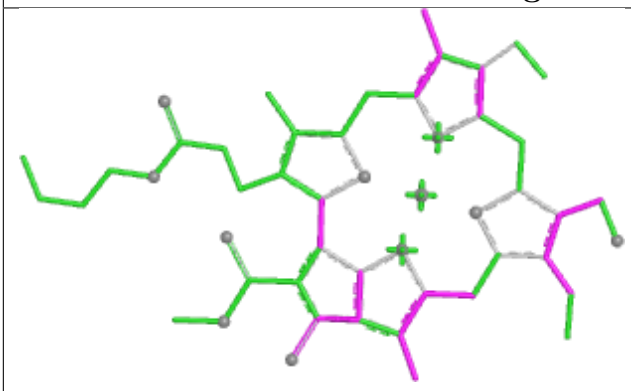


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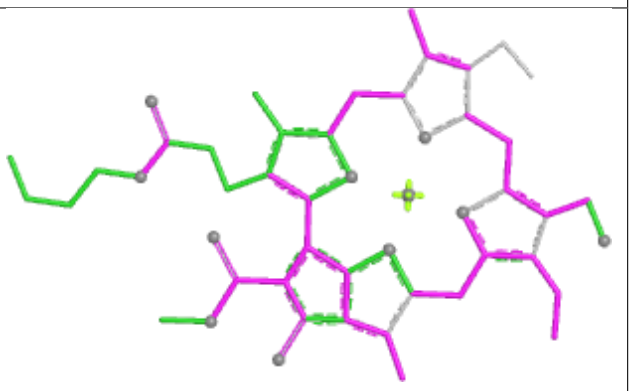


Rings

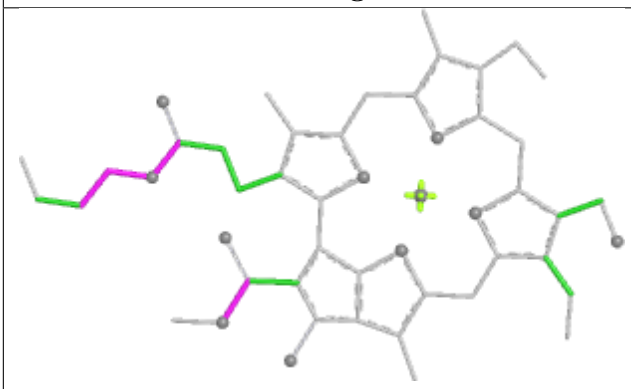
Ligand CHL R 309



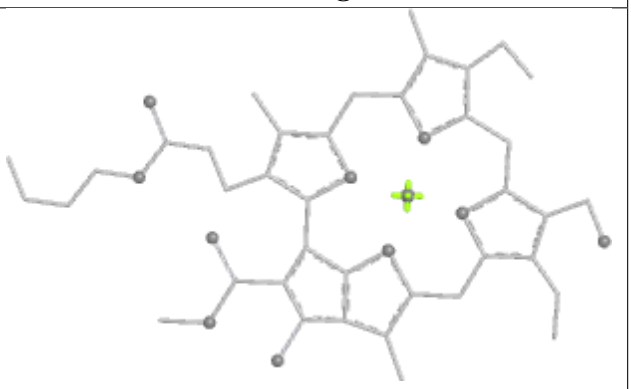
Bond lengths



Bond angles

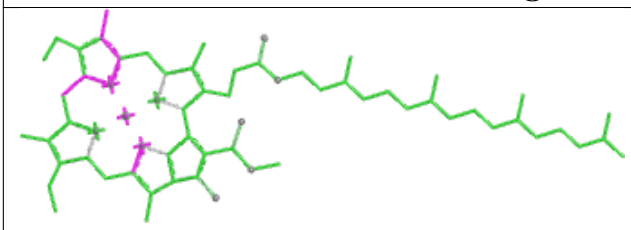


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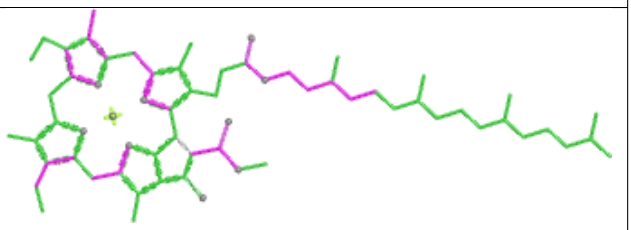


Rings

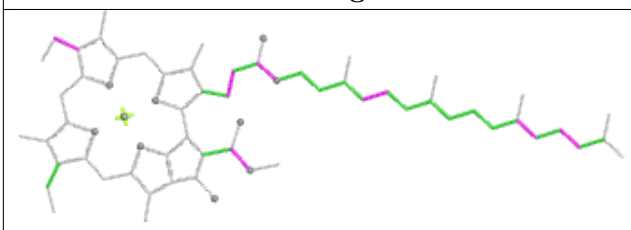
Ligand CLA A 823



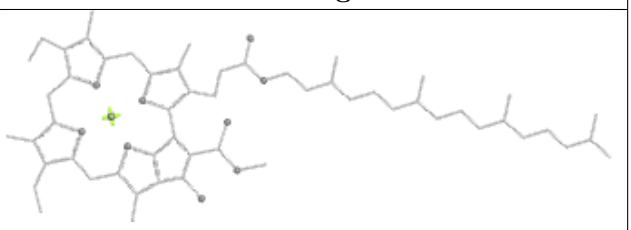
Bond lengths



Bond angles

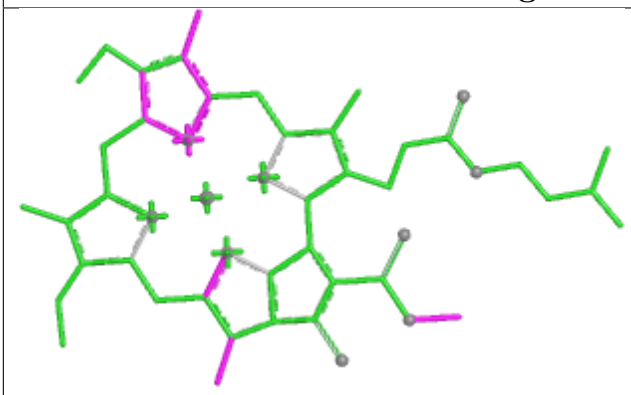


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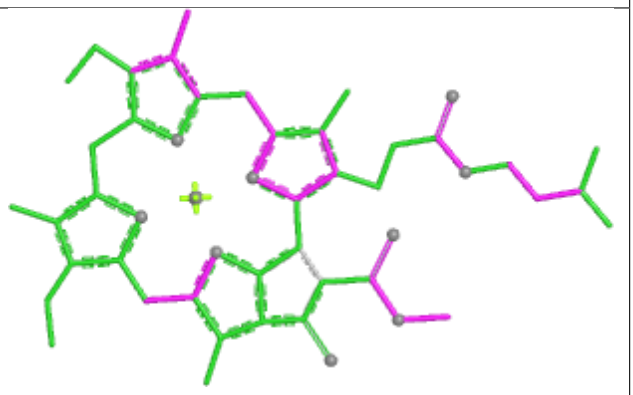


Rings

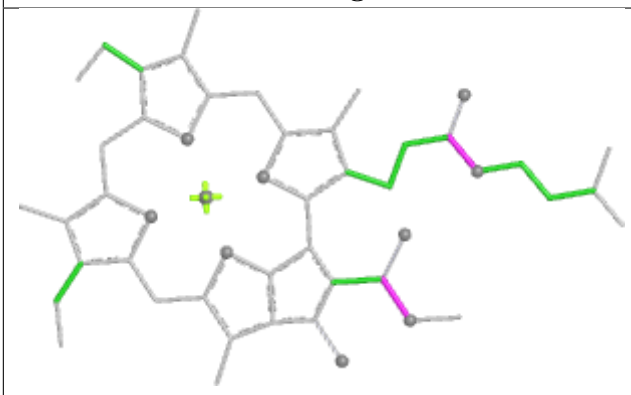
Ligand CLA W 303



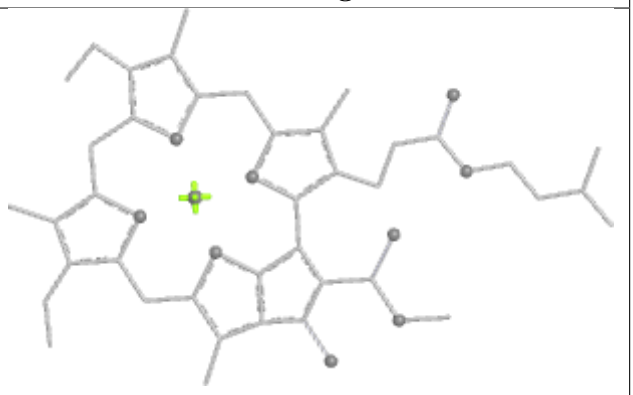
Bond lengths



Bond angles

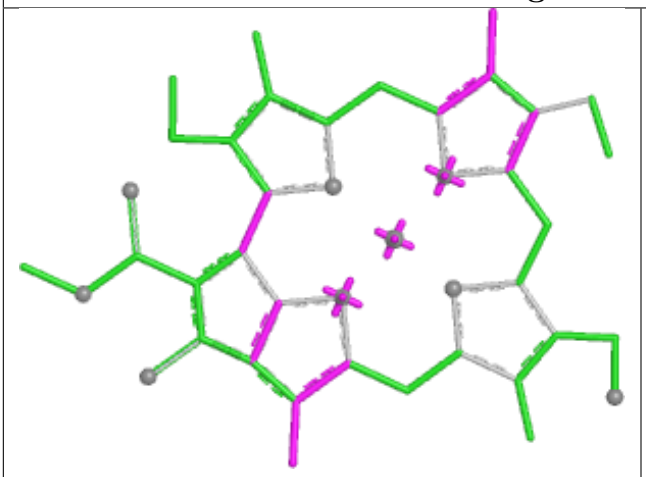


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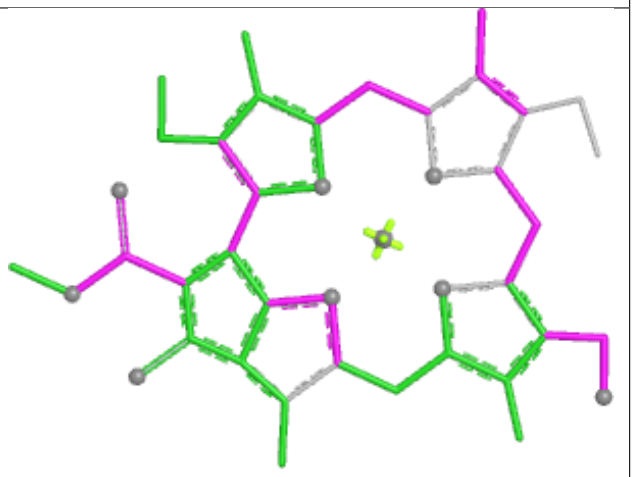


Rings

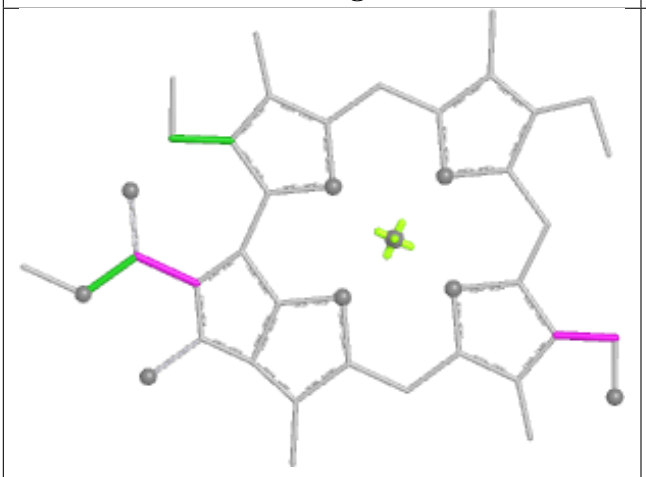
Ligand CHL 6 605



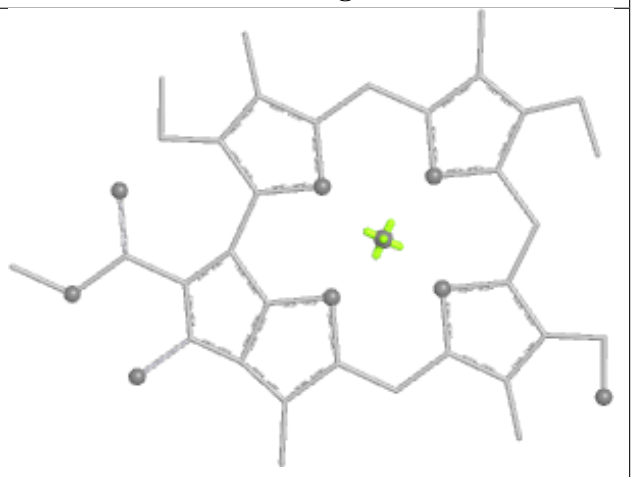
Bond lengths



Bond angles

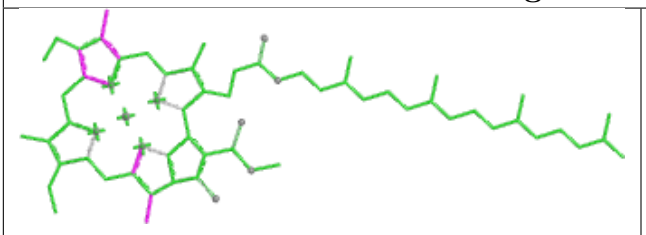


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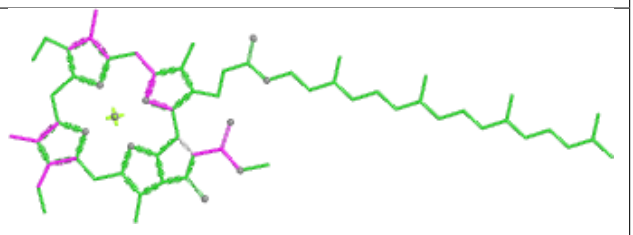


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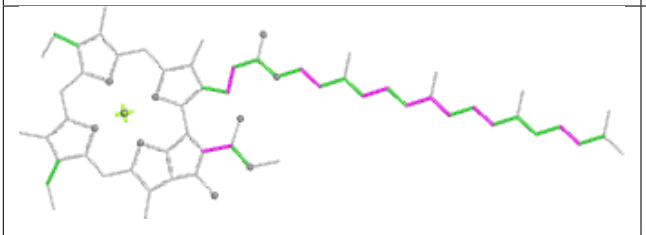
Ligand CLA B 814



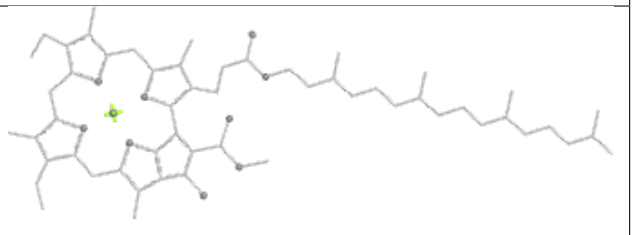
Bond lengths



Bond angles

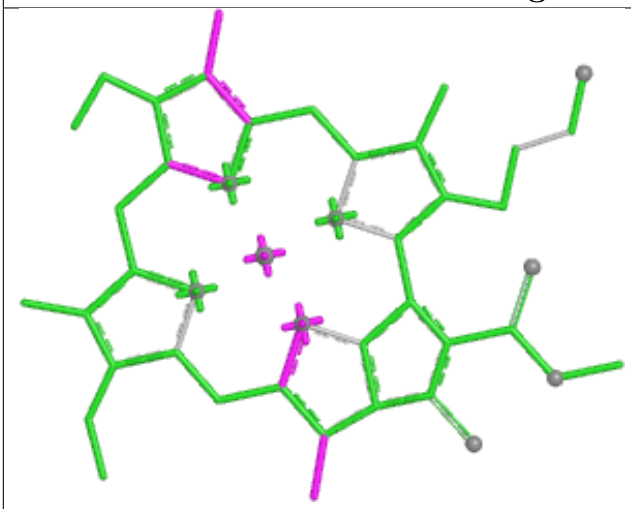


Torsions



Rings

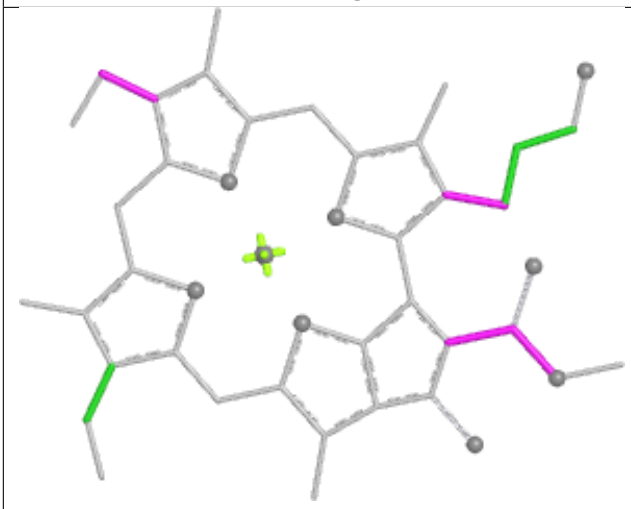
Ligand CLA 2 614



Bond lengths



Bond angles

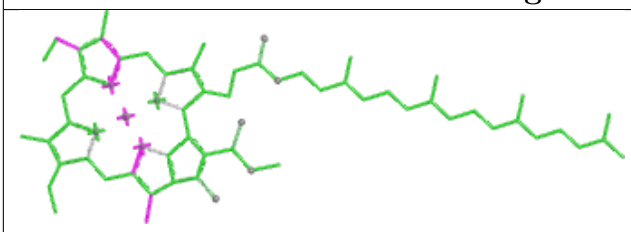


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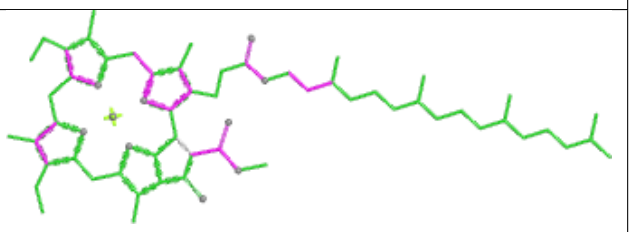


Rings

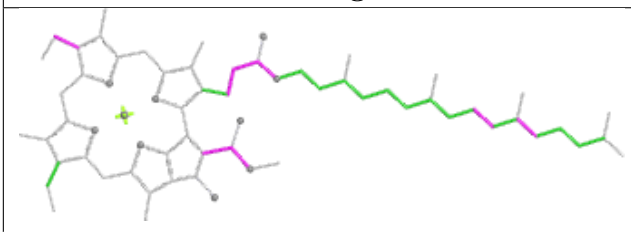
Ligand CLA B 812



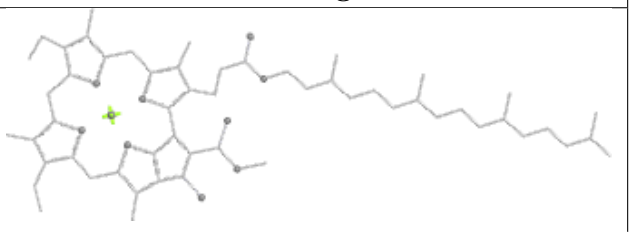
Bond lengths



Bond angles

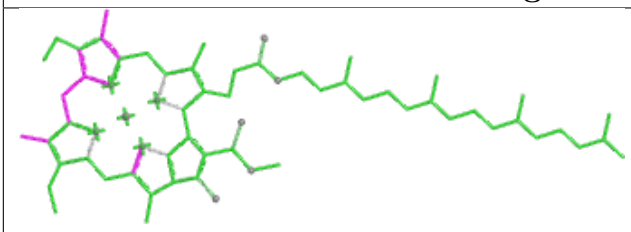


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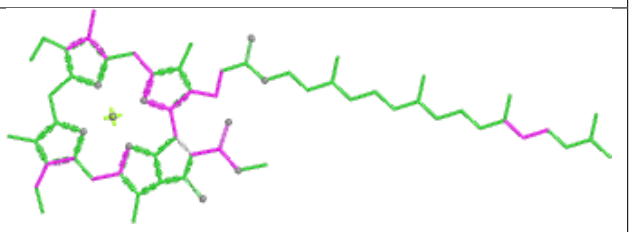


Rings

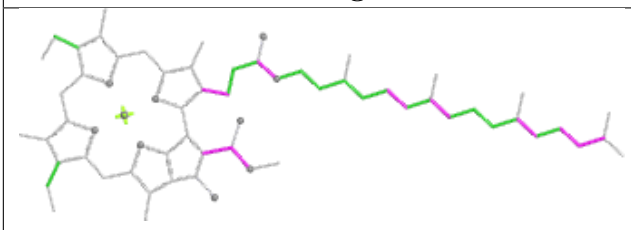
Ligand CLA A 821



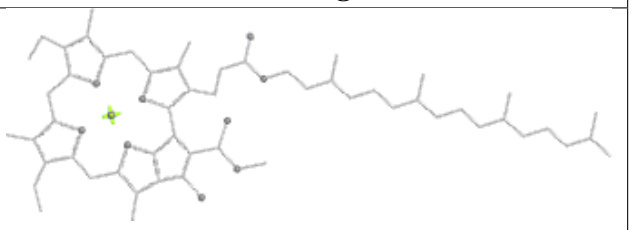
Bond lengths



Bond angles

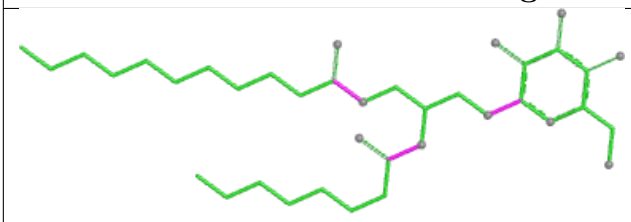


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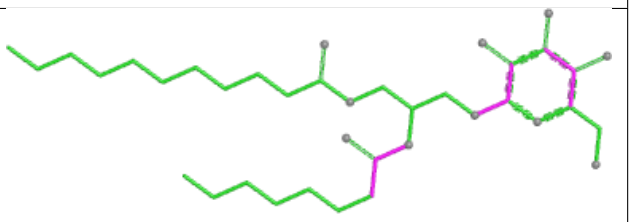


Rings

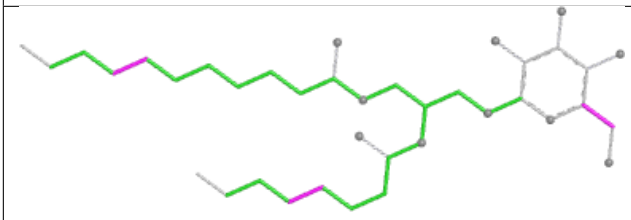
Ligand LMG B 801



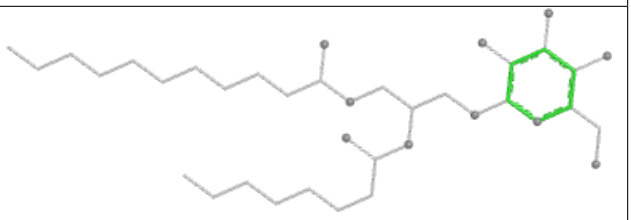
Bond lengths



Bond angles

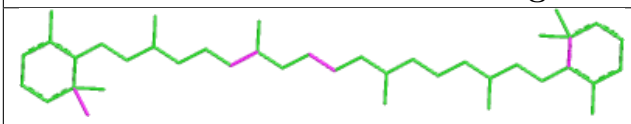


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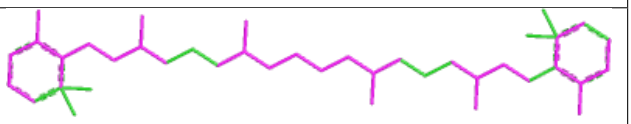


Rings

Ligand BCR I 101



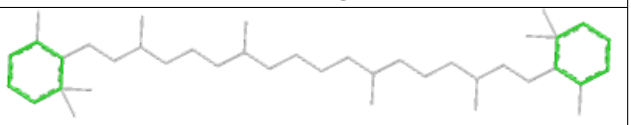
Bond lengths



Bond angles

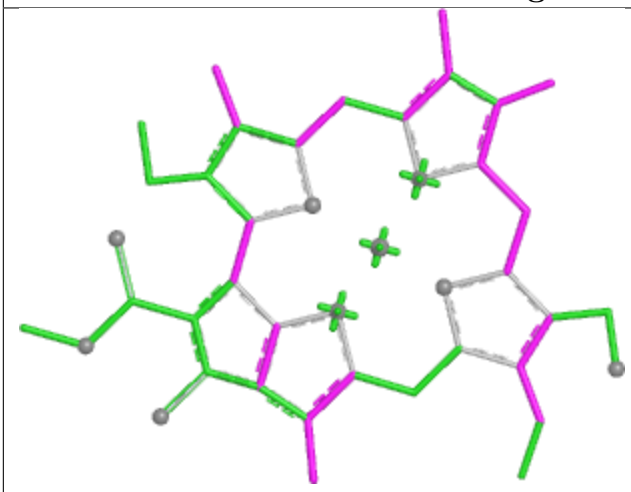


Torsions



Rings

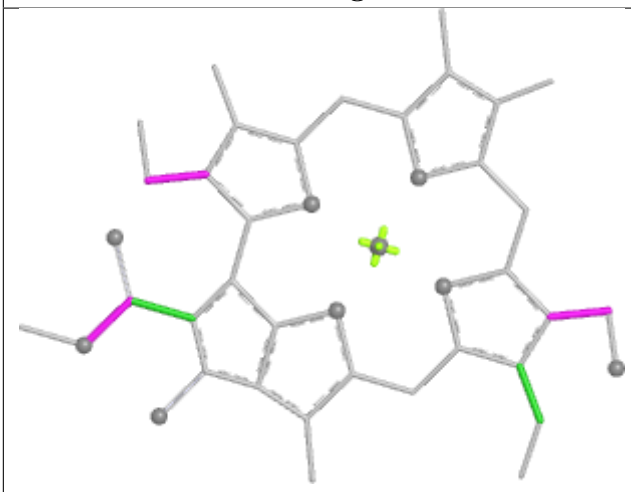
Ligand CHL 4 307



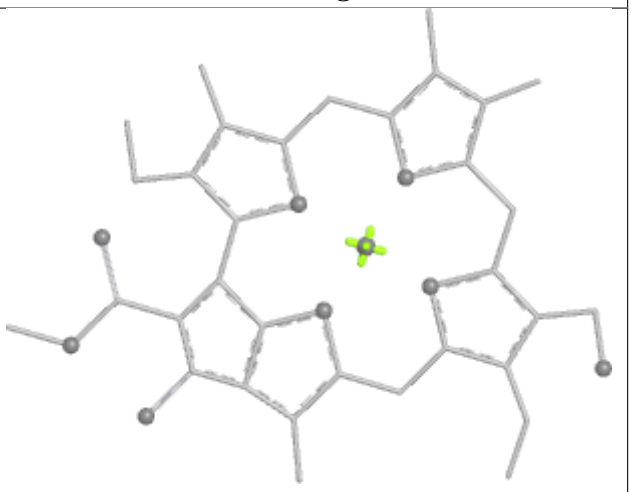
Bond lengths



Bond angles

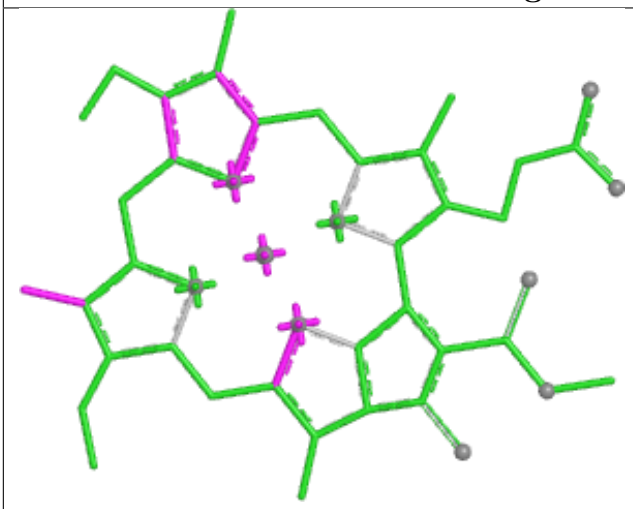


Torsions

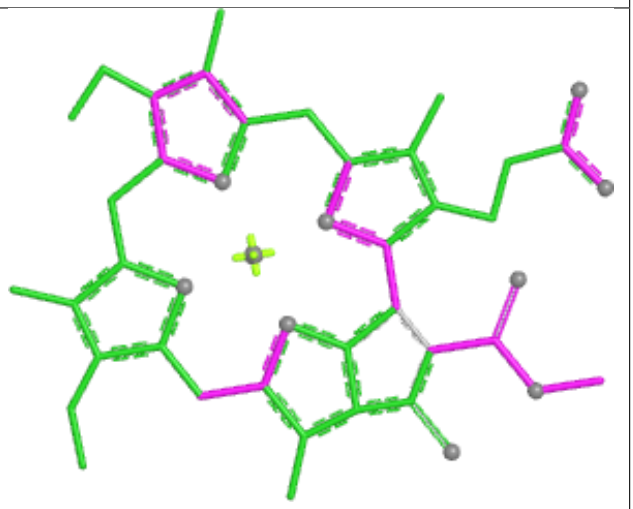


Rings

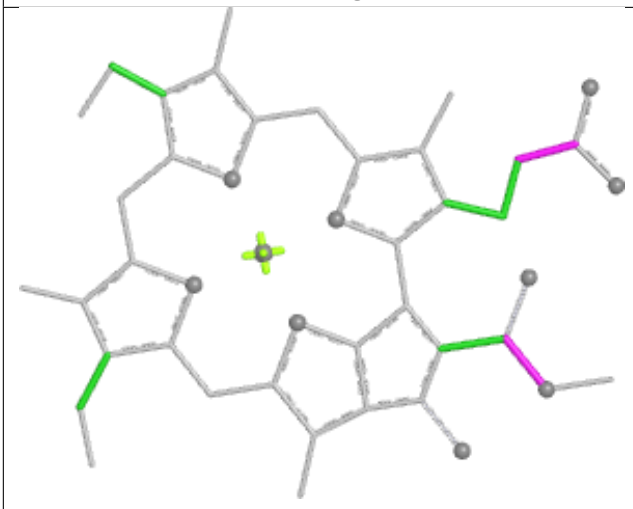
Ligand CLA B 825



Bond lengths



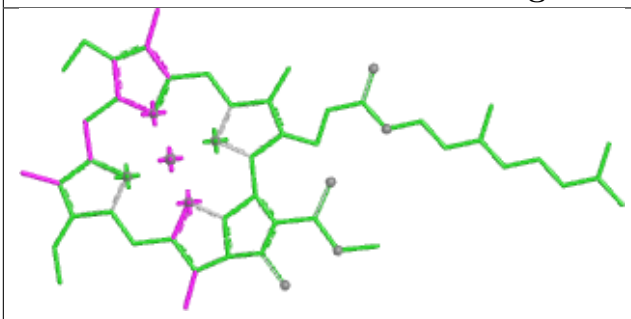
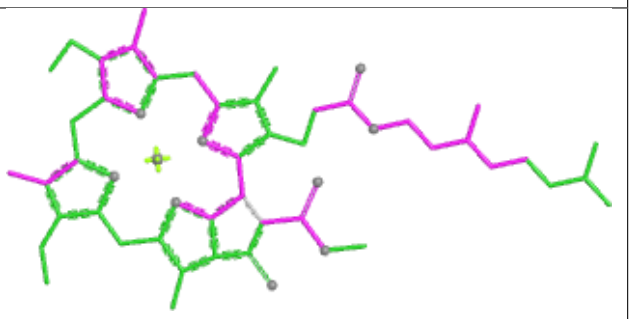
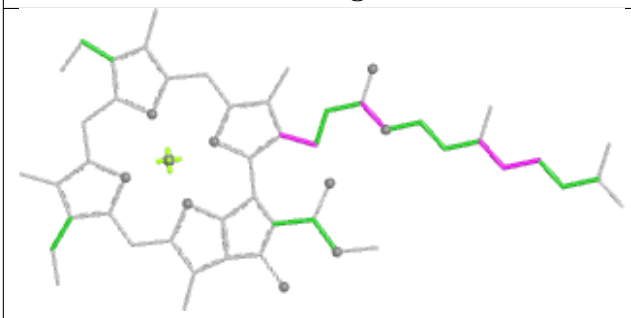
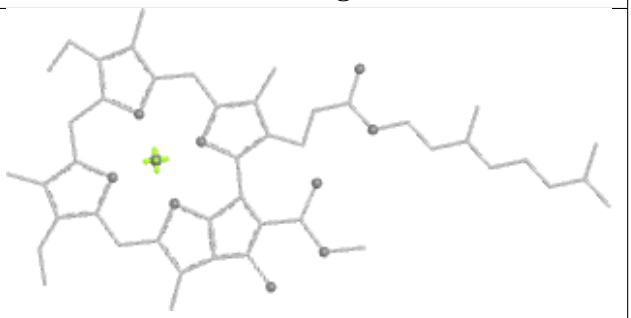
Bond angles

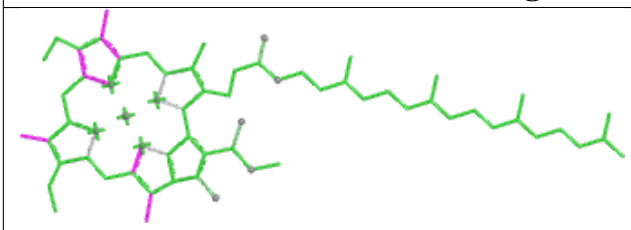
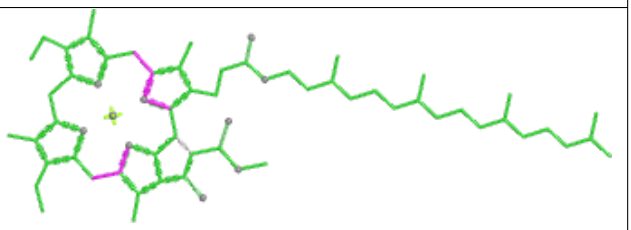
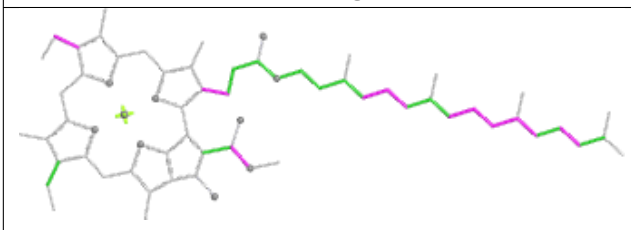
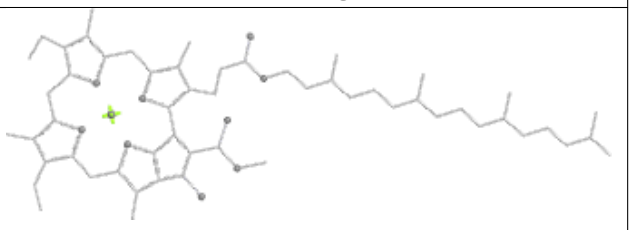


Torsions

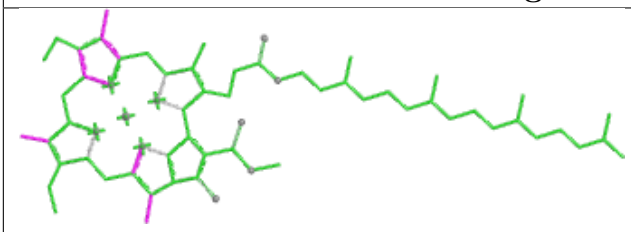


Rings

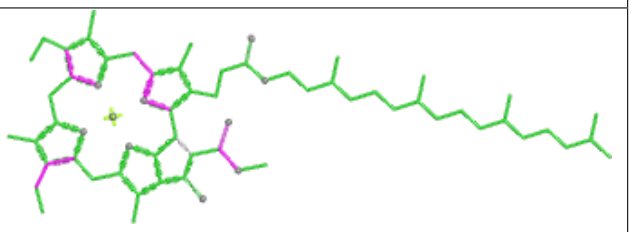
Ligand CLA 3 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

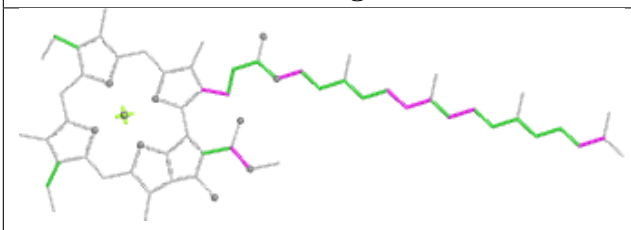
Ligand CLA T 302



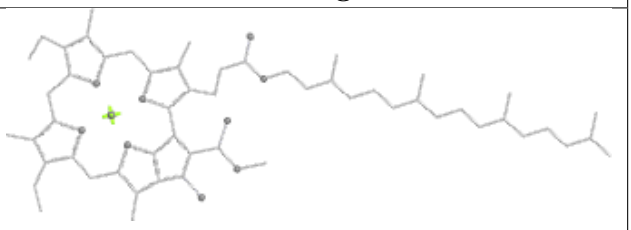
Bond lengths



Bond angles



Torsions



Rings

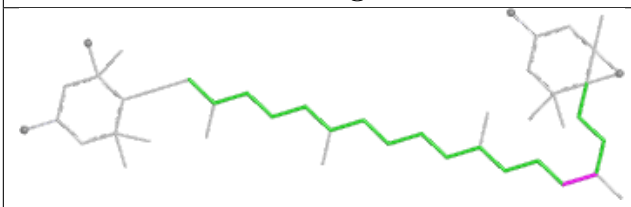
Ligand NEX W 317



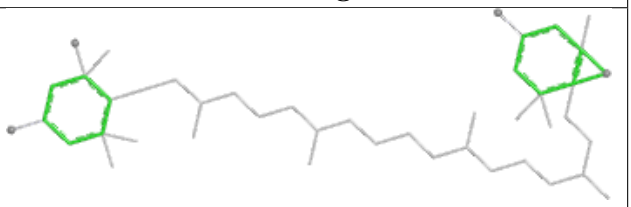
Bond lengths



Bond angles

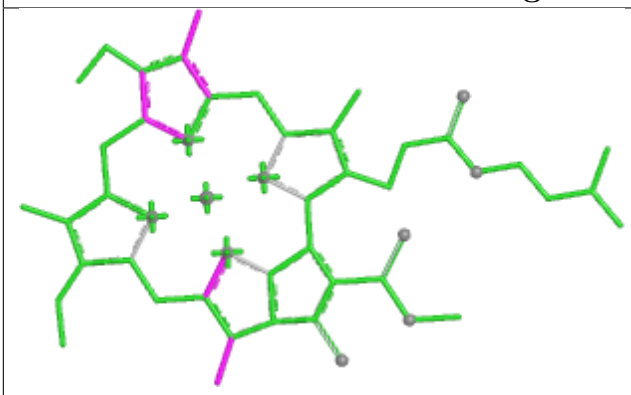


Torsions

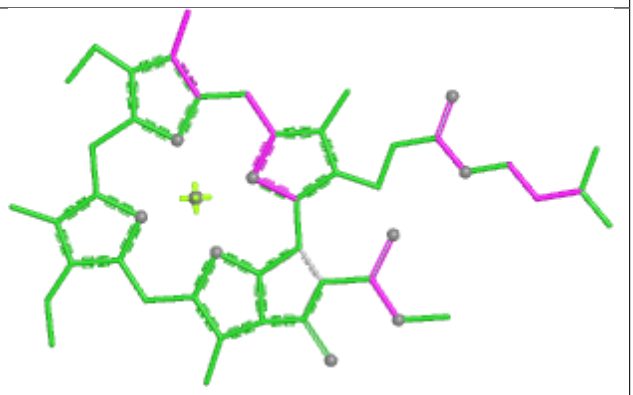


Rings

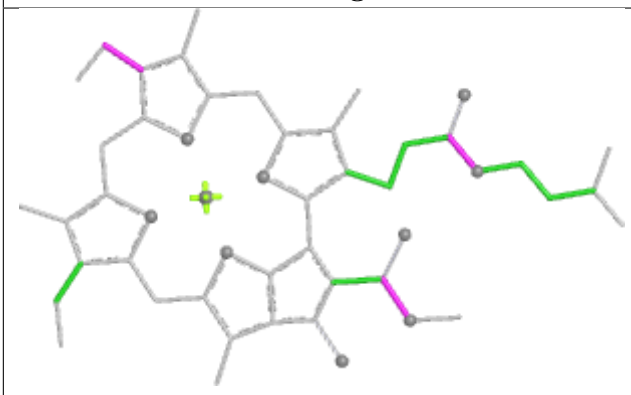
Ligand CLA U 303



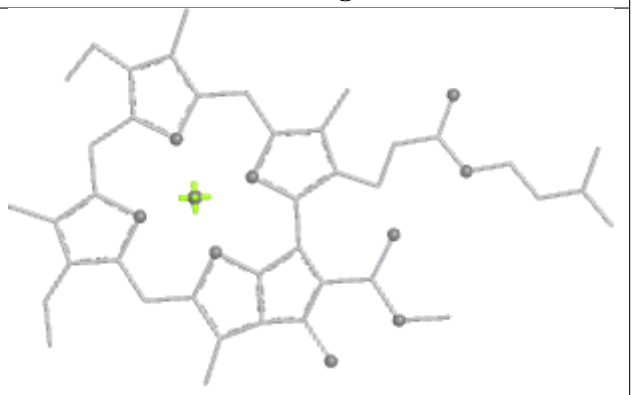
Bond lengths



Bond angles

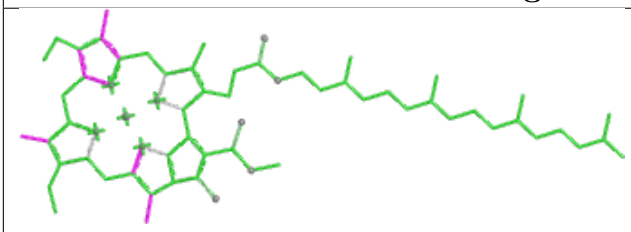


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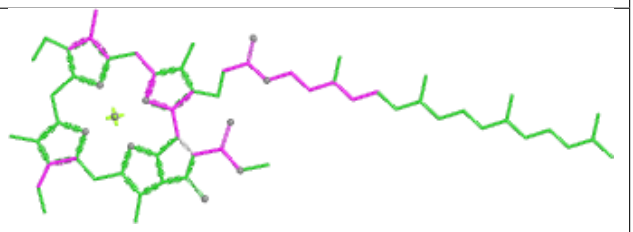


Rings

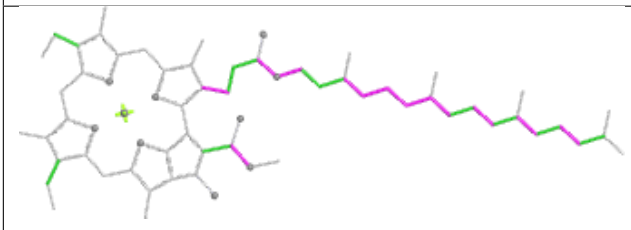
Ligand CLA A 830



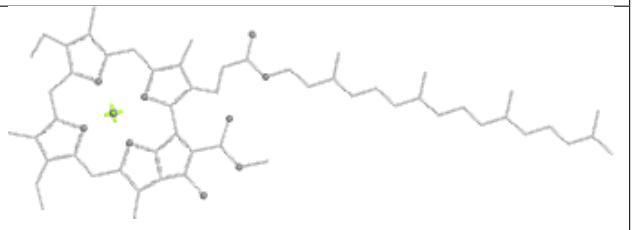
Bond lengths



Bond angles

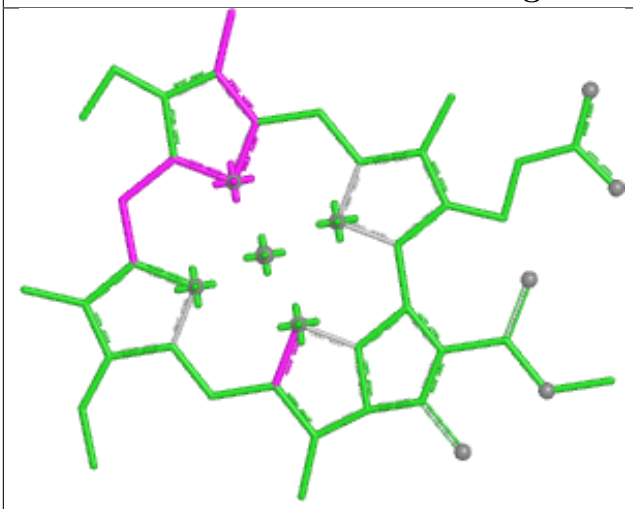


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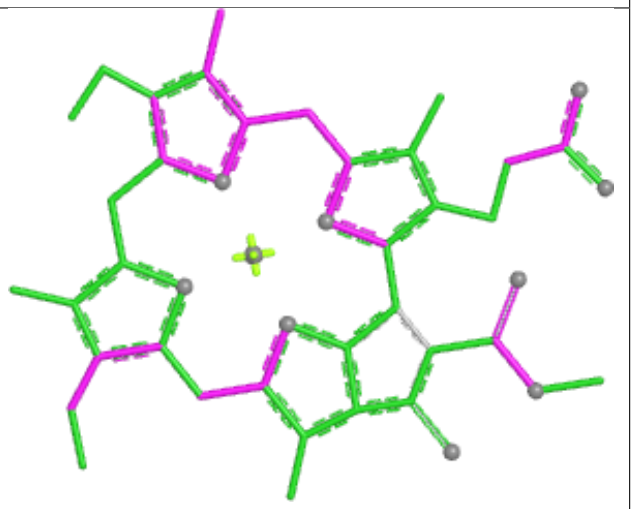


Rings

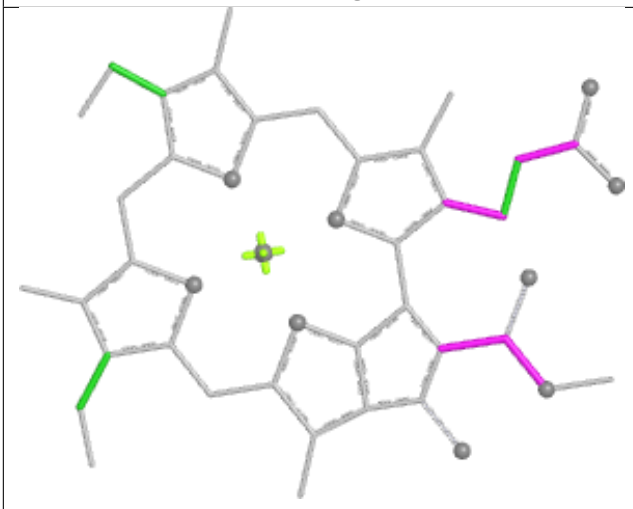
Ligand CLA G 204



Bond lengths



Bond angles

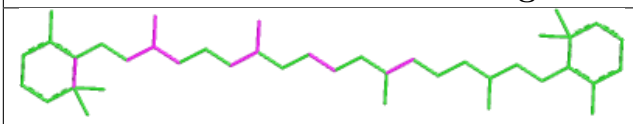


Torsions

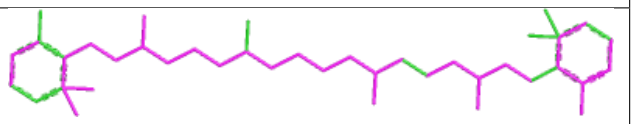


Rings

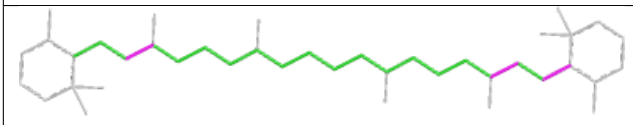
Ligand BCR M 101



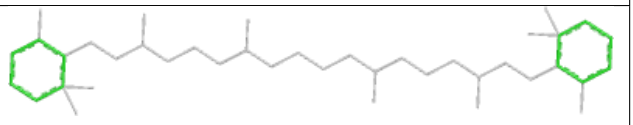
Bond lengths



Bond angles

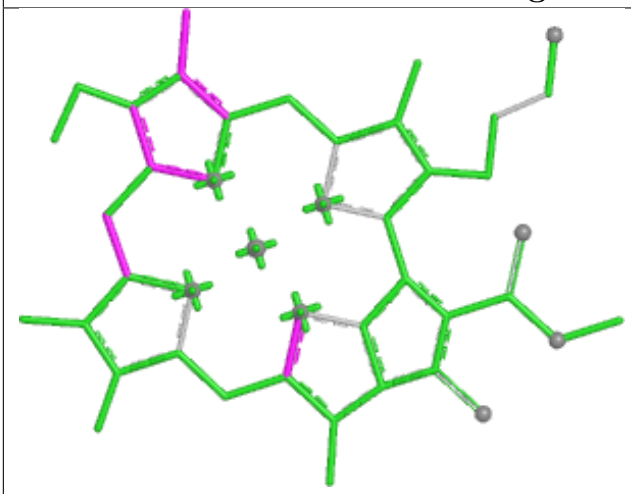


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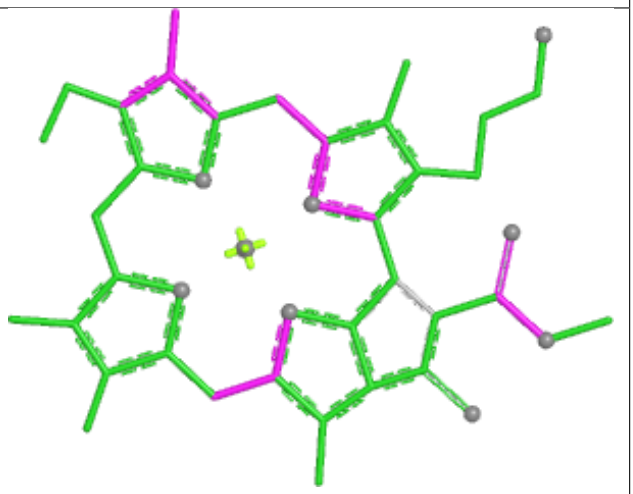


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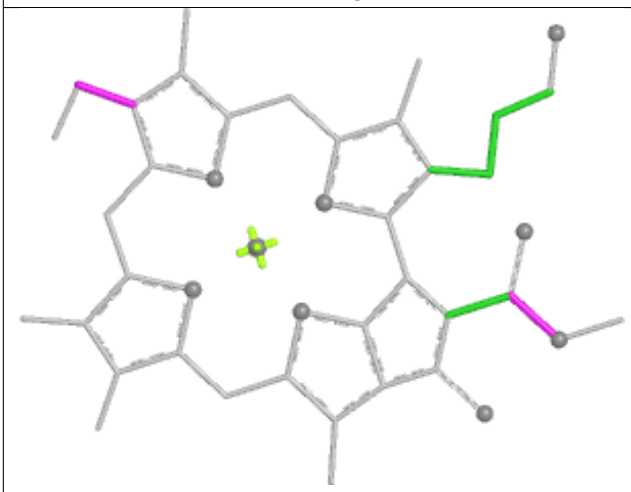
Ligand CLA 6 604



Bond lengths



Bond angles

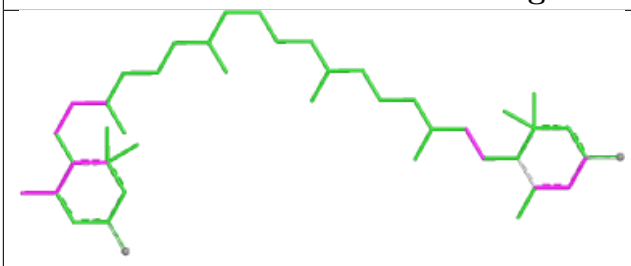


Torsions

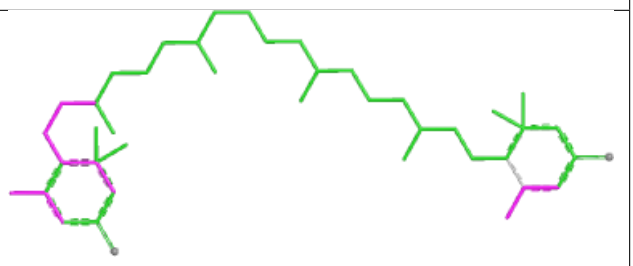


Rings

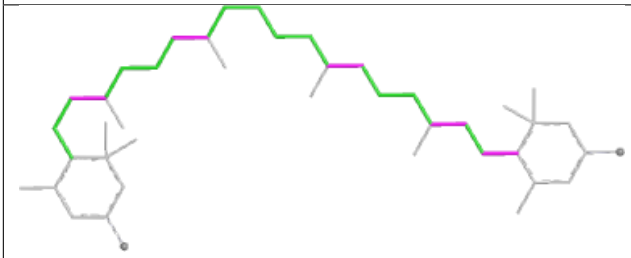
Ligand Q6L R 319



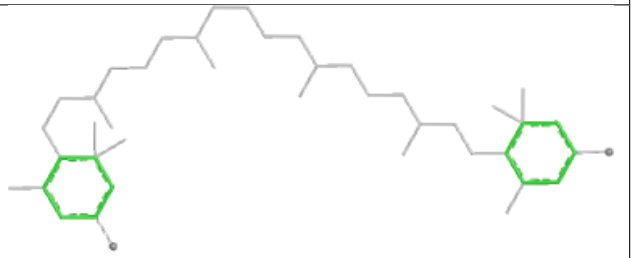
Bond lengths



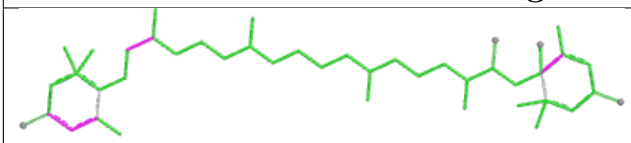
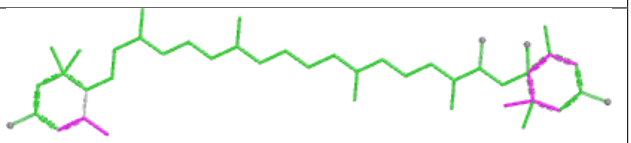
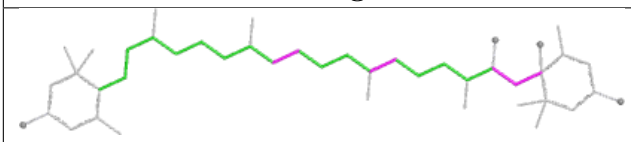
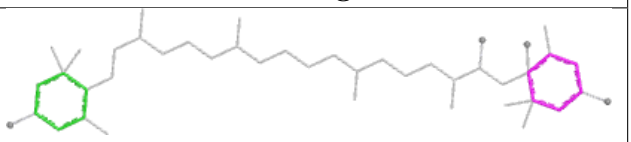
Bond angles

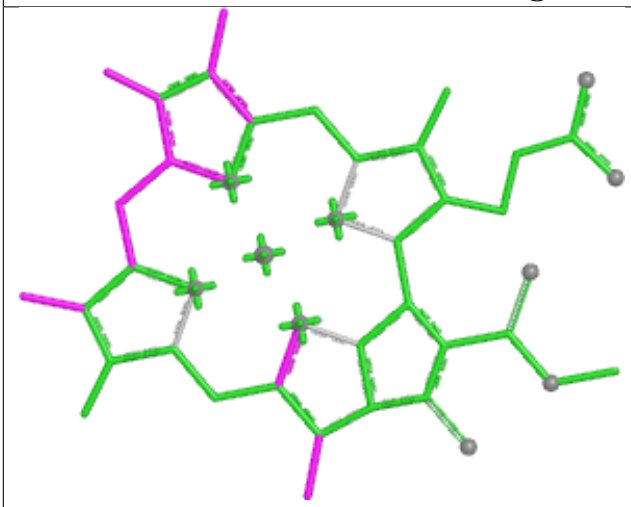
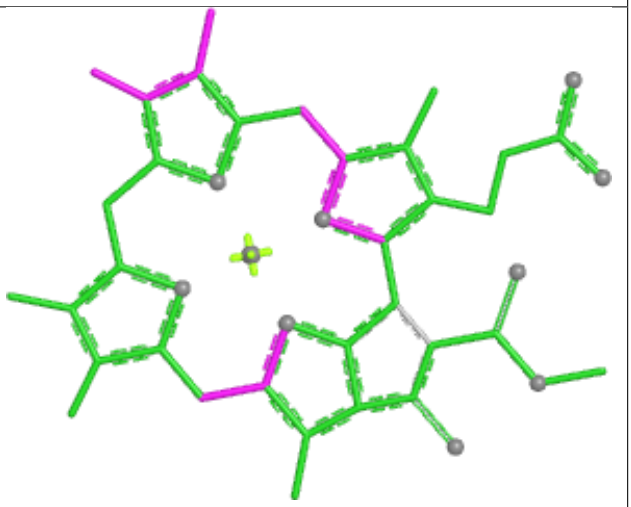
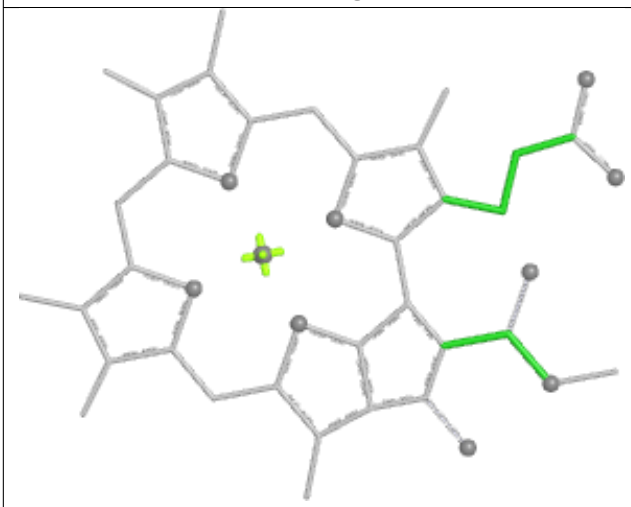


Torsions

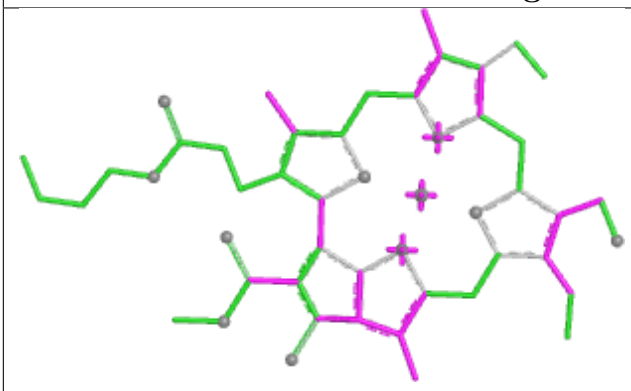


Rings

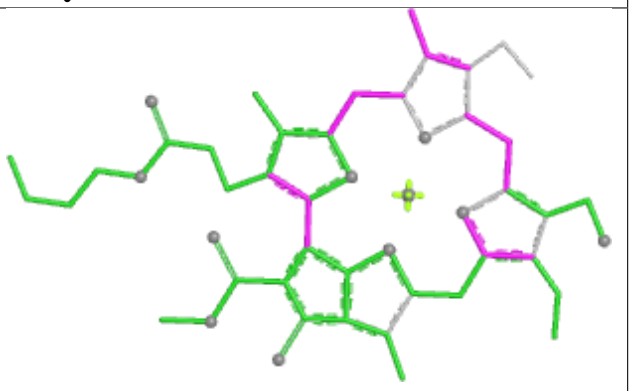
Ligand IWJ R 322	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

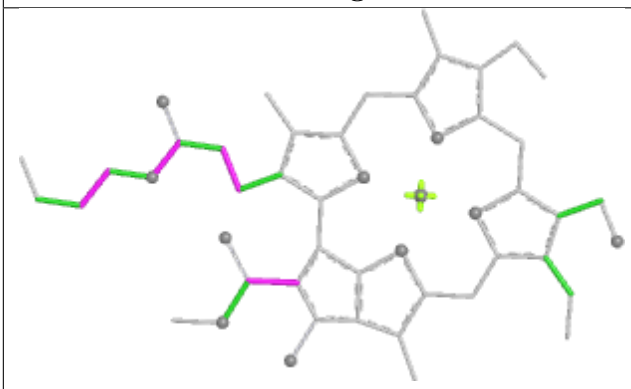
Ligand CHL Q 308



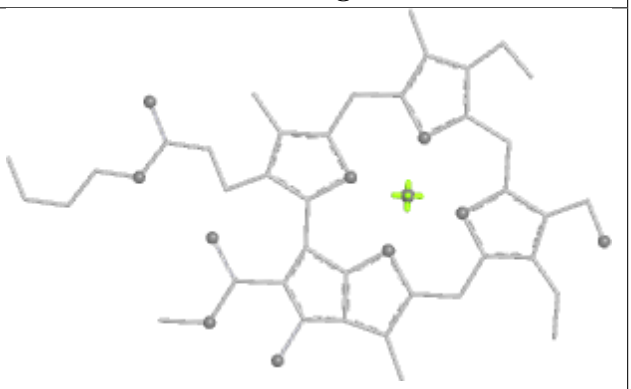
Bond lengths



Bond angles

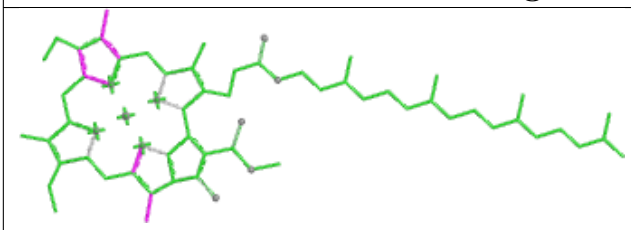


Torsions

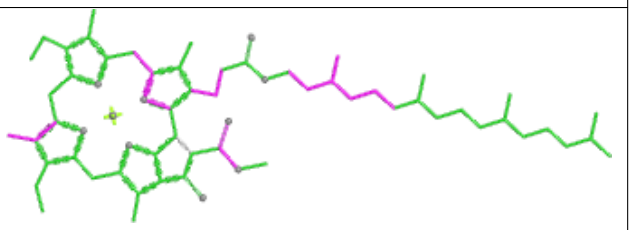


Rings

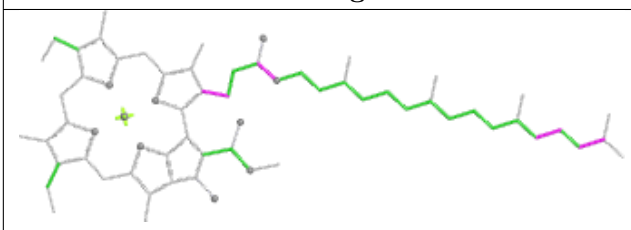
Ligand CLA A 843



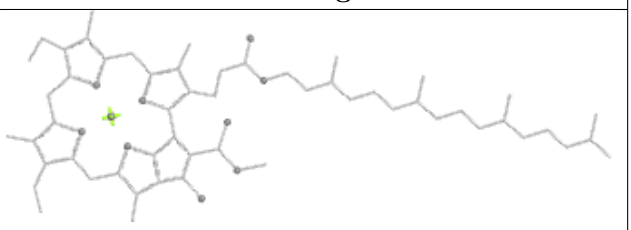
Bond lengths



Bond angles

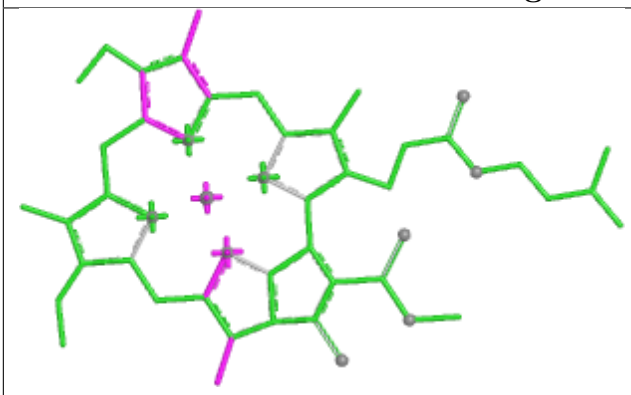


Torsions

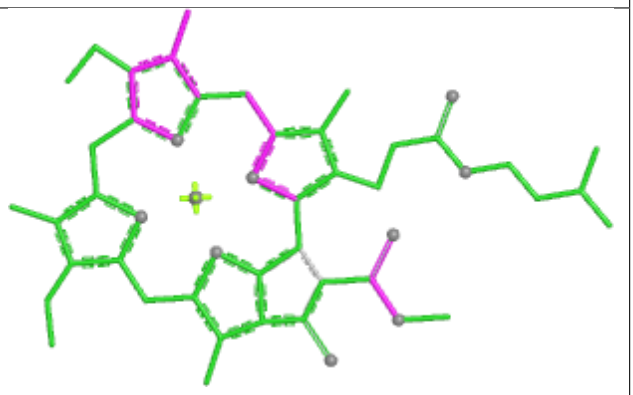


Rings

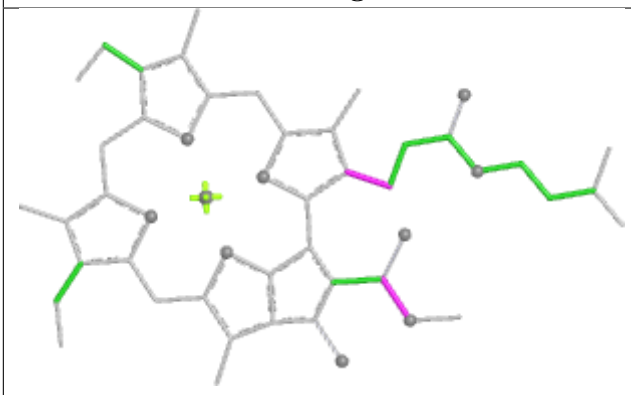
Ligand CLA T 303



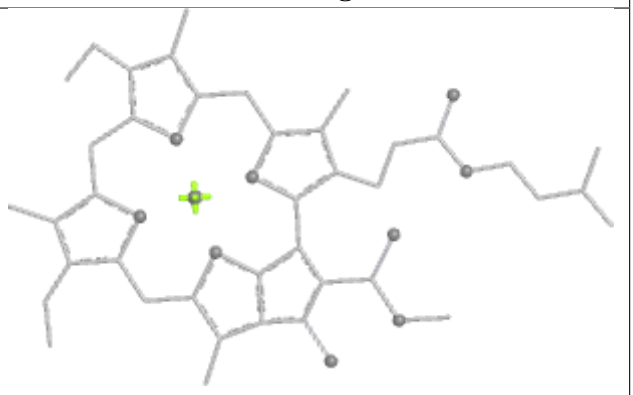
Bond lengths



Bond angles

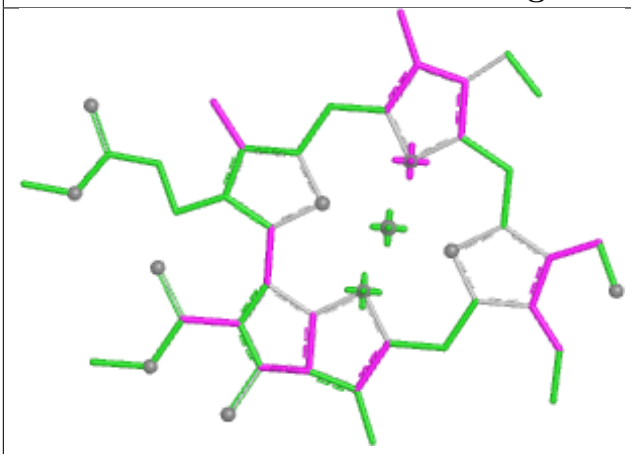


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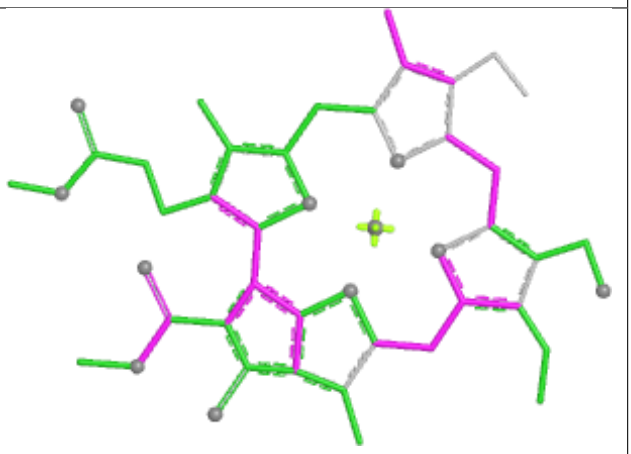


Rings

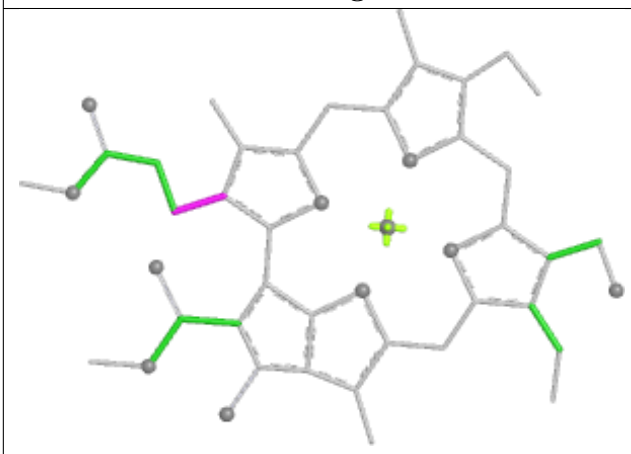
Ligand CHL 2 601



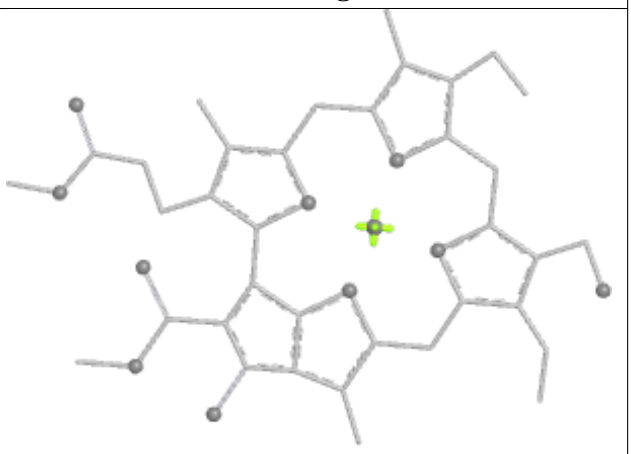
Bond lengths



Bond angles

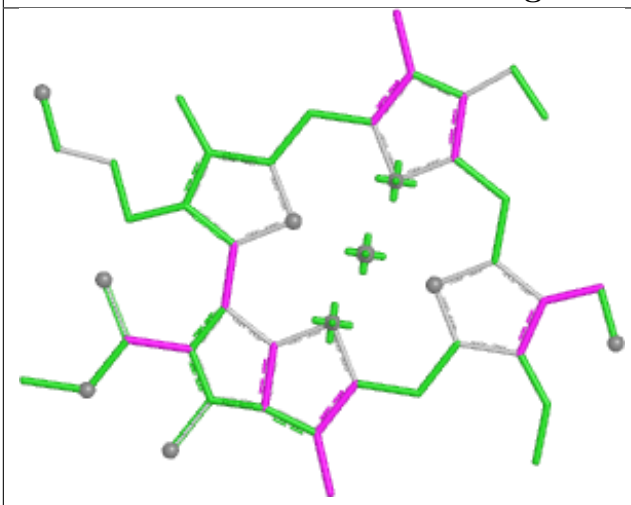


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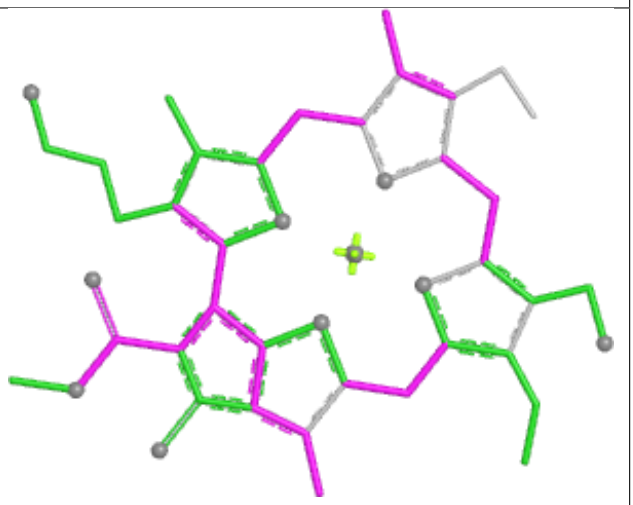


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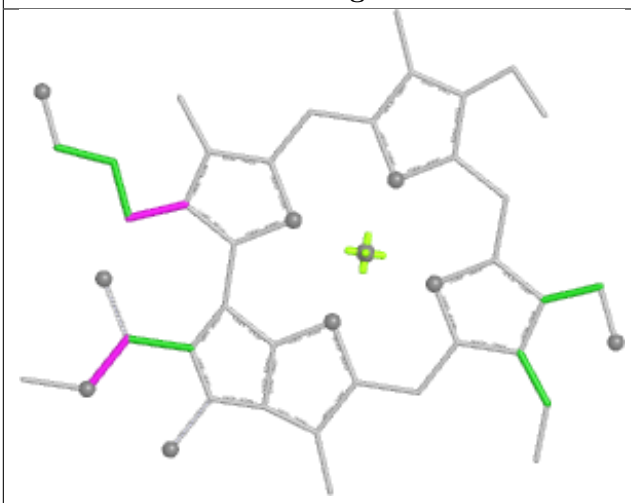
Ligand CHL P 314



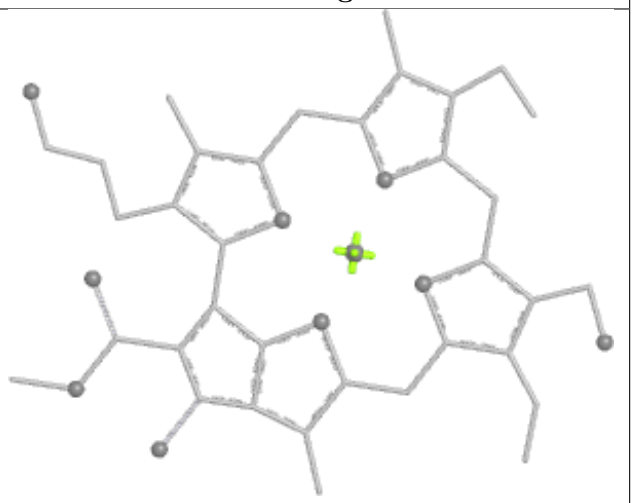
Bond lengths



Bond angles

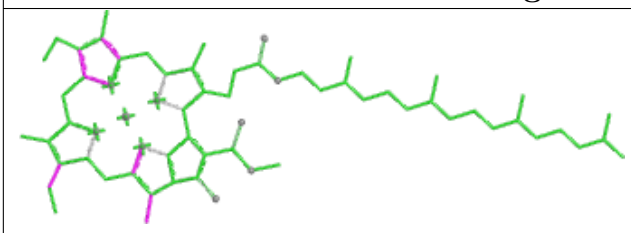


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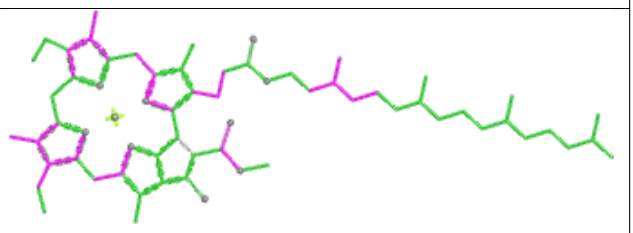


Rings

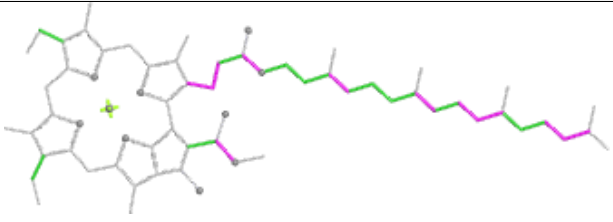
Ligand CLA A 825



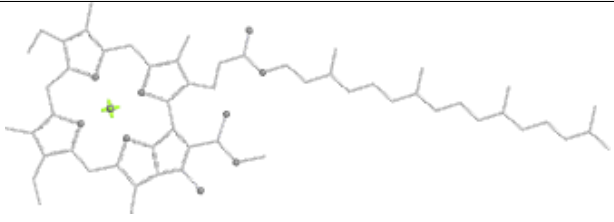
Bond lengths



Bond angles

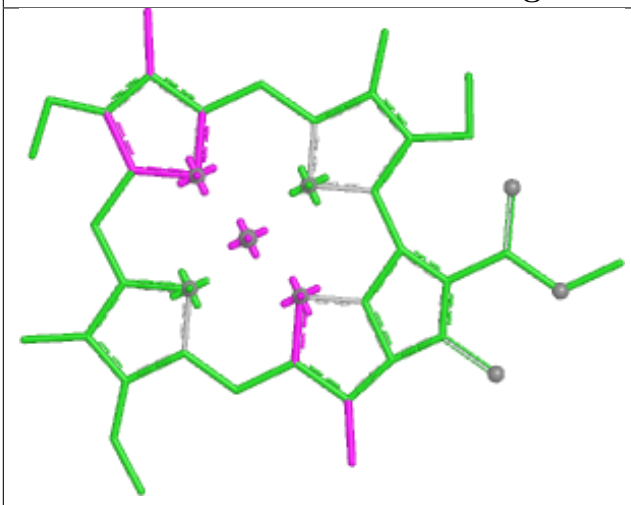


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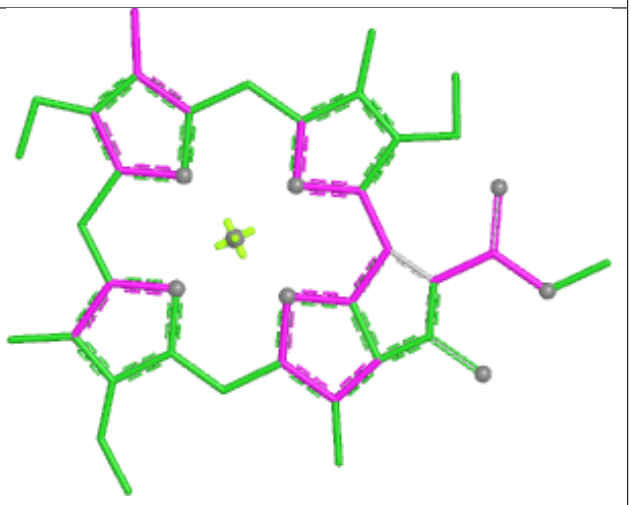


Rings

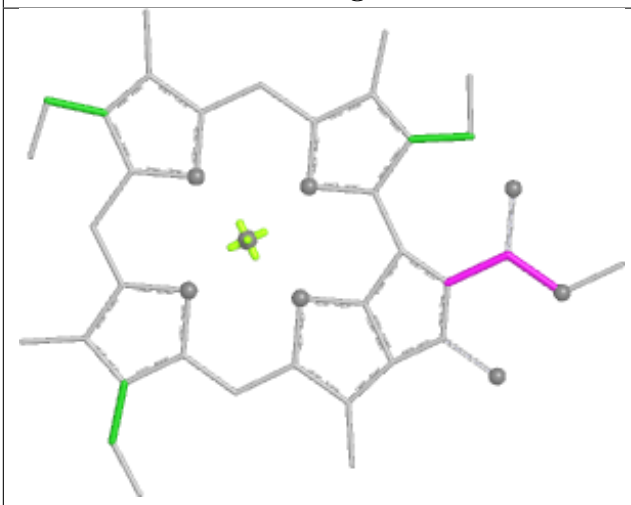
Ligand CLA N 203



Bond lengths



Bond angles

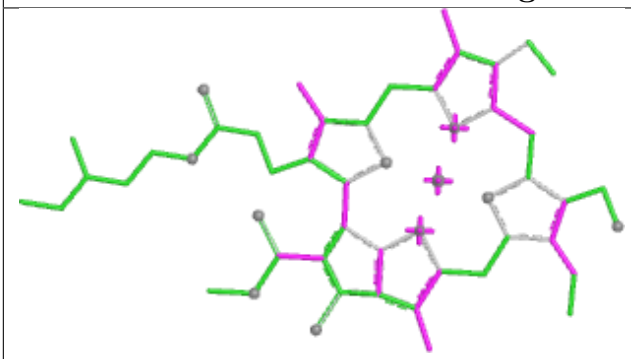


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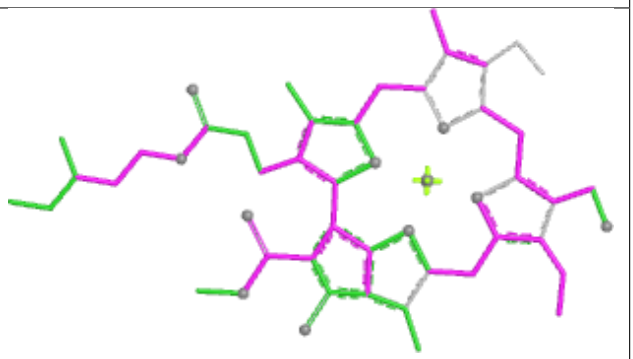


Rings

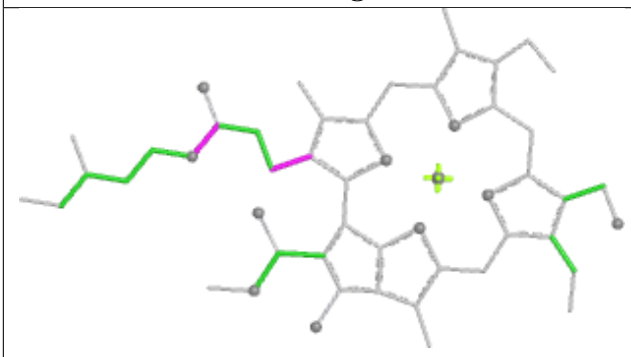
Ligand CHL W 306



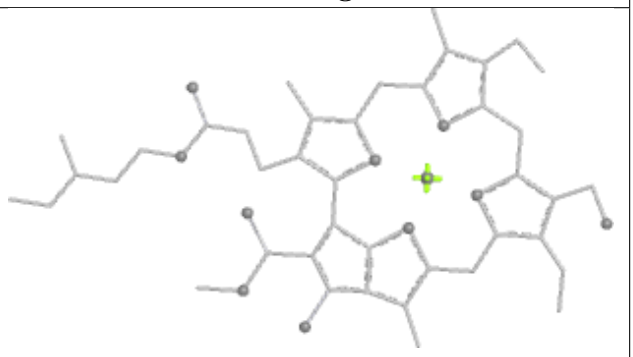
Bond lengths



Bond angles

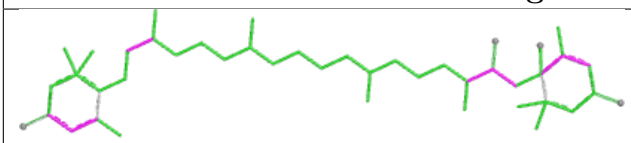


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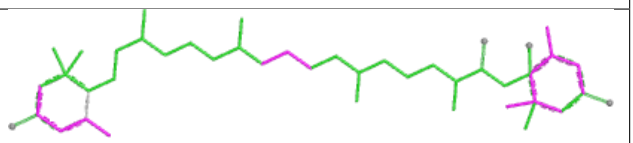


Rings

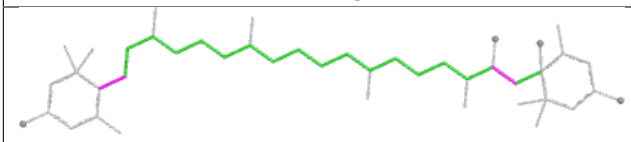
Ligand IWJ U 316



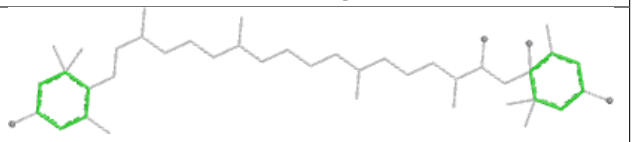
Bond lengths



Bond angles

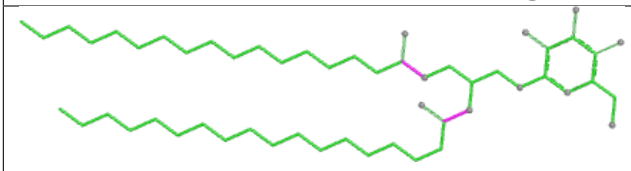


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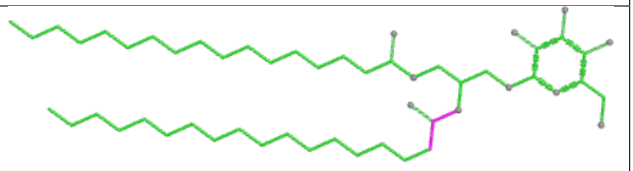


Rings

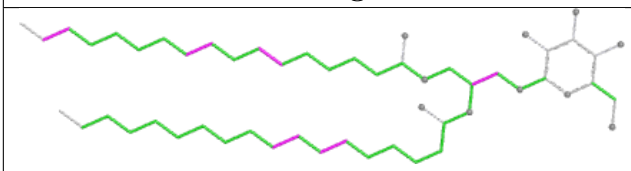
Ligand LMG 5 613



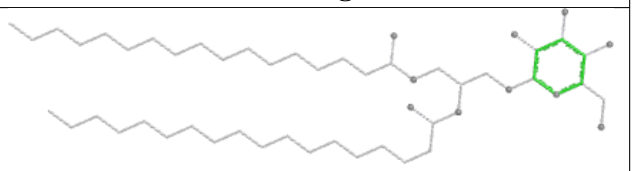
Bond lengths



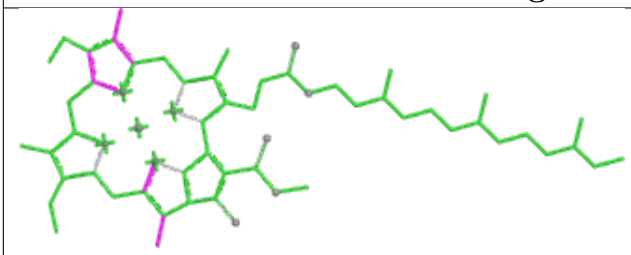
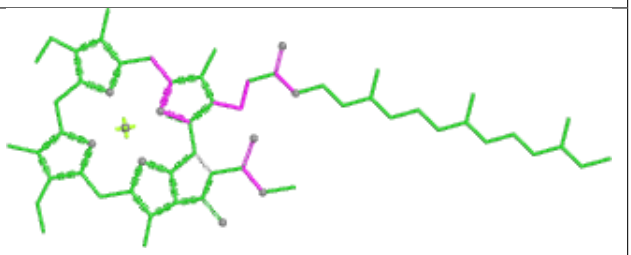
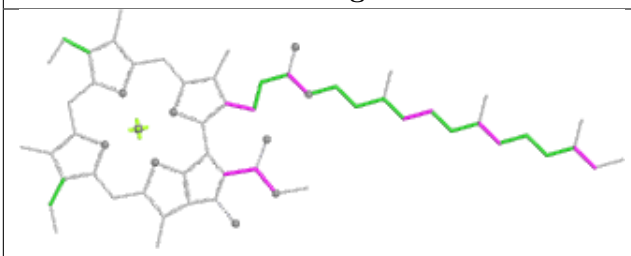
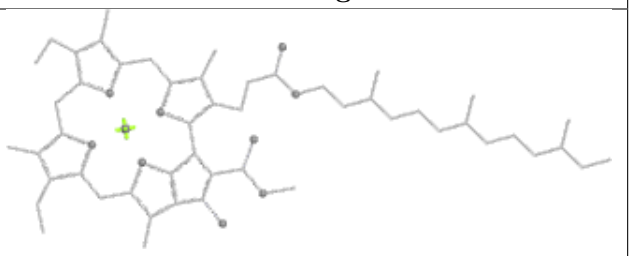
Bond angles

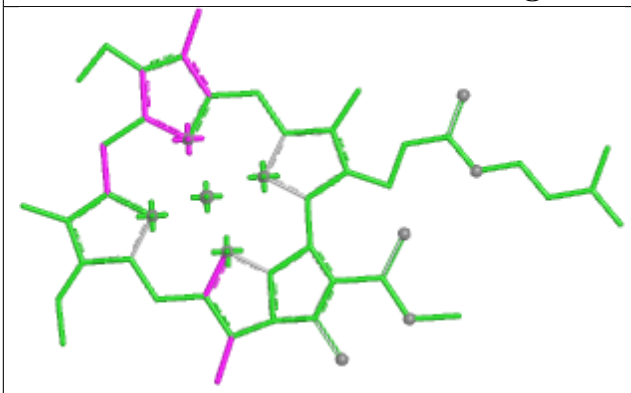
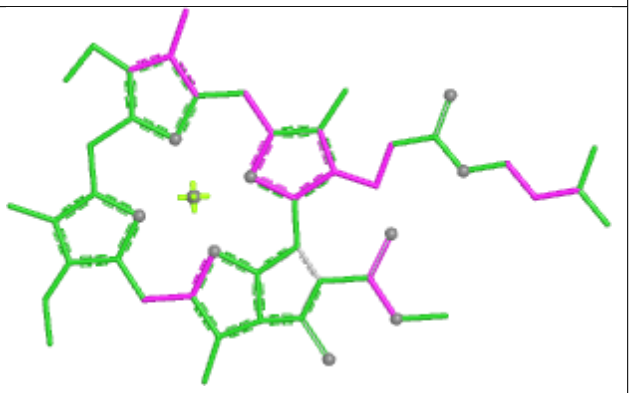
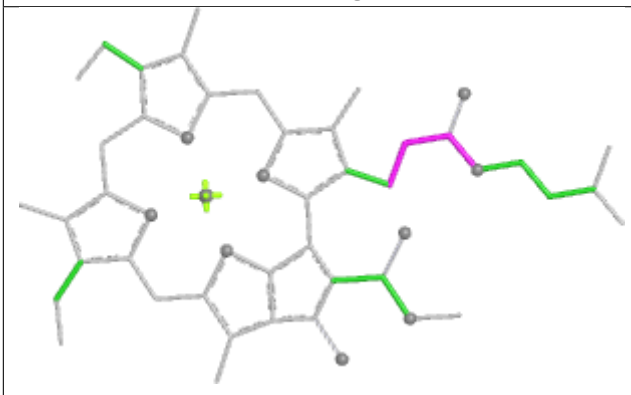
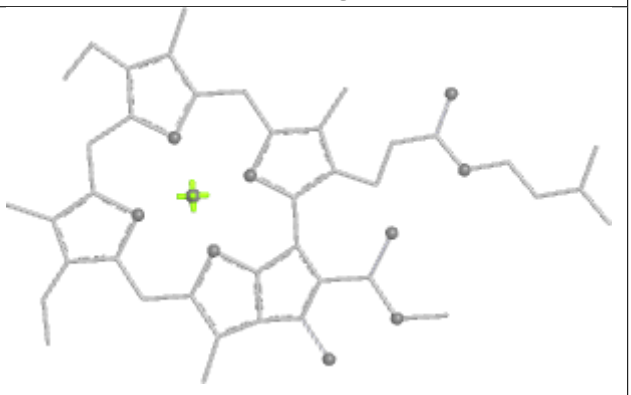


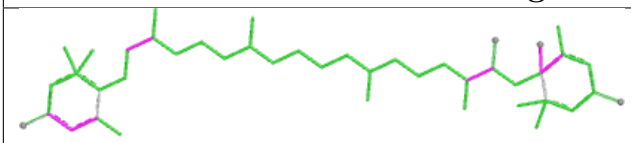
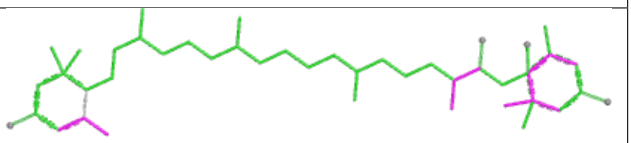
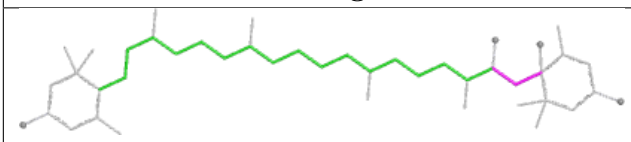
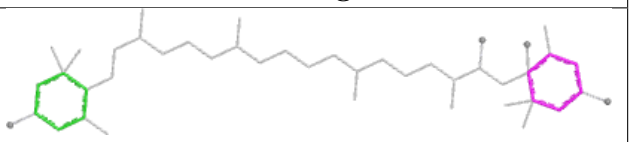
Torsions

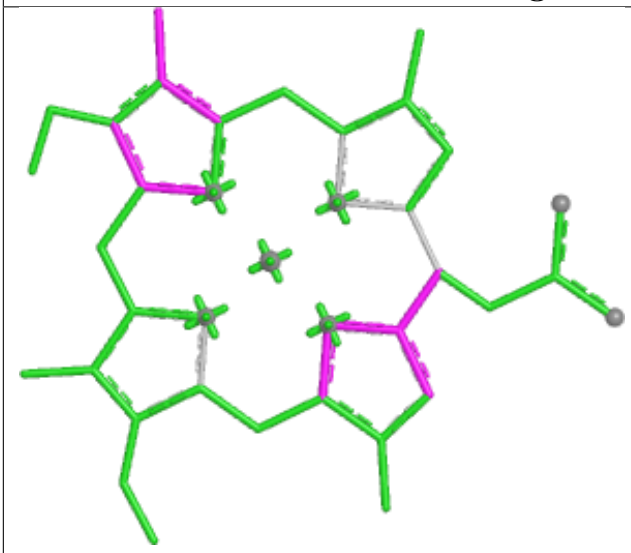
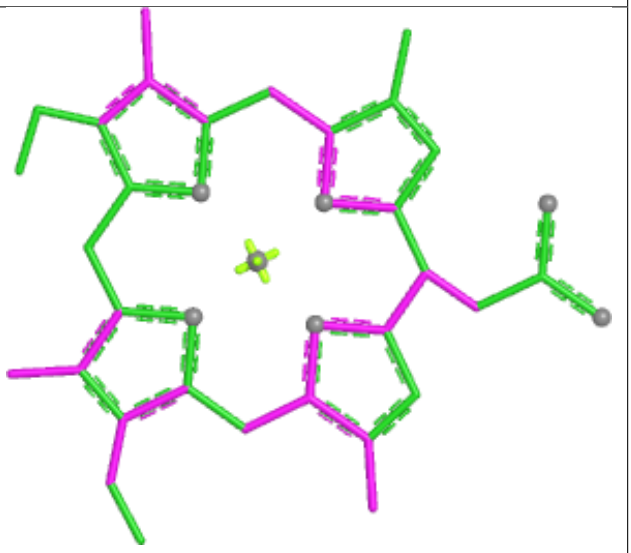
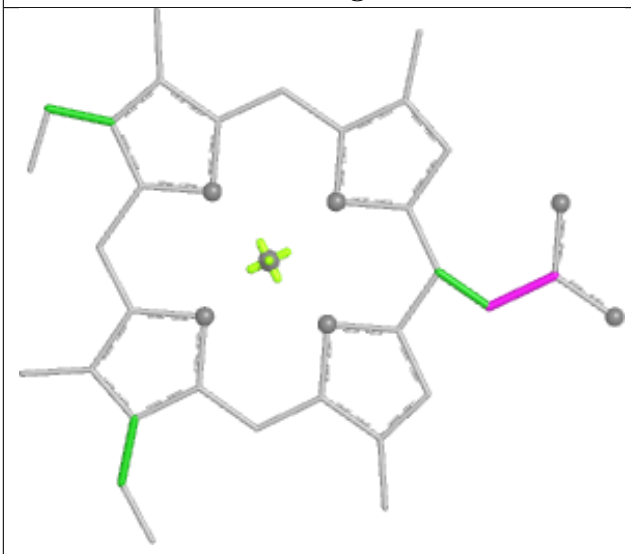
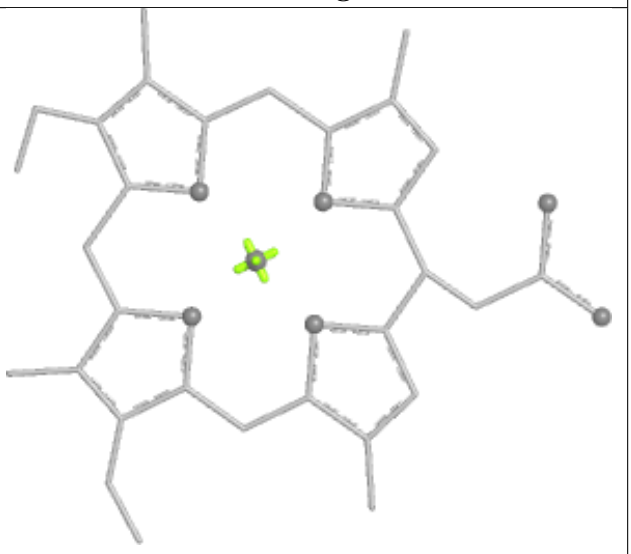


Rings

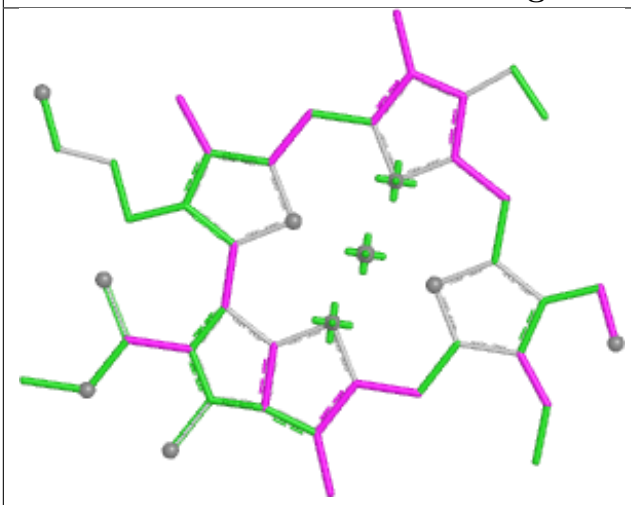
Ligand CLA 6 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

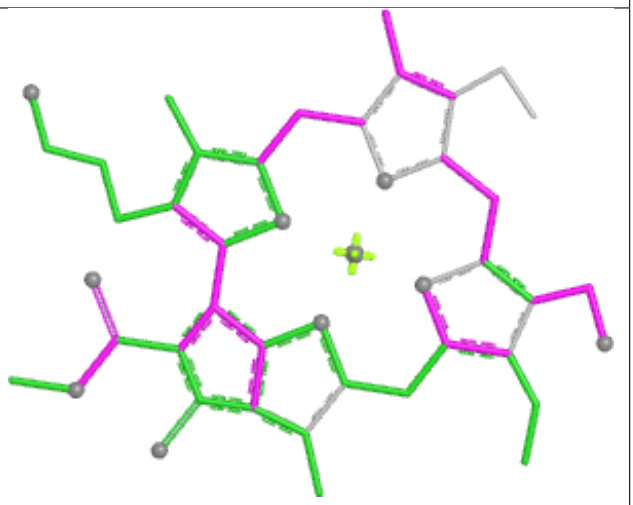
Ligand IWJ T 321	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

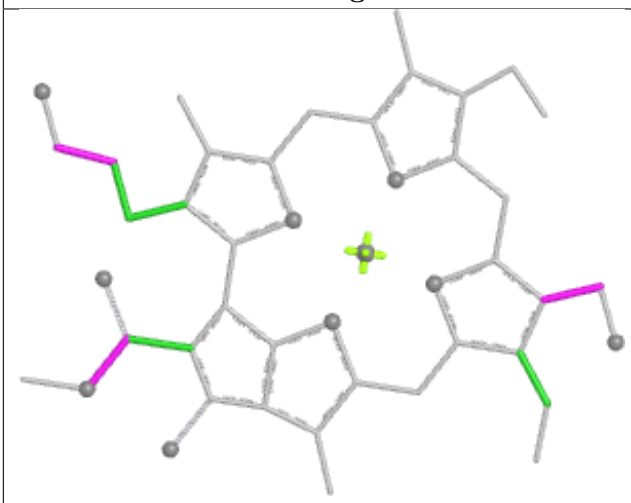
Ligand CHL 2 607



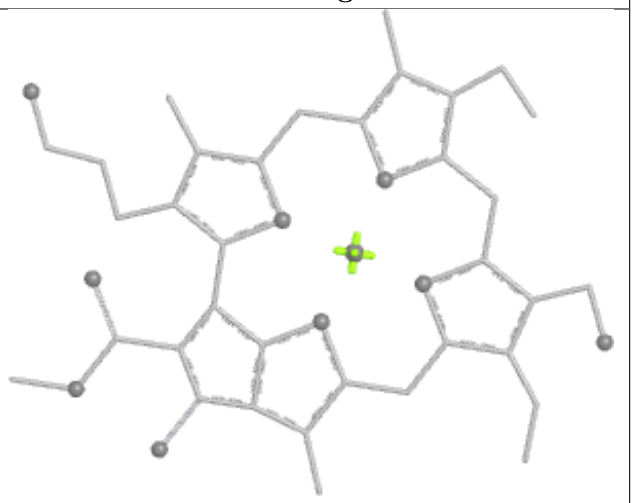
Bond lengths



Bond angles

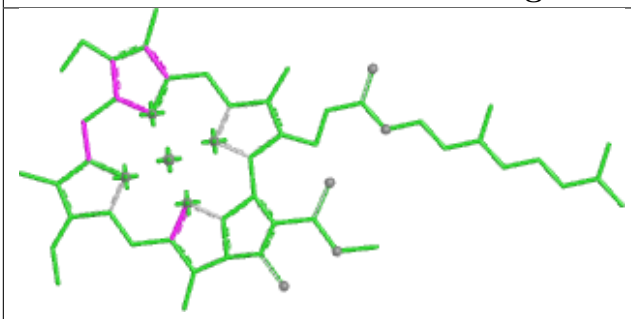


Torsions

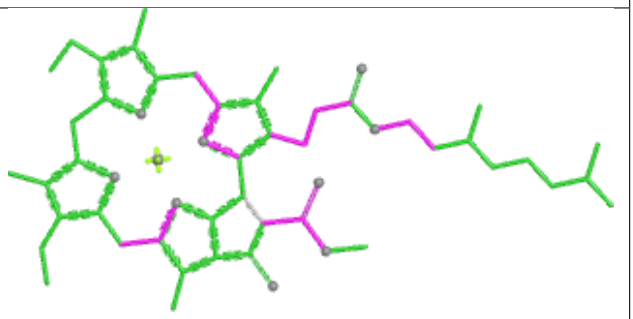


Rings

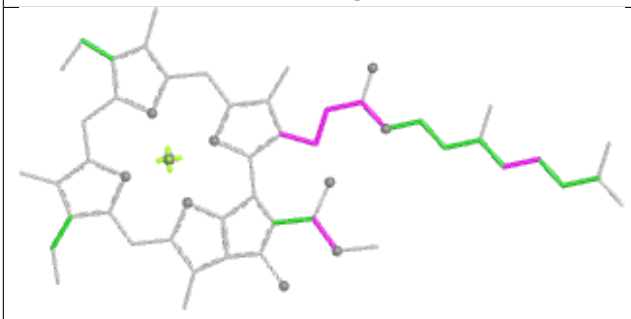
Ligand CLA P 312



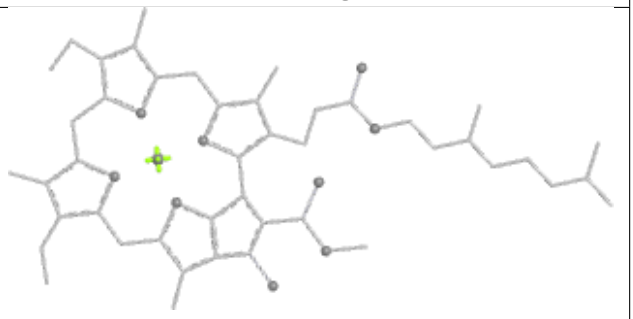
Bond lengths



Bond angles

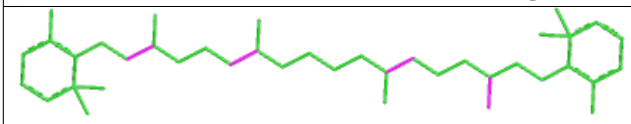


Torsions



Rings

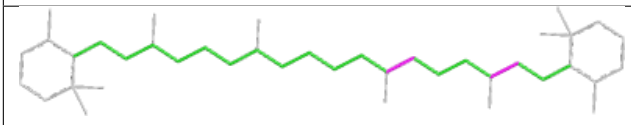
Ligand BCR F 801



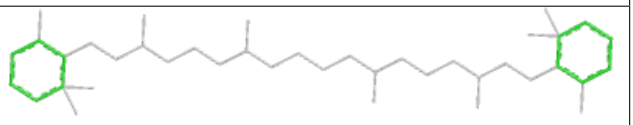
Bond lengths



Bond angles

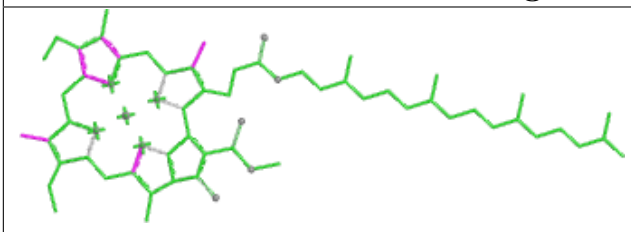


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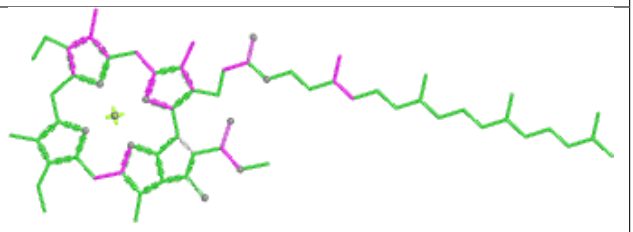


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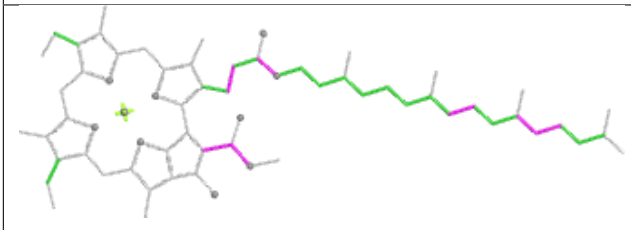
Ligand CLA A 815



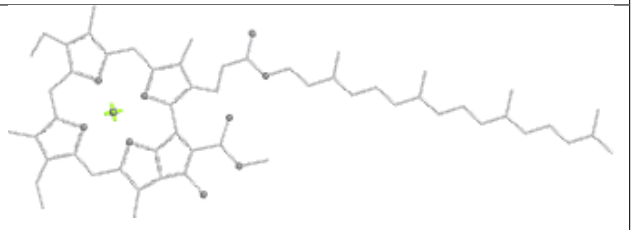
Bond lengths



Bond angles

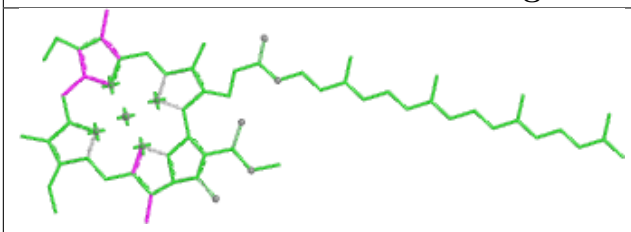


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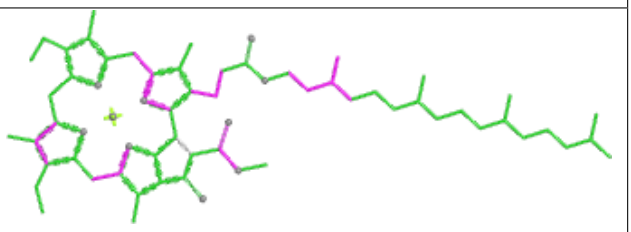


Rings

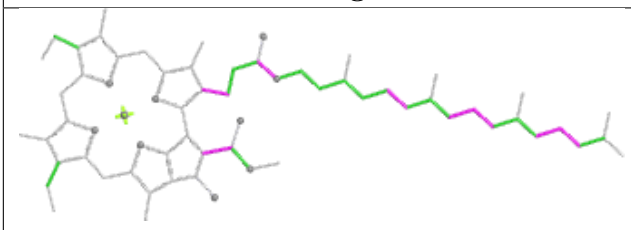
Ligand CLA H 302



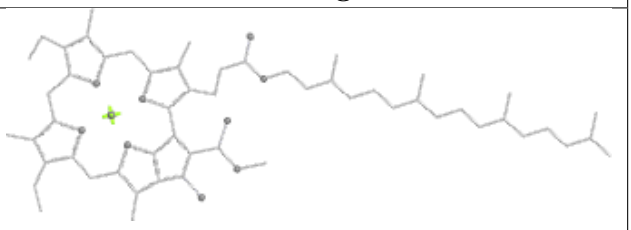
Bond lengths



Bond angles

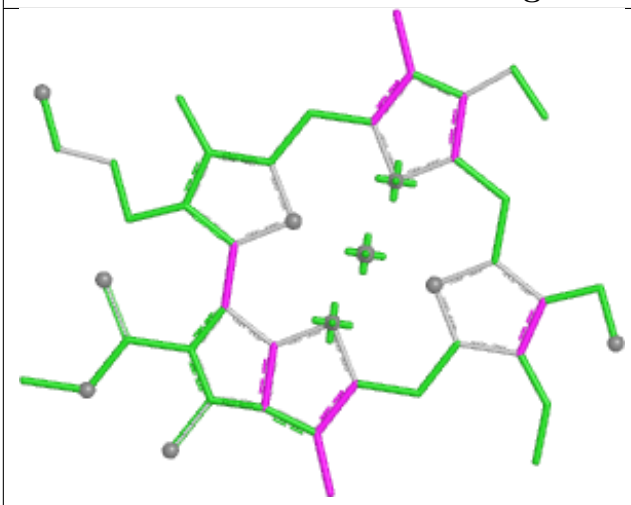


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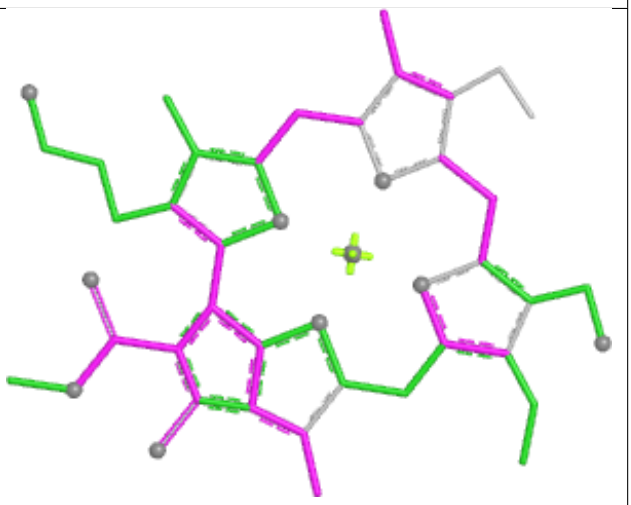


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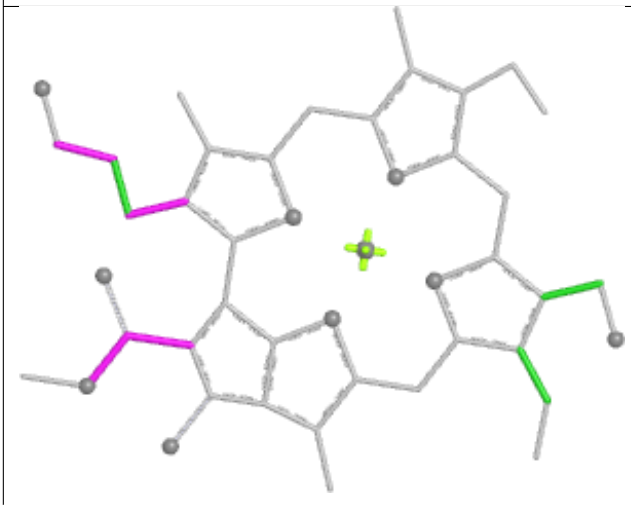
Ligand CHL X 315



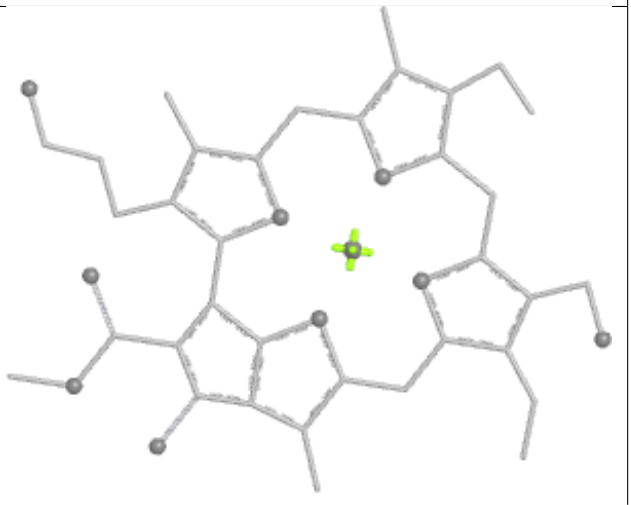
Bond lengths



Bond angles

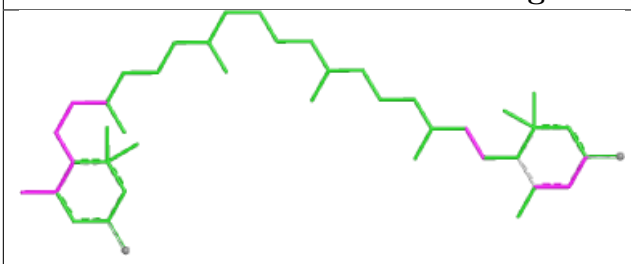


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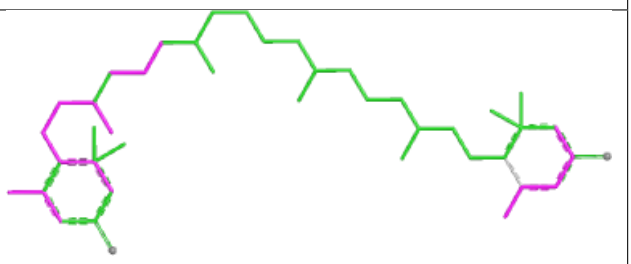


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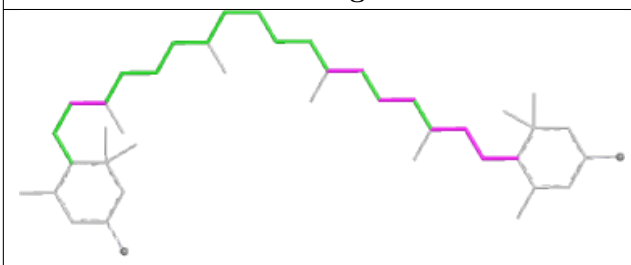
Ligand Q6L X 319



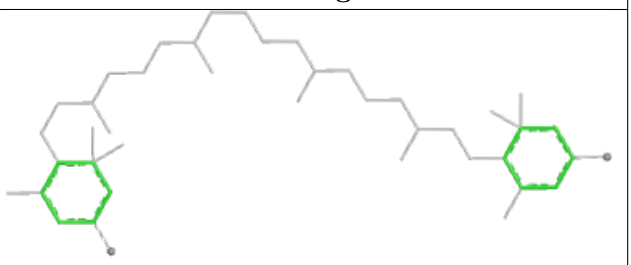
Bond lengths



Bond angles

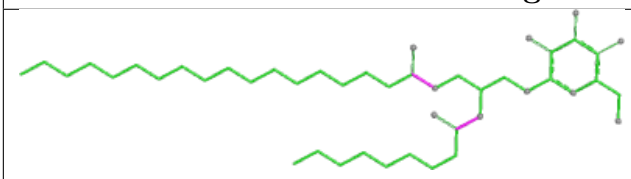


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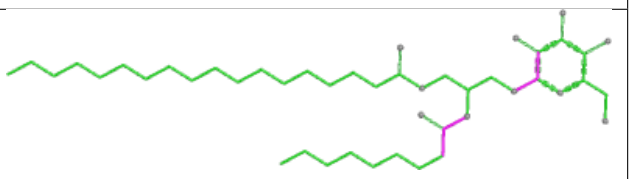


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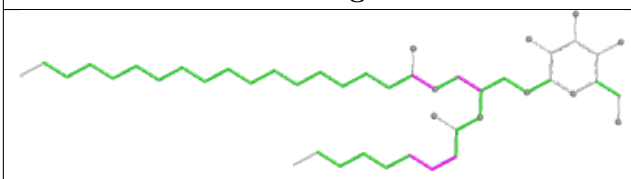
Ligand LMG J 104



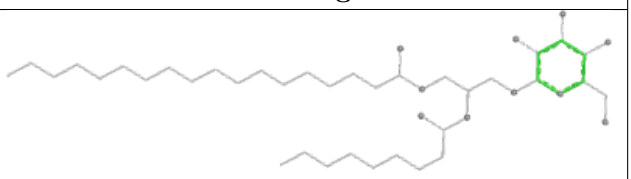
Bond lengths



Bond angles

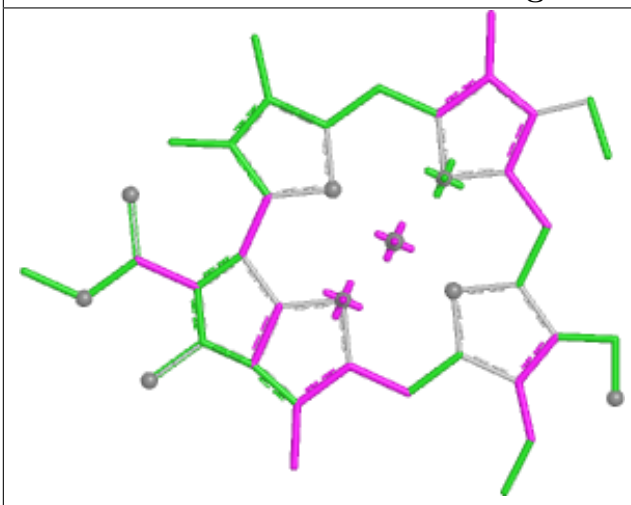


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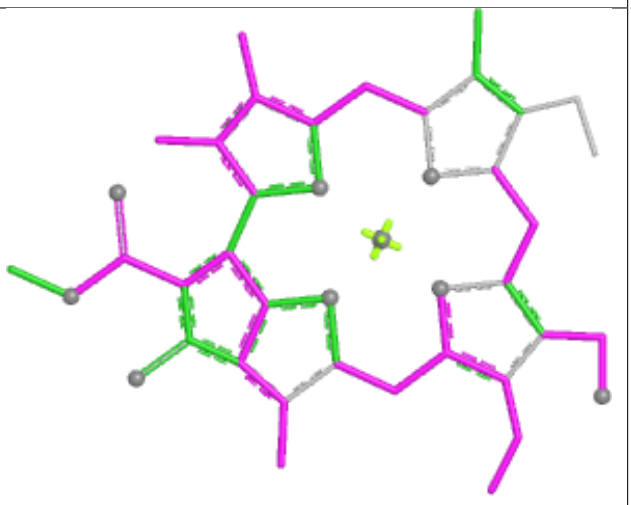


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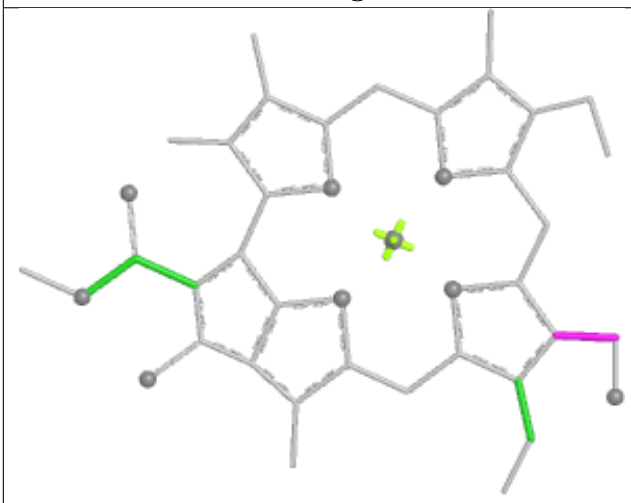
Ligand CHL S 304



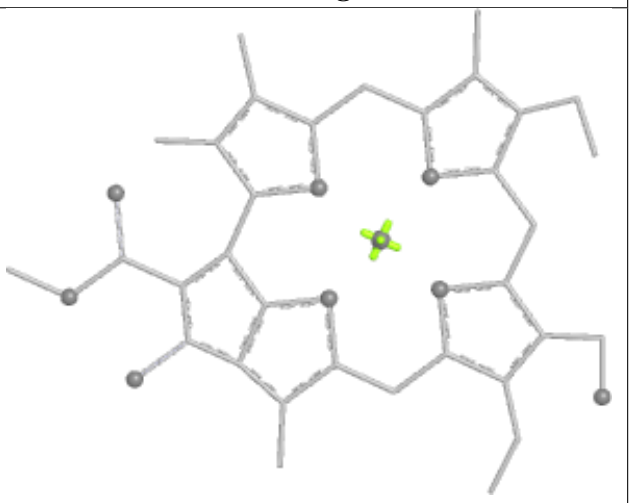
Bond lengths



Bond angles

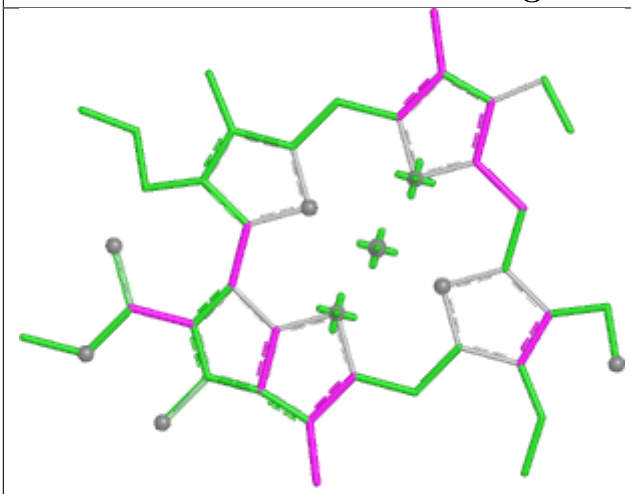


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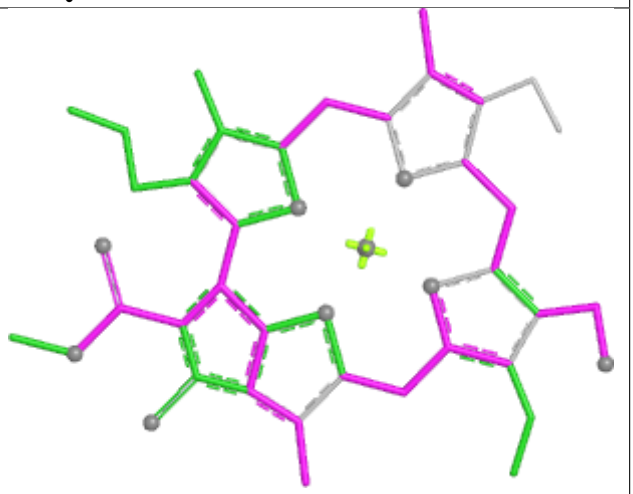


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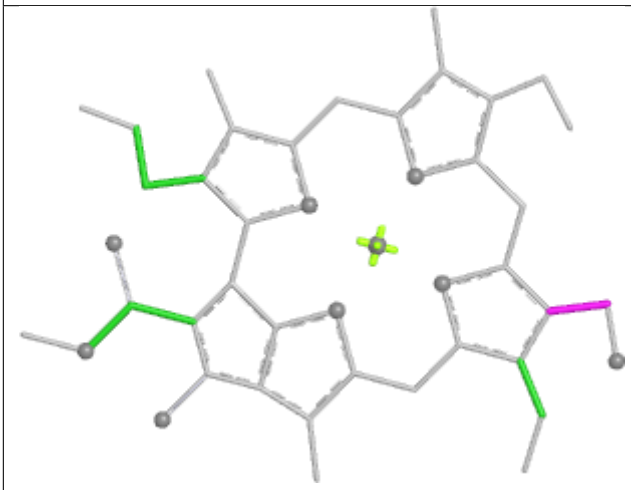
Ligand CHL Q 309



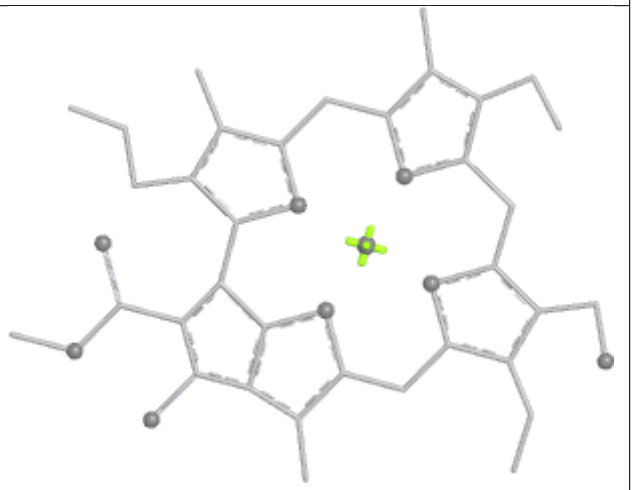
Bond lengths



Bond angles

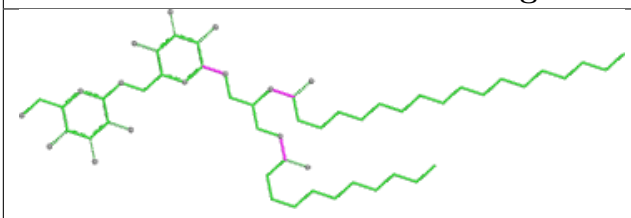


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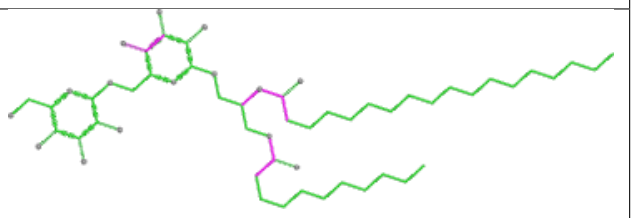


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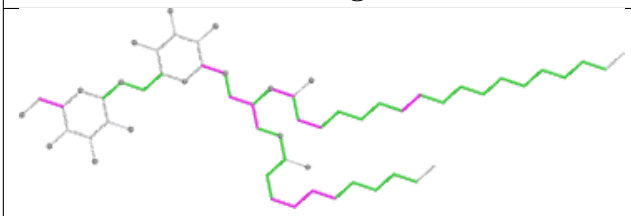
Ligand DGD B 850



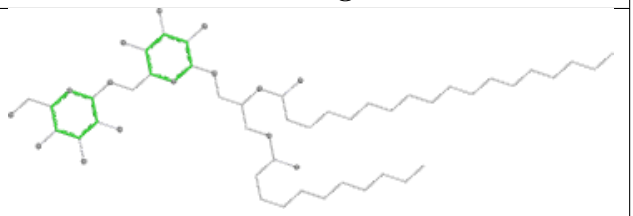
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Bond angles

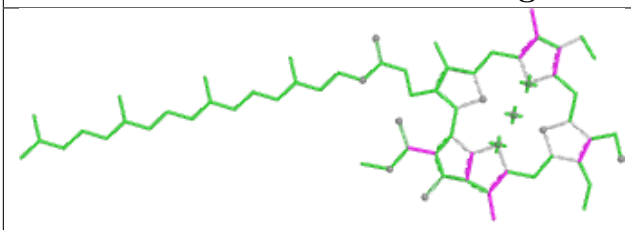


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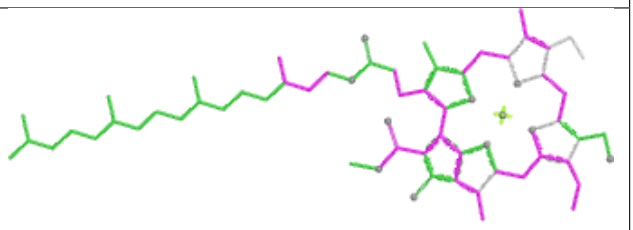


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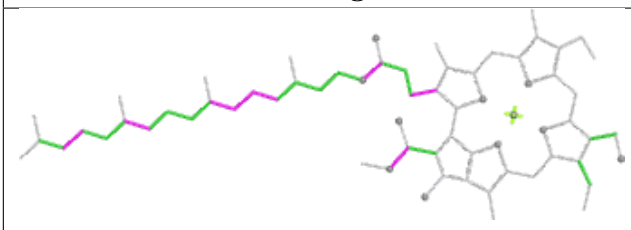
Ligand CHL W 307



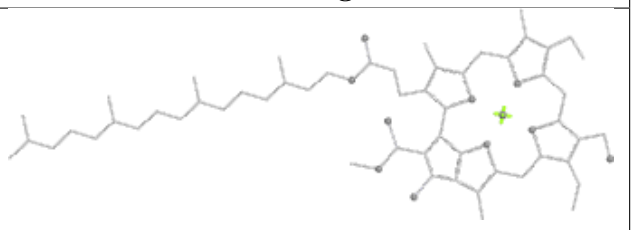
Bond lengths



Bond angles

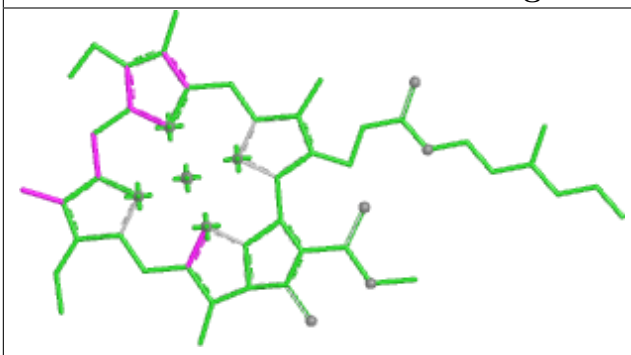


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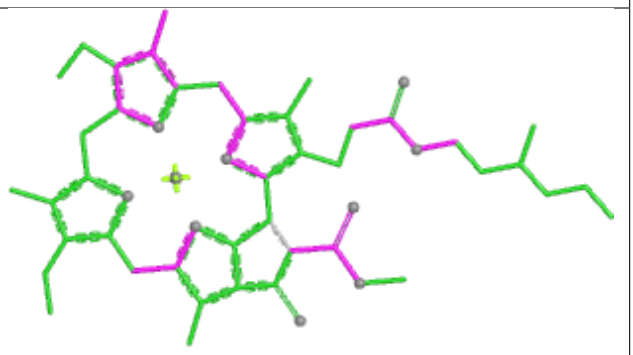


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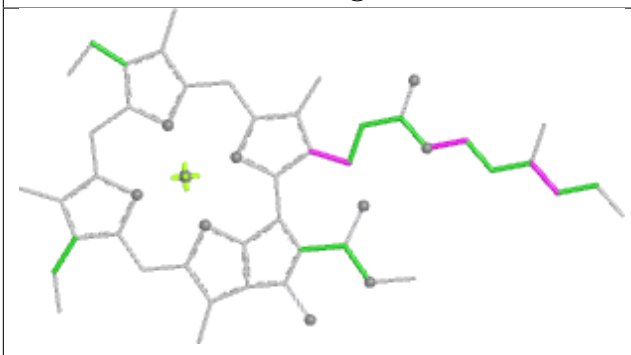
Ligand CLA A 806



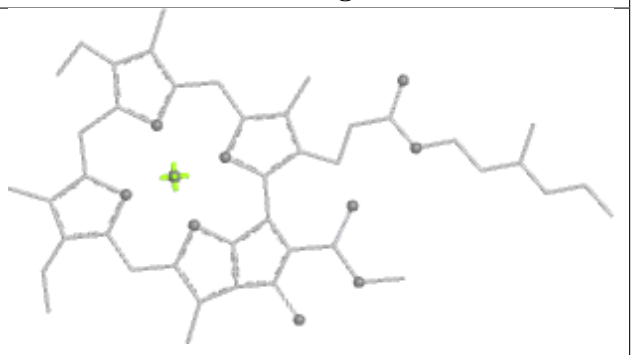
Bond lengths



Bond angles

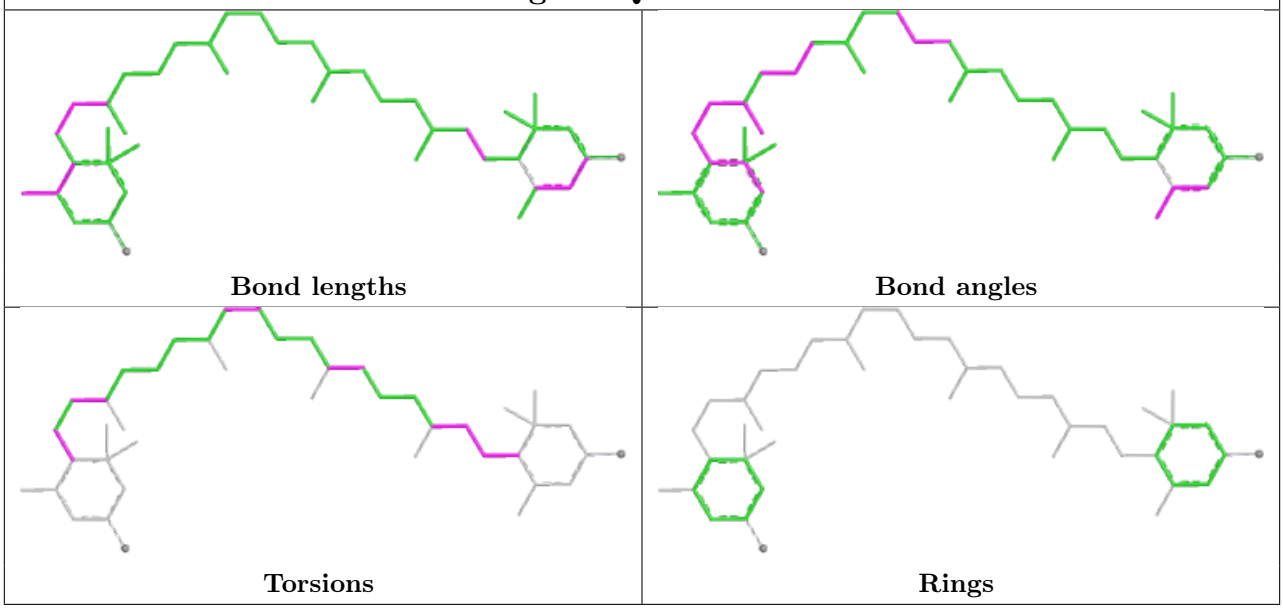


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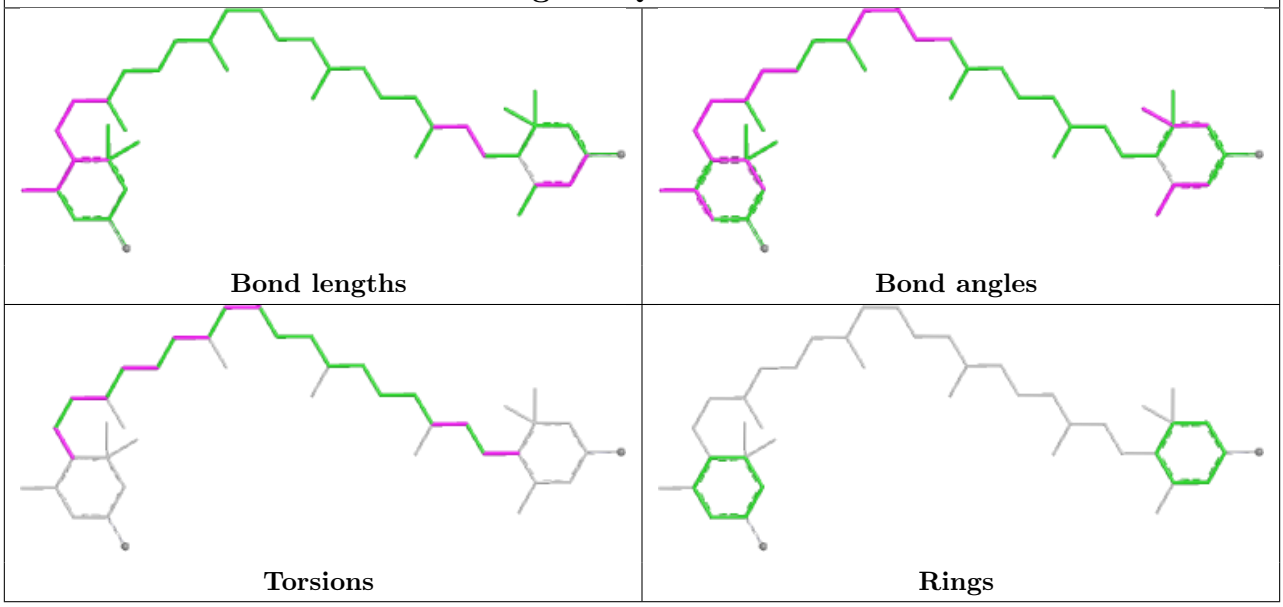


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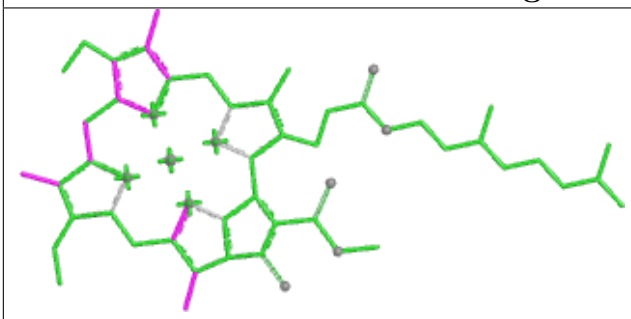
Ligand Q6L R 301



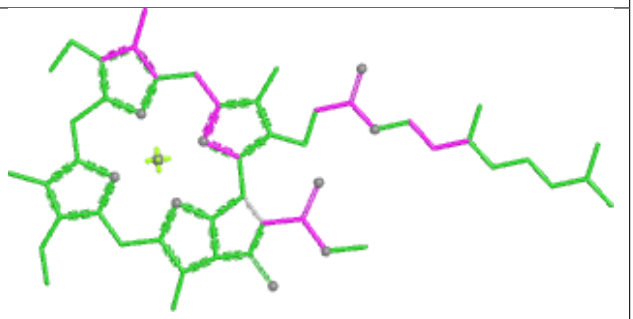
Ligand Q6L S 321



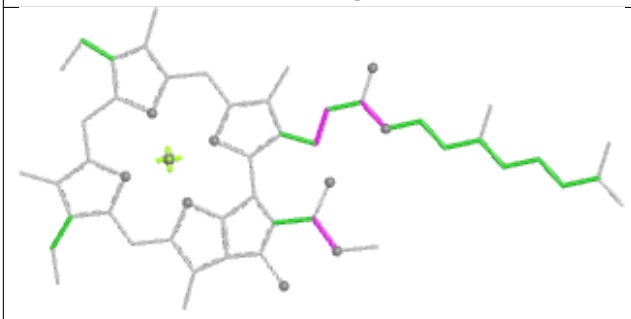
Ligand CLA U 311



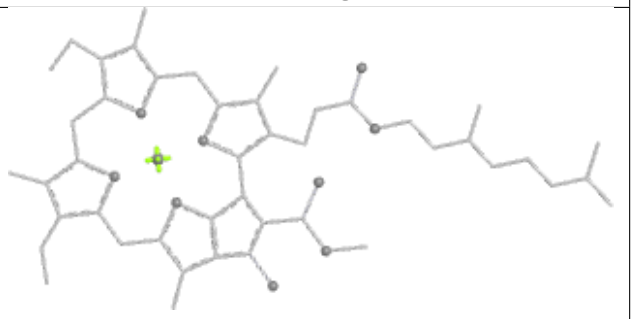
Bond lengths



Bond angles

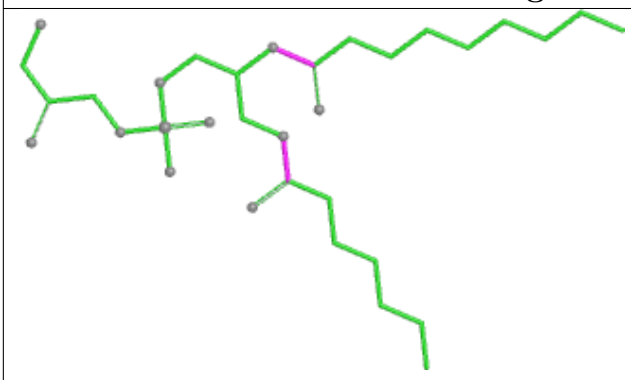


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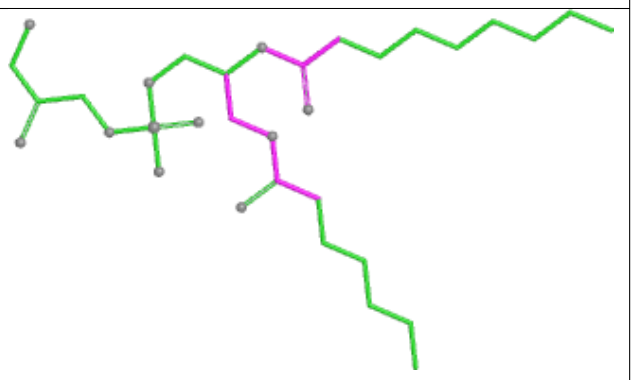


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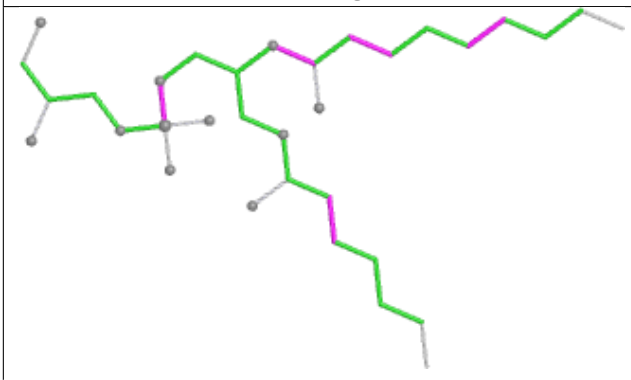
Ligand LHG 2 619



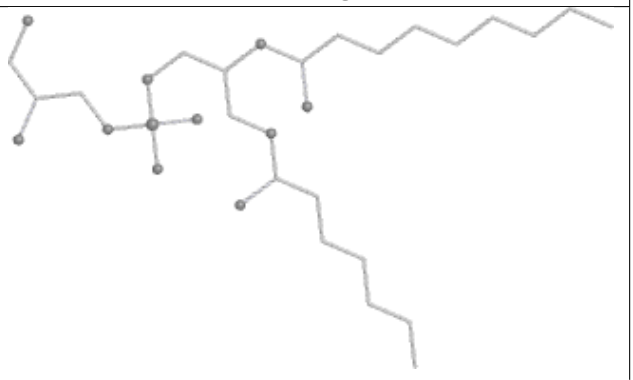
Bond lengths



Bond angles

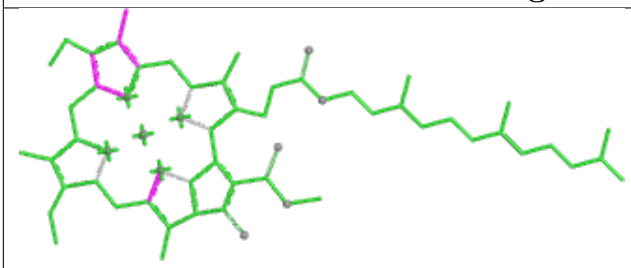


Torsions

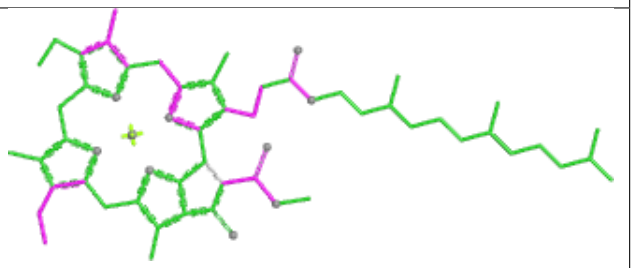


Rings

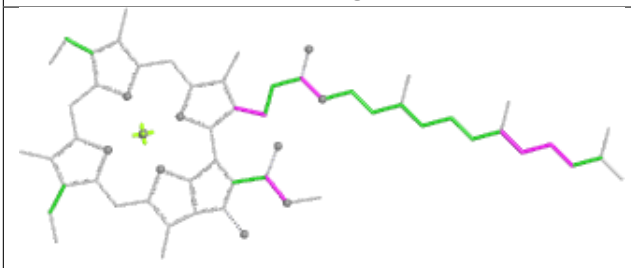
Ligand CLA 5 602



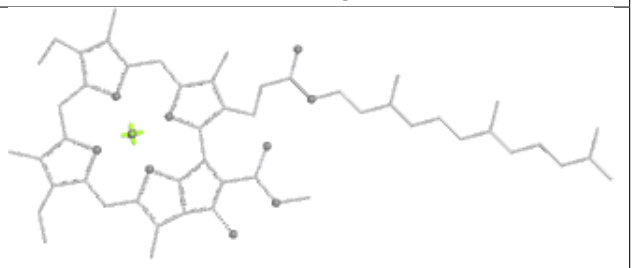
Bond lengths



Bond angles

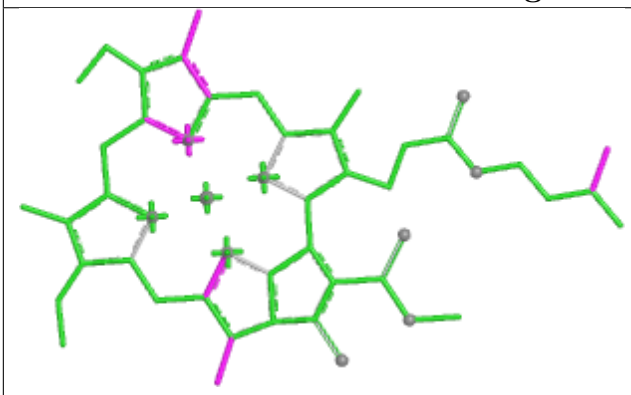


Torsions

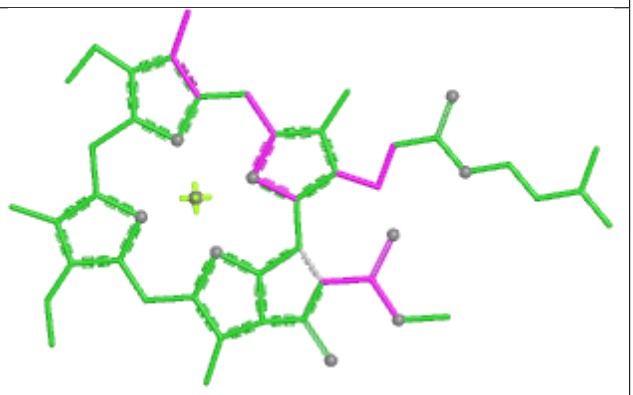


Rings

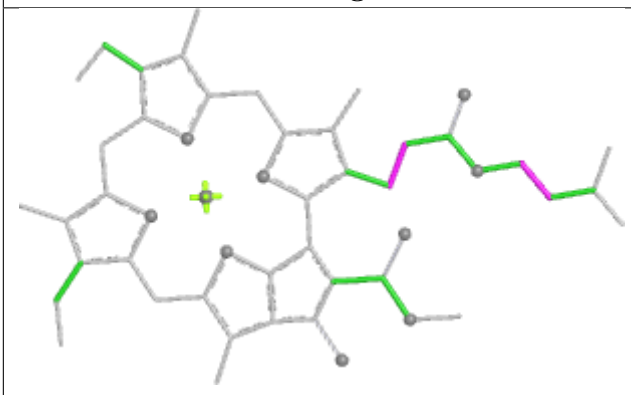
Ligand CLA B 822



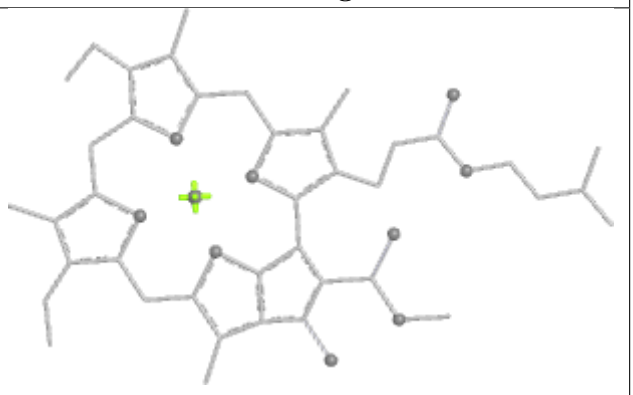
Bond lengths



Bond angles

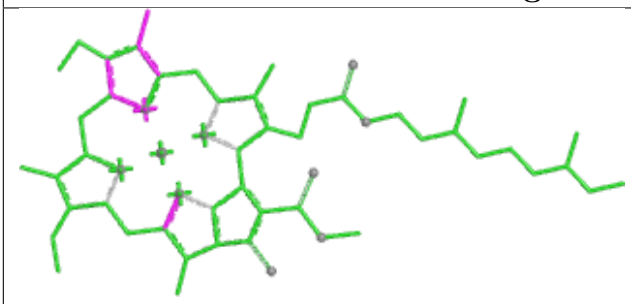


Torsions

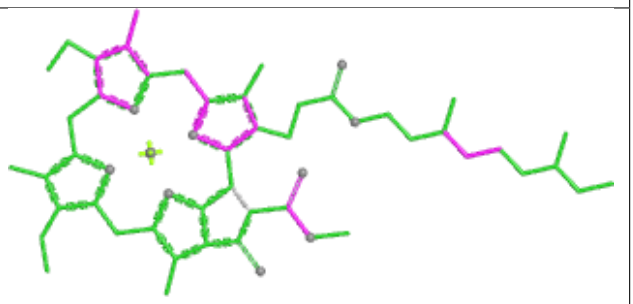


Rings

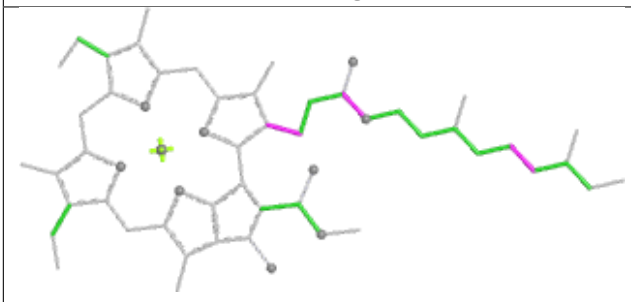
Ligand CLA A 834



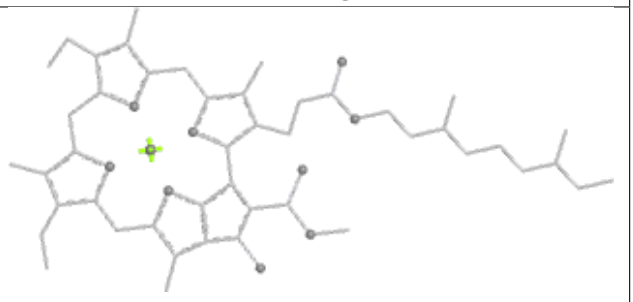
Bond lengths



Bond angles

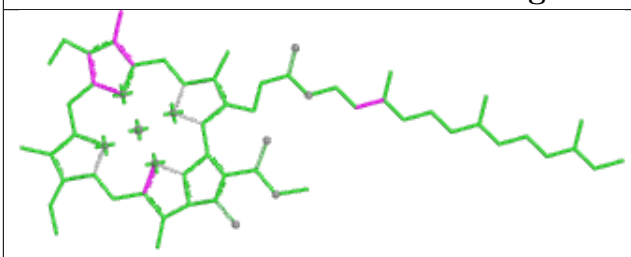


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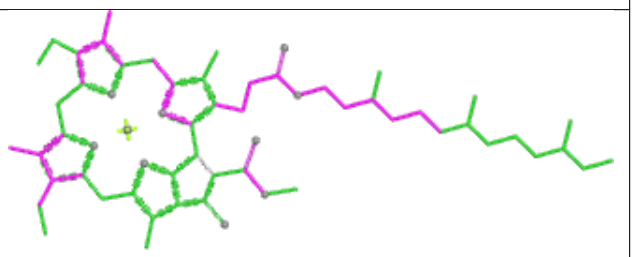


Rings

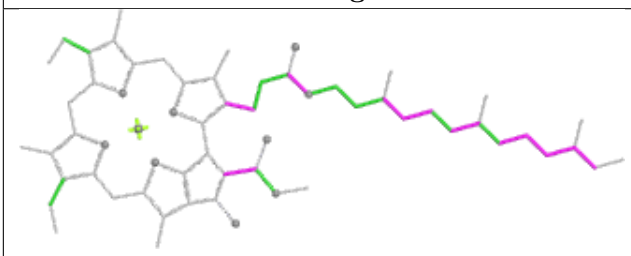
Ligand CLA 2 602



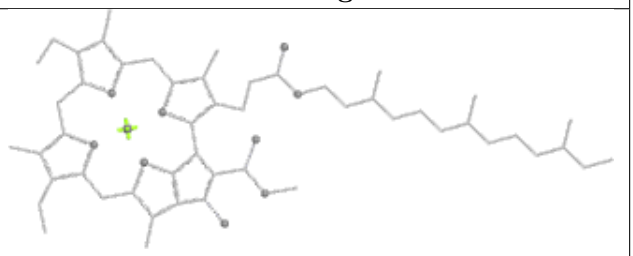
Bond lengths



Bond angles

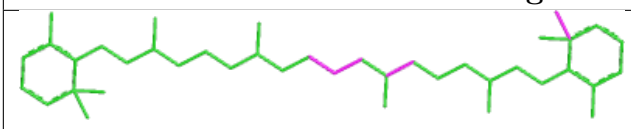


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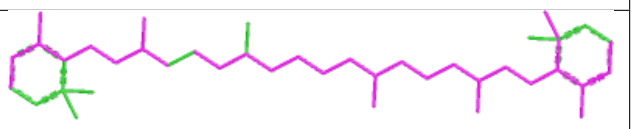


Rings

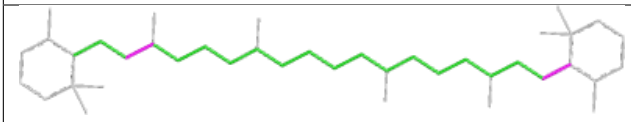
Ligand BCR J 101



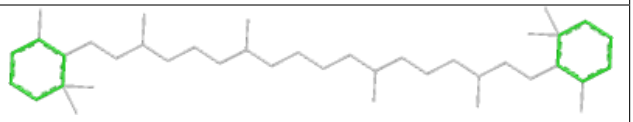
Bond lengths



Bond angles

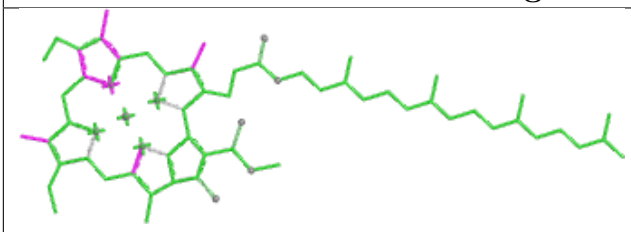


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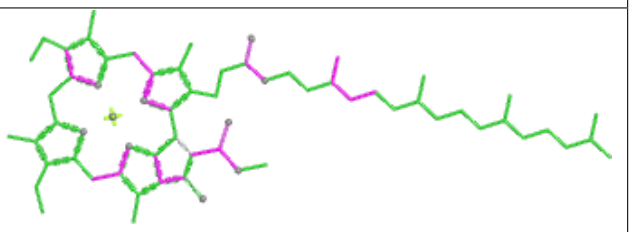


Rings

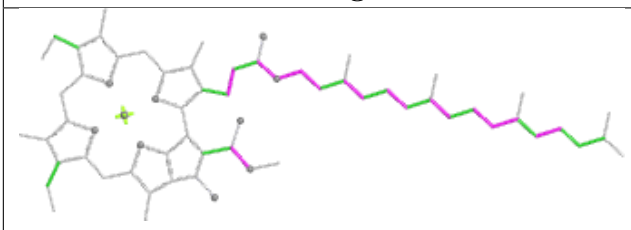
Ligand CLA B 805



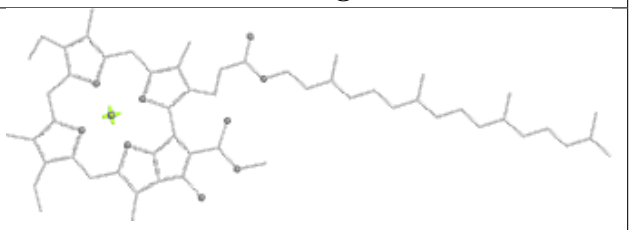
Bond lengths



Bond angles

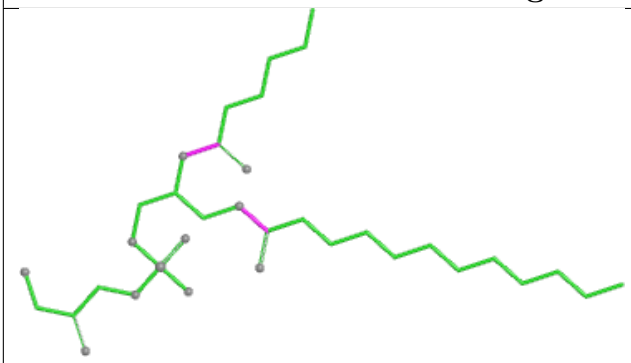


Torsions

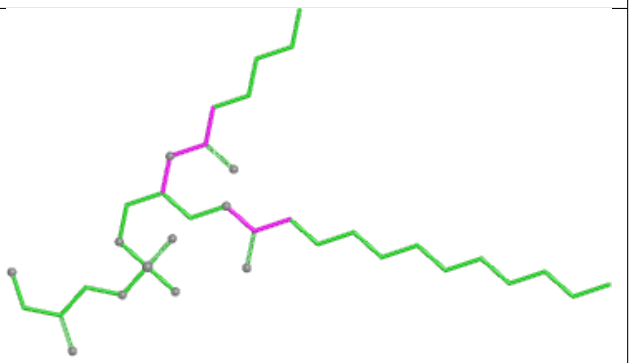


Rings

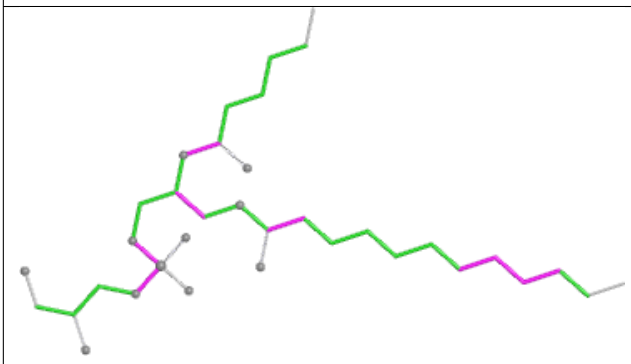
Ligand LHG 1 614



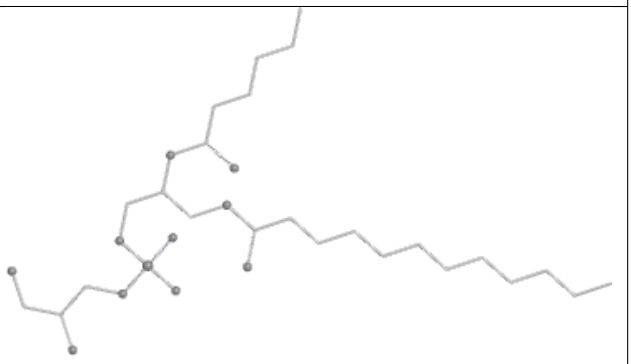
Bond lengths



Bond angles

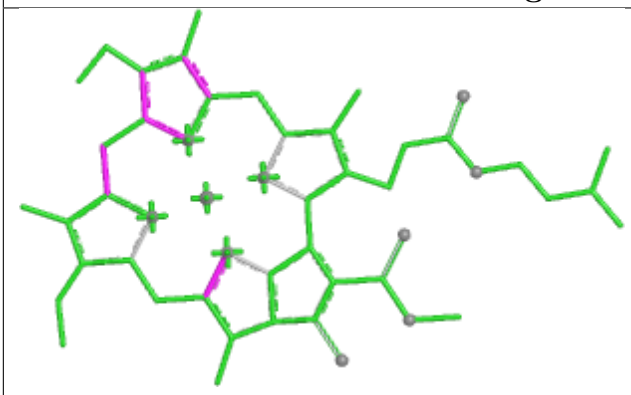


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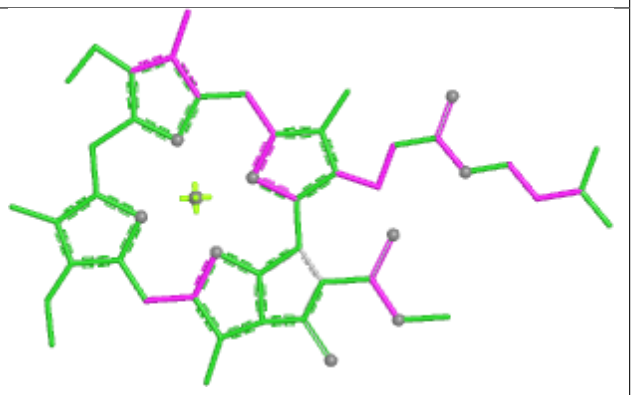


Rings

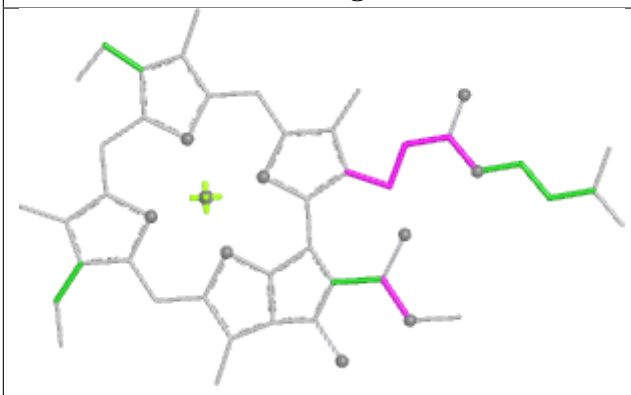
Ligand CLA P 303



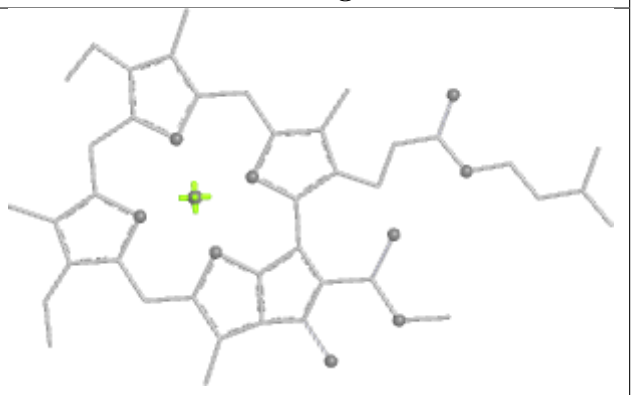
Bond lengths



Bond angles

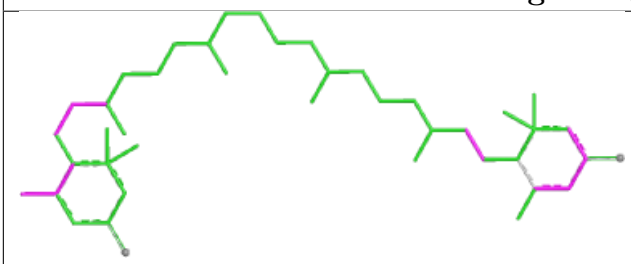


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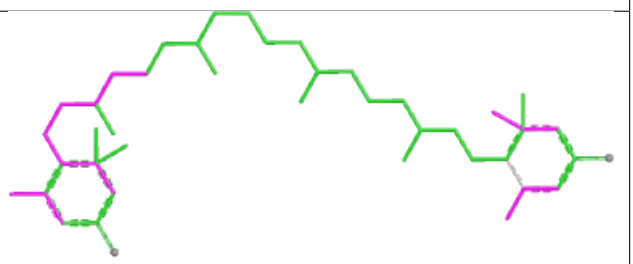


Rings

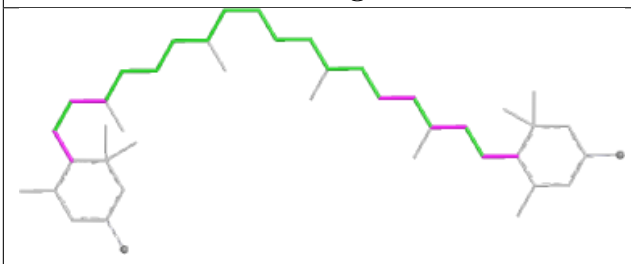
Ligand Q6L V 321



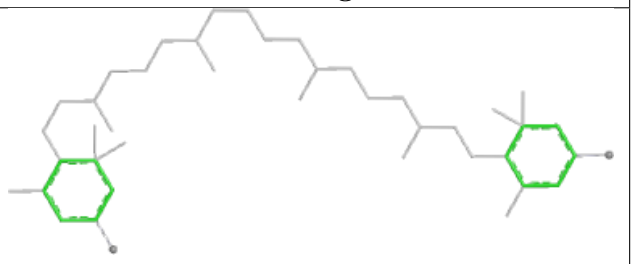
Bond lengths



Bond angles

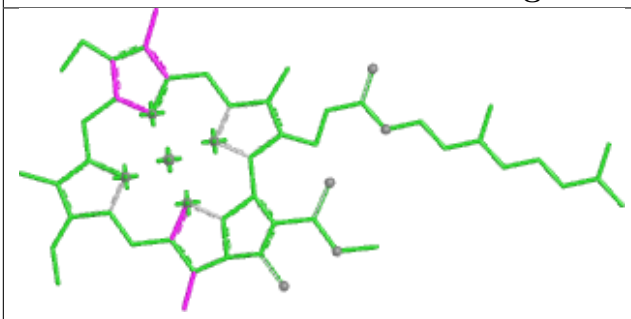


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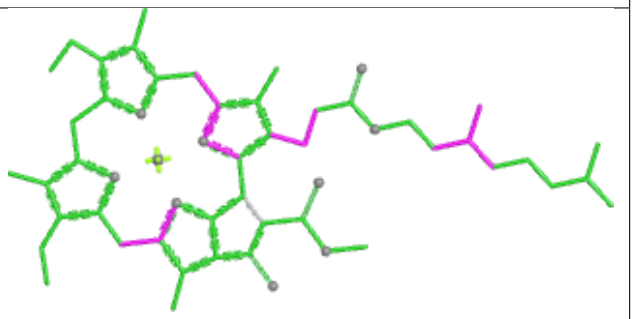


Rings

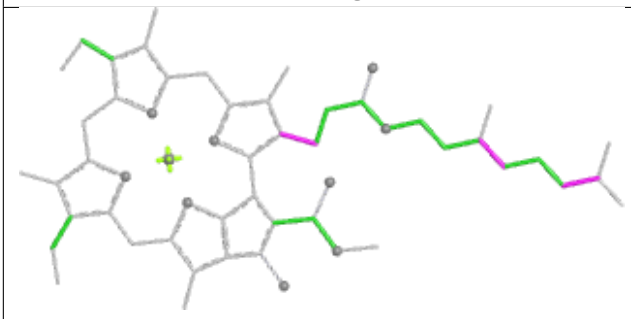
Ligand CLA A 840



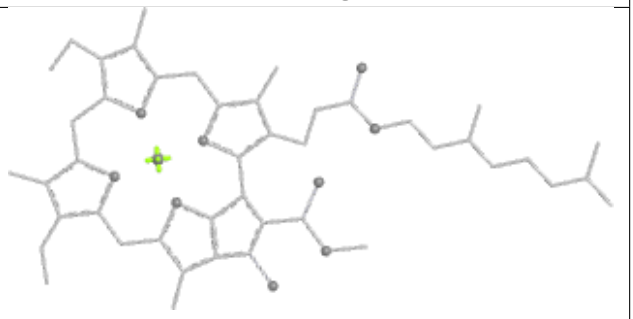
Bond lengths



Bond angles

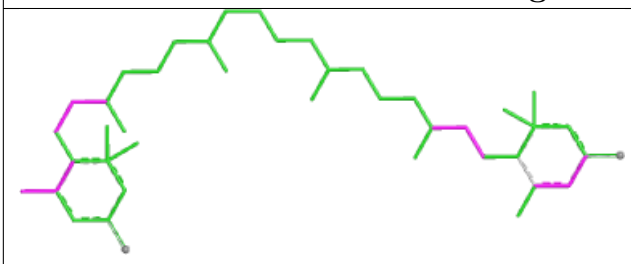


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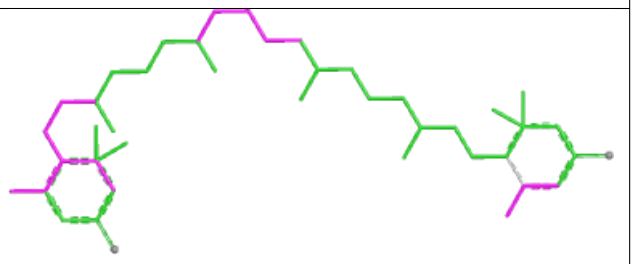


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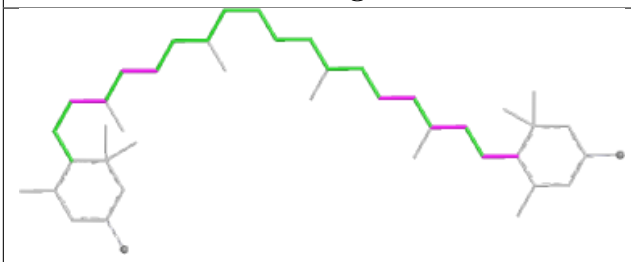
Ligand Q6L P 321



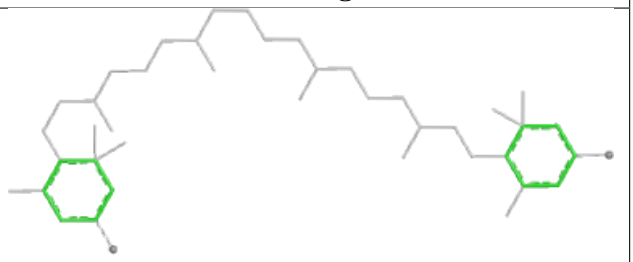
Bond lengths



Bond angles

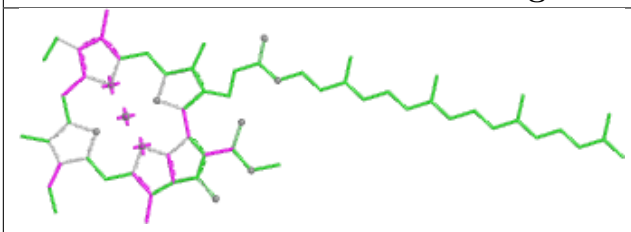


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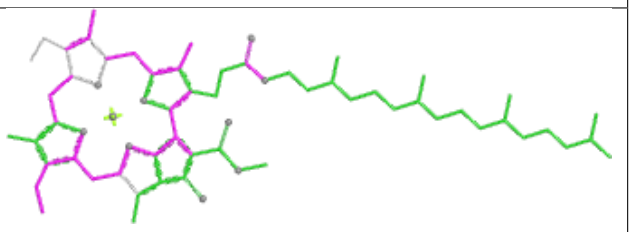


Rings

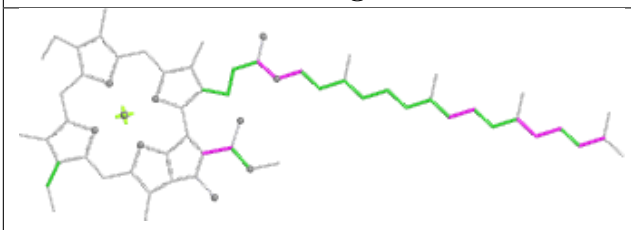
Ligand CL0 A 802



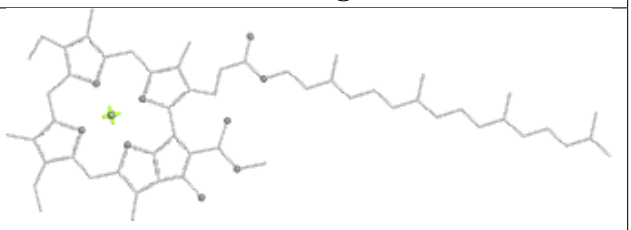
Bond lengths



Bond angles

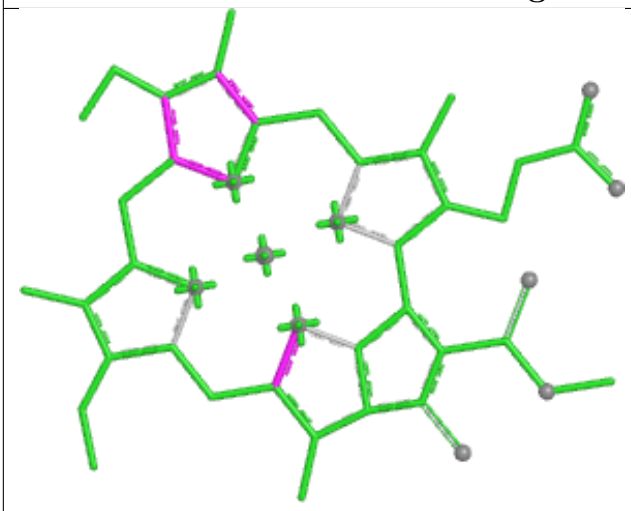


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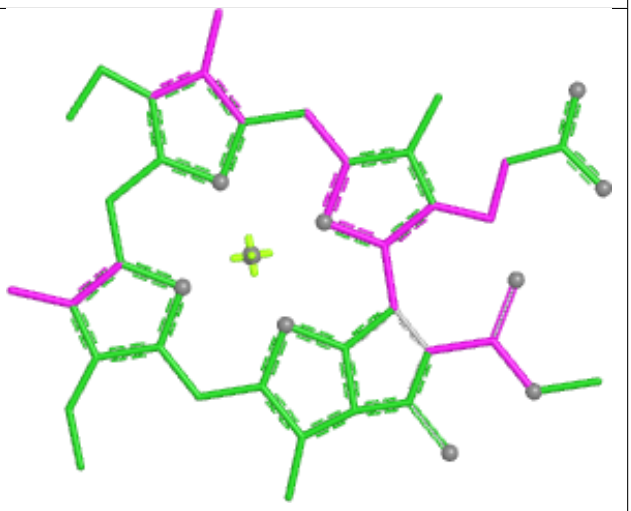


Rings

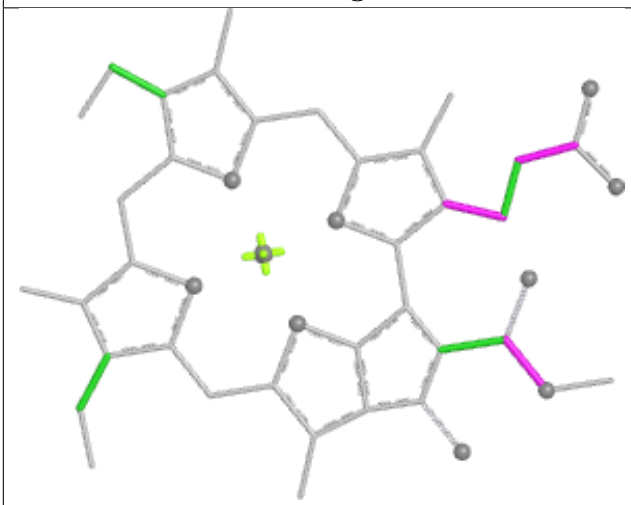
Ligand CLA 2 608



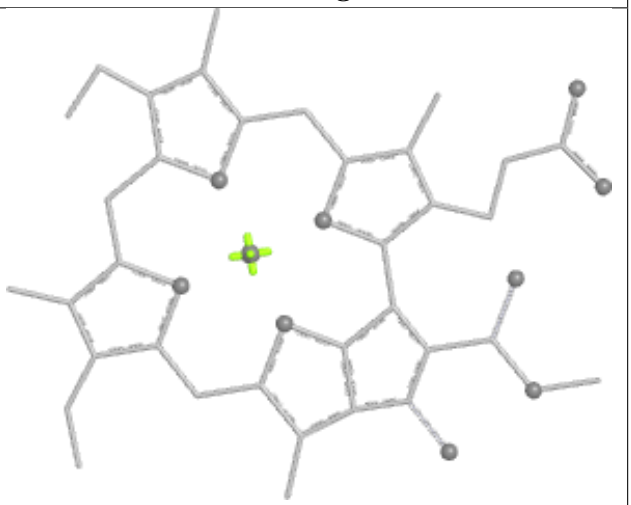
Bond lengths



Bond angles

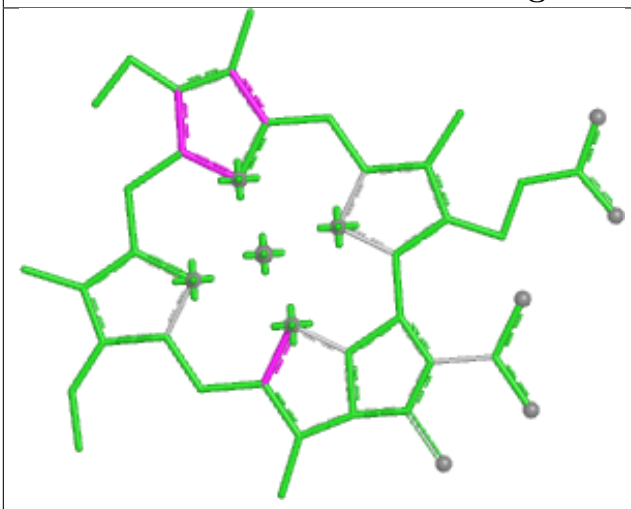


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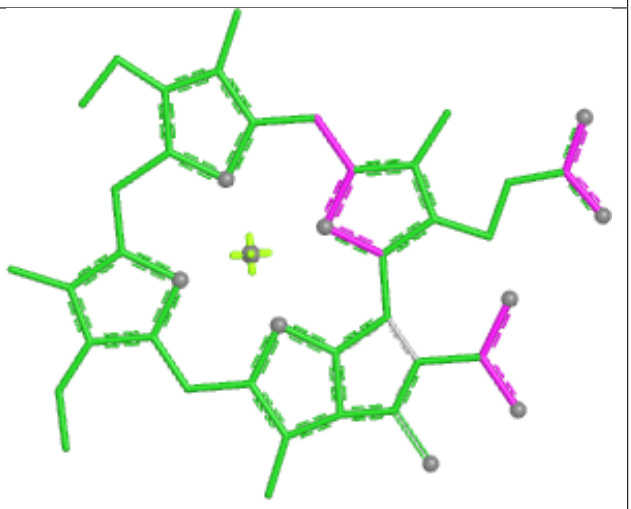


Rings

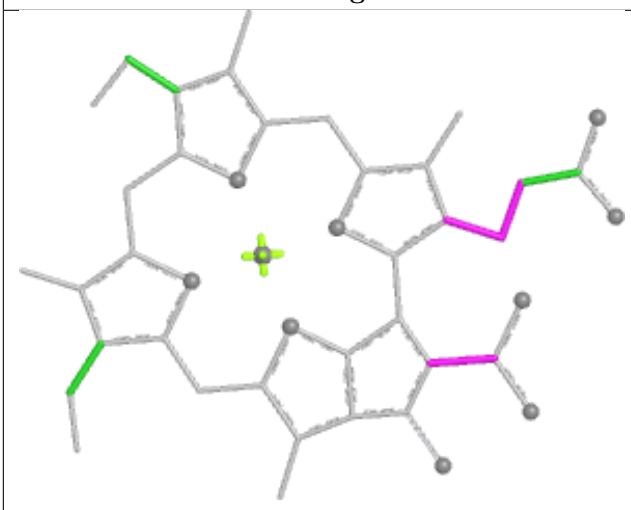
Ligand CLA 2 611



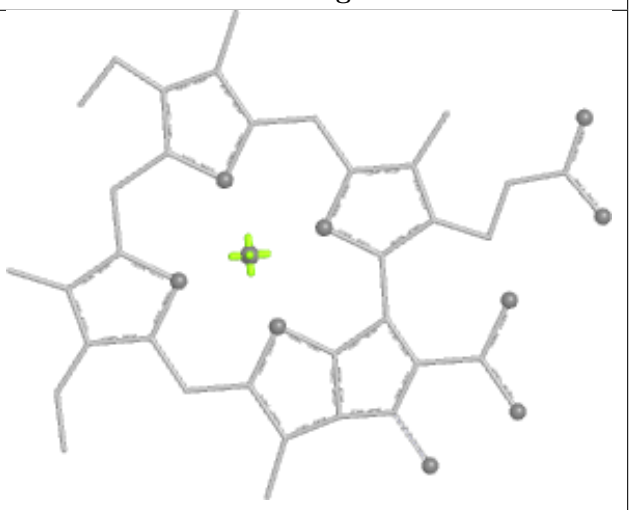
Bond lengths



Bond angles

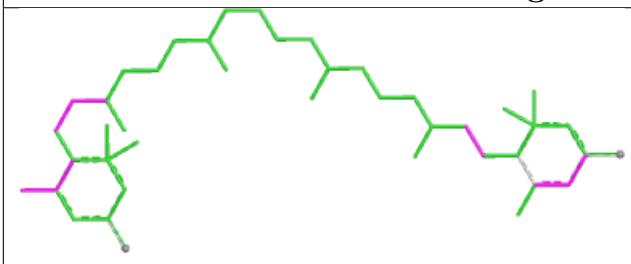


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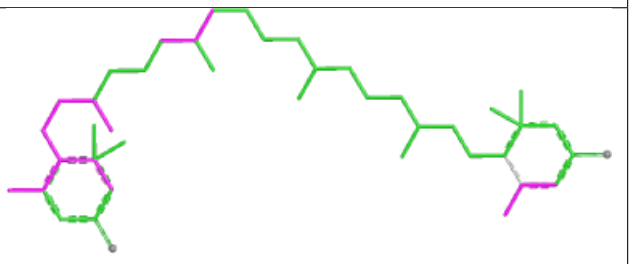


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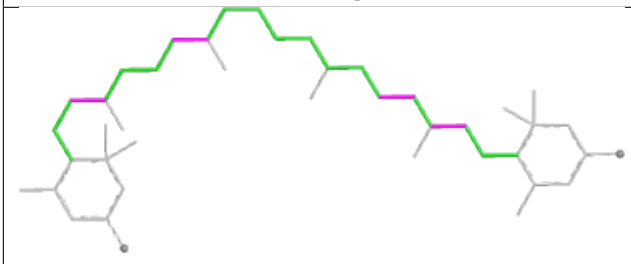
Ligand Q6L U 314



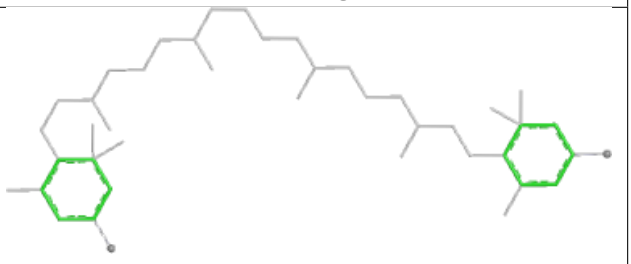
Bond lengths



Bond angles

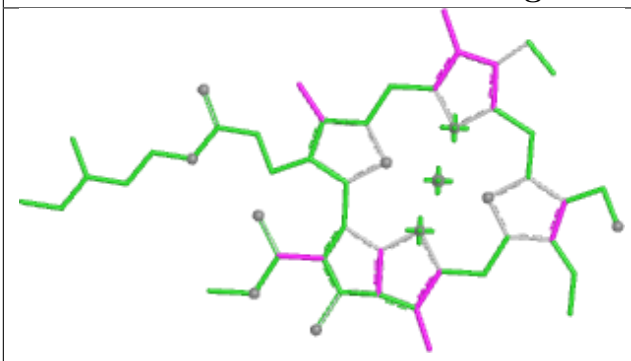


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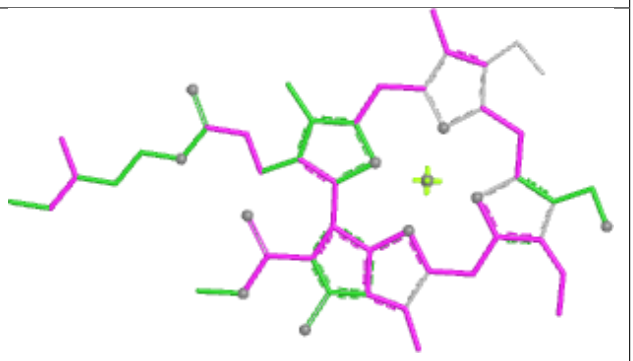


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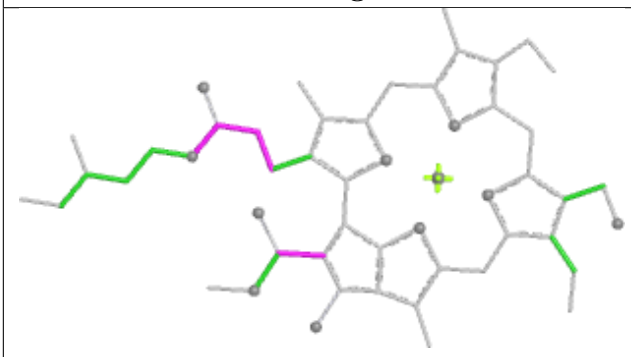
Ligand CHL T 320



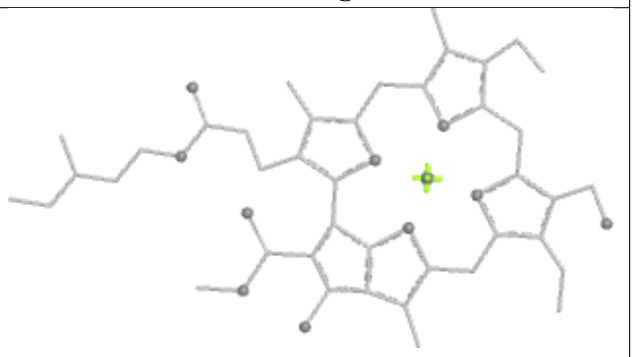
Bond lengths



Bond angles

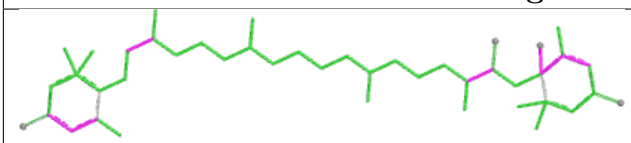


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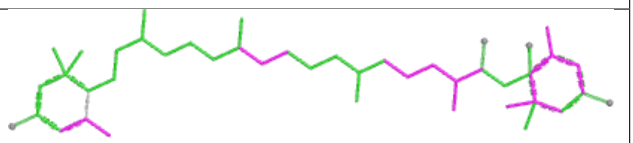


Rings

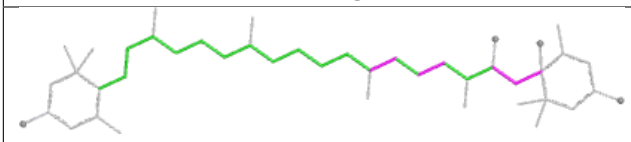
Ligand IWJ X 318



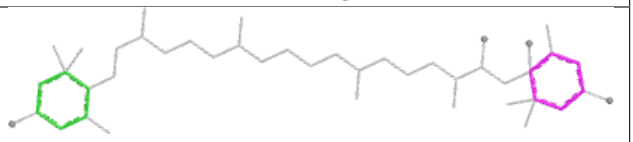
Bond lengths



Bond angles

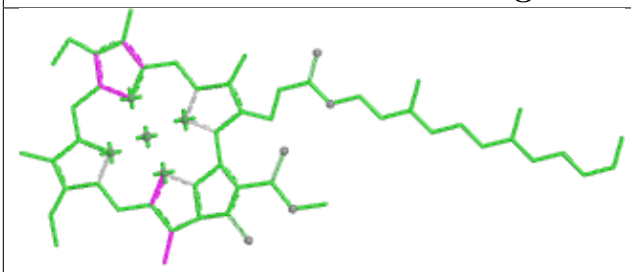


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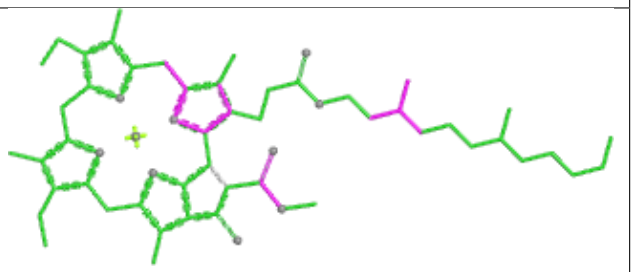


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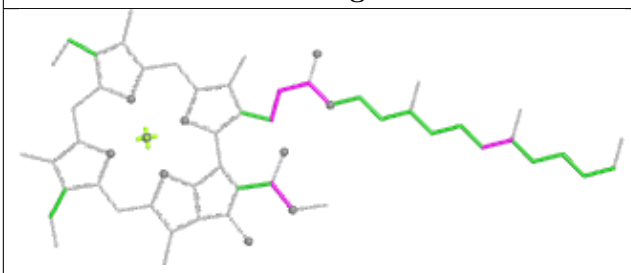
Ligand CLA O 2001



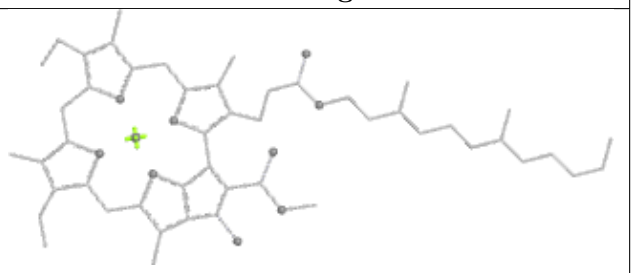
Bond lengths



Bond angles

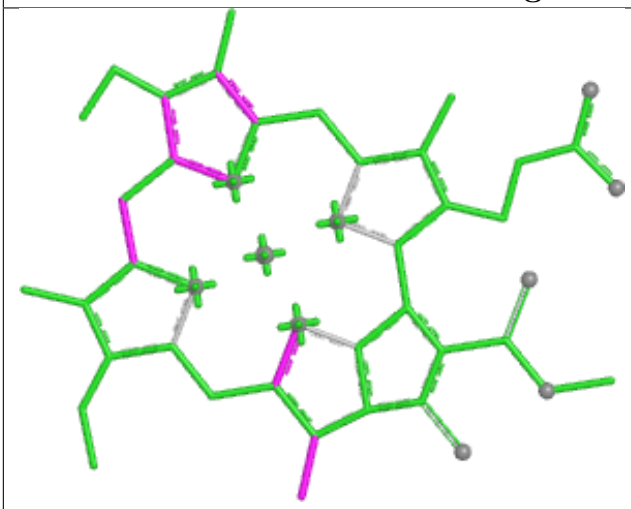


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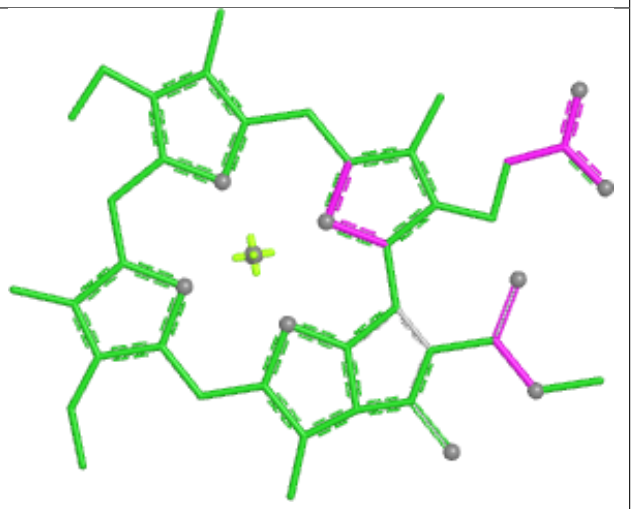


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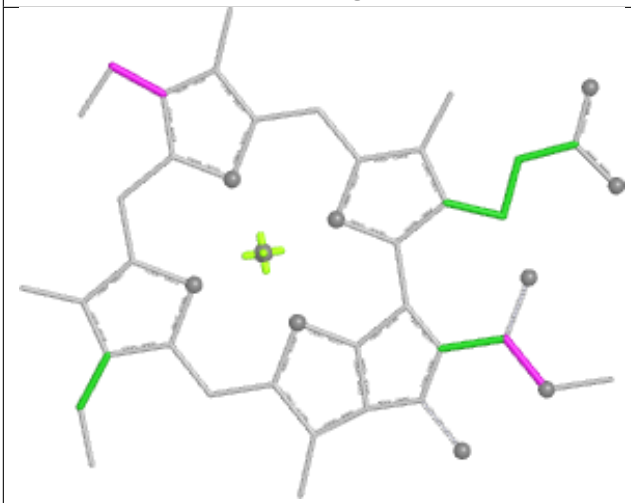
Ligand CLA B 835



Bond lengths



Bond angles

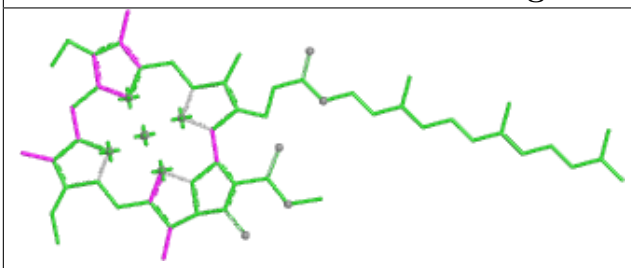


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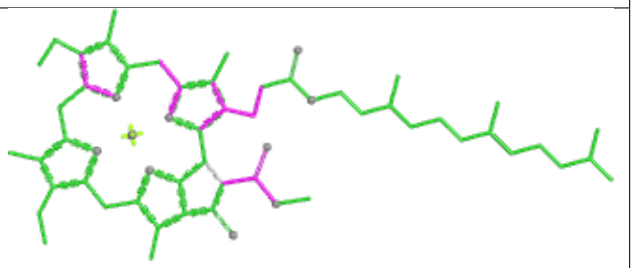


Rings

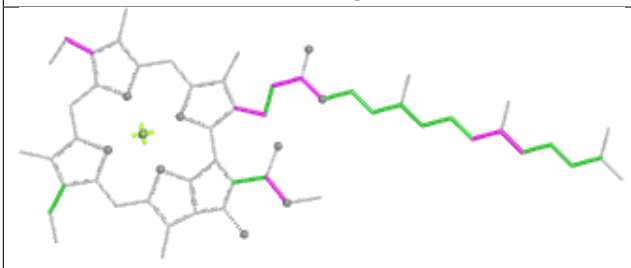
Ligand CLA S 309



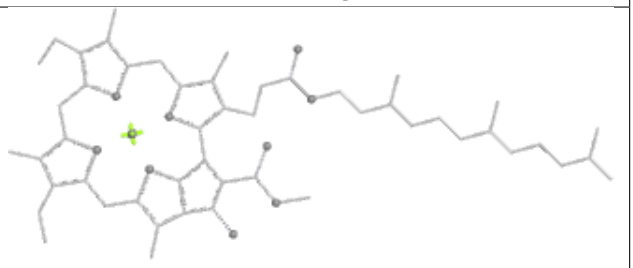
Bond lengths



Bond angles

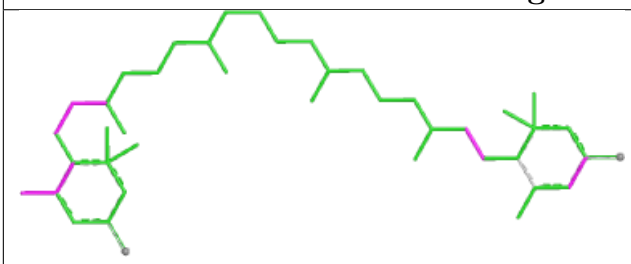


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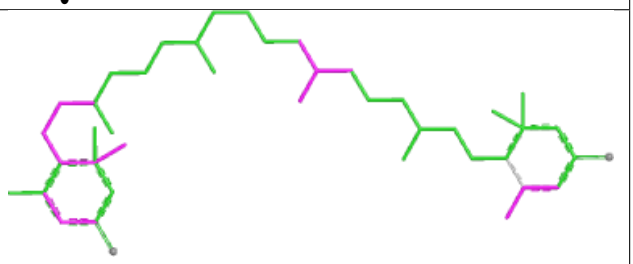


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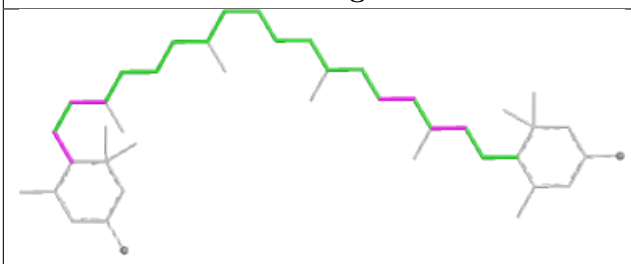
Ligand Q6L Q 318



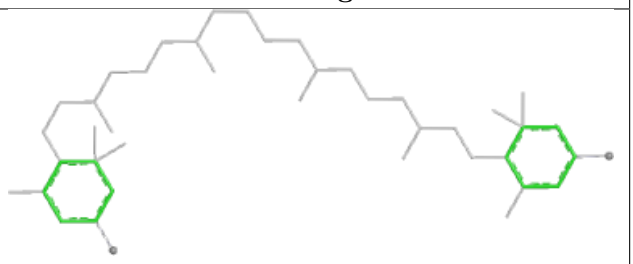
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Bond angles

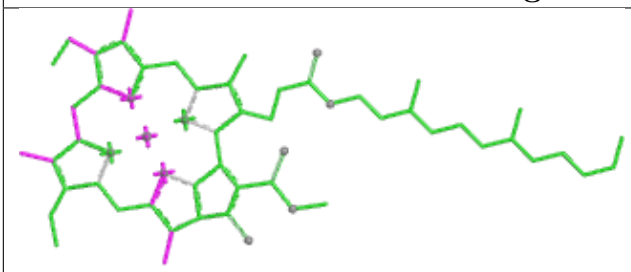


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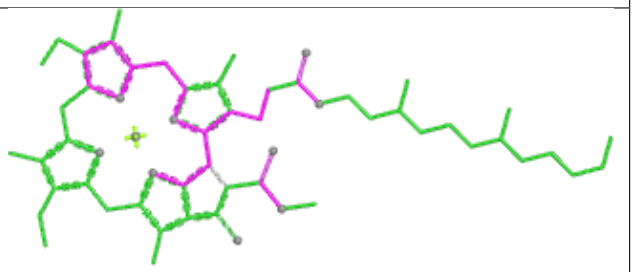


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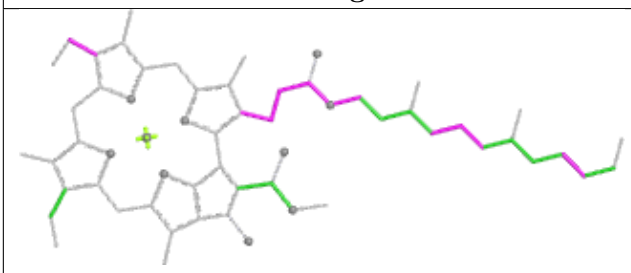
Ligand CLA A 820



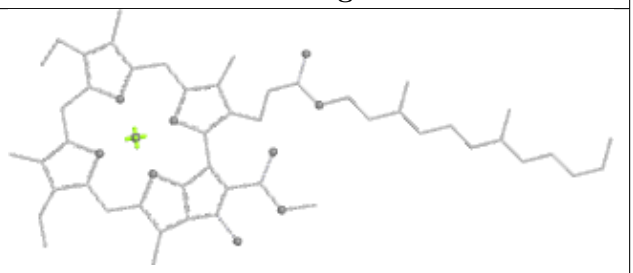
Bond lengths



Bond angles

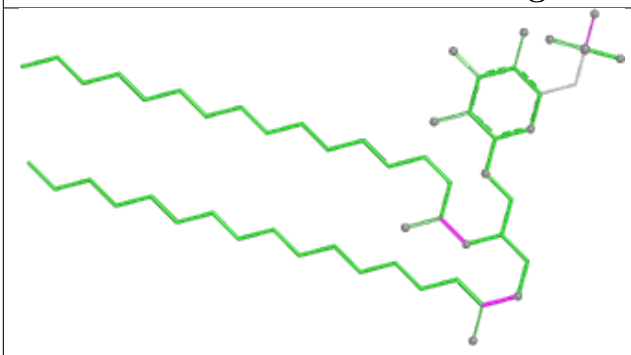


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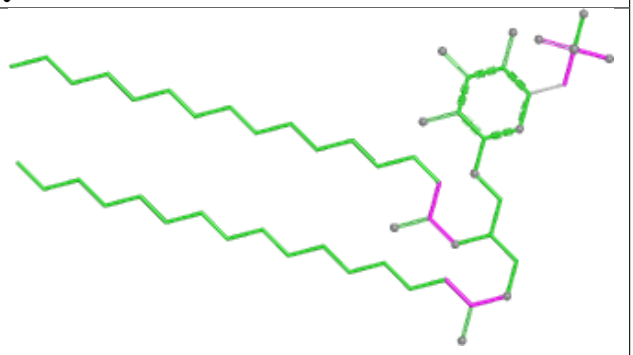


Rings

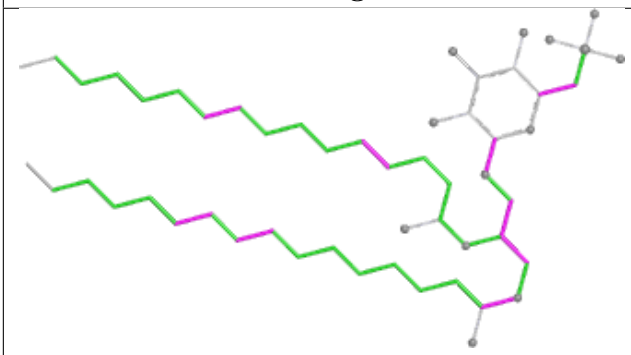
Ligand SQD 6 617



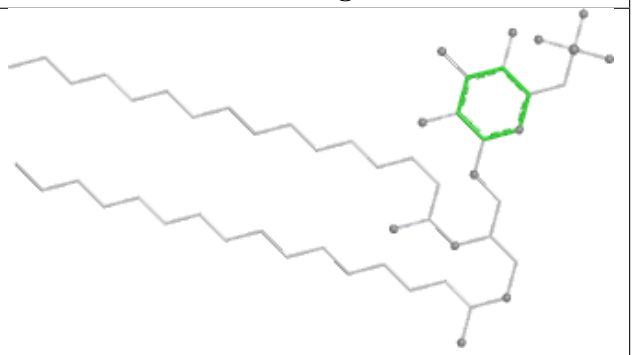
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Bond angles

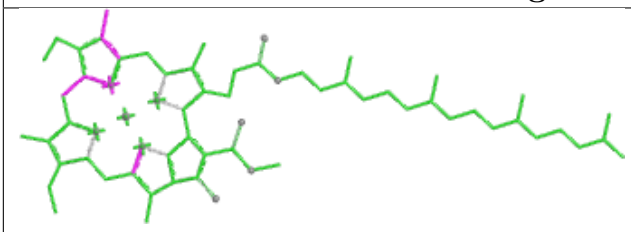


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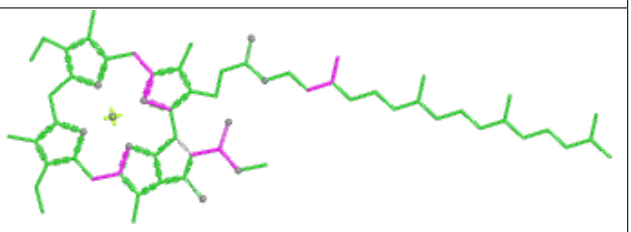


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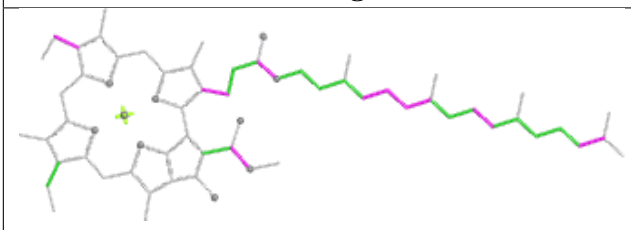
Ligand CLA 5 607



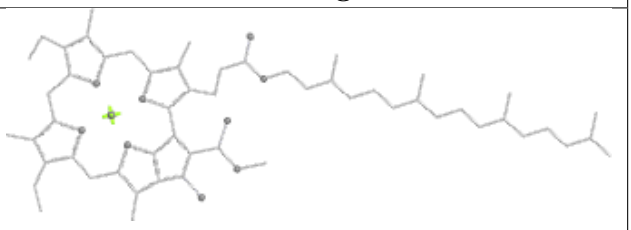
Bond lengths



Bond angles

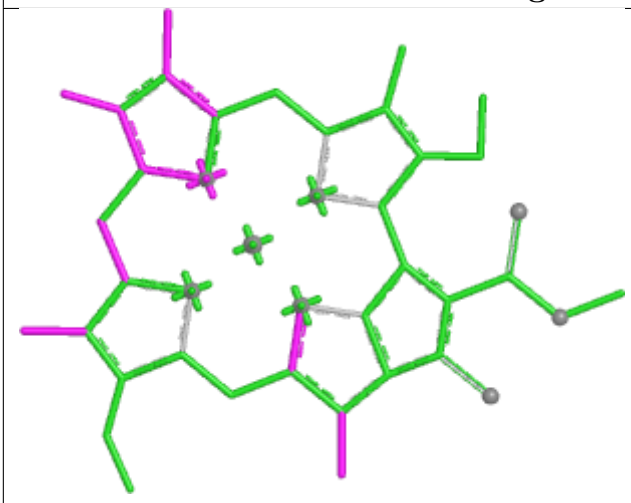


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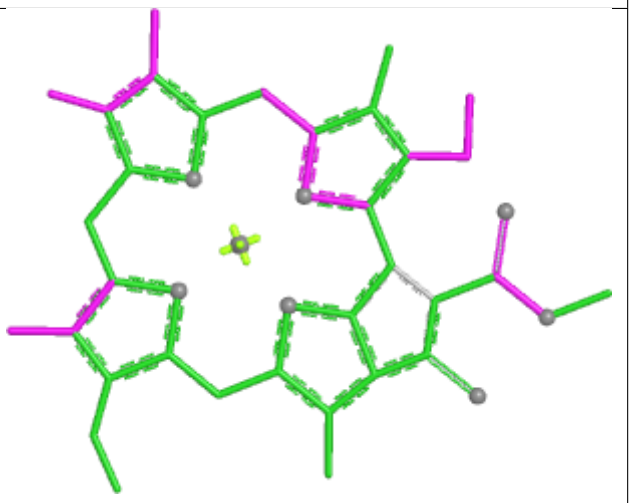


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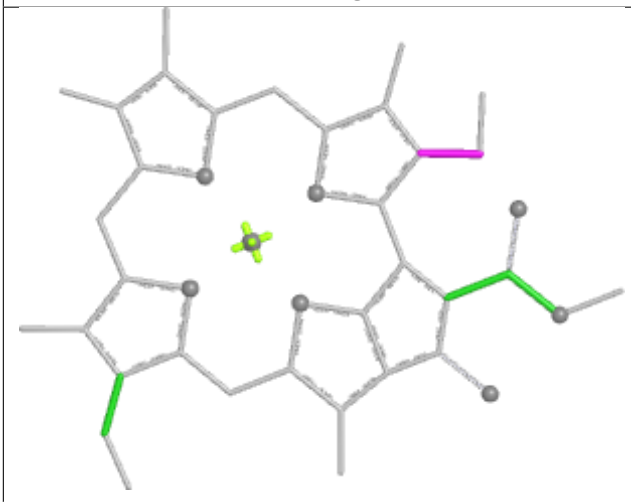
Ligand CLA 3 305



Bond lengths



Bond angles

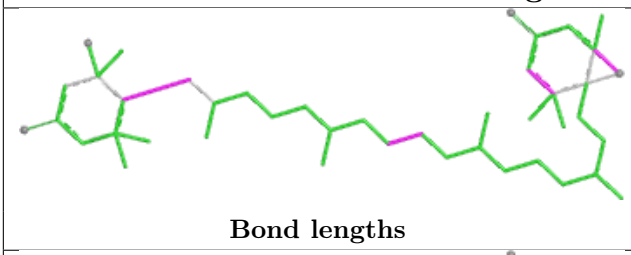


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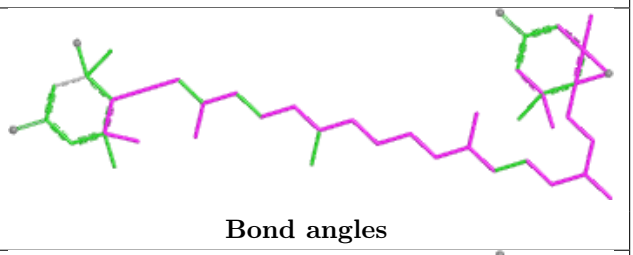


Rings

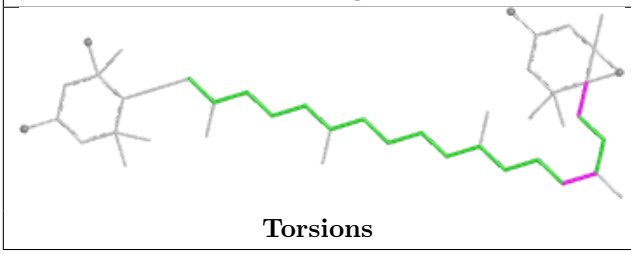
Ligand NEX S 317



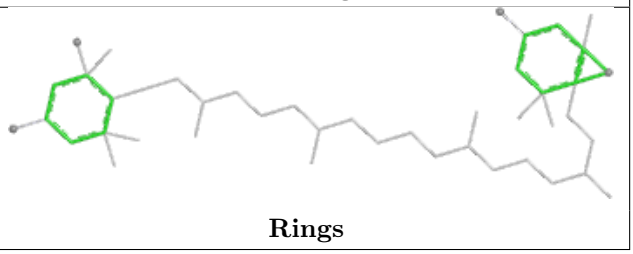
Bond lengths



Bond angles

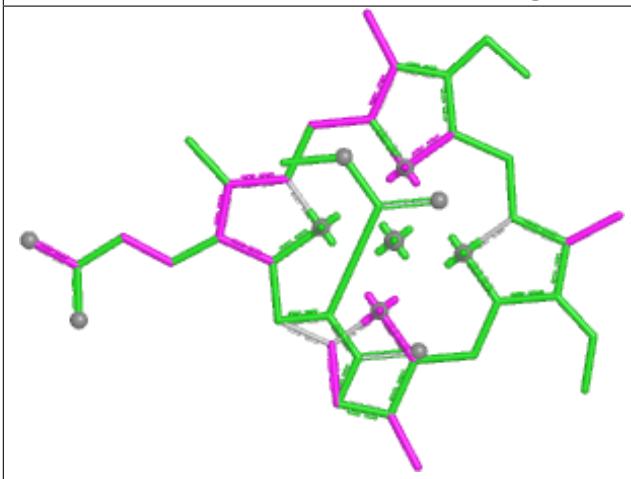


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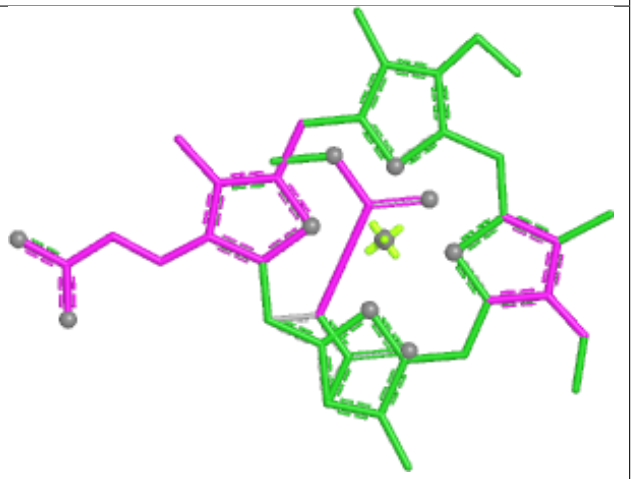


Rings

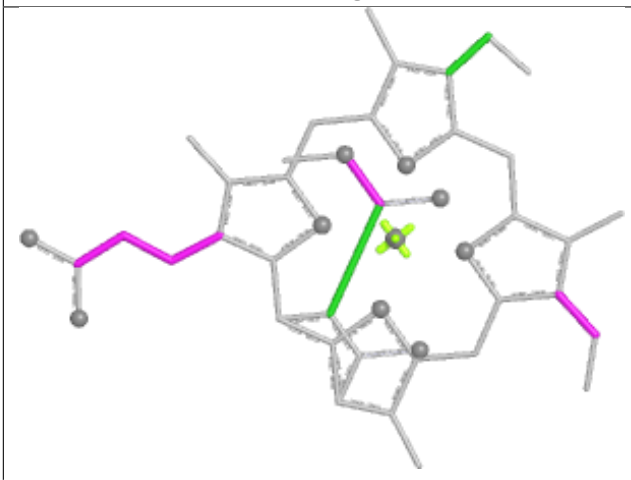
Ligand KC2 P 308



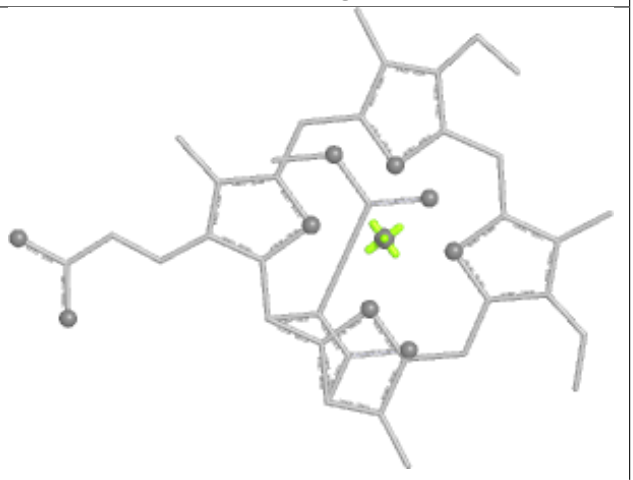
Bond lengths



Bond angles

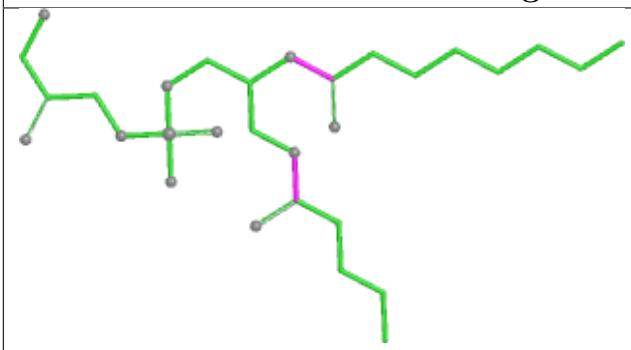


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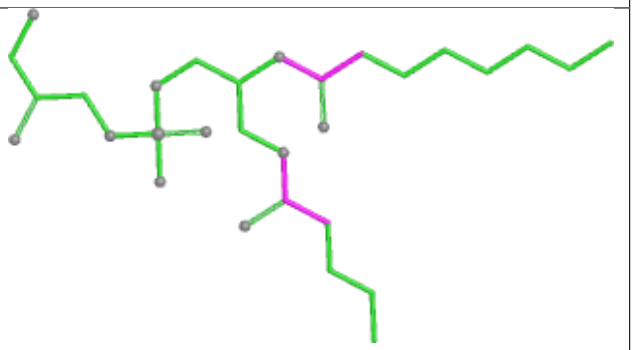


Rings

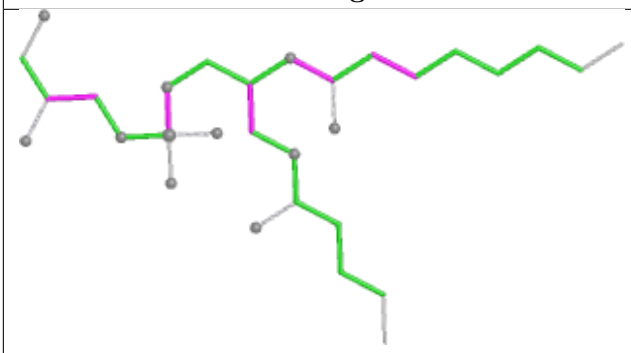
Ligand LHG A 847



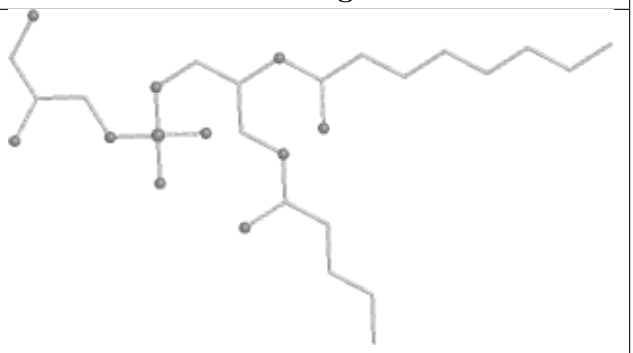
Bond lengths



Bond angles

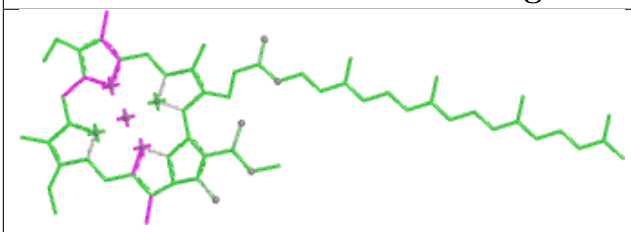


Torsions

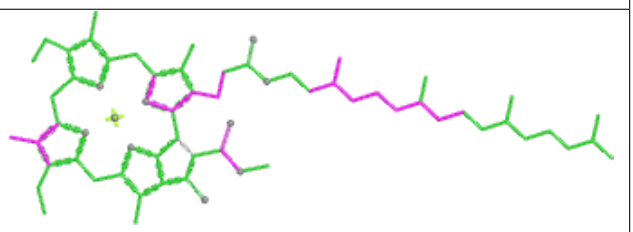


Rings

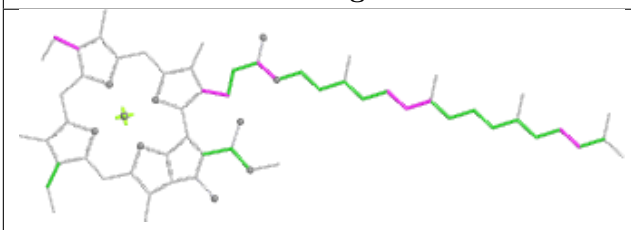
Ligand CLA B 809



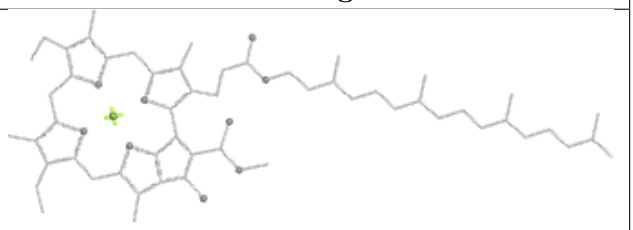
Bond lengths



Bond angles

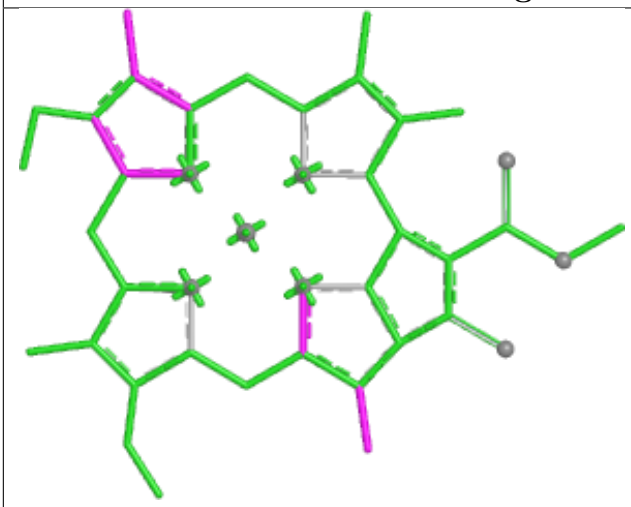


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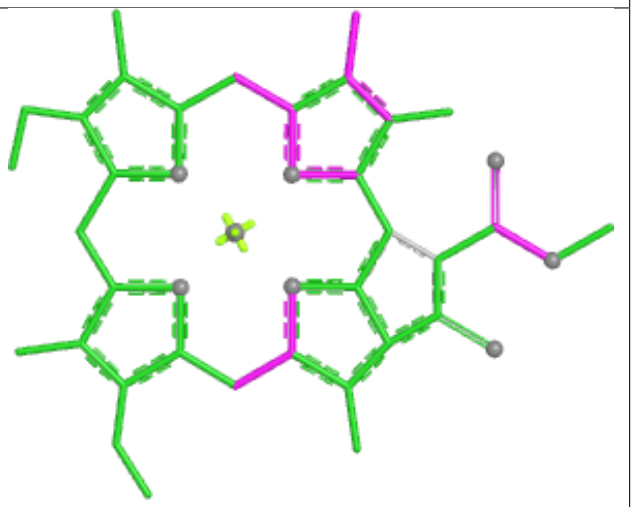


Rings

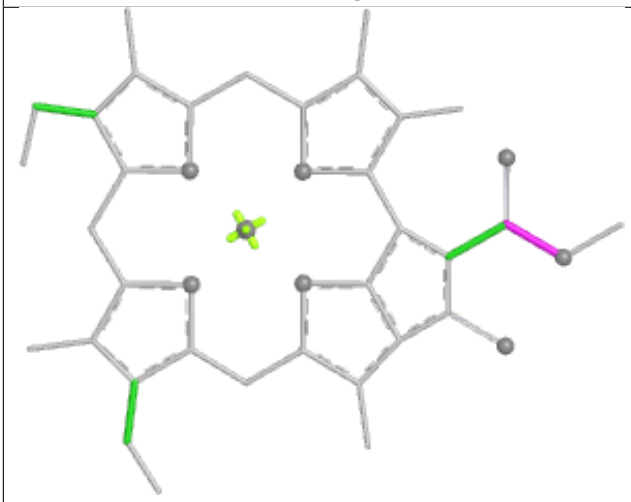
Ligand CLA O 2005



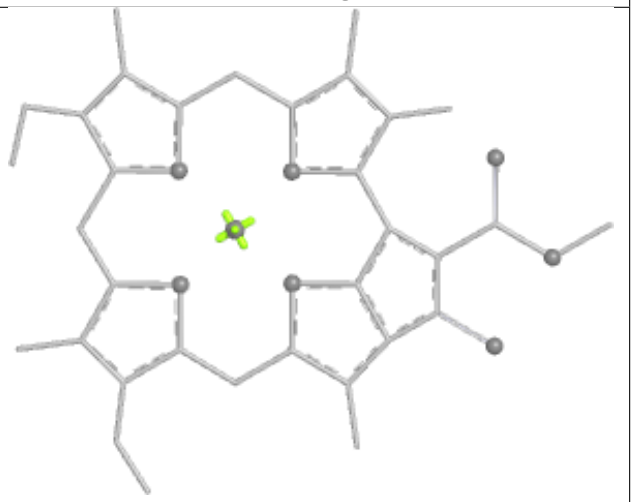
Bond lengths



Bond angles

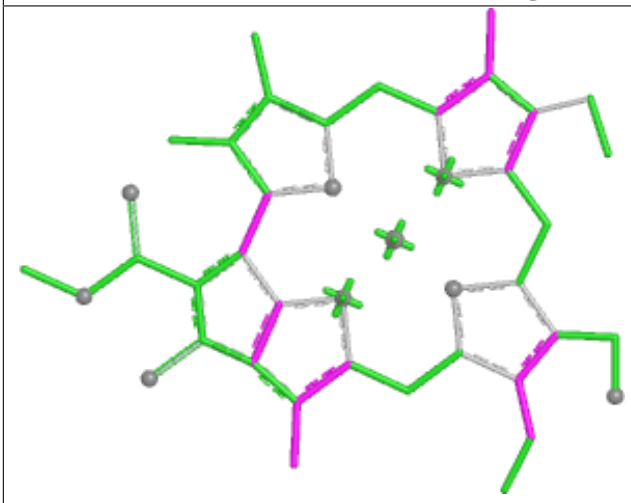


Torsions



Rings

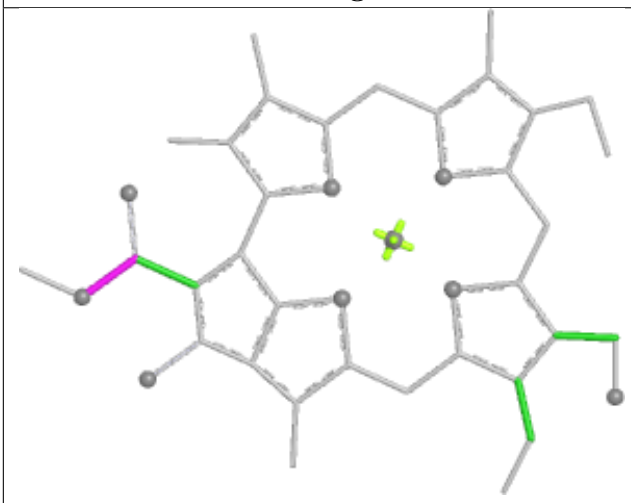
Ligand CHL T 314



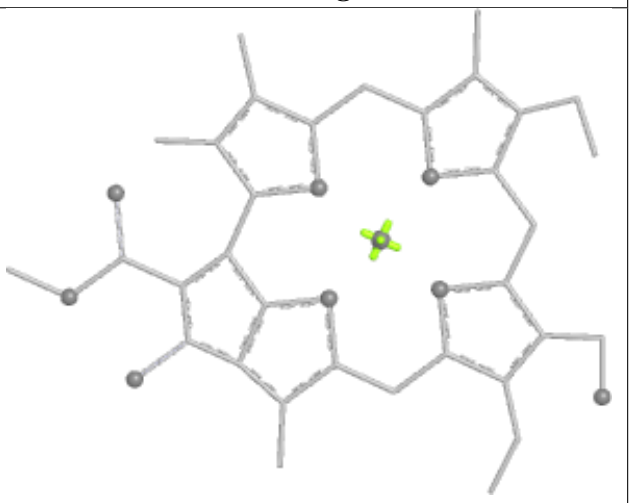
Bond lengths



Bond angles

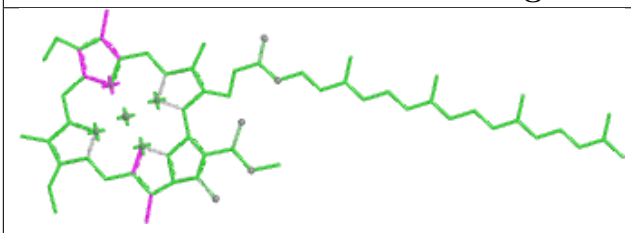


Torsions

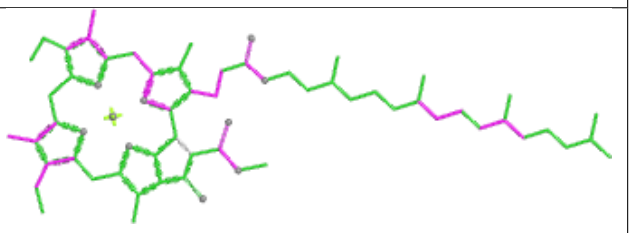


Rings

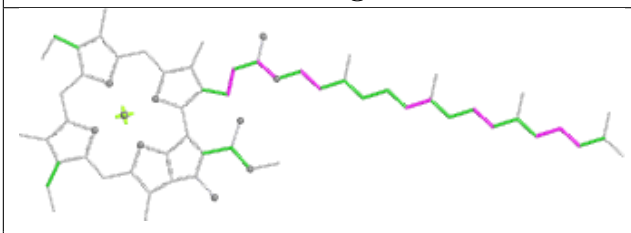
Ligand CLA B 802



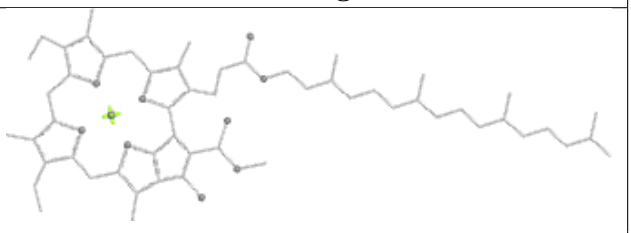
Bond lengths



Bond angles



Torsions

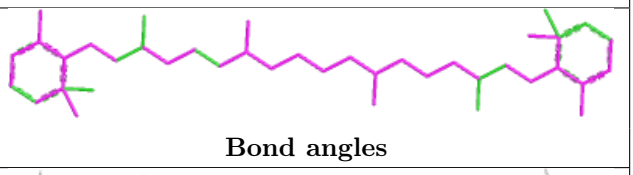


Rings

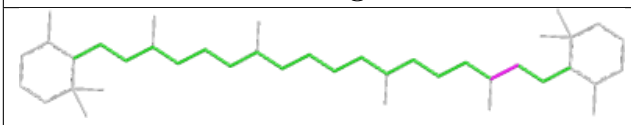
Ligand BCR 4 319



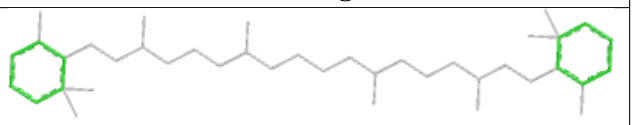
Bond lengths



Bond angles

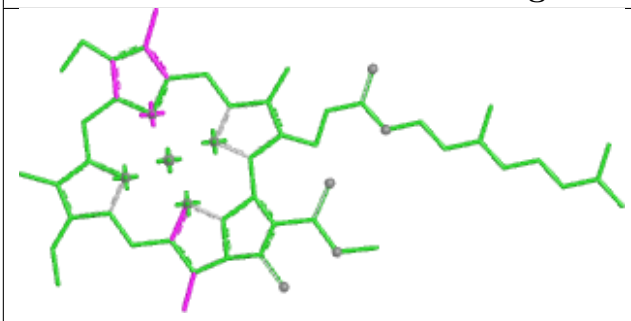


Torsions

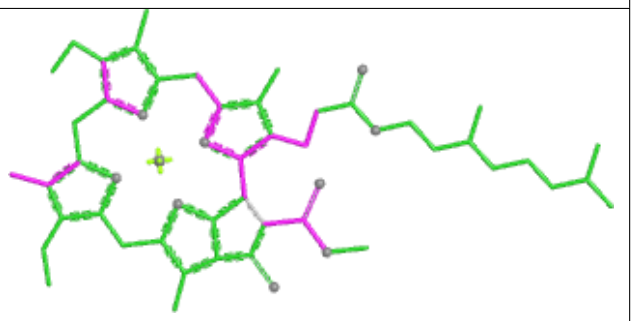


Rings

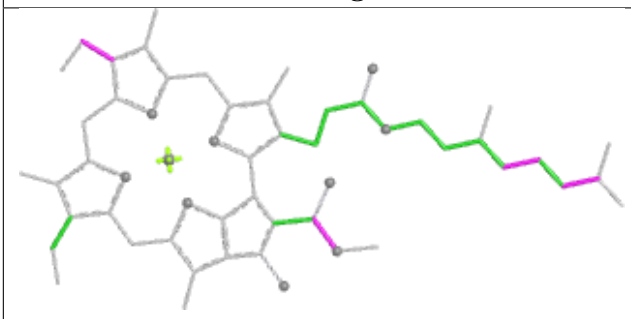
Ligand CLA 2 609



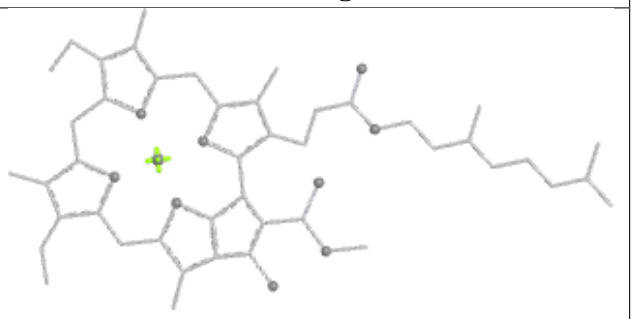
Bond lengths



Bond angles

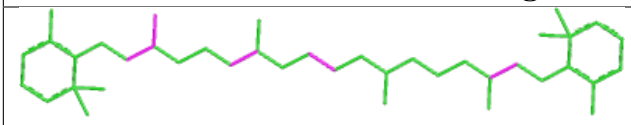


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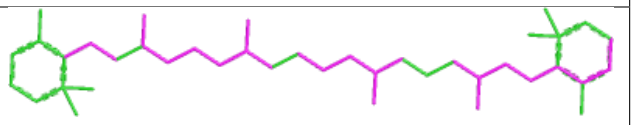


Rings

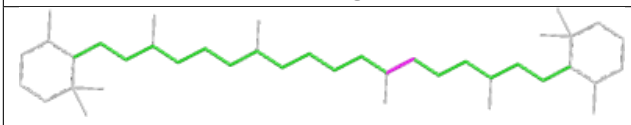
Ligand BCR G 205



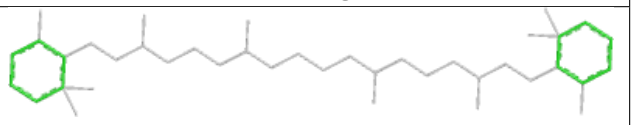
Bond lengths



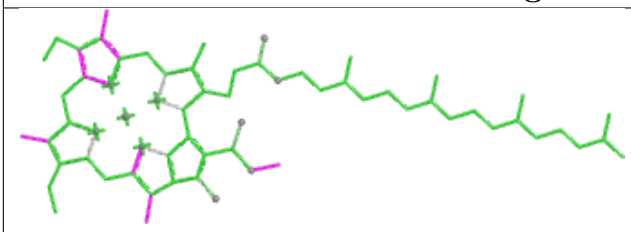
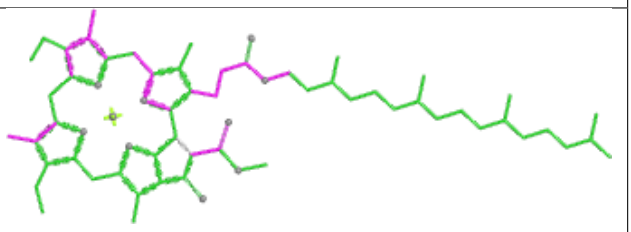
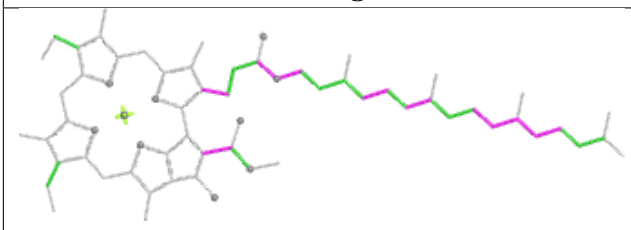
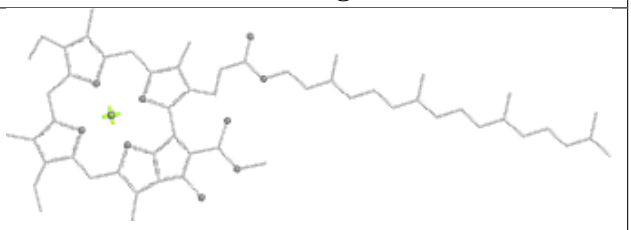
Bond angles

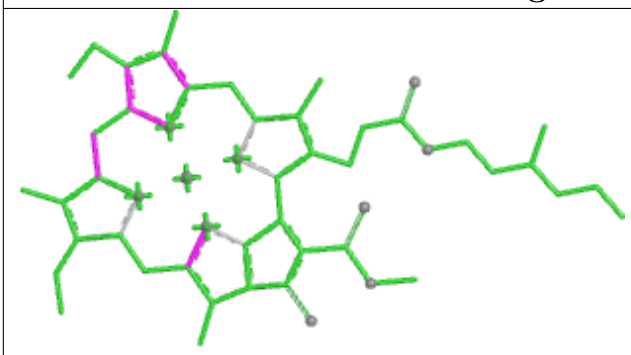
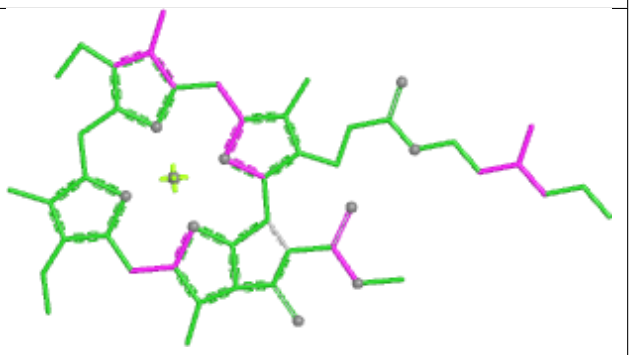
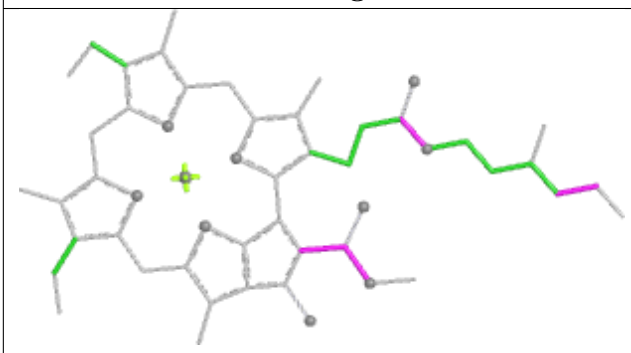
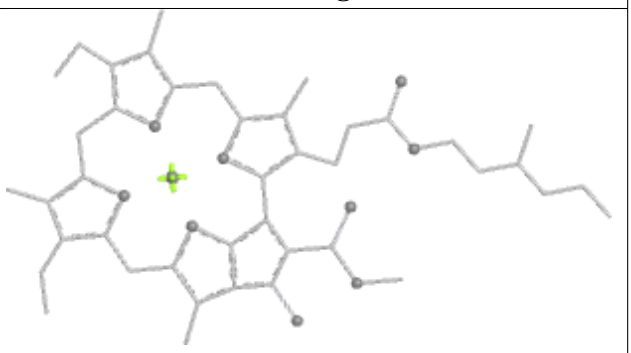


Torsions

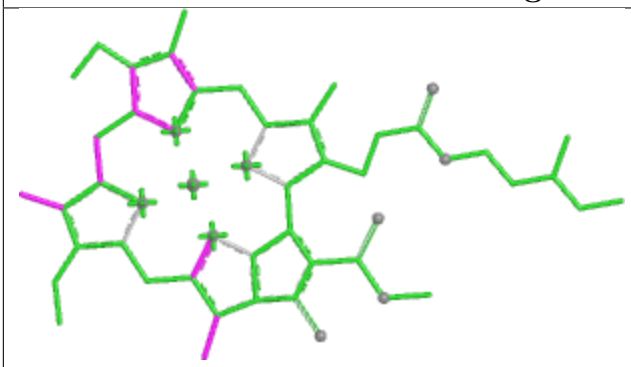


Rings

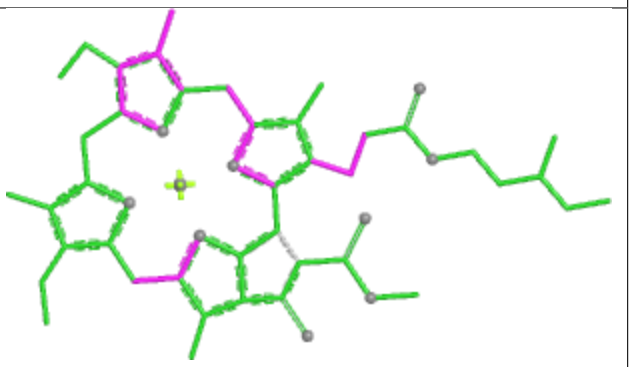
Ligand CLA B 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

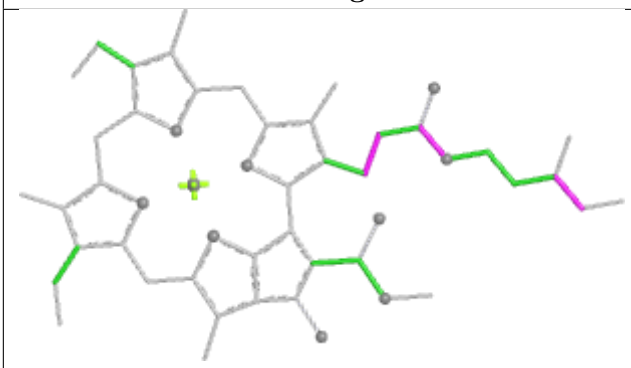
Ligand CLA B 816



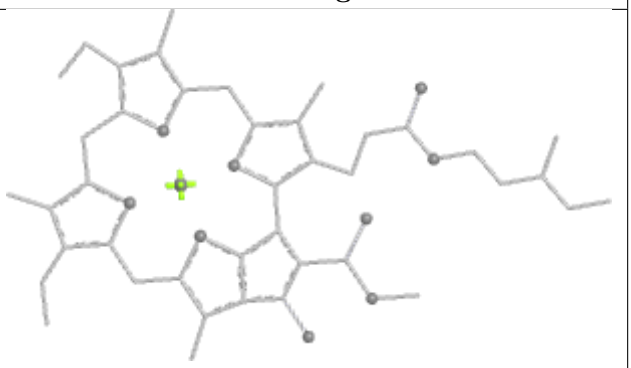
Bond lengths



Bond angles

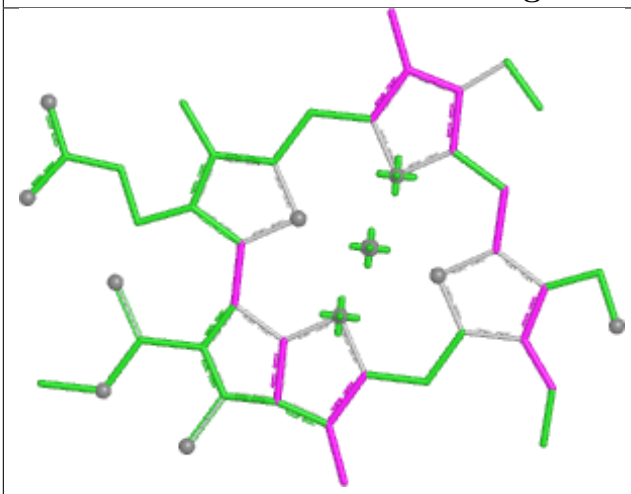


Torsions

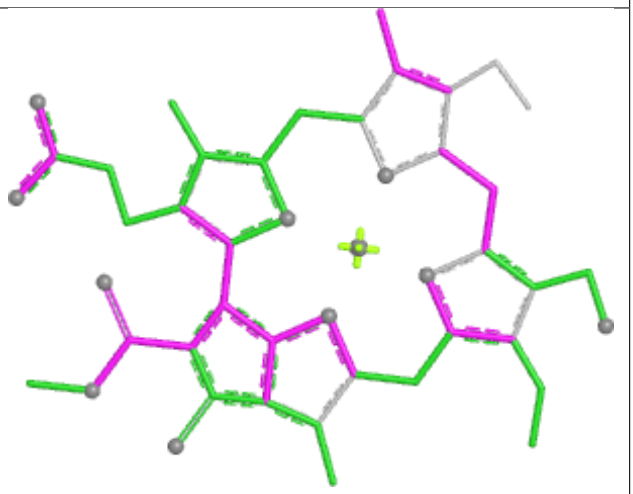


Rings

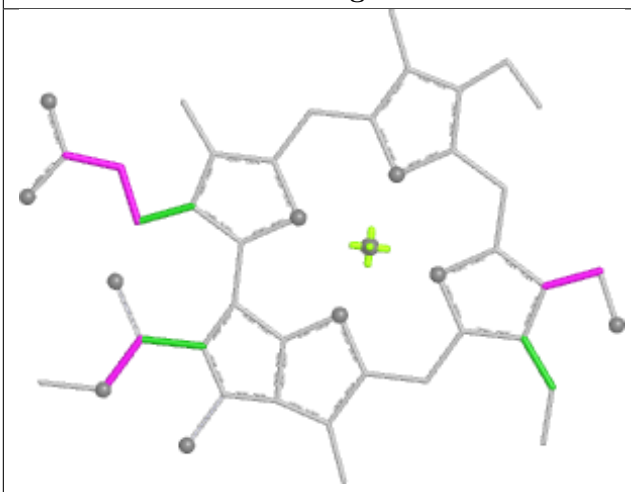
Ligand CHL V 304



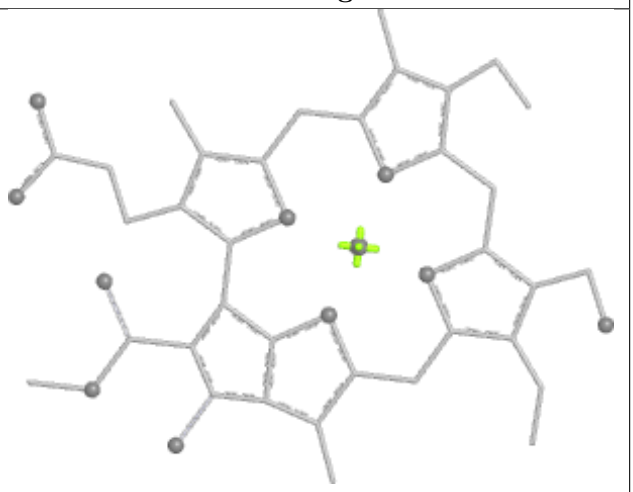
Bond lengths



Bond angles

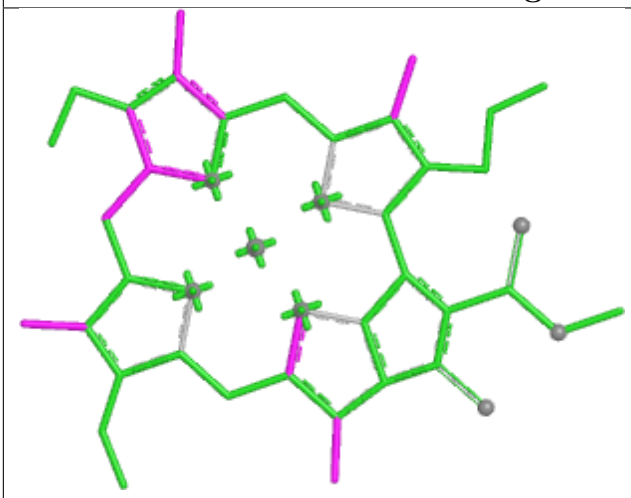


Torsions

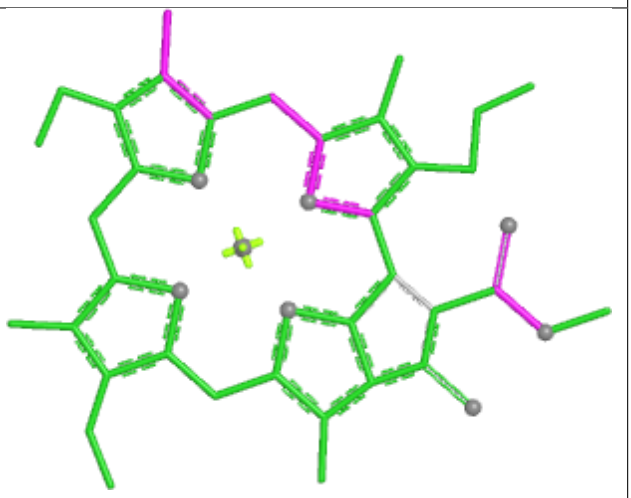


Rings

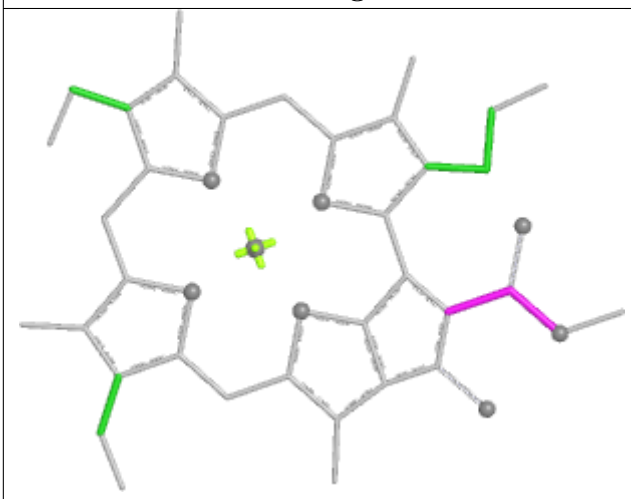
Ligand CLA B 817



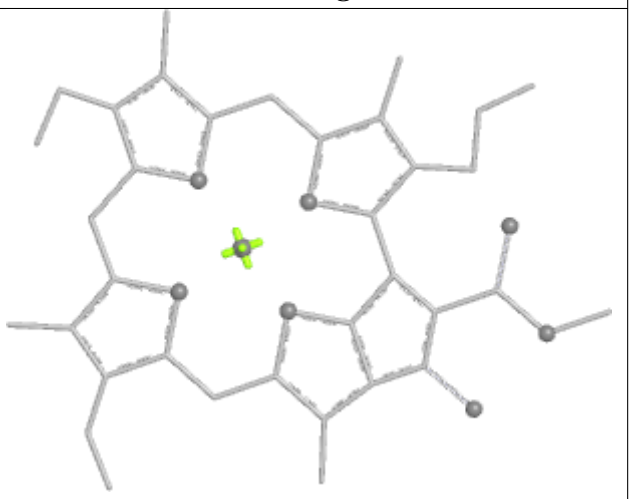
Bond lengths



Bond angles

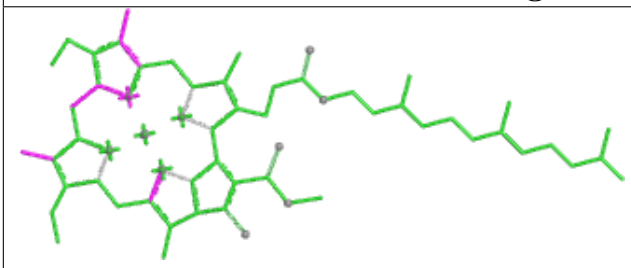


Torsions

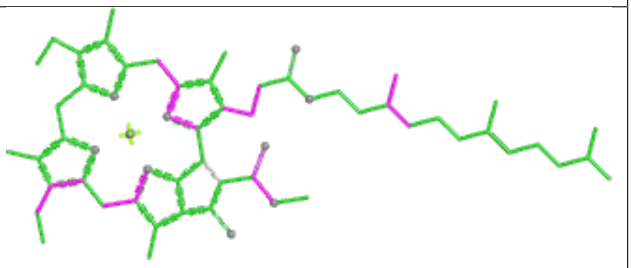


Rings

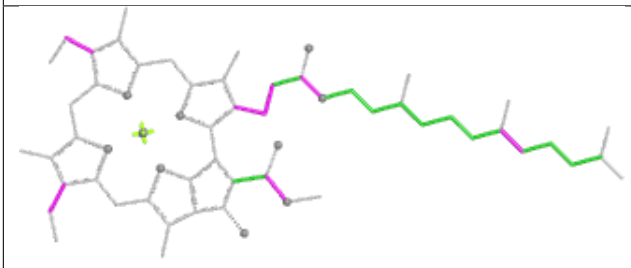
Ligand CLA L 302



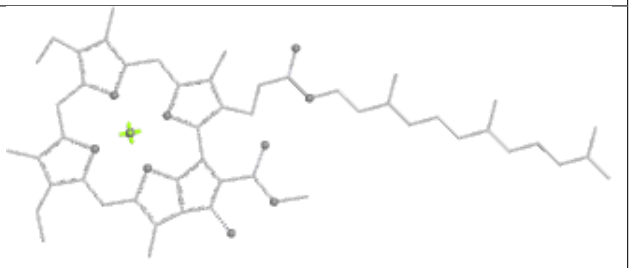
Bond lengths



Bond angles

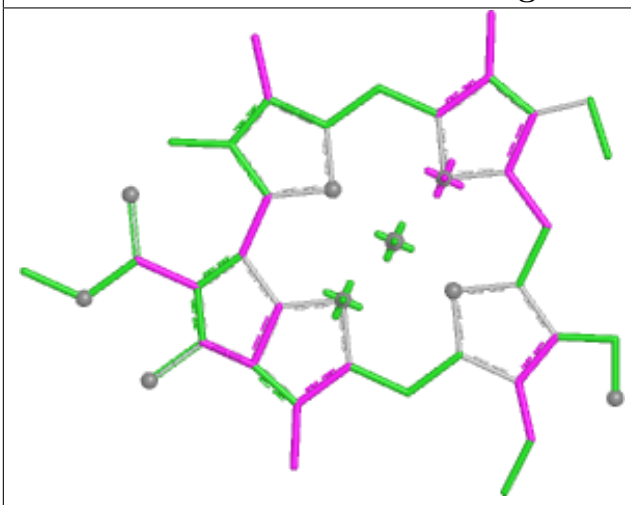


Torsions

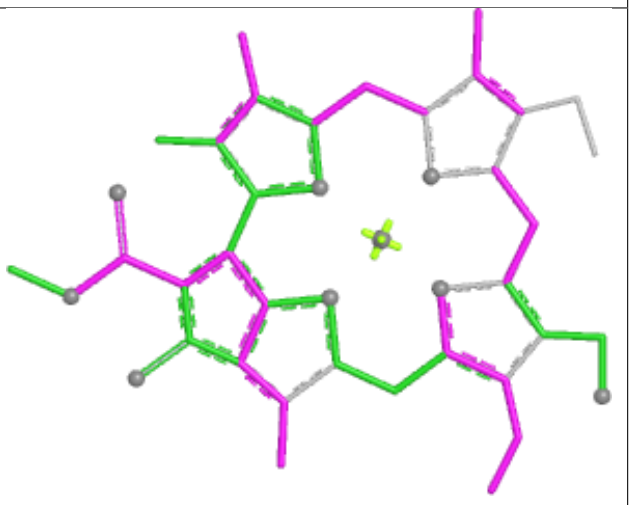


Rings

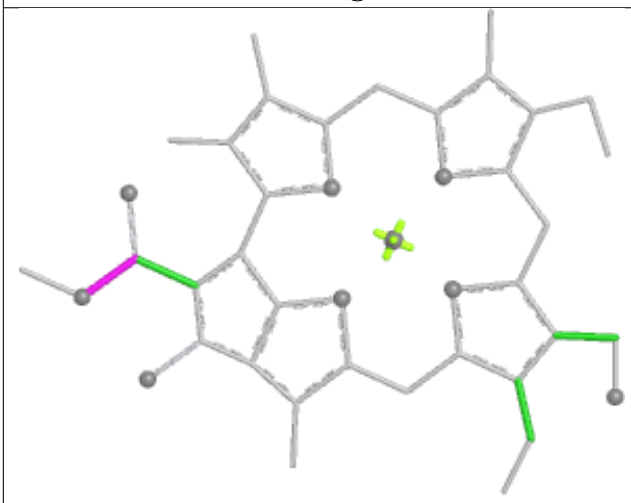
Ligand CHL W 305



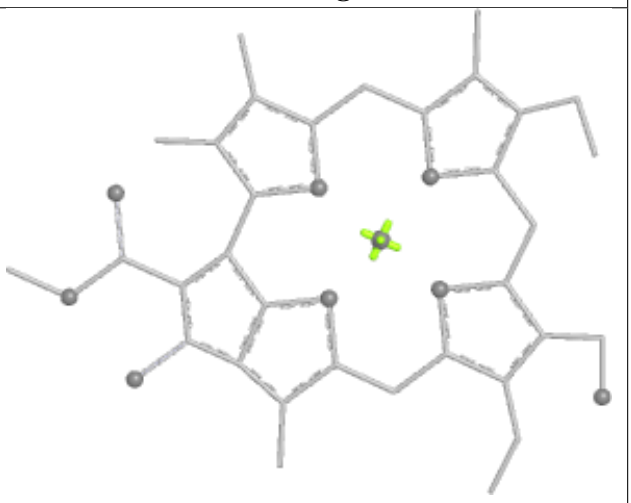
Bond lengths



Bond angles

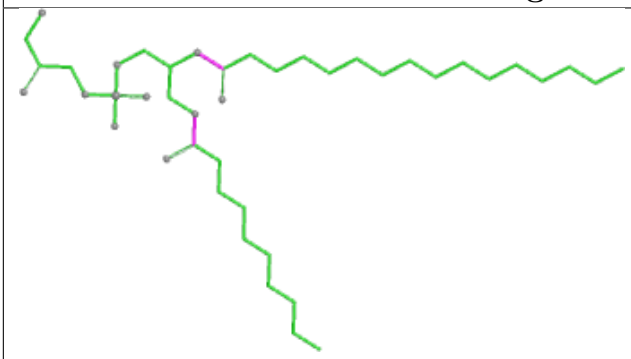


Torsions

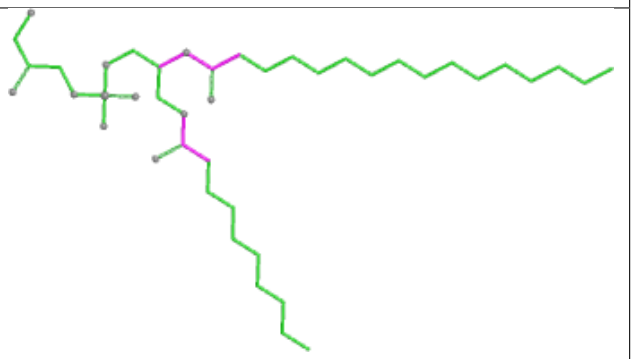


Rings

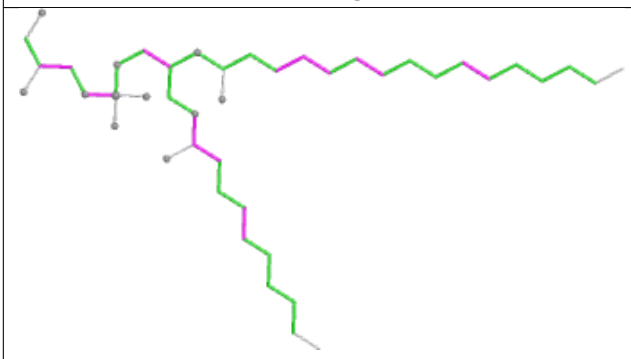
Ligand LHG 3 323



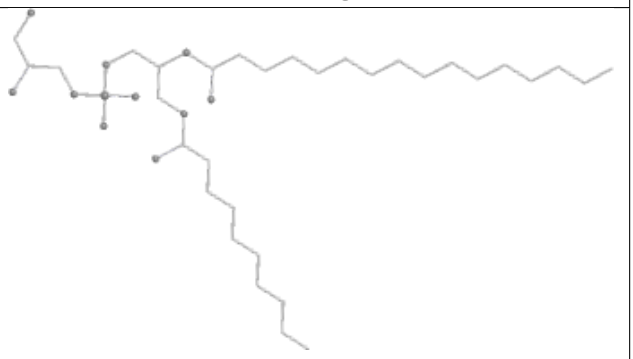
Bond lengths



Bond angles

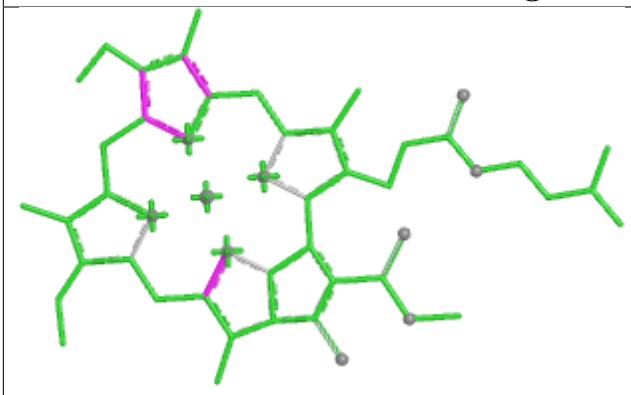


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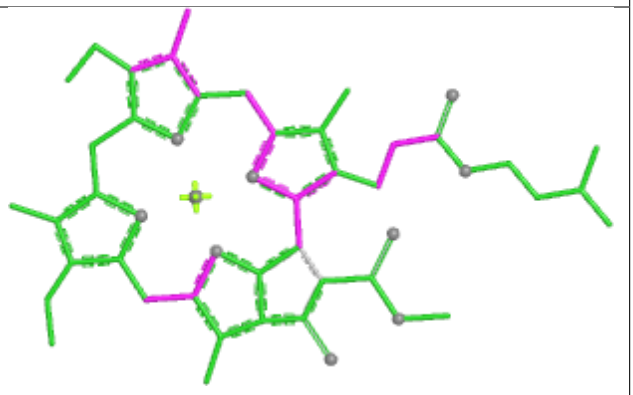


Rings

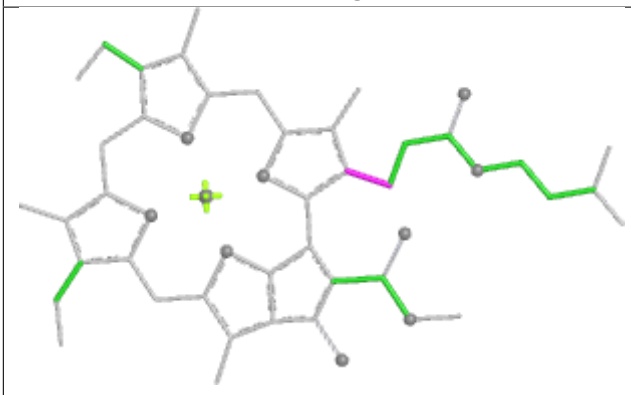
Ligand CLA A 811



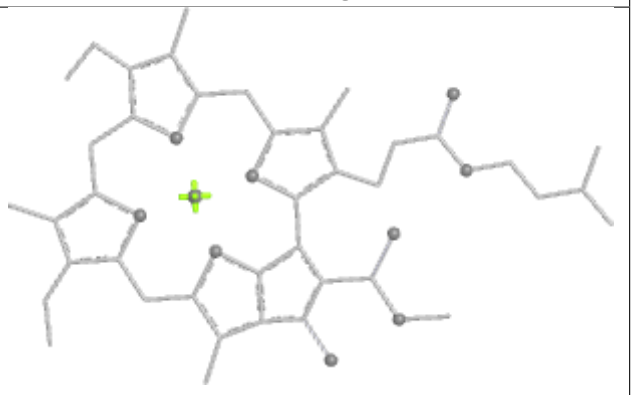
Bond lengths



Bond angles

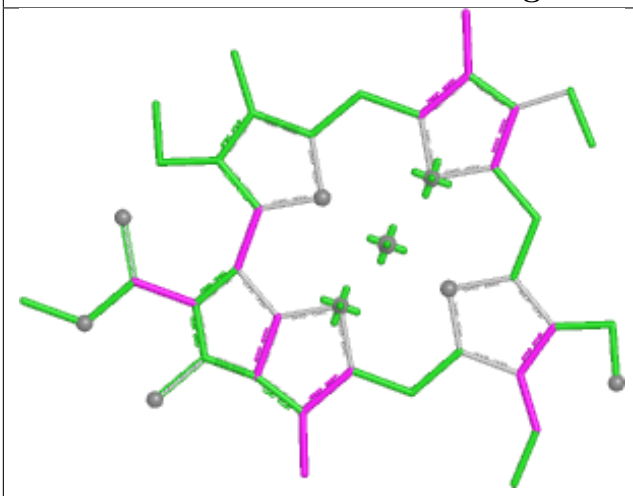


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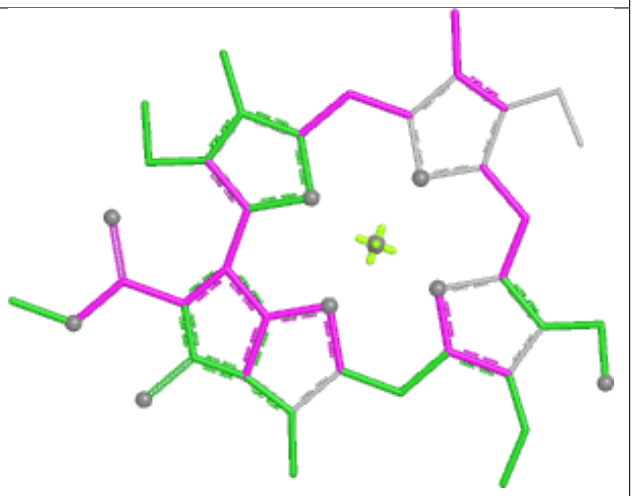


Rings

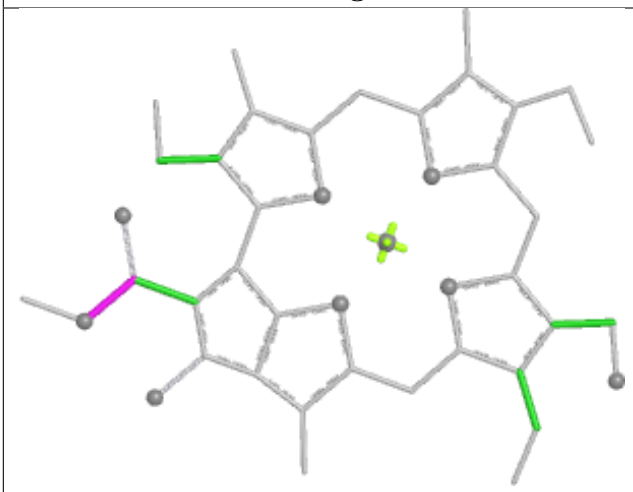
Ligand CHL U 313



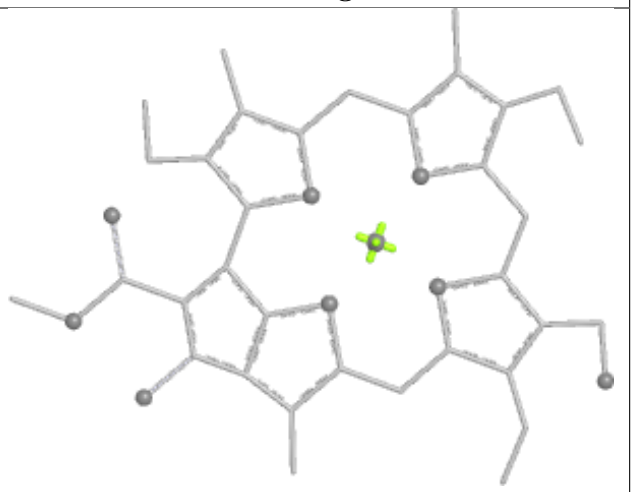
Bond lengths



Bond angles

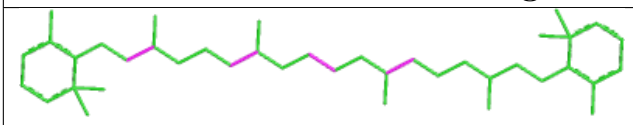


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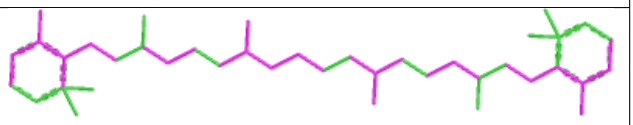


Rings

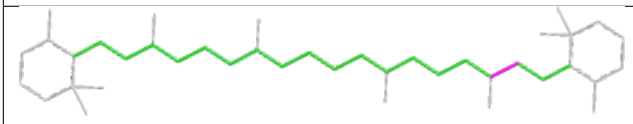
Ligand BCR K 205



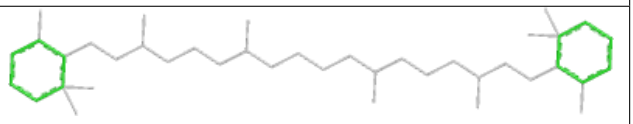
Bond lengths



Bond angles

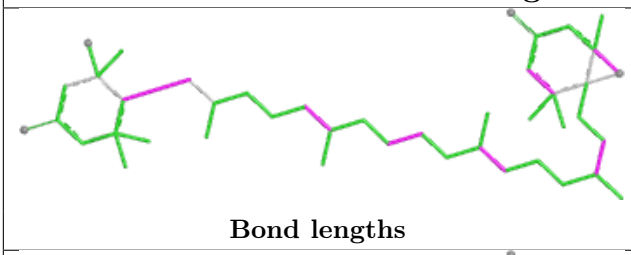


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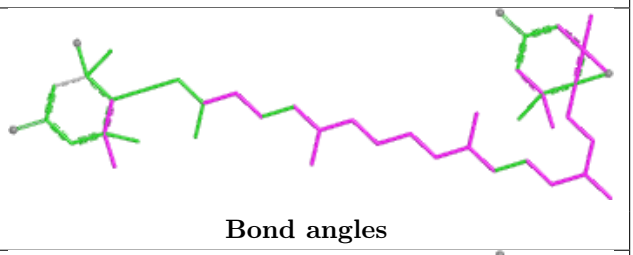


Rings

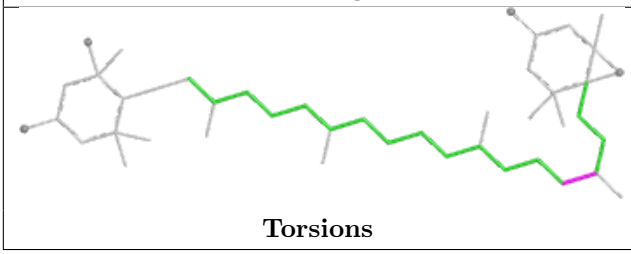
Ligand NEX P 317



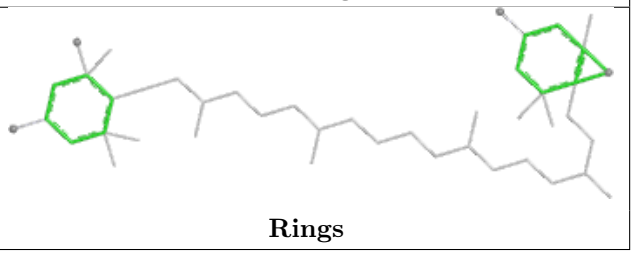
Bond lengths



Bond angles

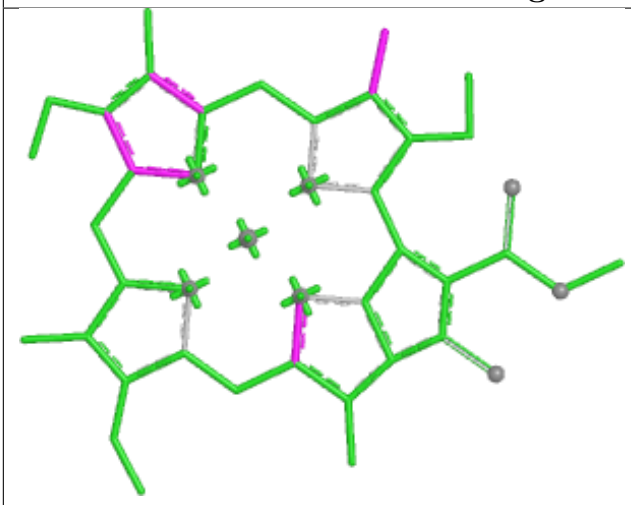


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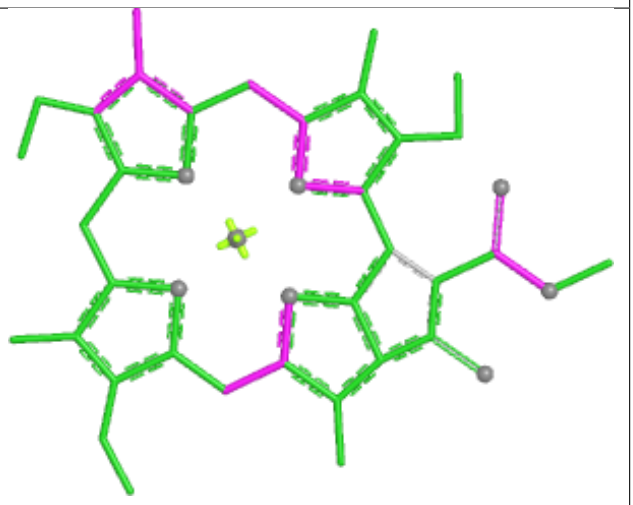


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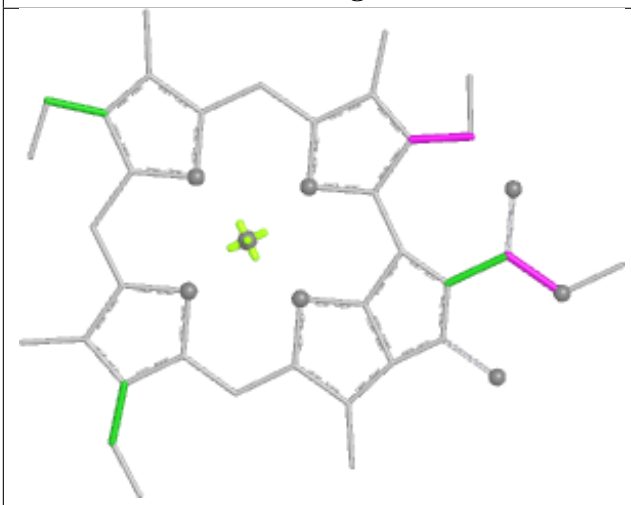
Ligand CLA 6 608



Bond lengths



Bond angles

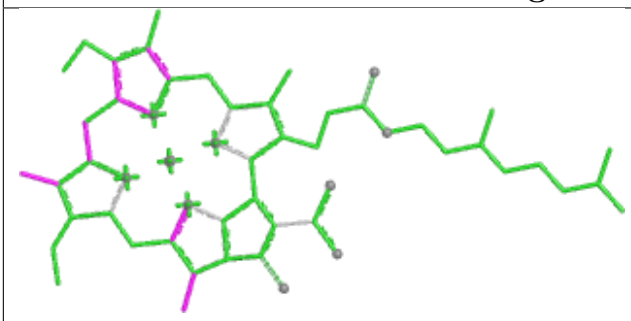


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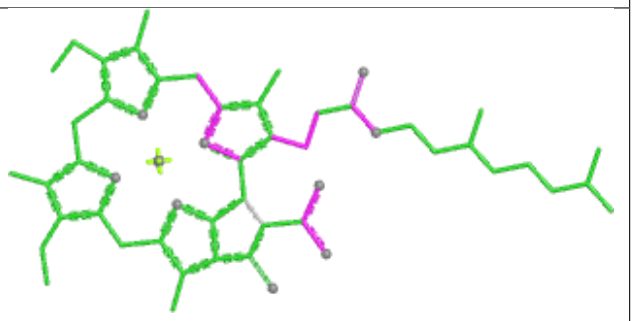


Rings

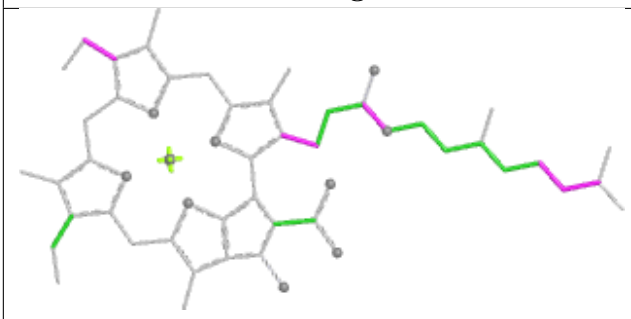
Ligand CLA 5 609



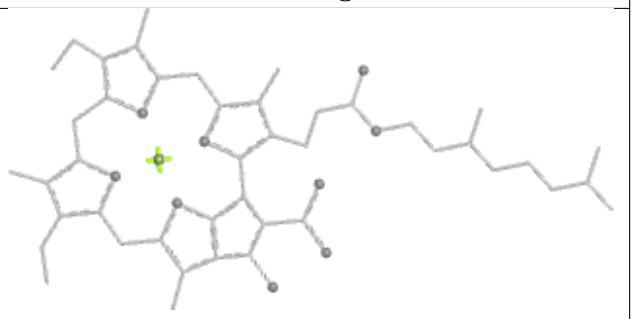
Bond lengths



Bond angles

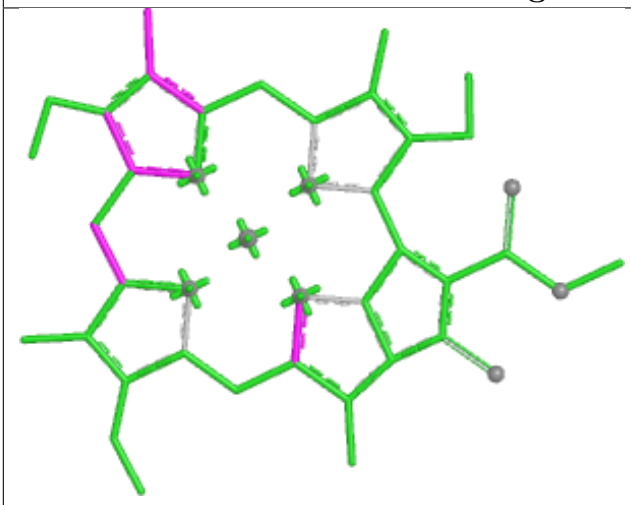


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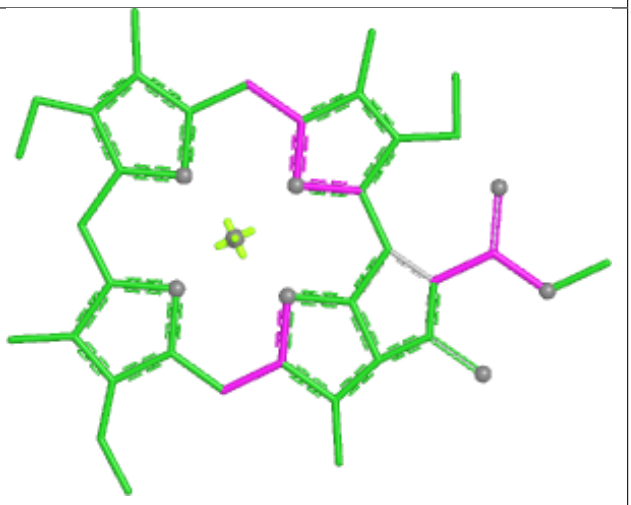


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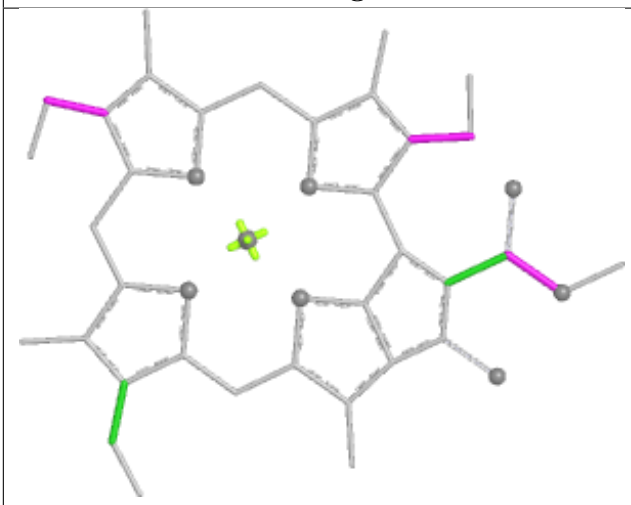
Ligand CLA 2 610



Bond lengths



Bond angles

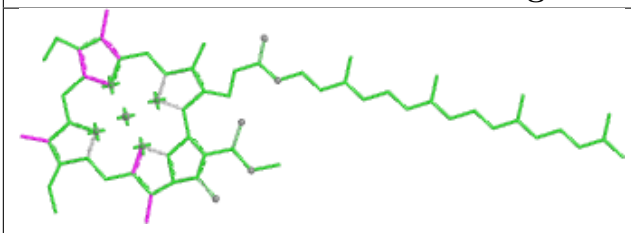


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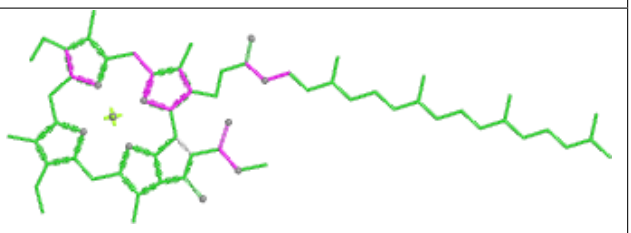


Rings

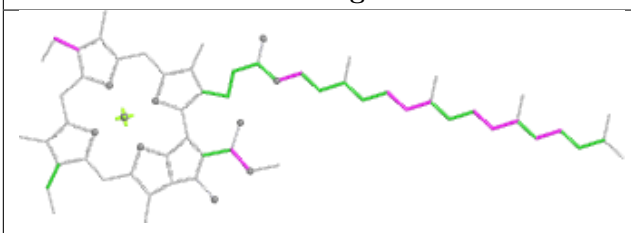
Ligand CLA S 302



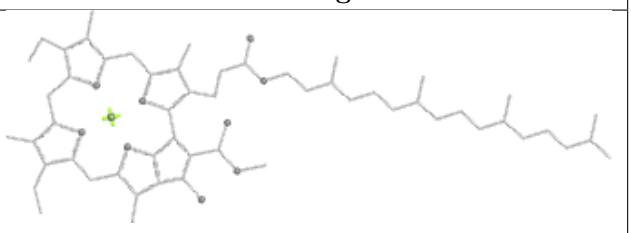
Bond lengths



Bond angles

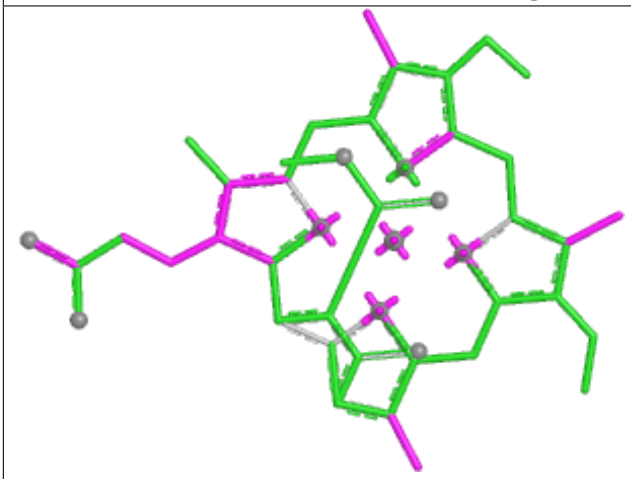


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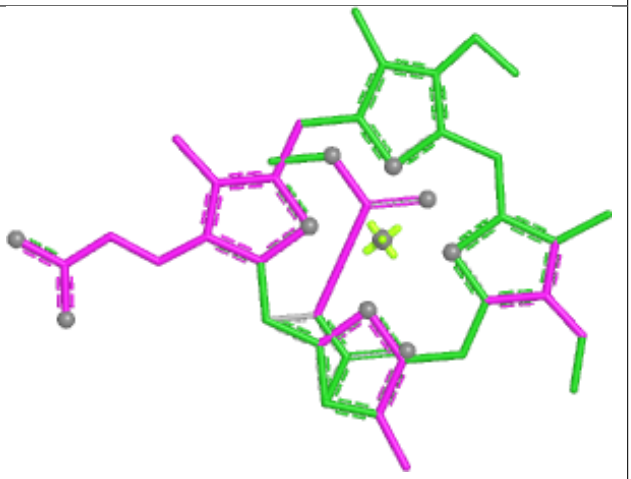


Rings

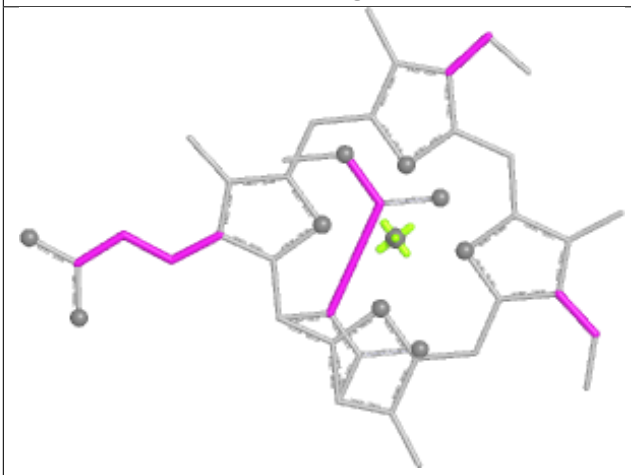
Ligand KC2 V 308



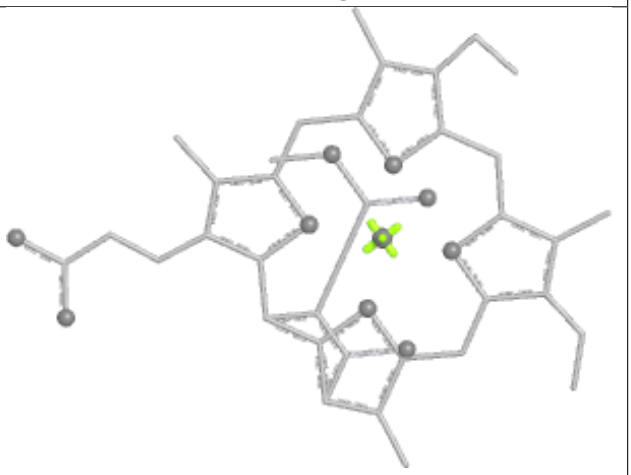
Bond lengths



Bond angles

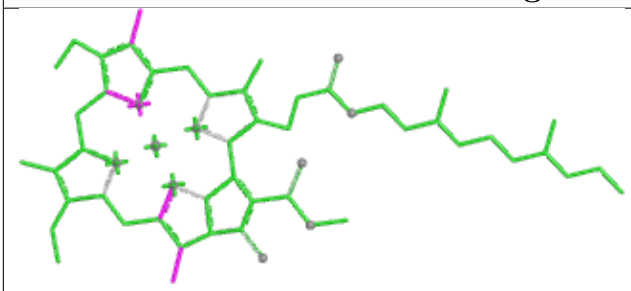


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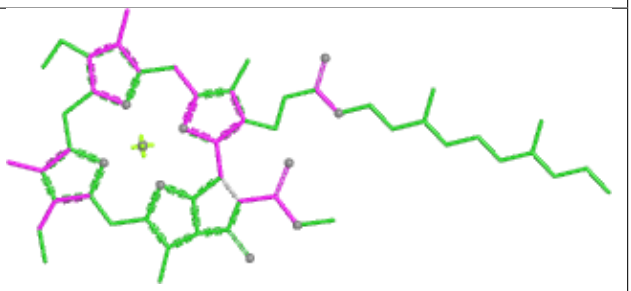


Rings

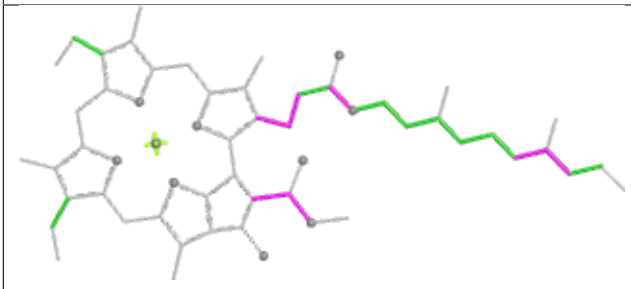
Ligand CLA A 856



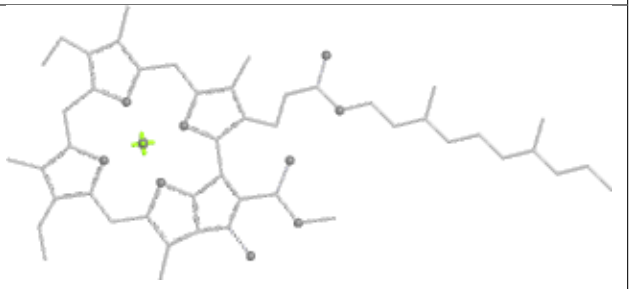
Bond lengths



Bond angles

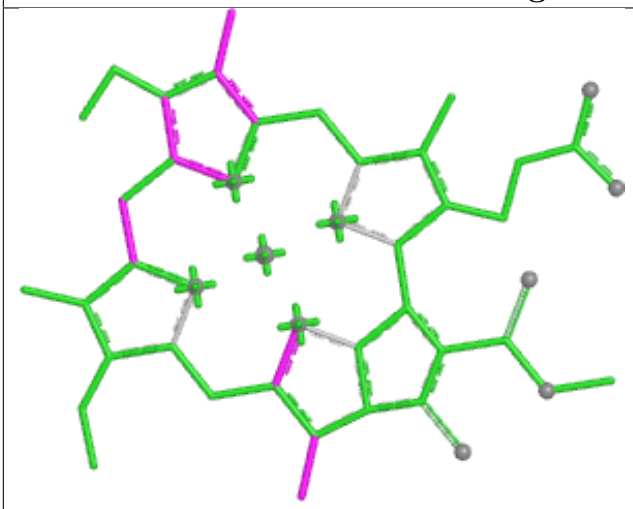


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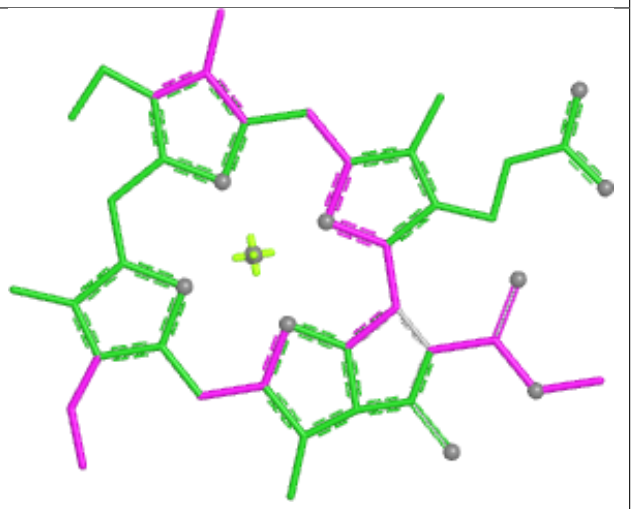


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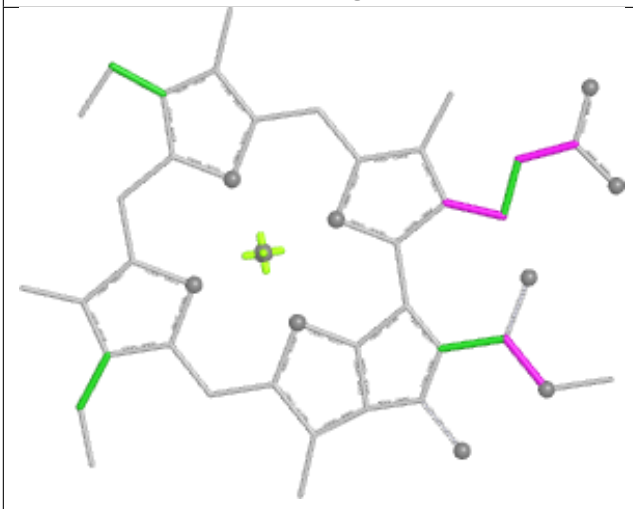
Ligand CLA 4 309



Bond lengths



Bond angles

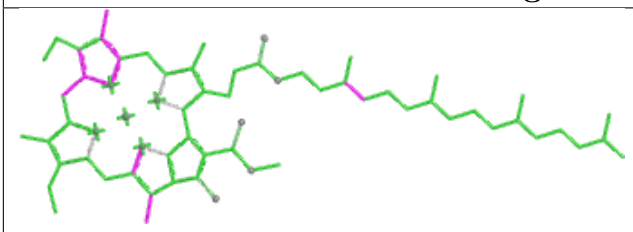


Torsions

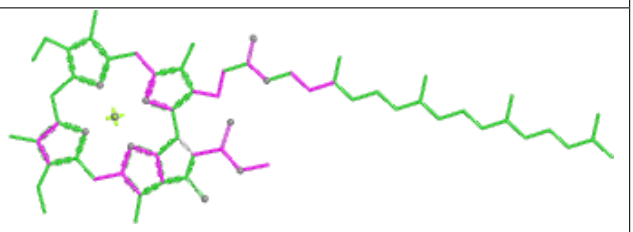


Rings

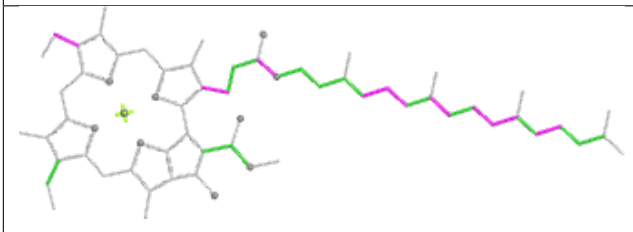
Ligand CLA A 842



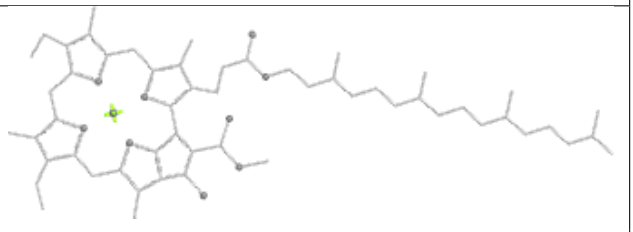
Bond lengths



Bond angles

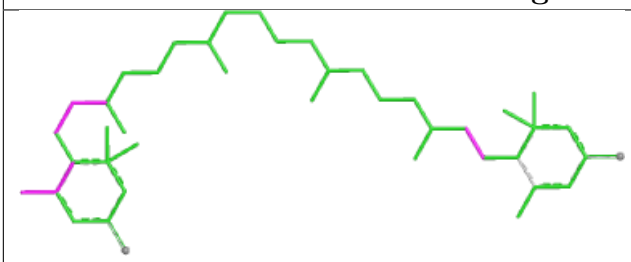


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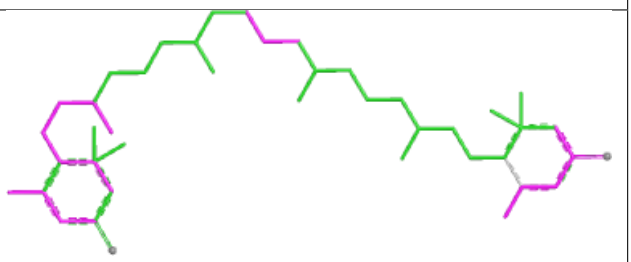


Rings

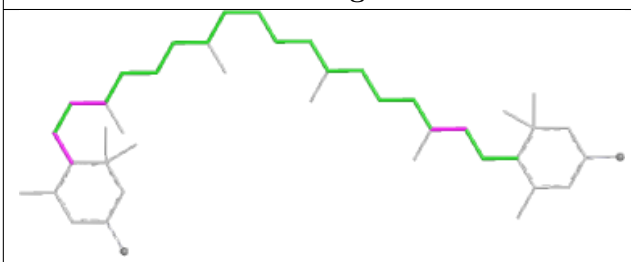
Ligand Q6L S 315



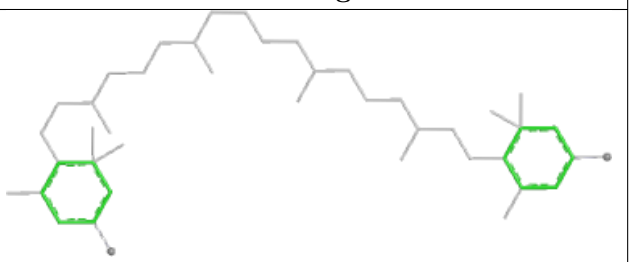
Bond lengths



Bond angles

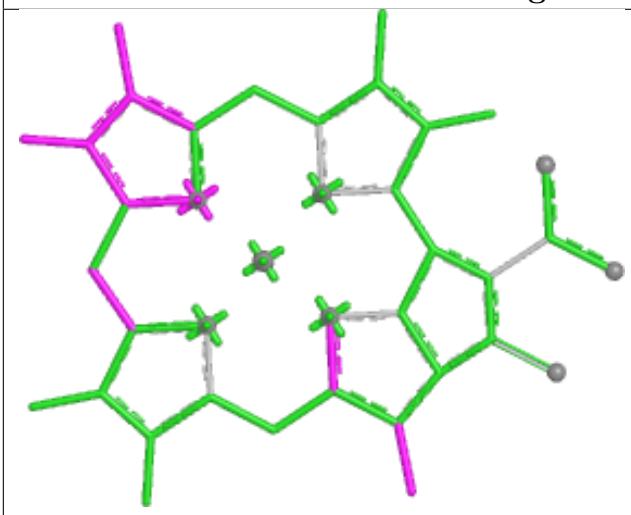


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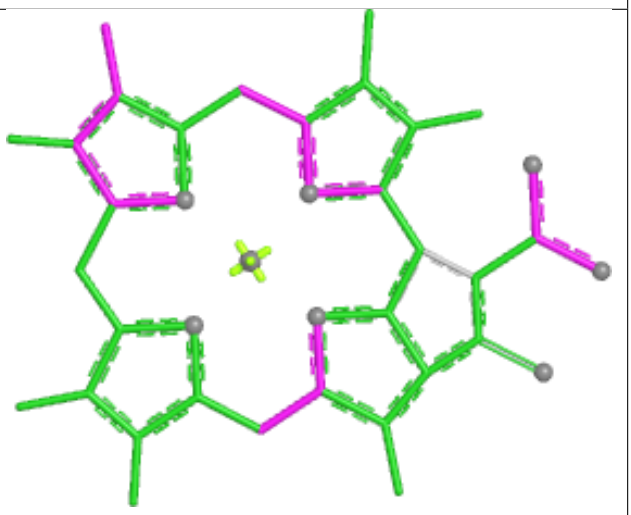


Rings

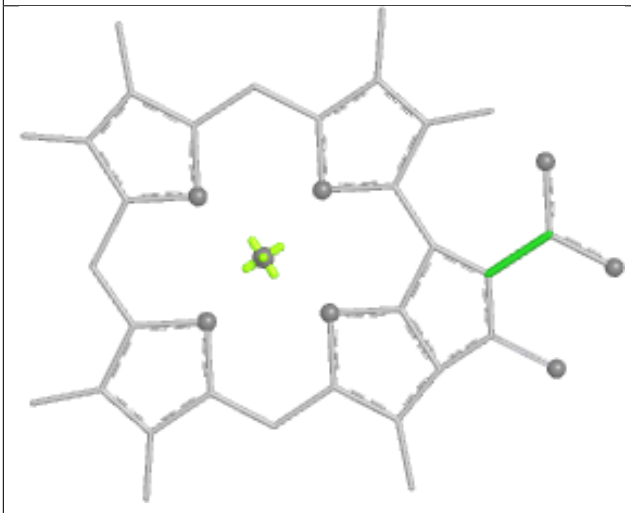
Ligand CLA 5 604



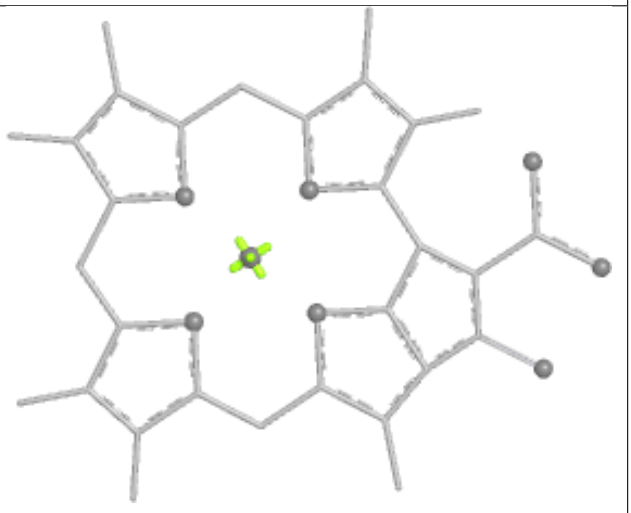
Bond lengths



Bond angles

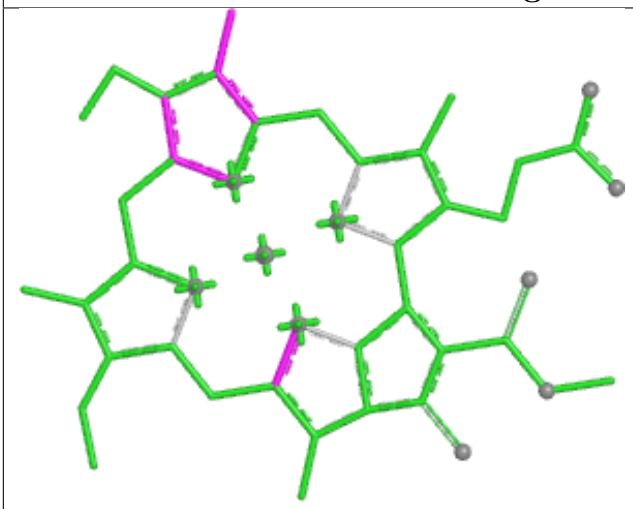


Torsions

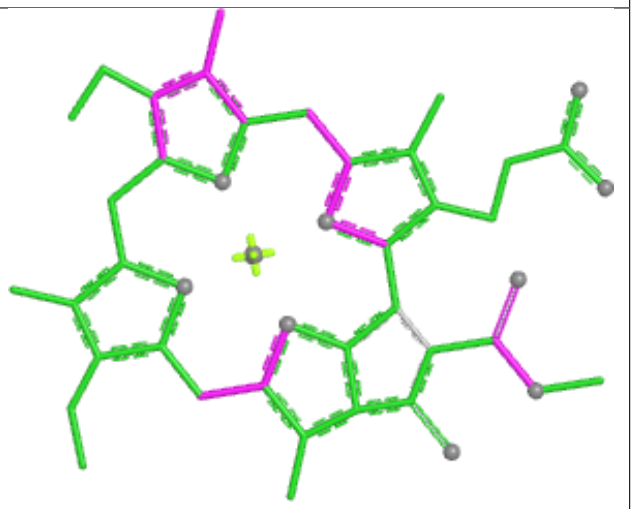


Rings

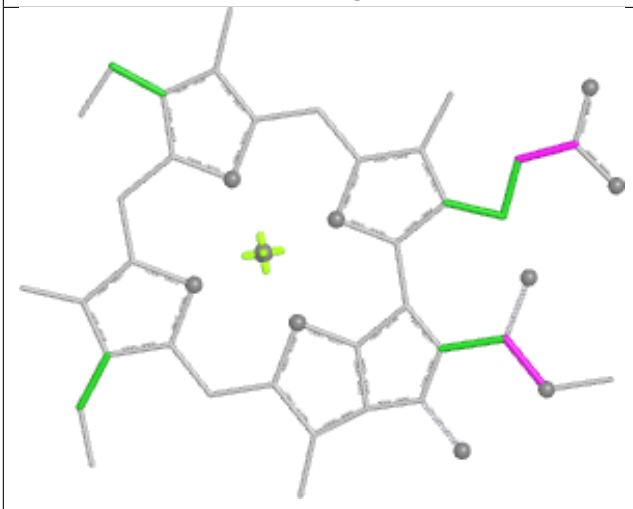
Ligand CLA A 818



Bond lengths



Bond angles

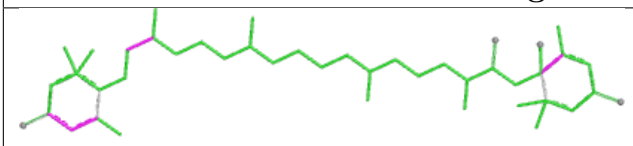


Torsions

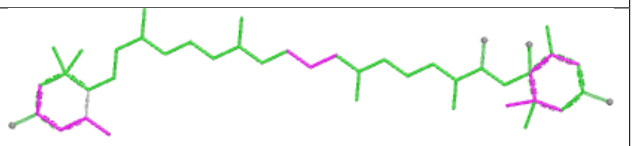


Rings

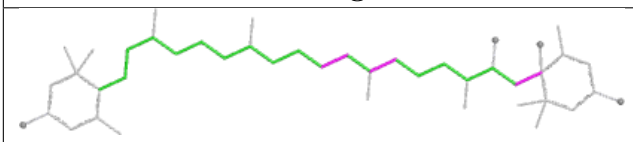
Ligand IWJ T 318



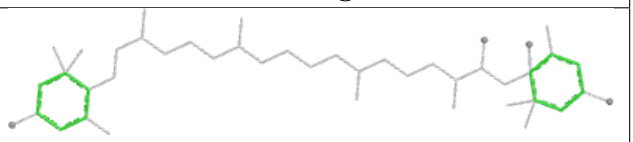
Bond lengths



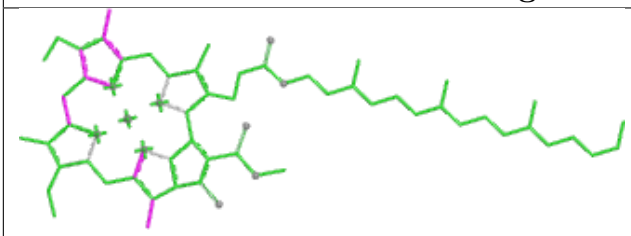
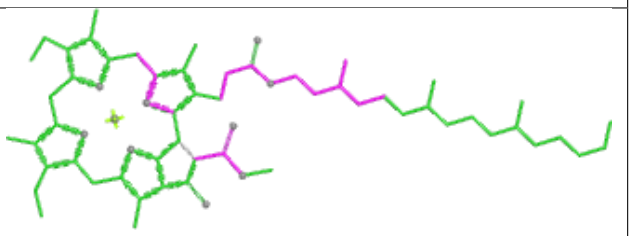
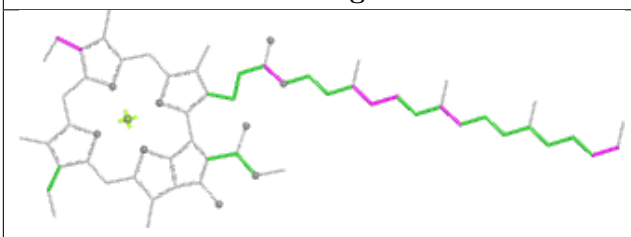
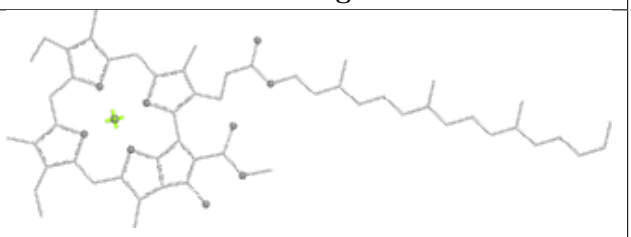
Bond angles

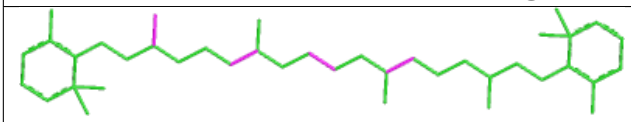
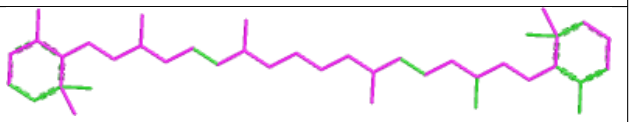
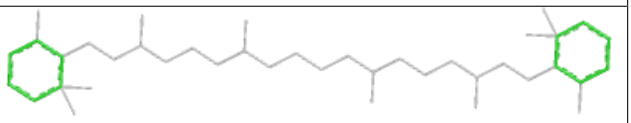


Torsions

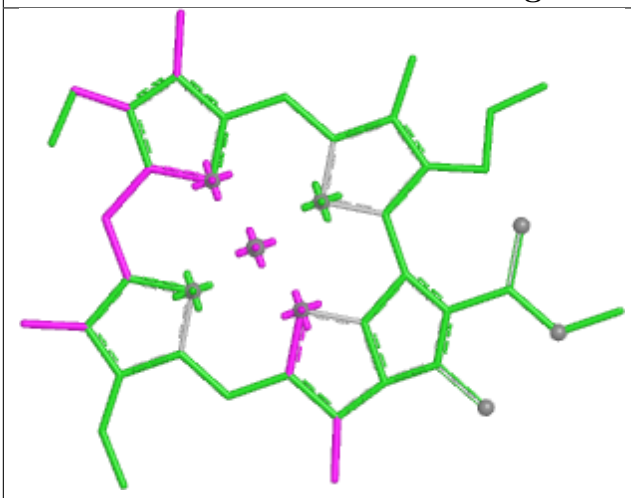


Rings

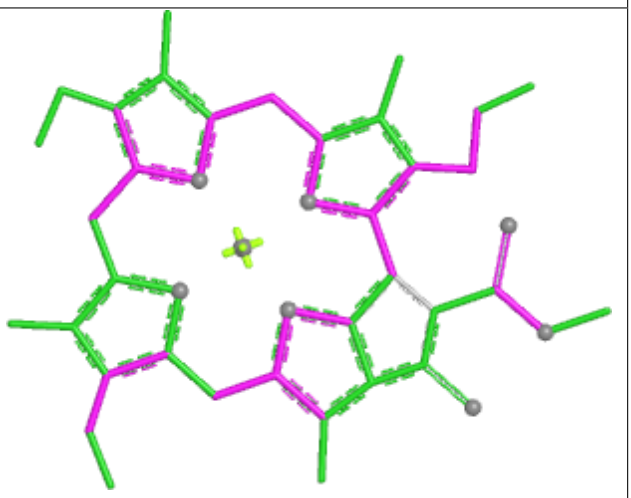
Ligand CLA W 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

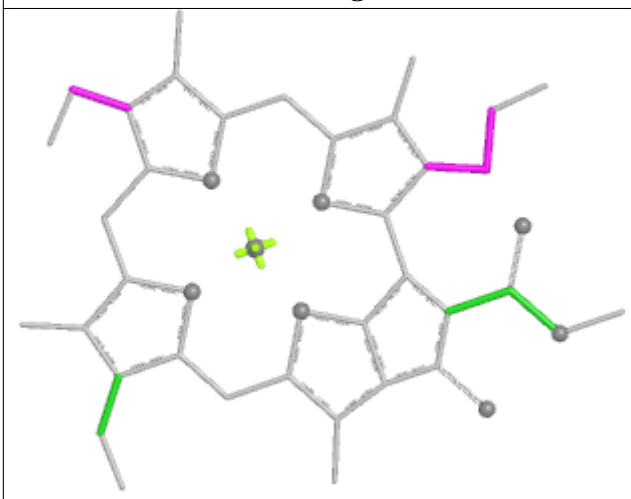
Ligand CLA B 832



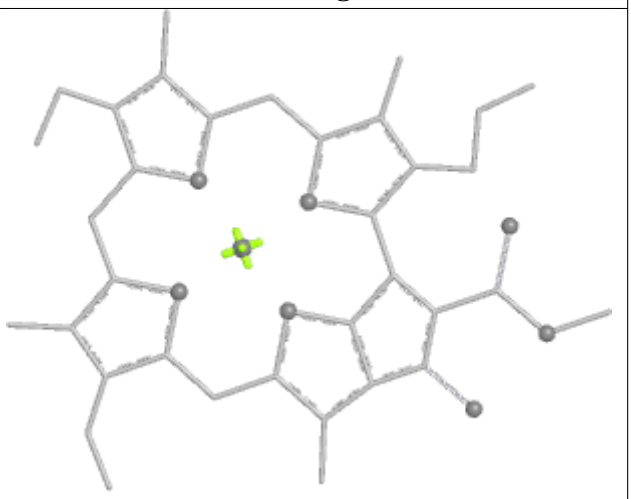
Bond lengths



Bond angles

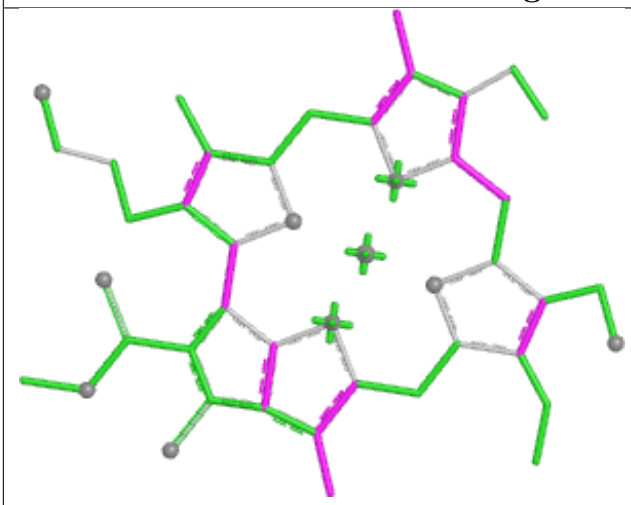


Torsions

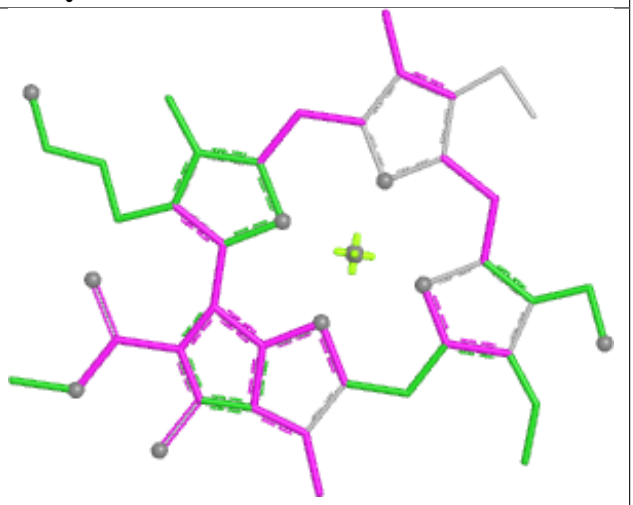


Rings

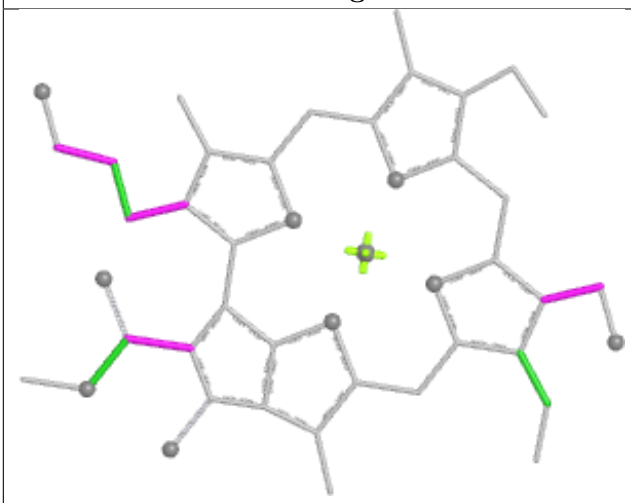
Ligand CHL Q 316



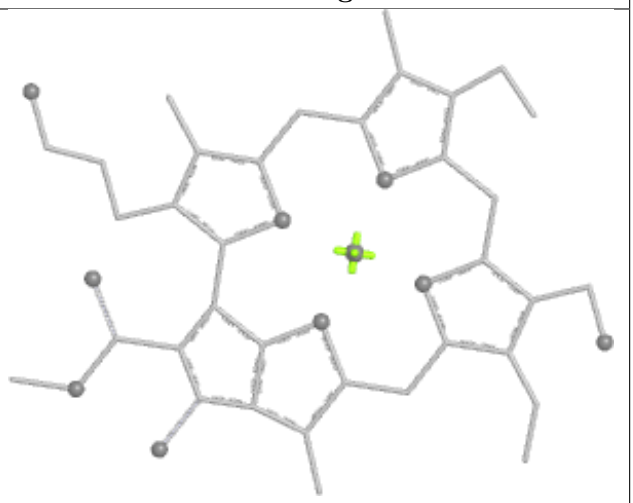
Bond lengths



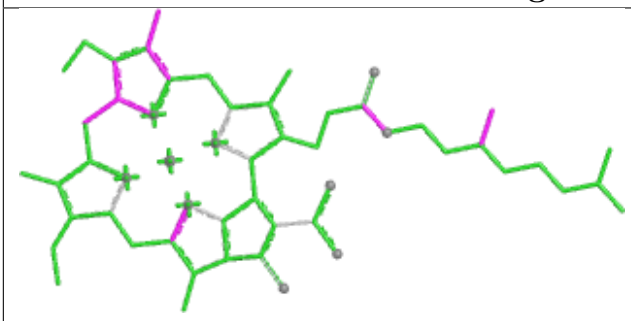
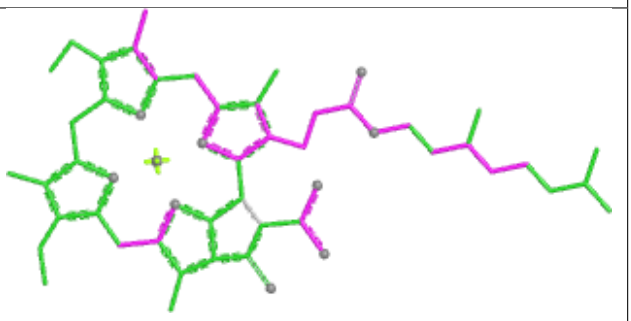
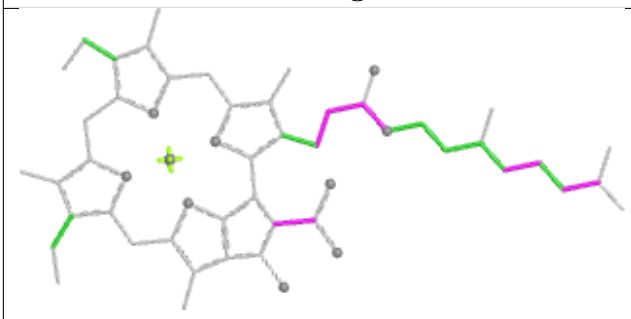
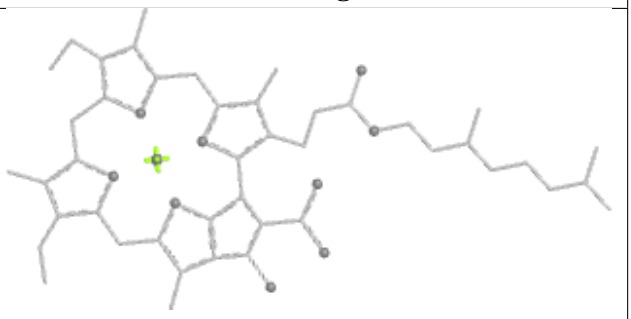
Bond angles

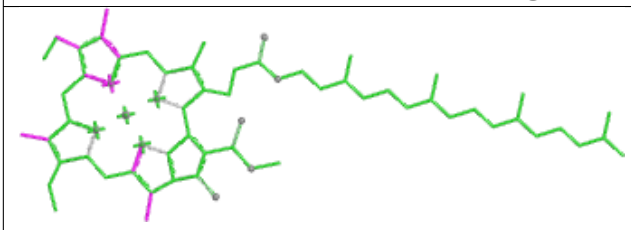
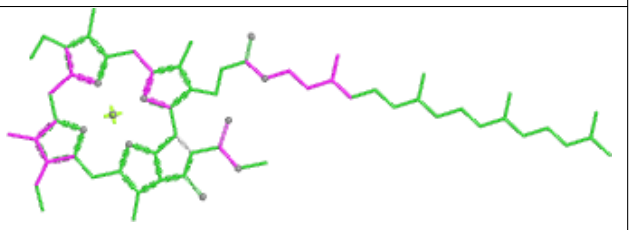
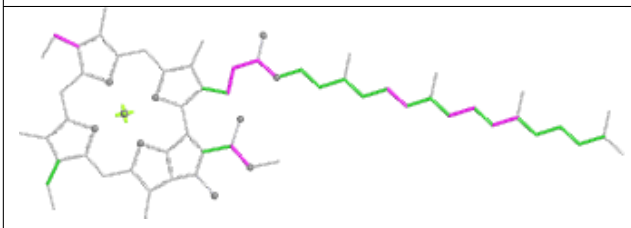
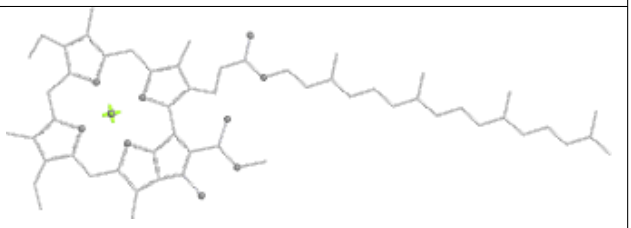


Torsions

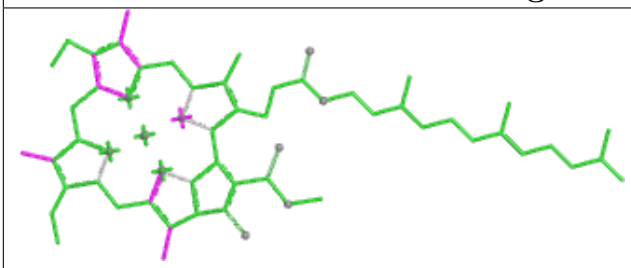


Rings

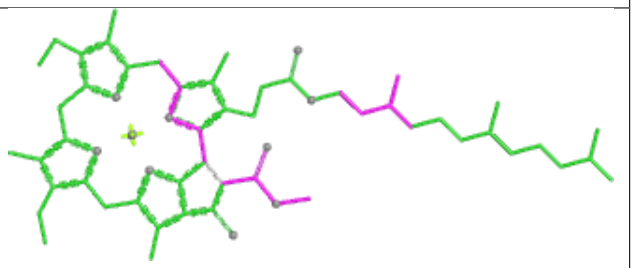
Ligand CLA 3 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

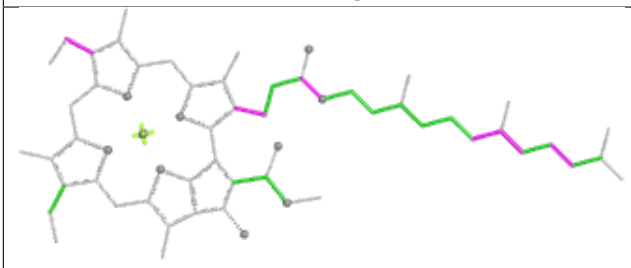
Ligand CLA S 310



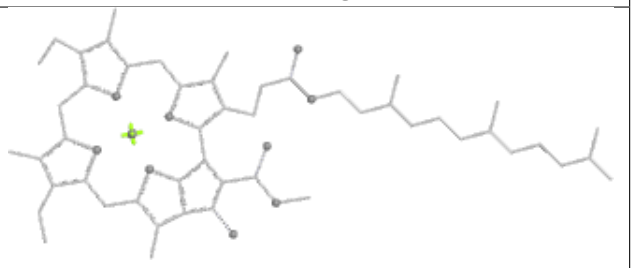
Bond lengths



Bond angles

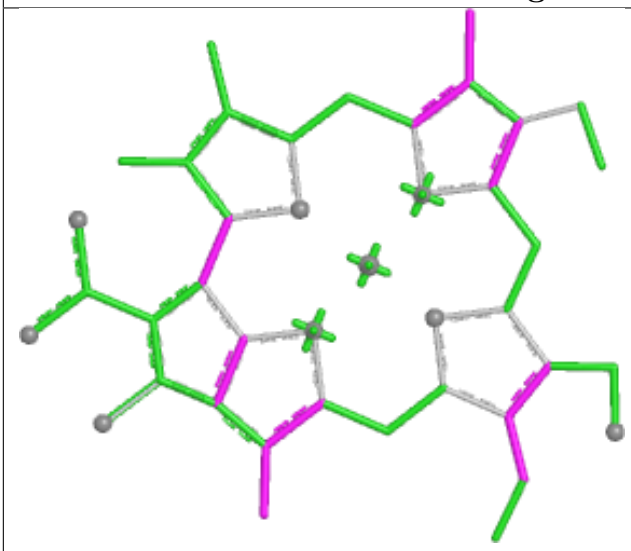


Torsions

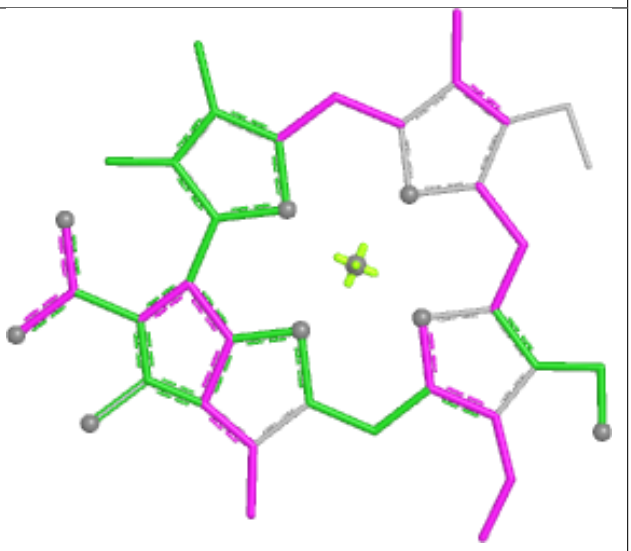


Rings

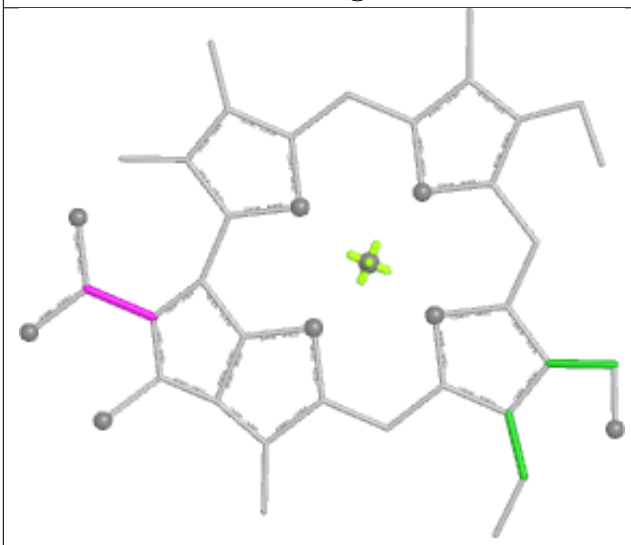
Ligand CHL 5 605



Bond lengths



Bond angles

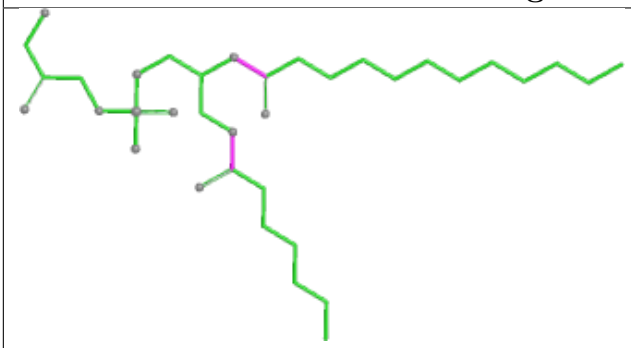


Torsions

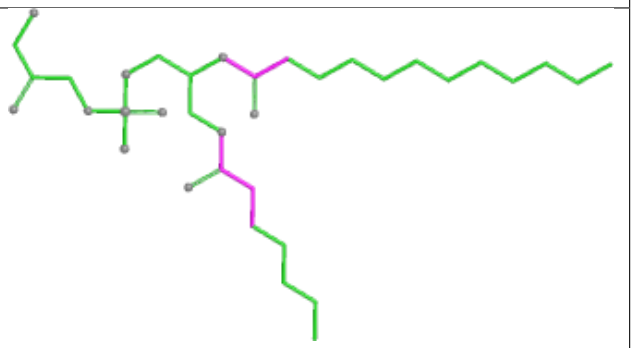


Rings

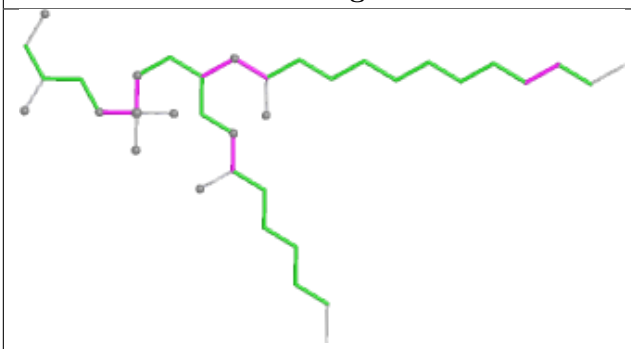
Ligand LHG 3 322



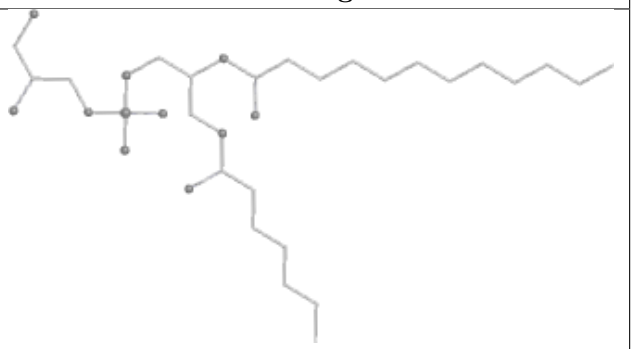
Bond lengths



Bond angles

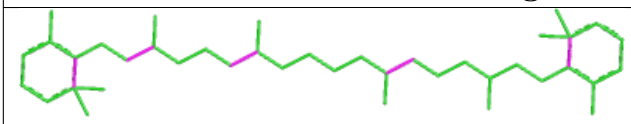


Torsions

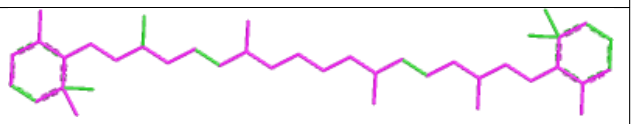


Rings

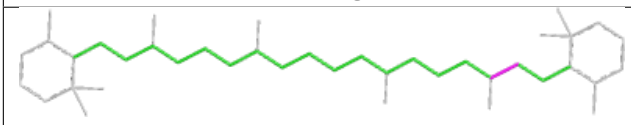
Ligand BCR A 850



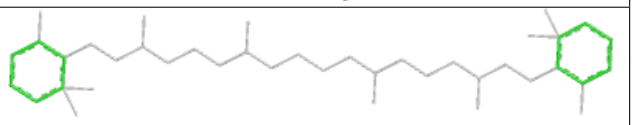
Bond lengths



Bond angles

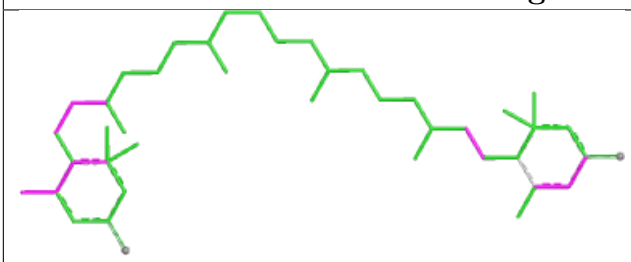


Torsions

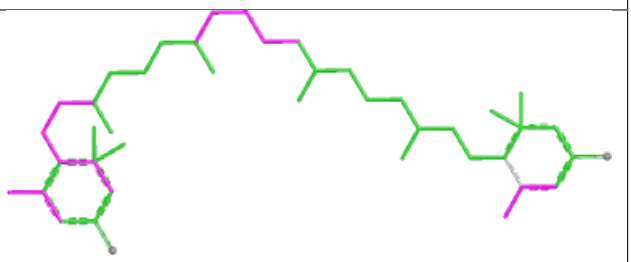


Rings

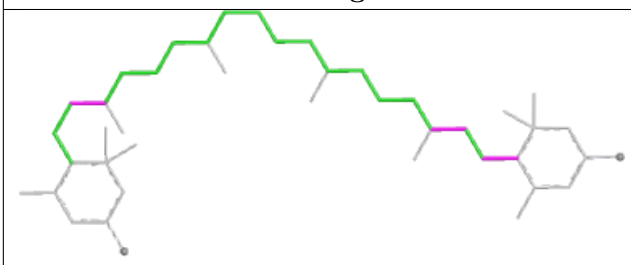
Ligand Q6L R 304



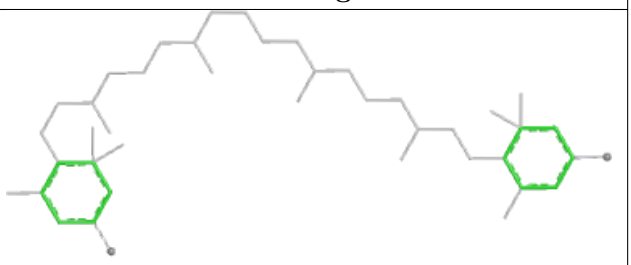
Bond lengths



Bond angles



Torsions

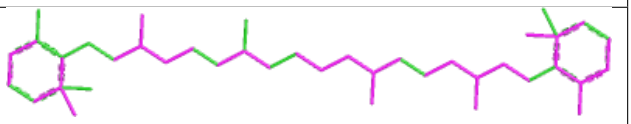


Rings

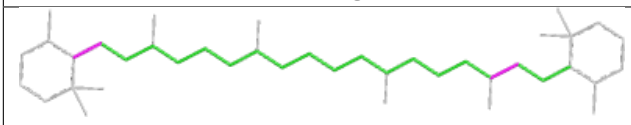
Ligand BCR L 305



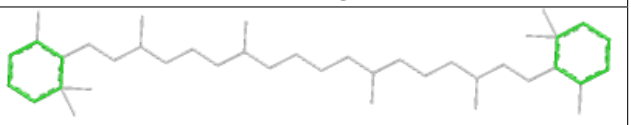
Bond lengths



Bond angles

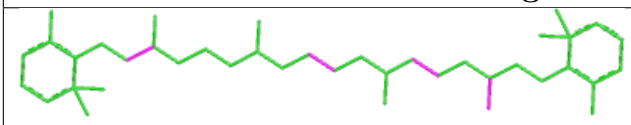


Torsions

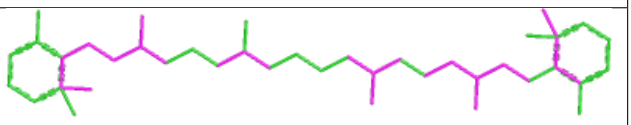


Rings

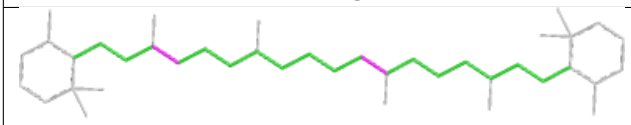
Ligand BCR A 852



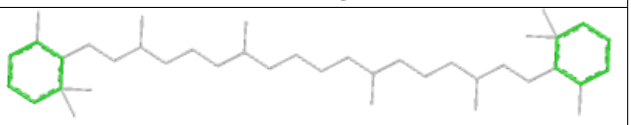
Bond lengths



Bond angles

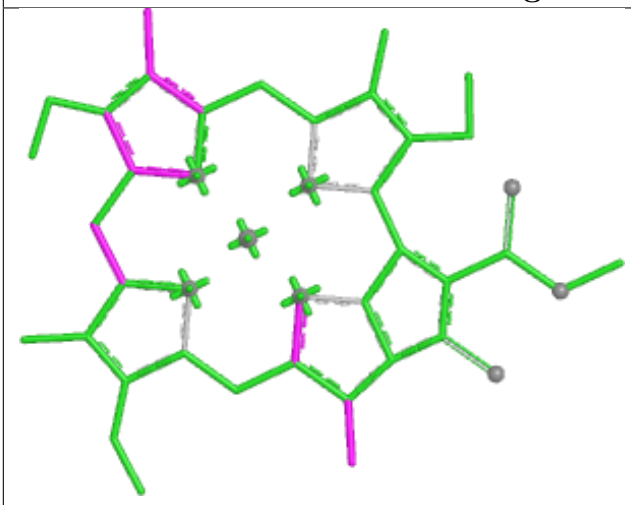


Torsions

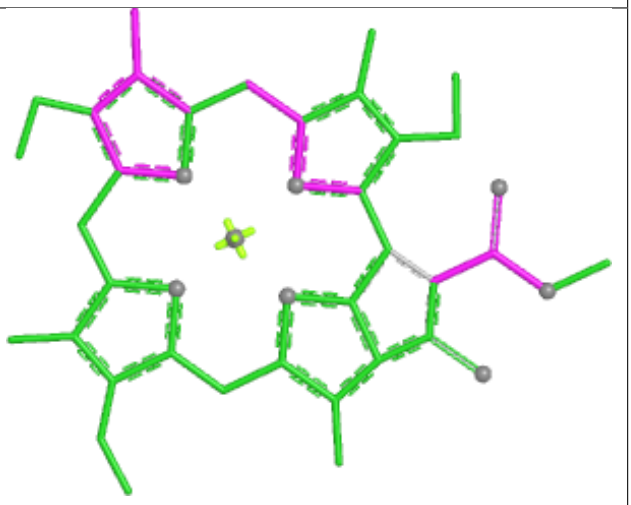


Rings

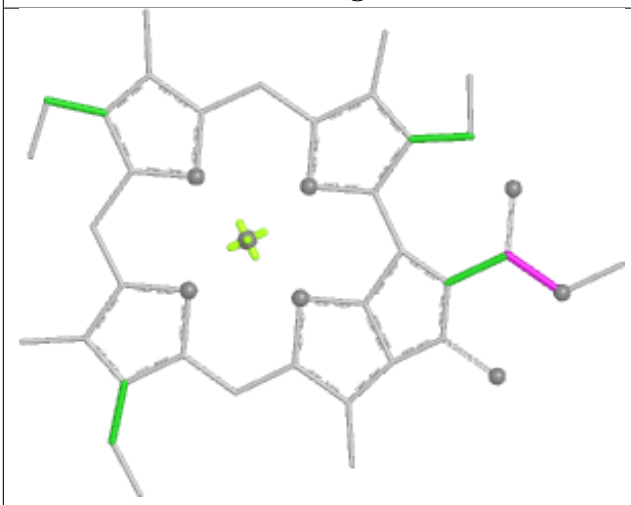
Ligand CLA X 310



Bond lengths



Bond angles

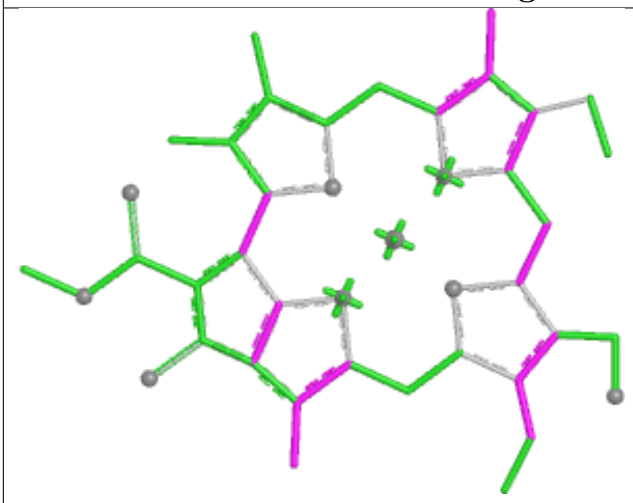


Torsions



Rings

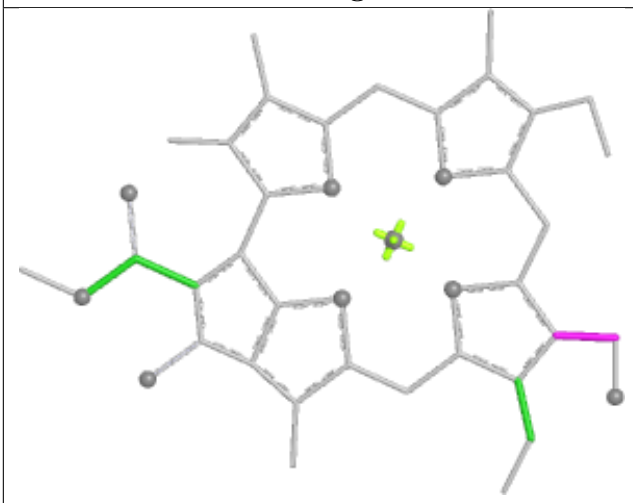
Ligand CHL W 304



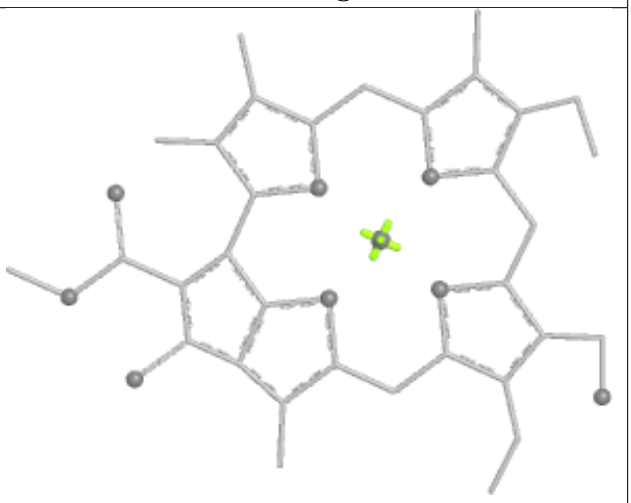
Bond lengths



Bond angles

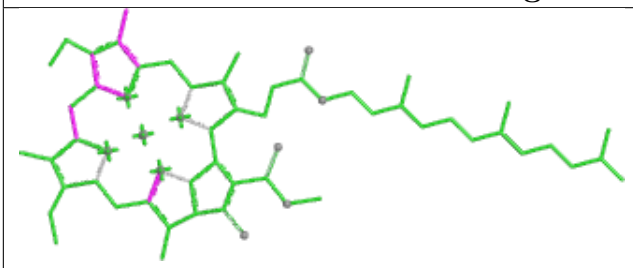


Torsions

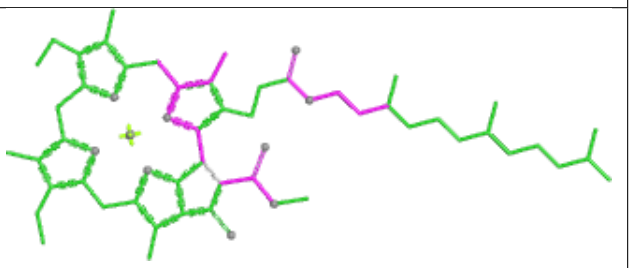


Rings

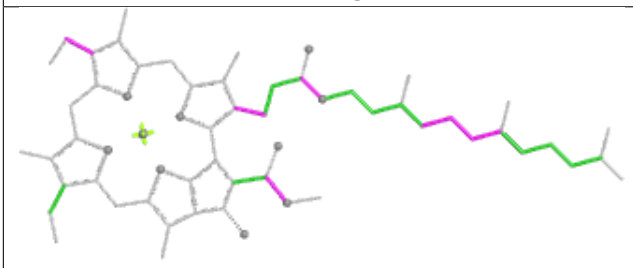
Ligand CLA R 314



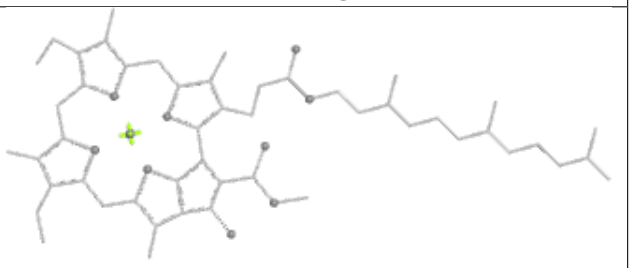
Bond lengths



Bond angles

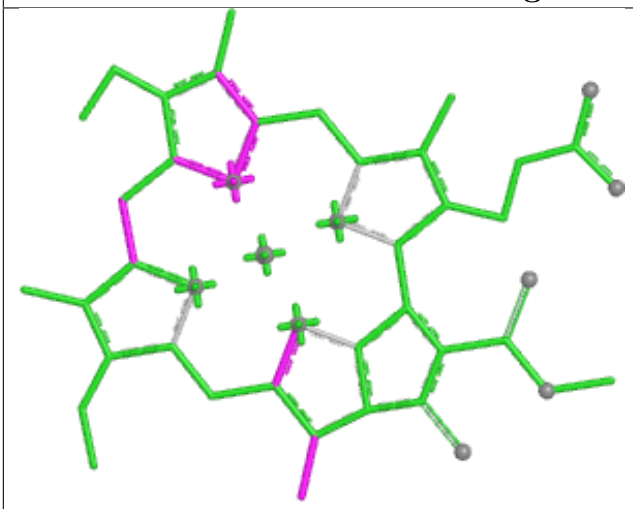


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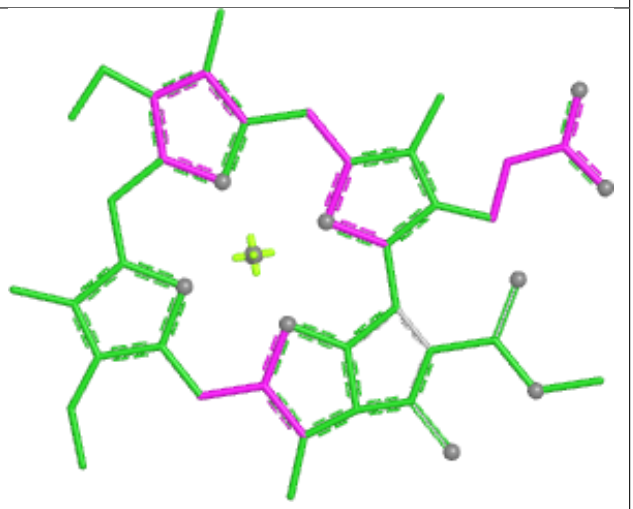


Rings

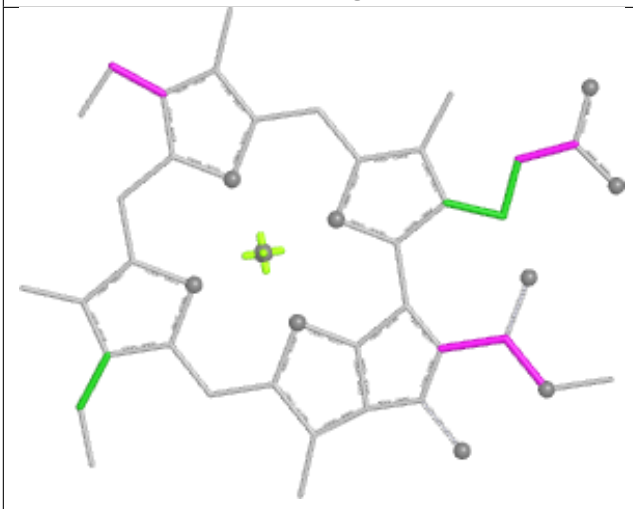
Ligand CLA A 816



Bond lengths



Bond angles

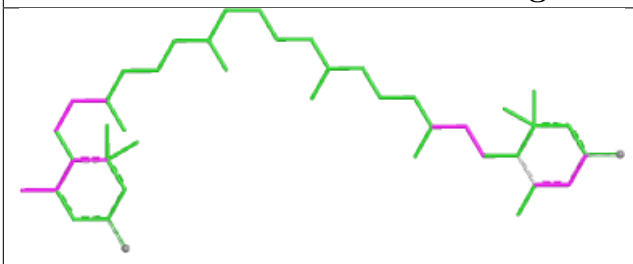


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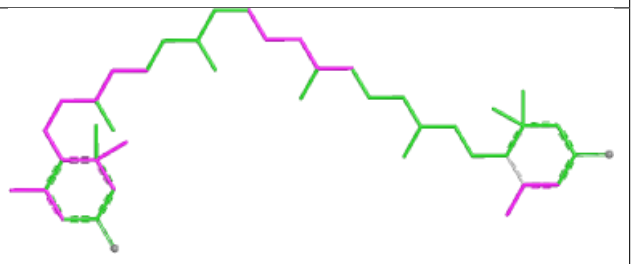


Rings

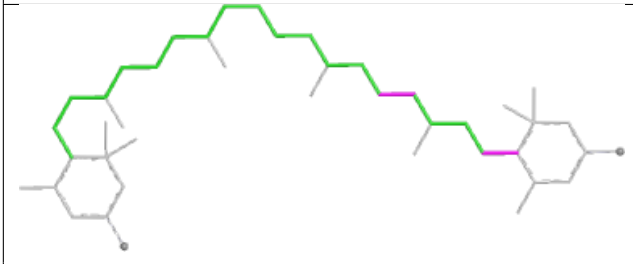
Ligand Q6L P 316



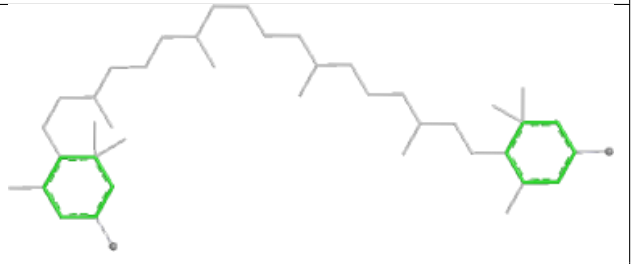
Bond lengths



Bond angles

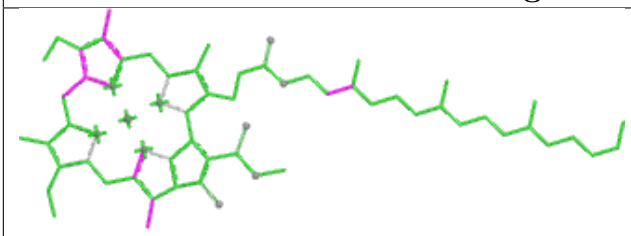


Torsions

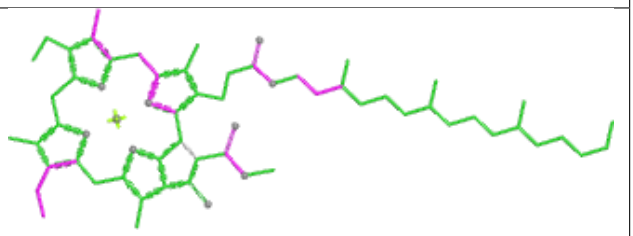


Rings

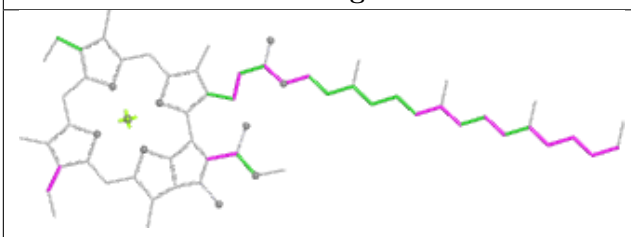
Ligand CLA A 807



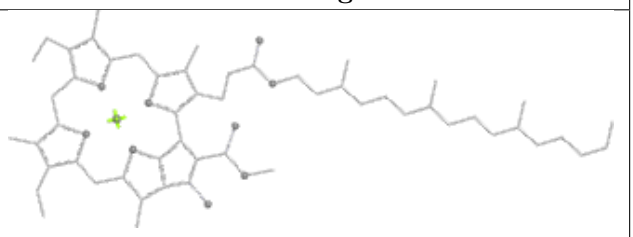
Bond lengths



Bond angles

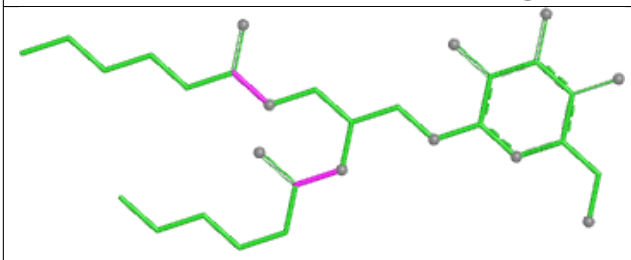


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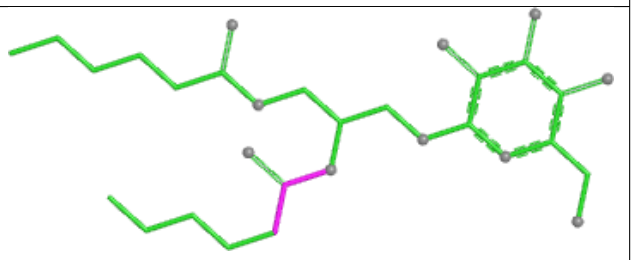


Rings

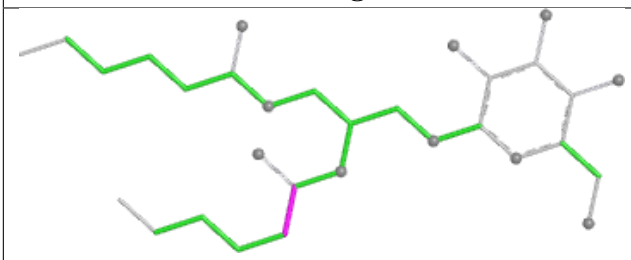
Ligand LMG A 801



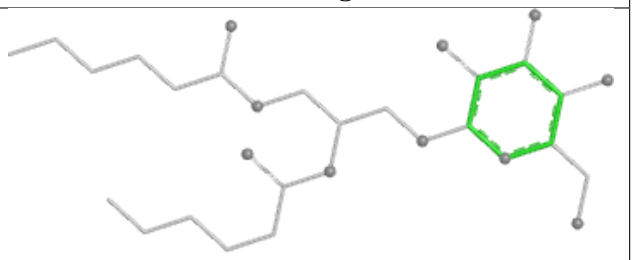
Bond lengths



Bond angles

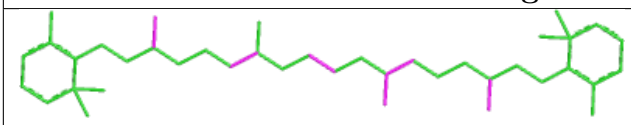


Torsions

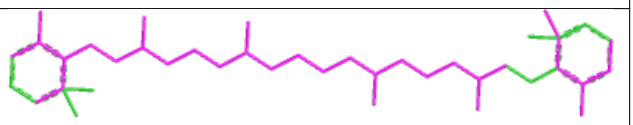


Rings

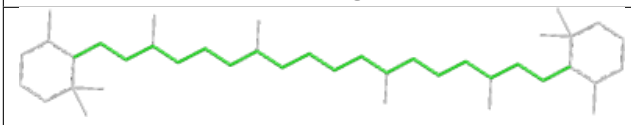
Ligand BCR K 202



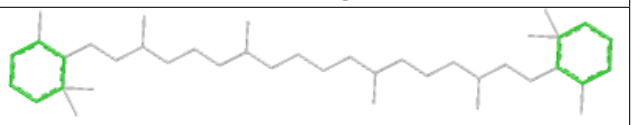
Bond lengths



Bond angles

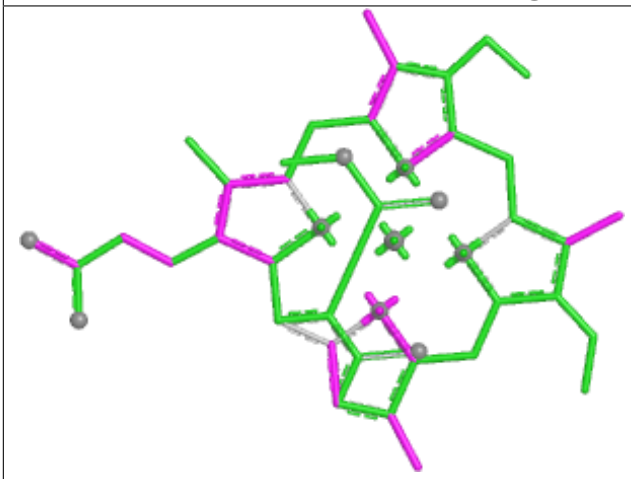


Torsions

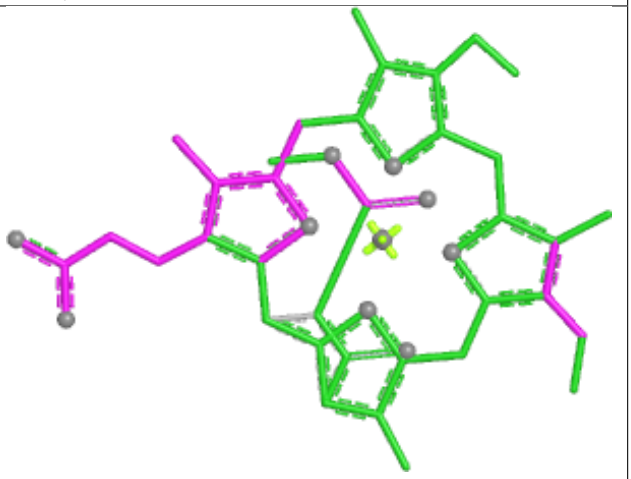


Rings

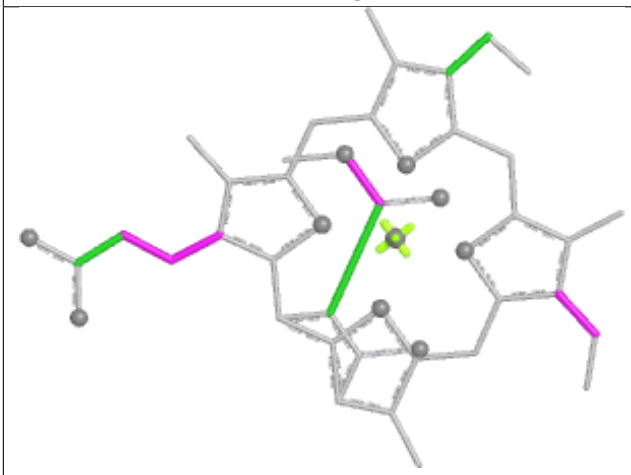
Ligand KC2 Q 310



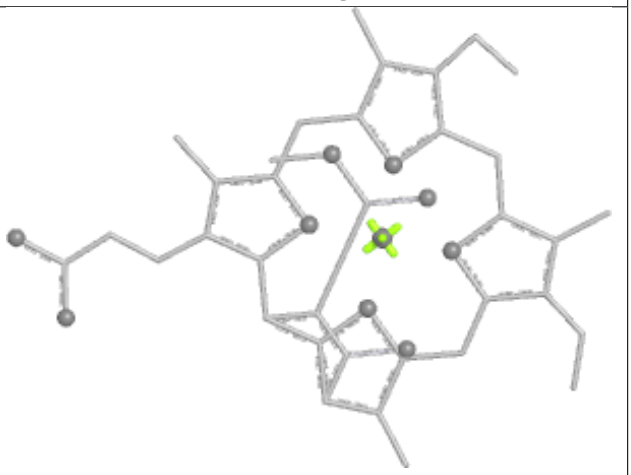
Bond lengths



Bond angles

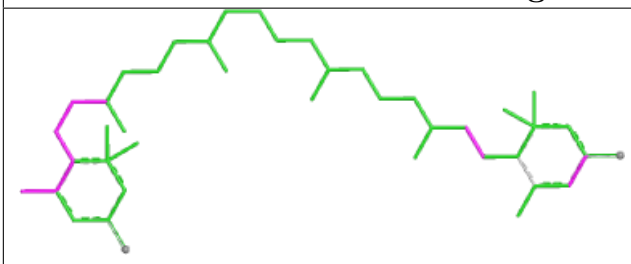


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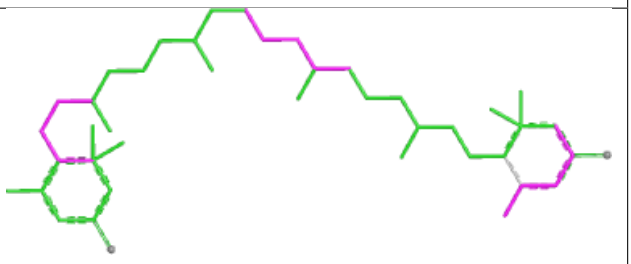


Rings

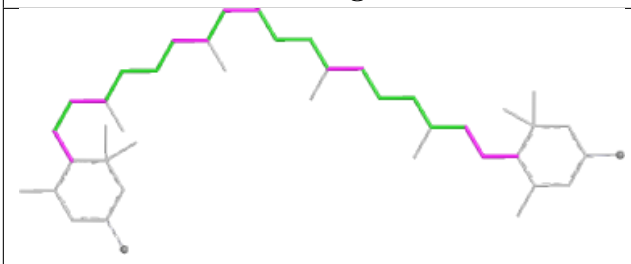
Ligand Q6L V 315



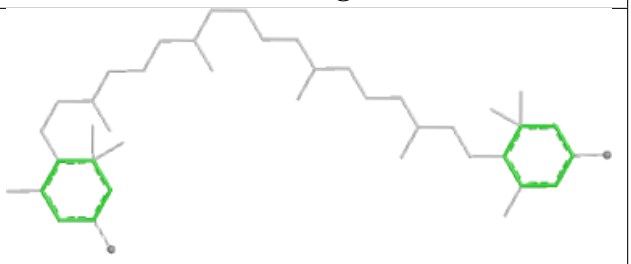
Bond lengths



Bond angles

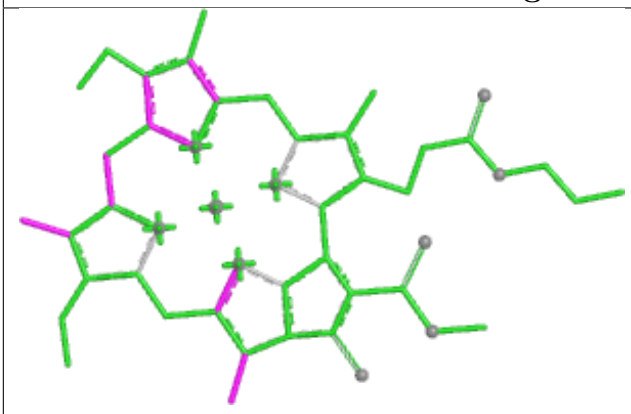


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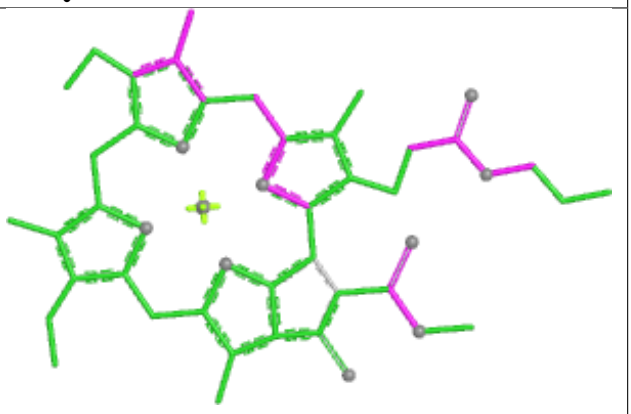


Rings

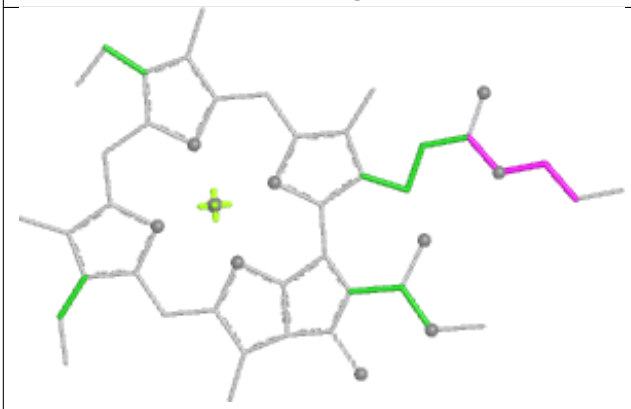
Ligand CLA Q 315



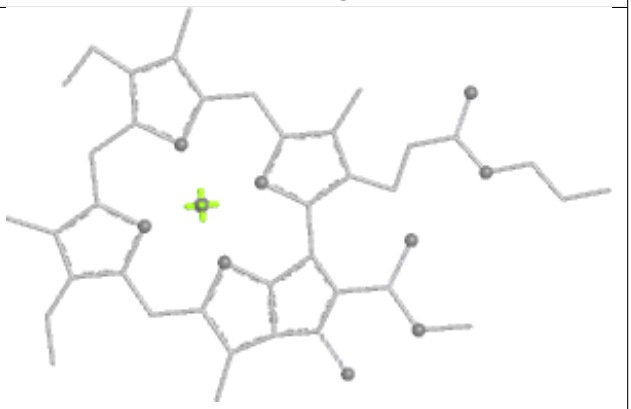
Bond lengths



Bond angles

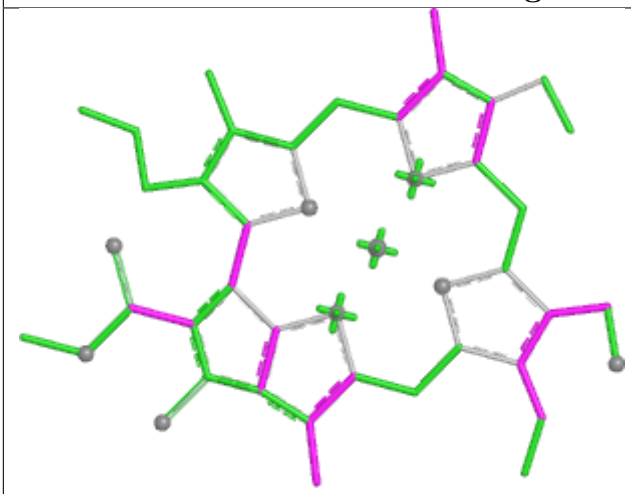


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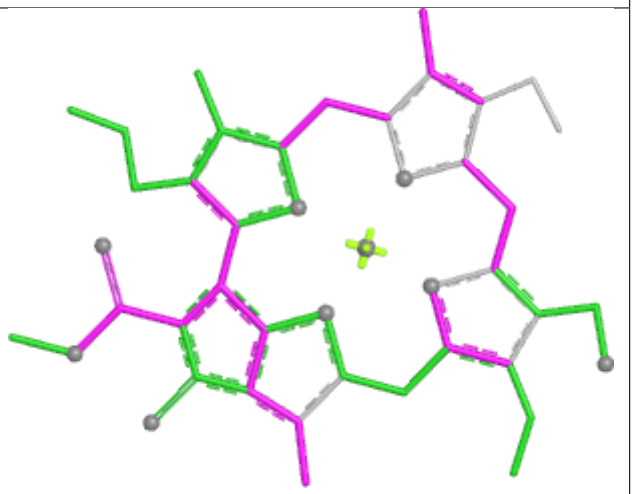


Rings

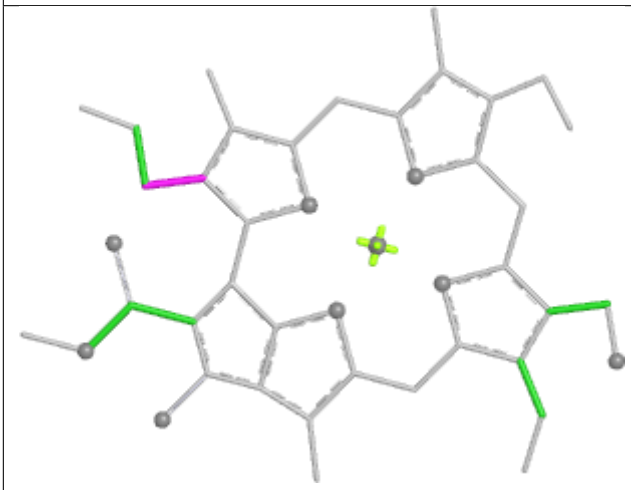
Ligand CHL P 307



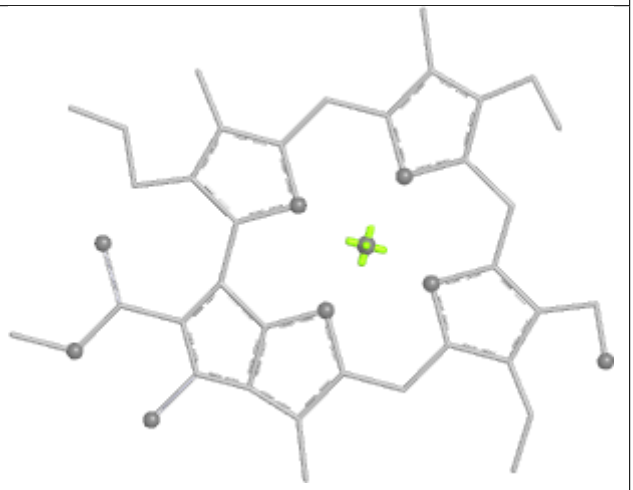
Bond lengths



Bond angles

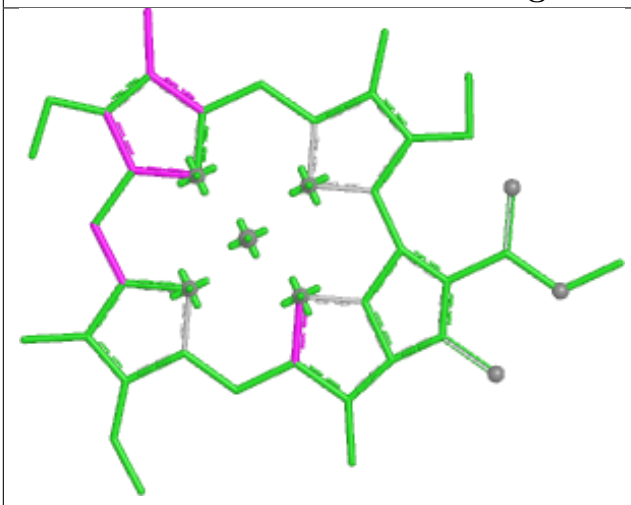


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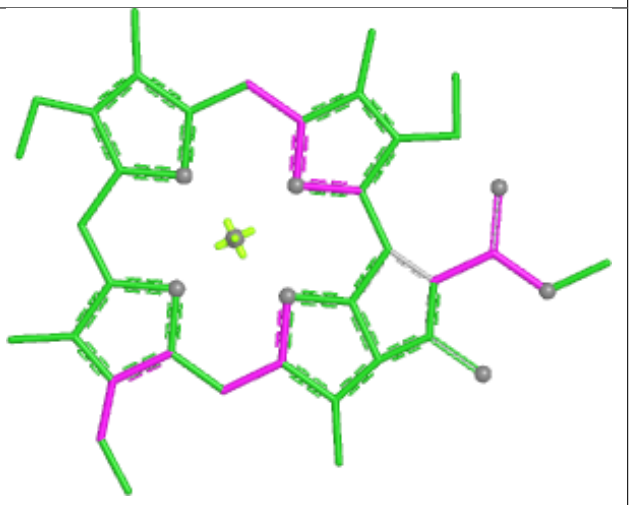


Rings

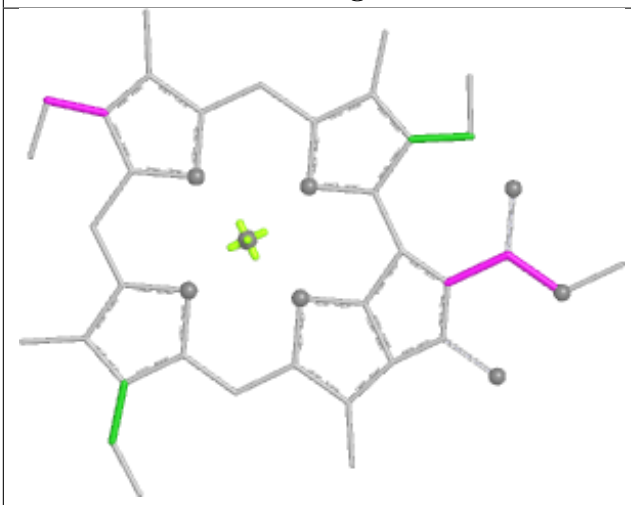
Ligand CLA 3 309



Bond lengths



Bond angles

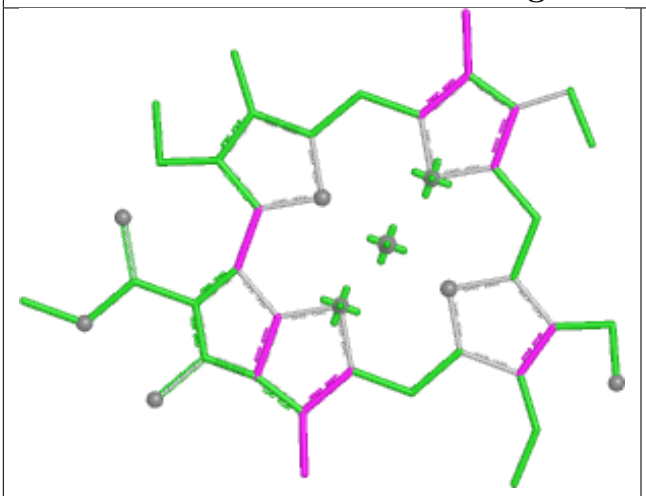


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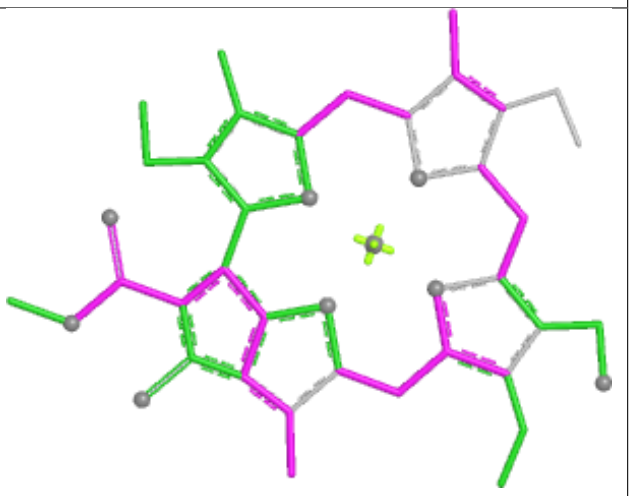


Rings

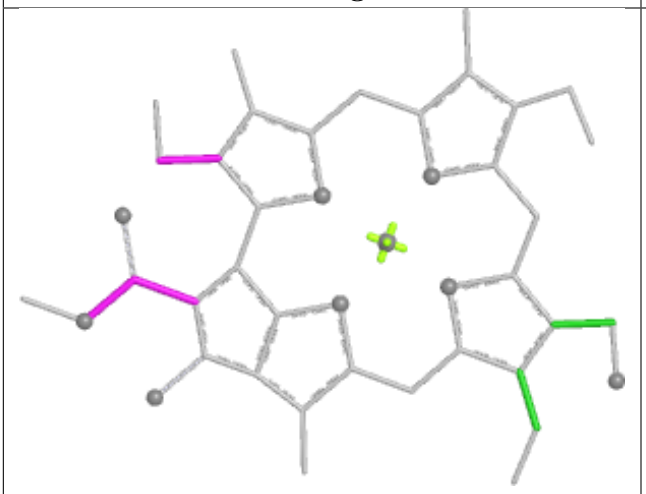
Ligand CHL 6 606



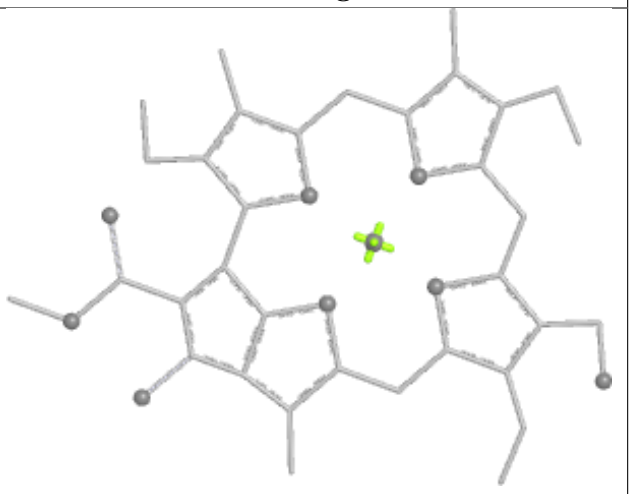
Bond lengths



Bond angles

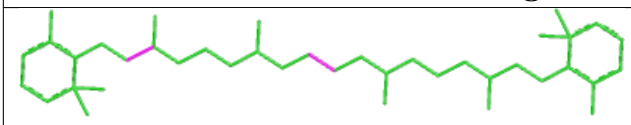


Torsions

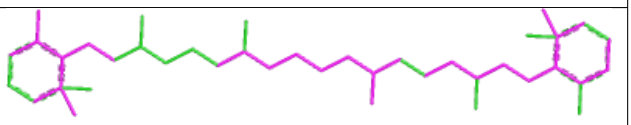


Rings

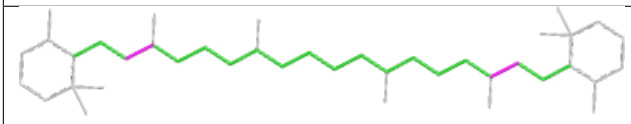
Ligand BCR B 849



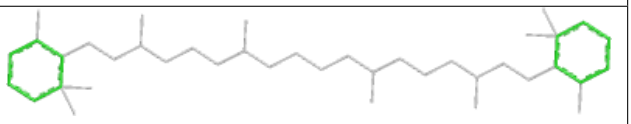
Bond lengths



Bond angles

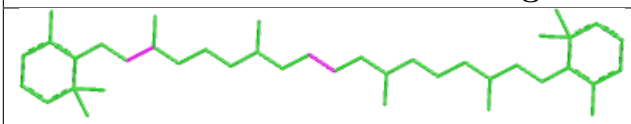


Torsions

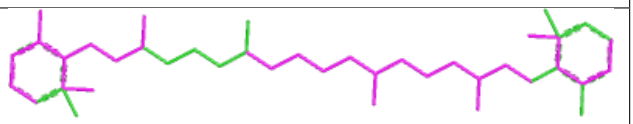


Rings

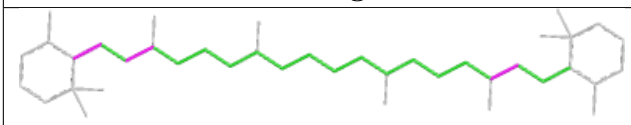
Ligand BCR A 851



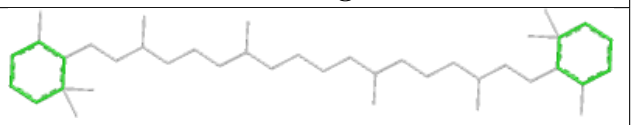
Bond lengths



Bond angles

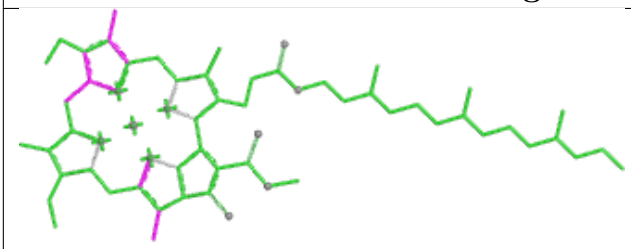


Torsions

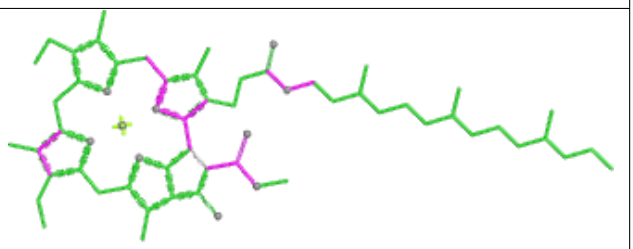


Rings

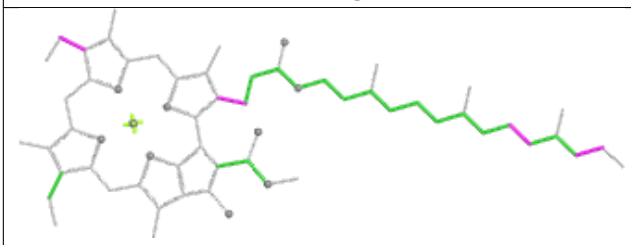
Ligand CLA K 203



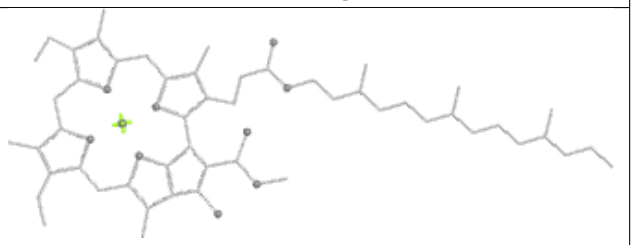
Bond lengths



Bond angles

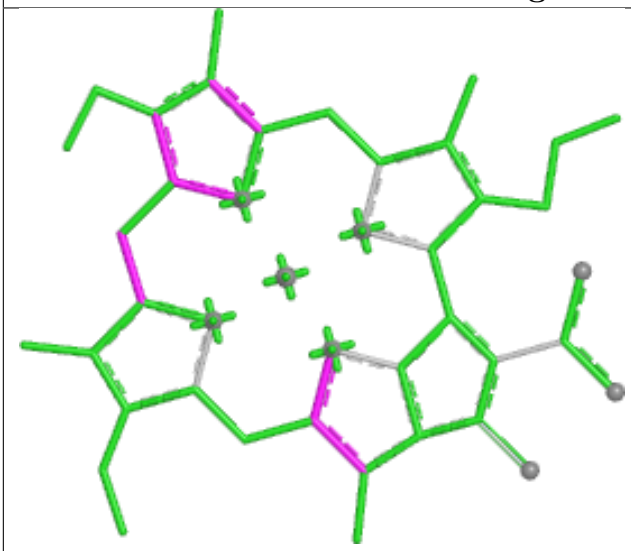


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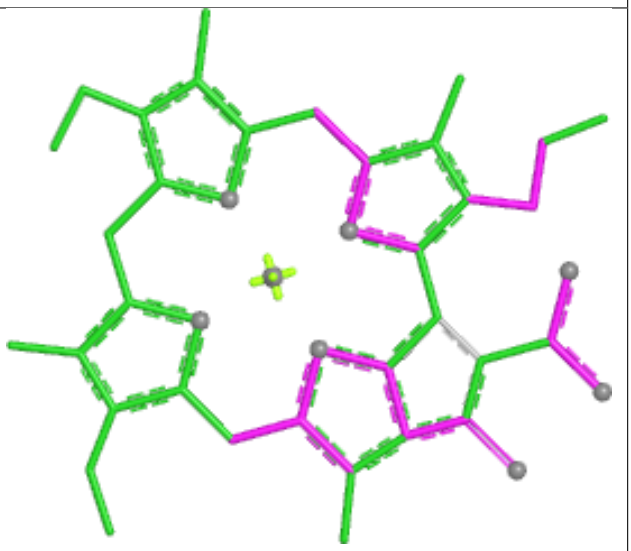


Rings

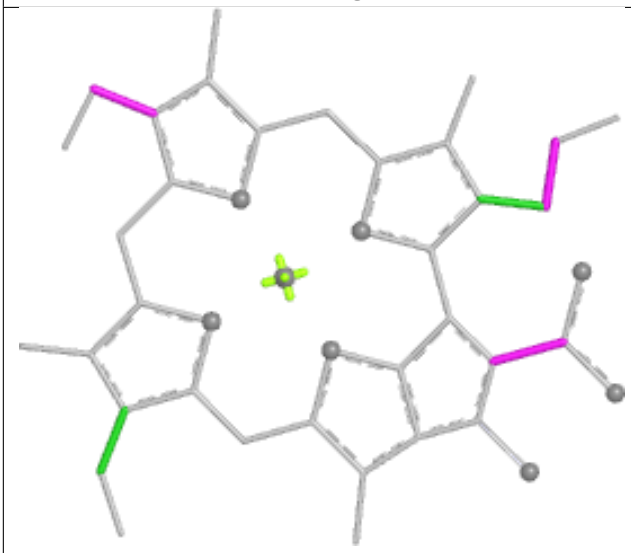
Ligand CLA 2 613



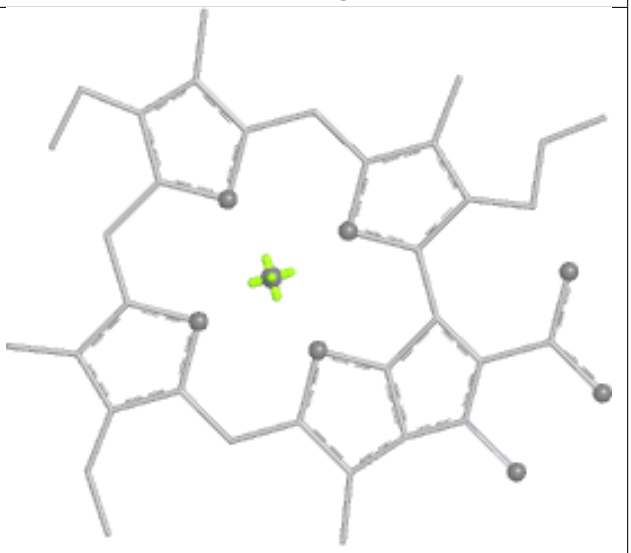
Bond lengths



Bond angles

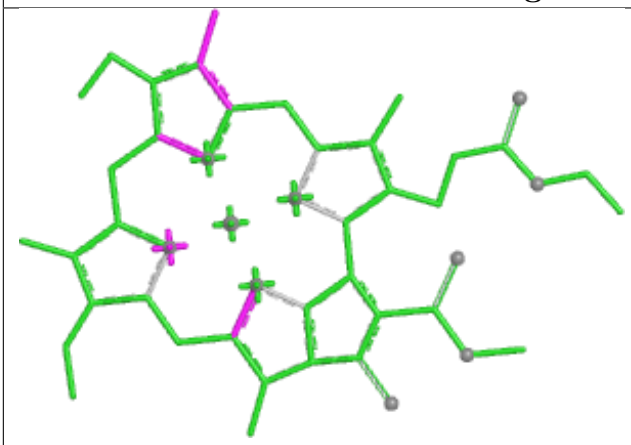


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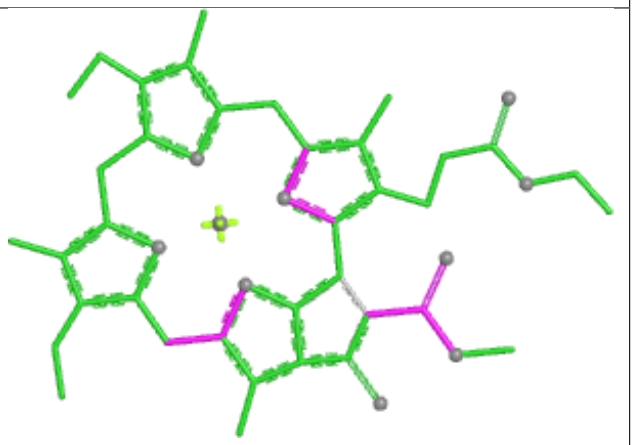


Rings

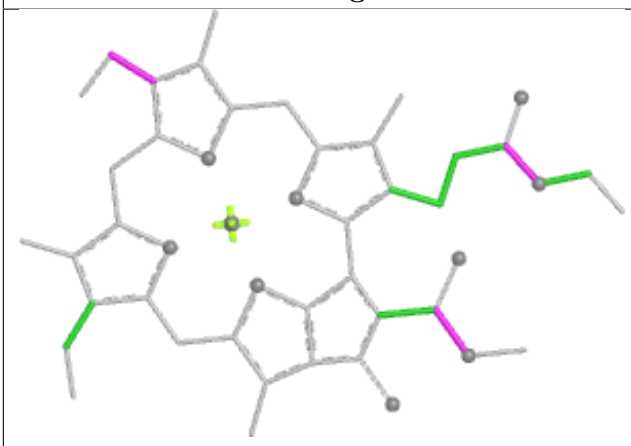
Ligand CLA B 823



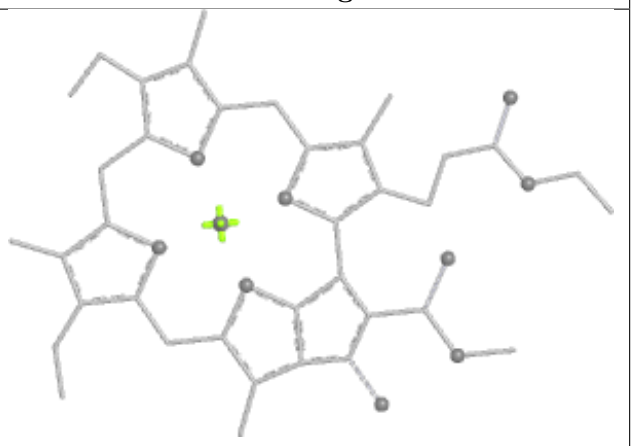
Bond lengths



Bond angles

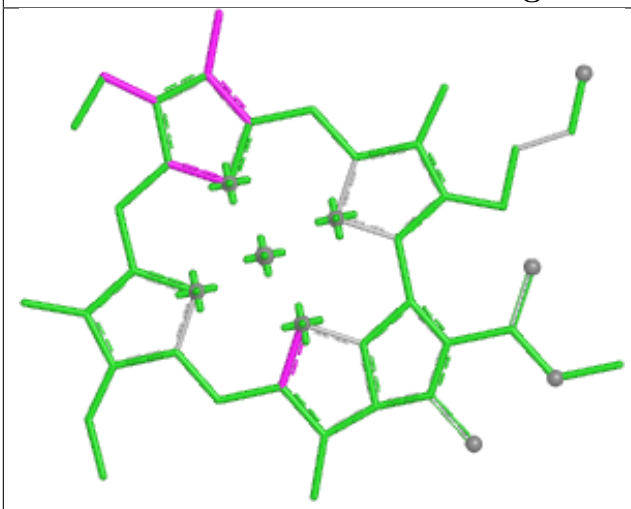


Torsions

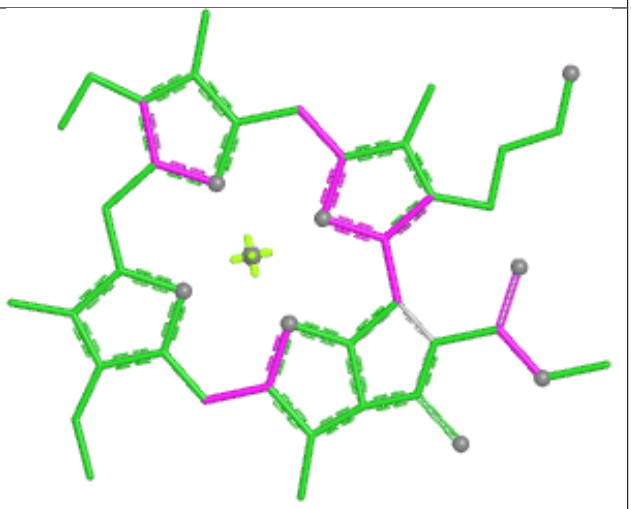


Rings

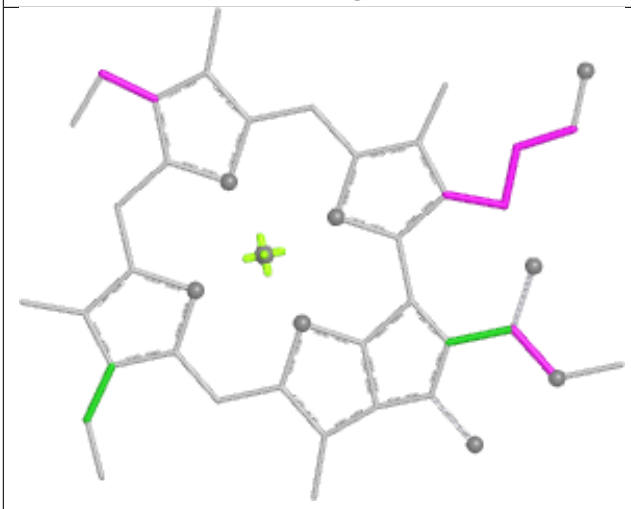
Ligand CLA H 301



Bond lengths



Bond angles

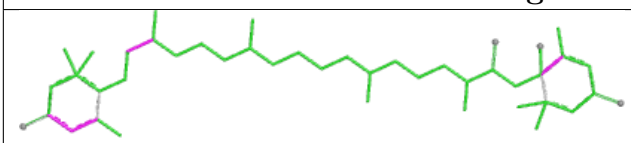


Torsions

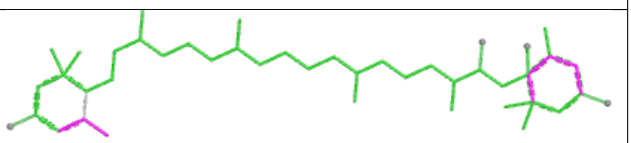


Rings

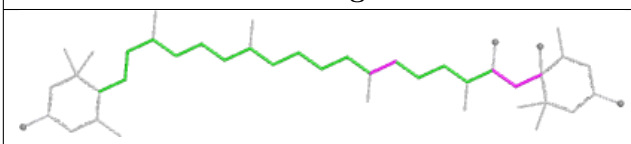
Ligand IWJ V 317



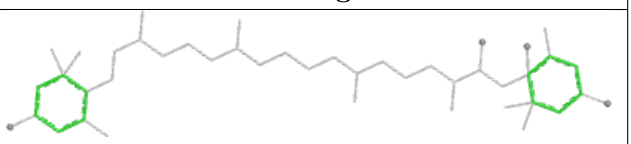
Bond lengths



Bond angles



Torsions

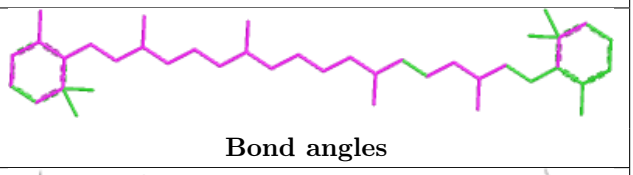


Rings

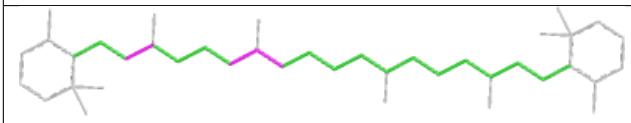
Ligand BCR F 804



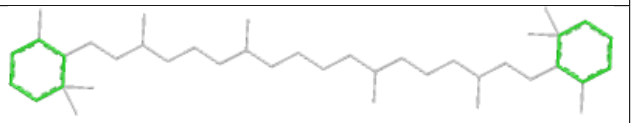
Bond lengths



Bond angles

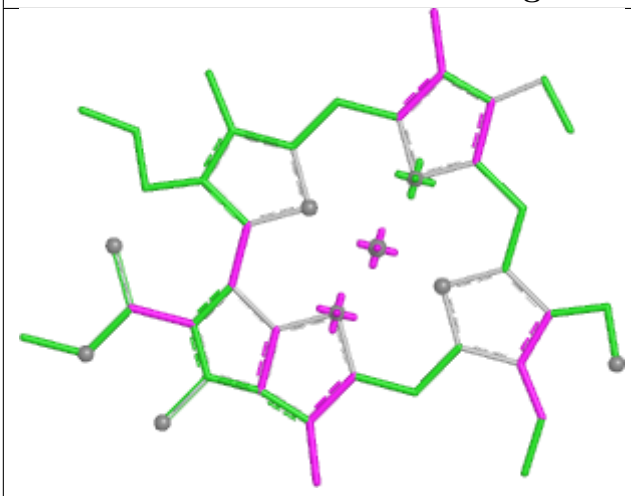


Torsions

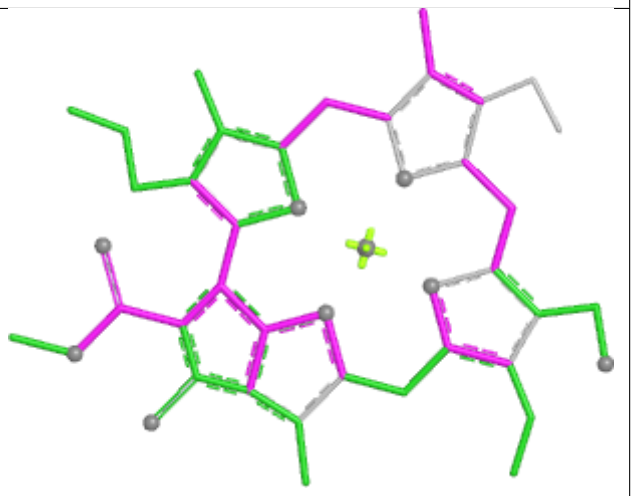


Rings

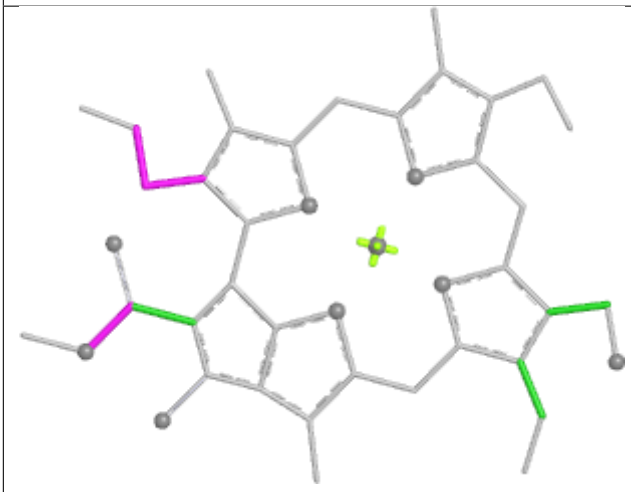
Ligand CHL V 314



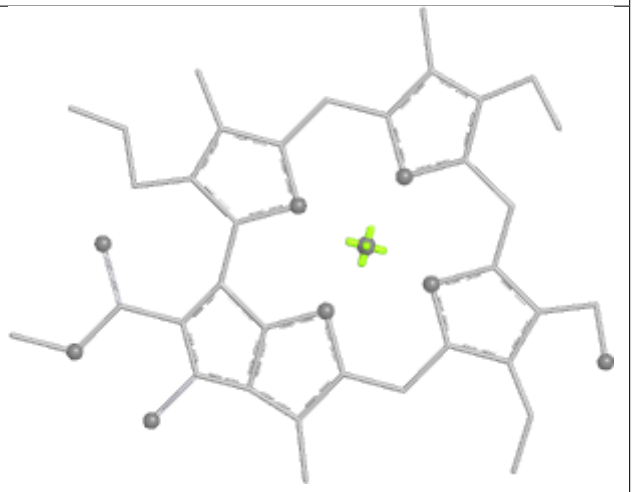
Bond lengths



Bond angles

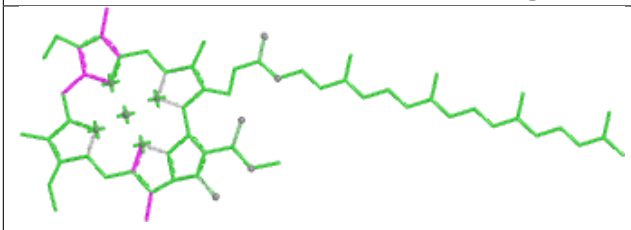


Torsions

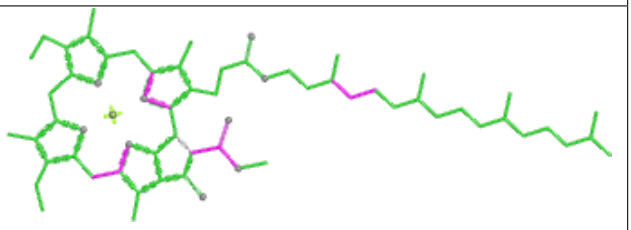


Rings

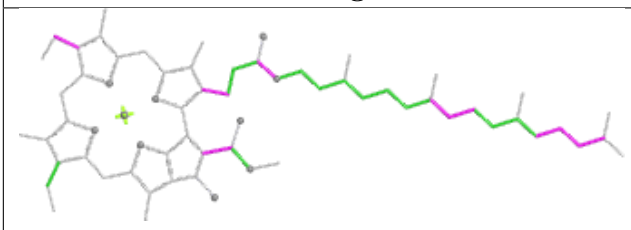
Ligand CLA A 813



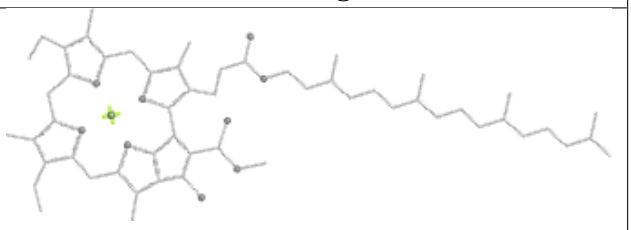
Bond lengths



Bond angles

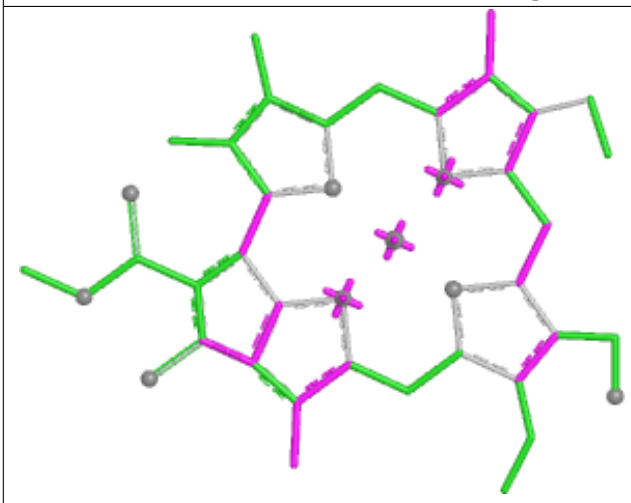


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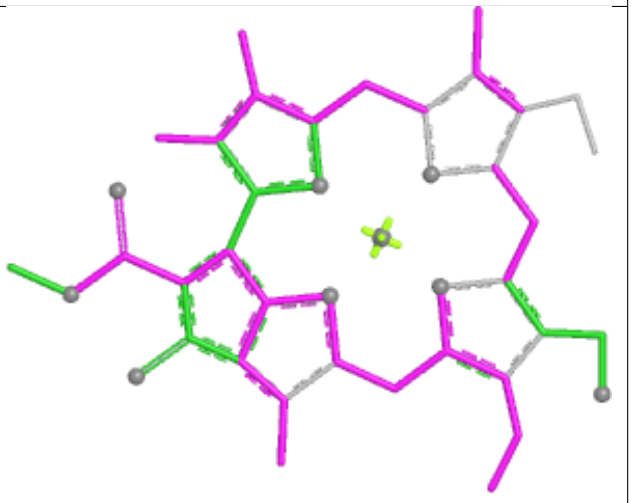


Rings

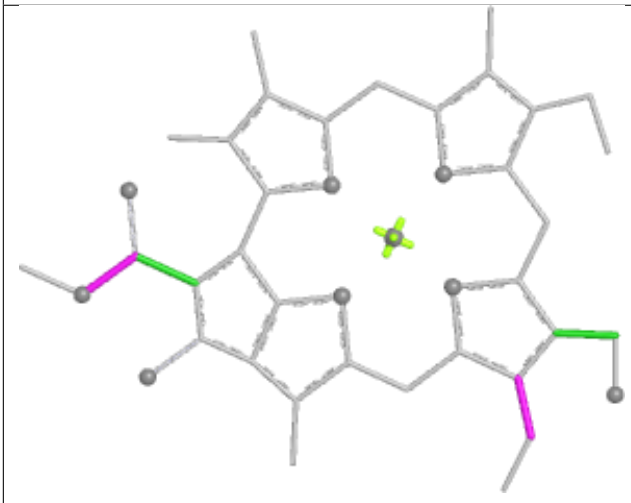
Ligand CHL S 305



Bond lengths



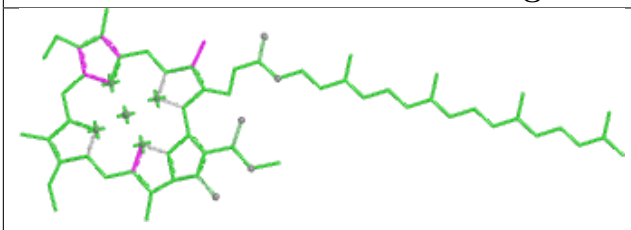
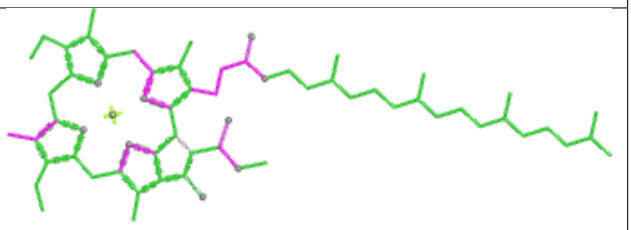
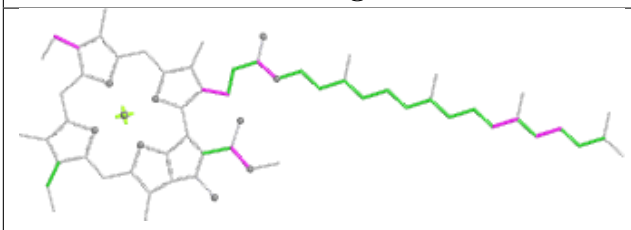
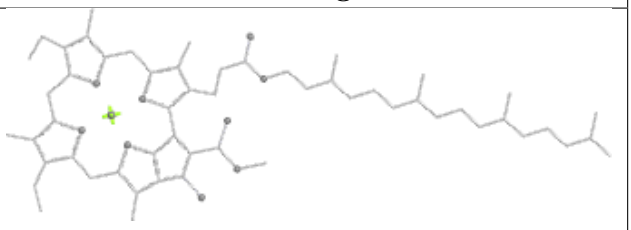
Bond angles

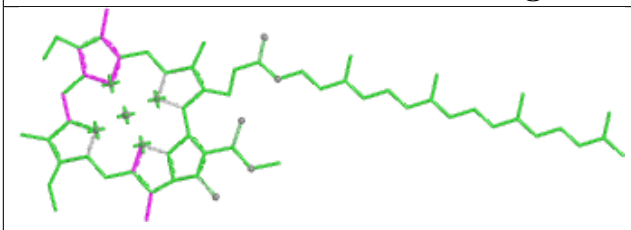
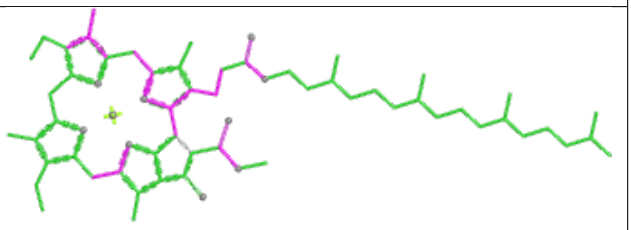
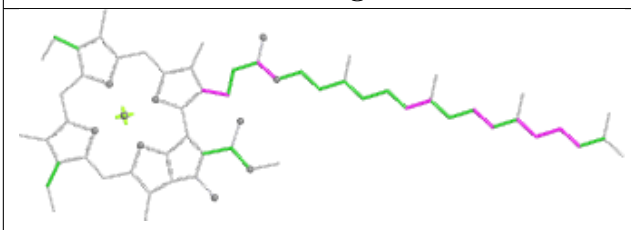
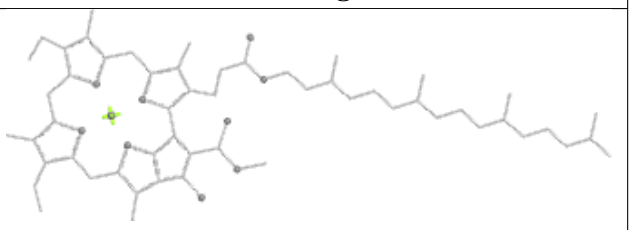


Torsions

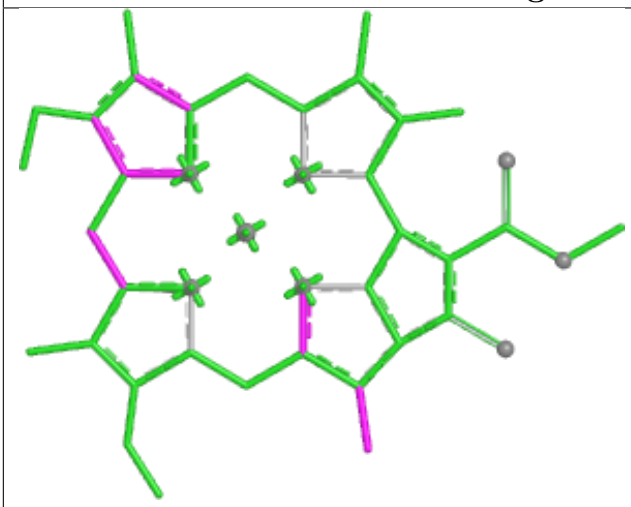


Rings

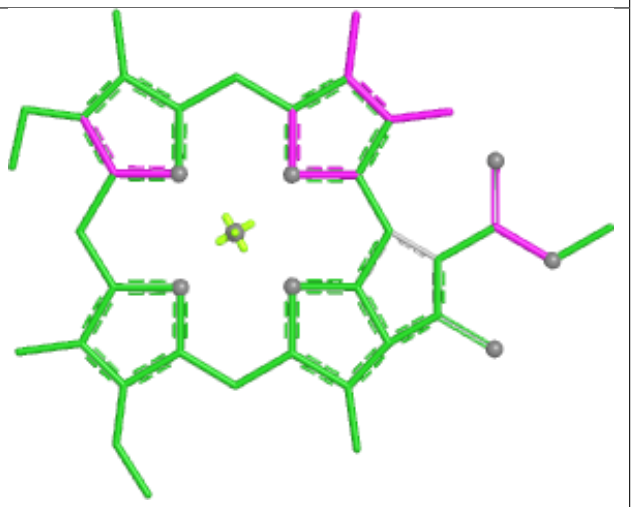
Ligand CLA R 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

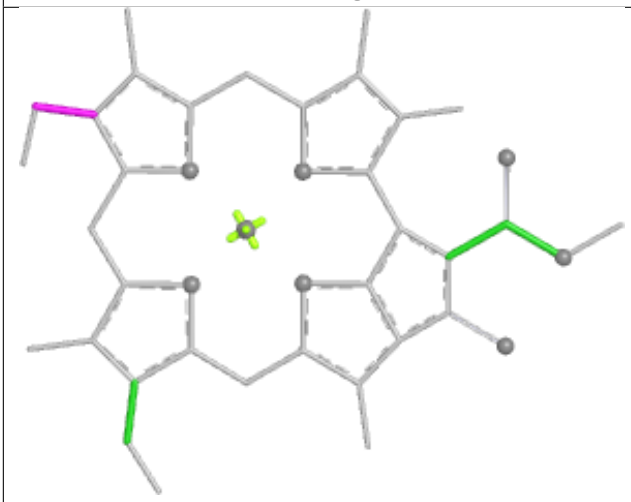
Ligand CLA S 313



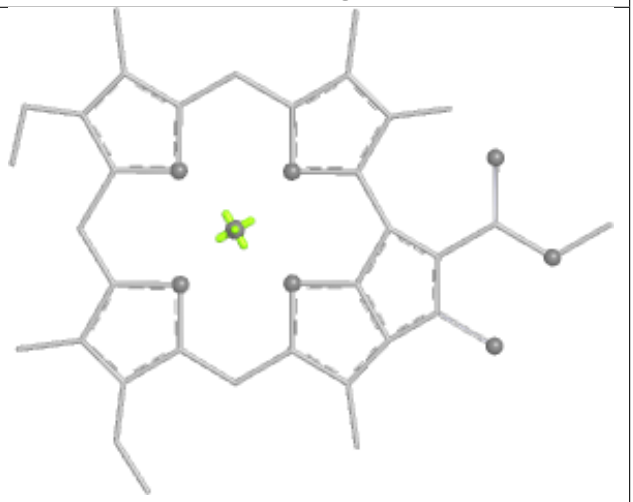
Bond lengths



Bond angles

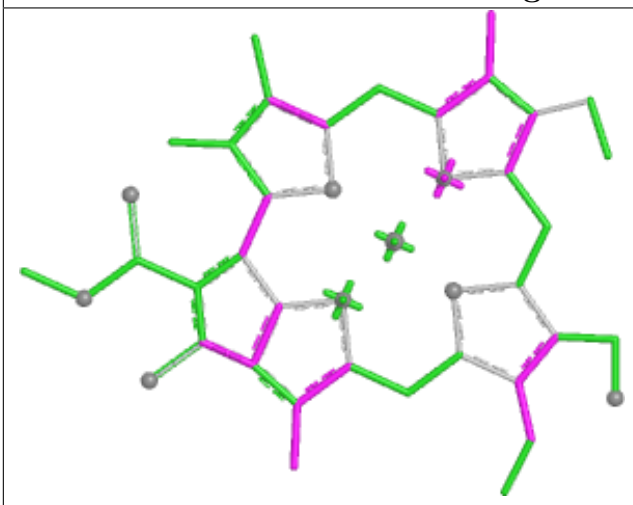


Torsions

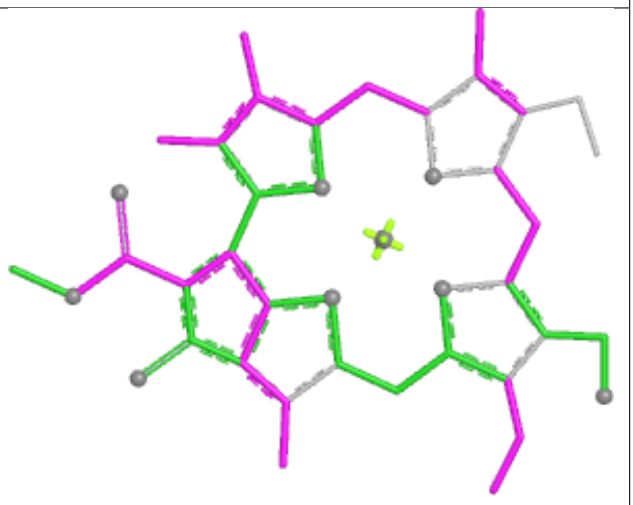


Rings

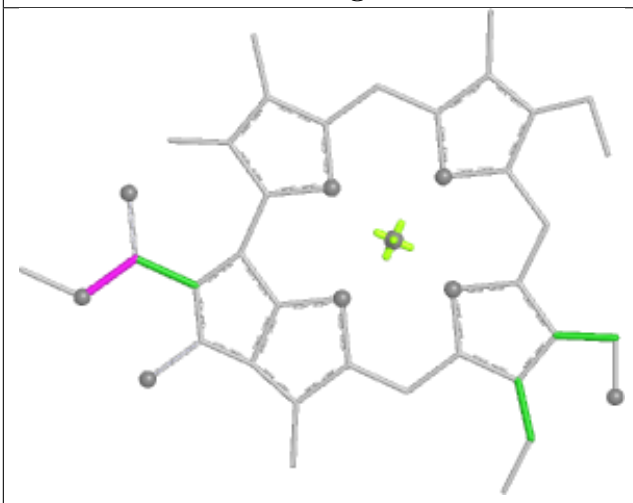
Ligand CHL X 306



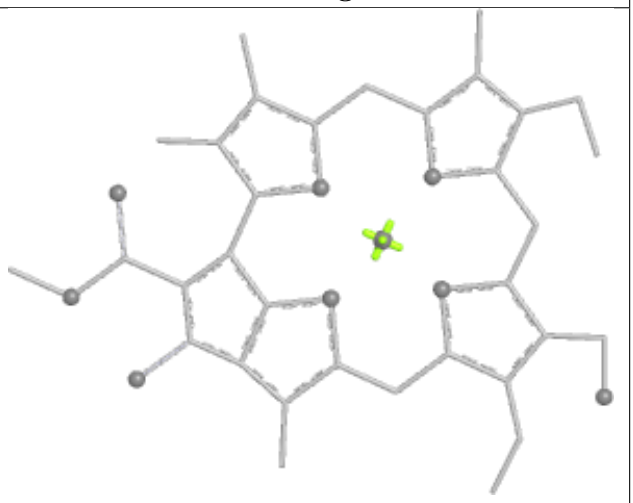
Bond lengths



Bond angles

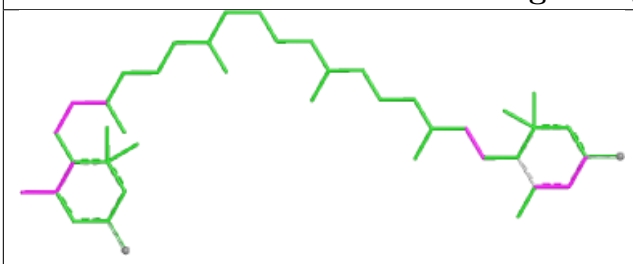


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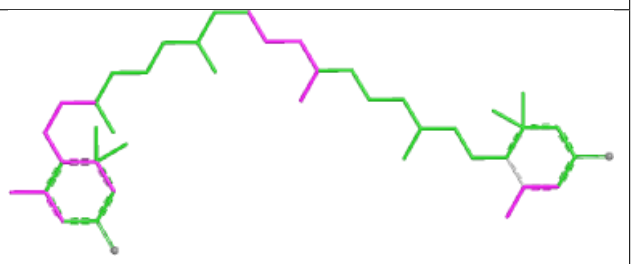


Rings

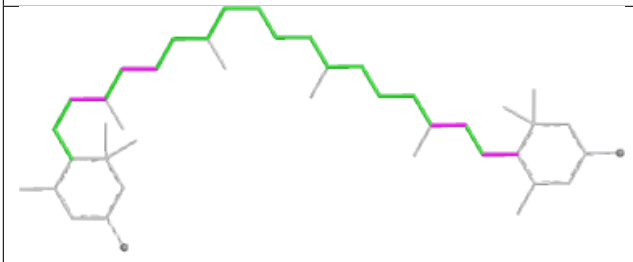
Ligand Q6L P 319



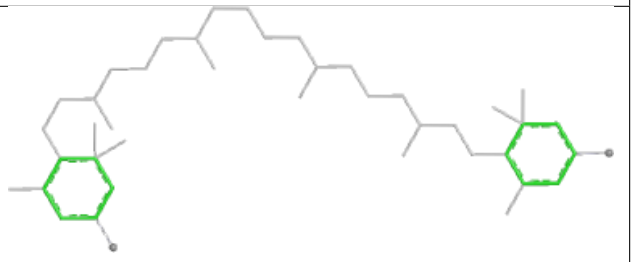
Bond lengths



Bond angles

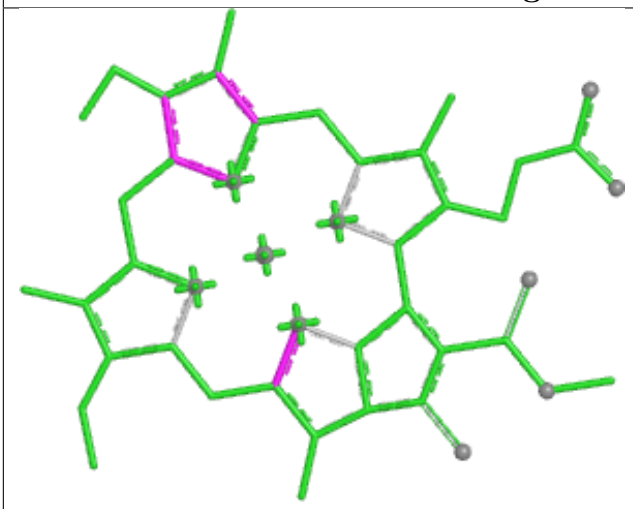


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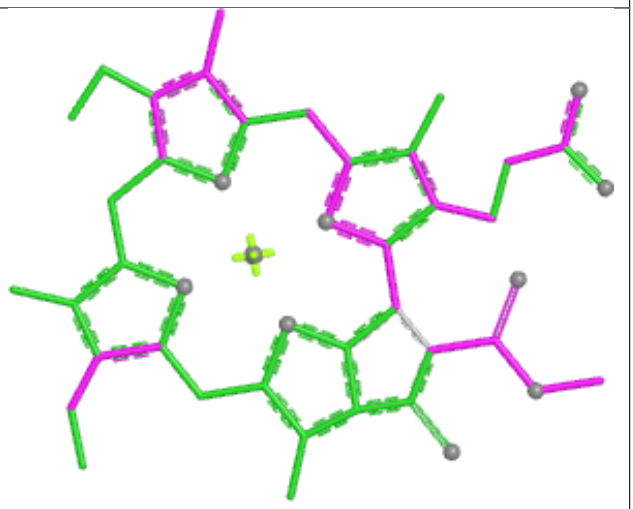


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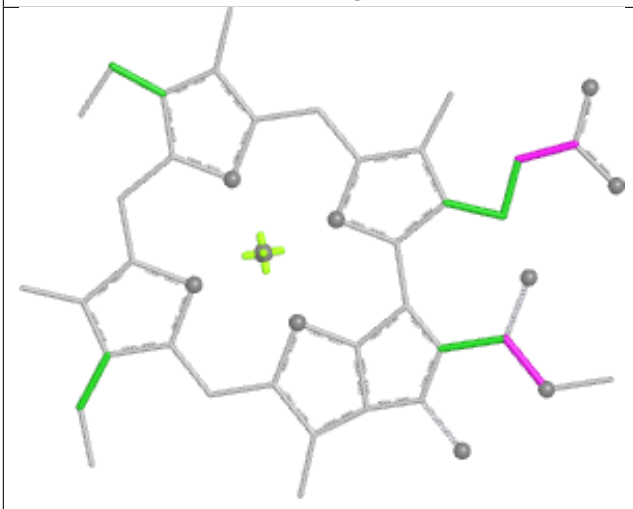
Ligand CLA K 201



Bond lengths



Bond angles

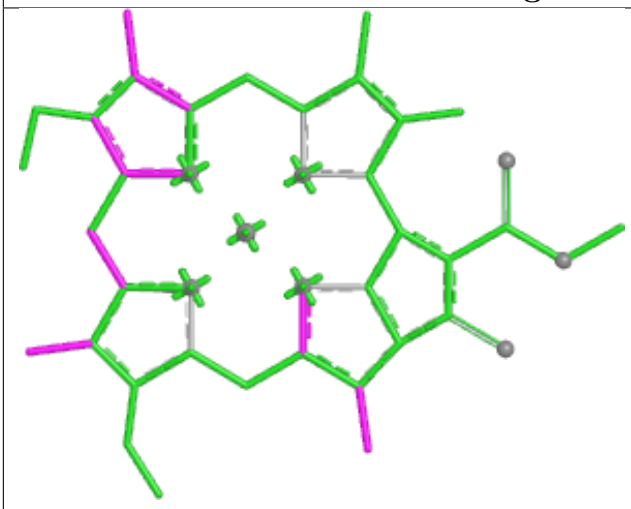


Torsions

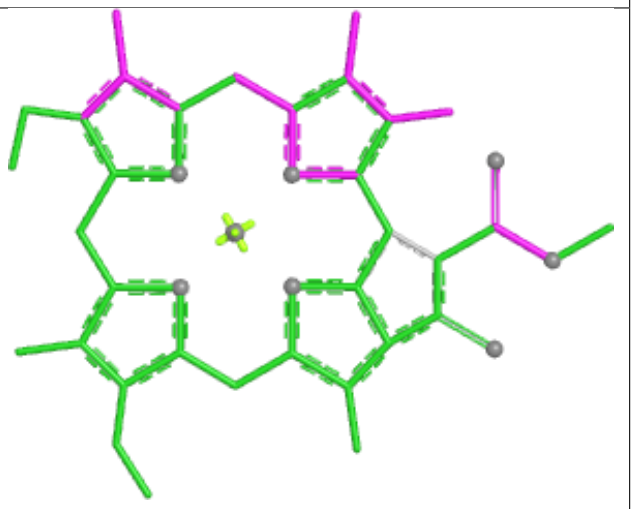


Rings

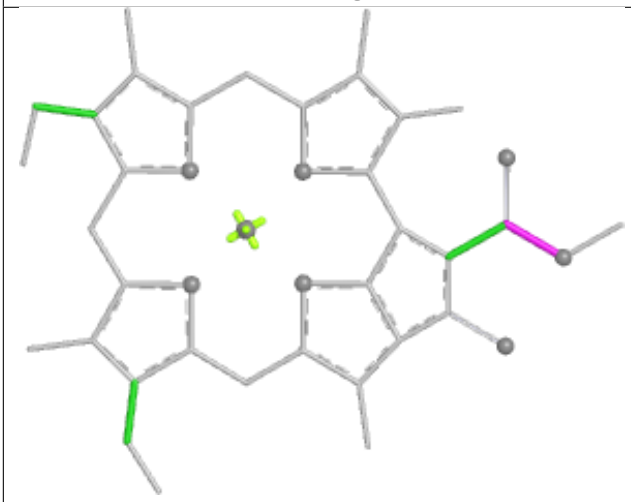
Ligand CLA X 313



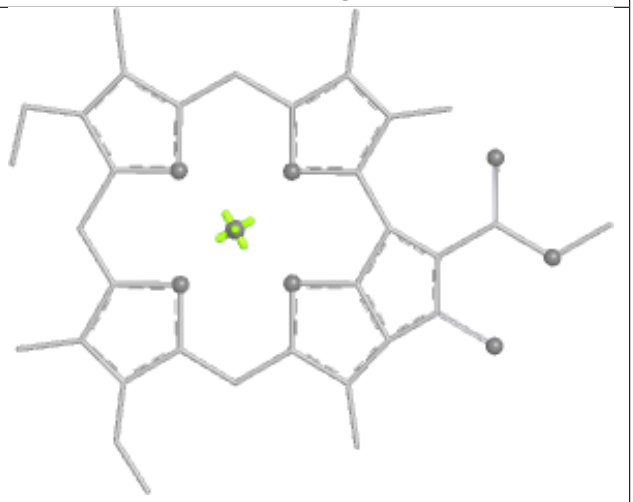
Bond lengths



Bond angles

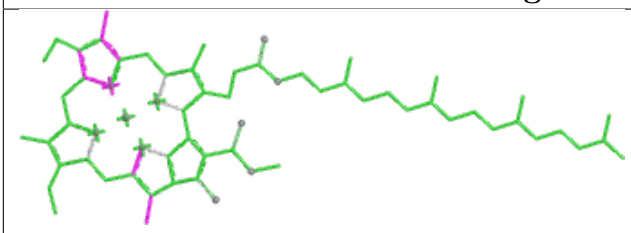


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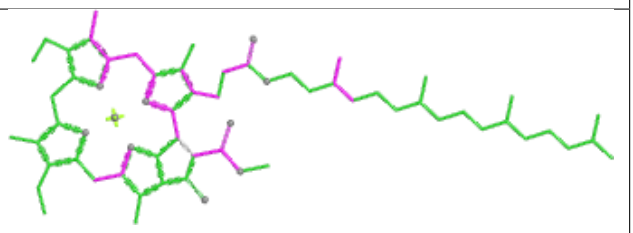


Rings

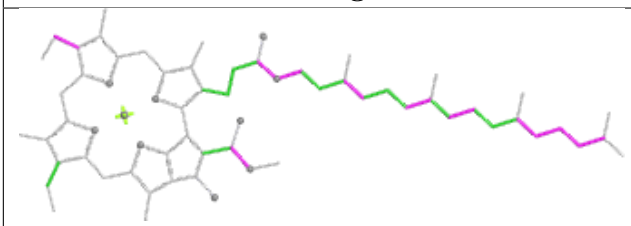
Ligand CLA A 838



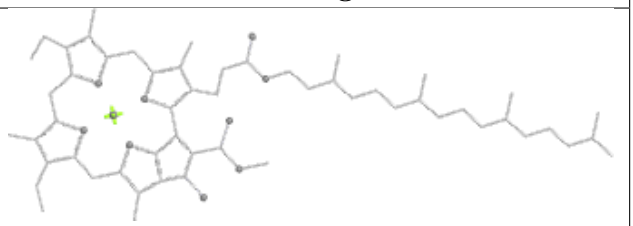
Bond lengths



Bond angles

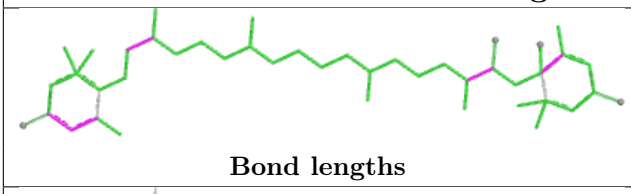


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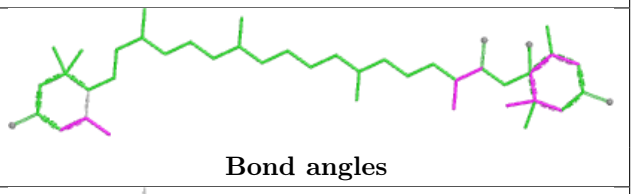


Rings

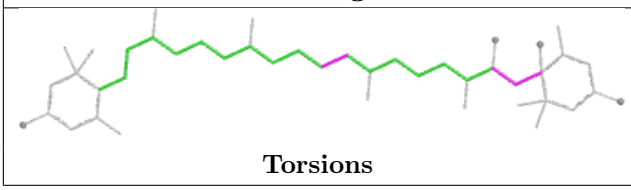
Ligand IWJ S 322



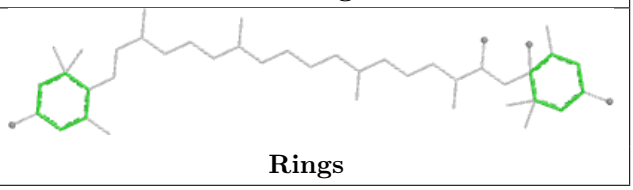
Bond lengths



Bond angles

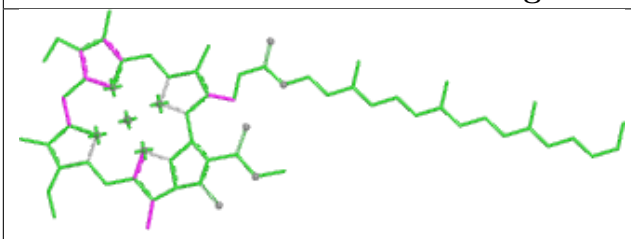


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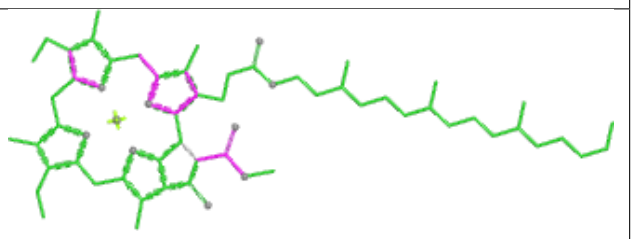


Rings

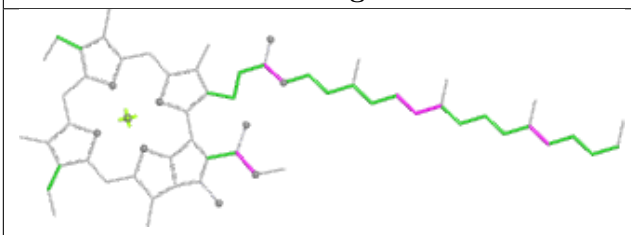
Ligand CLA A 812



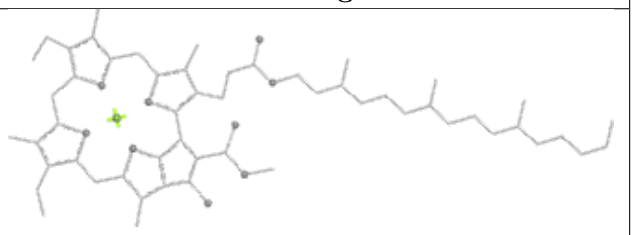
Bond lengths



Bond angles

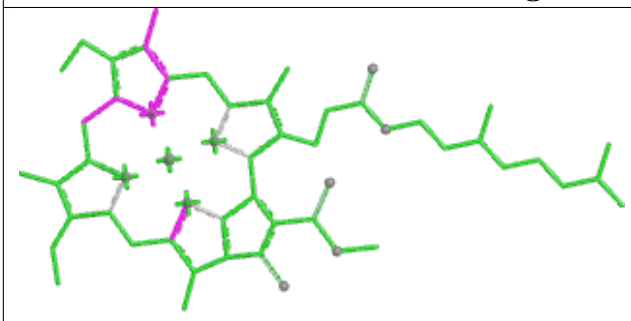


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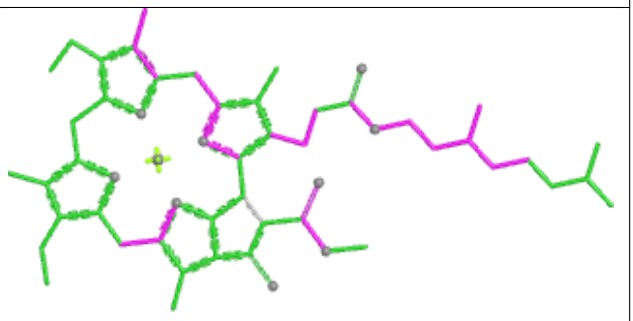


Rings

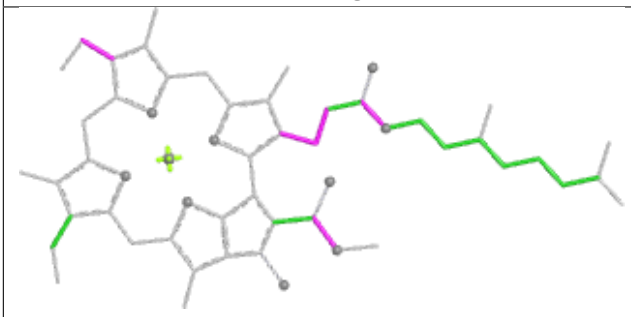
Ligand CLA B 821



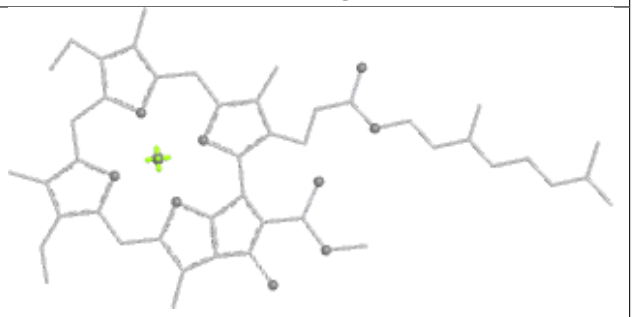
Bond lengths



Bond angles

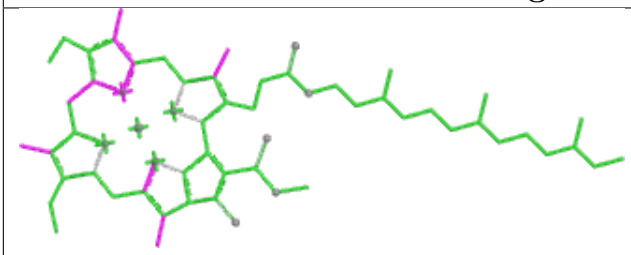


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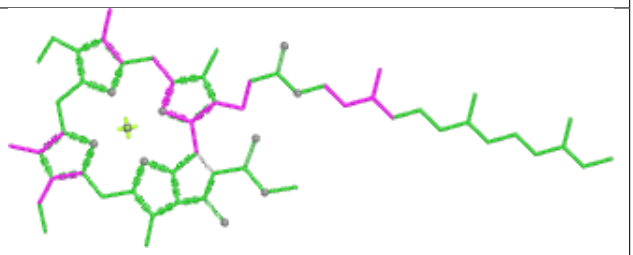


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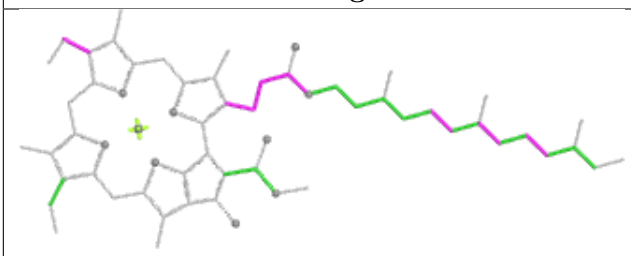
Ligand CLA 3 307



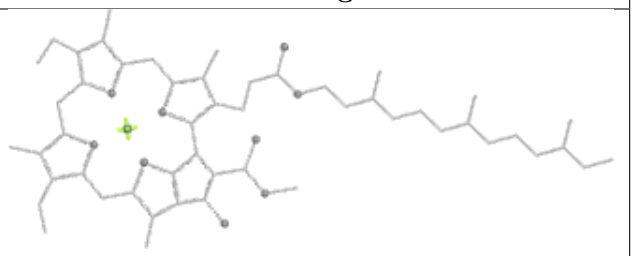
Bond lengths



Bond angles

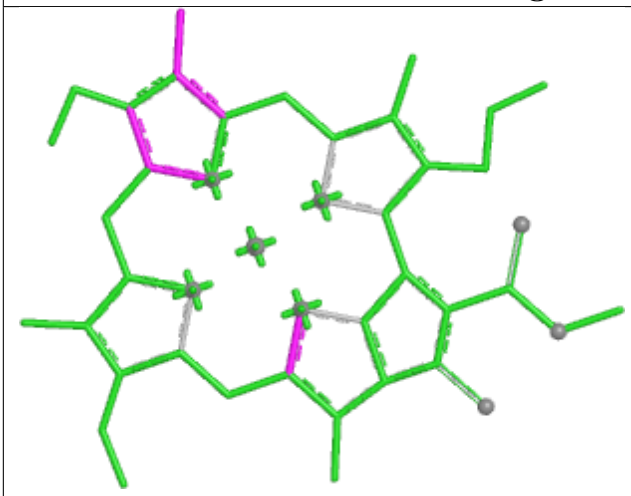


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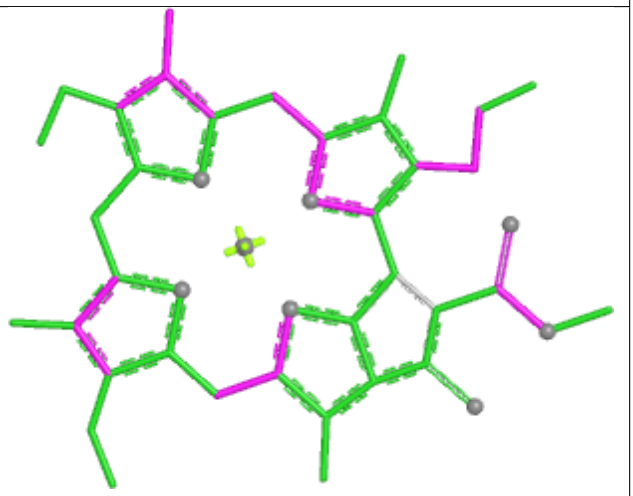


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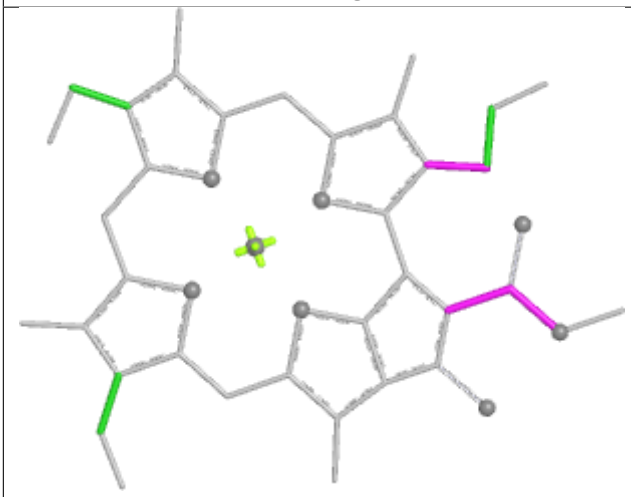
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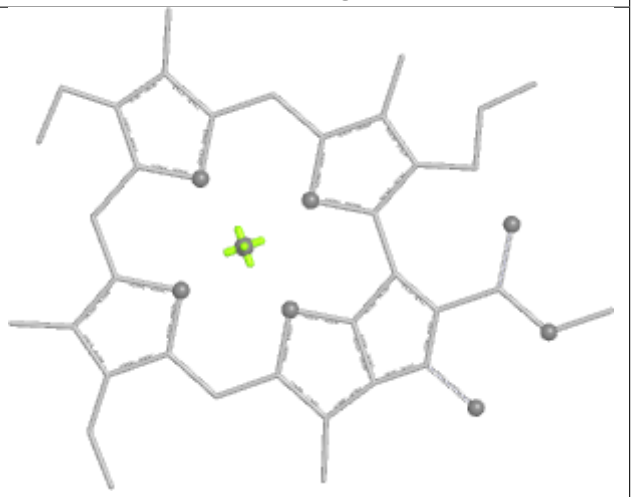
Bond lengths



Bond angles

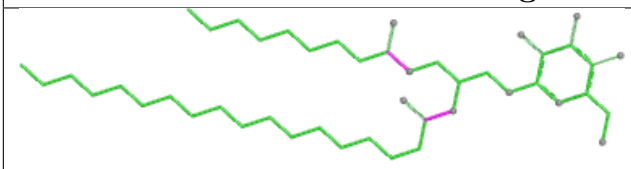


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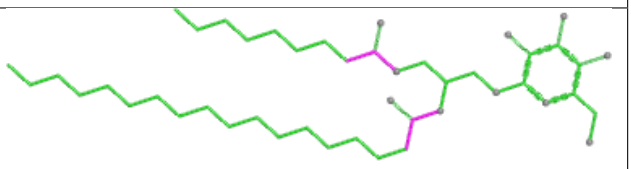


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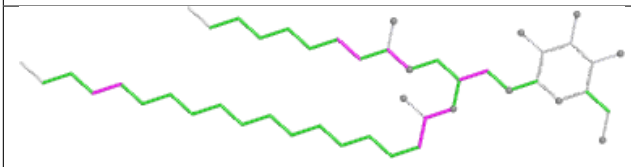
Ligand LMG A 857



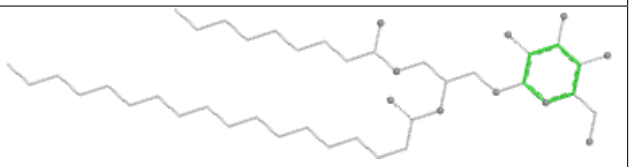
Bond lengths



Bond angles

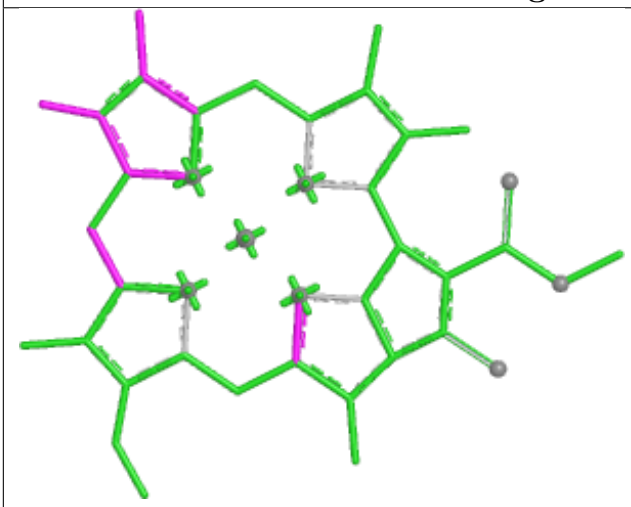


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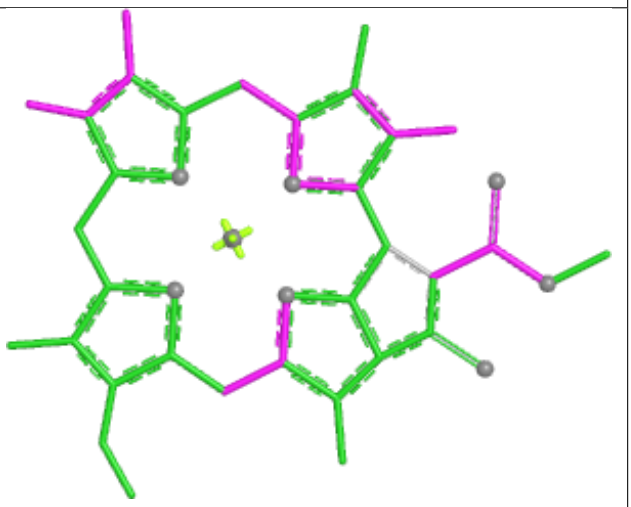


Rings

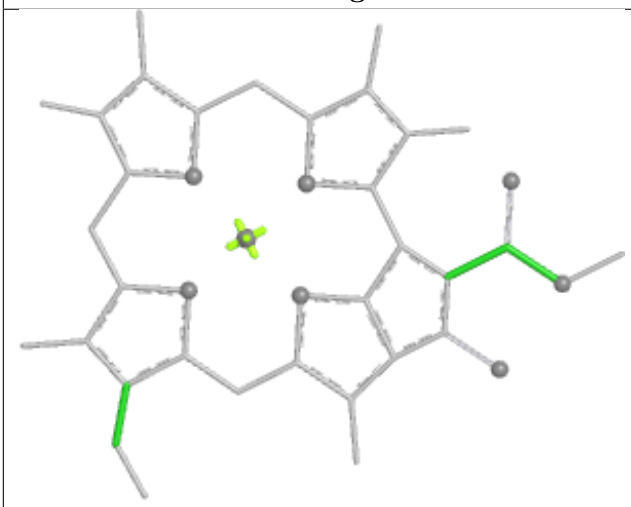
Ligand CLA 5 606



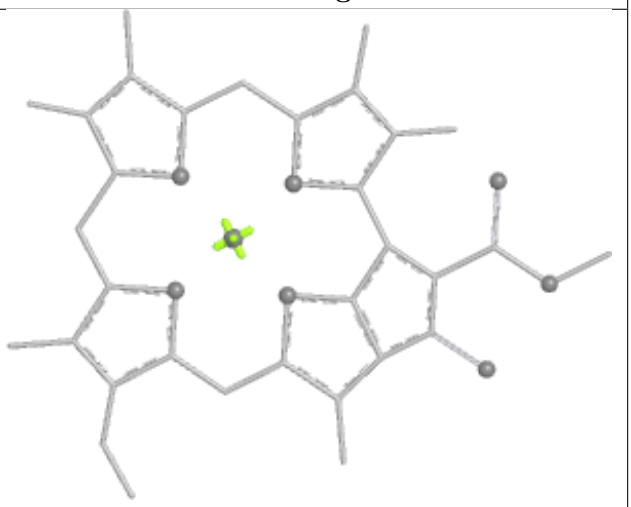
Bond lengths



Bond angles

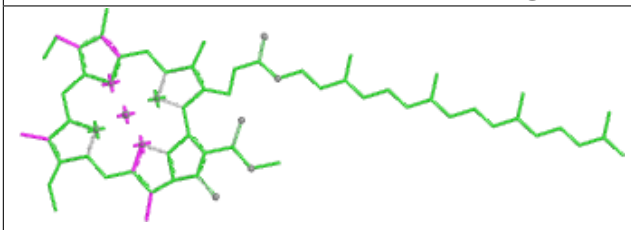


Torsions

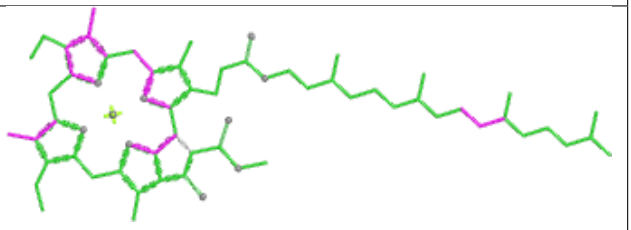


Rings

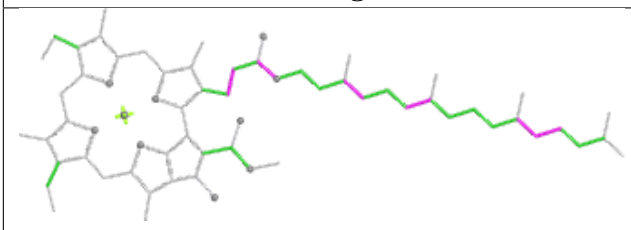
Ligand CLA A 808



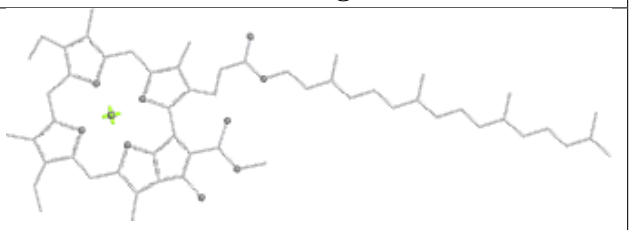
Bond lengths



Bond angles

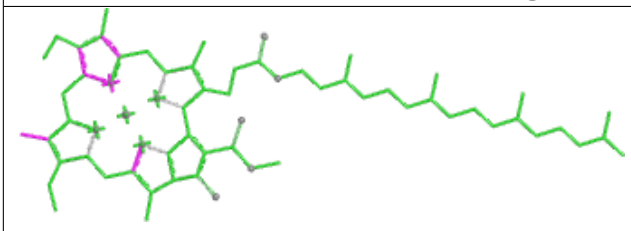


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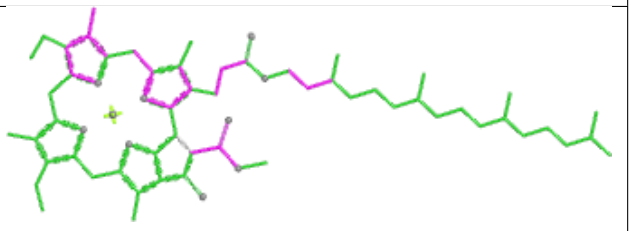


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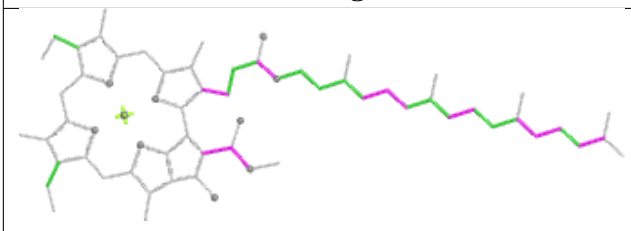
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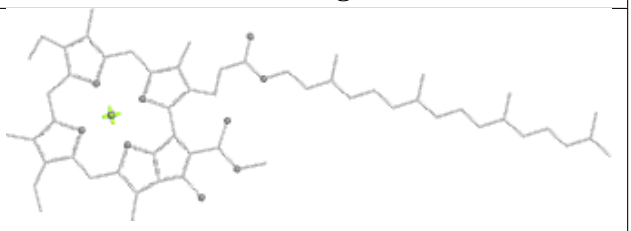
Bond lengths



Bond angles

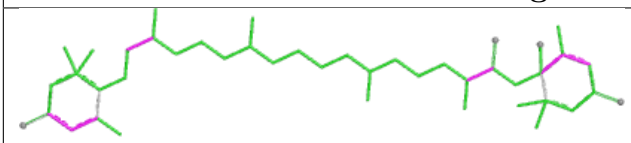


Torsions

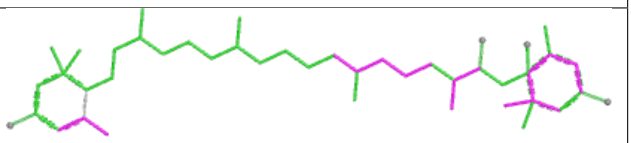


Rings

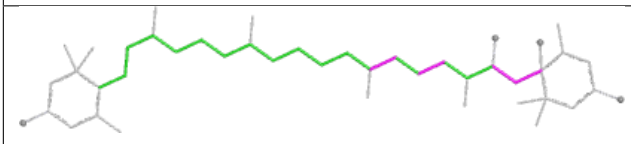
Ligand IWJ S 319



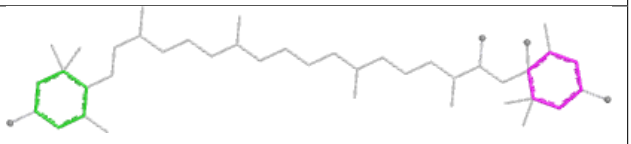
Bond lengths



Bond angles

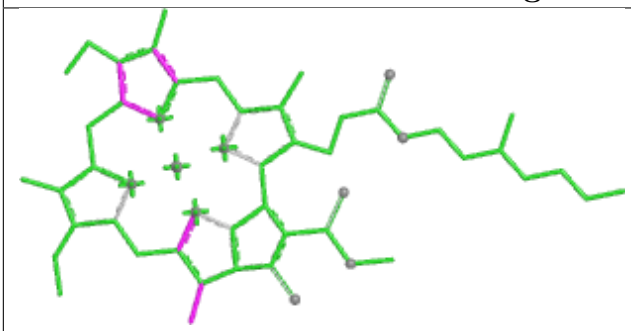


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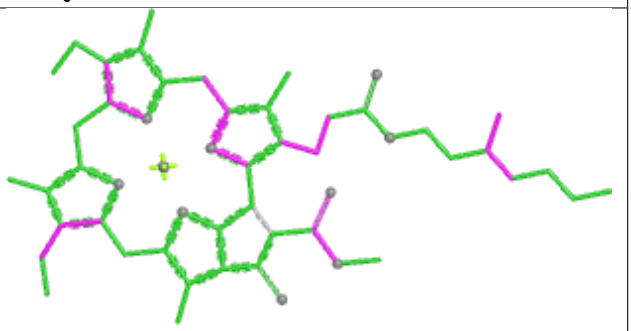


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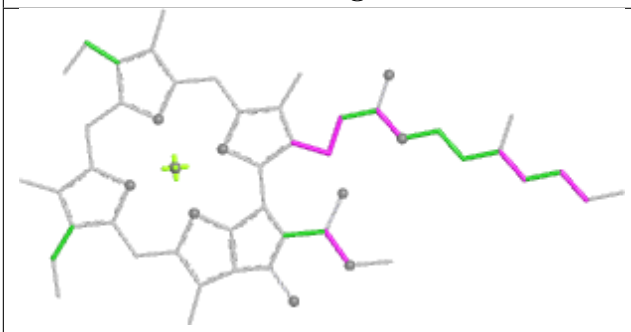
Ligand CLA Q 314



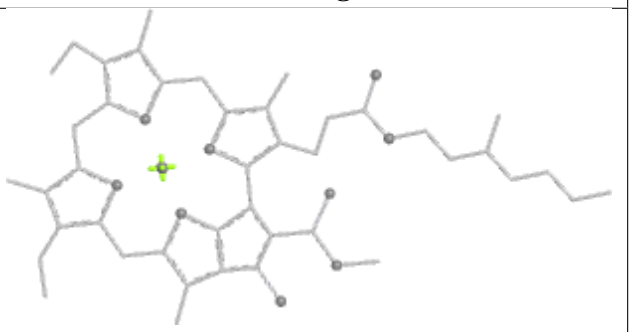
Bond lengths



Bond angles

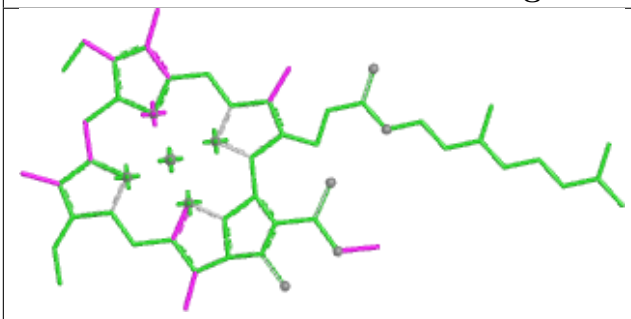


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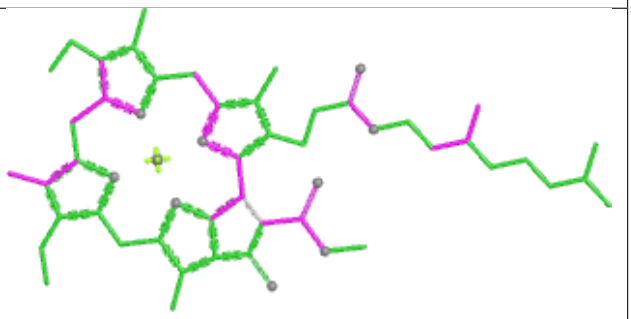


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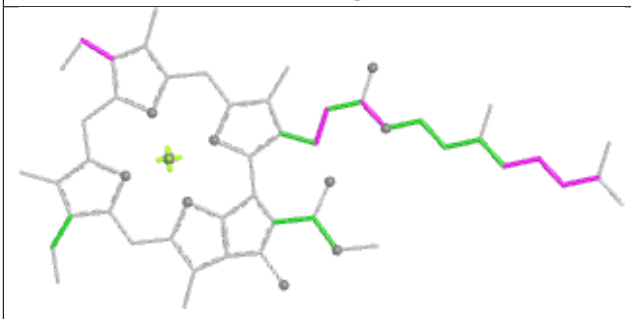
Ligand CLA X 302



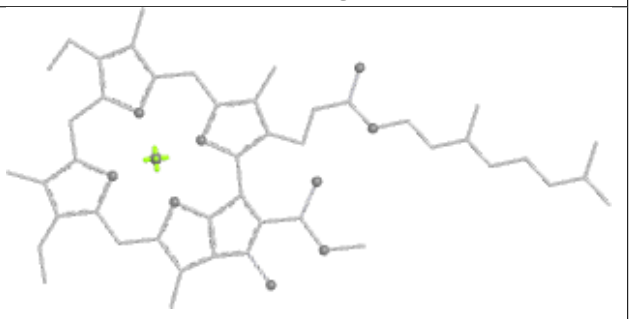
Bond lengths



Bond angles

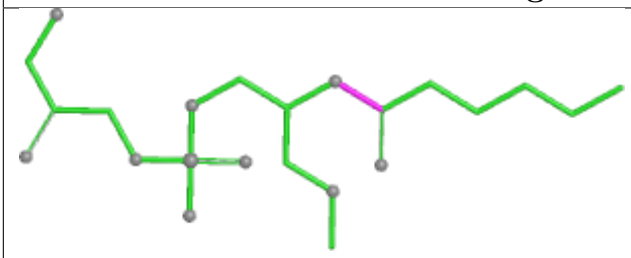


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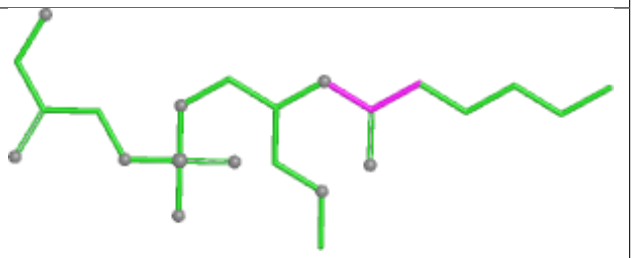


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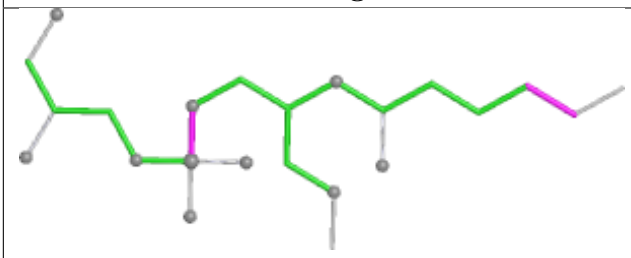
Ligand LHG 3 320



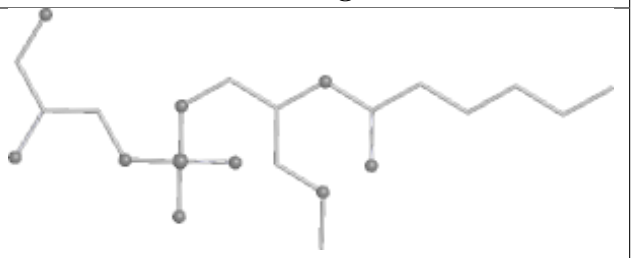
Bond lengths



Bond angles

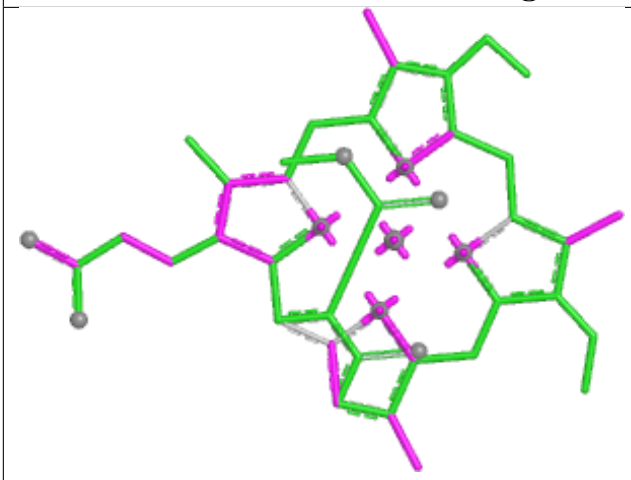


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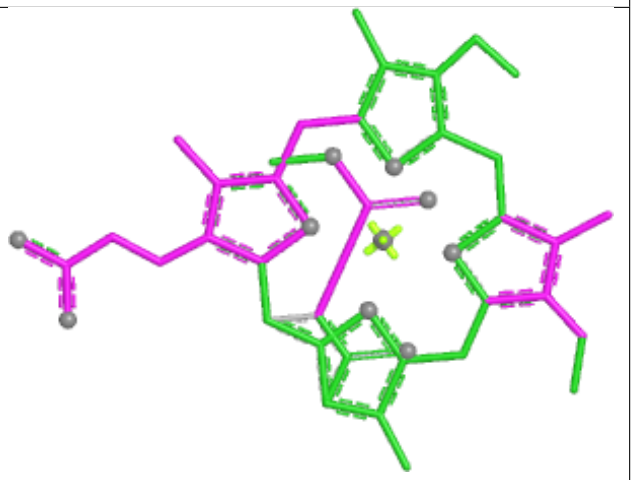


Rings

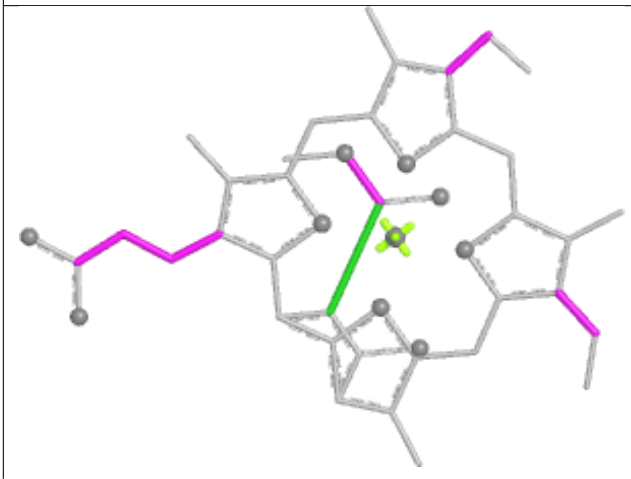
Ligand KC2 W 308



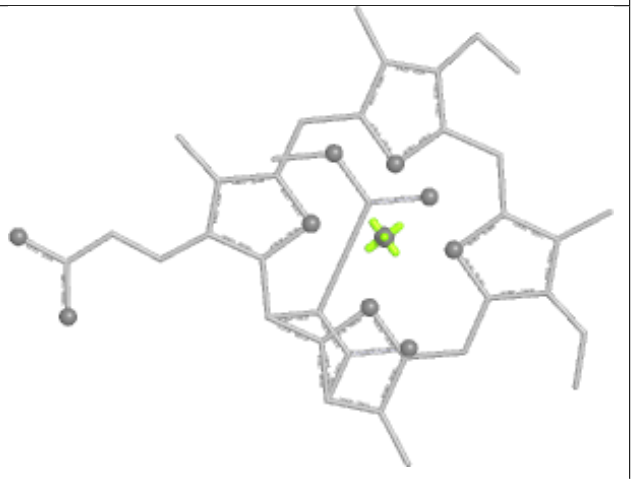
Bond lengths



Bond angles

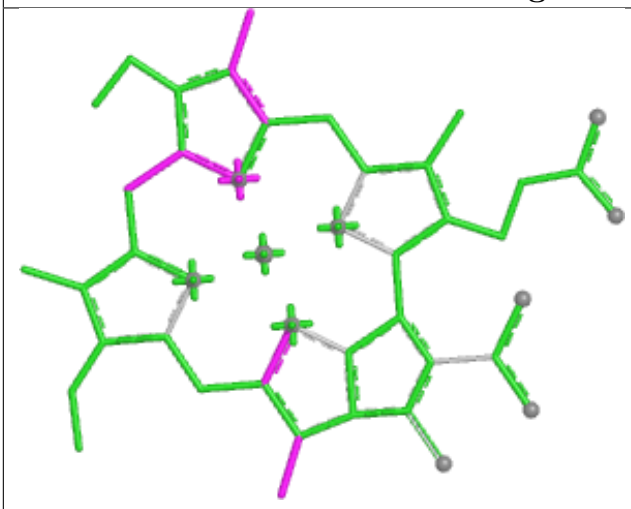


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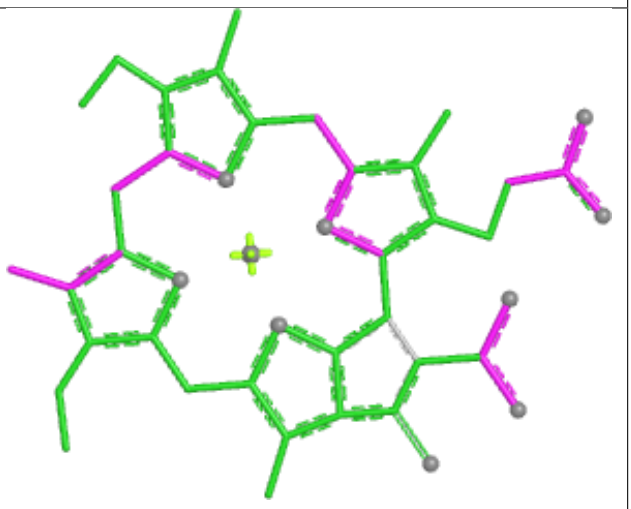


Rings

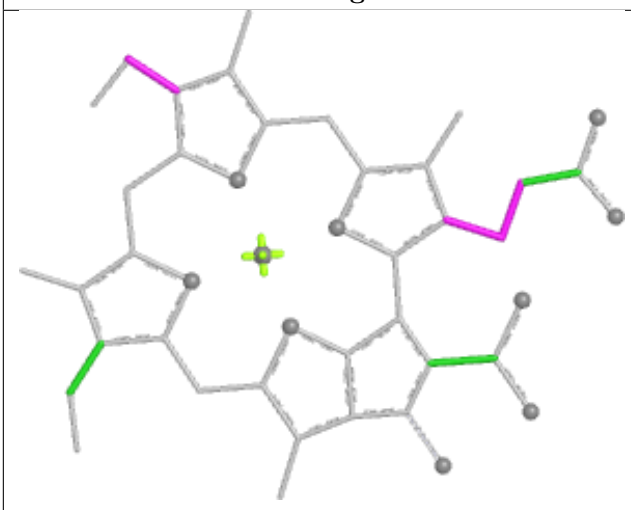
Ligand CLA 2 603



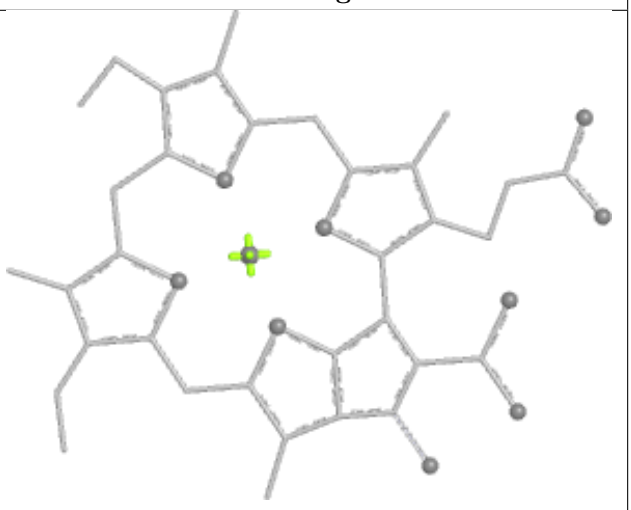
Bond lengths



Bond angles

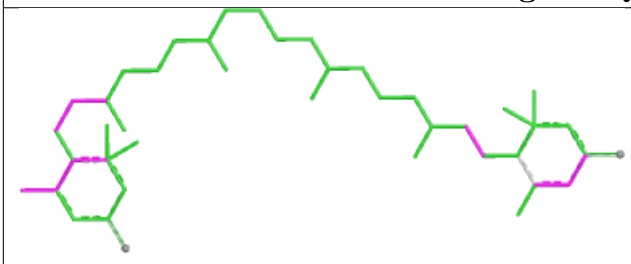


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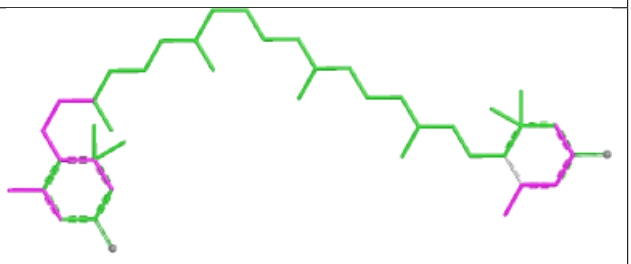


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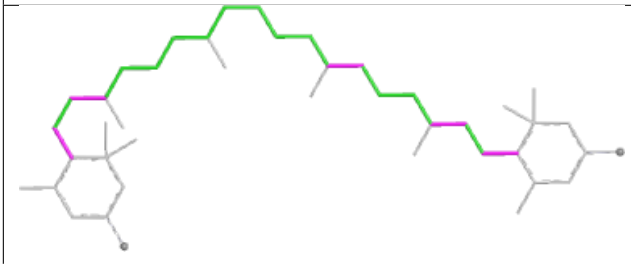
Ligand Q6L O 2006



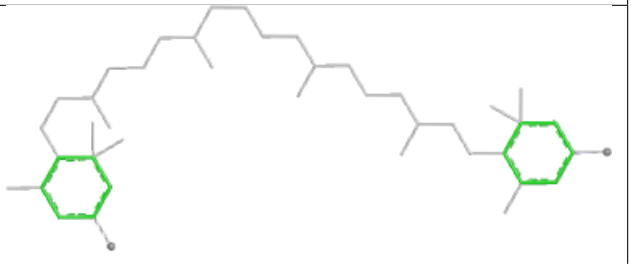
Bond lengths



Bond angles

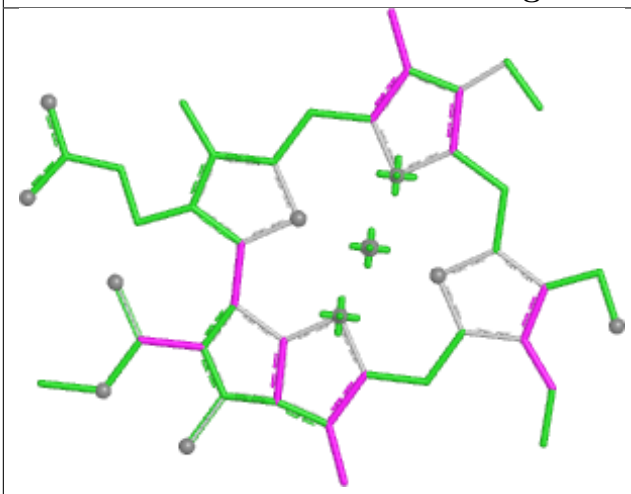


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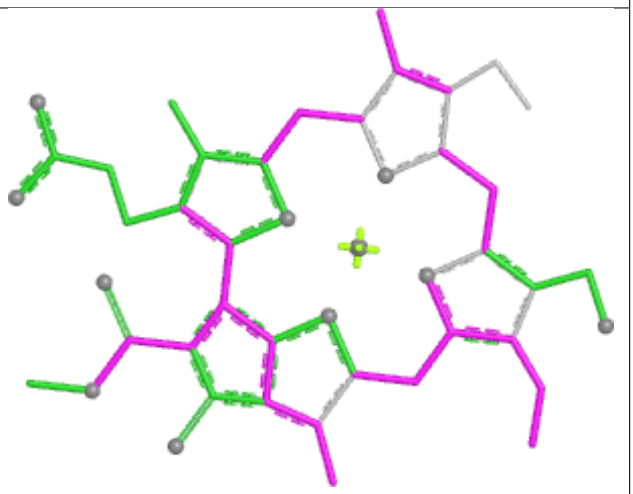


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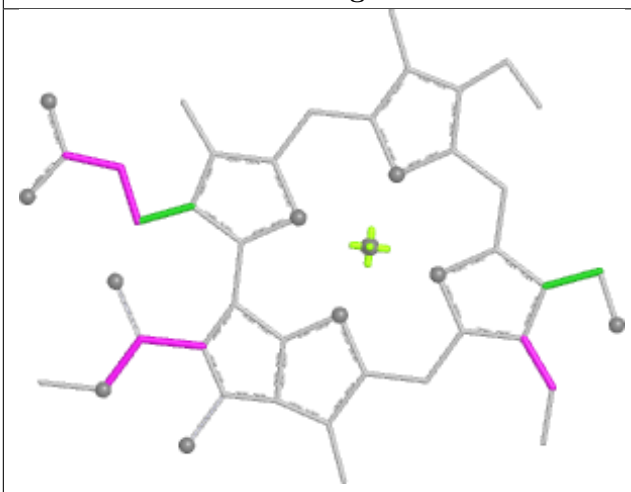
Ligand CHL U 305



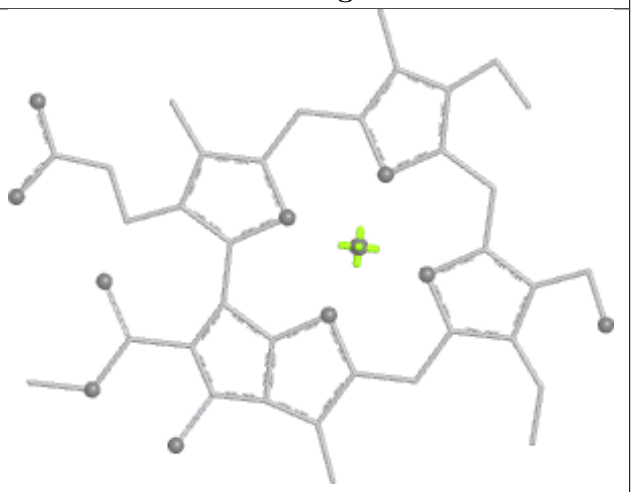
Bond lengths



Bond angles

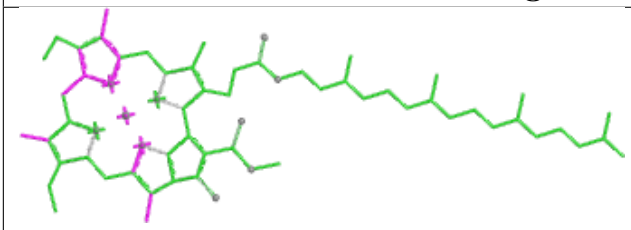


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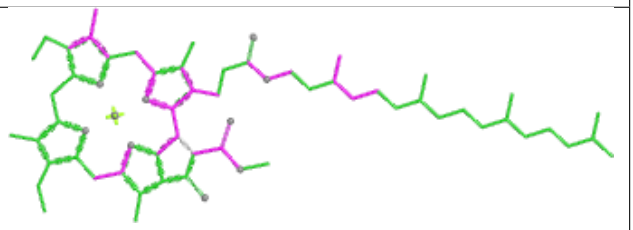


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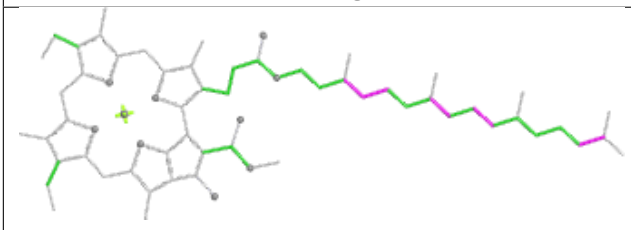
Ligand CLA B 826



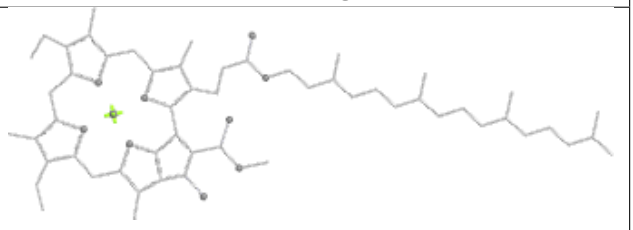
Bond lengths



Bond angles

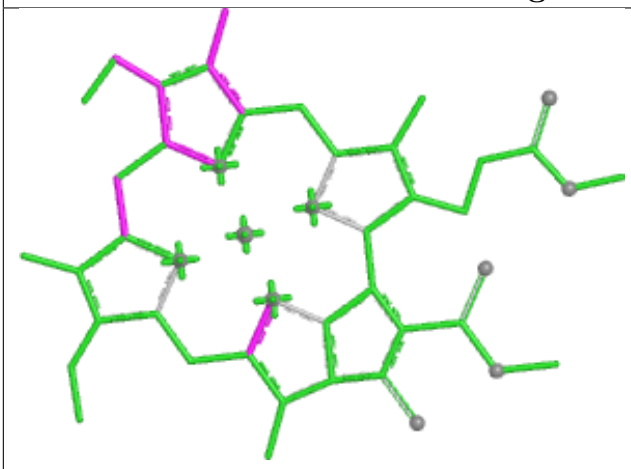


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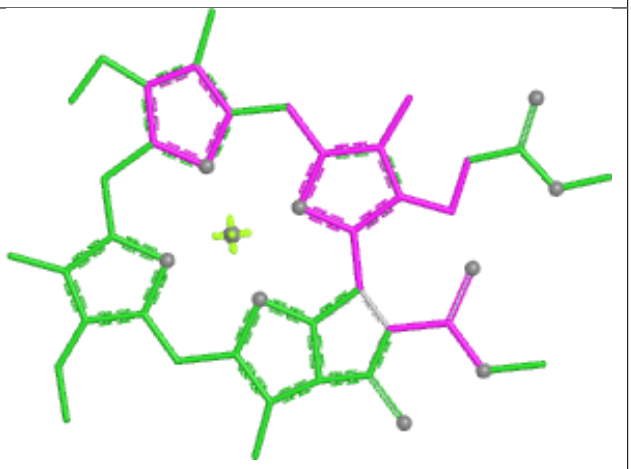


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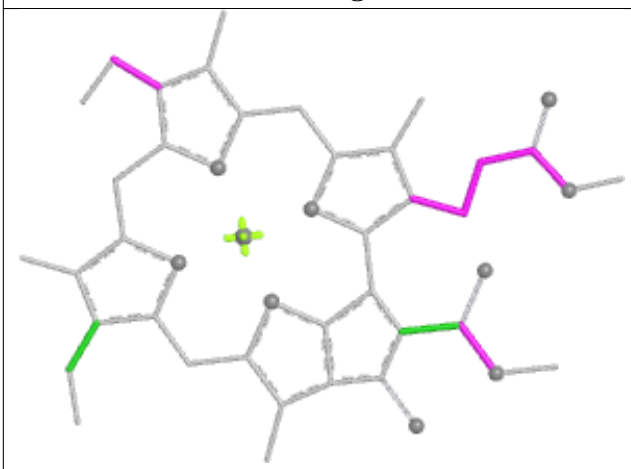
Ligand CLA 5 601



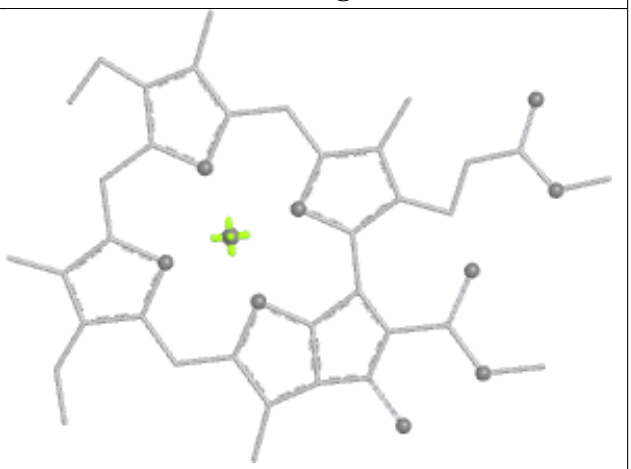
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Bond angles

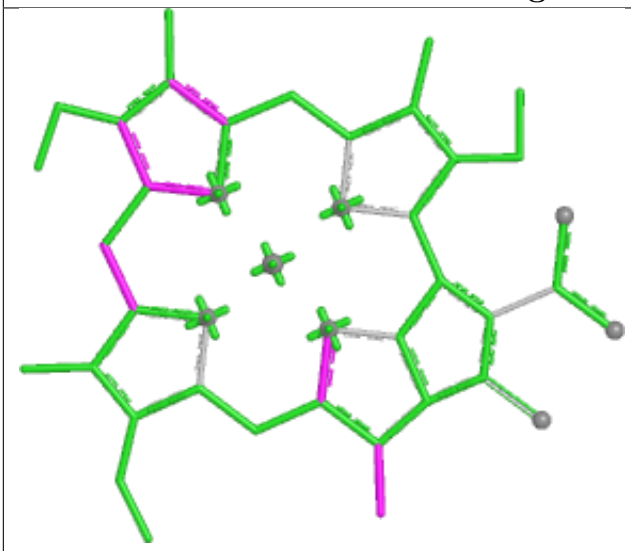


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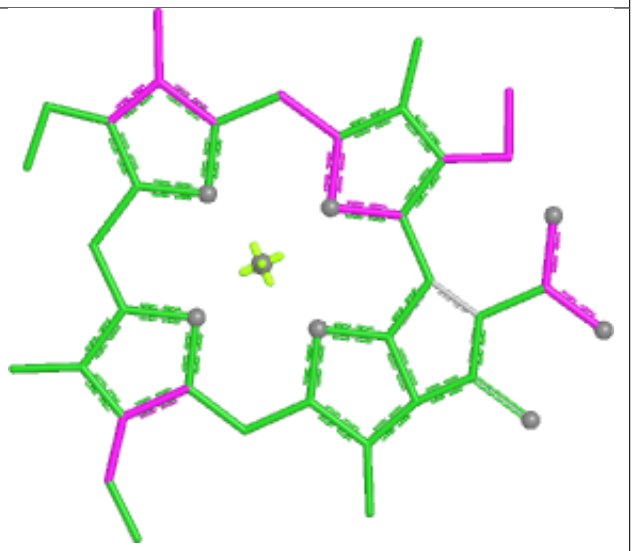


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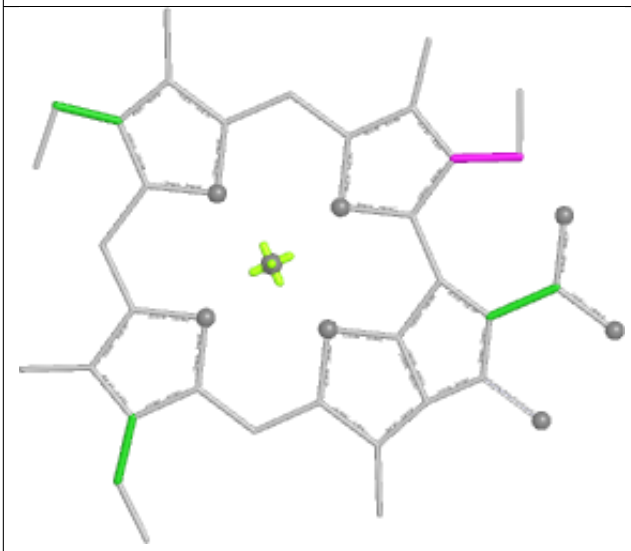
Ligand CLA 4 312



Bond lengths



Bond angles

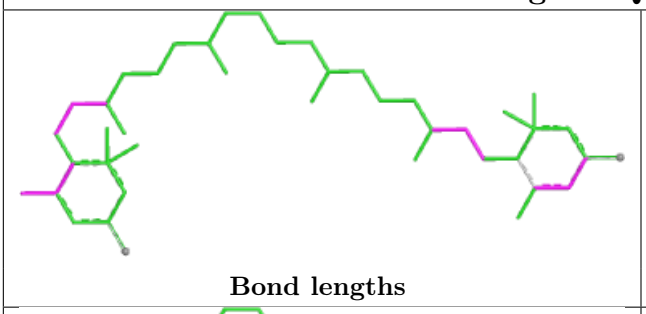


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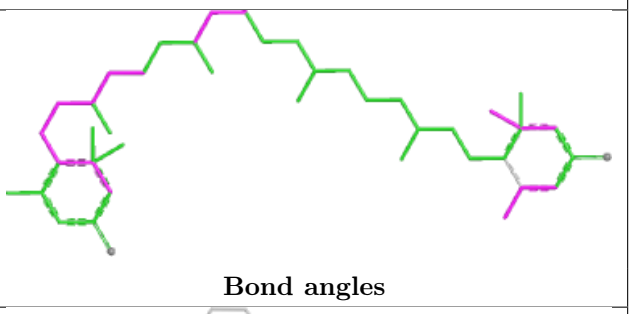


Rings

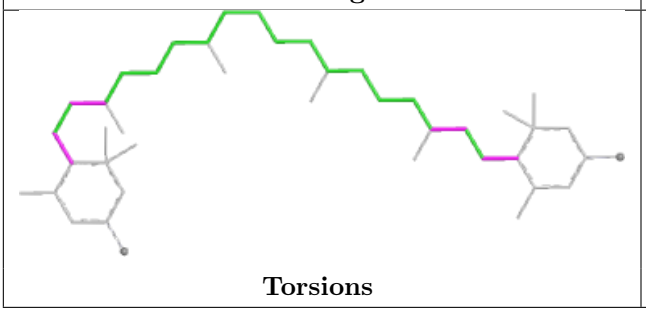
Ligand Q6L T 322



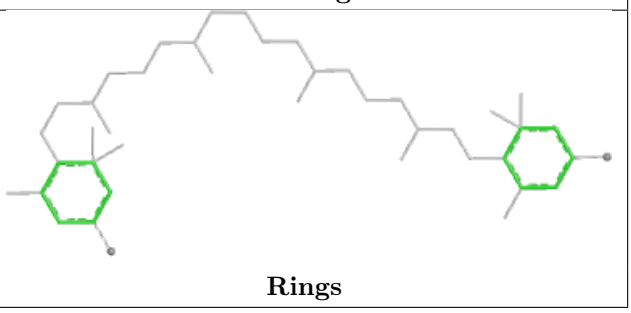
Bond lengths



Bond angles

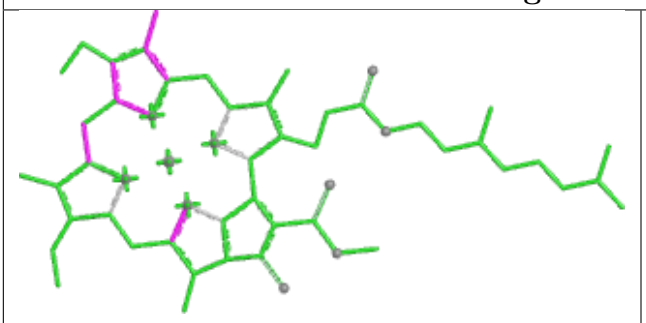


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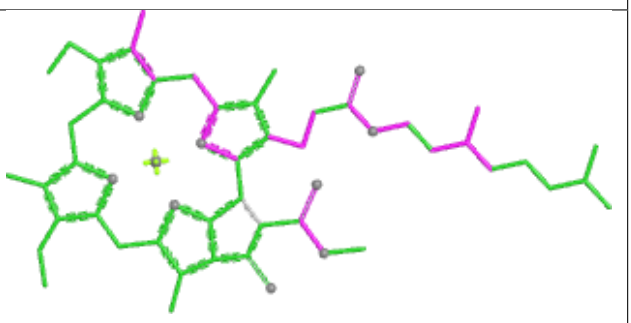


Rings

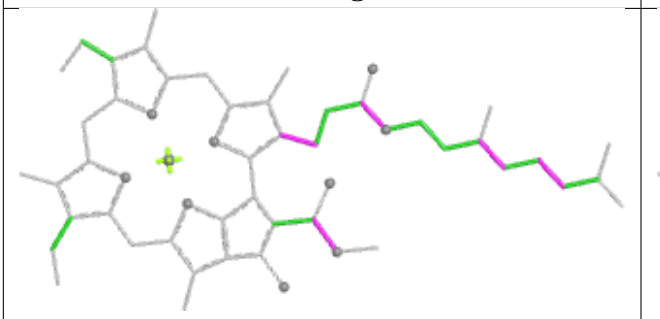
Ligand CLA R 316



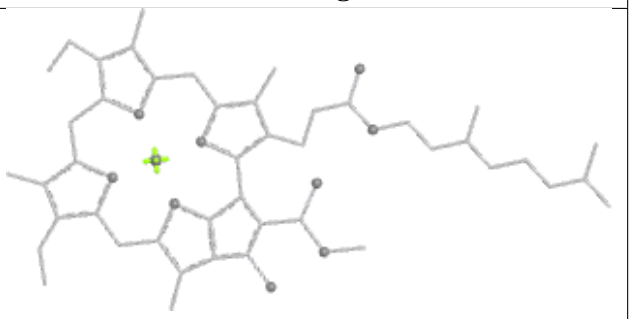
Bond lengths



Bond angles

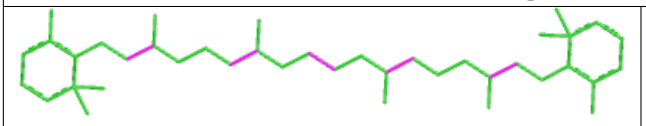


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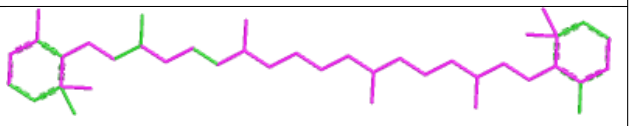


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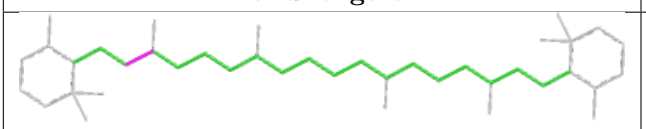
Ligand BCR A 848



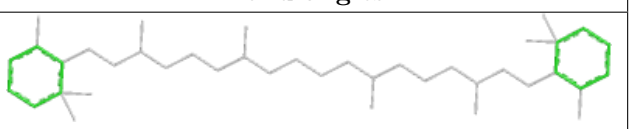
Bond lengths



Bond angles

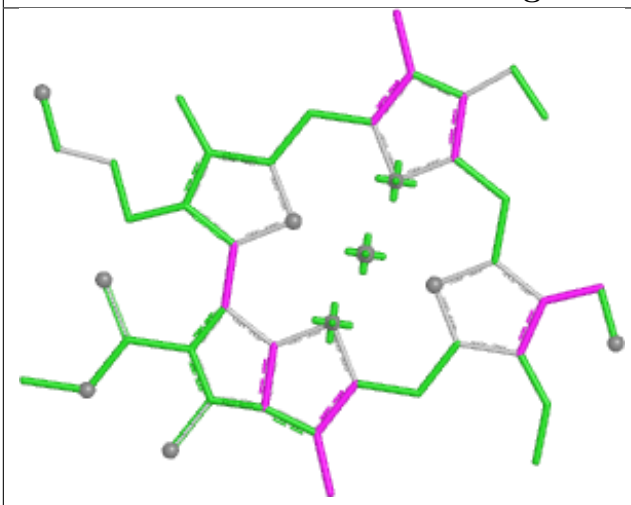


Torsions

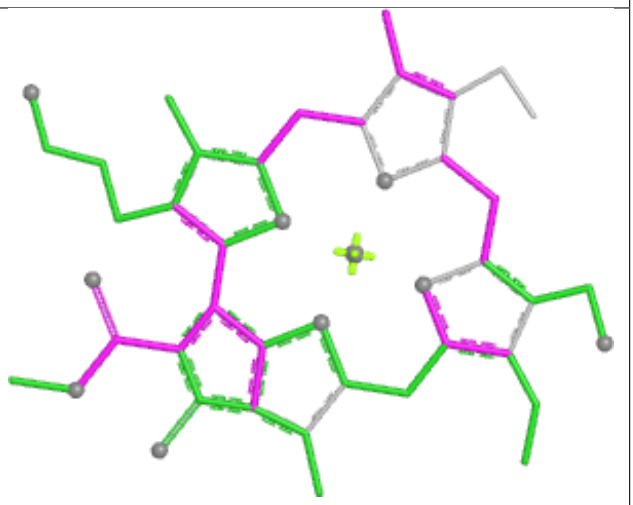


Rings

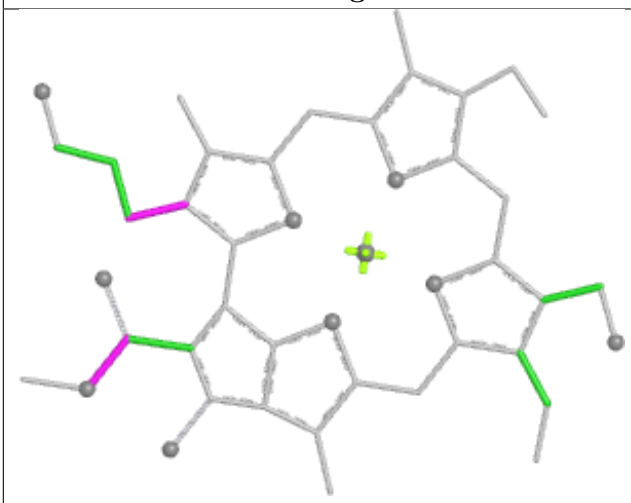
Ligand CHL R 318



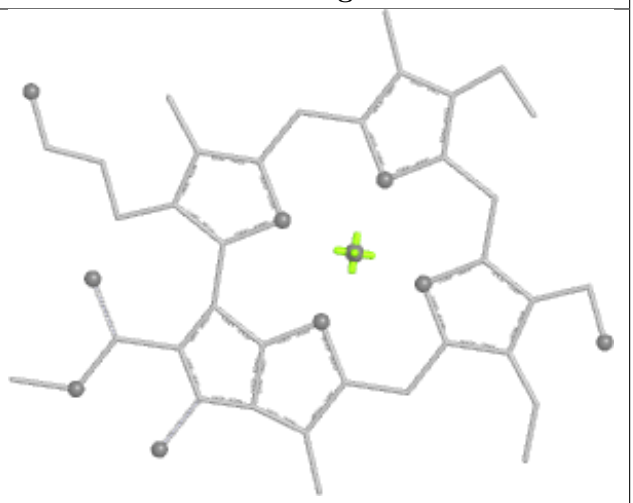
Bond lengths



Bond angles

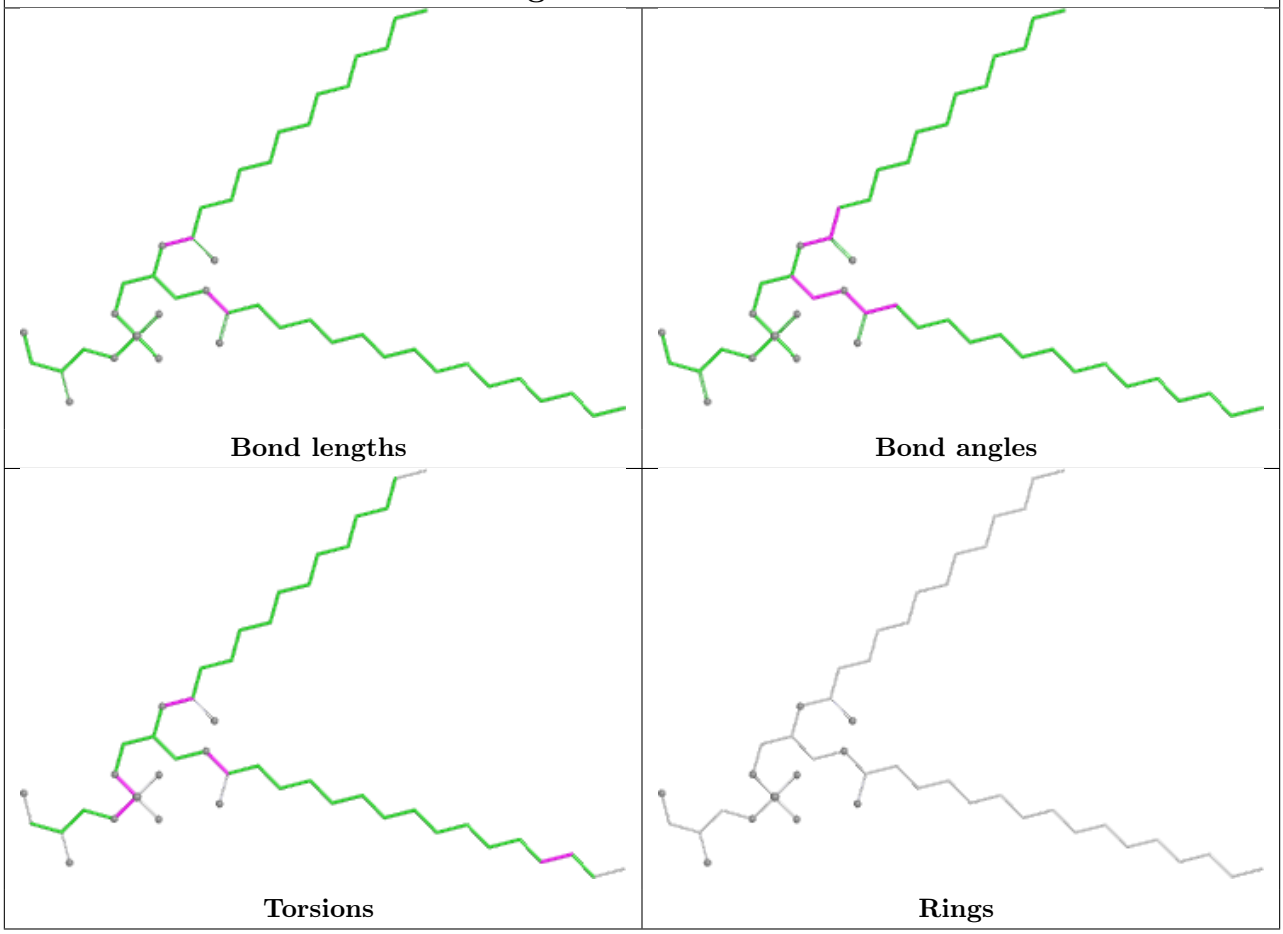


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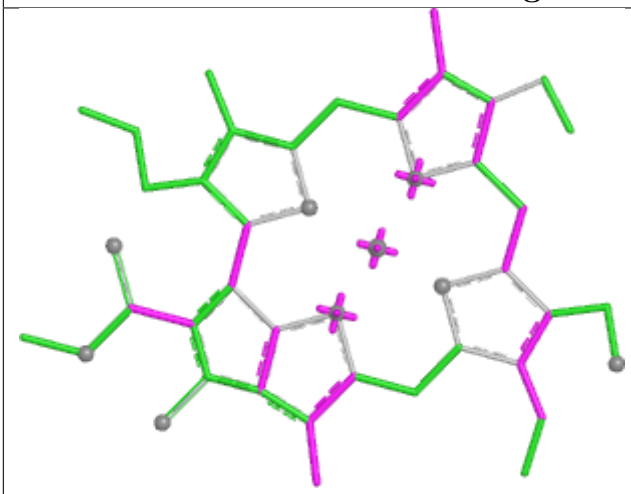


Rings

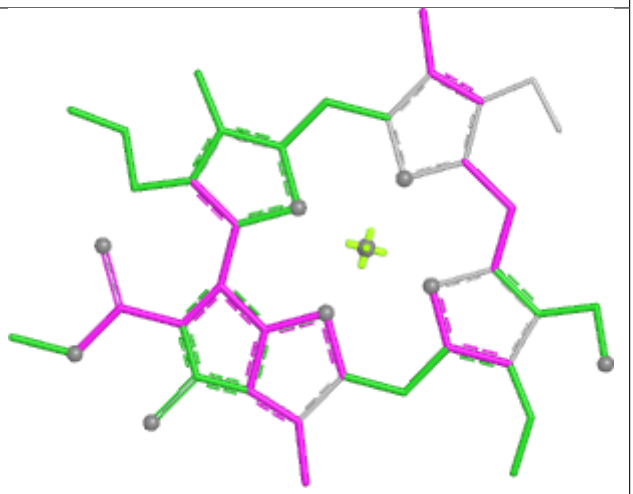
Ligand LHG 6 616



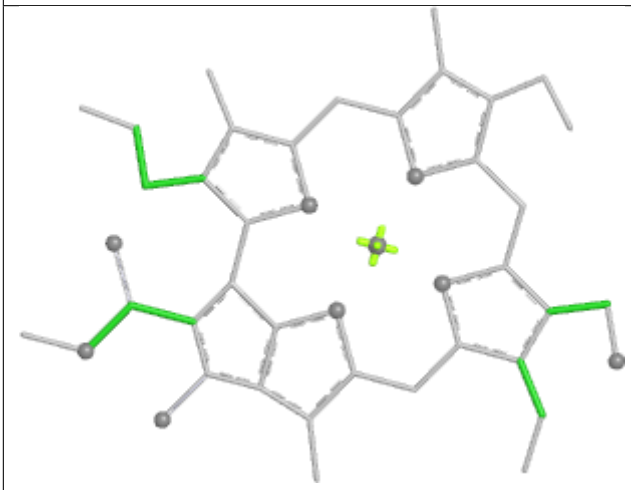
Ligand CHL V 306



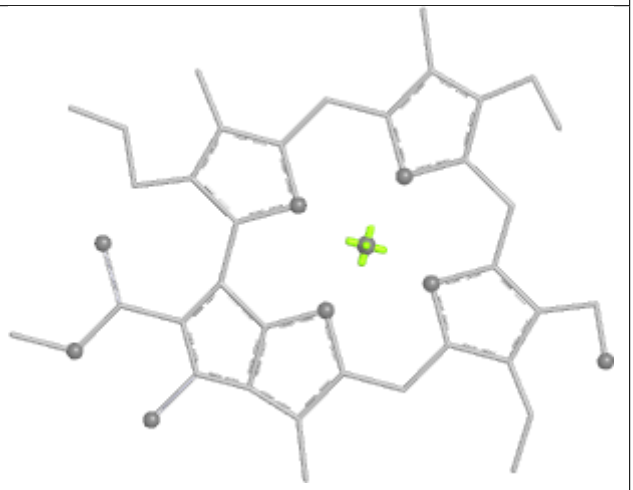
Bond lengths



Bond angles

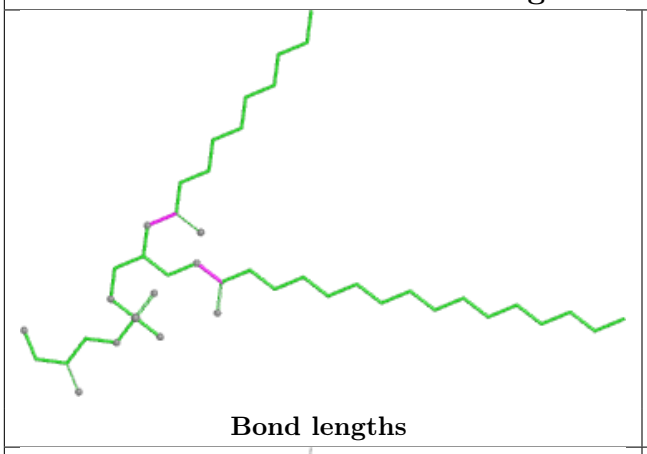


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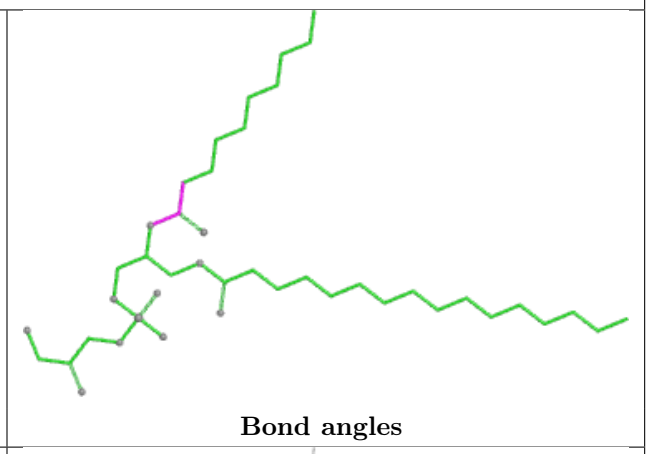


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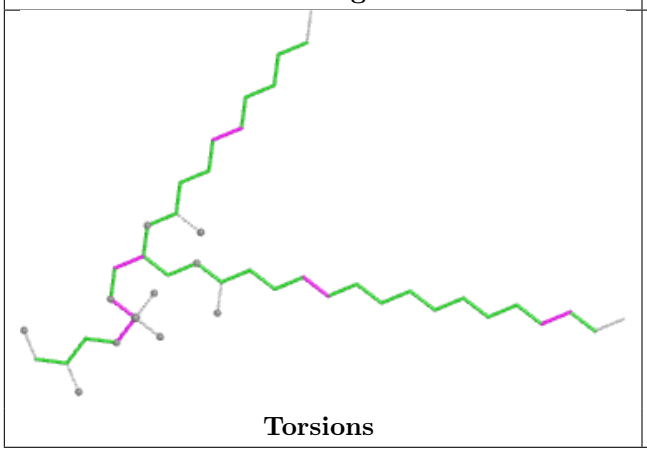
Ligand LHG 3 321



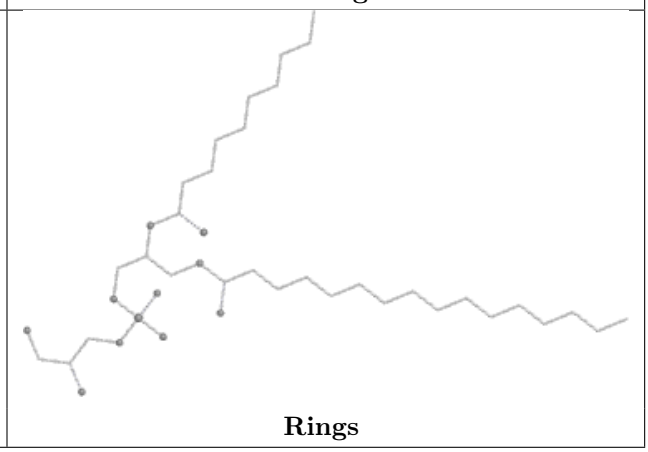
Bond lengths



Bond angles

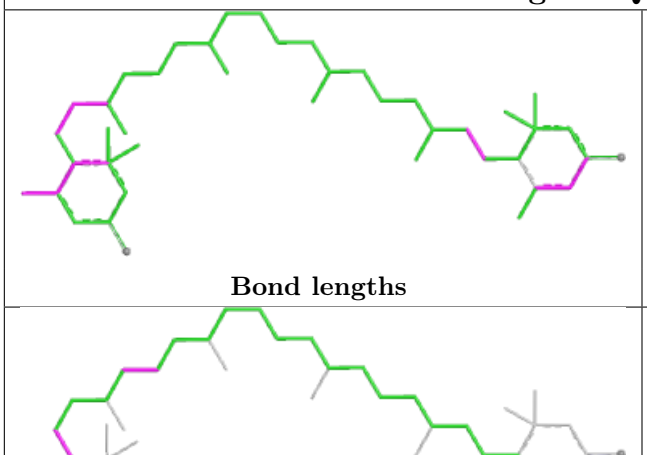


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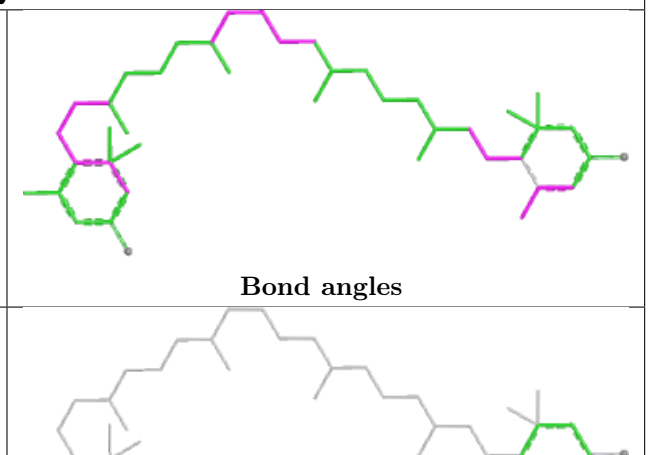


Rings

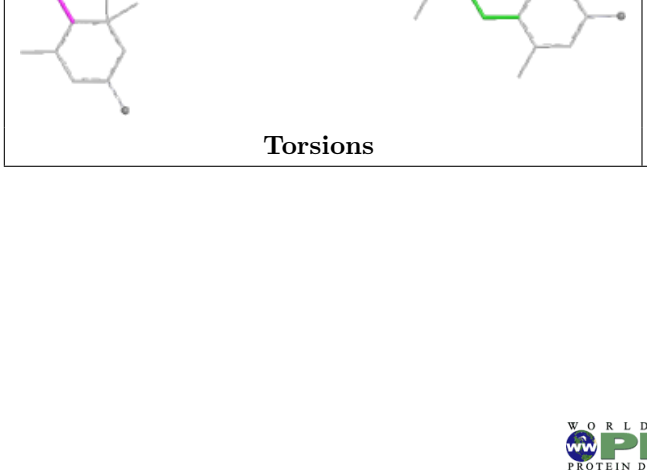
Ligand Q6L X 317



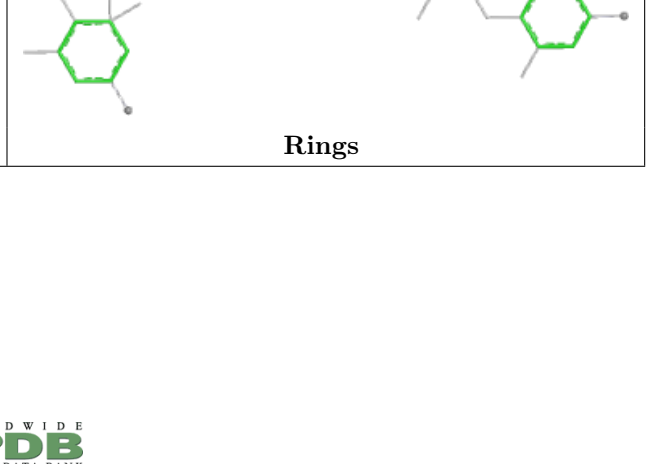
Bond lengths



Bond angles

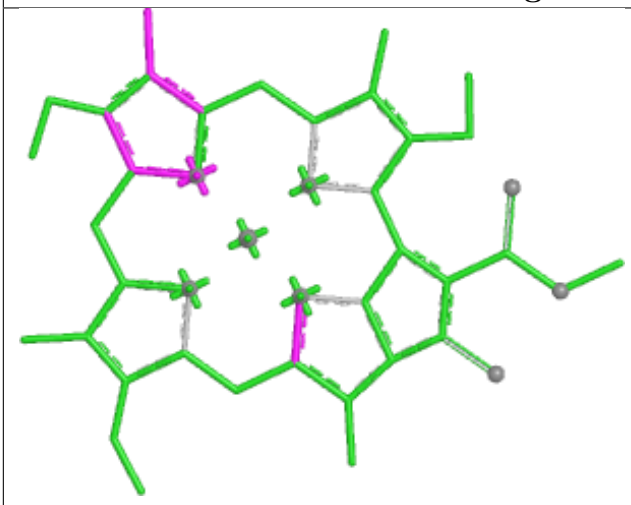


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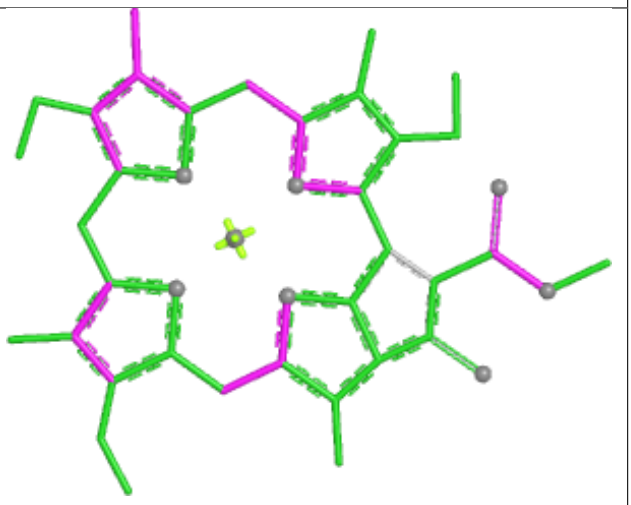


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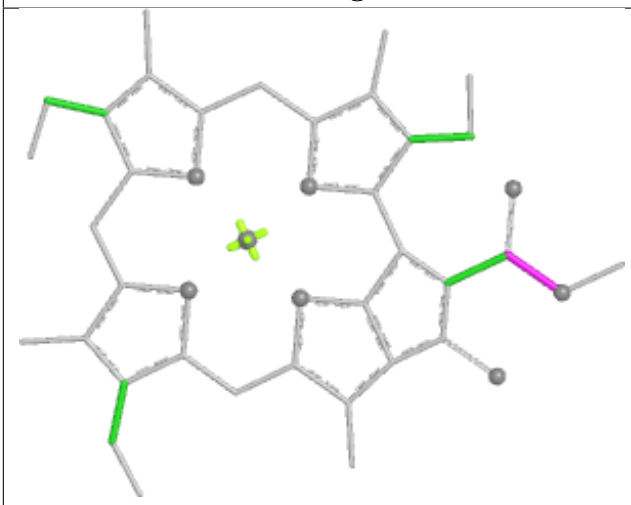
Ligand CLA B 837



Bond lengths



Bond angles

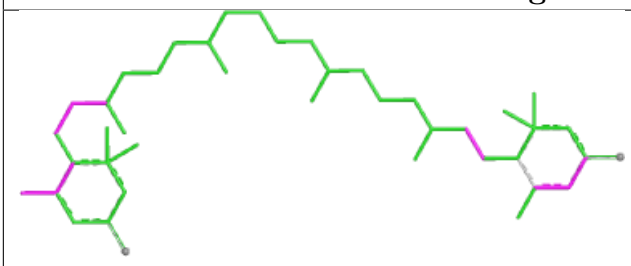


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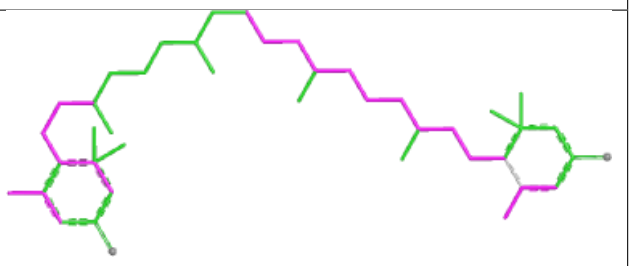


Rings

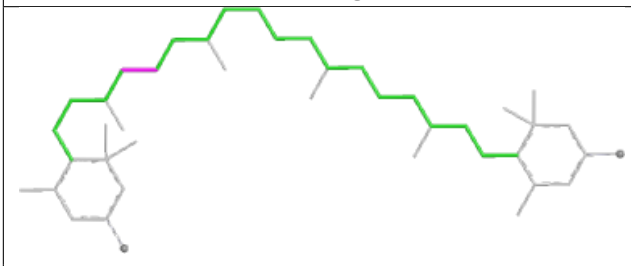
Ligand Q6L T 316



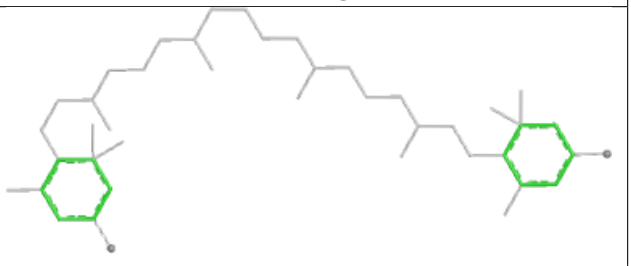
Bond lengths



Bond angles

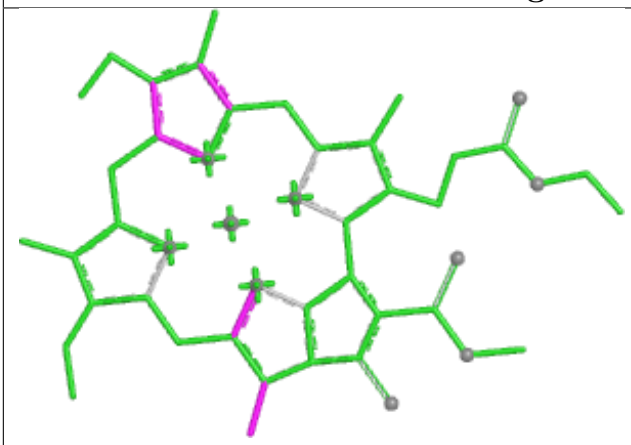


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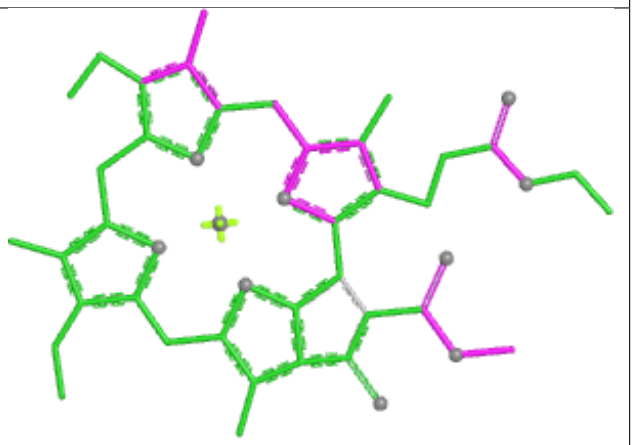


Rings

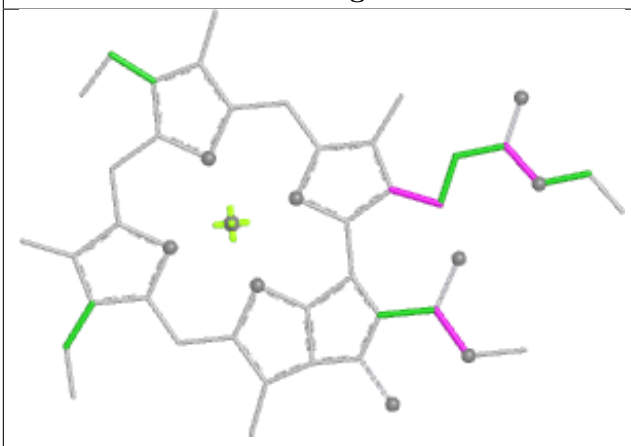
Ligand CLA S 311



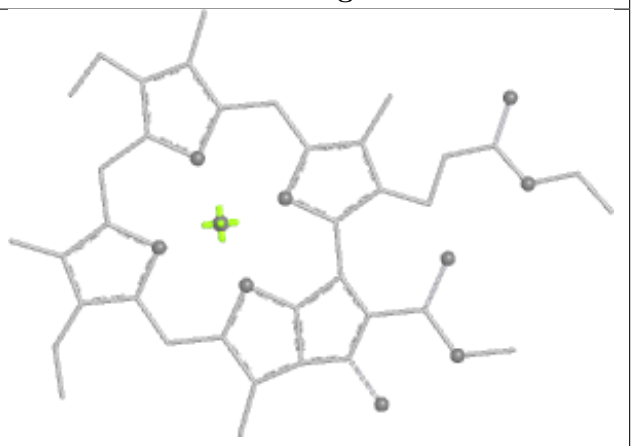
Bond lengths



Bond angles

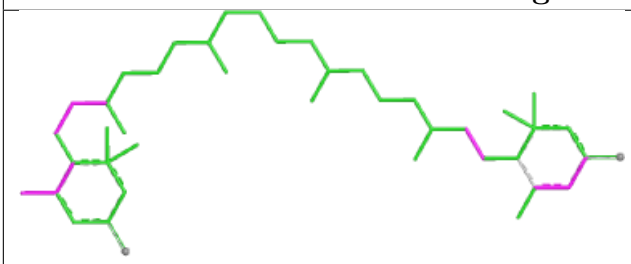


Torsions



Rings

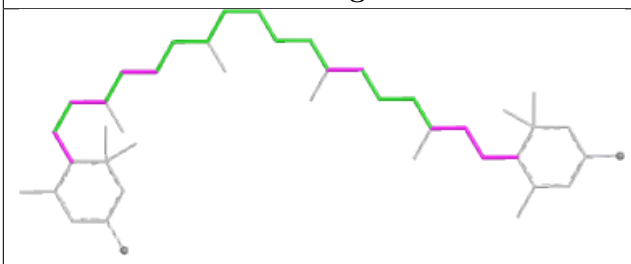
Ligand Q6L 2 616



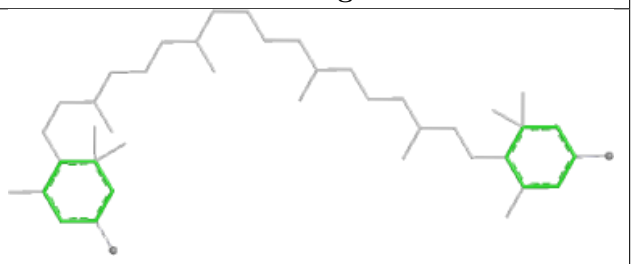
Bond lengths



Bond angles

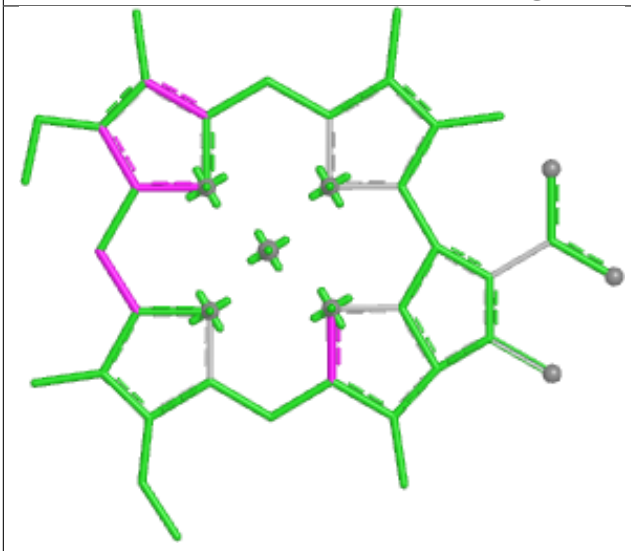


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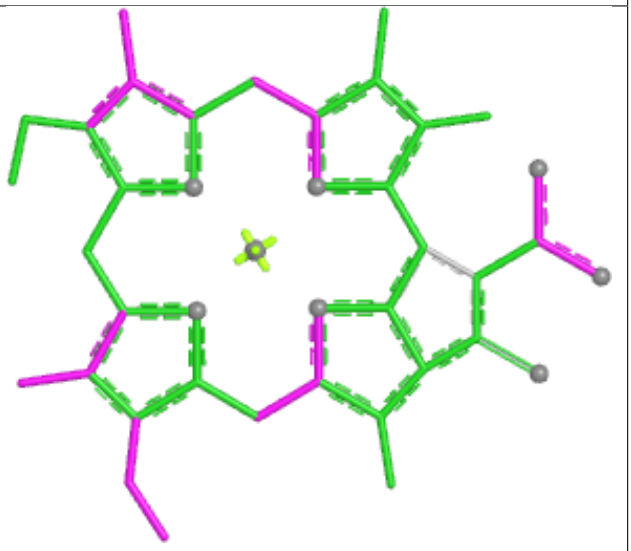


Rings

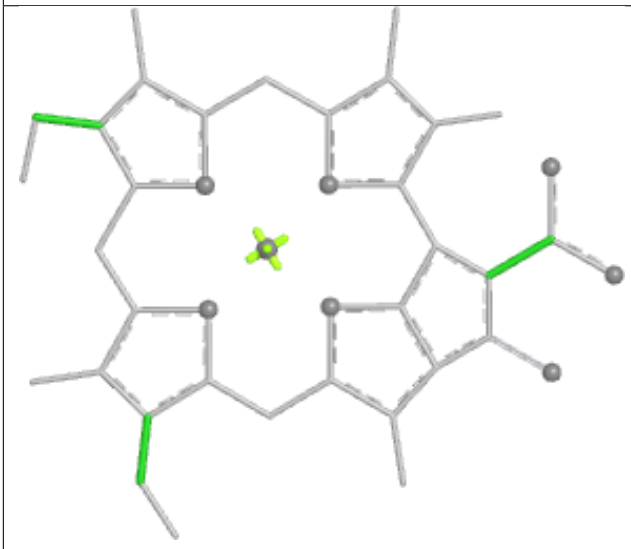
Ligand CLA 3 314



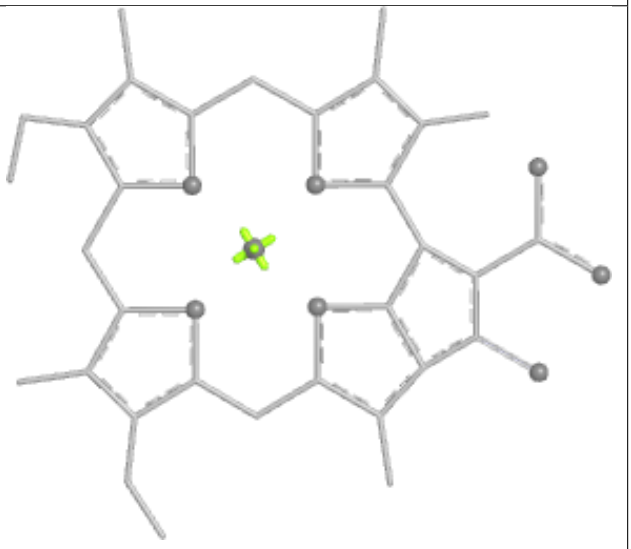
Bond lengths



Bond angles

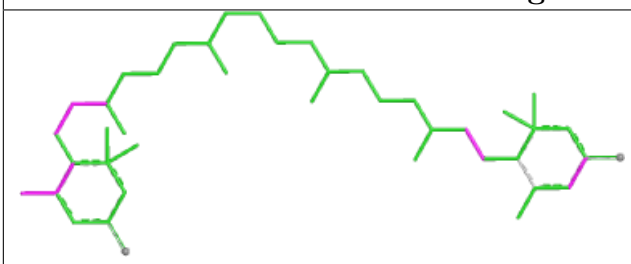


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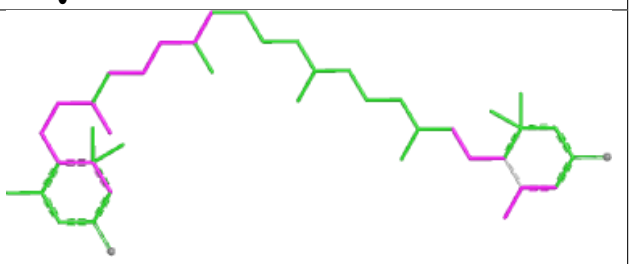


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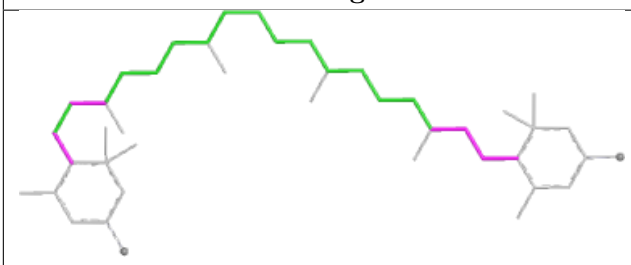
Ligand Q6L Q 317



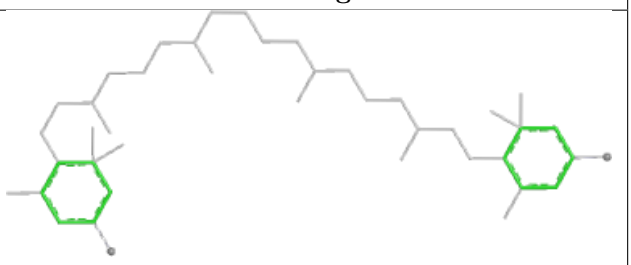
Bond lengths



Bond angles

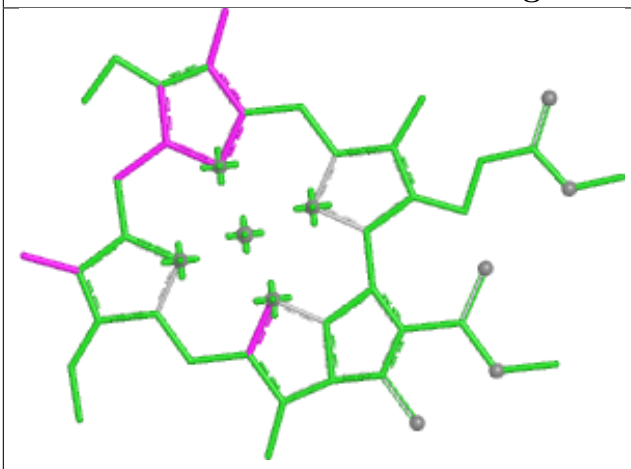


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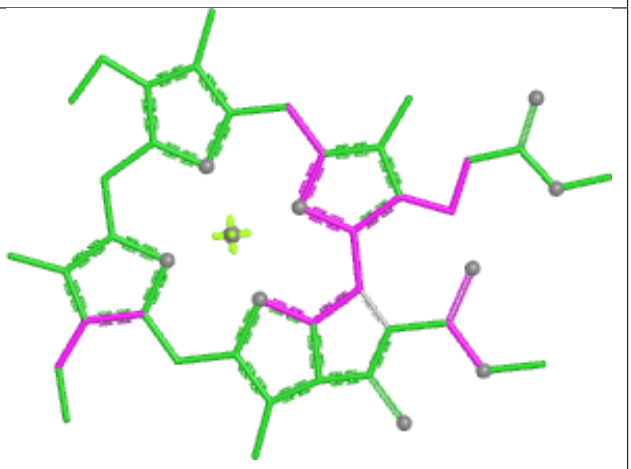


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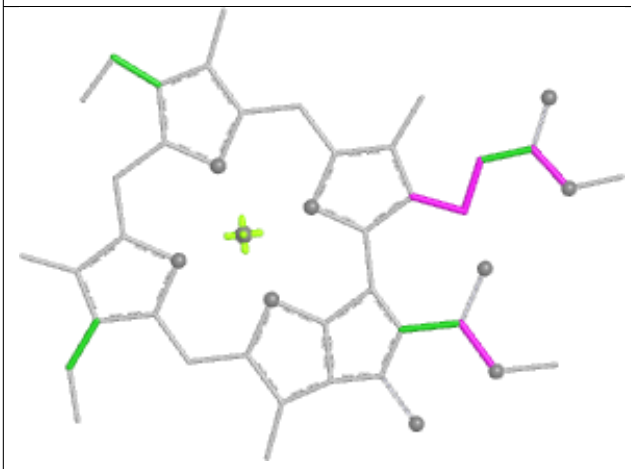
Ligand CLA K 204



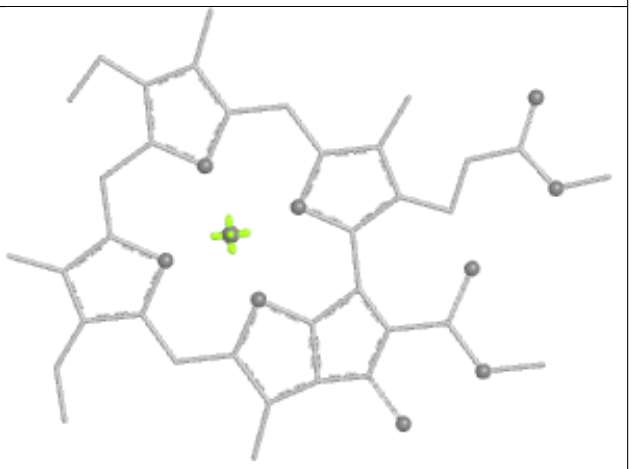
Bond lengths



Bond angles

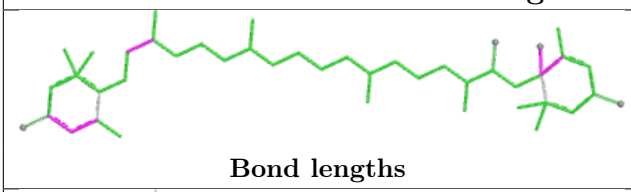


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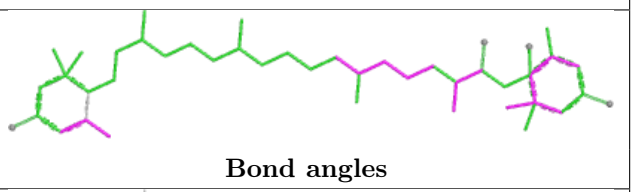


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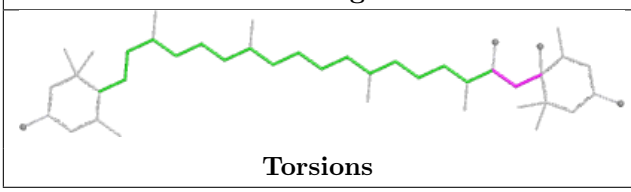
Ligand IWJ R 303



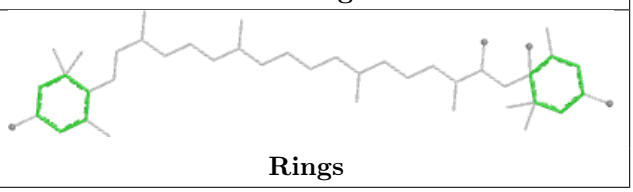
Bond lengths



Bond angles

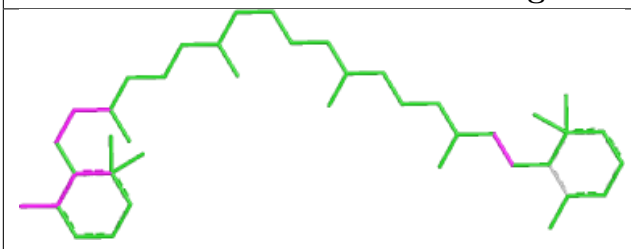


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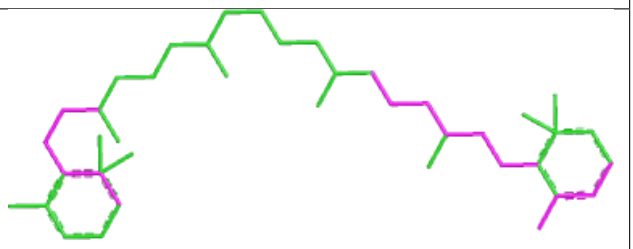


Rings

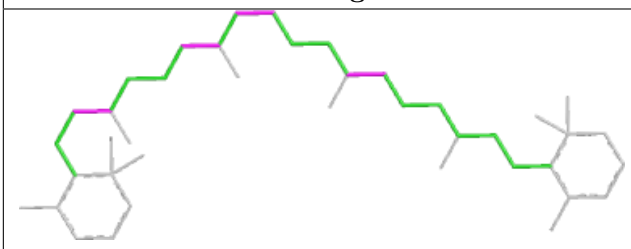
Ligand Q6L X 316



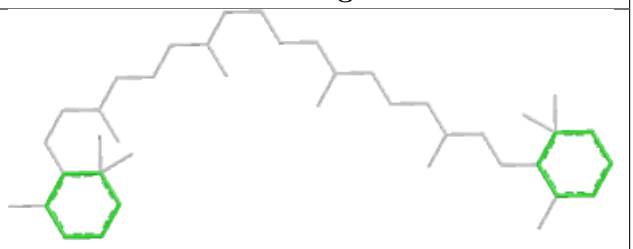
Bond lengths



Bond angles

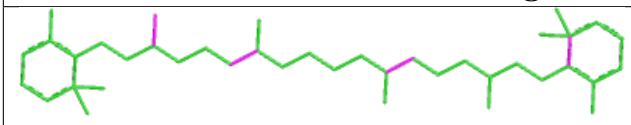


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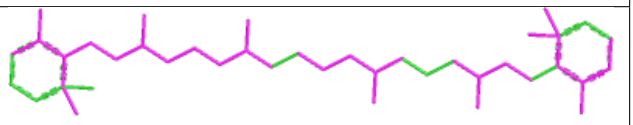


Rings

Ligand BCR B 845



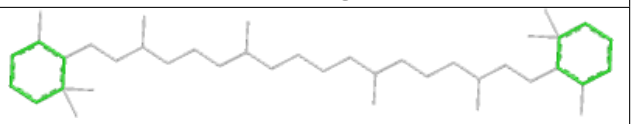
Bond lengths



Bond angles

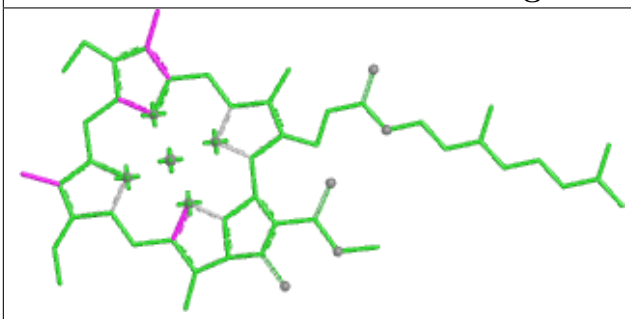


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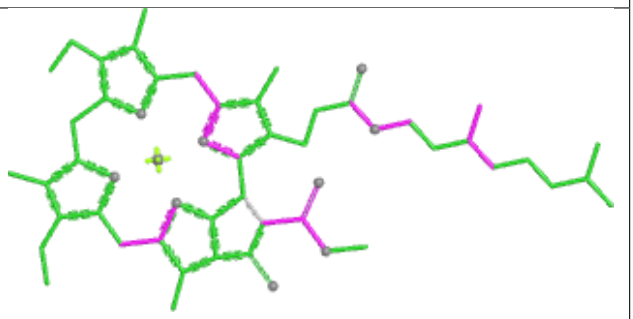


Rings

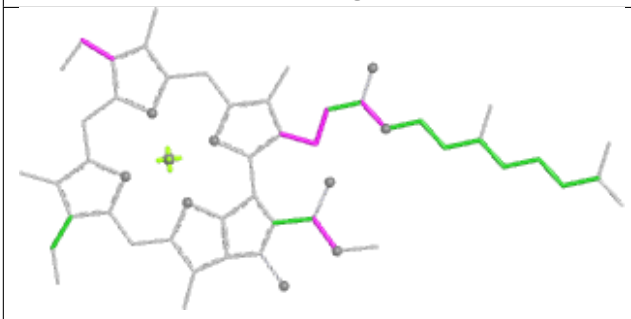
Ligand CLA A 826



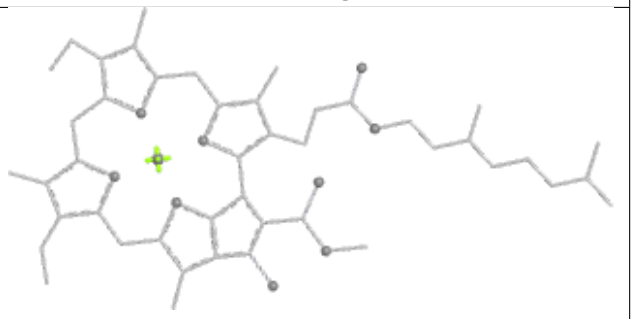
Bond lengths



Bond angles

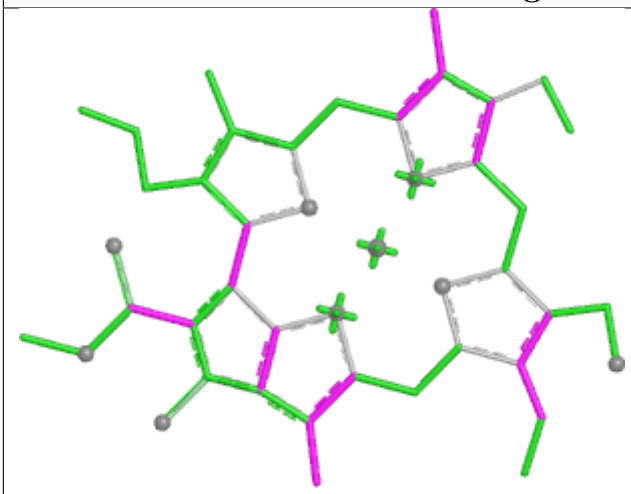


Torsions

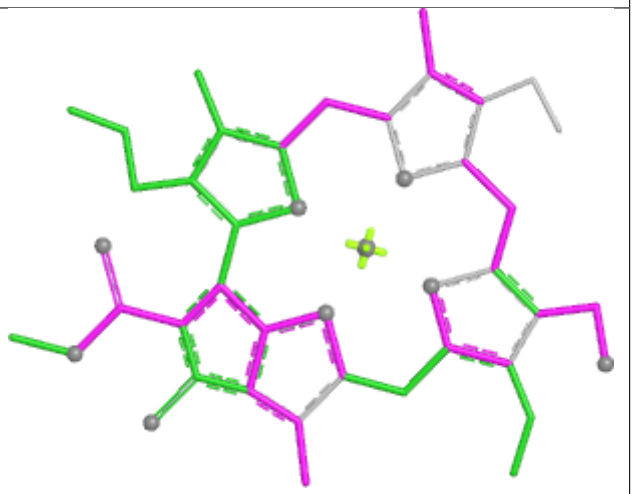


Rings

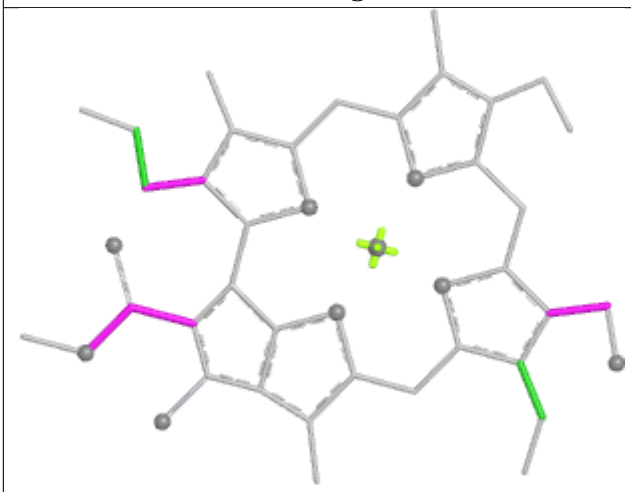
Ligand CHL X 308



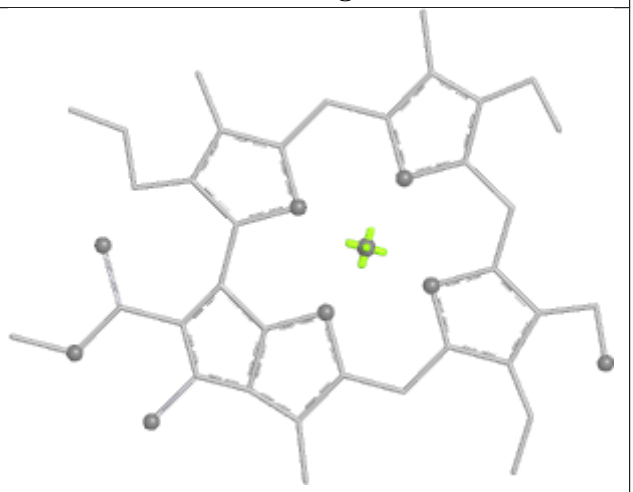
Bond lengths



Bond angles

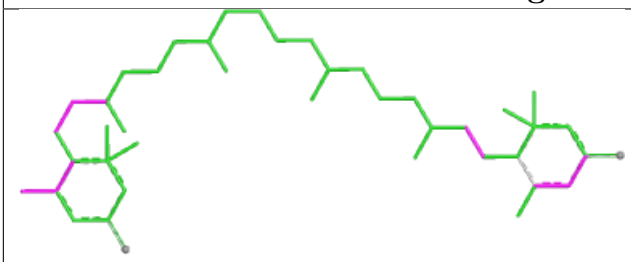


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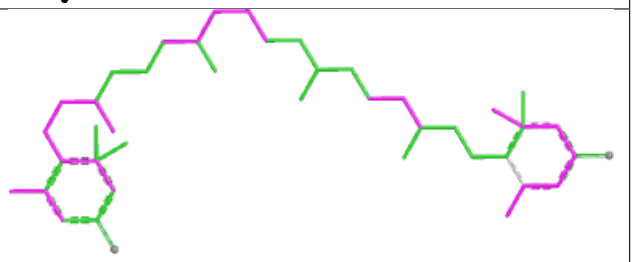


Rings

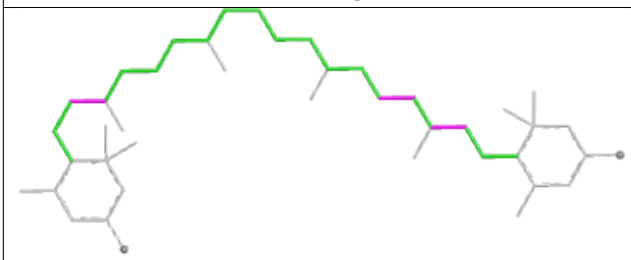
Ligand Q6L Q 319



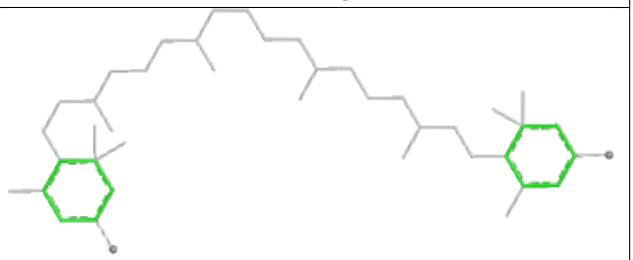
Bond lengths



Bond angles

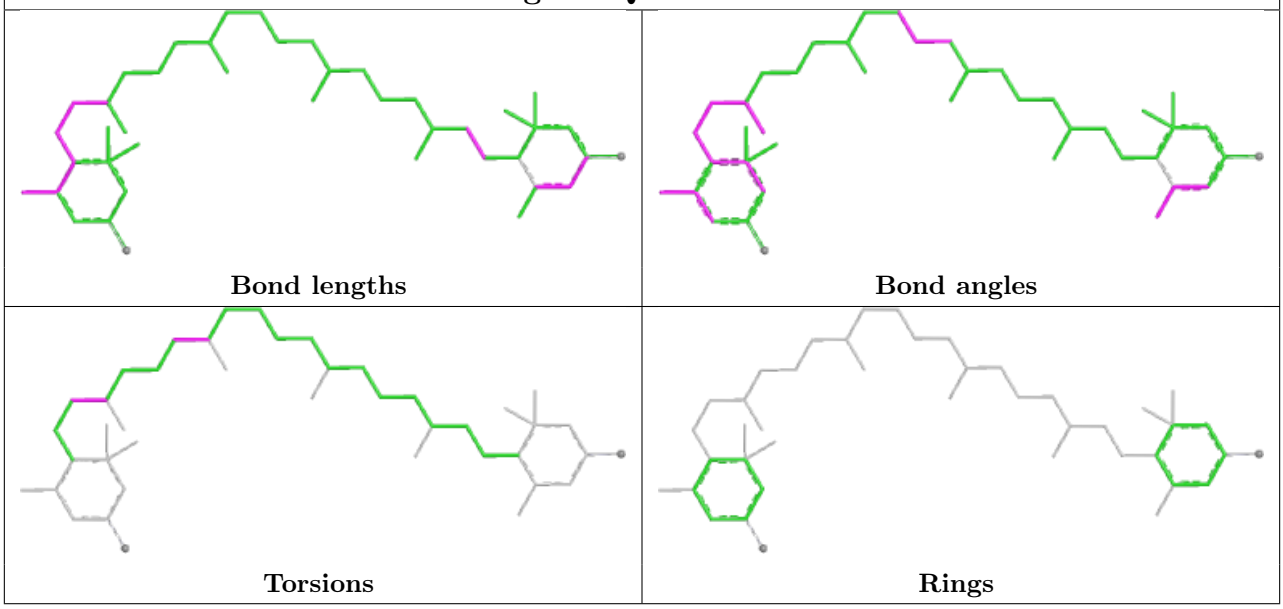


Torsions

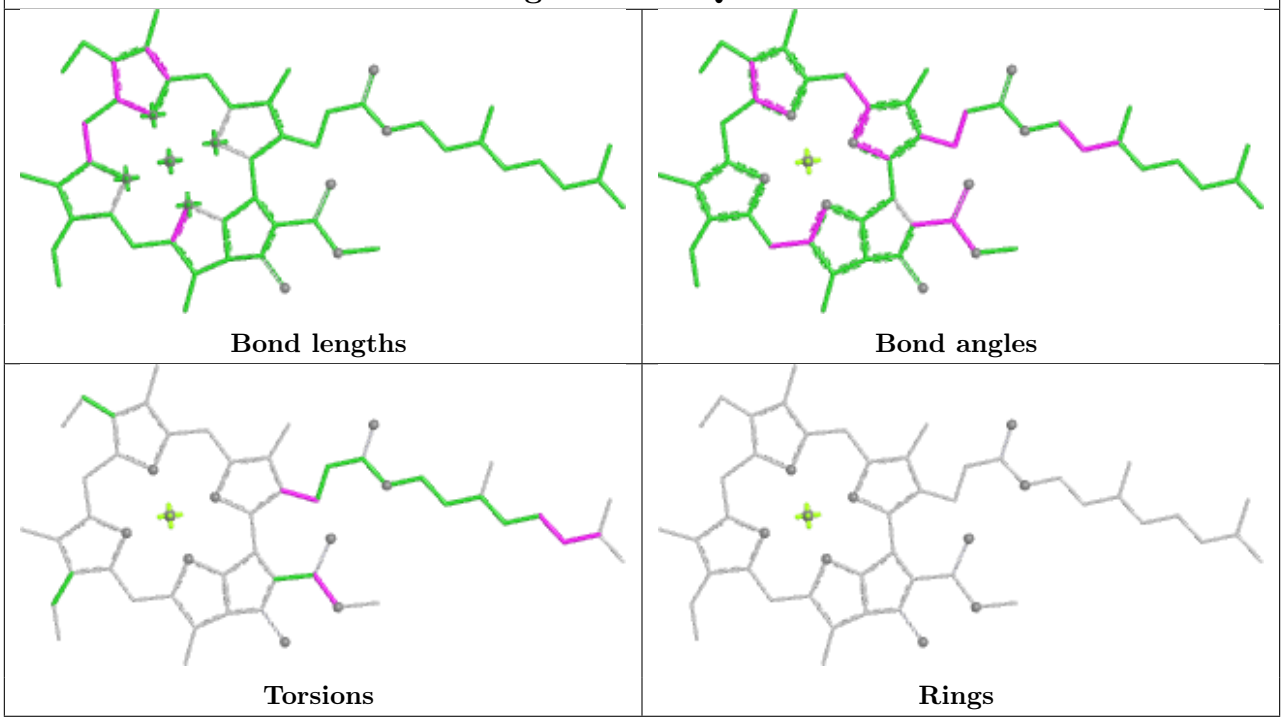


Rings

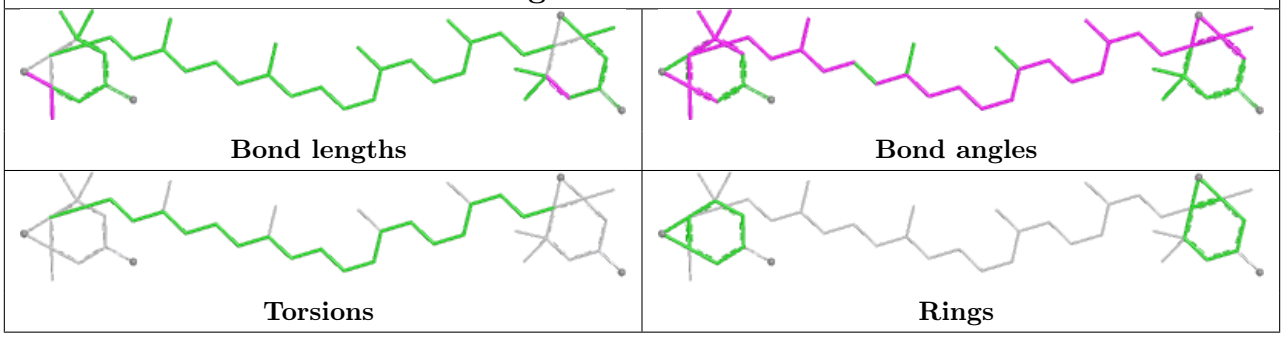
Ligand Q6L W 315



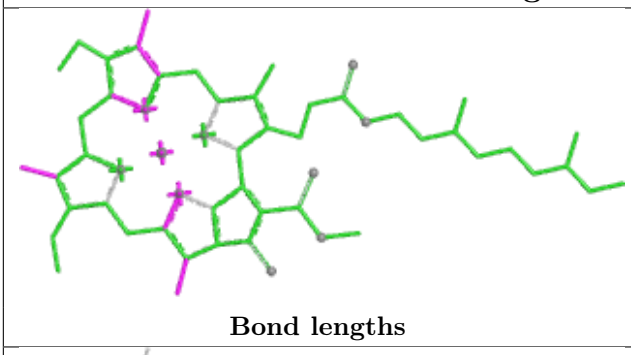
Ligand CLA Q 311



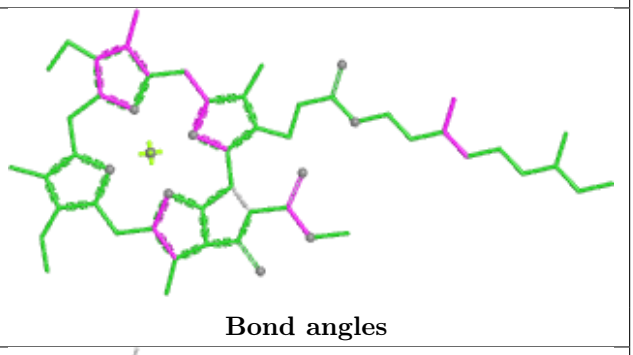
Ligand XAT 6 615



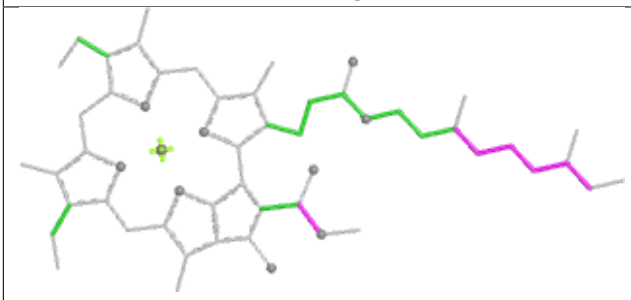
Ligand CLA U 302



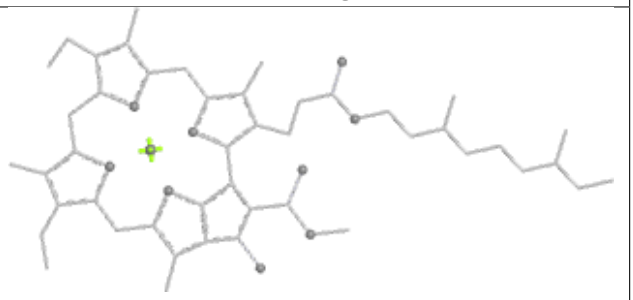
Bond lengths



Bond angles

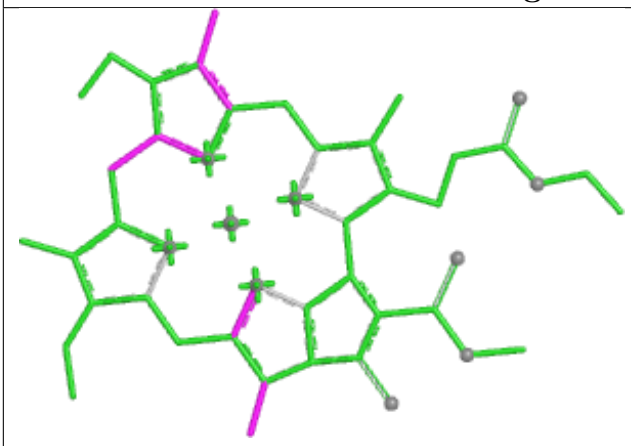


Torsions

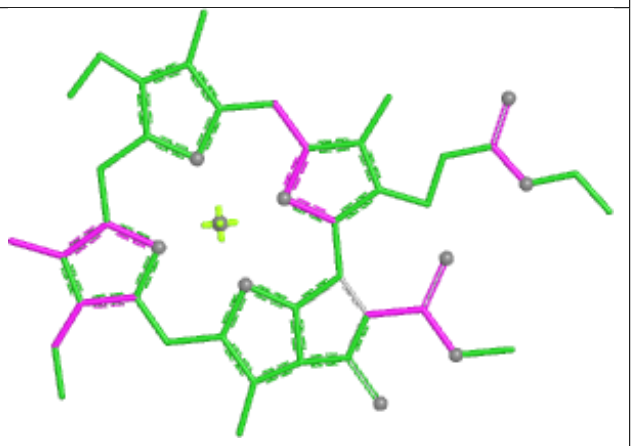


Rings

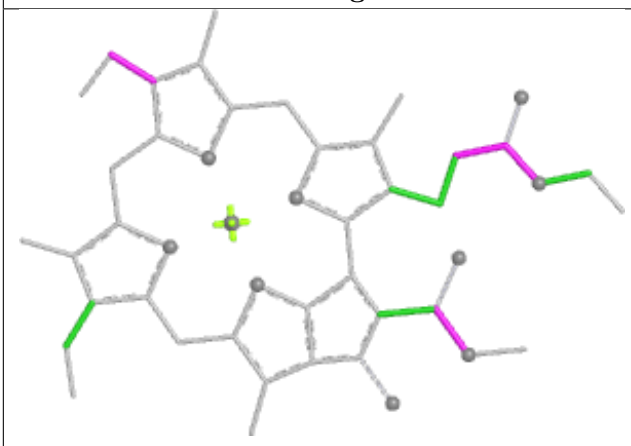
Ligand CLA V 310



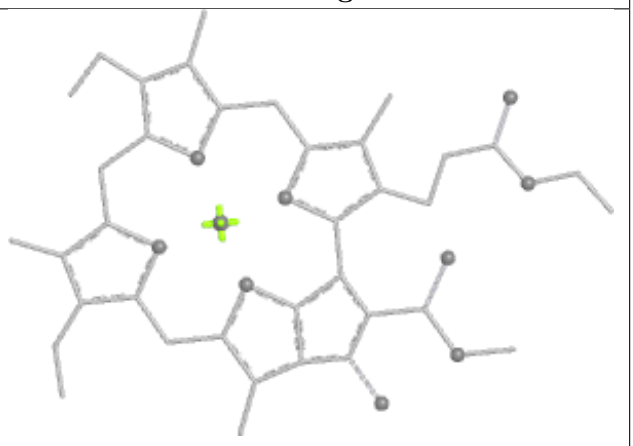
Bond lengths



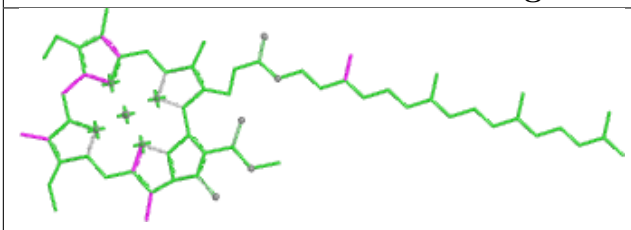
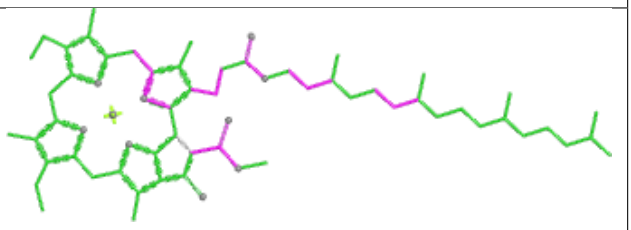
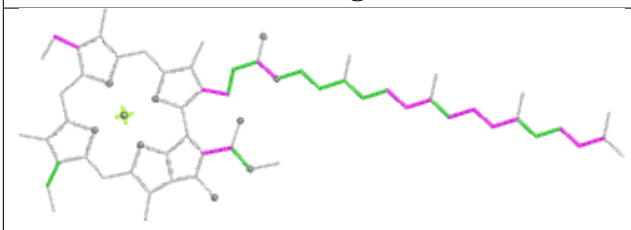
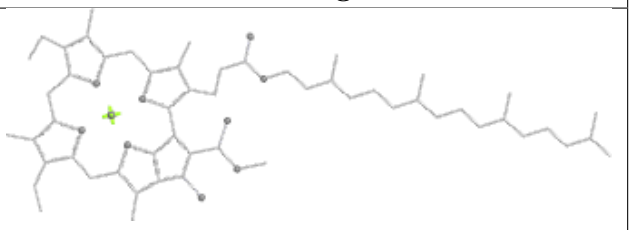
Bond angles

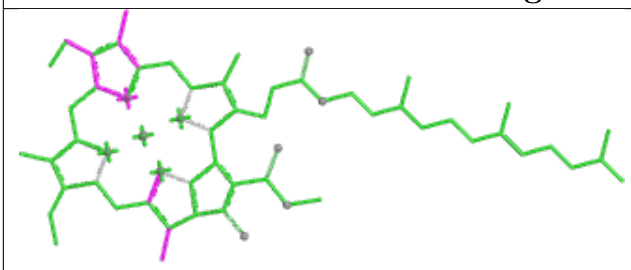
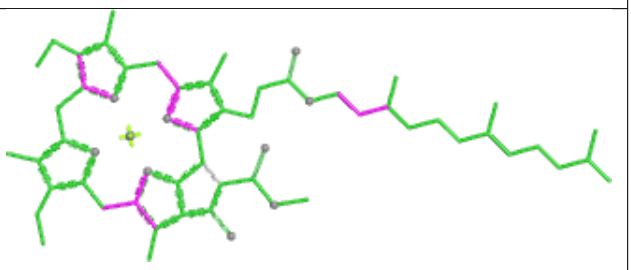
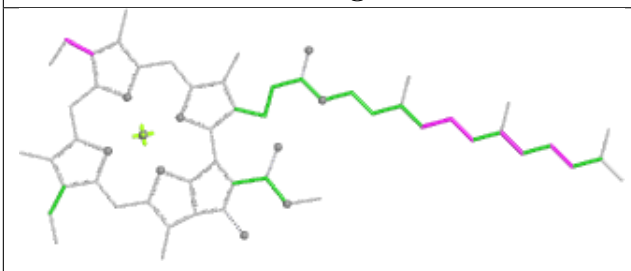
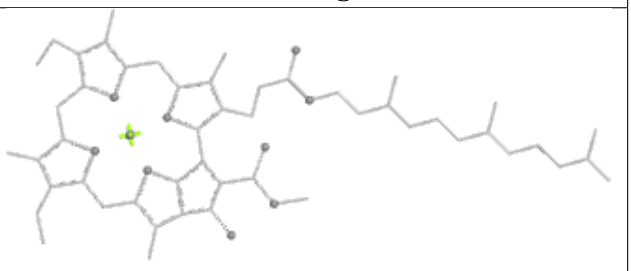


Torsions

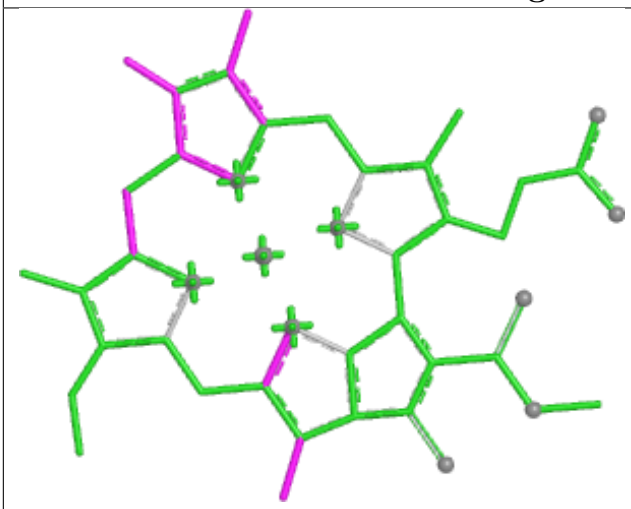


Rings

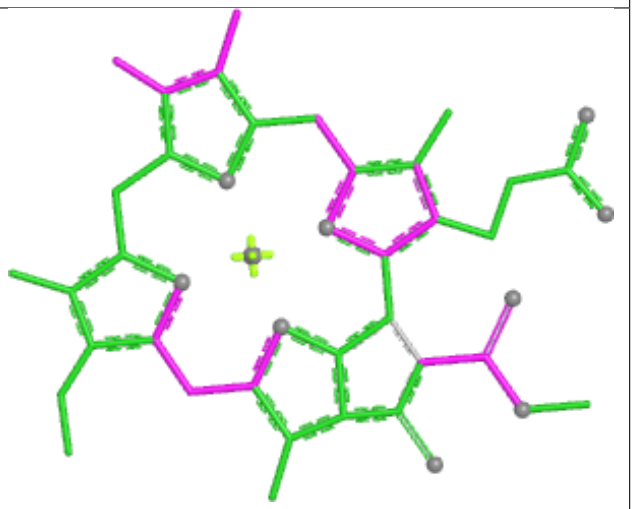
Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

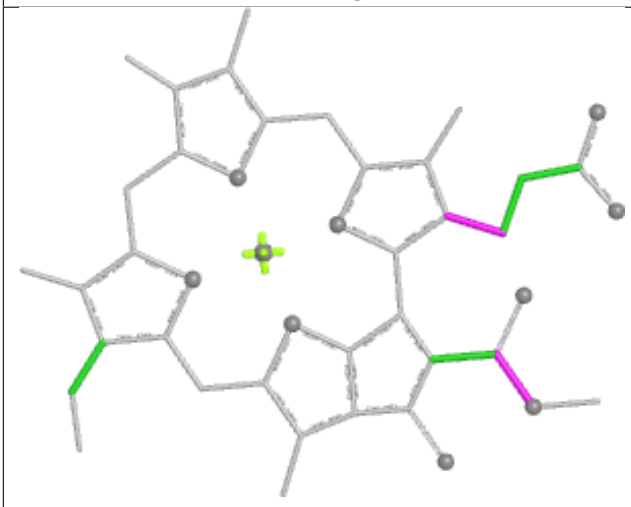
Ligand CLA 4 304



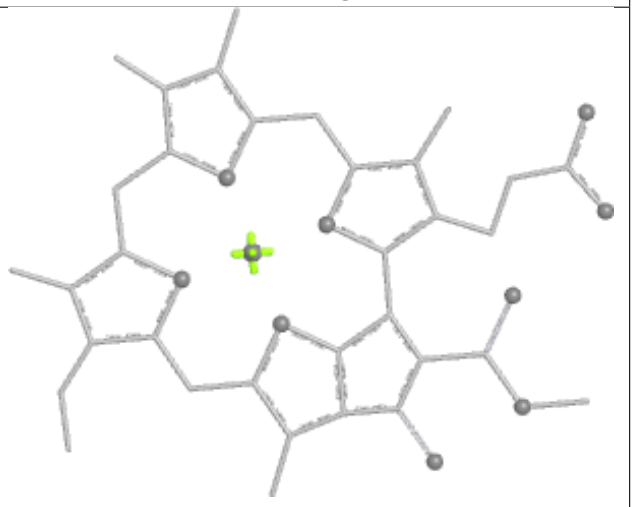
Bond lengths



Bond angles

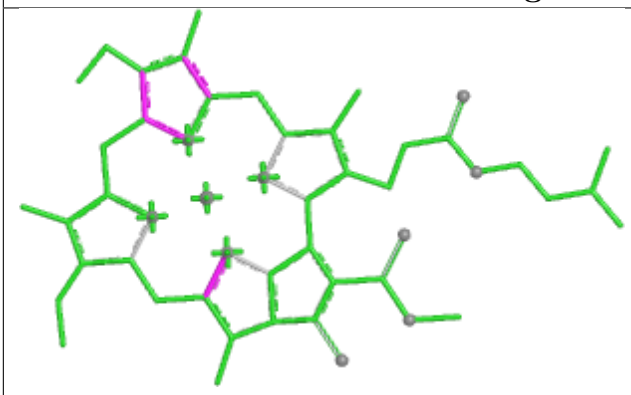


Torsions

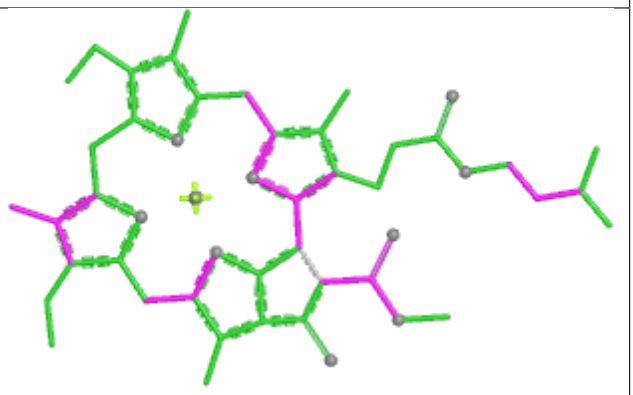


Rings

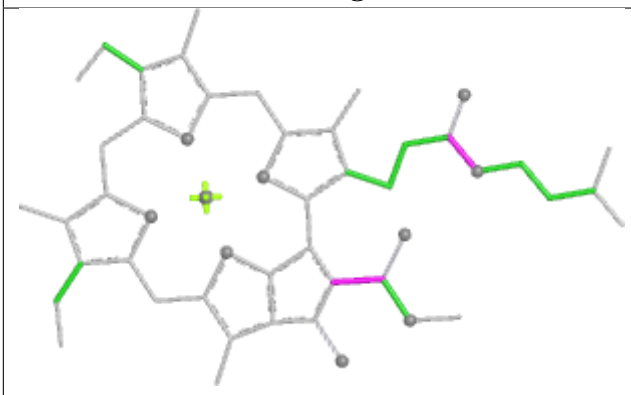
Ligand CLA B 827



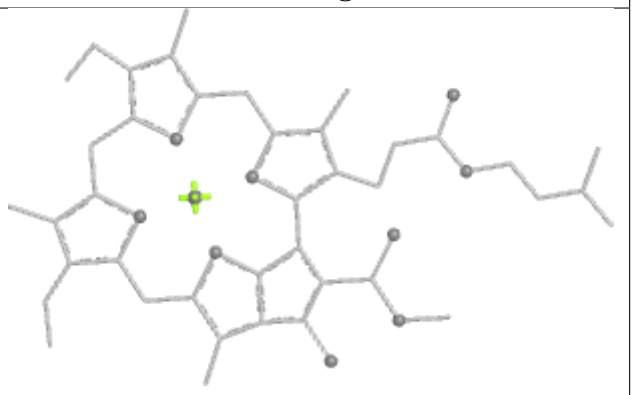
Bond lengths



Bond angles

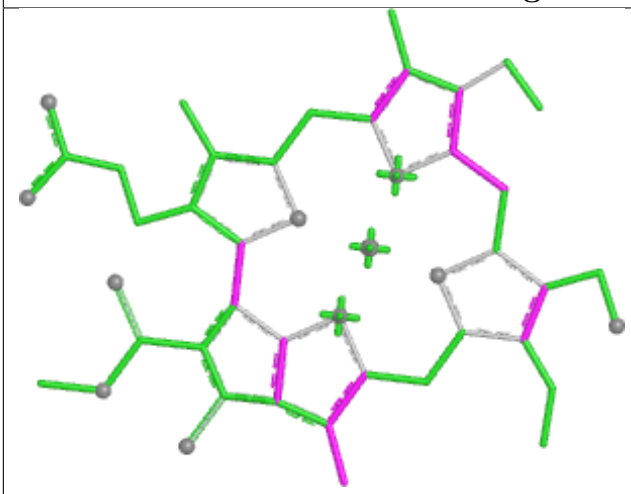


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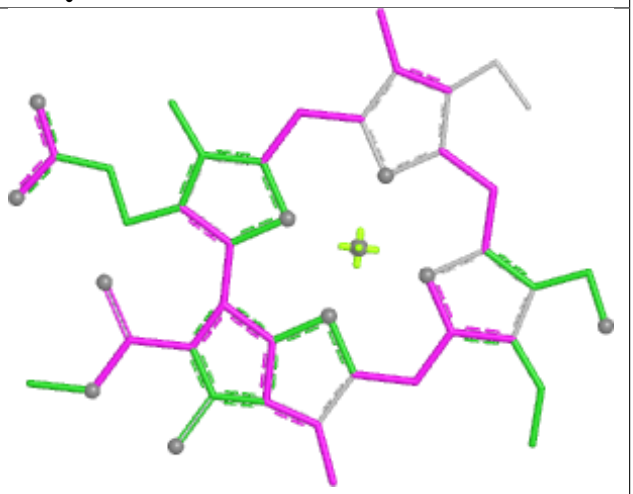


Rings

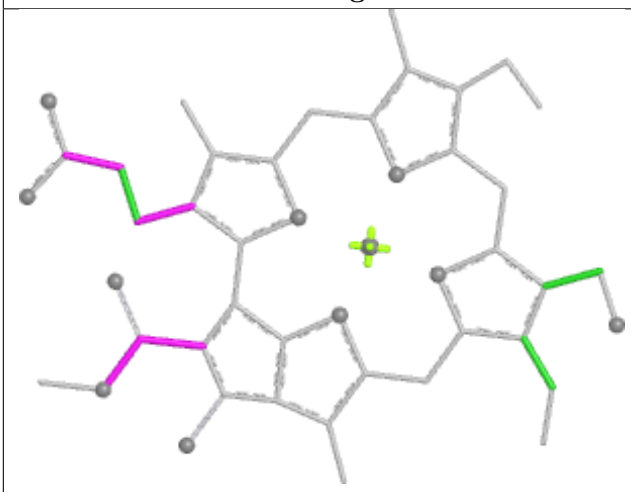
Ligand CHL Q 307



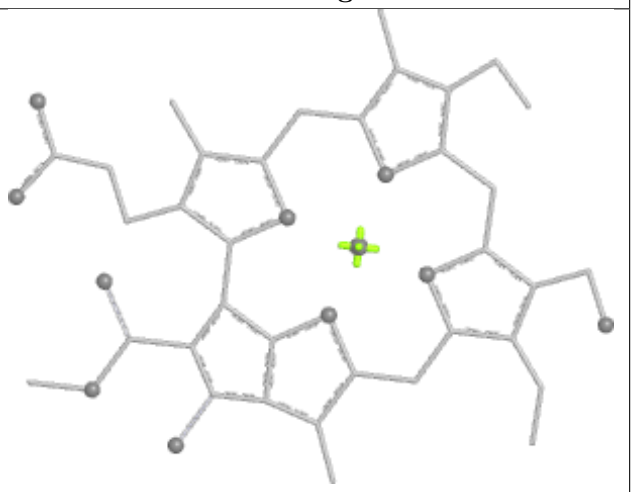
Bond lengths



Bond angles

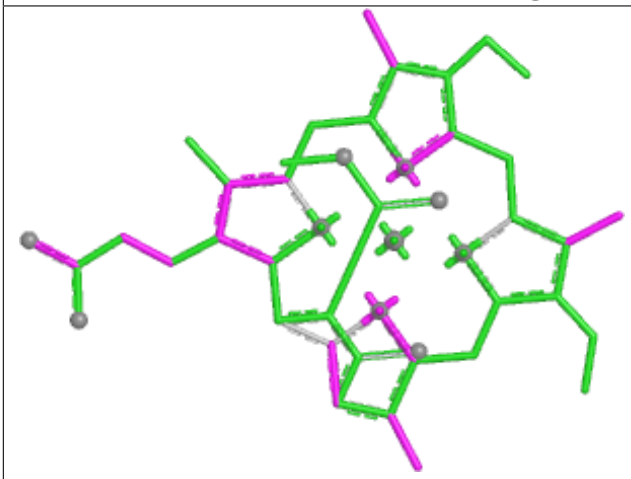


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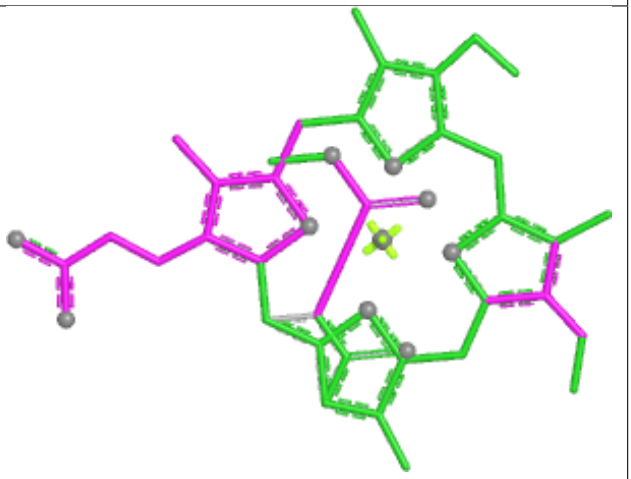


Rings

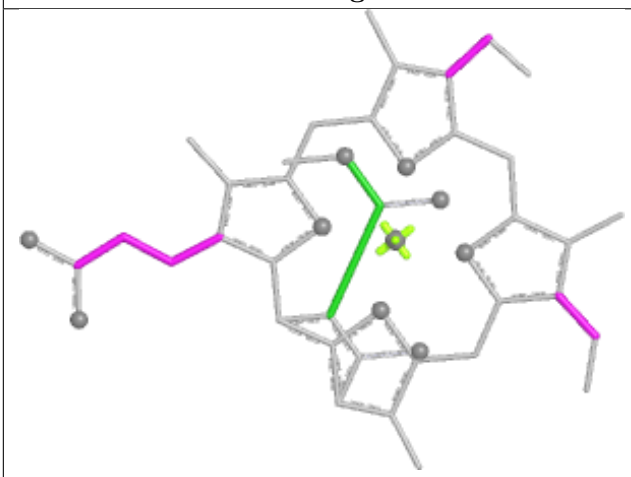
Ligand KC2 T 308



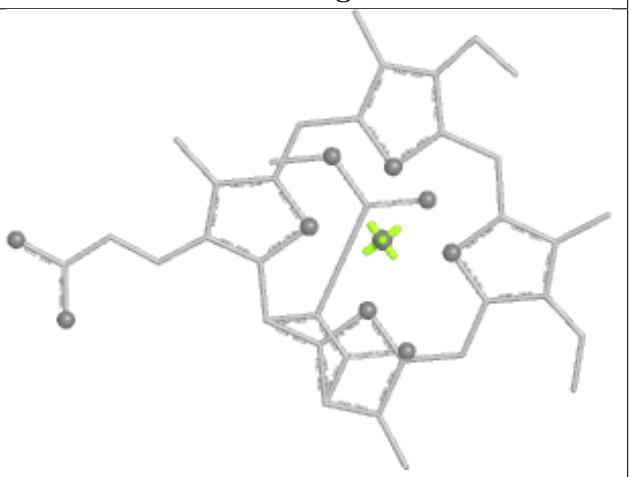
Bond lengths



Bond angles

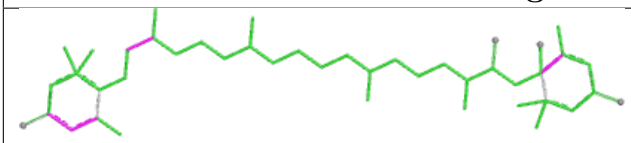


Torsions

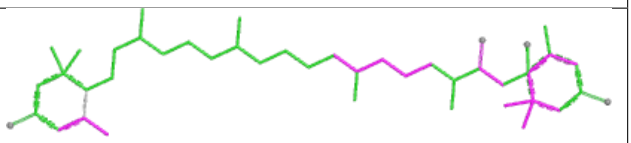


Rings

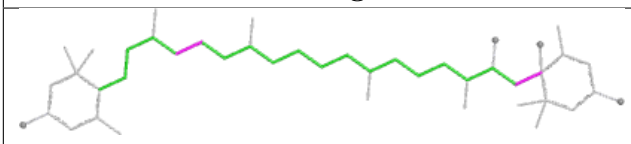
Ligand IWJ V 318



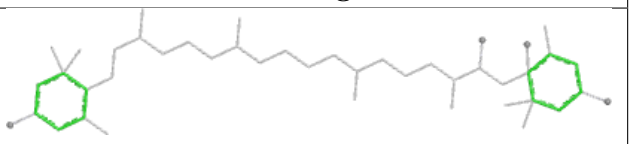
Bond lengths



Bond angles

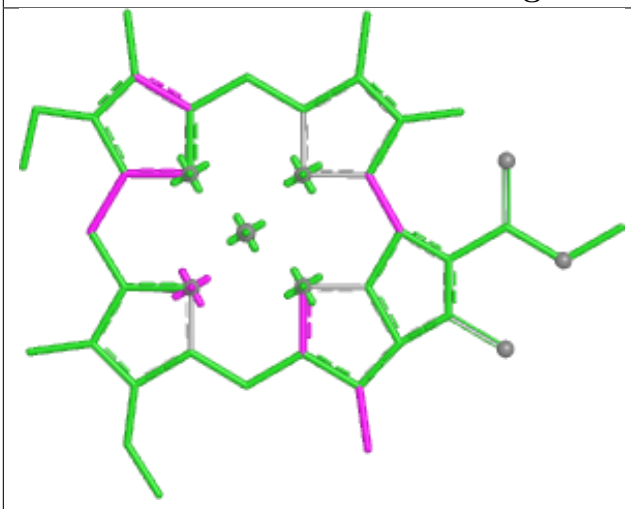


Torsions

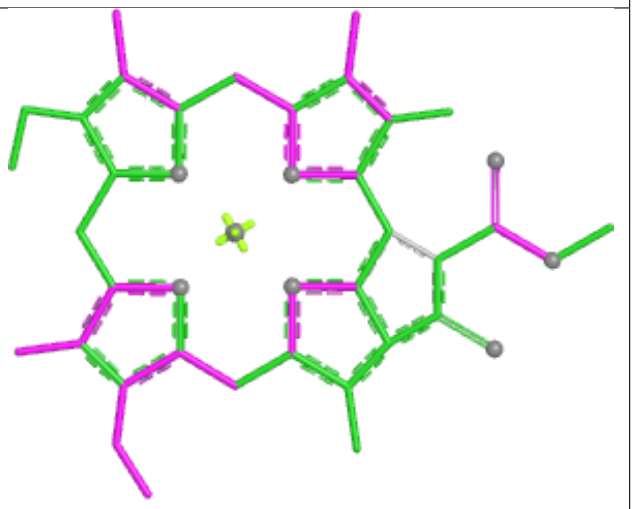


Rings

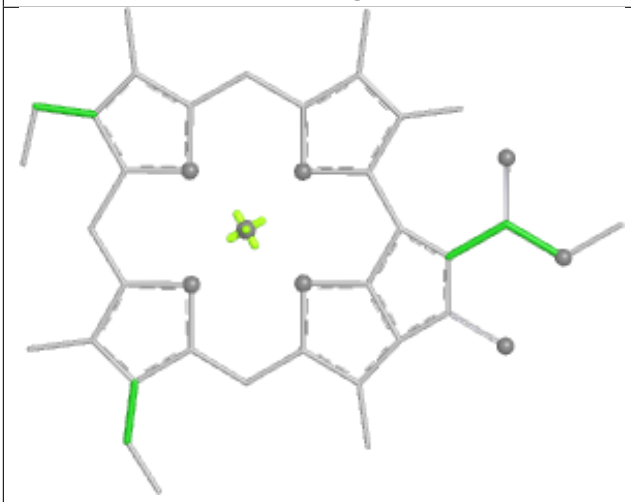
Ligand CLA U 308



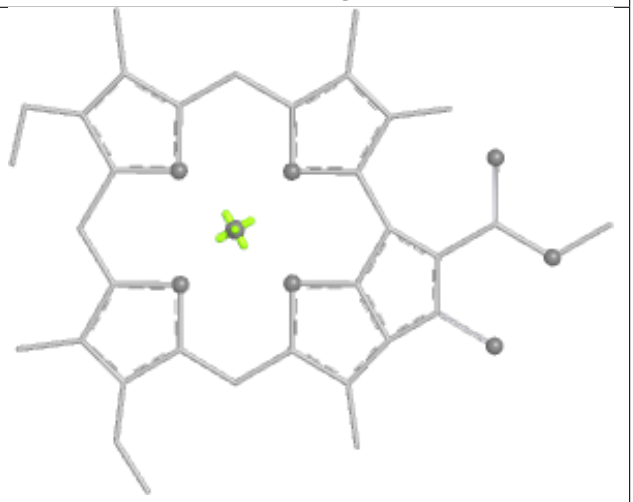
Bond lengths



Bond angles

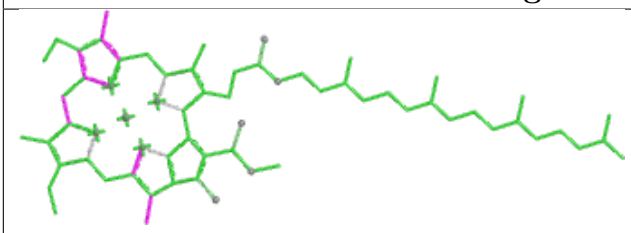


Torsions

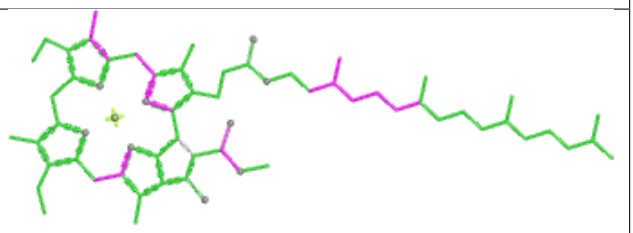


Rings

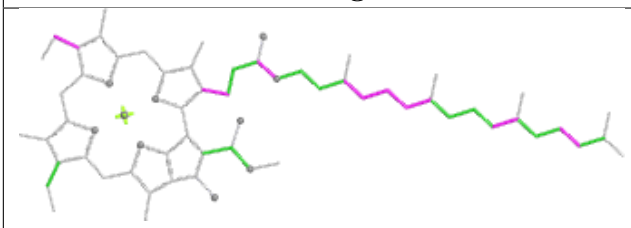
Ligand CLA A 837



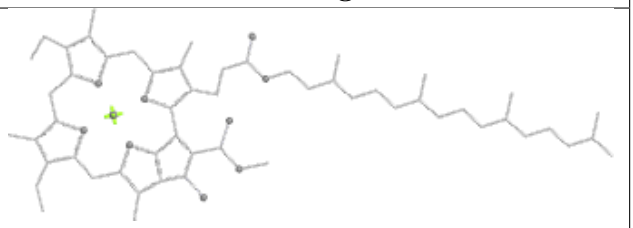
Bond lengths



Bond angles

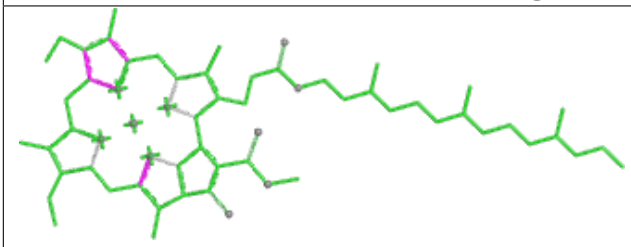


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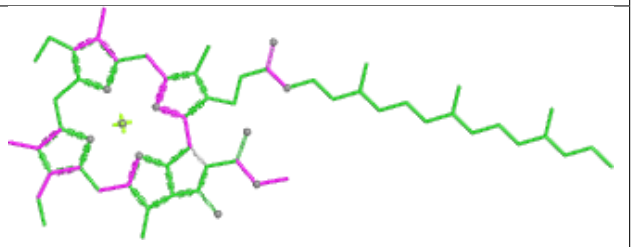


Rings

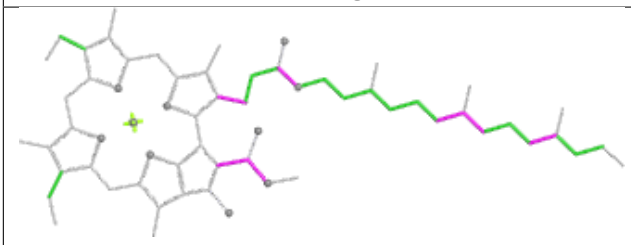
Ligand CLA 6 602



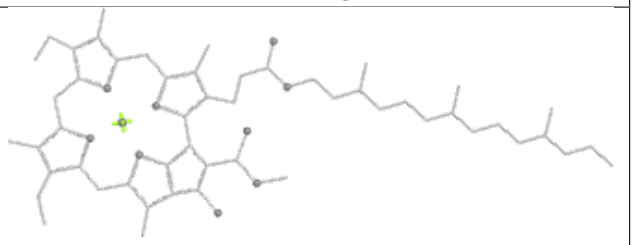
Bond lengths



Bond angles

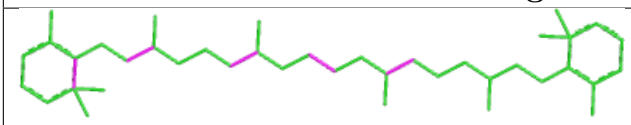


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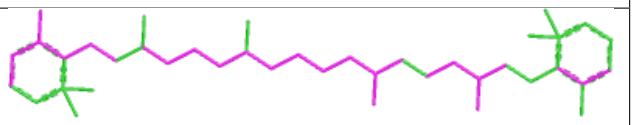


Rings

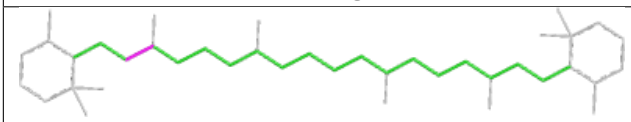
Ligand BCR 3 319



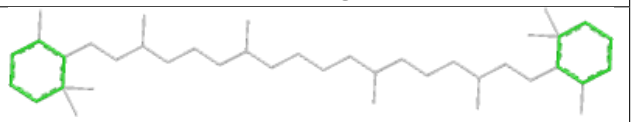
Bond lengths



Bond angles

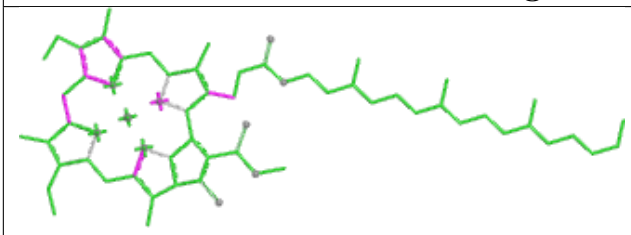


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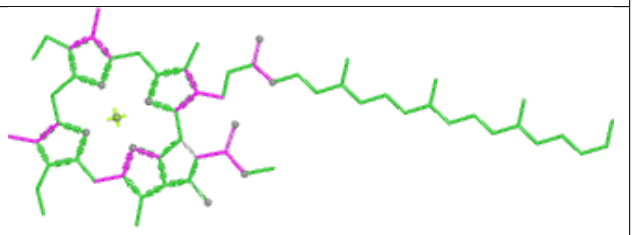


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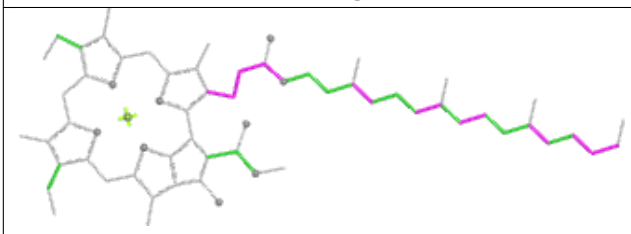
Ligand CLA R 313



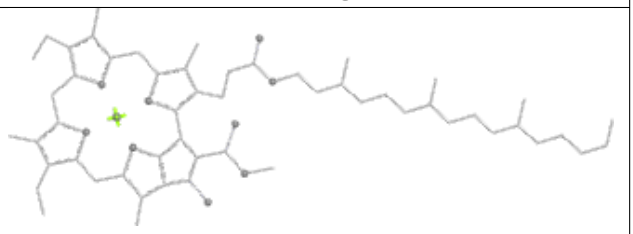
Bond lengths



Bond angles

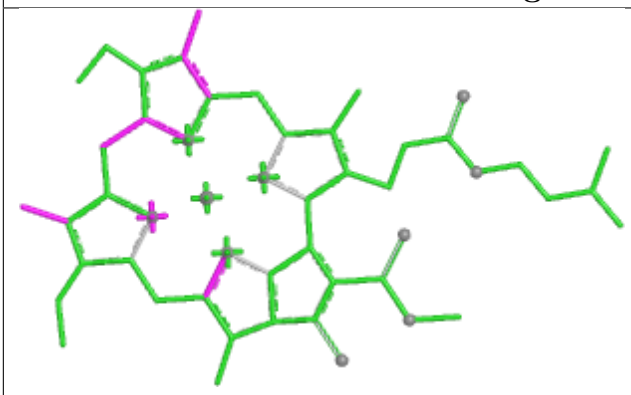


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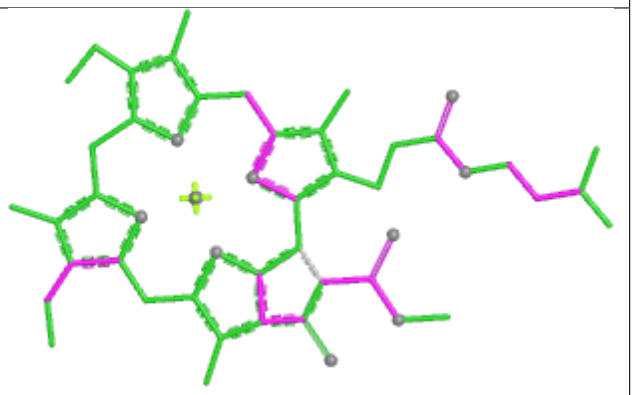


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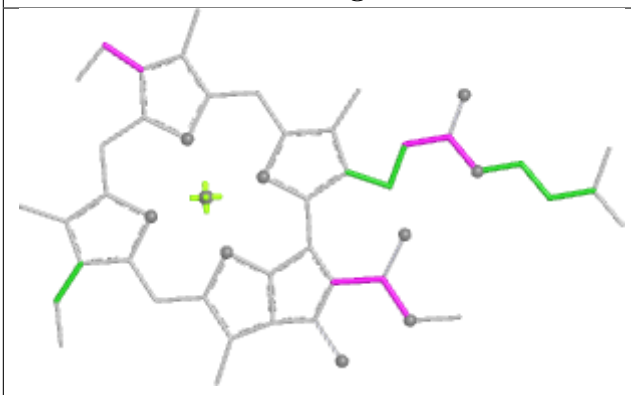
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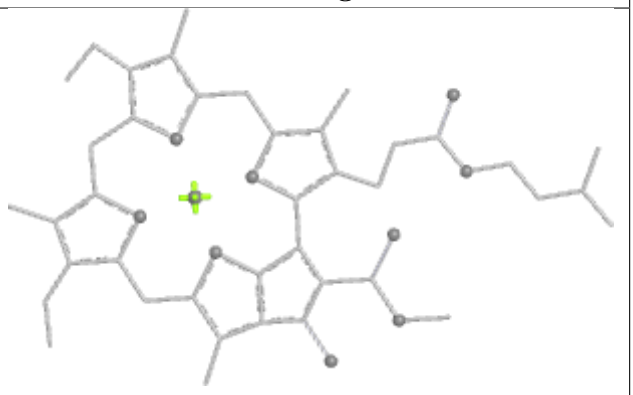
Bond lengths



Bond angles

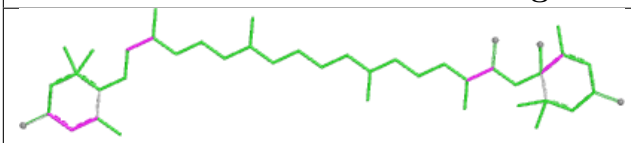


Torsions



Rings

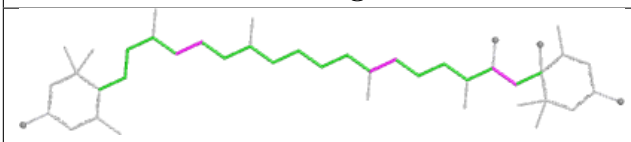
Ligand IWJ 1 611



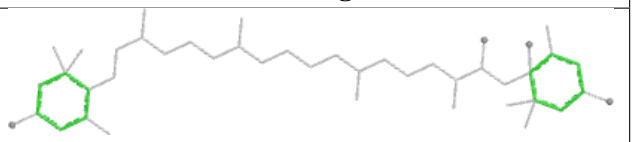
Bond lengths



Bond angles

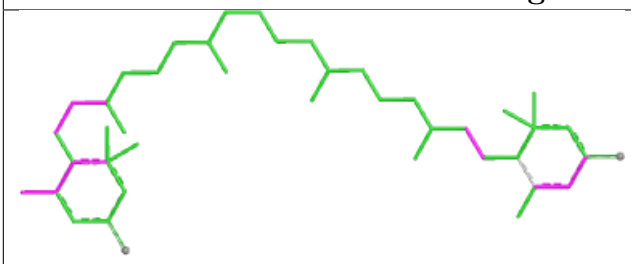


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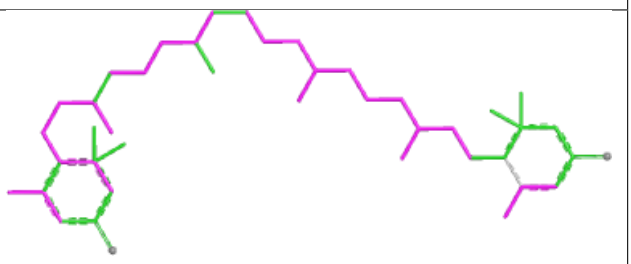


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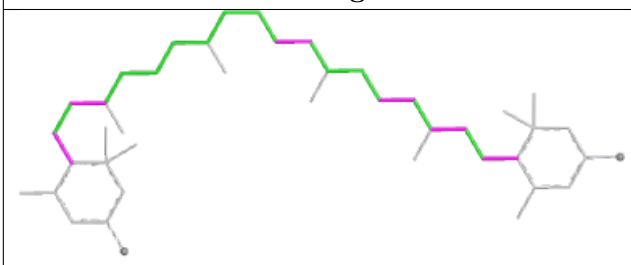
Ligand Q6L V 319



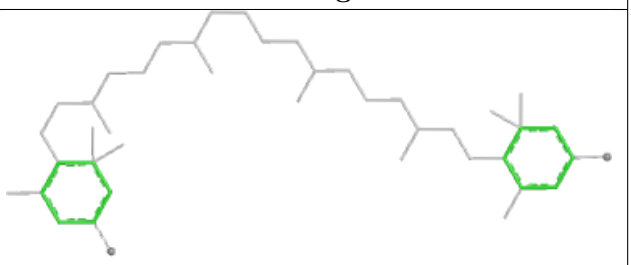
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Bond angles

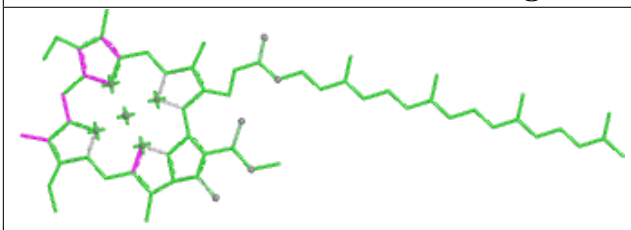


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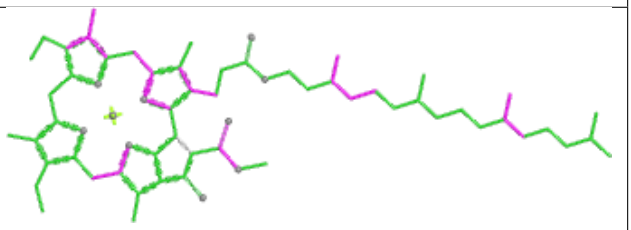


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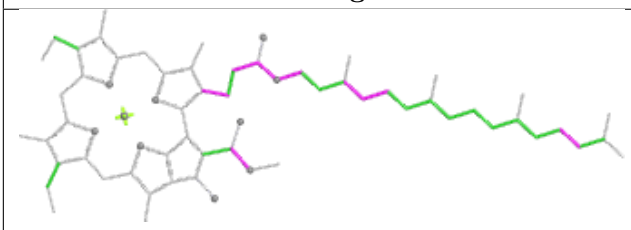
Ligand CLA K 206



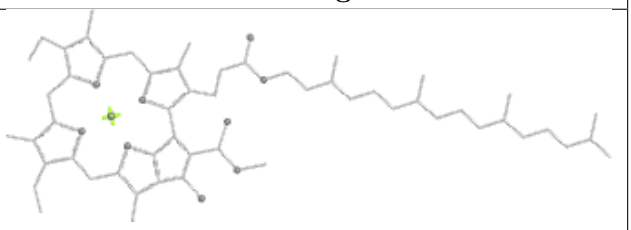
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Bond angles

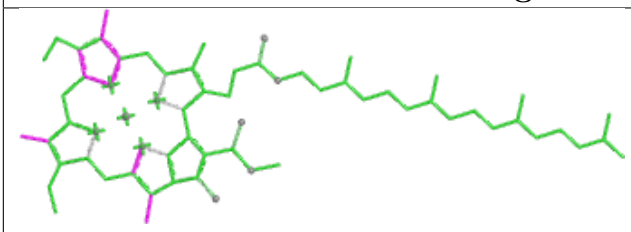


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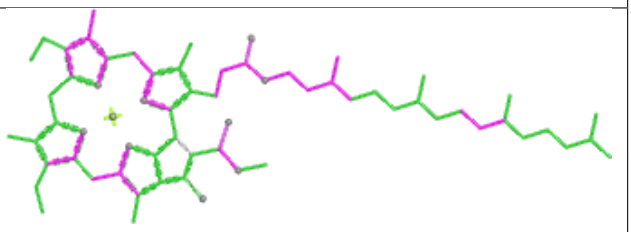


Rings

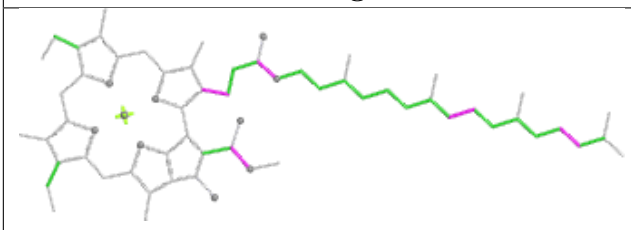
Ligand CLA O 2002



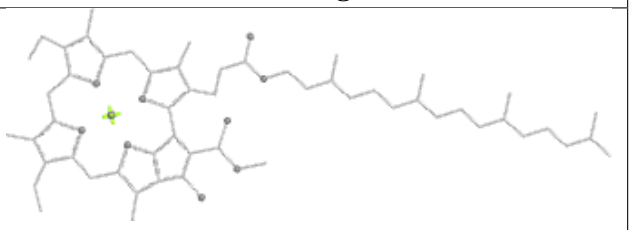
Bond lengths



Bond angles

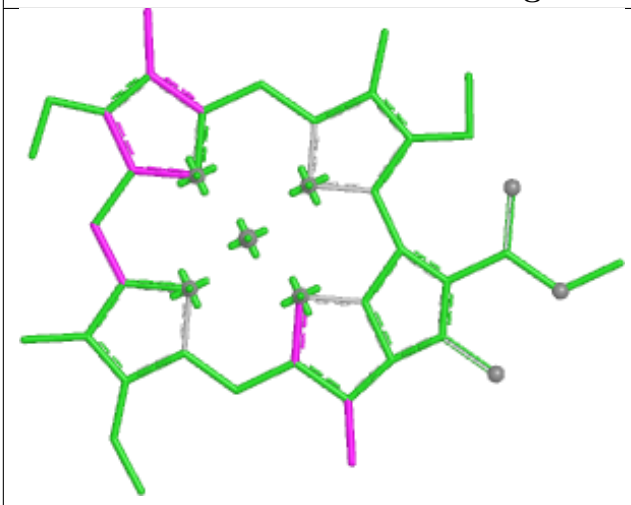


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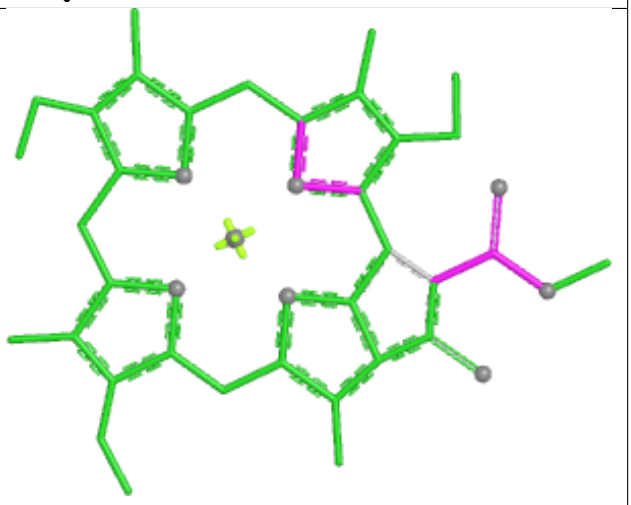


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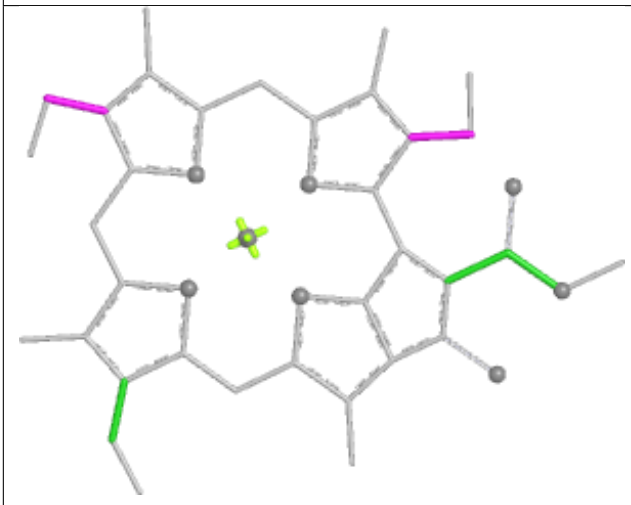
Ligand CLA Q 312



Bond lengths



Bond angles

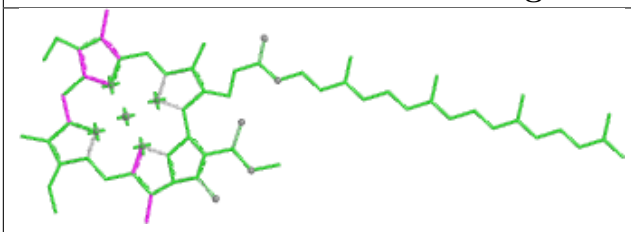


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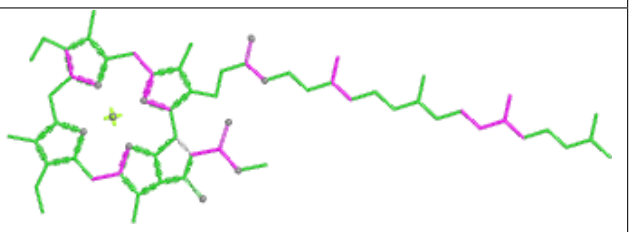


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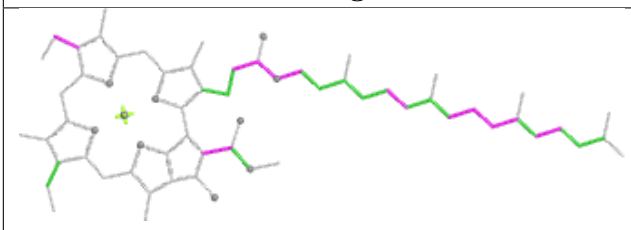
Ligand CLA P 302



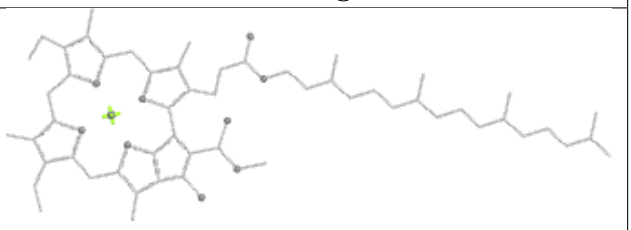
Bond lengths



Bond angles

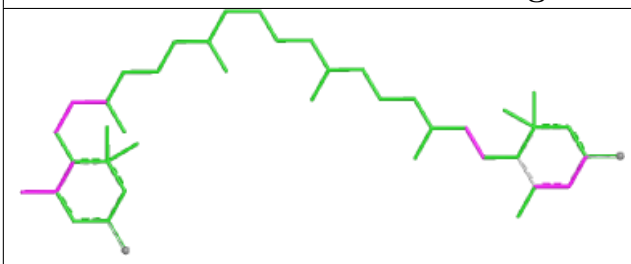


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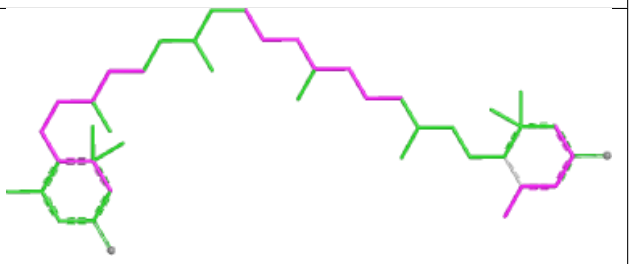


Rings

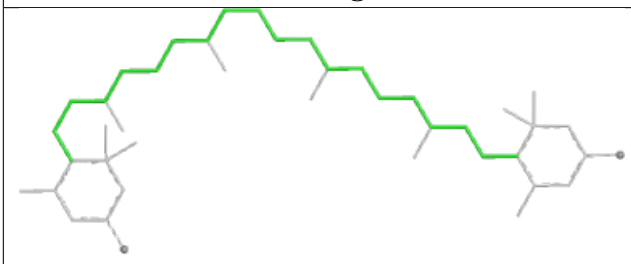
Ligand Q6L R 320



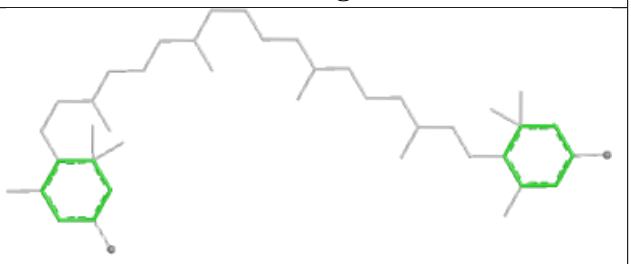
Bond lengths



Bond angles

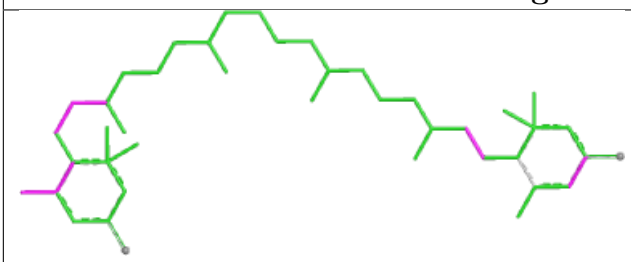


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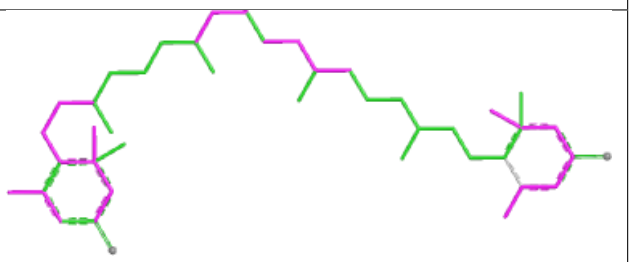


Rings

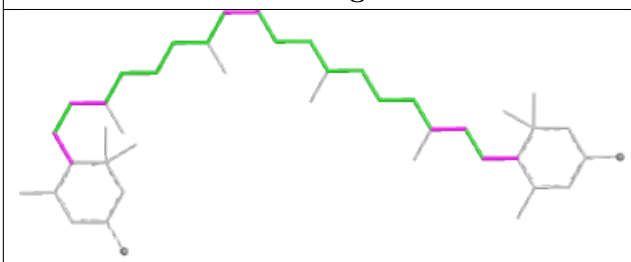
Ligand Q6L S 323



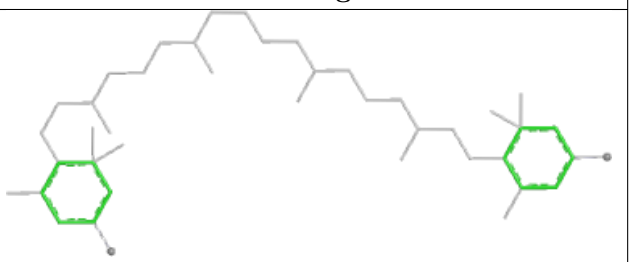
Bond lengths



Bond angles

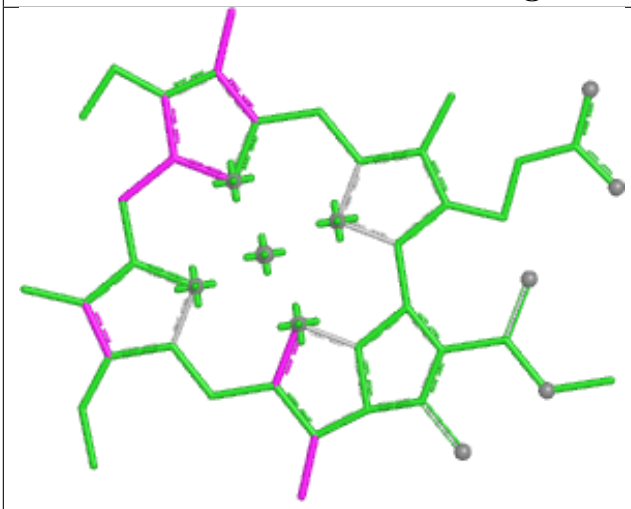


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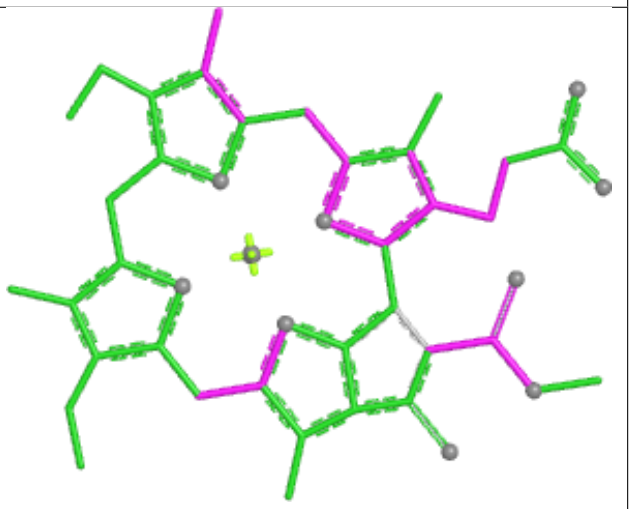


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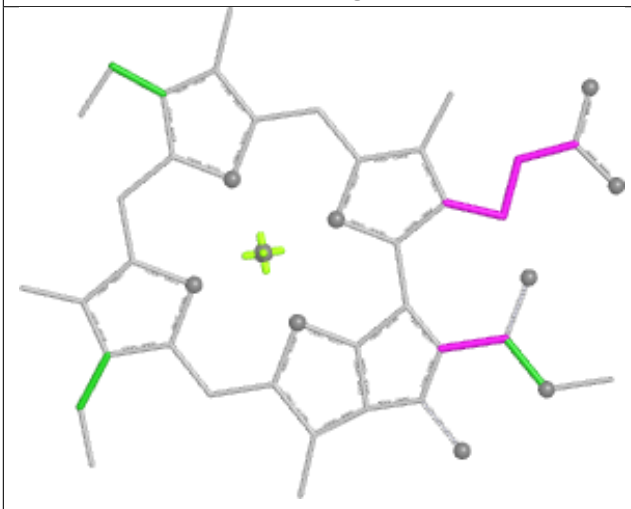
Ligand CLA H 304



Bond lengths



Bond angles

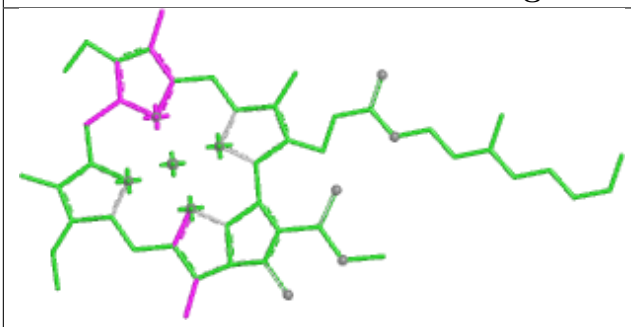


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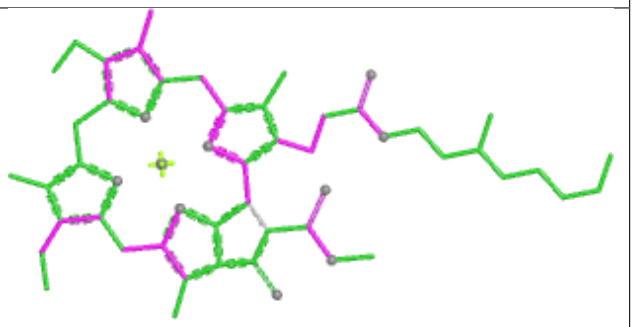


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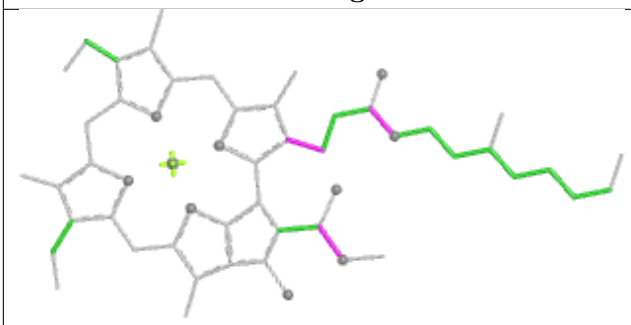
Ligand CLA A 814



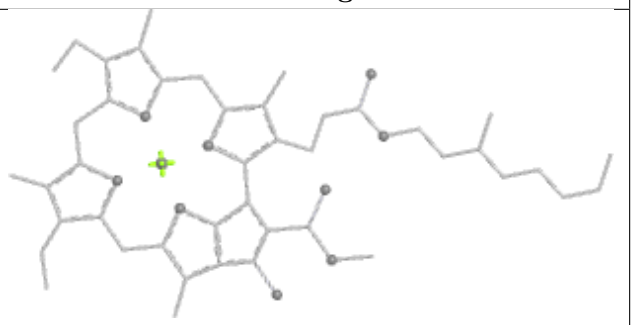
Bond lengths



Bond angles

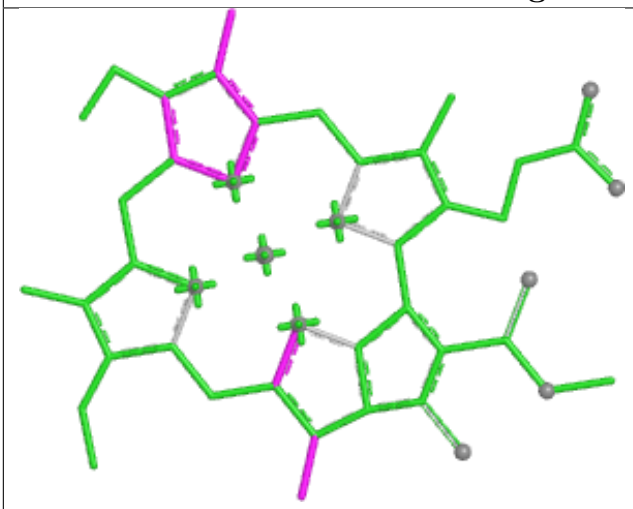


Torsions

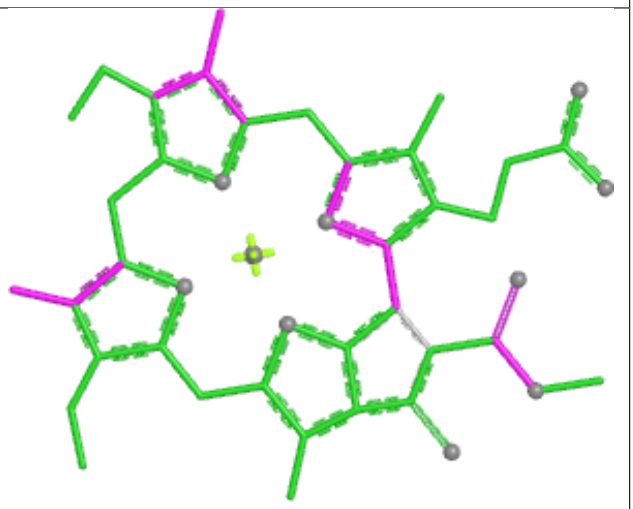


Rings

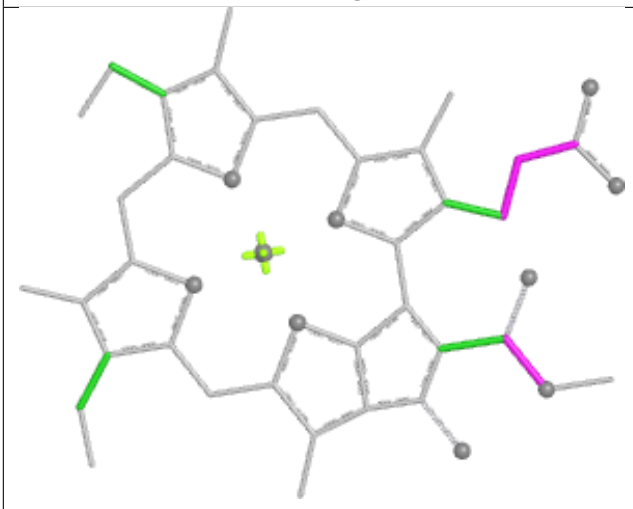
Ligand CLA 5 603



Bond lengths



Bond angles

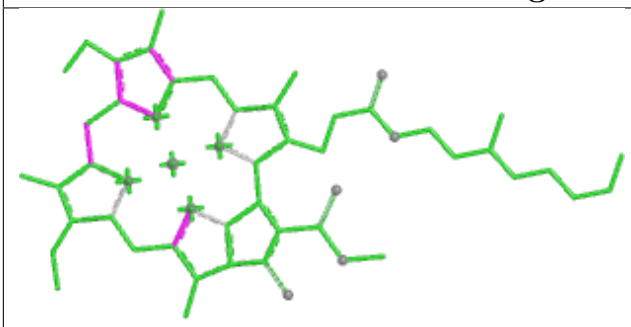


Torsions

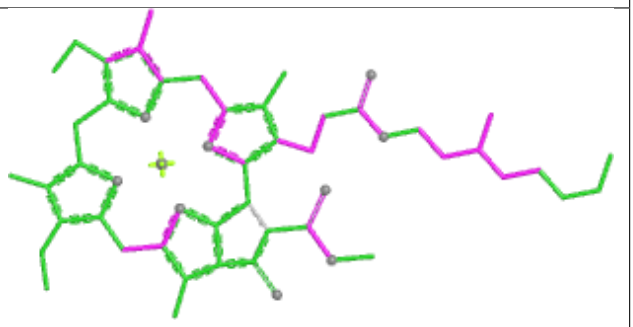


Rings

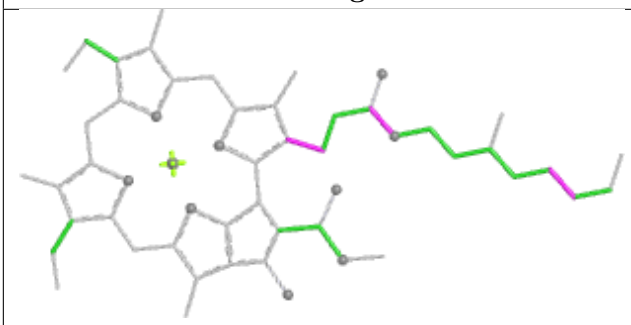
Ligand CLA 4 310



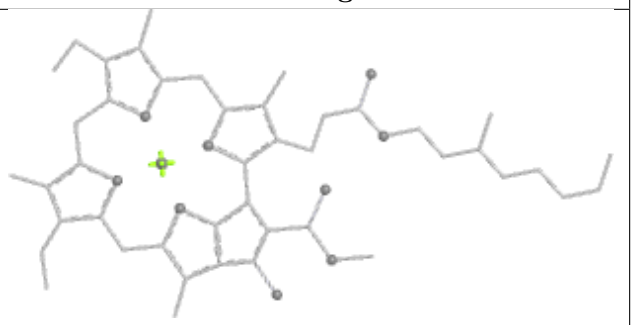
Bond lengths



Bond angles



Torsions

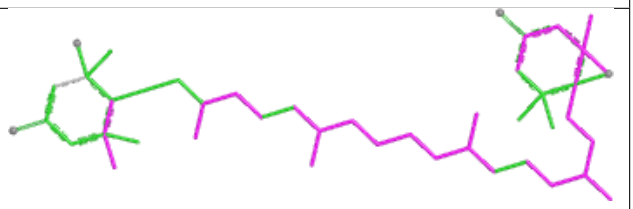


Rings

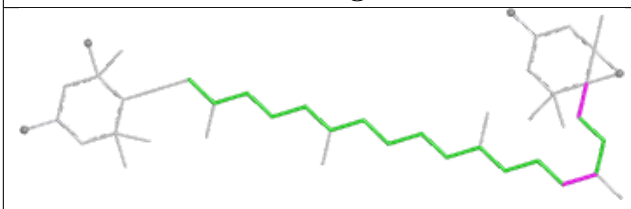
Ligand NEX H 306



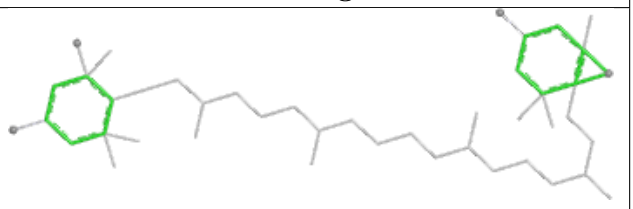
Bond lengths



Bond angles

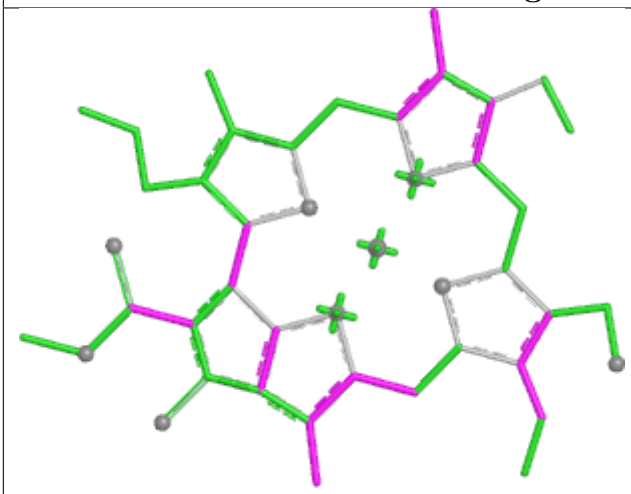


Torsions

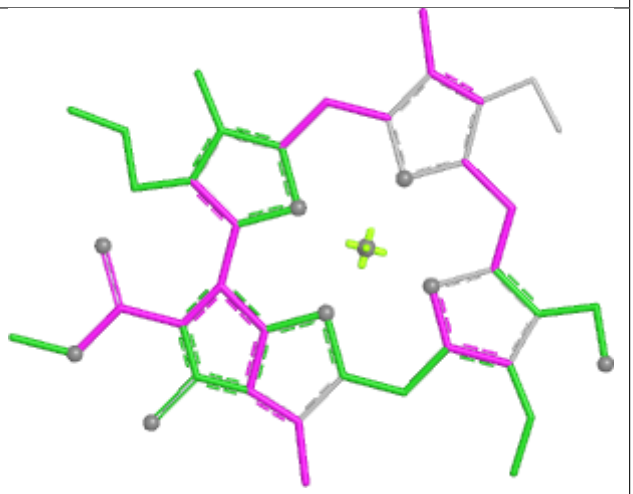


Rings

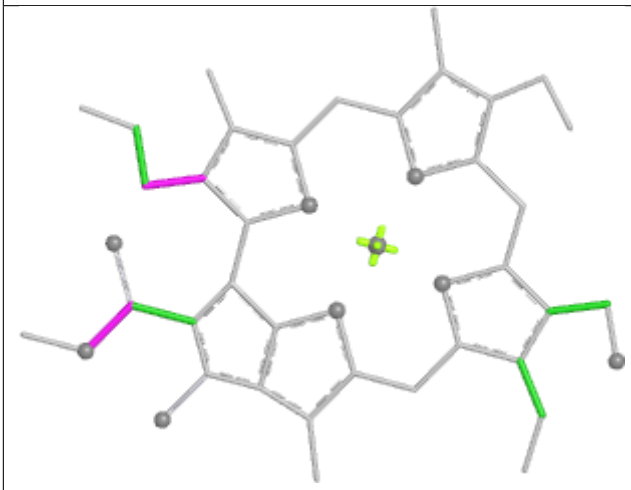
Ligand CHL T 307



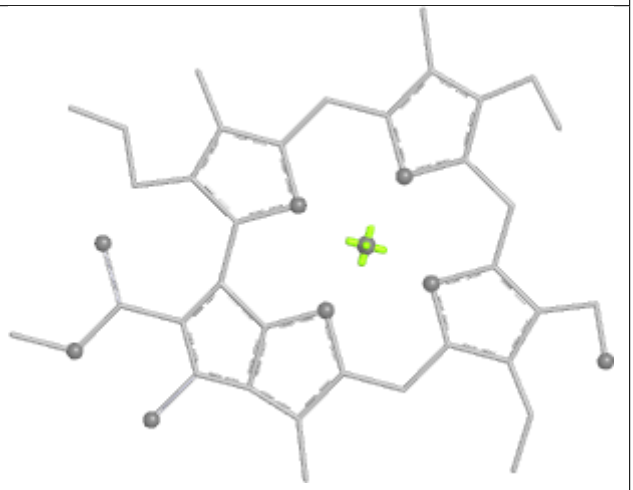
Bond lengths



Bond angles

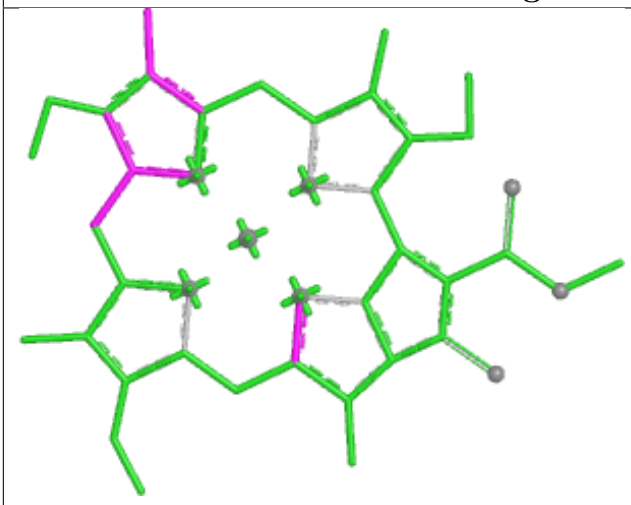


Torsions

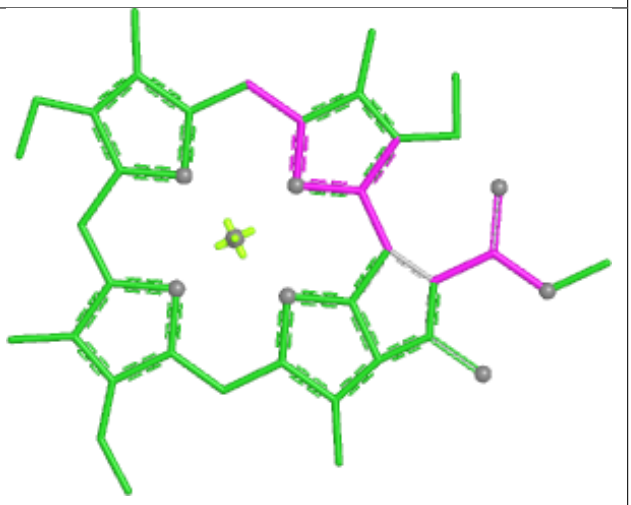


Rings

Ligand CLA G 203



Bond lengths



Bond angles

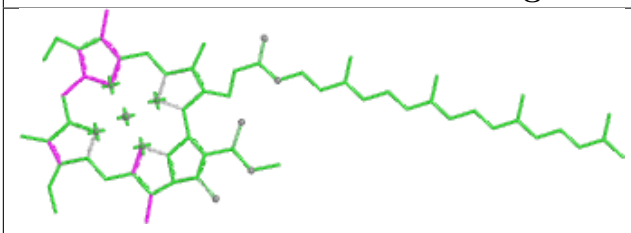


Torsions

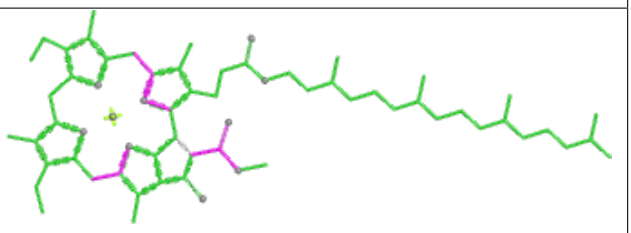


Rings

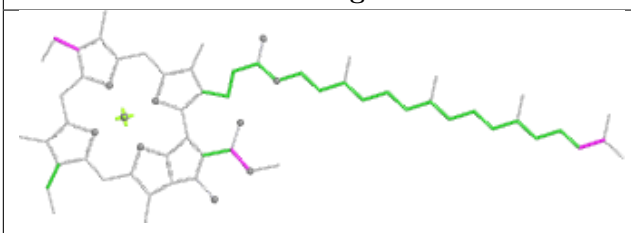
Ligand CLA A 836



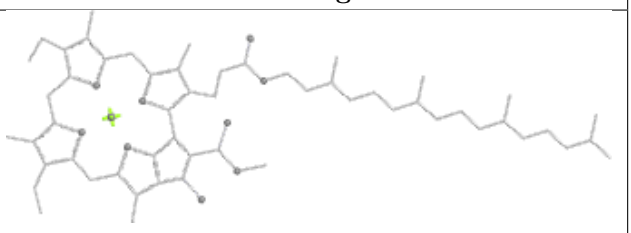
Bond lengths



Bond angles

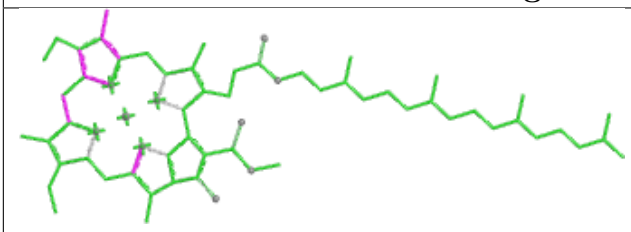


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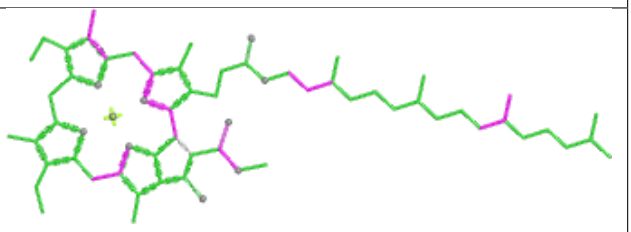


Rings

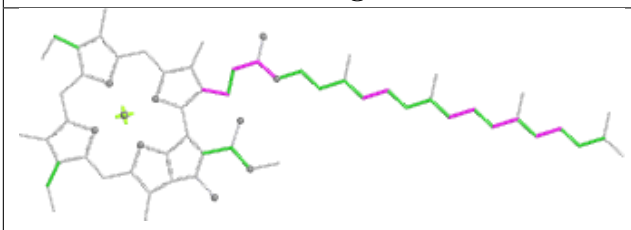
Ligand CLA A 817



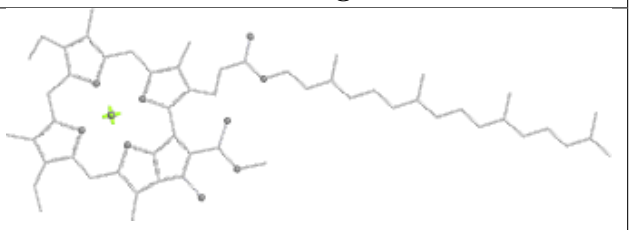
Bond lengths



Bond angles

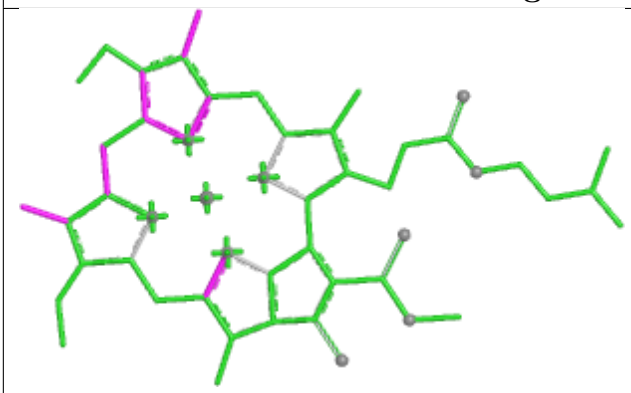


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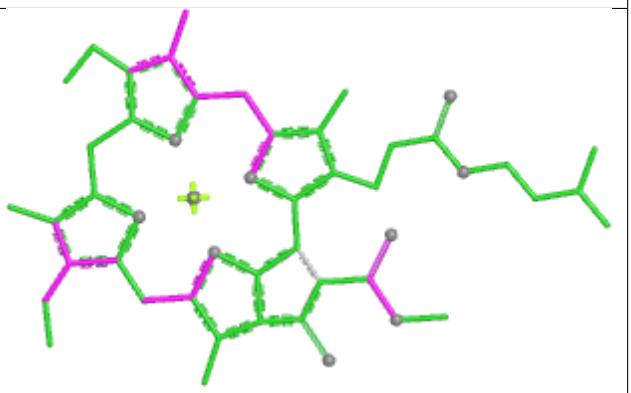


Rings

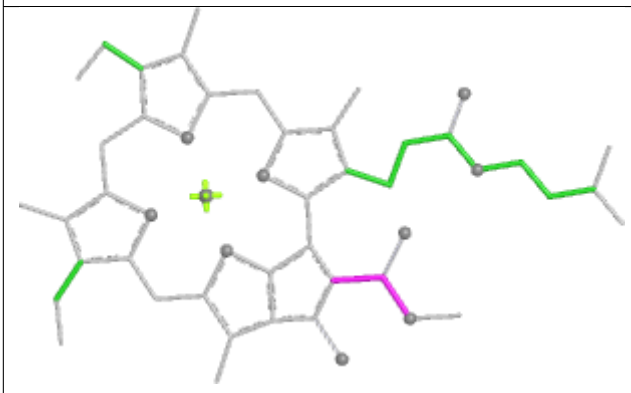
Ligand CLA V 303



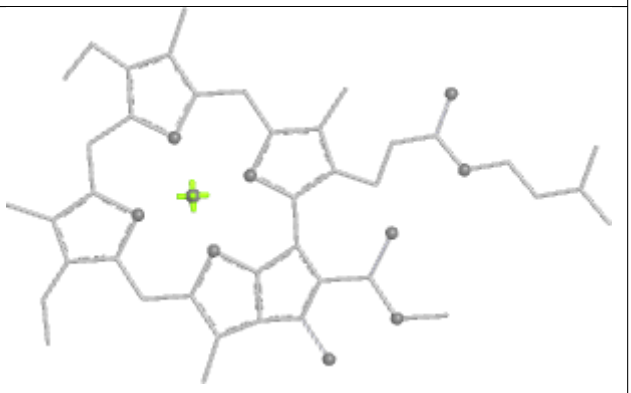
Bond lengths



Bond angles

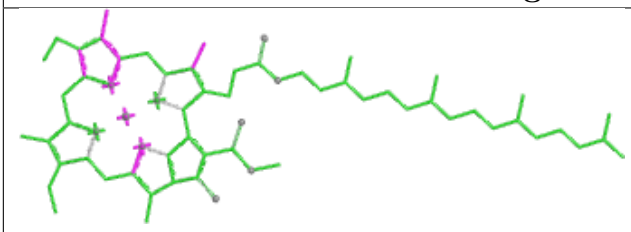


Torsions

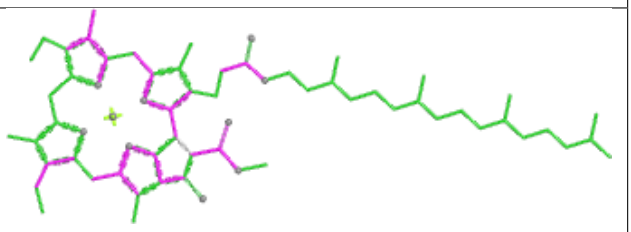


Rings

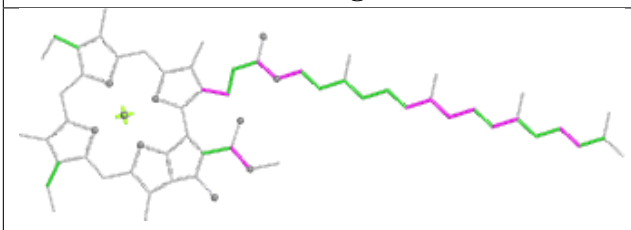
Ligand CLA A 804



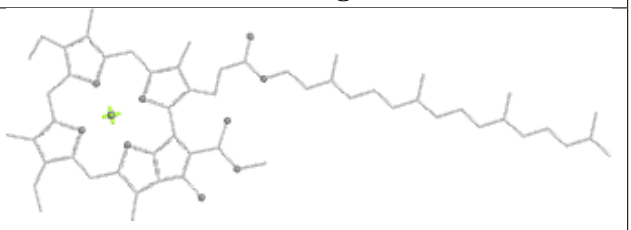
Bond lengths



Bond angles



Torsions



Rings

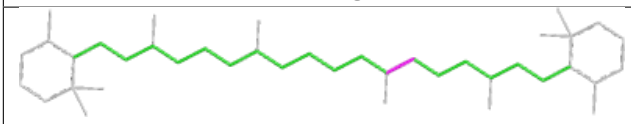
Ligand BCR J 103



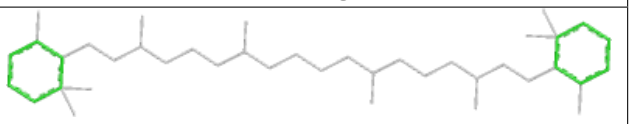
Bond lengths



Bond angles

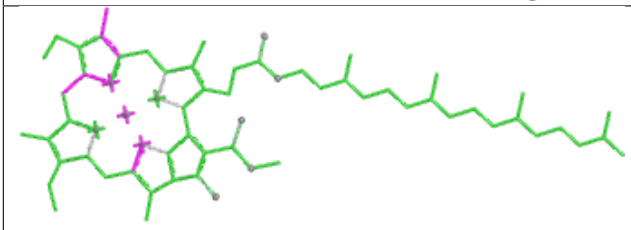


Torsions

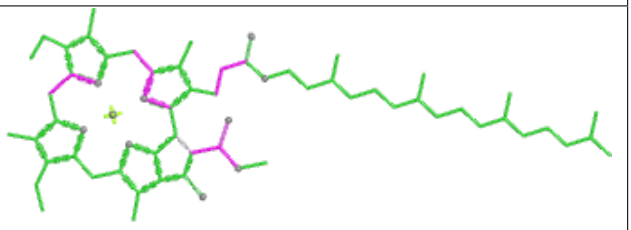


Rings

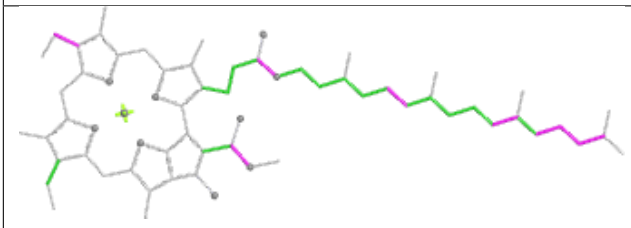
Ligand CLA A 835



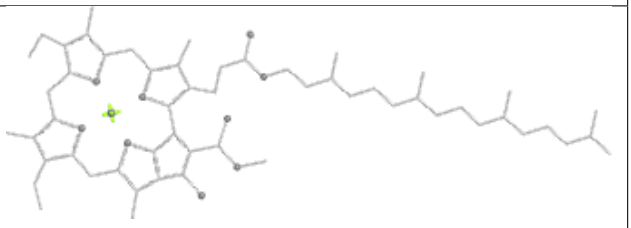
Bond lengths



Bond angles

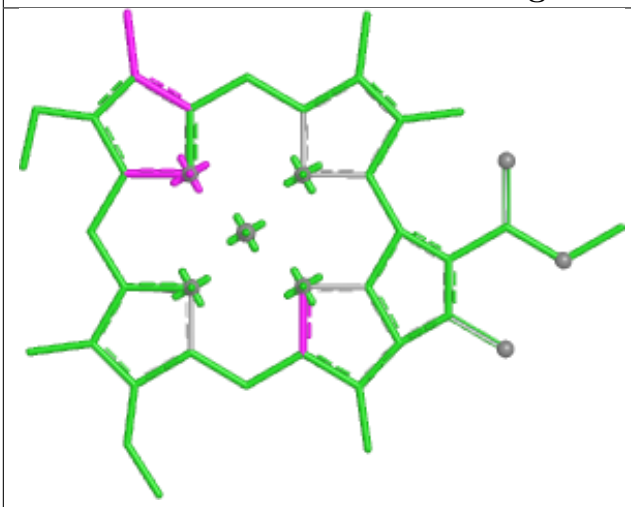


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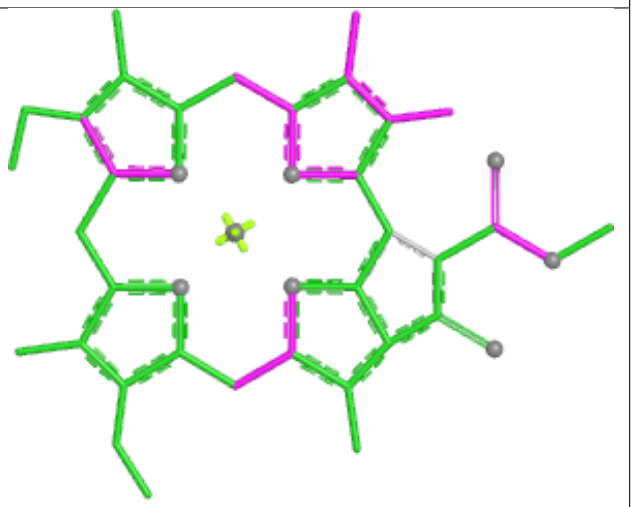


Rings

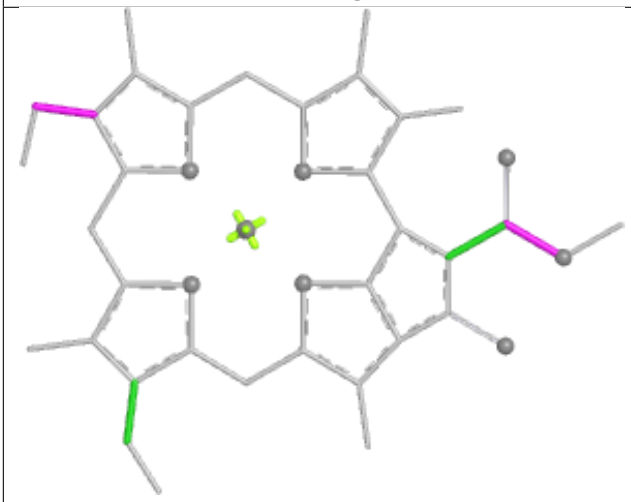
Ligand CLA 4 315



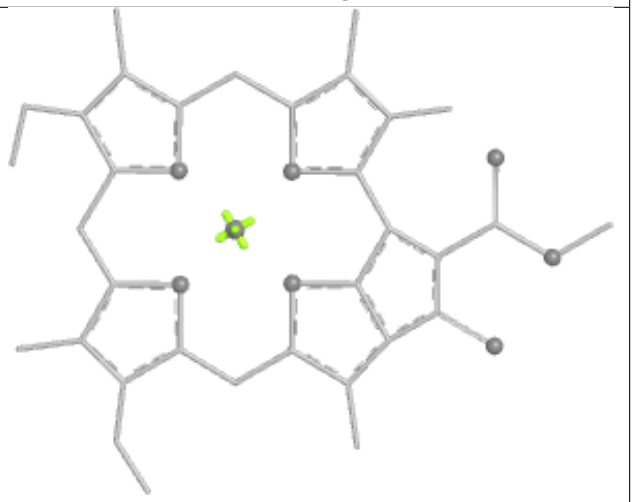
Bond lengths



Bond angles

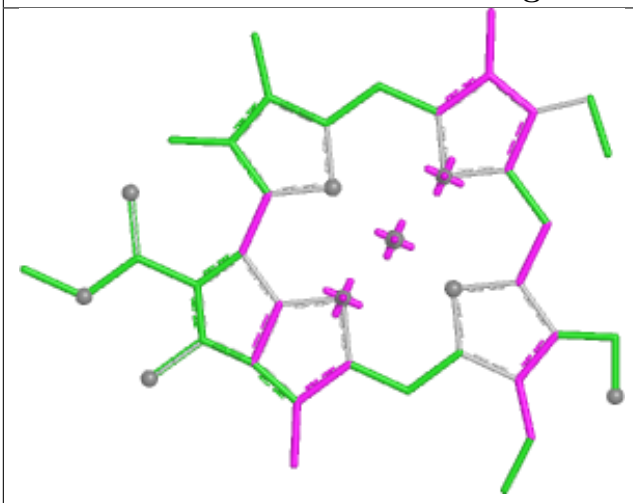


Torsions



Rings

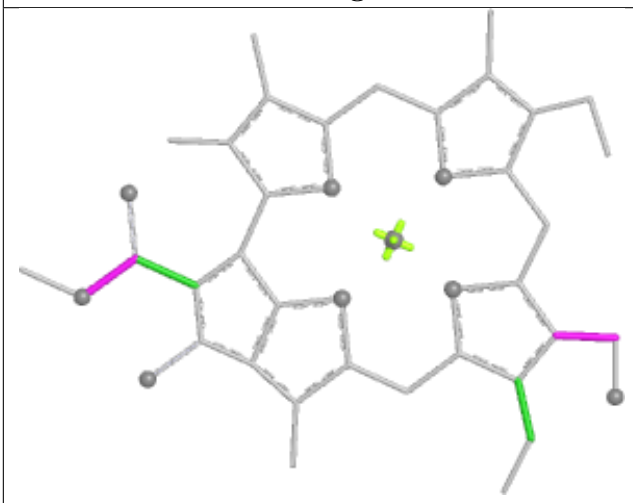
Ligand CHL U 304



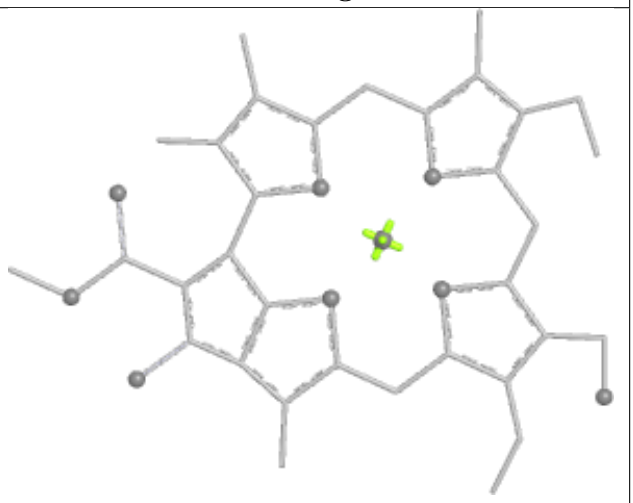
Bond lengths



Bond angles

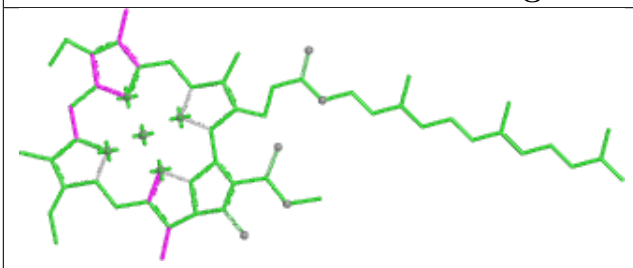


Torsions

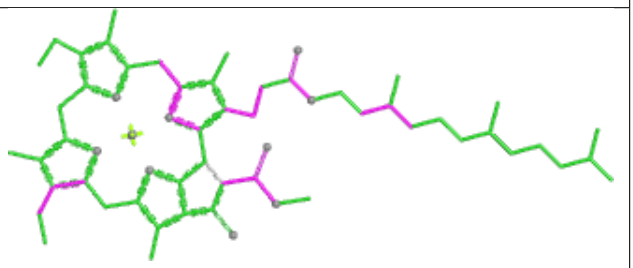


Rings

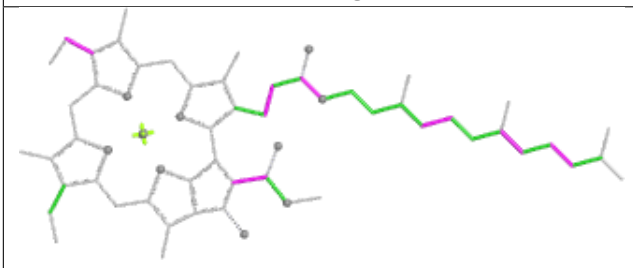
Ligand CLA R 315



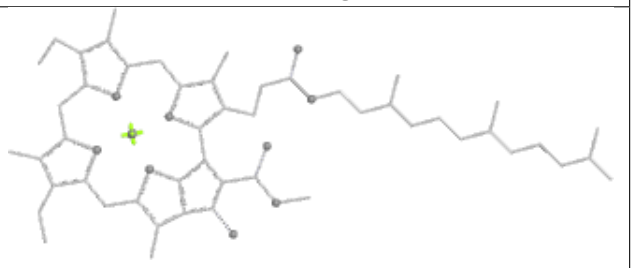
Bond lengths



Bond angles

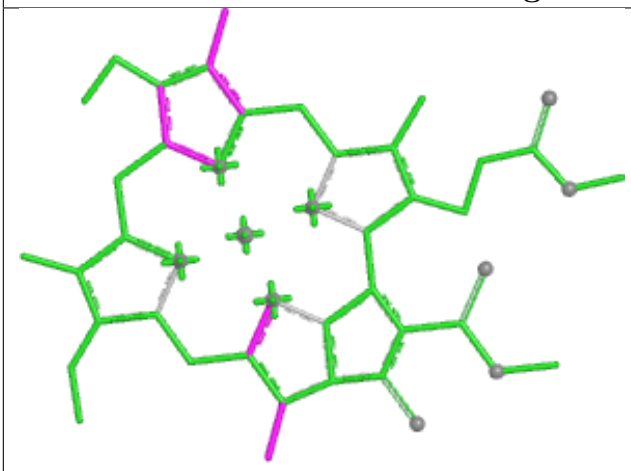


Torsions

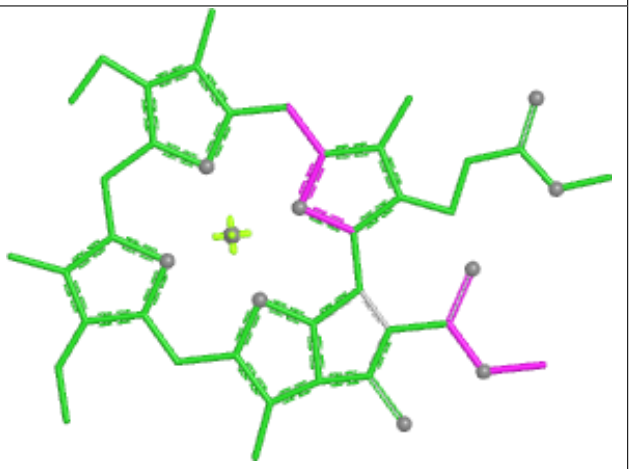


Rings

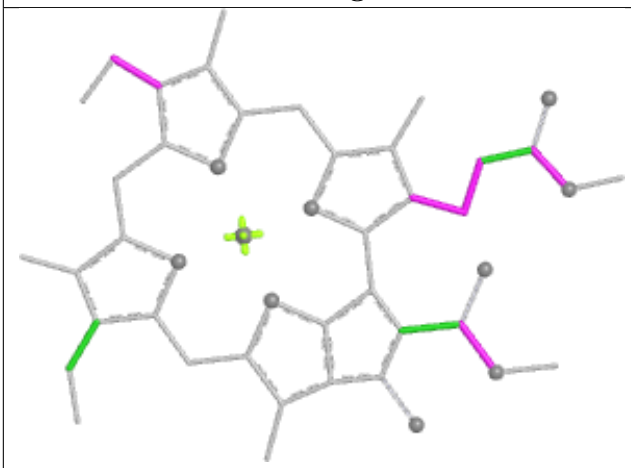
Ligand CLA U 309



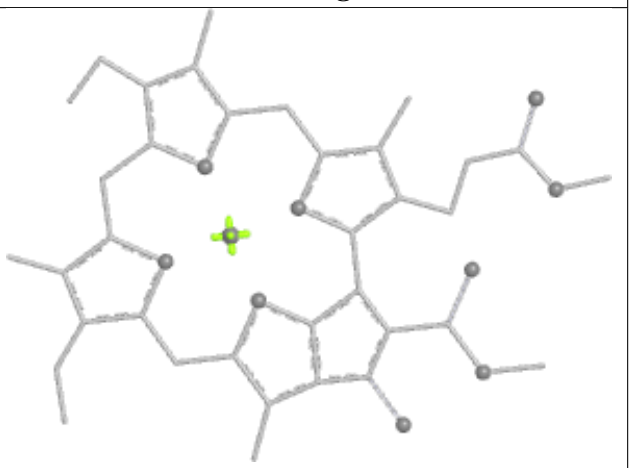
Bond lengths



Bond angles

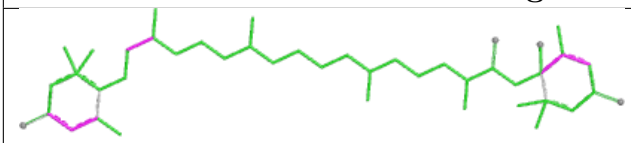


Torsions



Rings

Ligand IWJ V 320



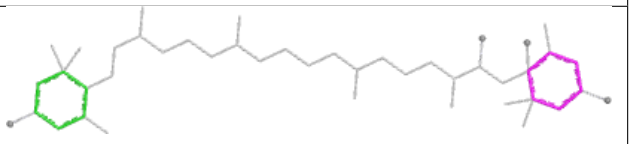
Bond lengths



Bond angles

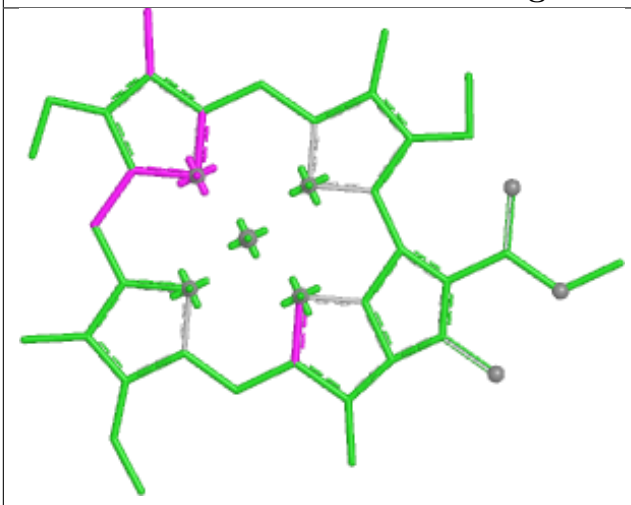


Torsions

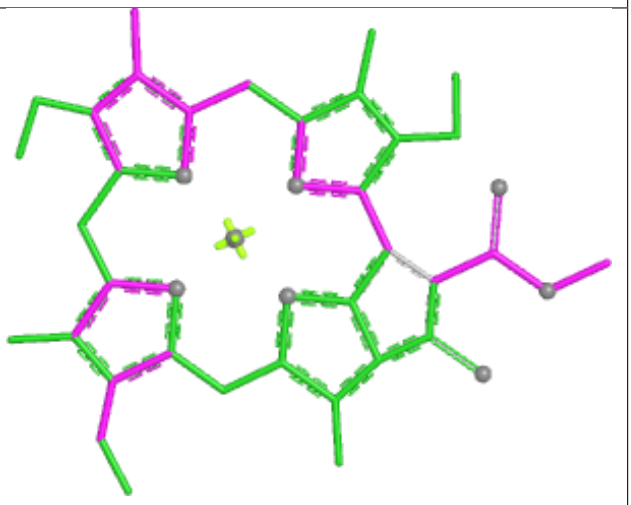


Rings

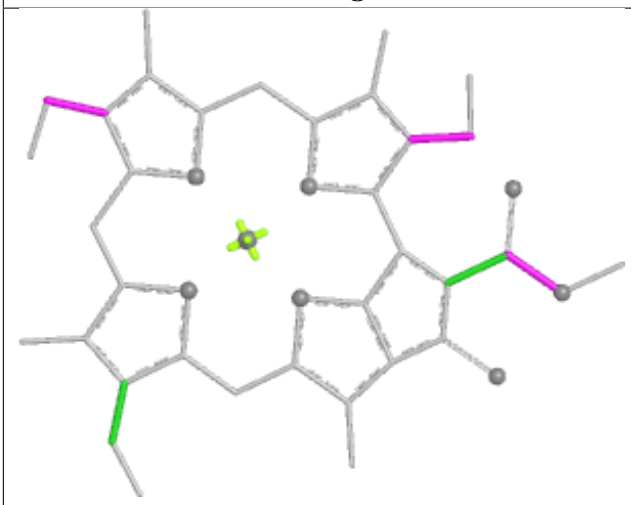
Ligand CLA 4 311



Bond lengths



Bond angles

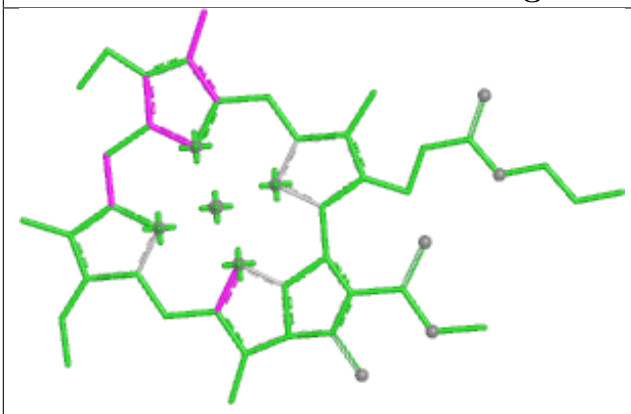


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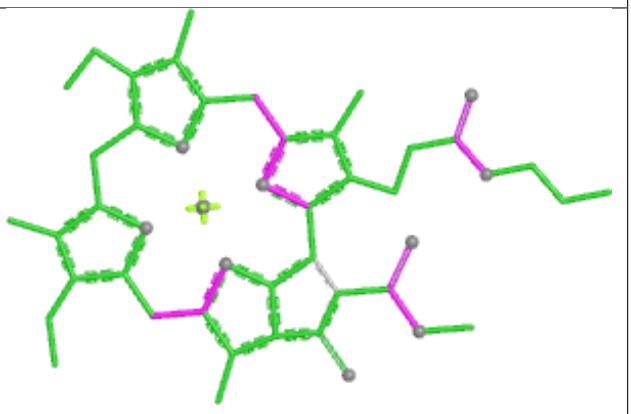


Rings

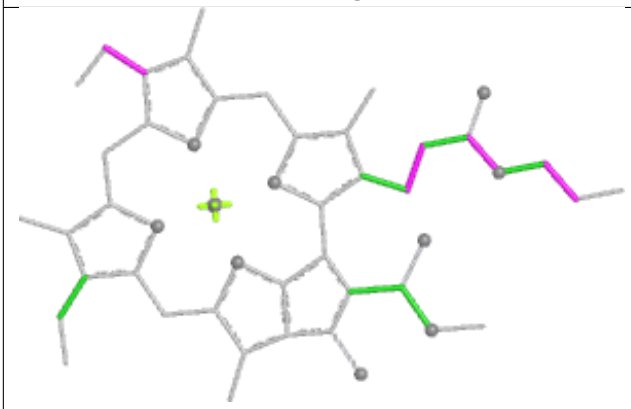
Ligand CLA V 313



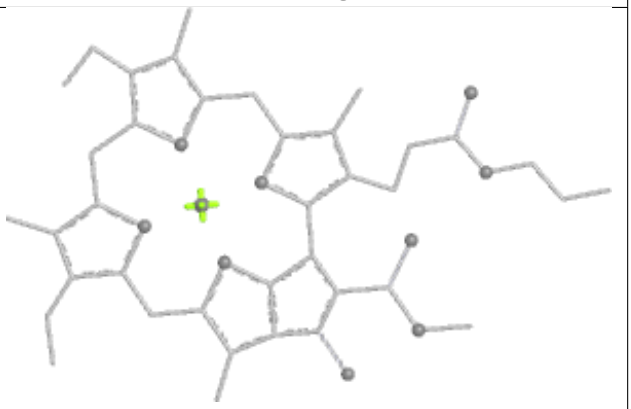
Bond lengths



Bond angles

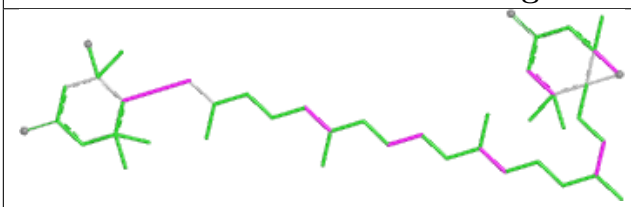


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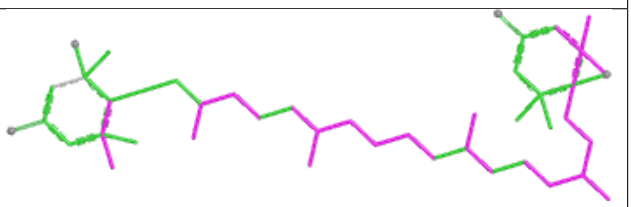


Rings

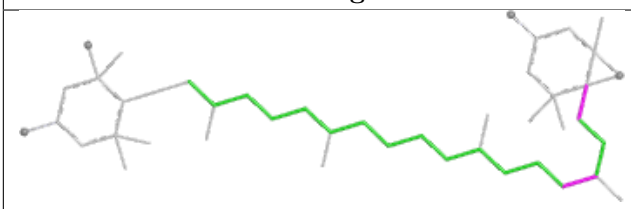
Ligand NEX R 321



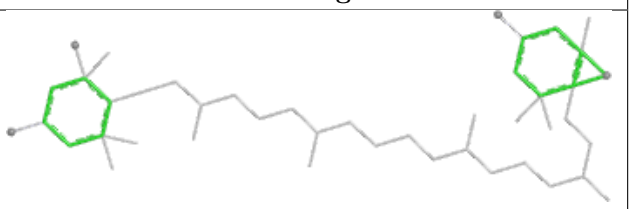
Bond lengths



Bond angles

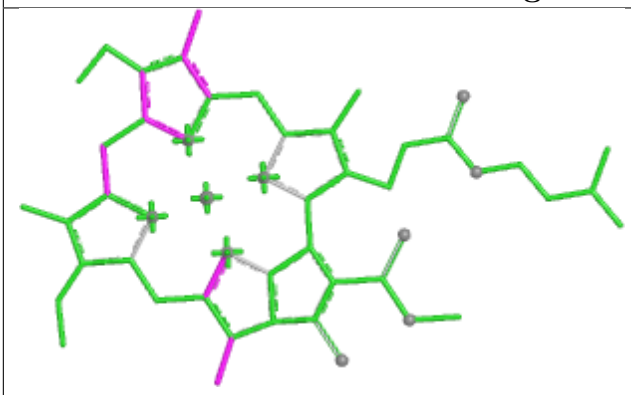


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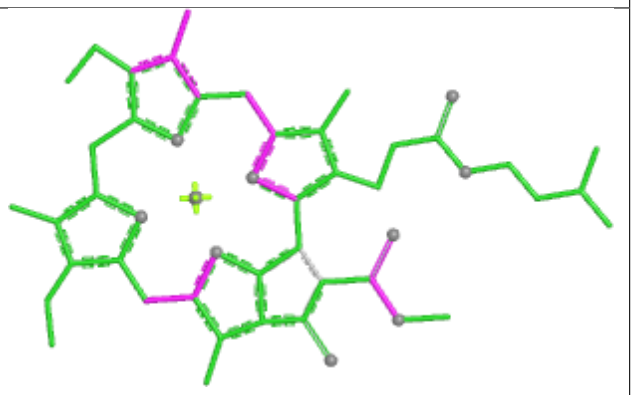


Rings

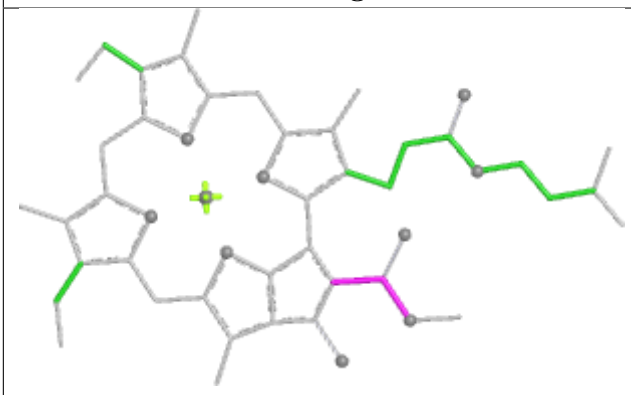
Ligand CLA R 307



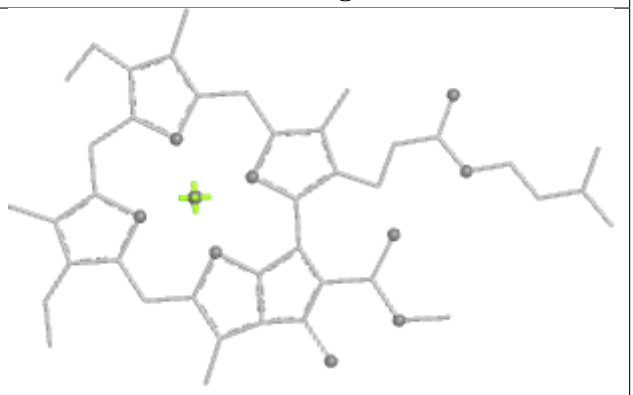
Bond lengths



Bond angles

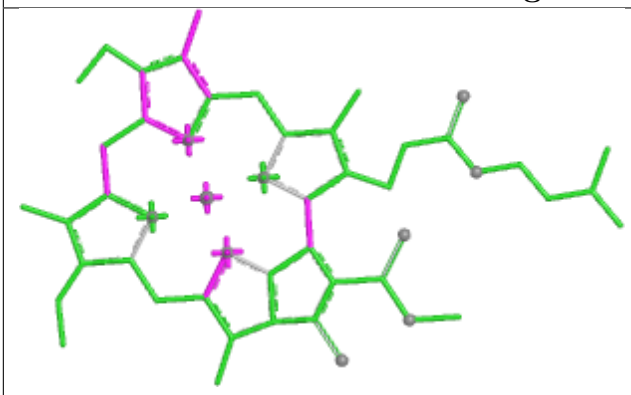


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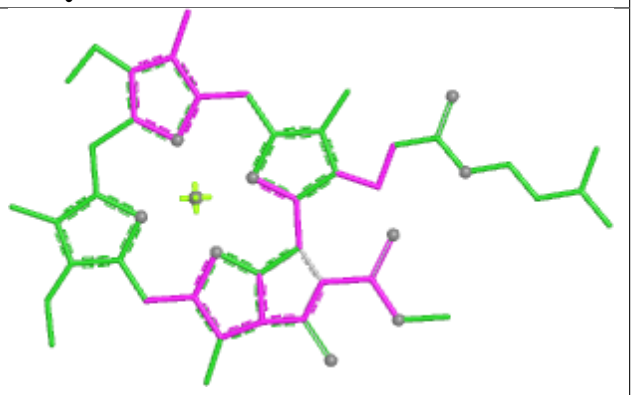


Rings

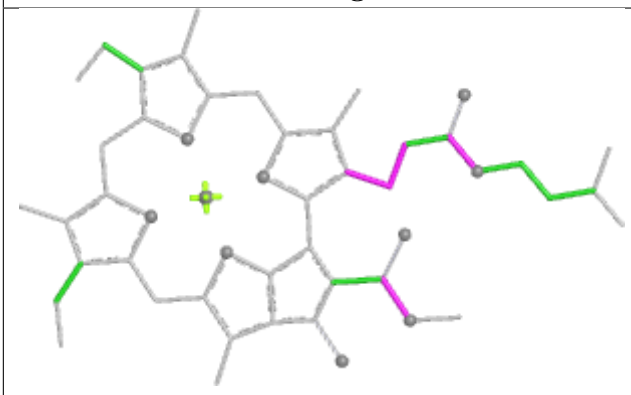
Ligand CLA Q 306



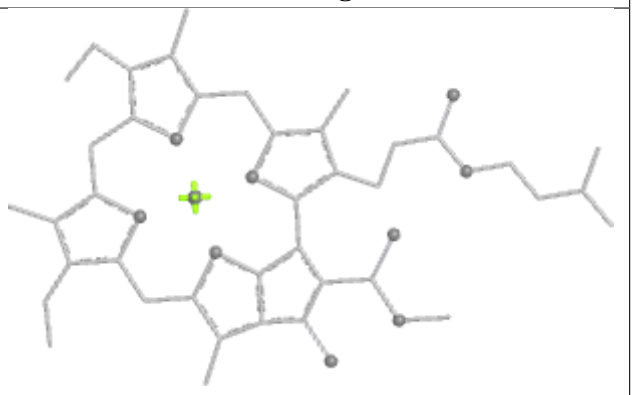
Bond lengths



Bond angles

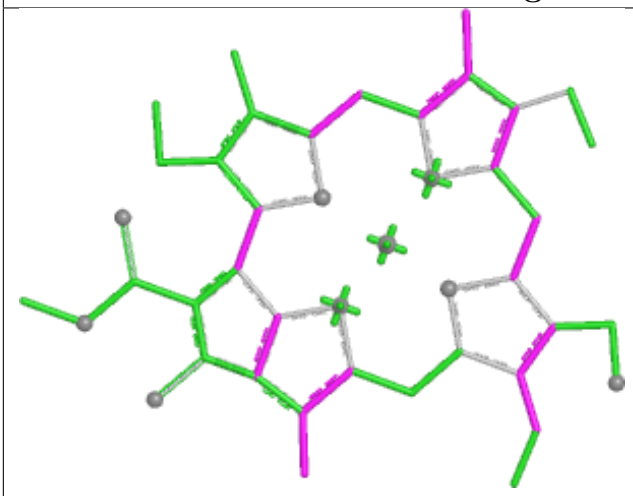


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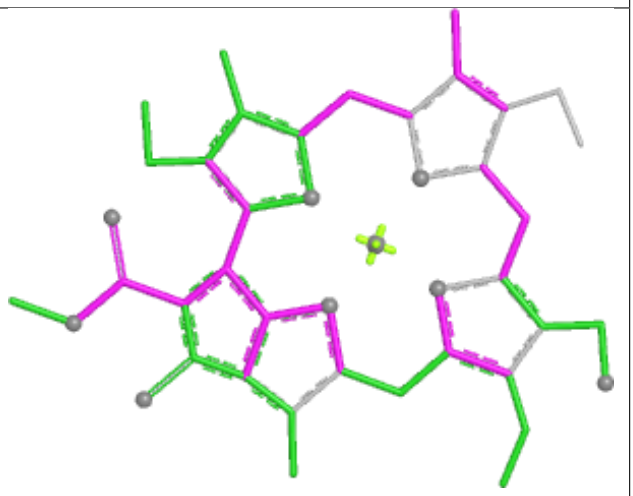


Rings

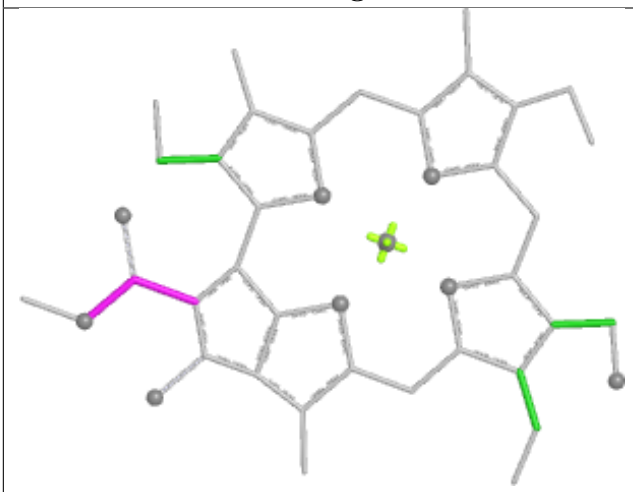
Ligand CHL T 304



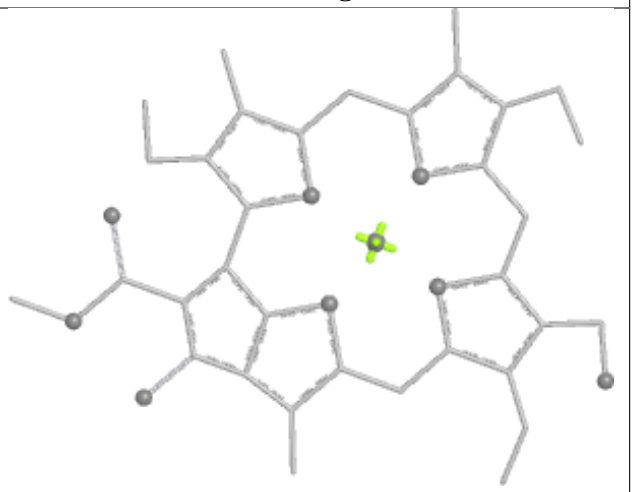
Bond lengths



Bond angles

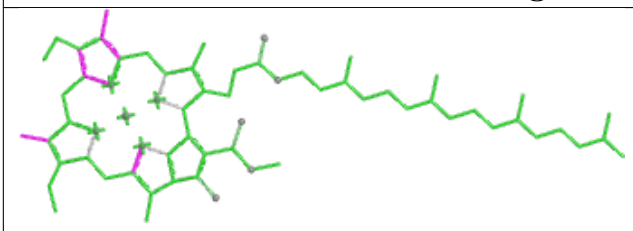


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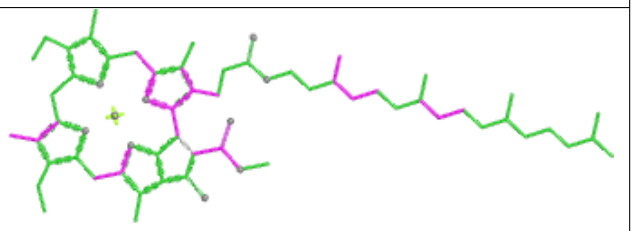


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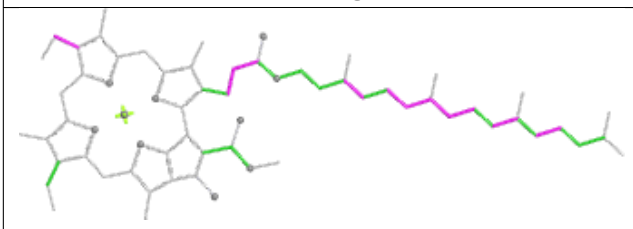
Ligand CLA 2 612



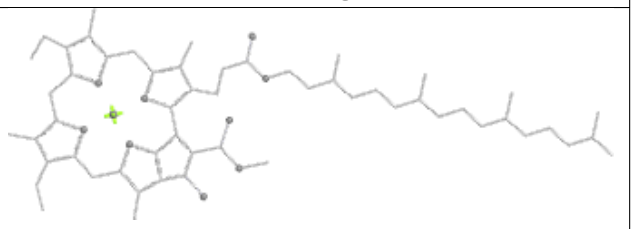
Bond lengths



Bond angles

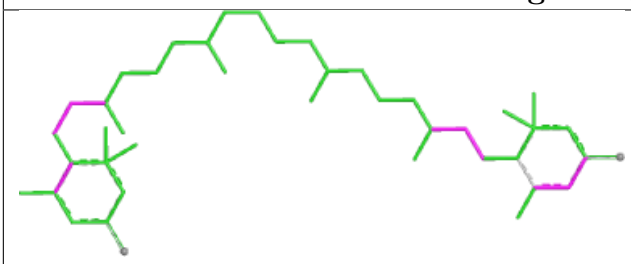


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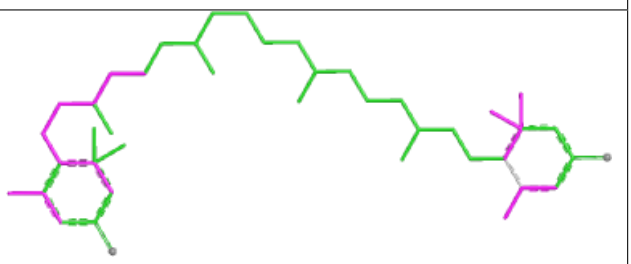


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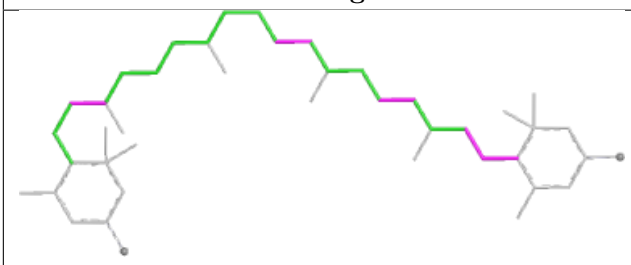
Ligand Q6L V 316



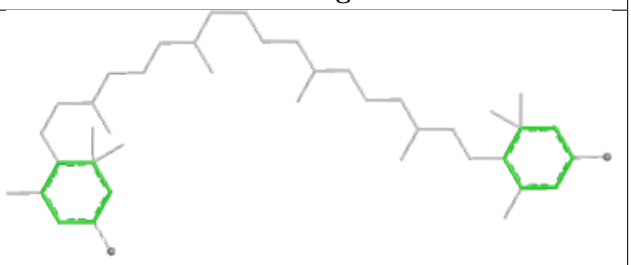
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Bond angles

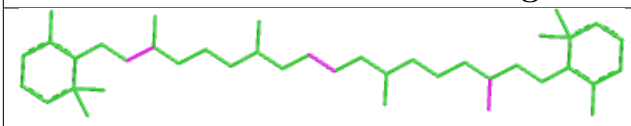


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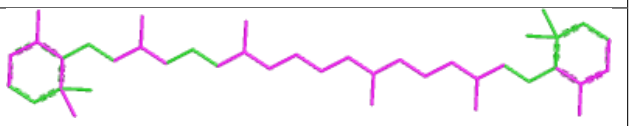


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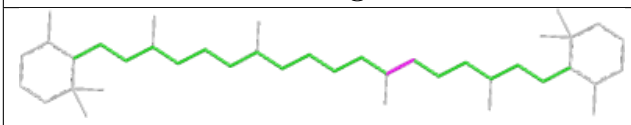
Ligand BCR G 201



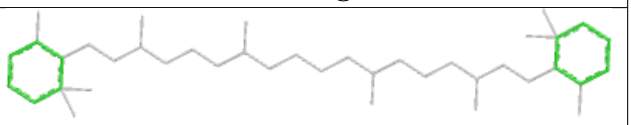
Bond lengths



Bond angles

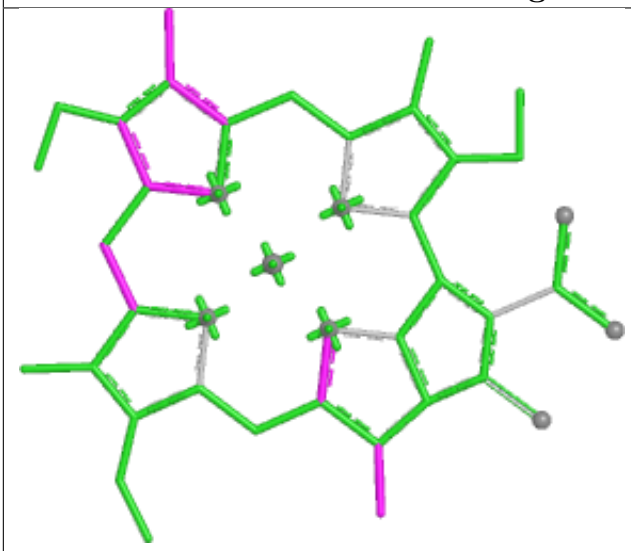


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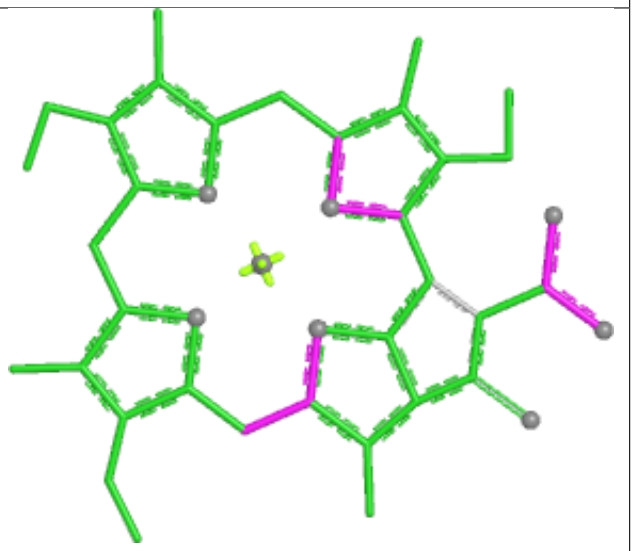


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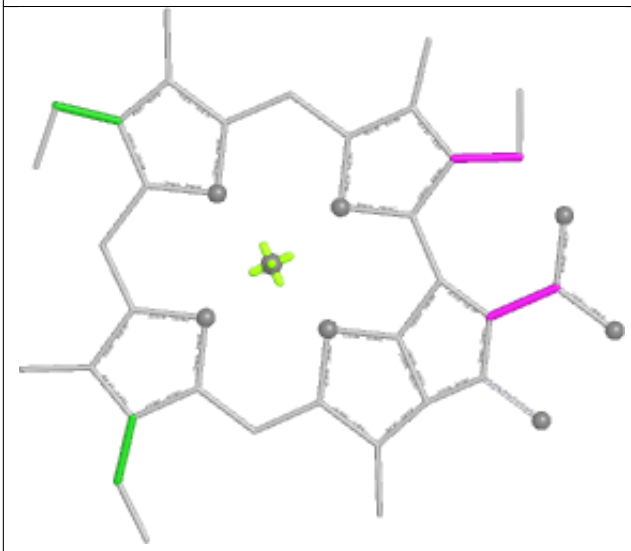
Ligand CLA 1 605



Bond lengths



Bond angles

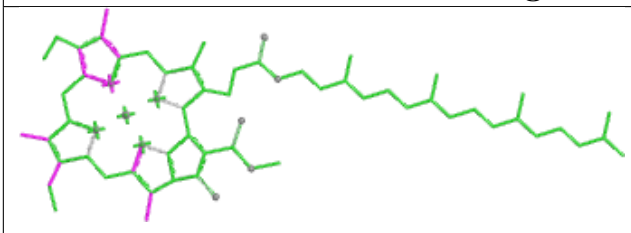


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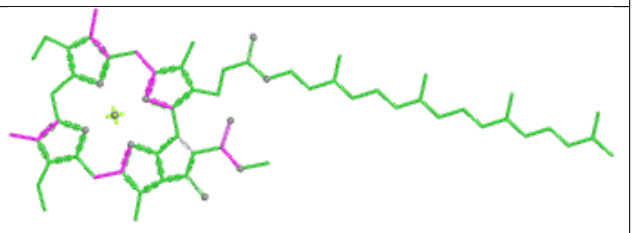


Rings

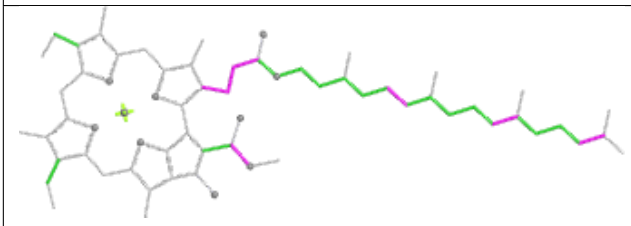
Ligand CLA B 811



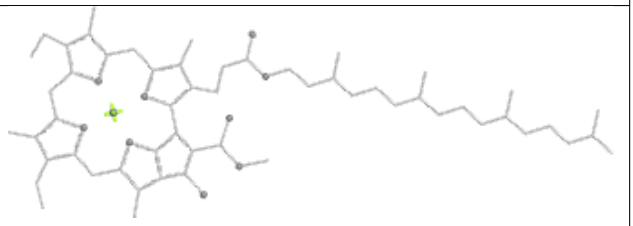
Bond lengths



Bond angles

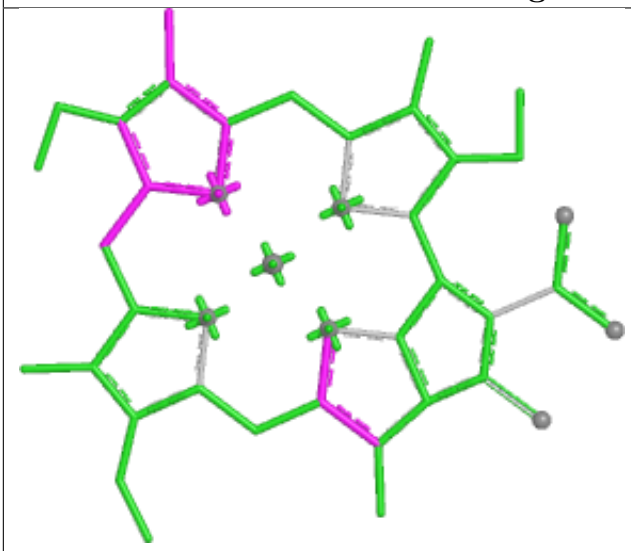


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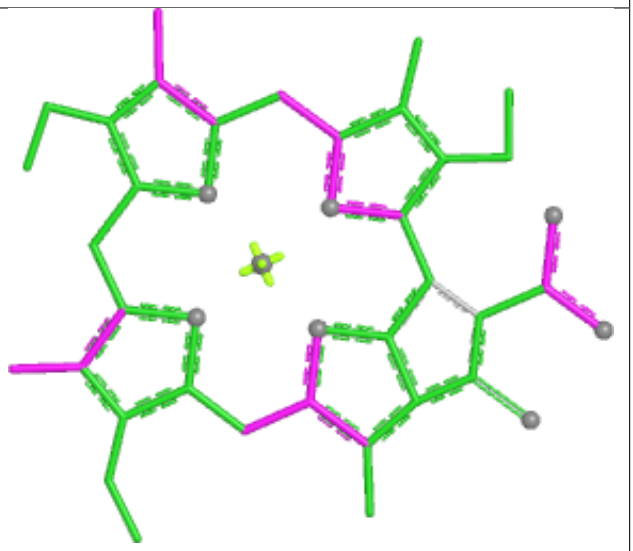


Rings

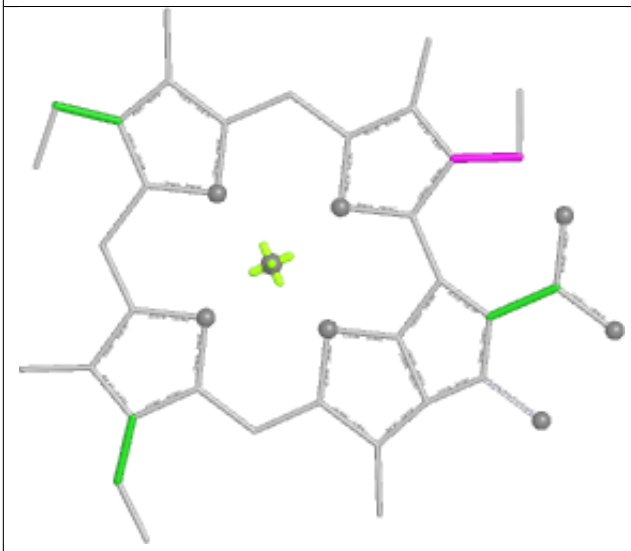
Ligand CLA 3 304



Bond lengths



Bond angles

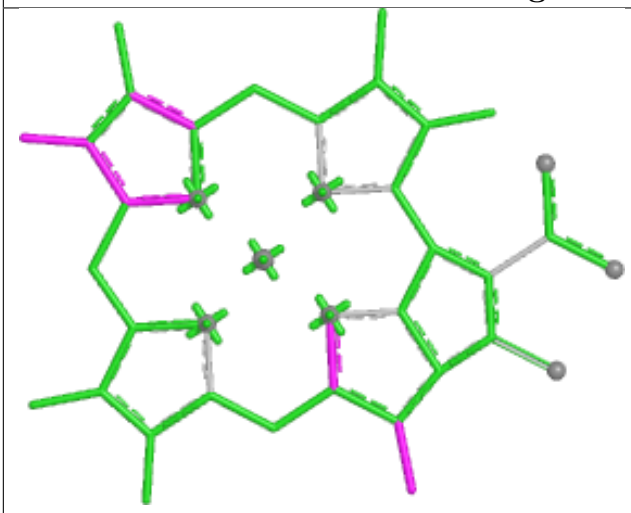


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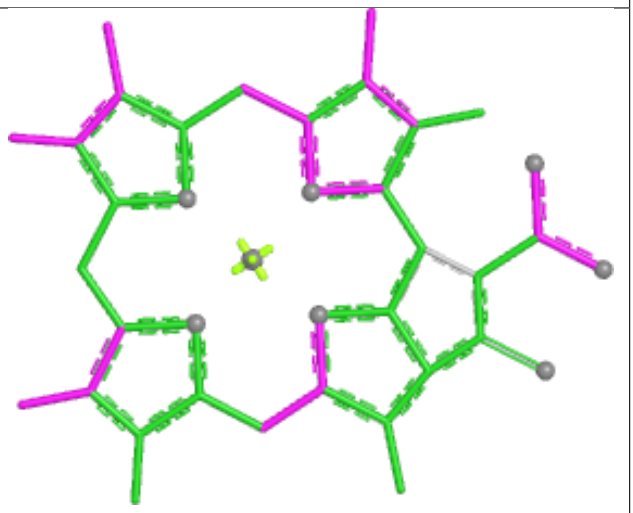


Rings

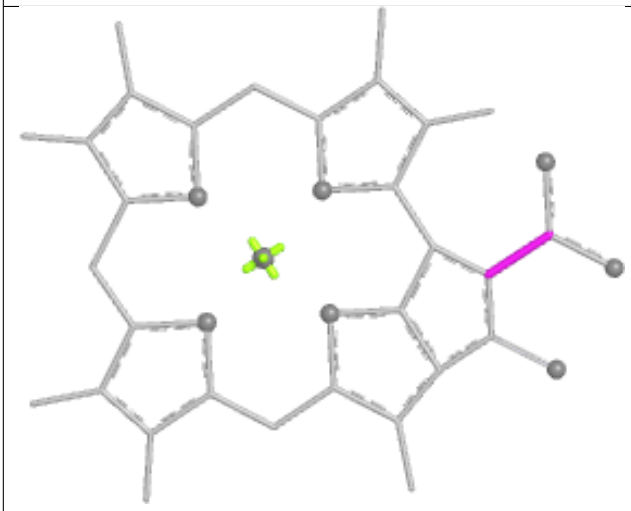
Ligand CLA 1 609



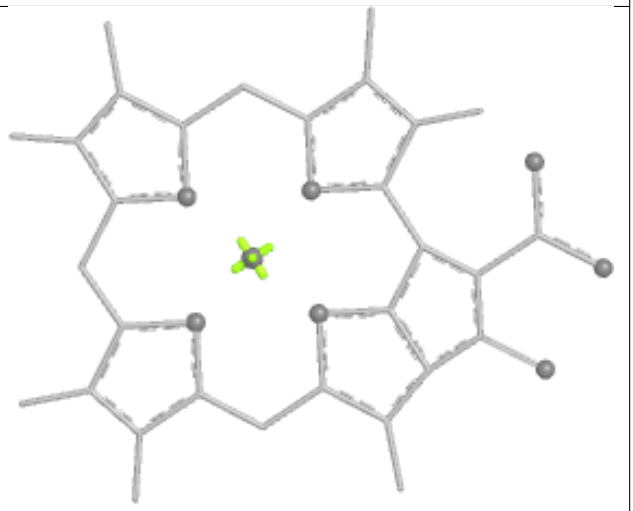
Bond lengths



Bond angles

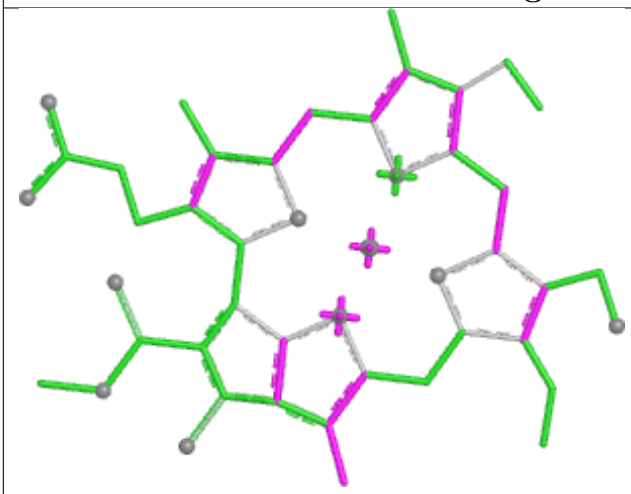


Torsions

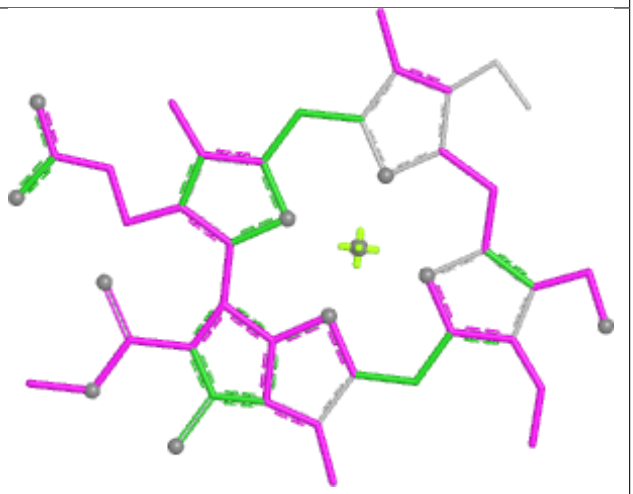


Rings

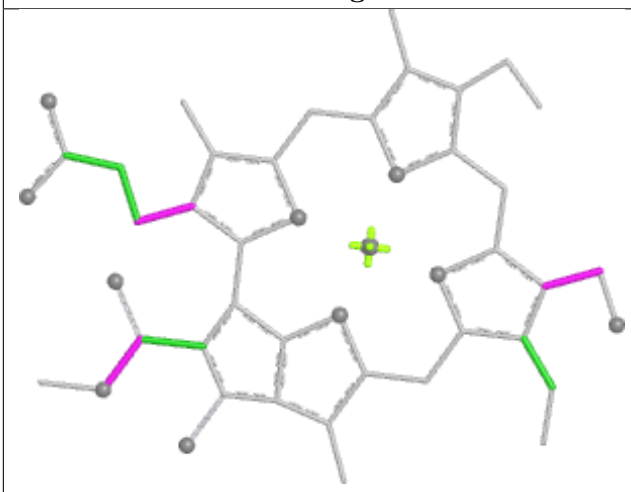
Ligand CHL P 304



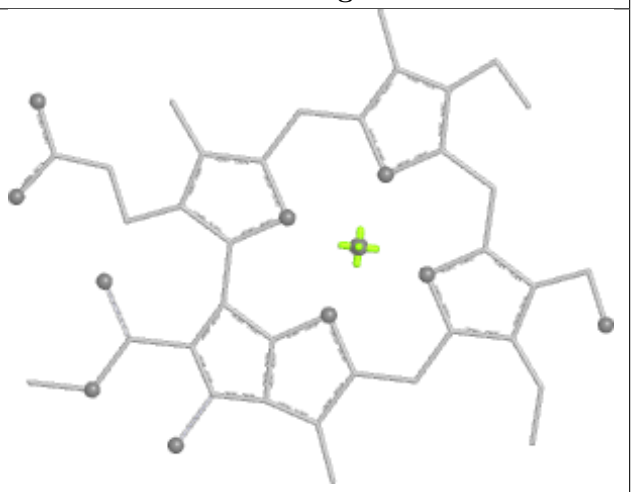
Bond lengths



Bond angles

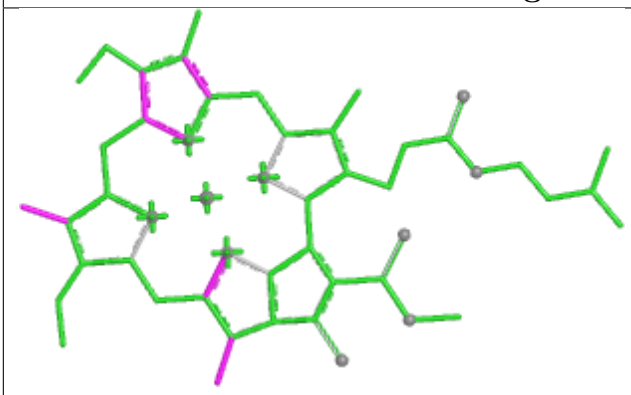


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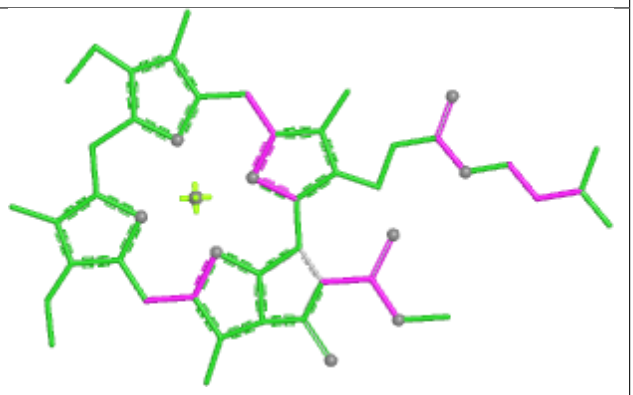


Rings

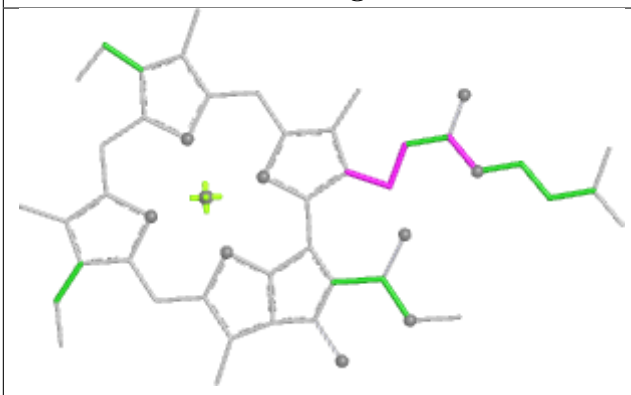
Ligand CLA A 845



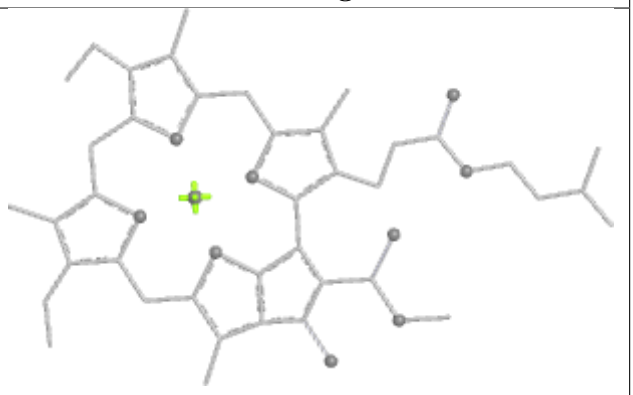
Bond lengths



Bond angles

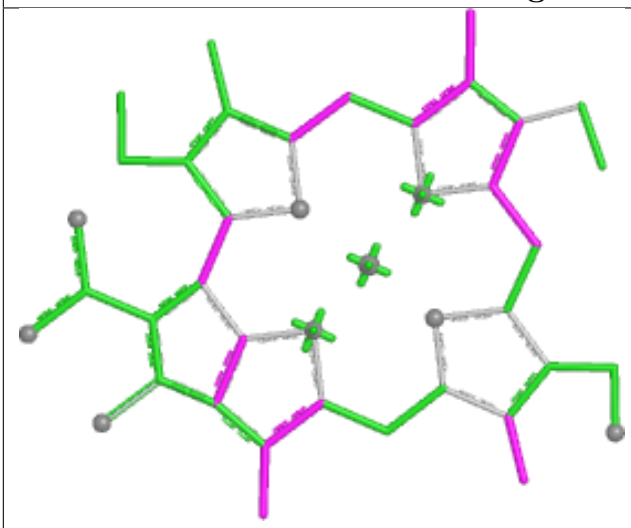


Torsions

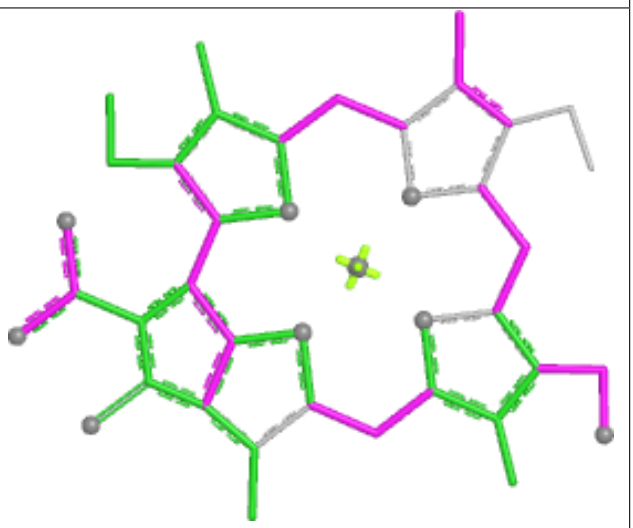


Rings

Ligand CHL 4 306



Bond lengths



Bond angles

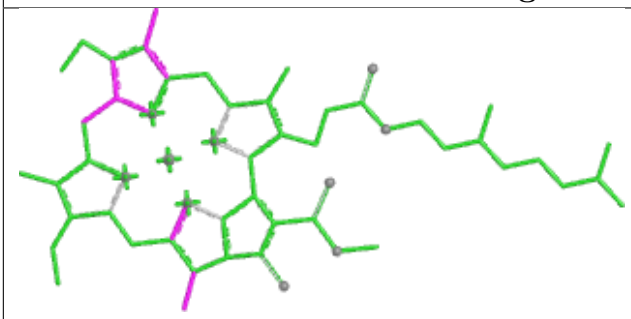


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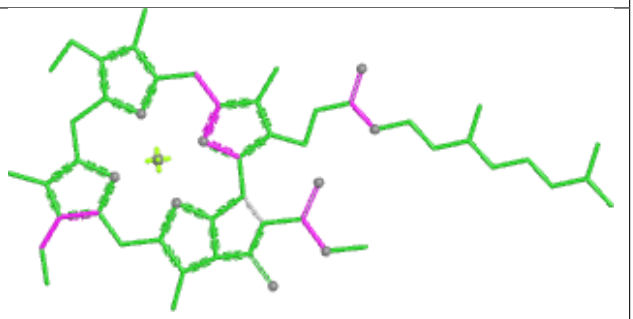


Rings

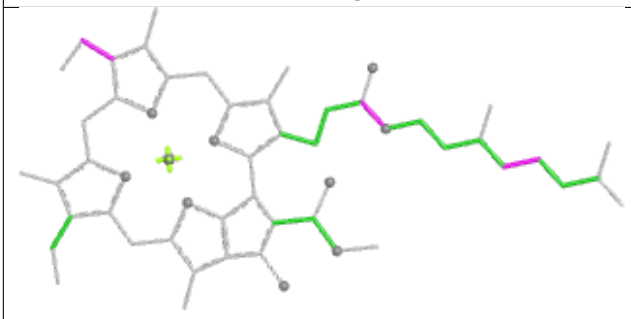
Ligand CLA W 302



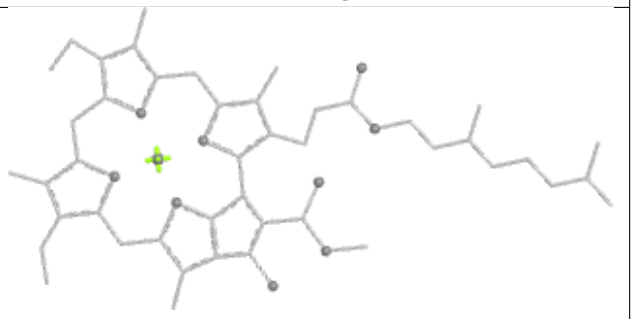
Bond lengths



Bond angles

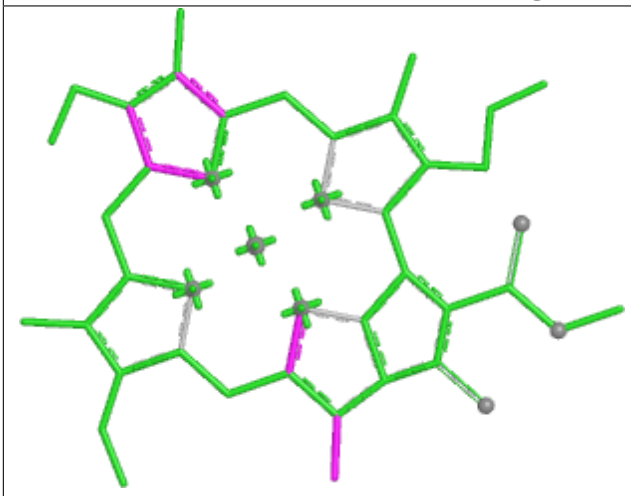


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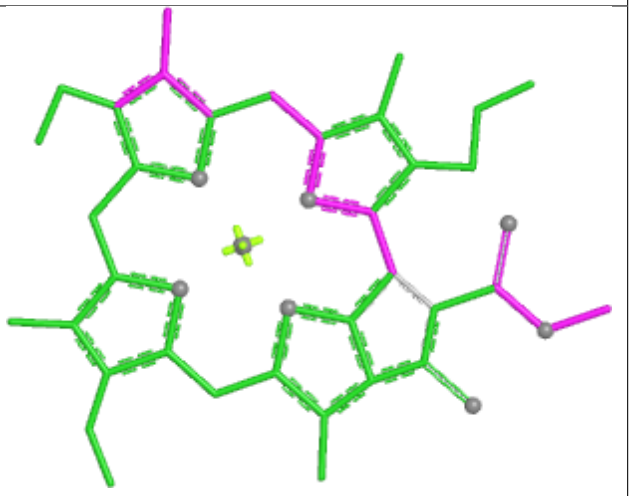


Rings

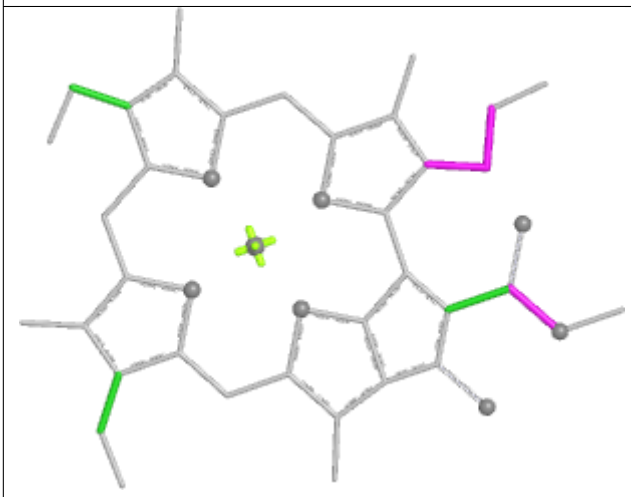
Ligand CLA 3 310



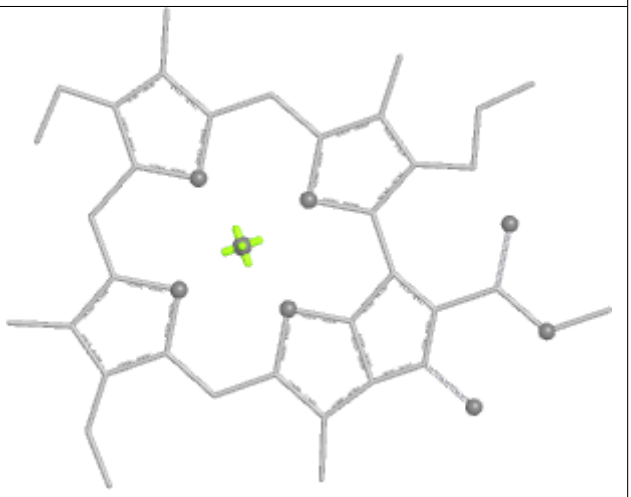
Bond lengths



Bond angles

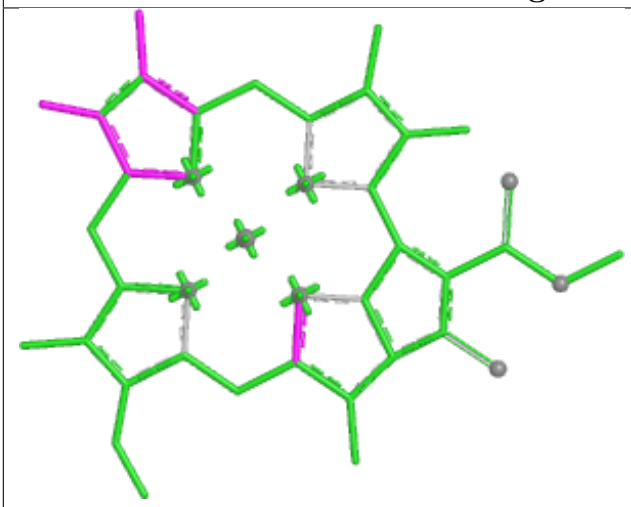


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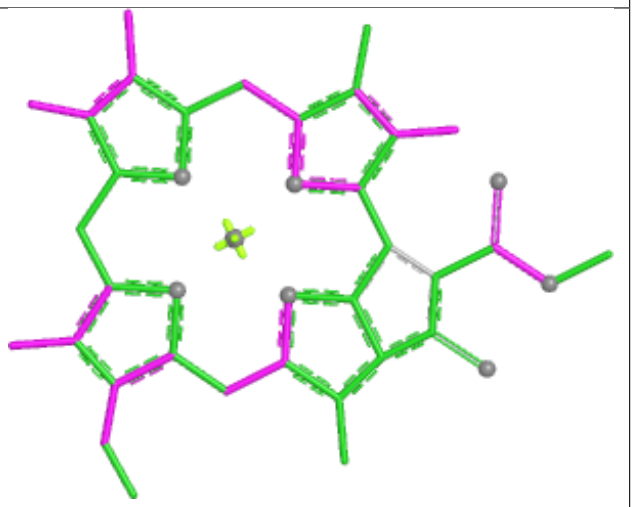


Rings

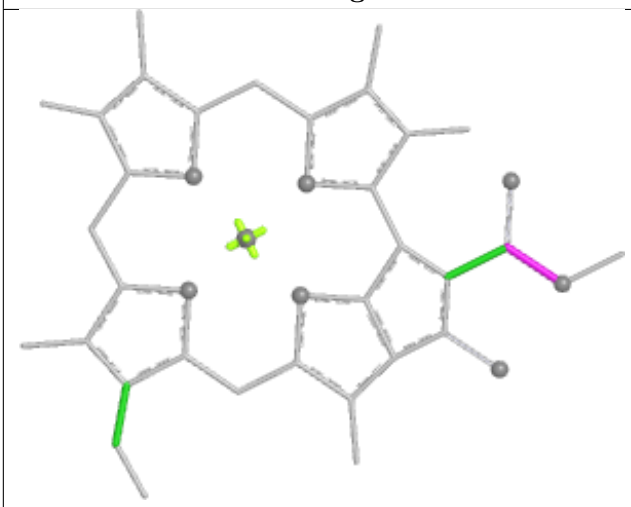
Ligand CLA 1 606



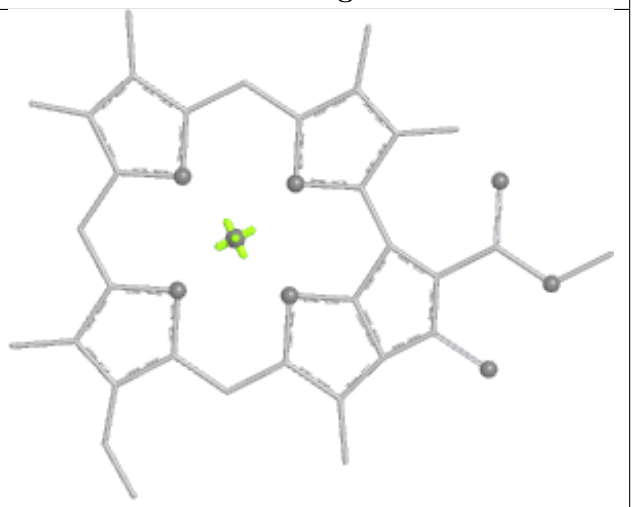
Bond lengths



Bond angles

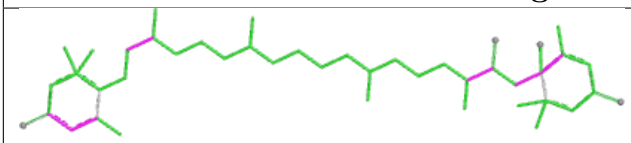


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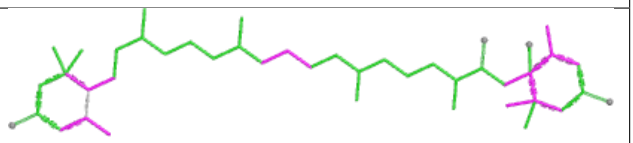


Rings

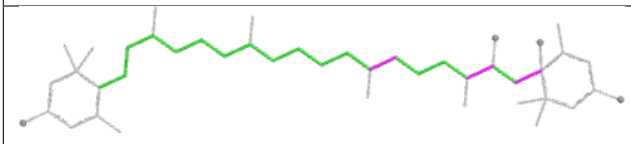
Ligand IWJ 4 317



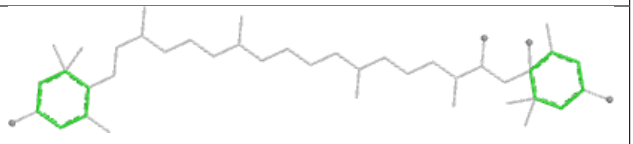
Bond lengths



Bond angles

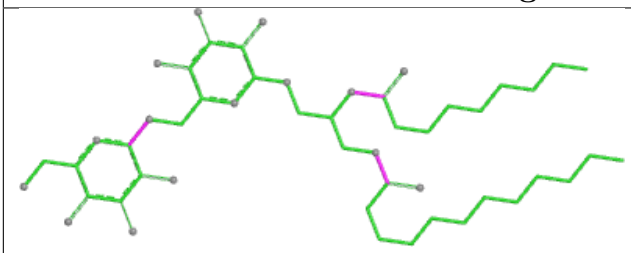


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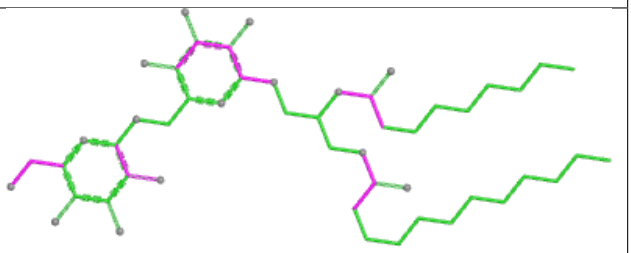


Rings

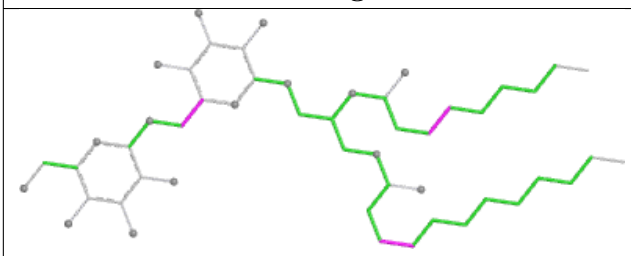
Ligand DGD A 854



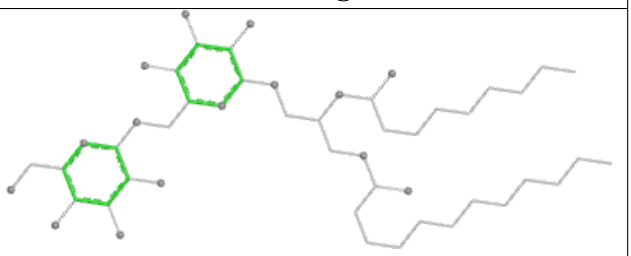
Bond lengths



Bond angles

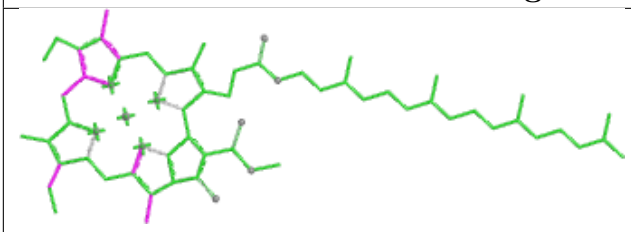


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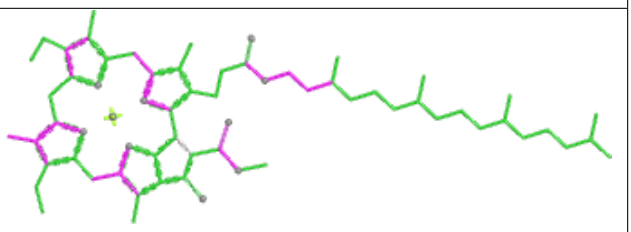


Rings

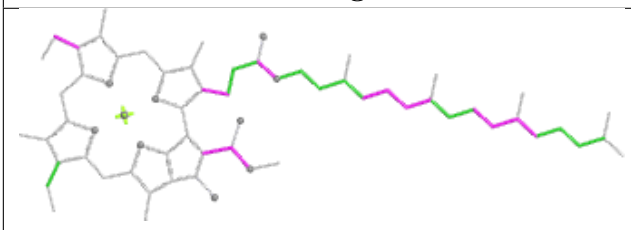
Ligand CLA B 842



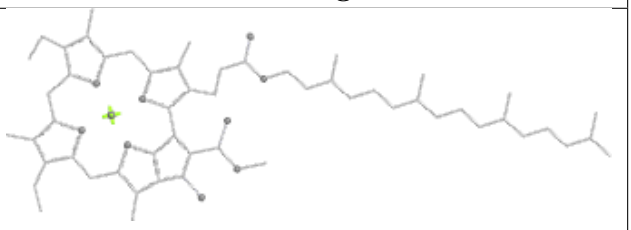
Bond lengths



Bond angles

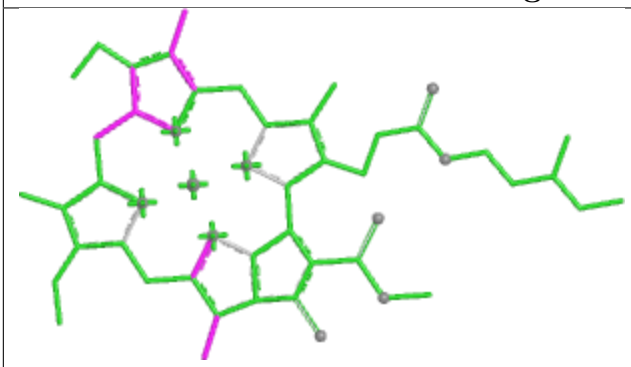


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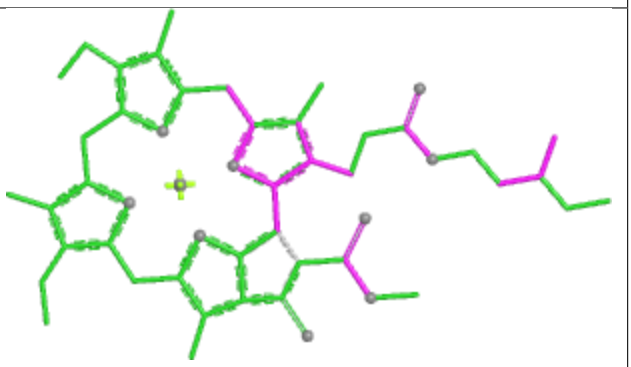


Rings

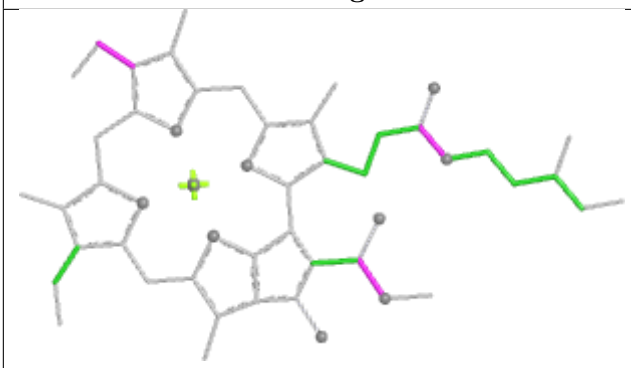
Ligand CLA X 312



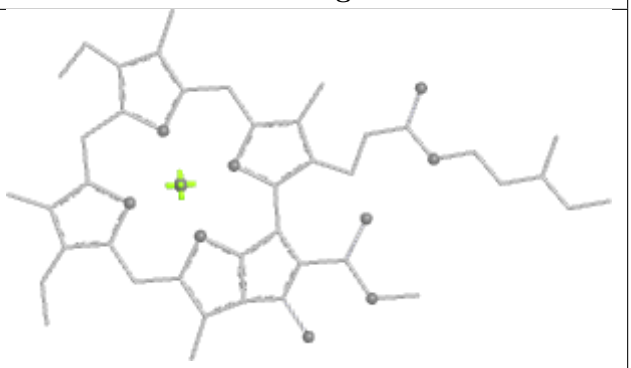
Bond lengths



Bond angles

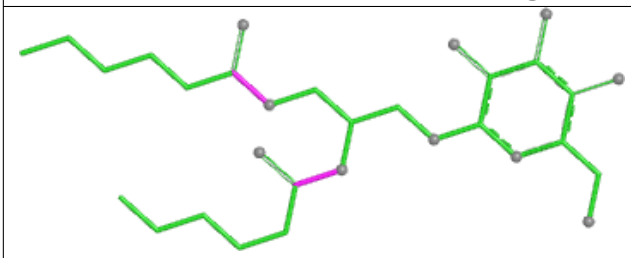


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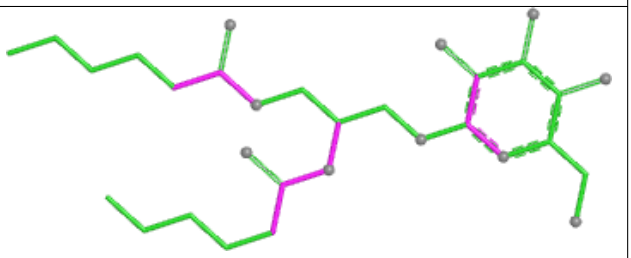


Rings

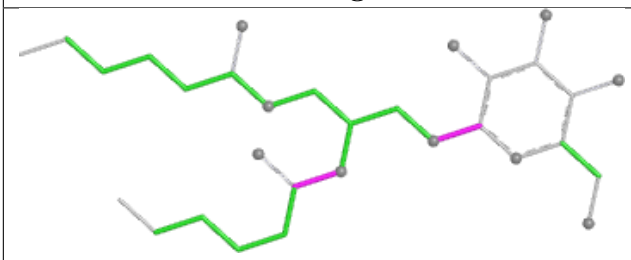
Ligand LMG 2 620



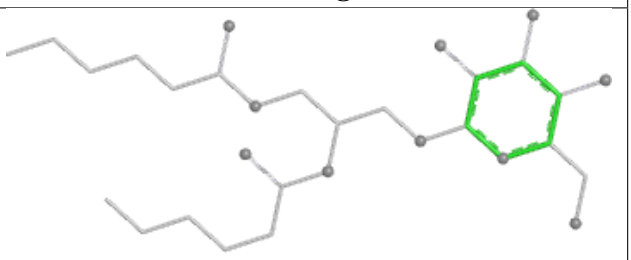
Bond lengths



Bond angles

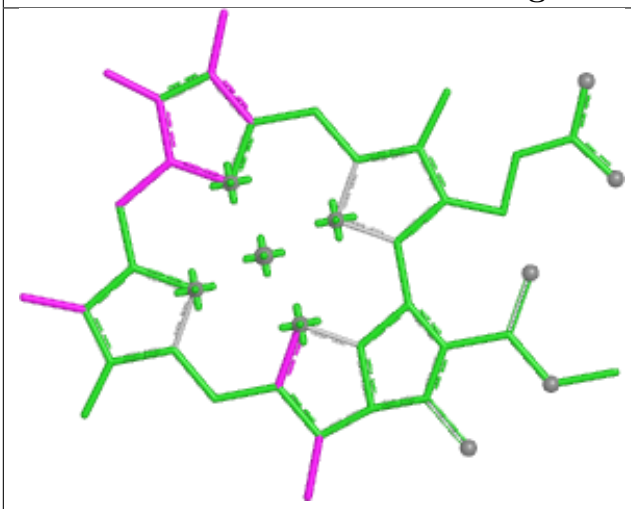


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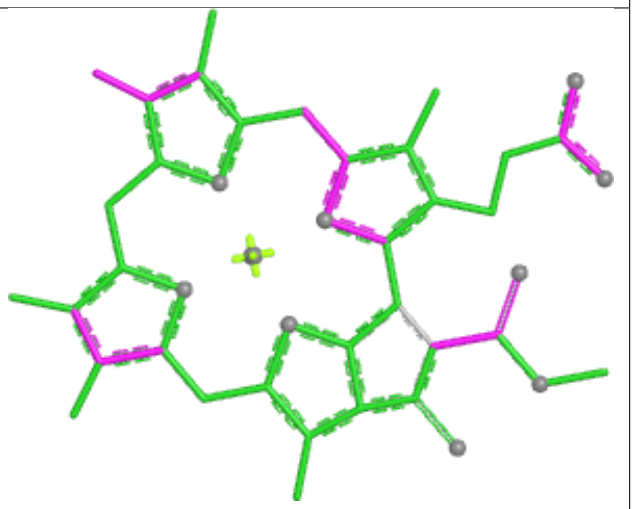


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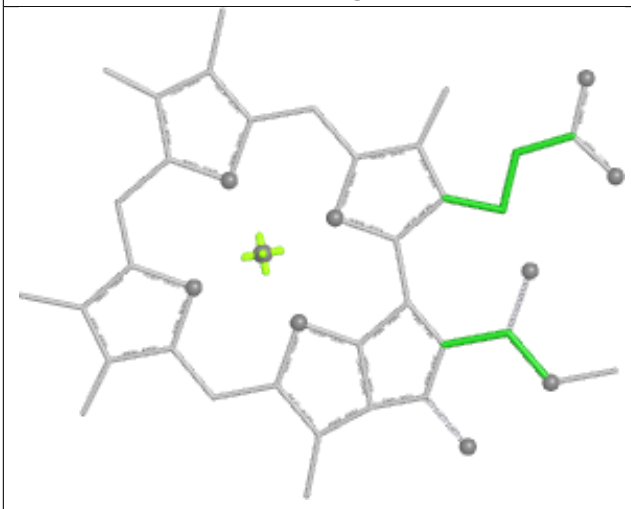
Ligand CLA 3 303



Bond lengths



Bond angles

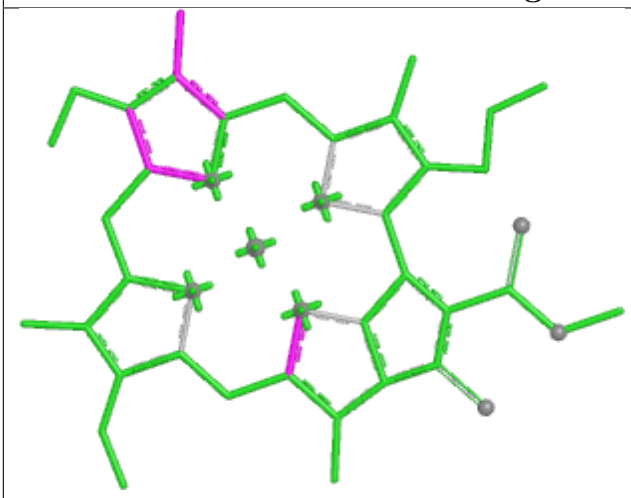


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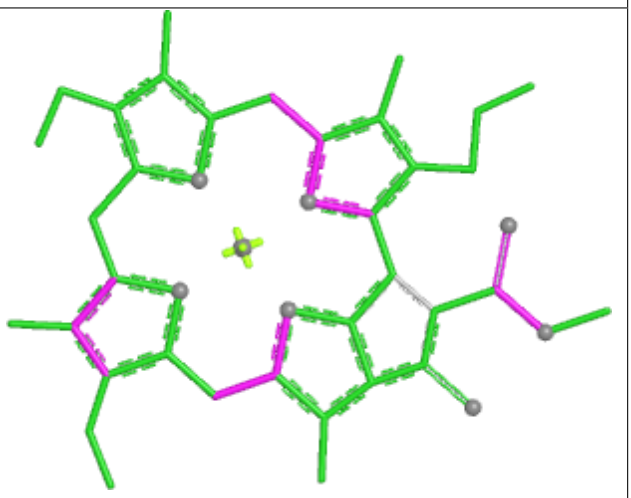


Rings

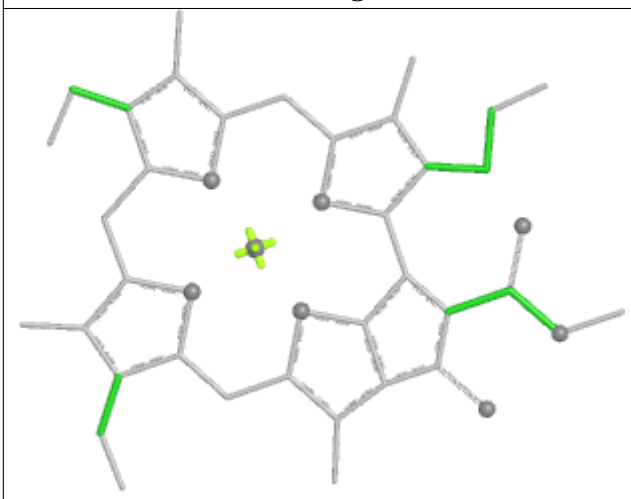
Ligand CLA B 833



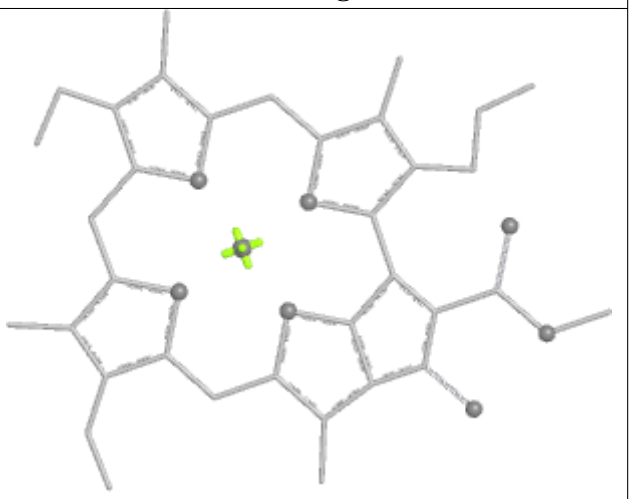
Bond lengths



Bond angles

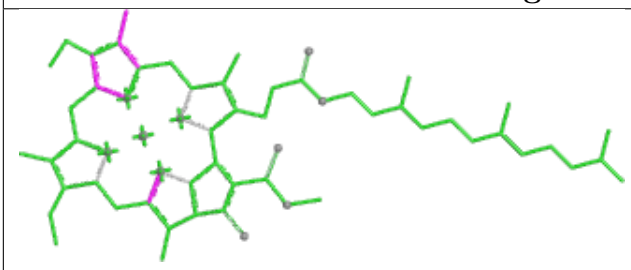


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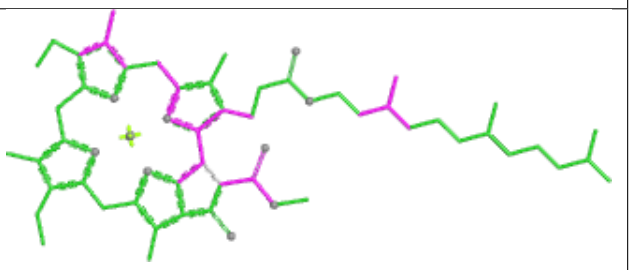


Rings

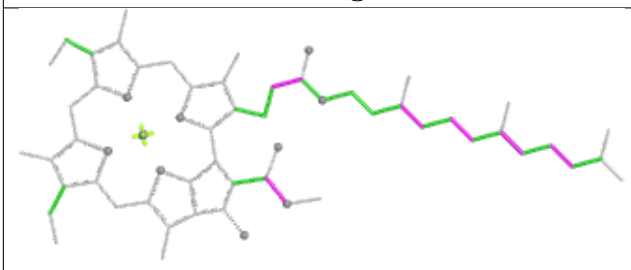
Ligand CLA V 301



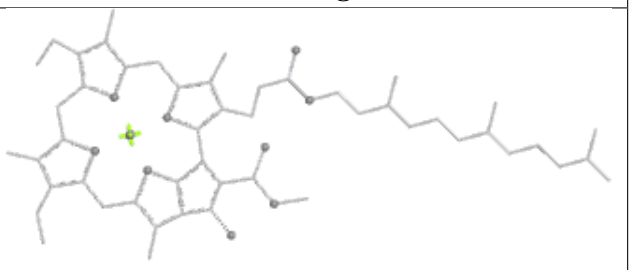
Bond lengths



Bond angles

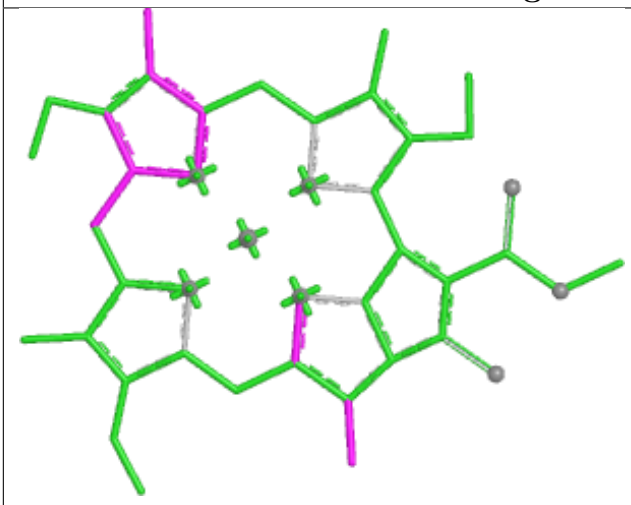


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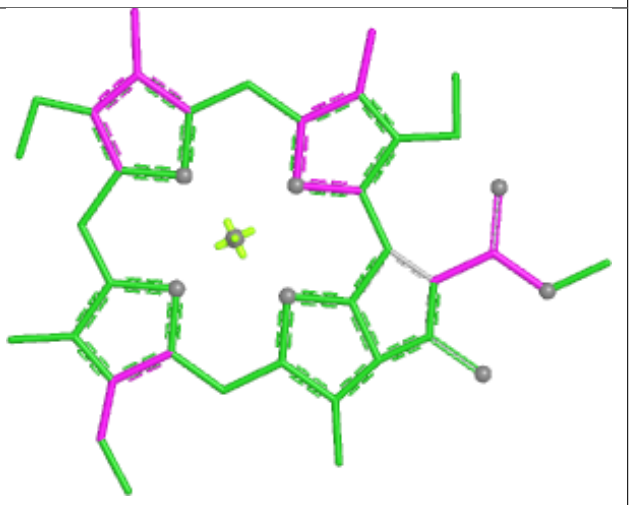


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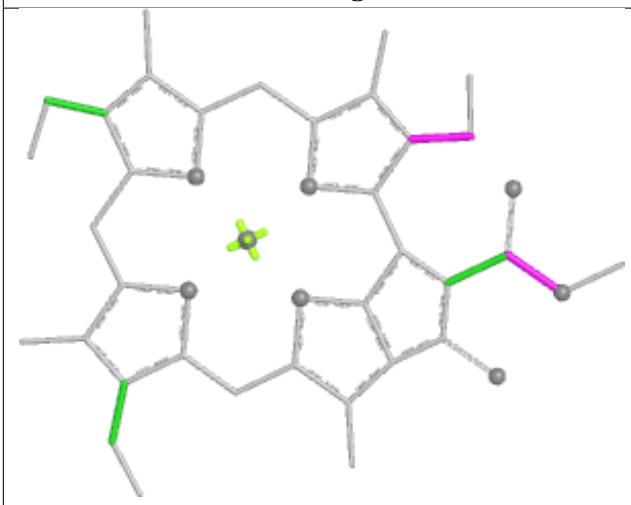
Ligand CLA X 304



Bond lengths



Bond angles

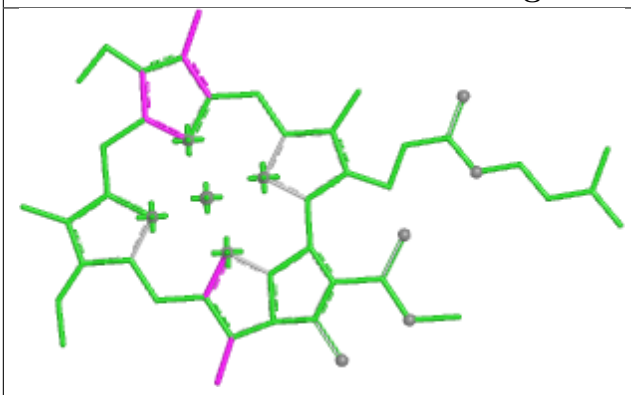


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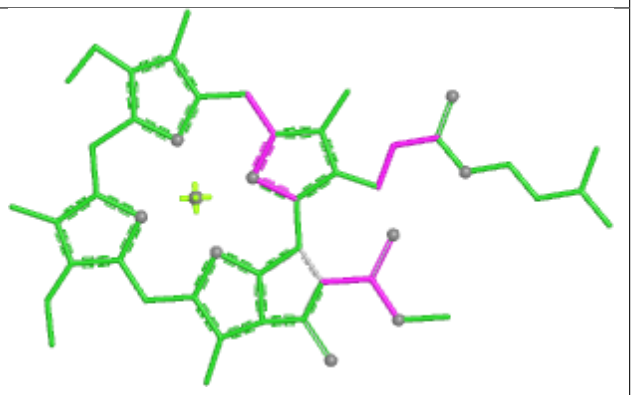


Rings

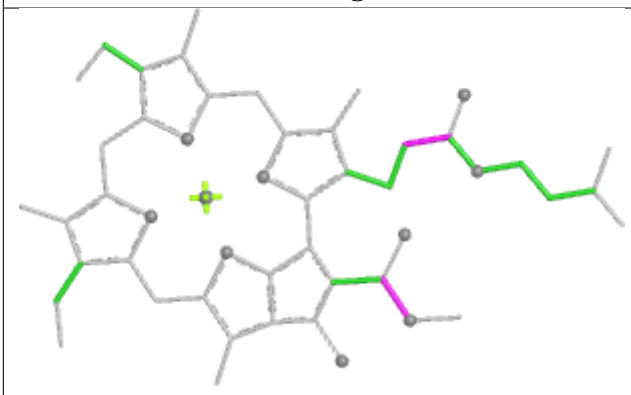
Ligand CLA A 841



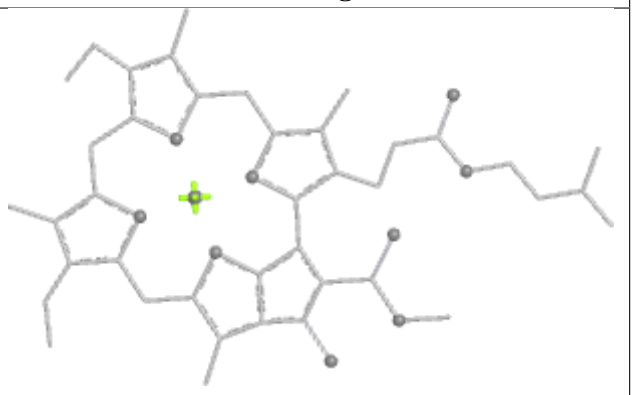
Bond lengths



Bond angles

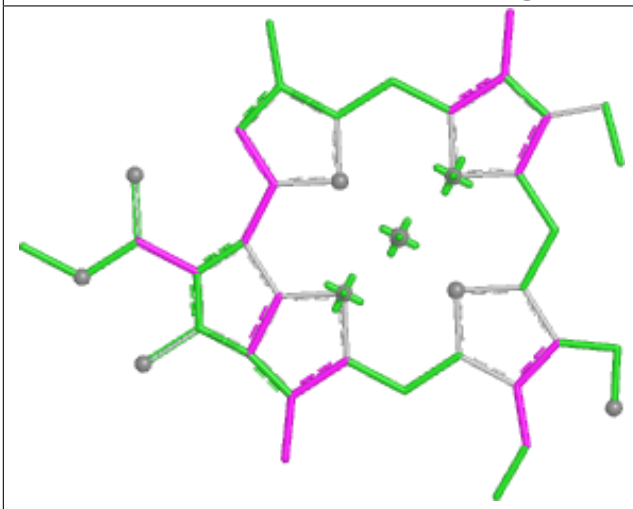


Torsions

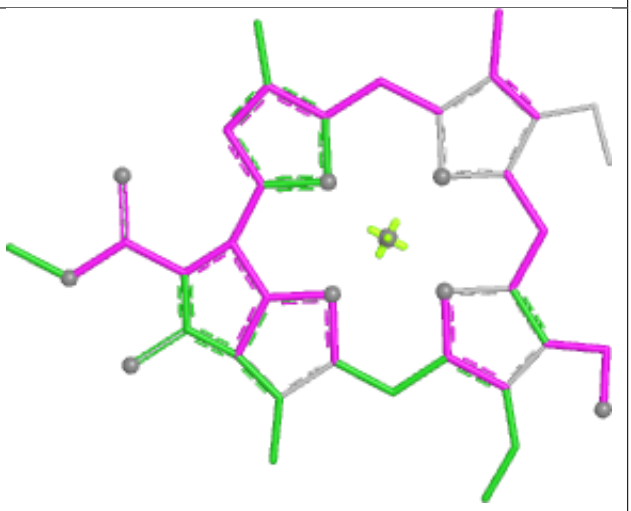


Rings

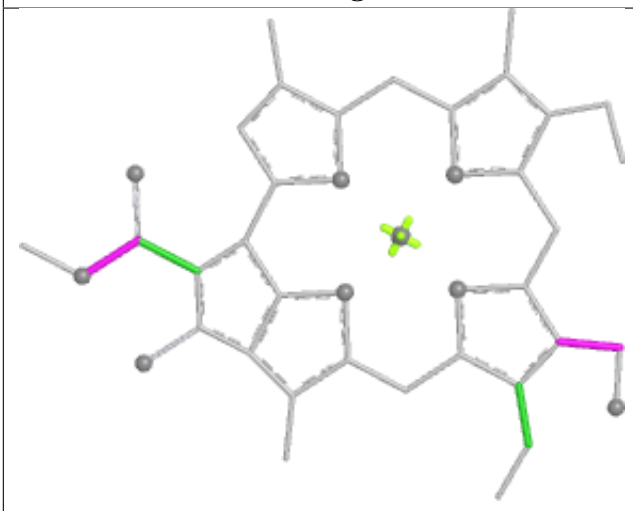
Ligand CHL W 314



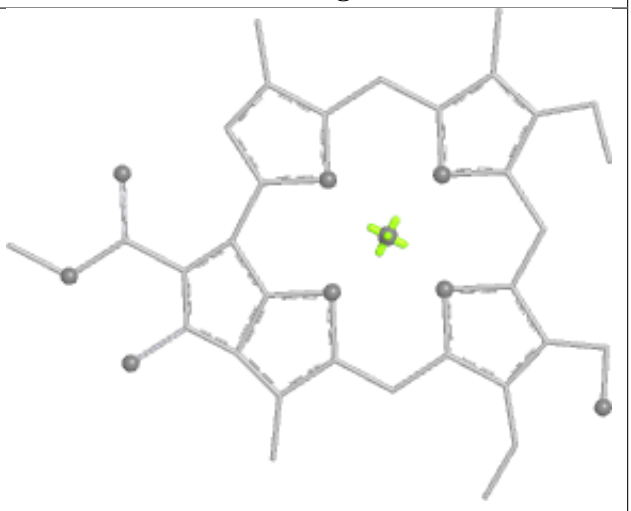
Bond lengths



Bond angles

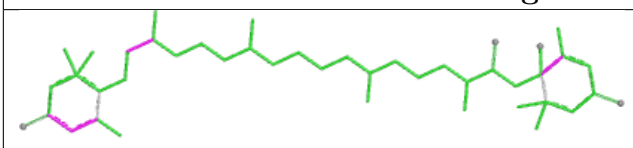


Torsions

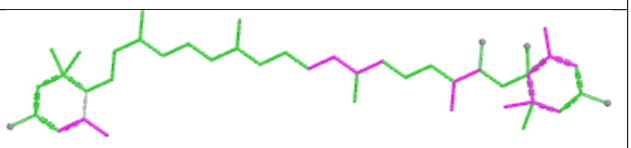


Rings

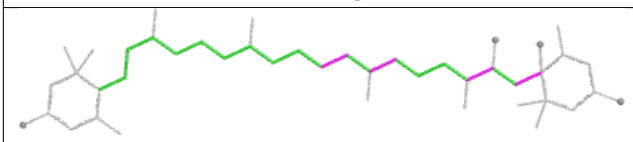
Ligand IWJ W 318



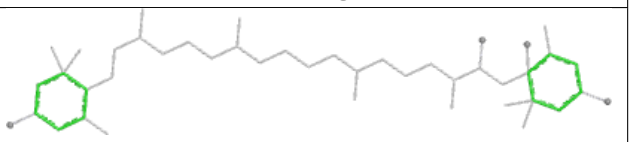
Bond lengths



Bond angles

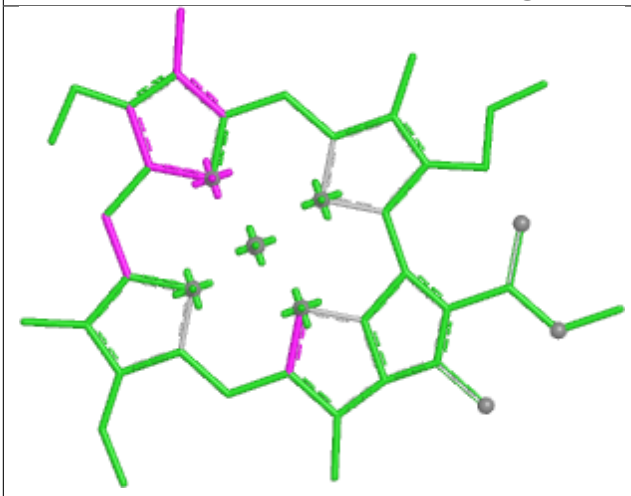


Torsions

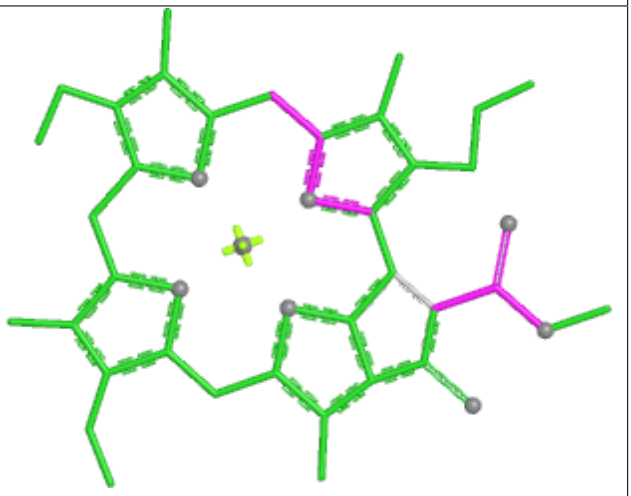


Rings

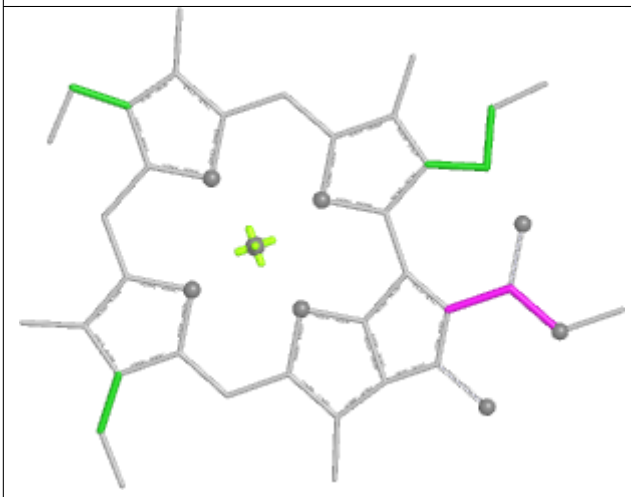
Ligand CLA W 313



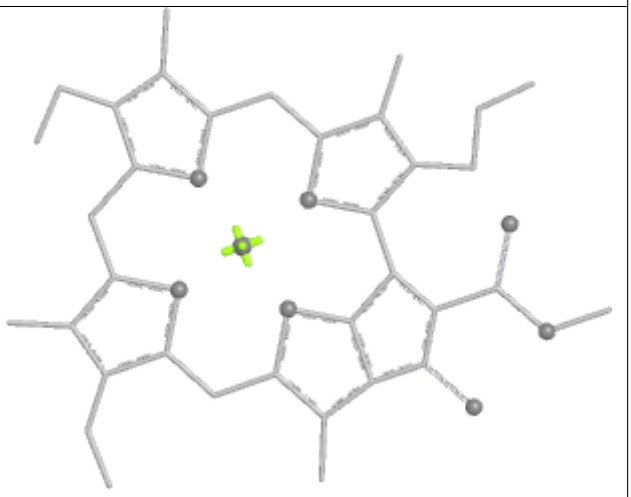
Bond lengths



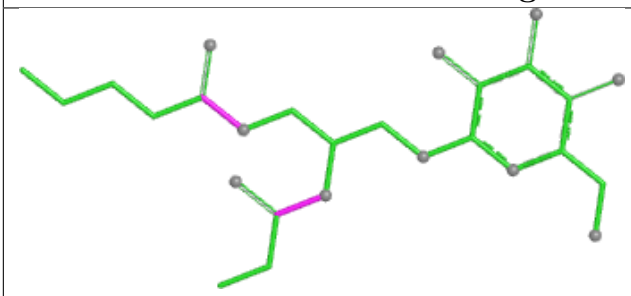
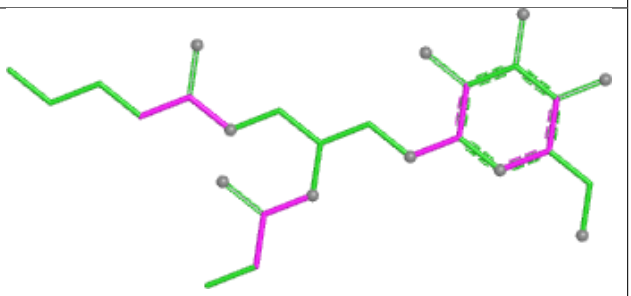
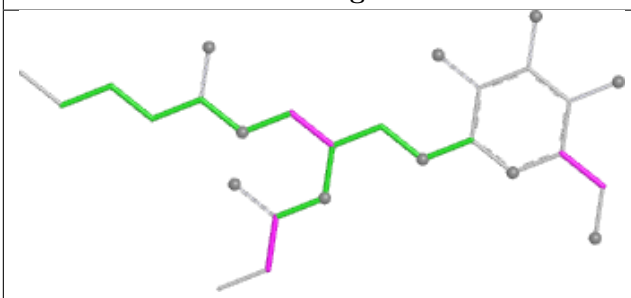
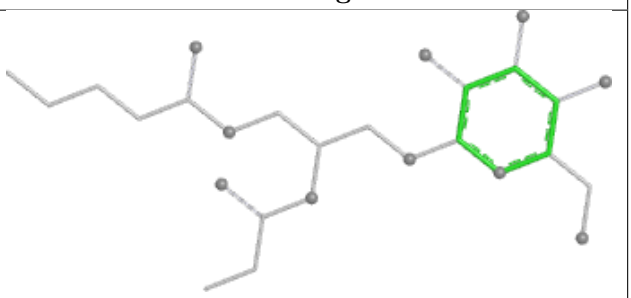
Bond angles

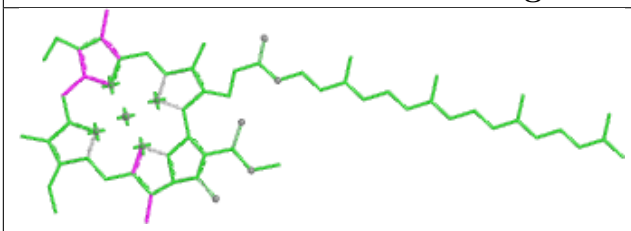
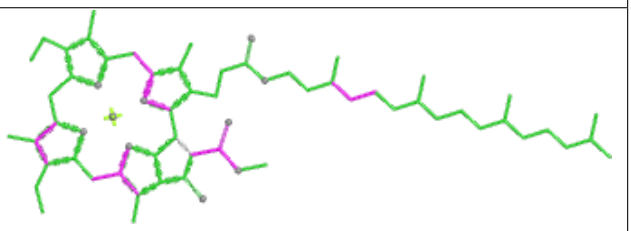
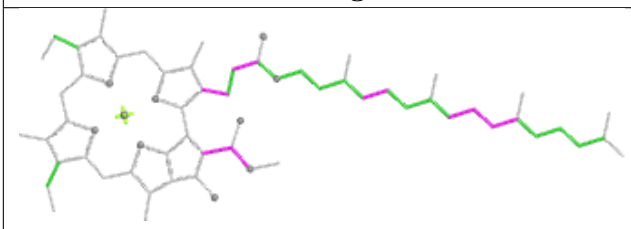
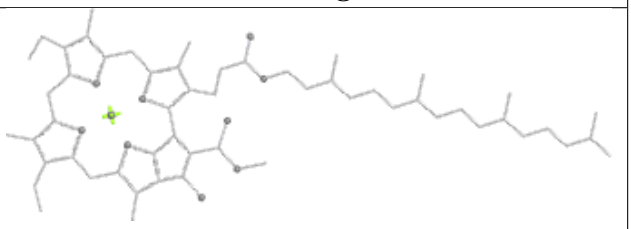


Torsions

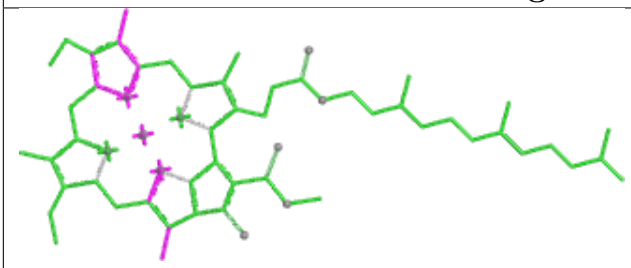


Rings

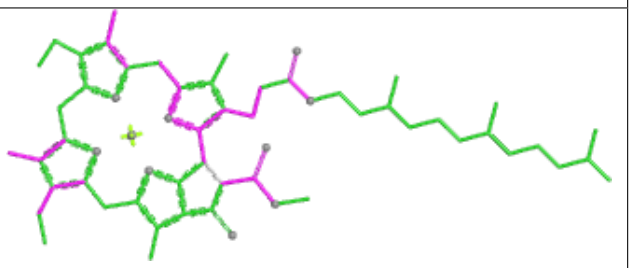
Ligand LMG A 855	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

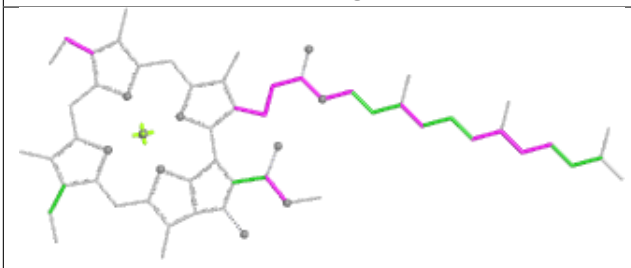
Ligand CLA 4 303



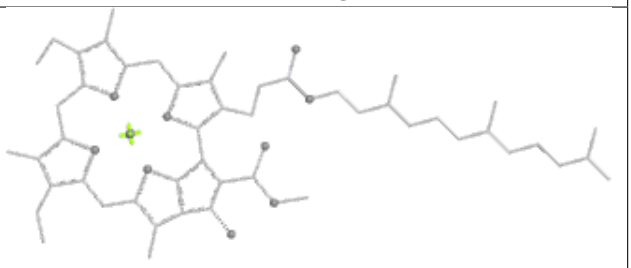
Bond lengths



Bond angles

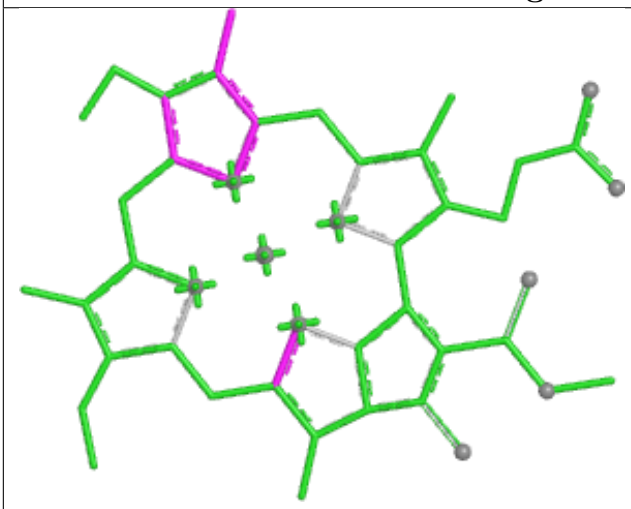


Torsions

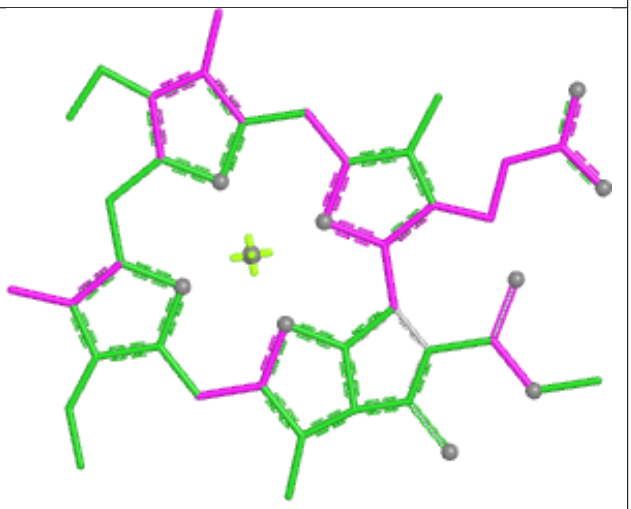


Rings

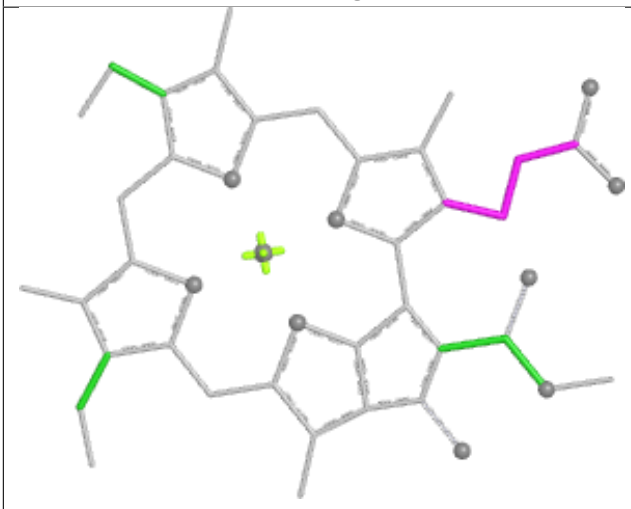
Ligand CLA L 303



Bond lengths



Bond angles

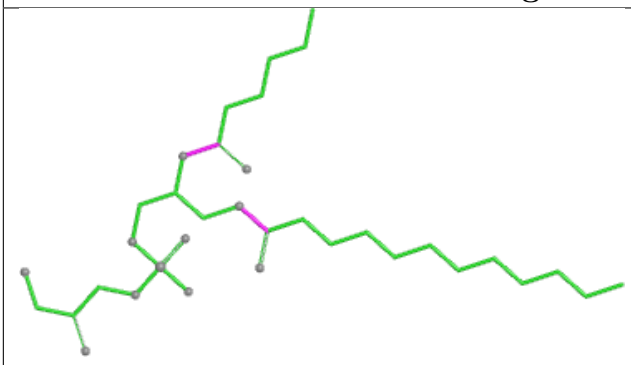


Torsions

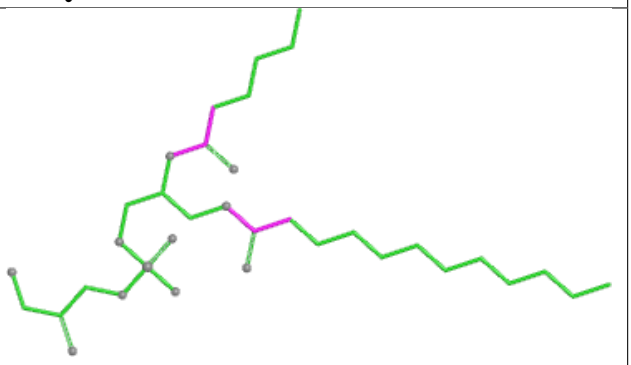


Rings

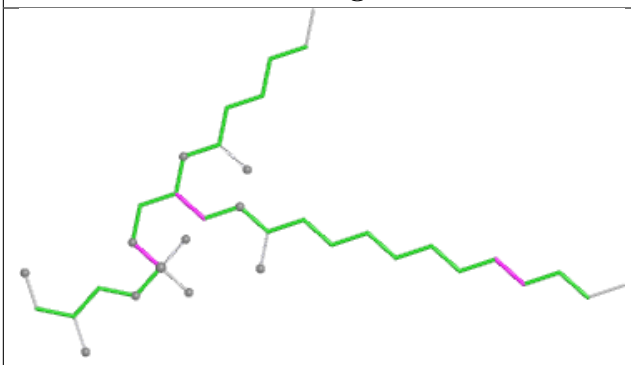
Ligand LHG Q 302



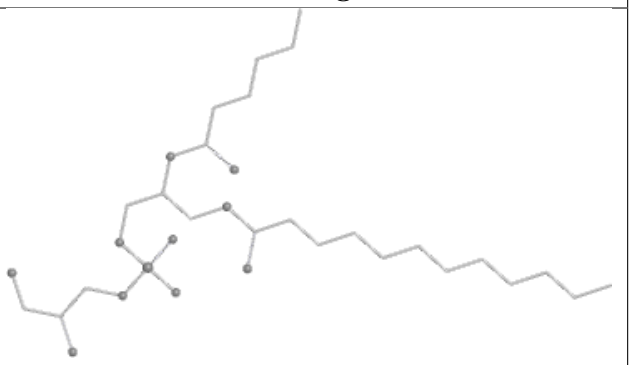
Bond lengths



Bond angles

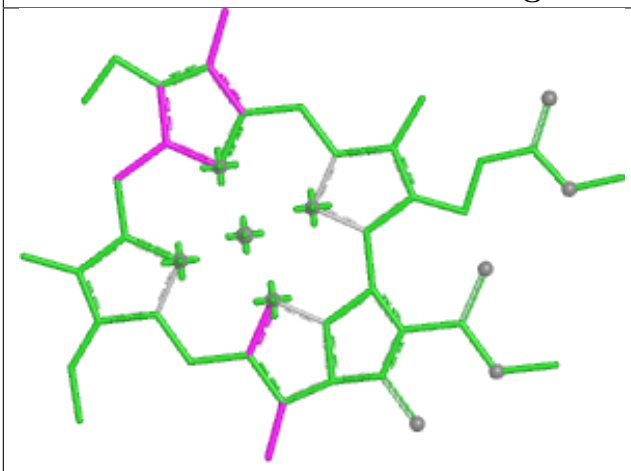


Torsions

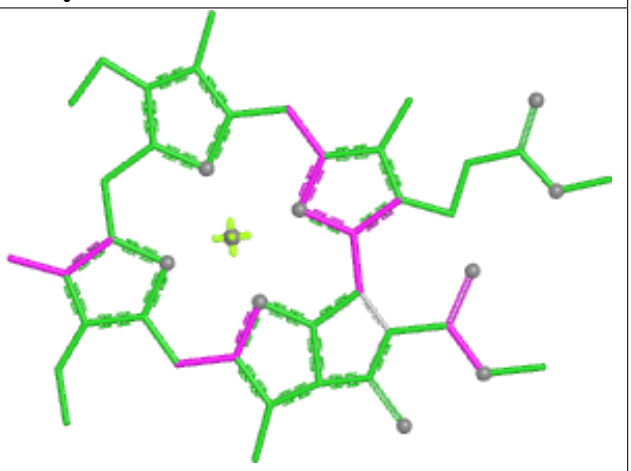


Rings

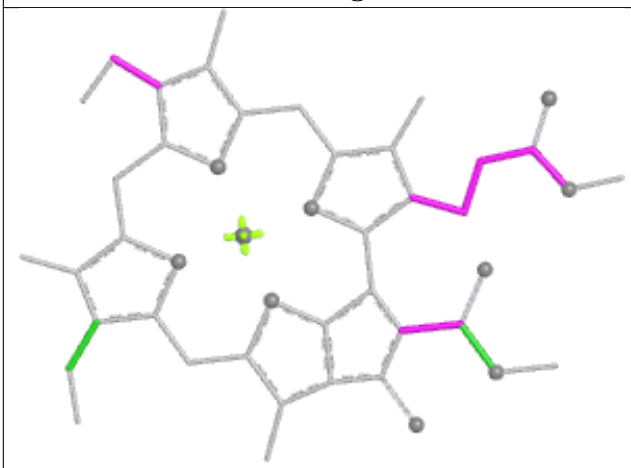
Ligand CLA Q 313



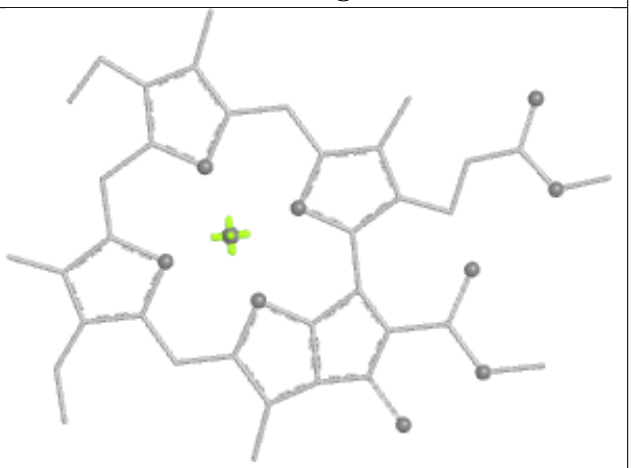
Bond lengths



Bond angles

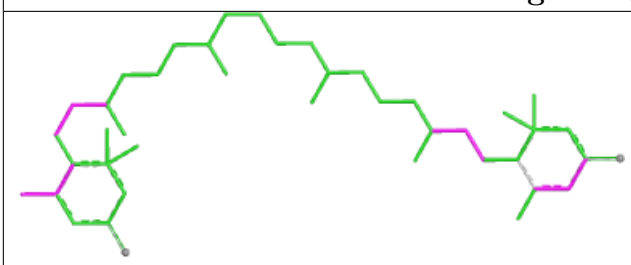


Torsions



Rings

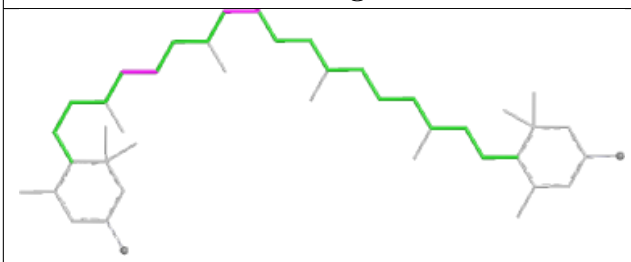
Ligand Q6L U 315



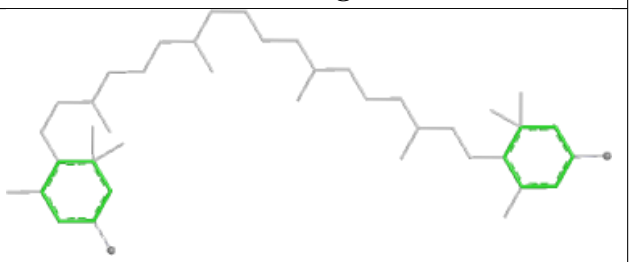
Bond lengths



Bond angles

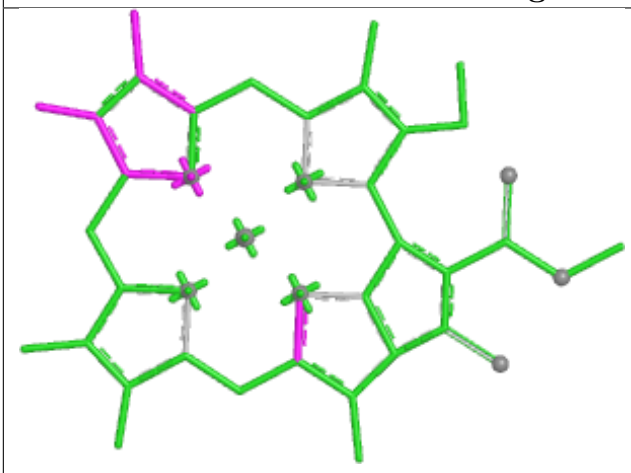


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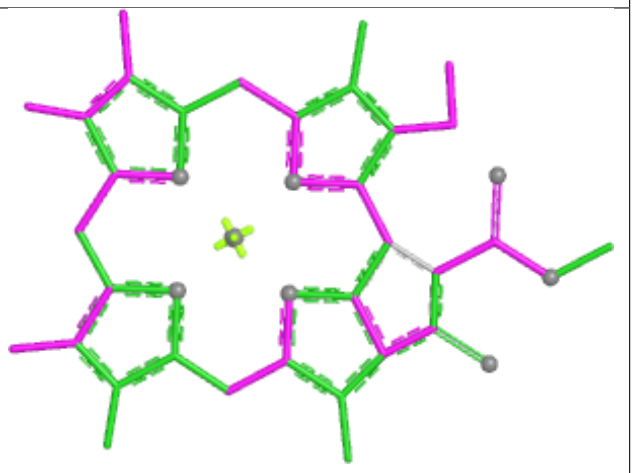


Rings

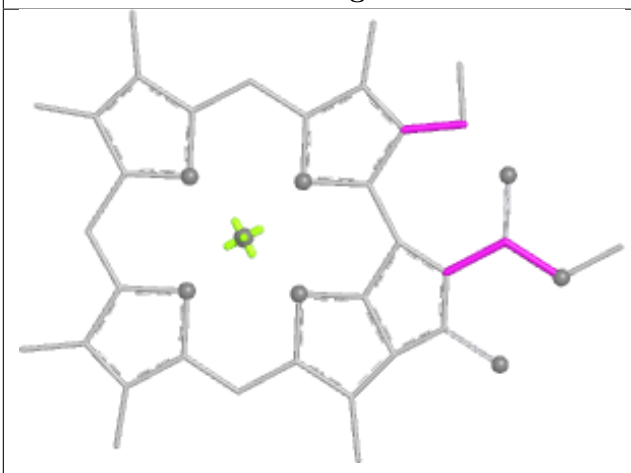
Ligand CLA 1 610



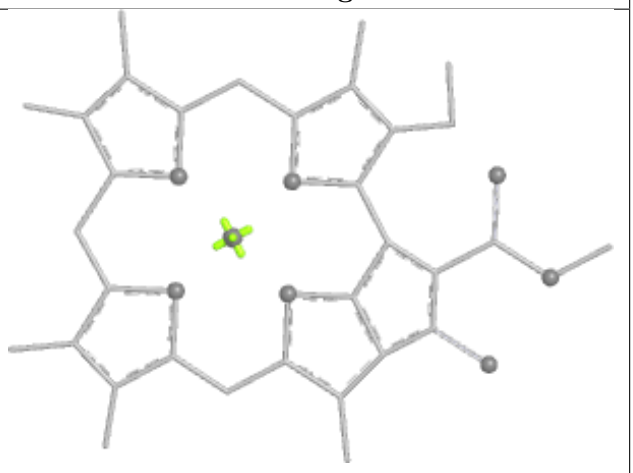
Bond lengths



Bond angles

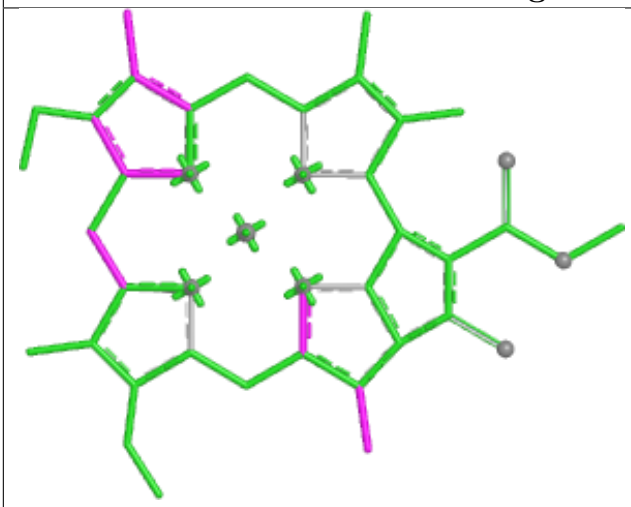


Torsions

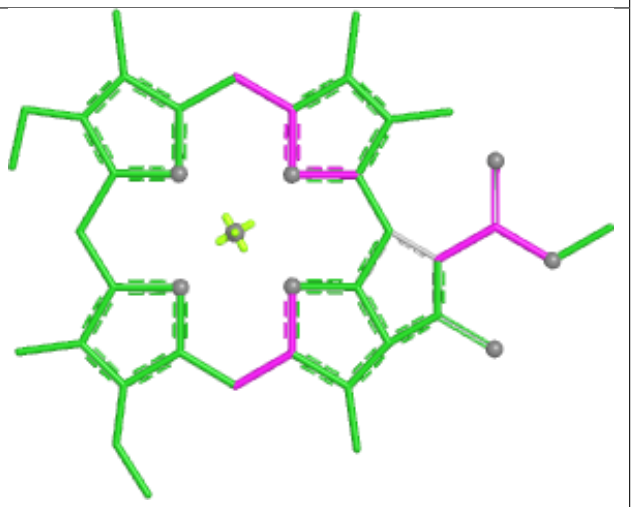


Rings

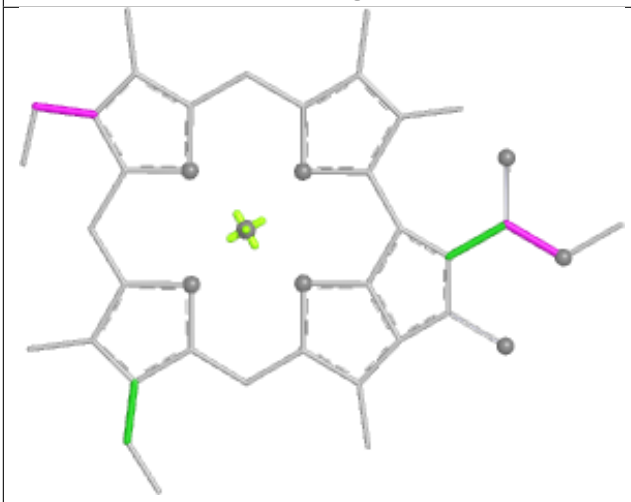
Ligand CLA 5 610



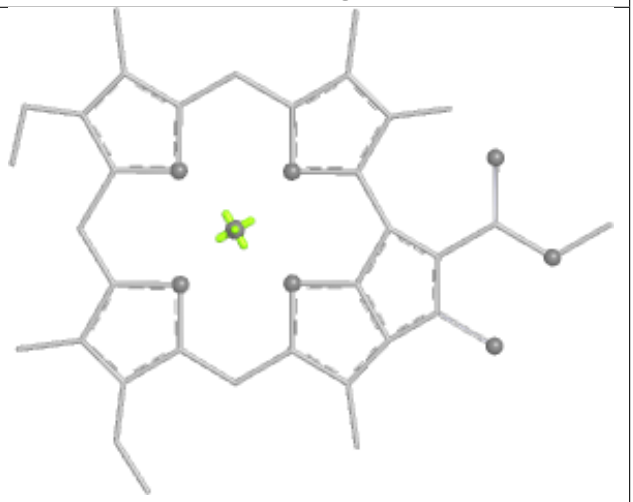
Bond lengths



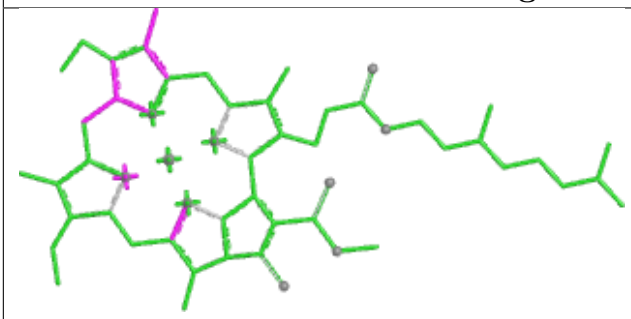
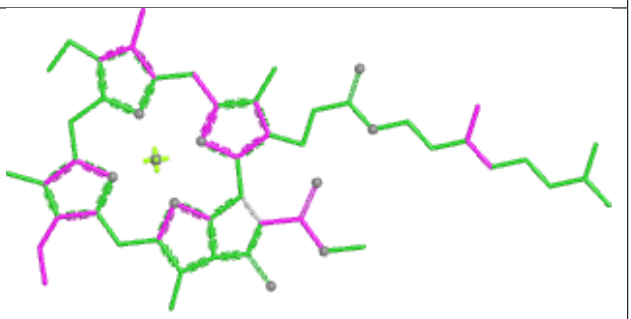
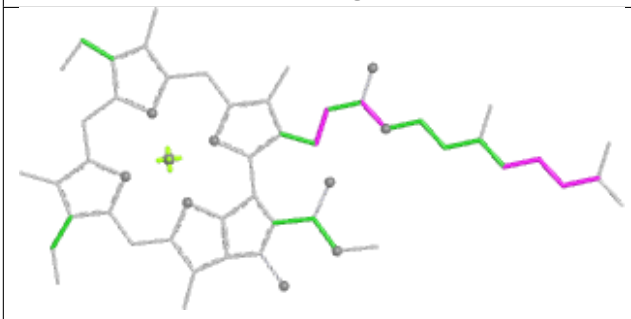
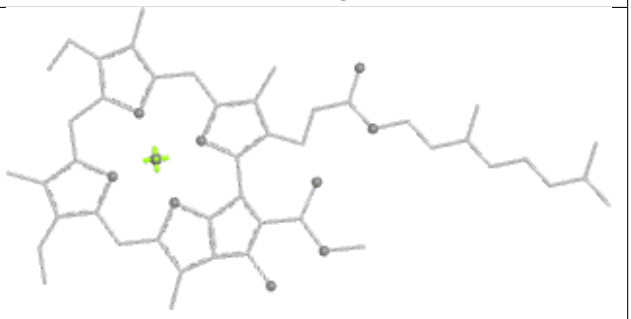
Bond angles

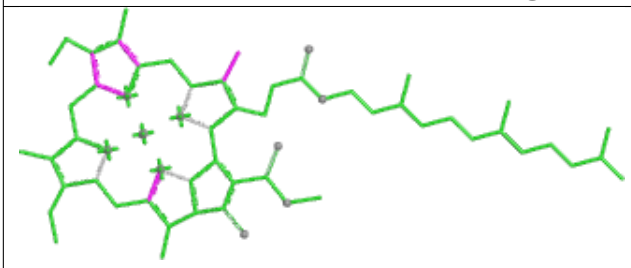
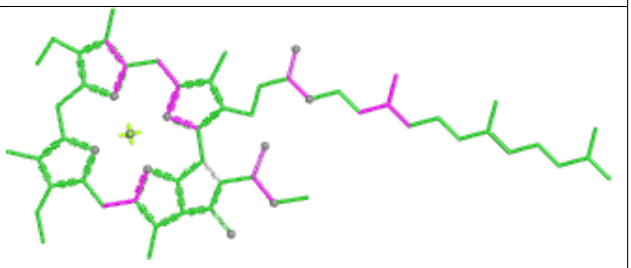
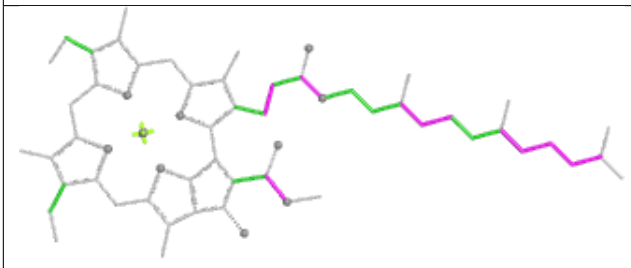
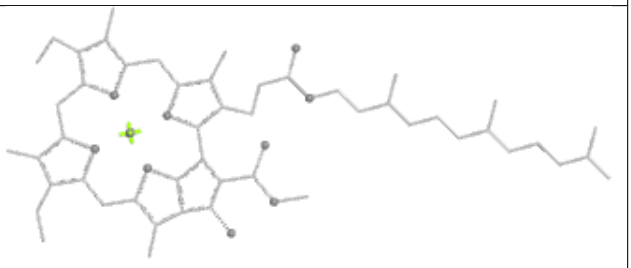


Torsions

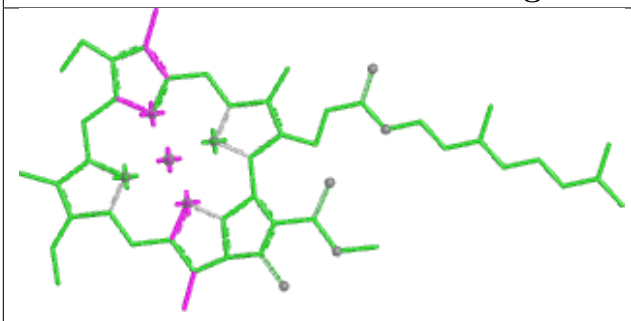


Rings

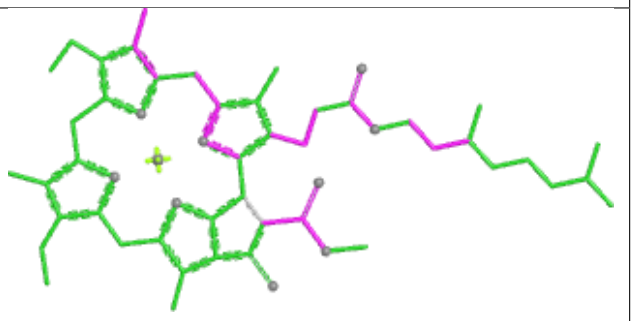
Ligand CLA W 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

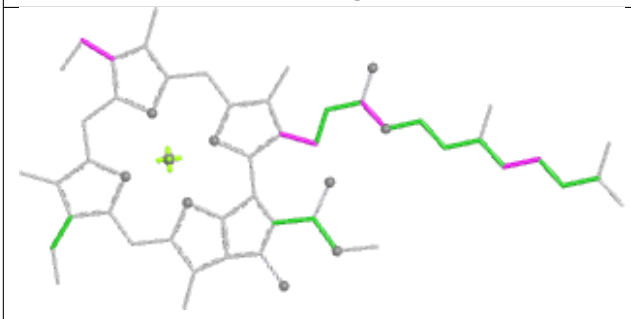
Ligand CLA V 312



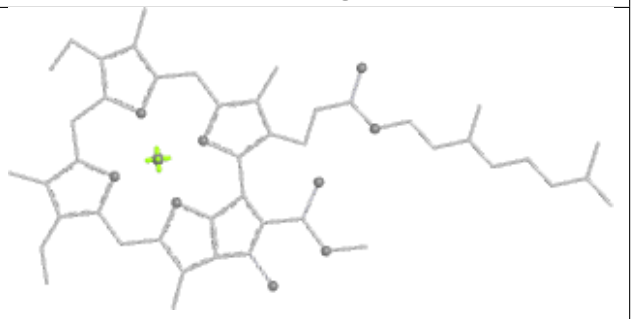
Bond lengths



Bond angles

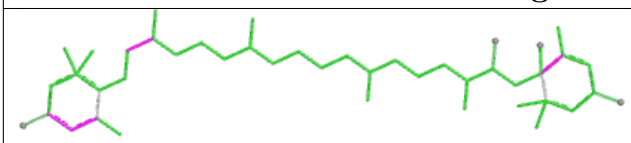


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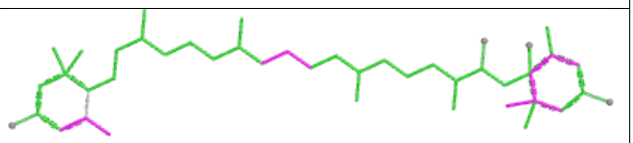


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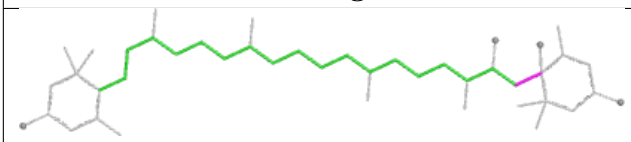
Ligand IWJ 6 614



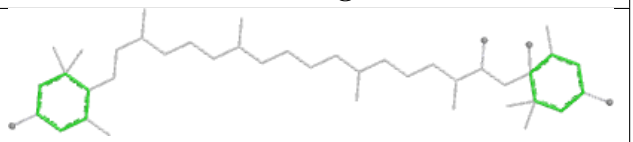
Bond lengths



Bond angles



Torsions

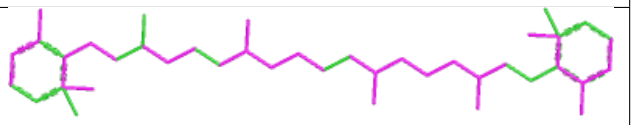


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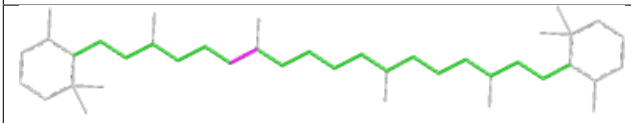
Ligand BCR 3 318



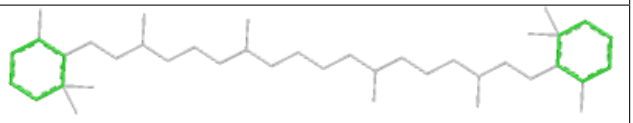
Bond lengths



Bond angles

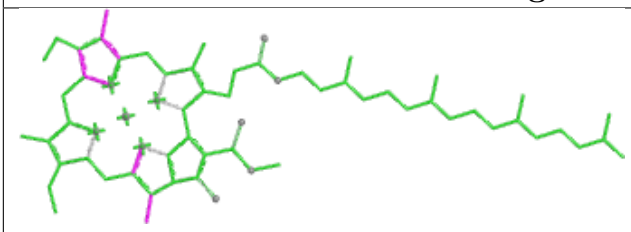


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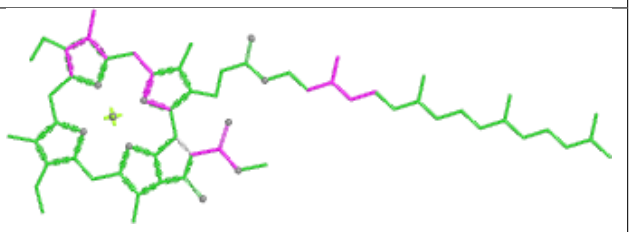


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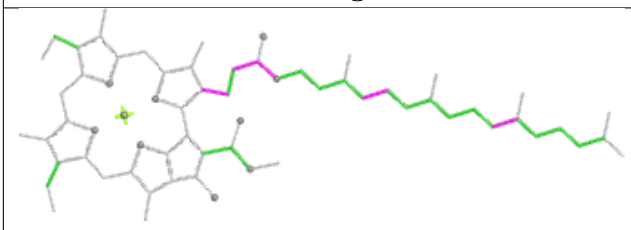
Ligand CLA 6 613



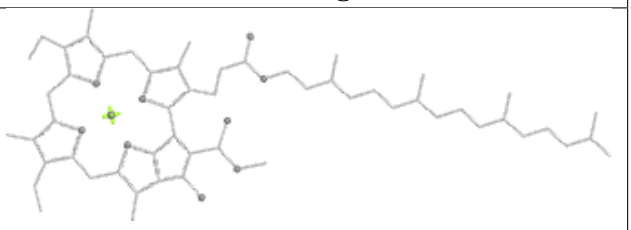
Bond lengths



Bond angles

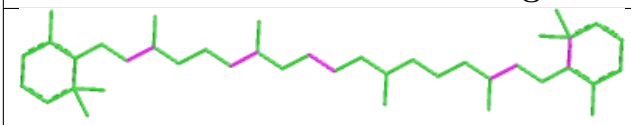


Torsions



Rings

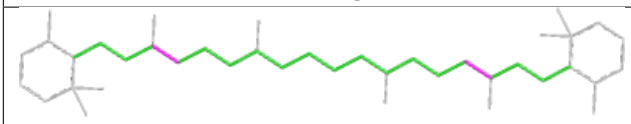
Ligand BCR B 846



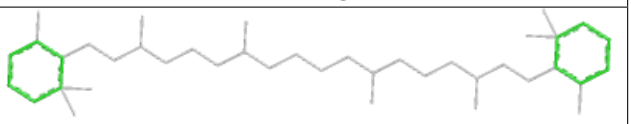
Bond lengths



Bond angles

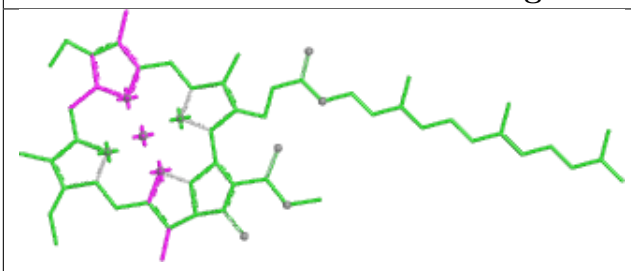


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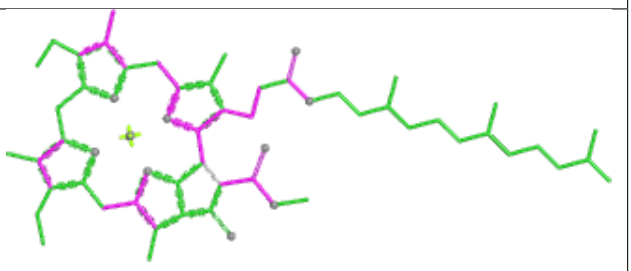


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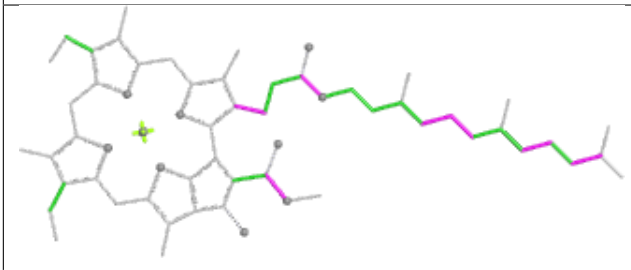
Ligand CLA B 820



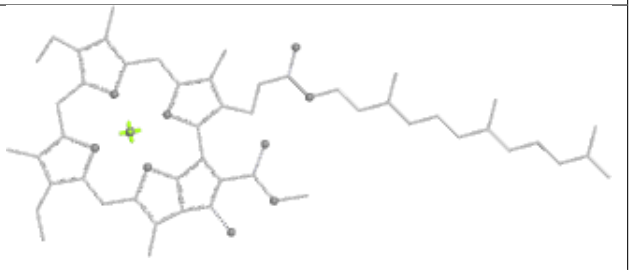
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Bond angles

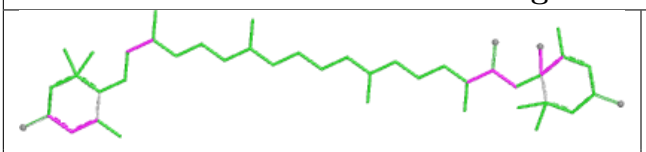


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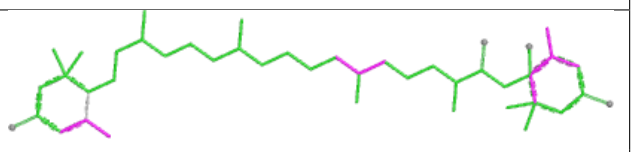


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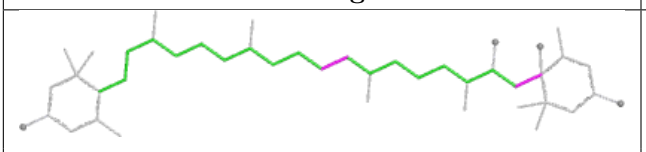
Ligand IWJ 3 315



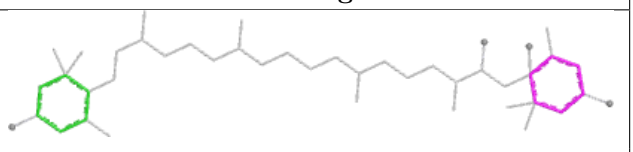
Bond lengths



Bond angles

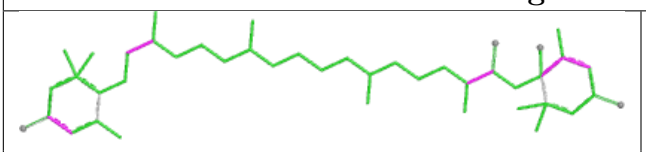


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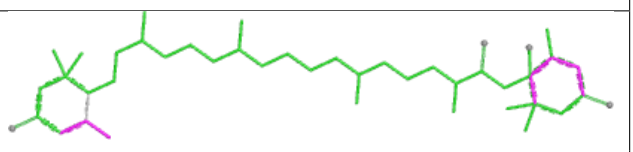


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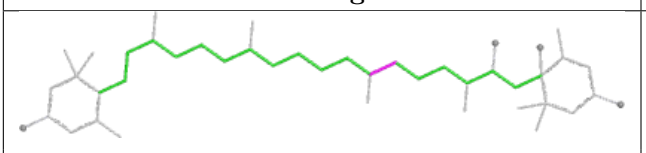
Ligand IWJ P 318



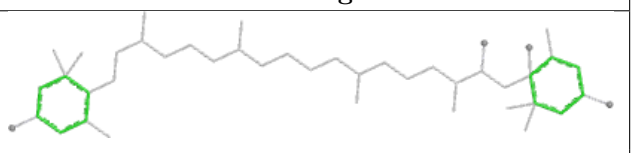
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Bond angles

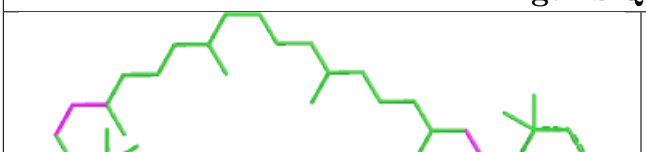


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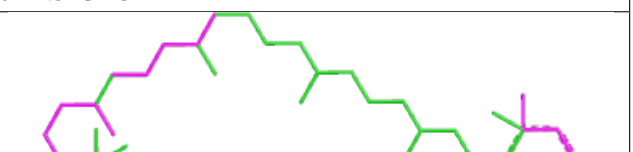


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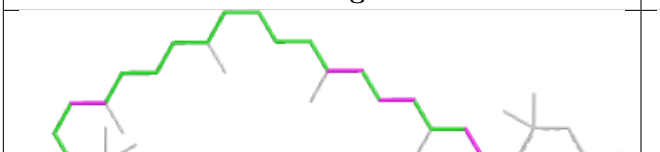
Ligand Q6L S 320



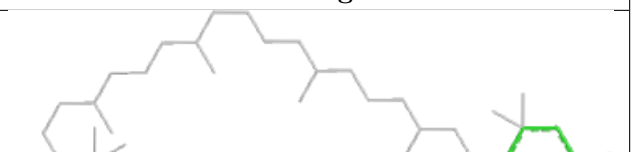
Bond lengths



Bond angles

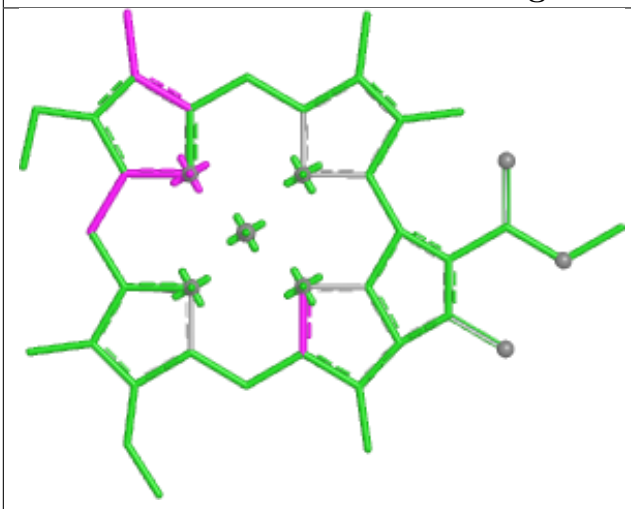


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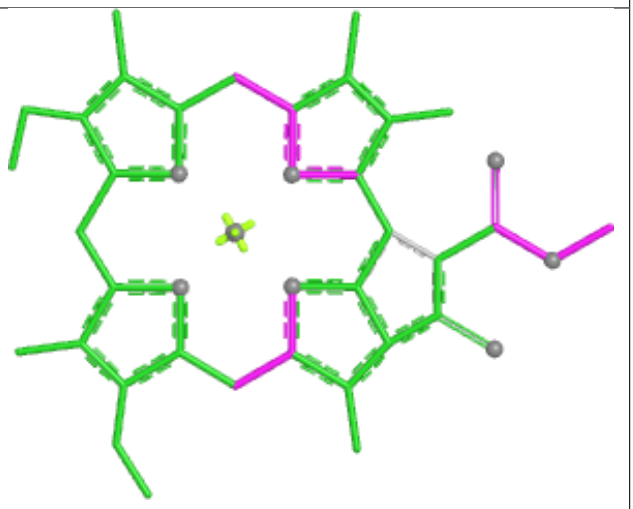


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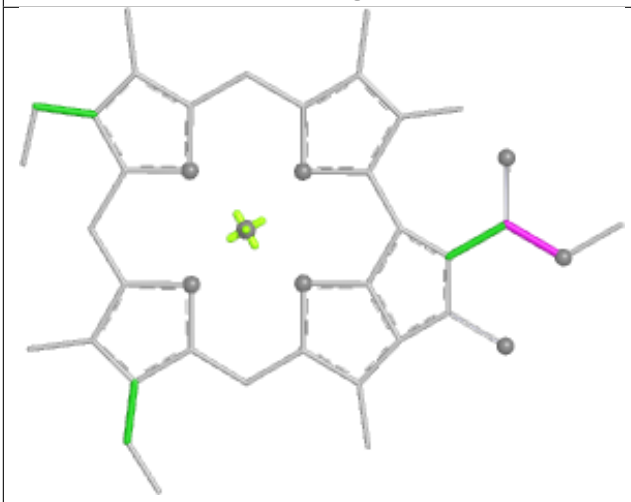
Ligand CLA 3 313



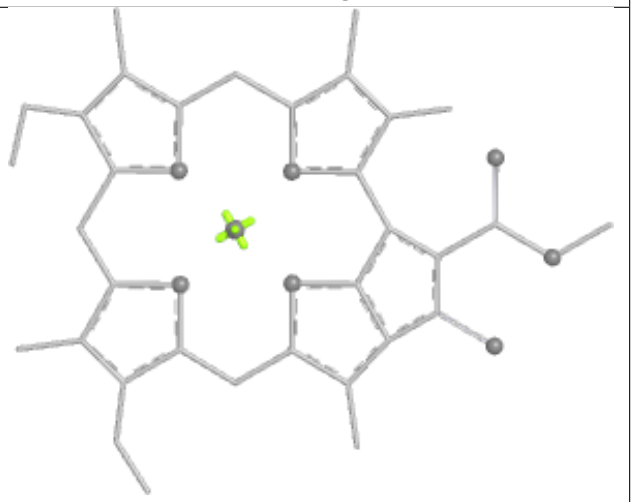
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Bond angles

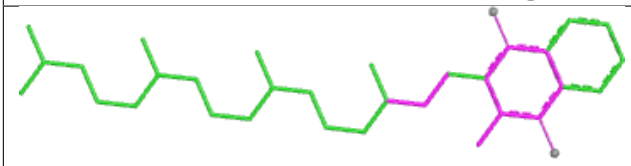


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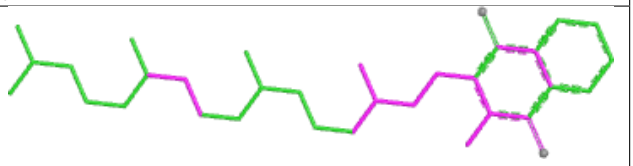


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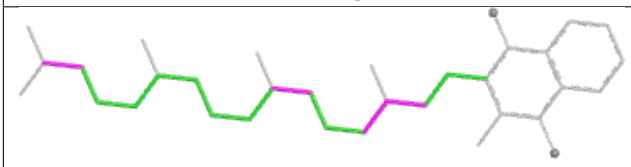
Ligand PQN B 844



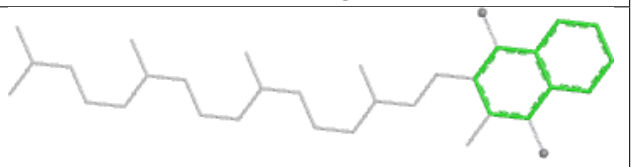
Bond lengths



Bond angles

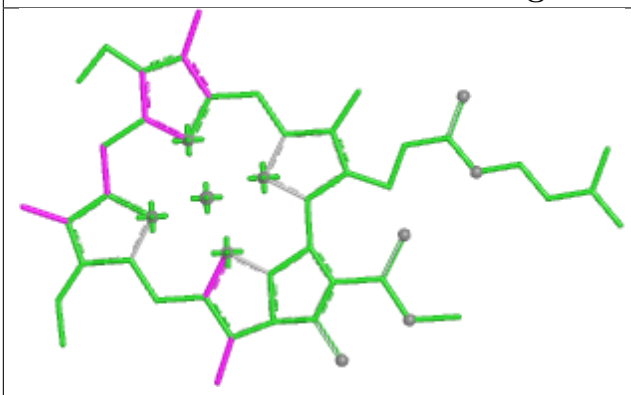


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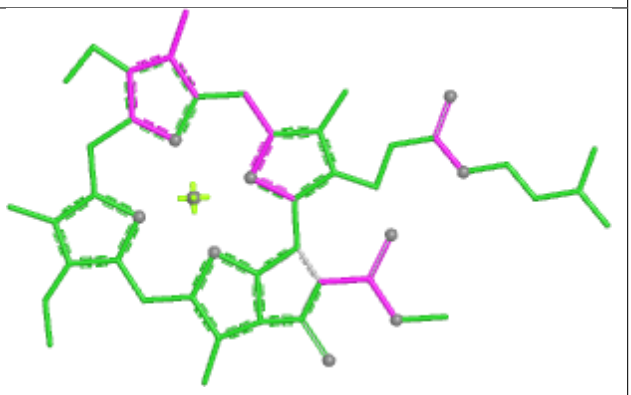


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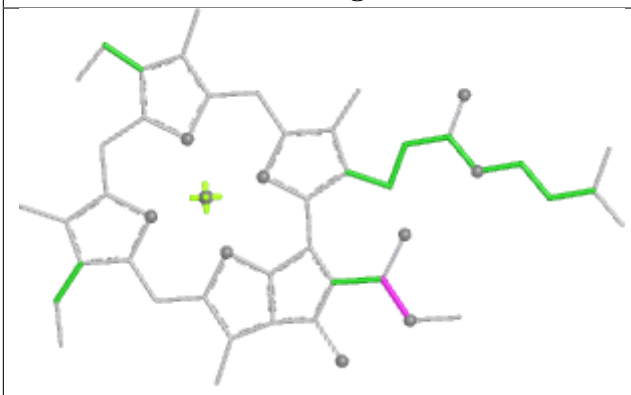
Ligand CLA S 303



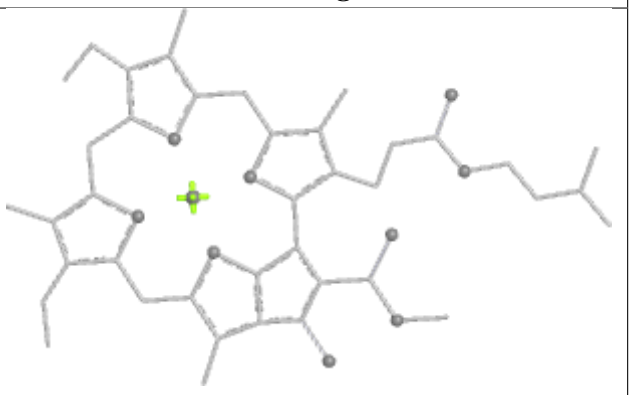
Bond lengths



Bond angles

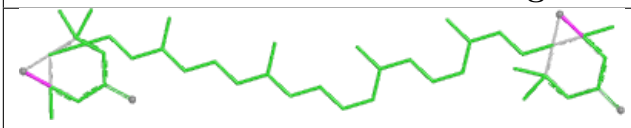


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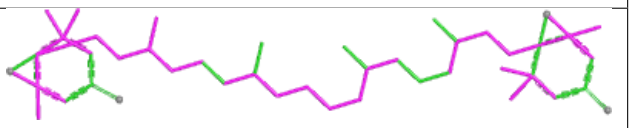


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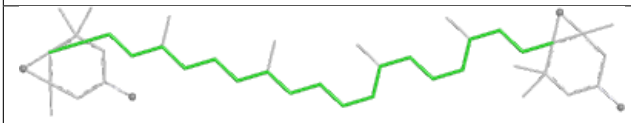
Ligand XAT 5 612



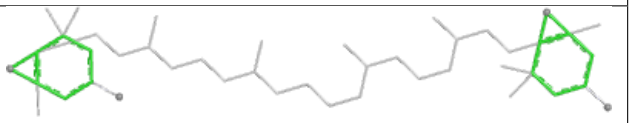
Bond lengths



Bond angles

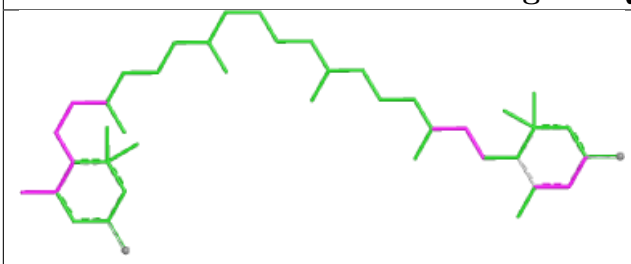


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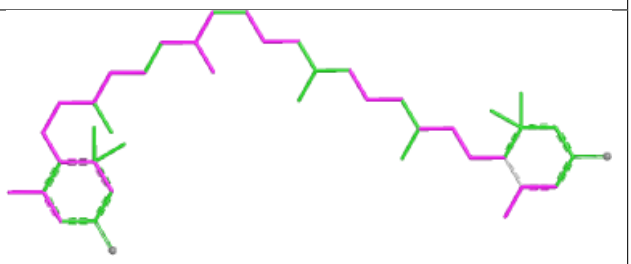


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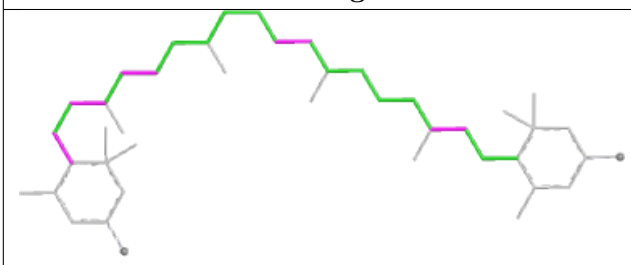
Ligand Q6L W 316



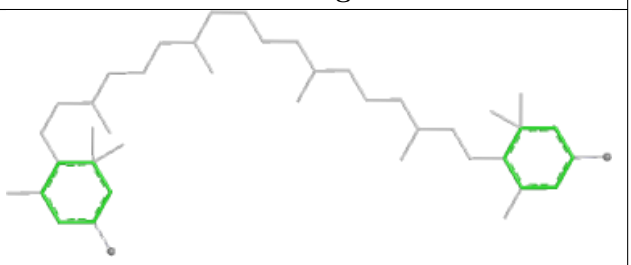
Bond lengths



Bond angles

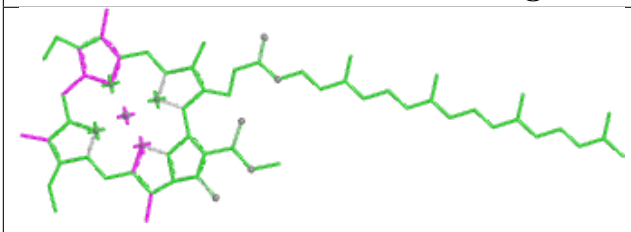


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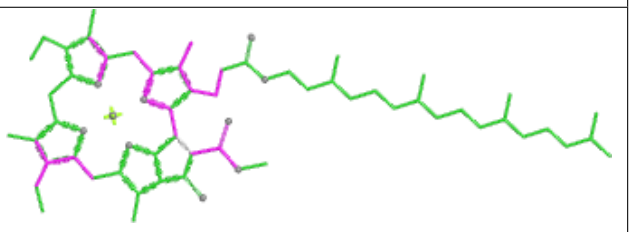


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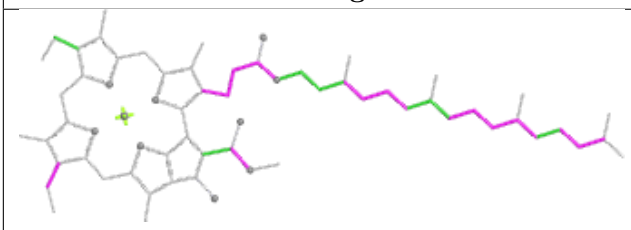
Ligand CLA B 808



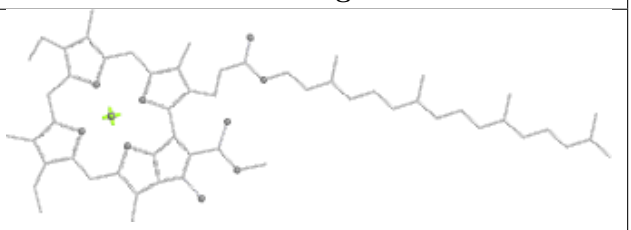
Bond lengths



Bond angles

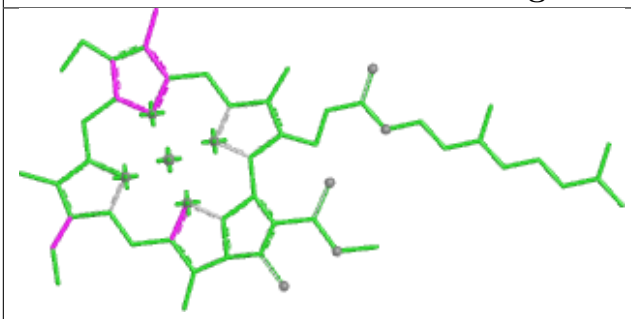


Torsions

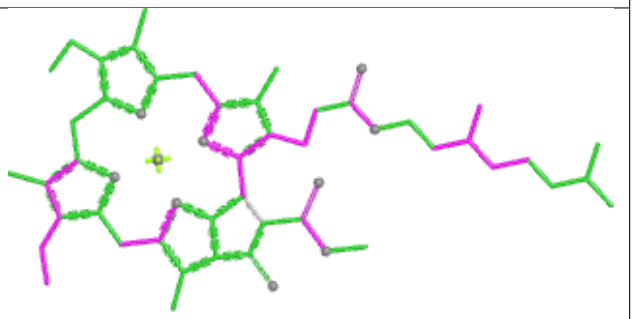


Rings

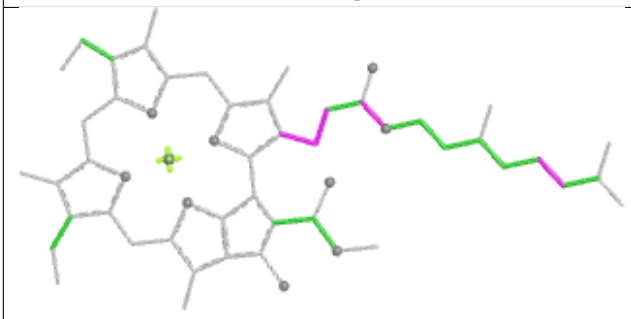
Ligand CLA 1 603



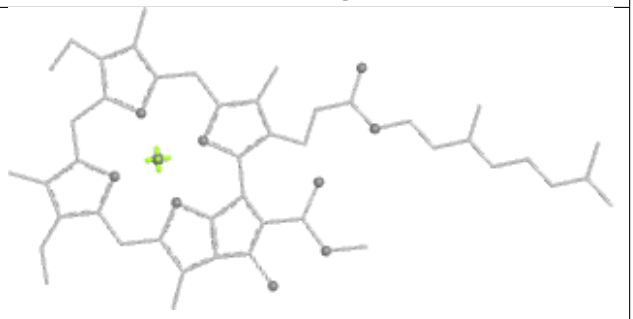
Bond lengths



Bond angles

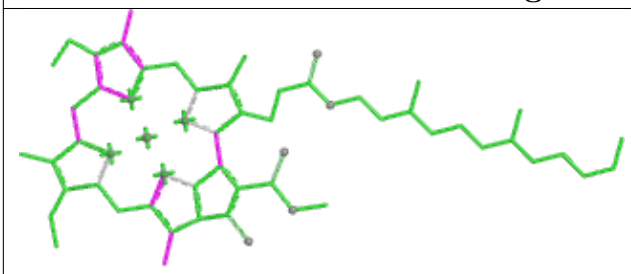


Torsions

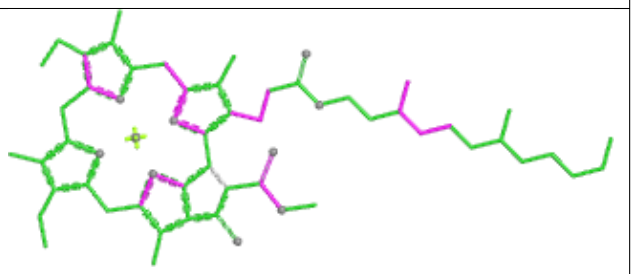


Rings

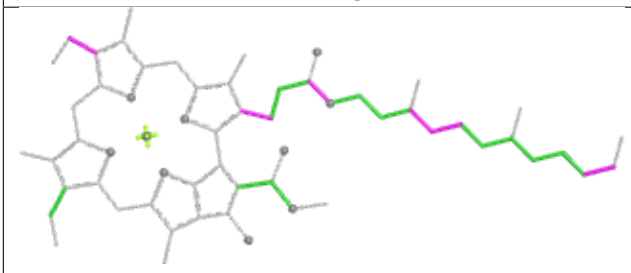
Ligand CLA T 309



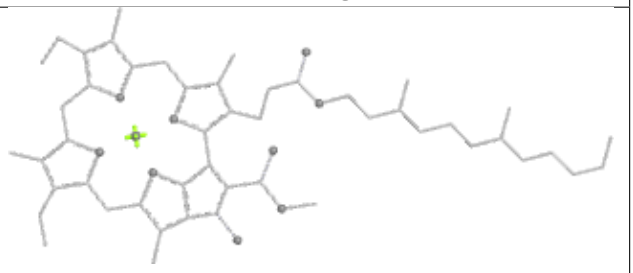
Bond lengths



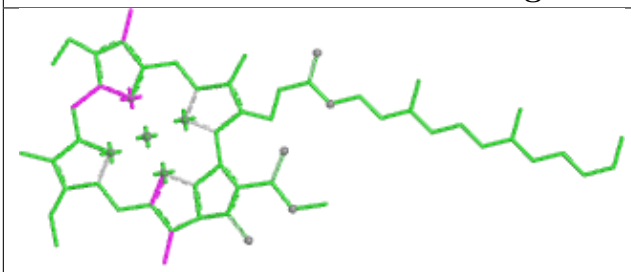
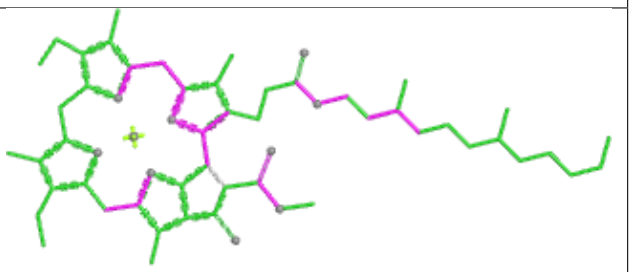
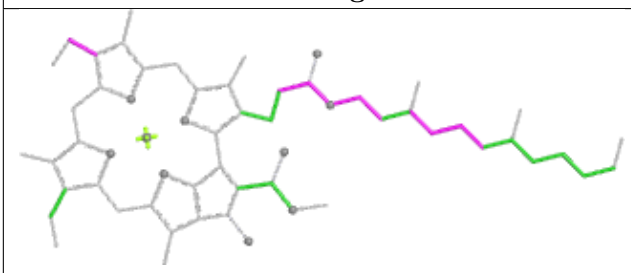
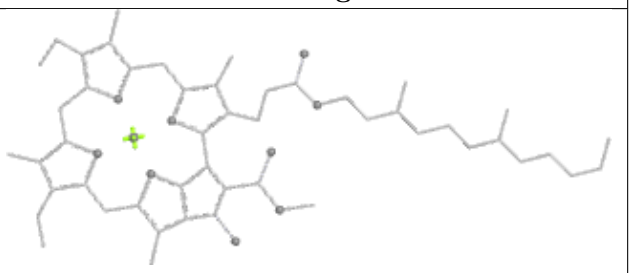
Bond angles

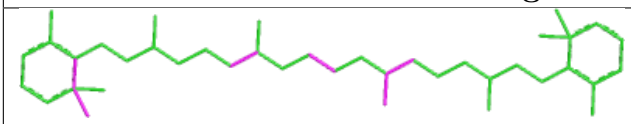
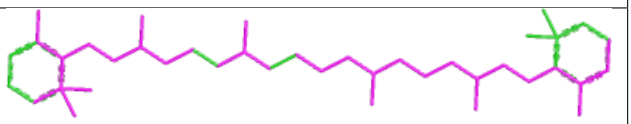
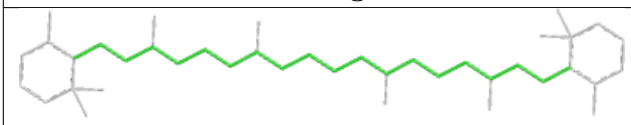
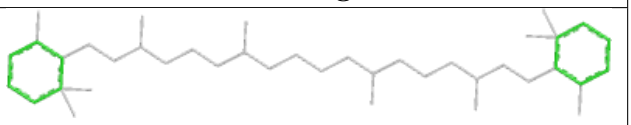


Torsions

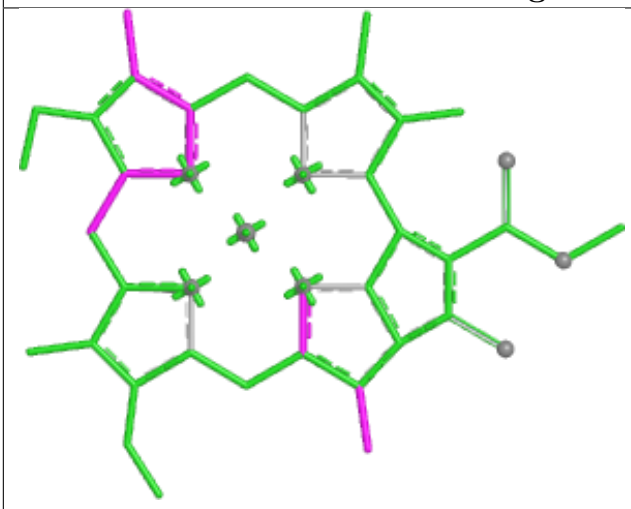


Rings

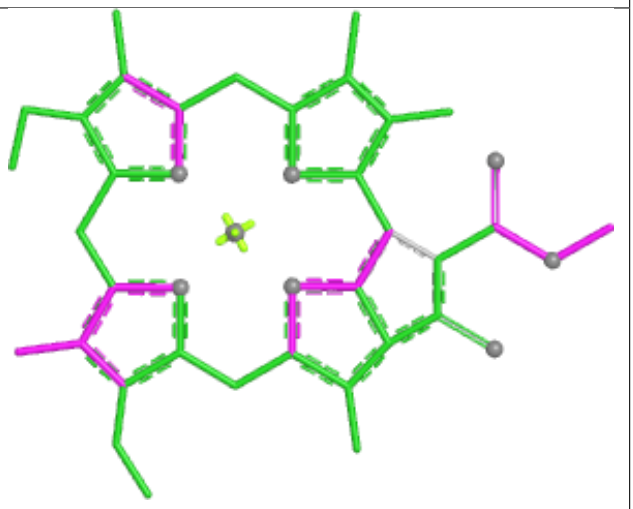
Ligand CLA B 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

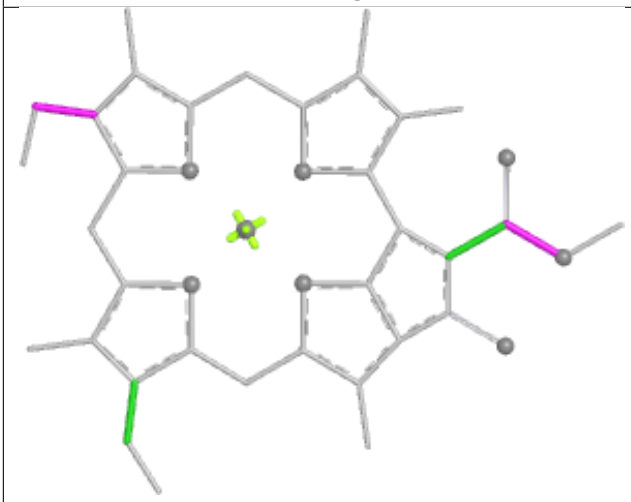
Ligand CLA 3 308



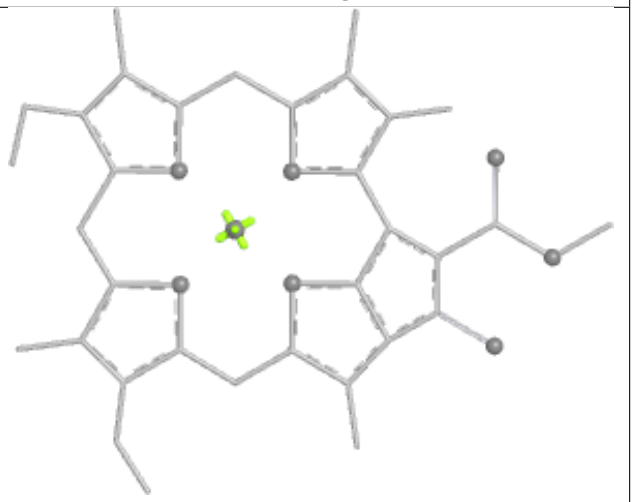
Bond lengths



Bond angles

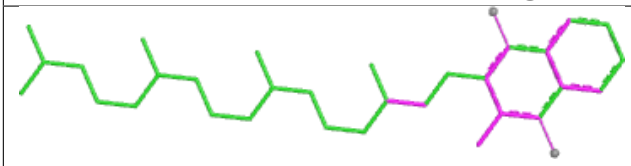


Torsions

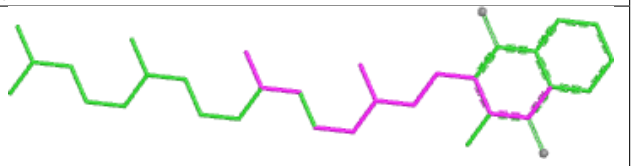


Rings

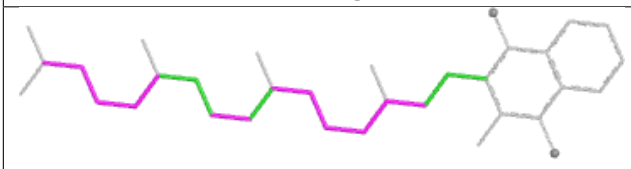
Ligand PQN A 844



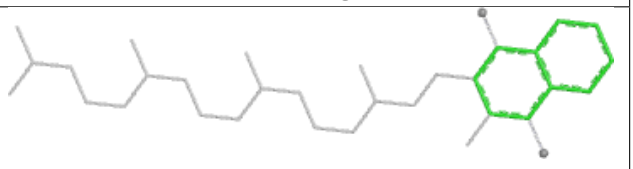
Bond lengths



Bond angles

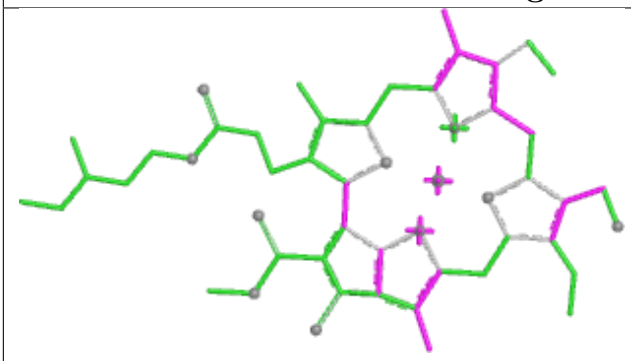


Torsions

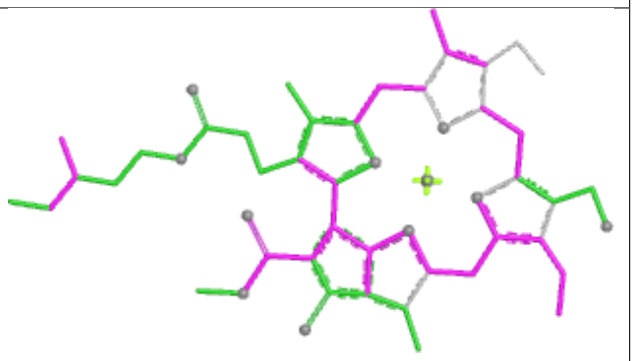


Rings

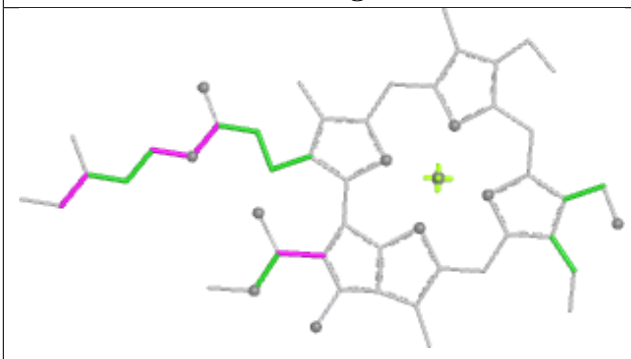
Ligand CHL S 306



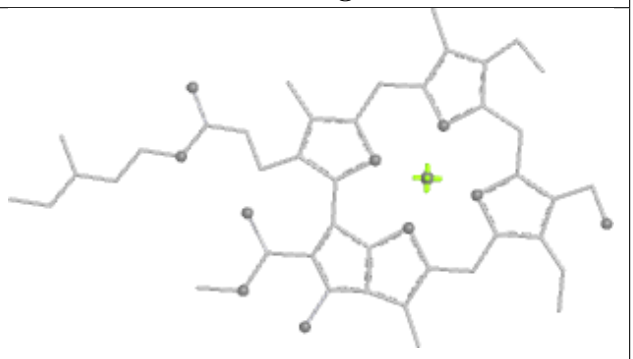
Bond lengths



Bond angles

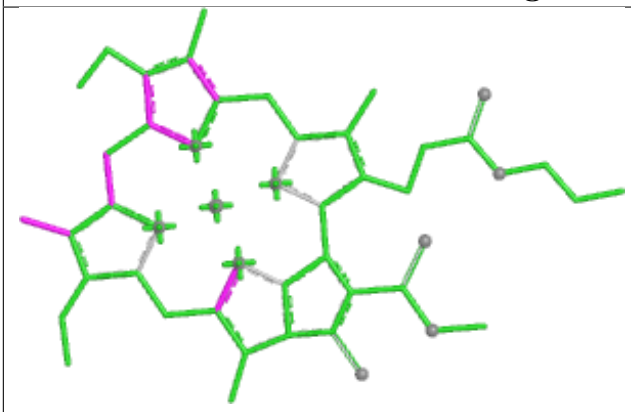


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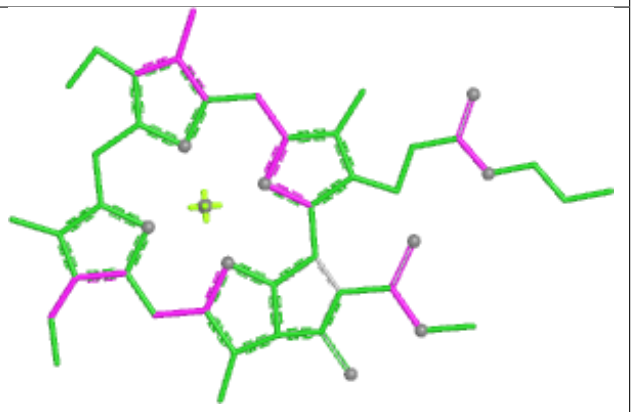


Rings

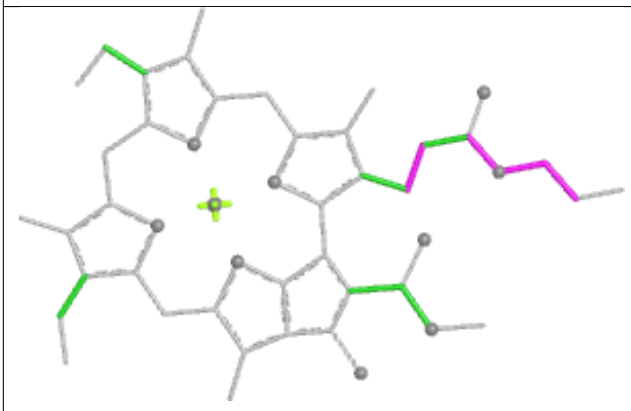
Ligand CLA R 317



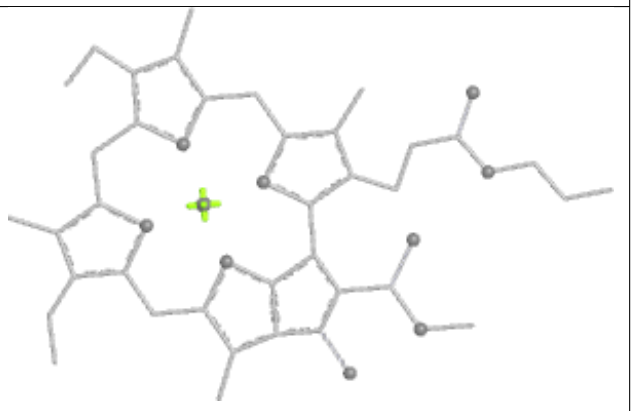
Bond lengths



Bond angles

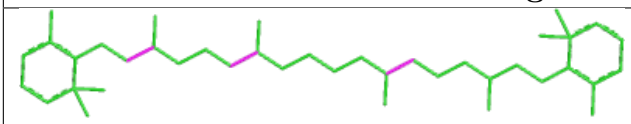


Torsions

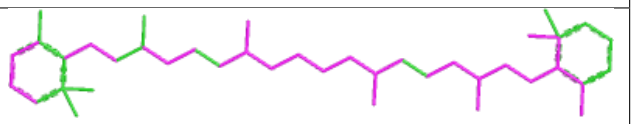


Rings

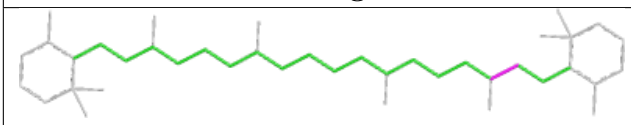
Ligand BCR 3 317



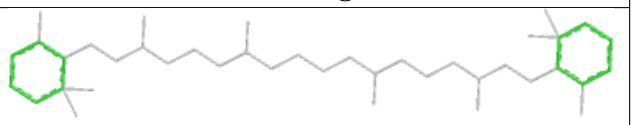
Bond lengths



Bond angles

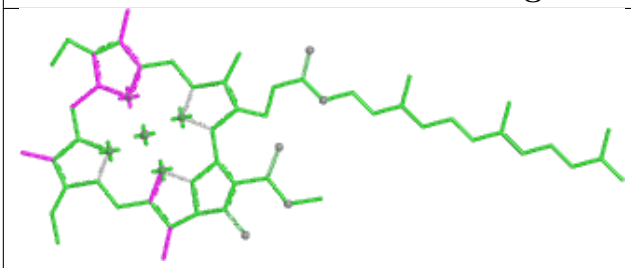


Torsions

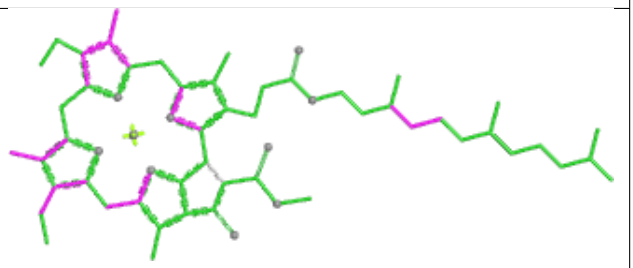


Rings

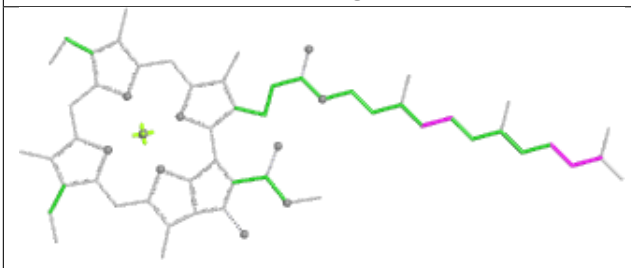
Ligand CLA B 824



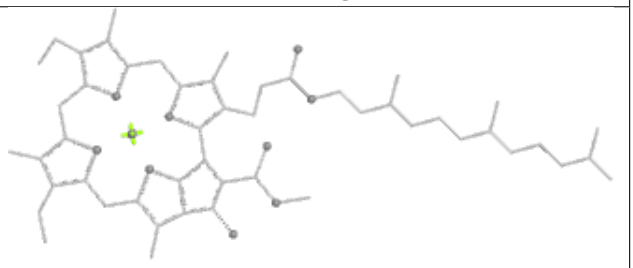
Bond lengths



Bond angles

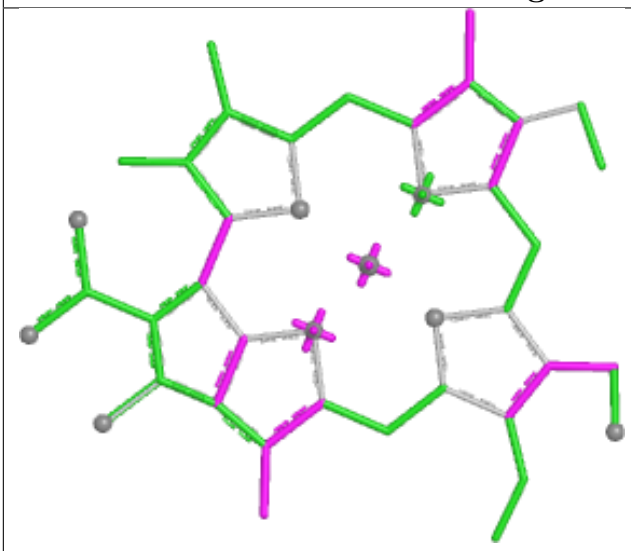


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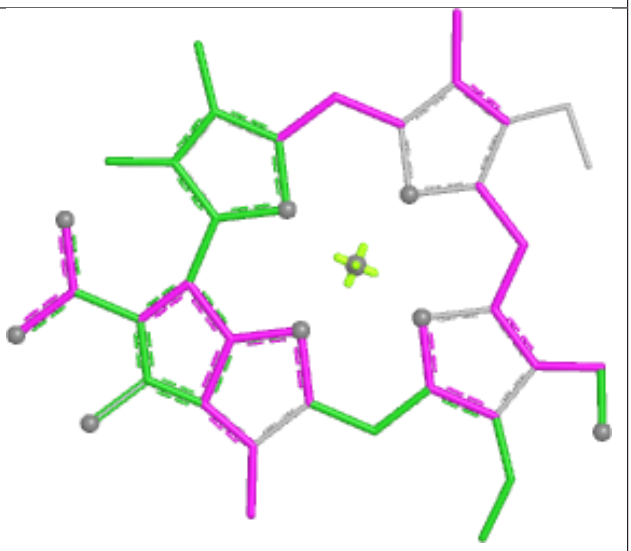


Rings

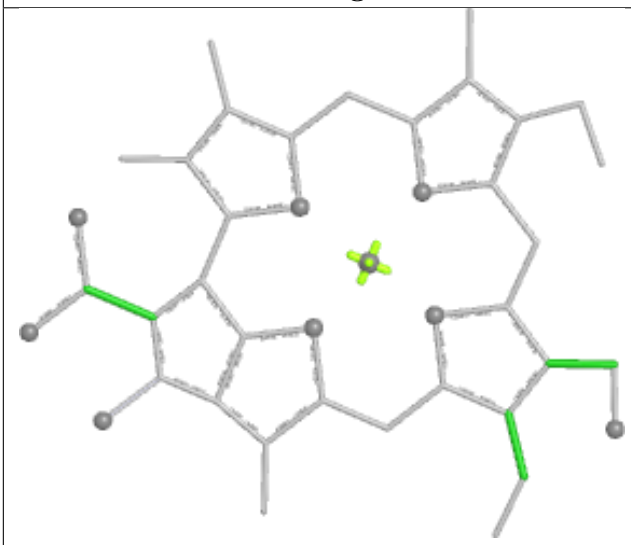
Ligand CHL 1 604



Bond lengths



Bond angles

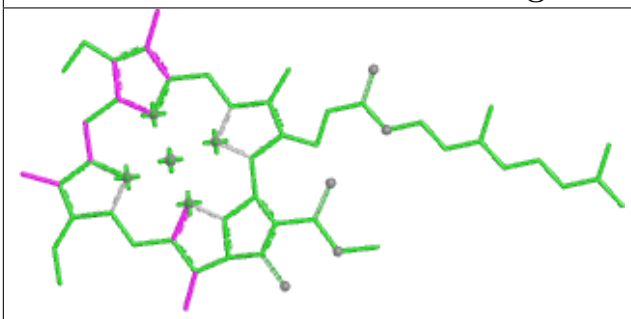


Torsions

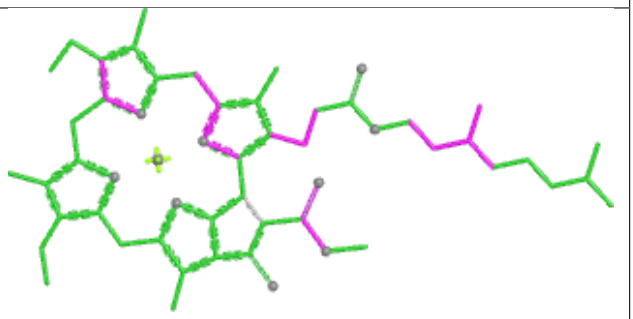


Rings

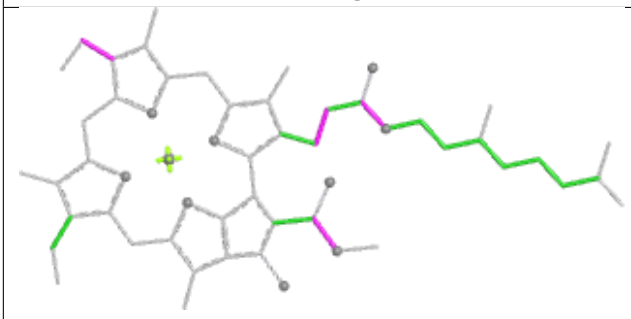
Ligand CLA S 312



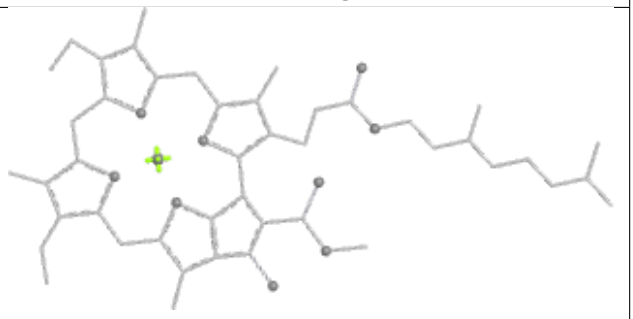
Bond lengths



Bond angles

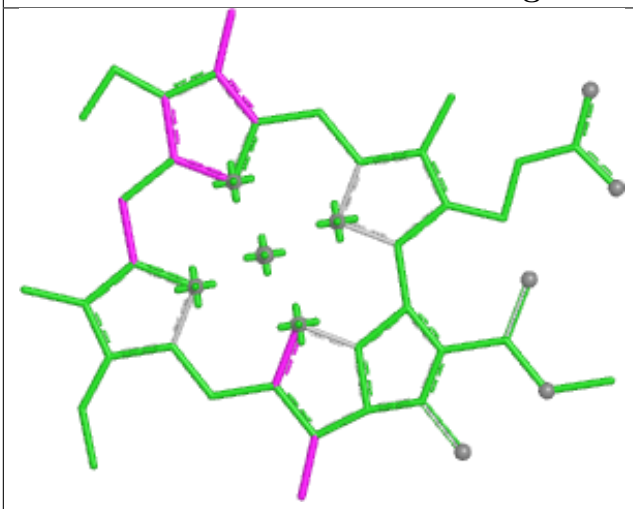


Torsions

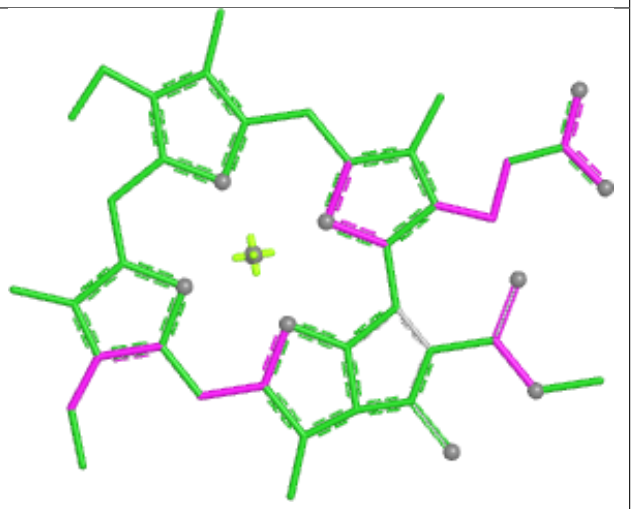


Rings

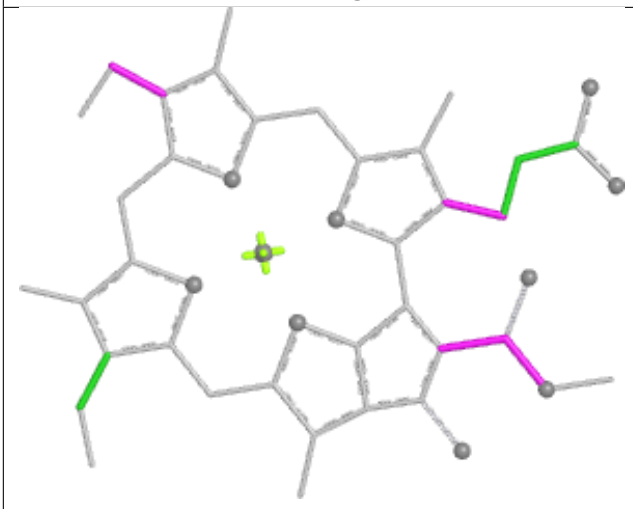
Ligand CLA G 202



Bond lengths



Bond angles

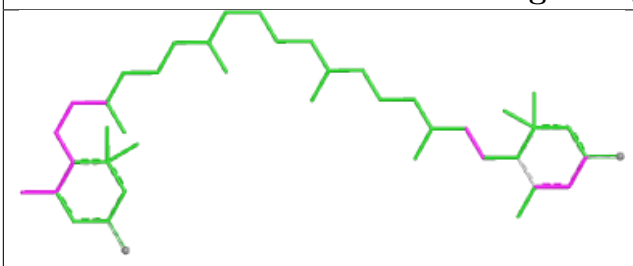


Torsions

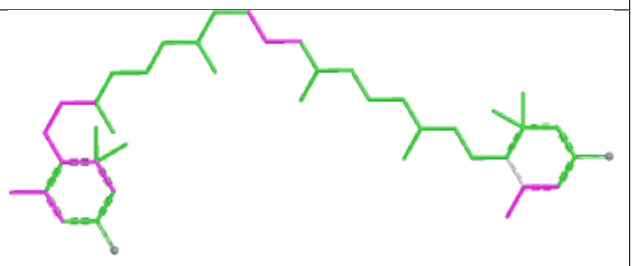


Rings

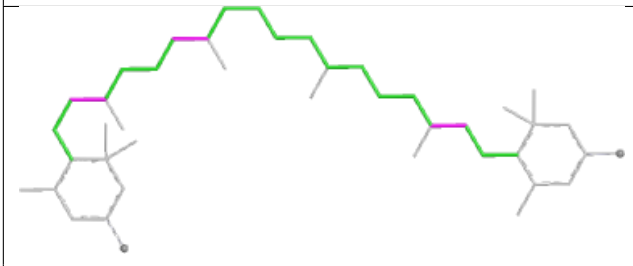
Ligand Q6L P 315



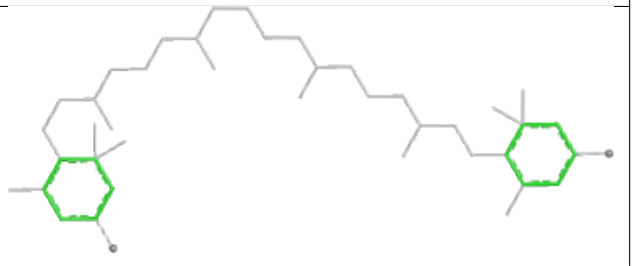
Bond lengths



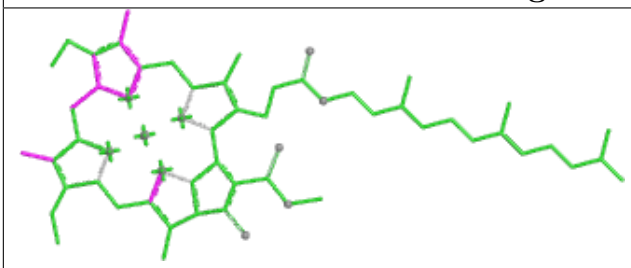
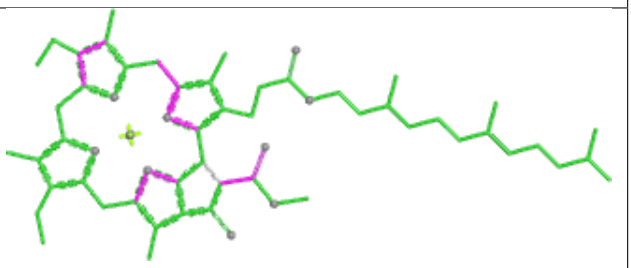
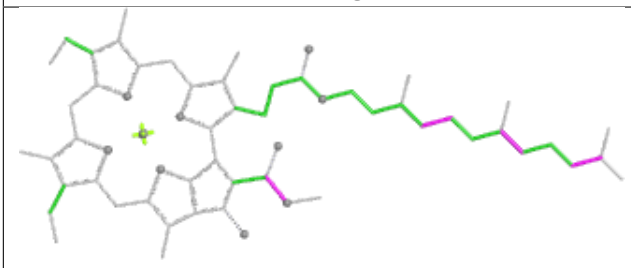
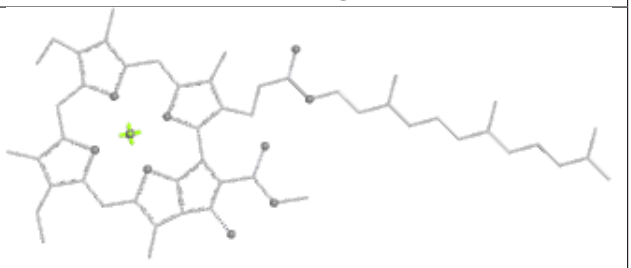
Bond angles

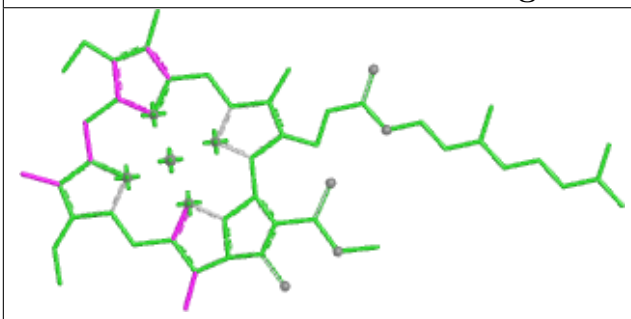
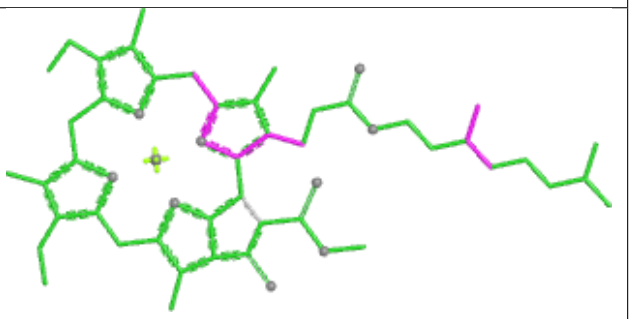
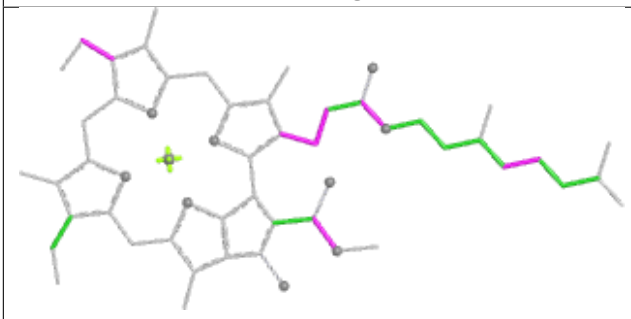
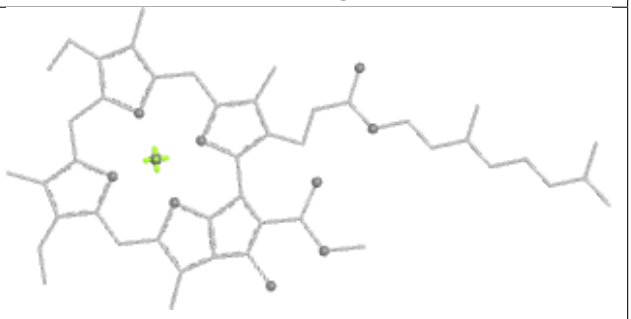


Torsions

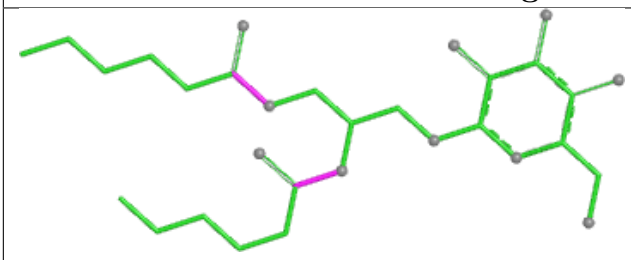


Rings

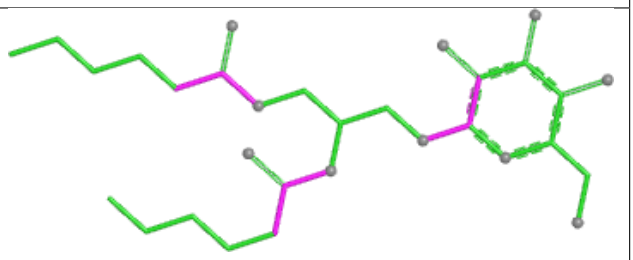
Ligand CLA 3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

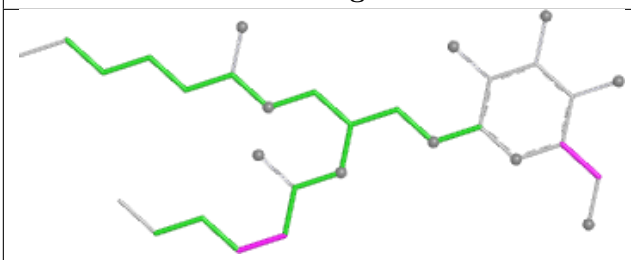
Ligand LMG F 805



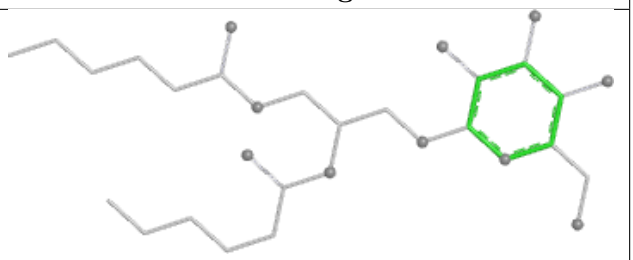
Bond lengths



Bond angles

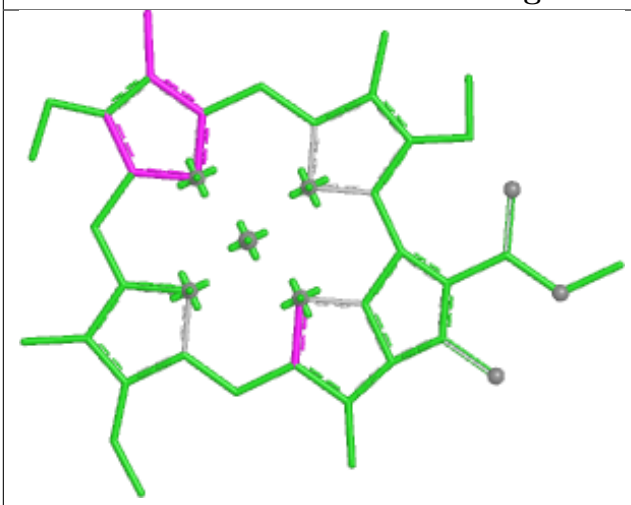


Torsions

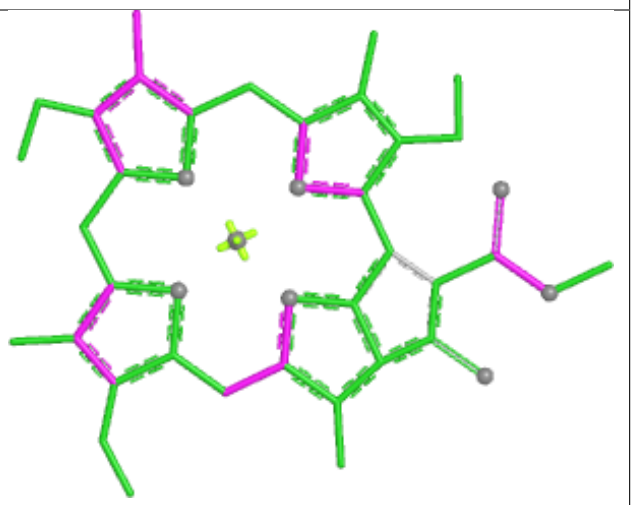


Rings

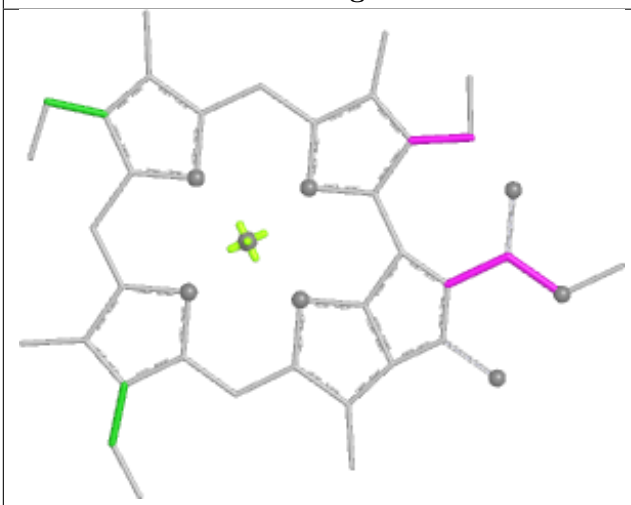
Ligand CLA A 824



Bond lengths



Bond angles

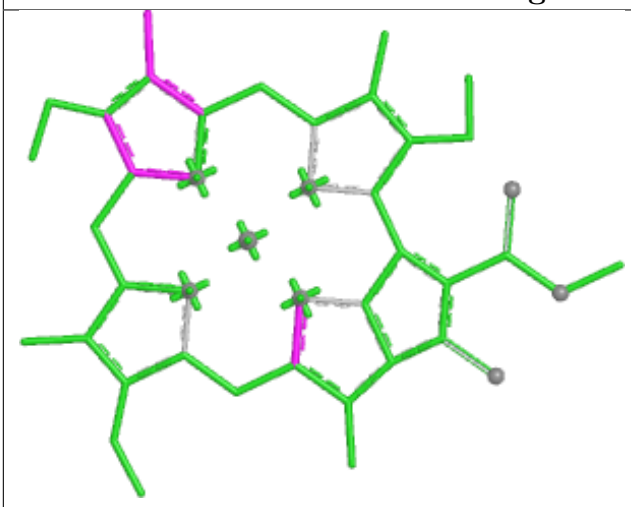


Torsions

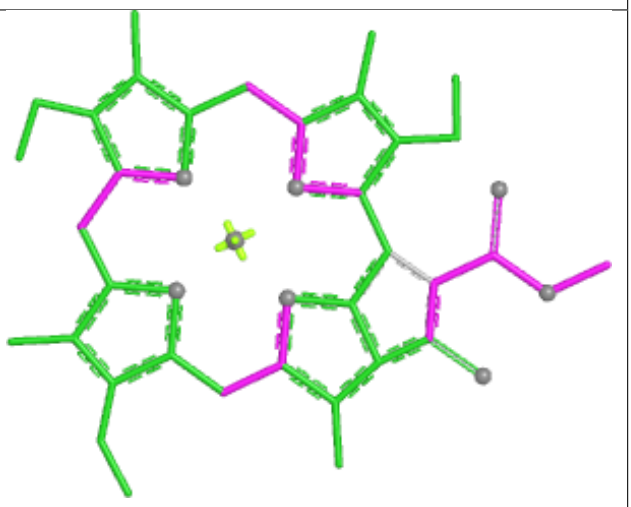


Rings

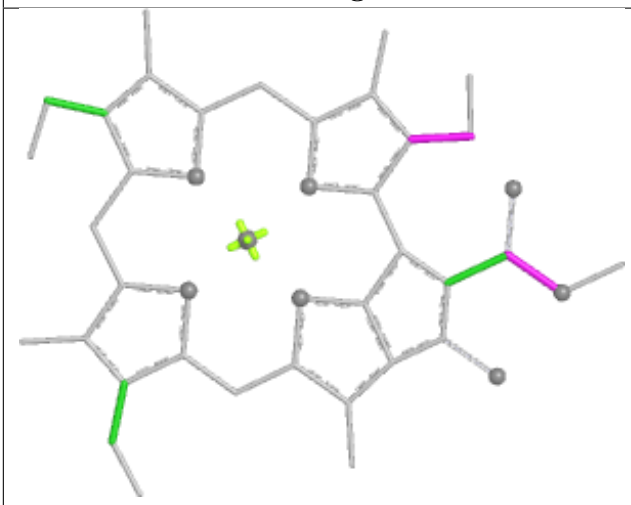
Ligand CLA 4 316



Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

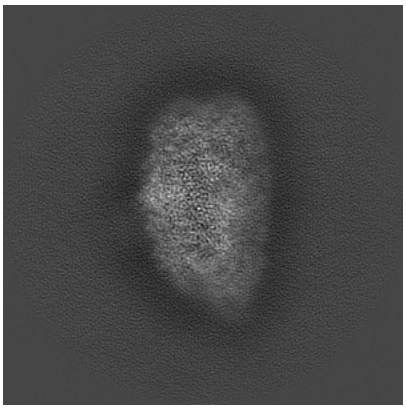
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33737. These allow visual inspection of the internal detail of the map and identification of artifacts.

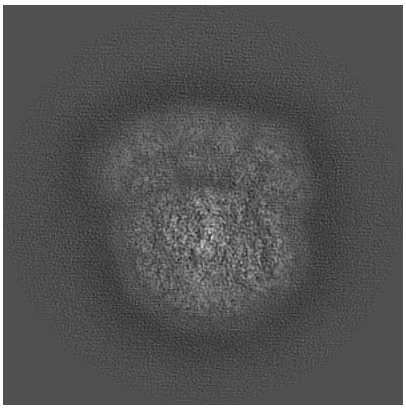
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

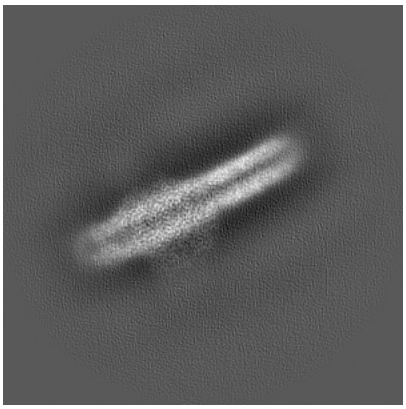
6.1.1 Primary map



X

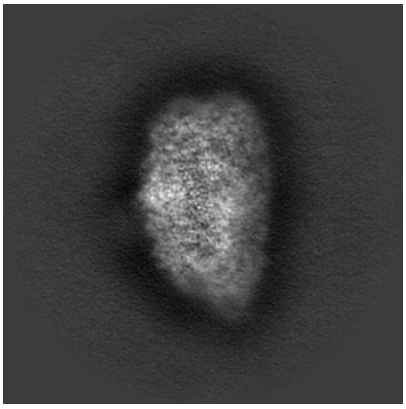


Y

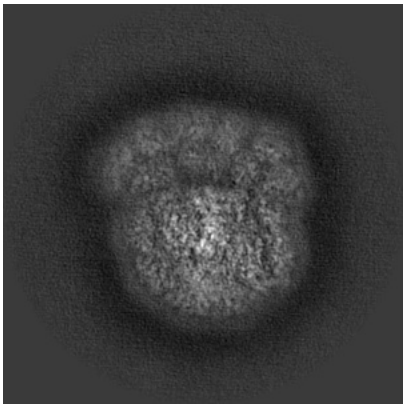


Z

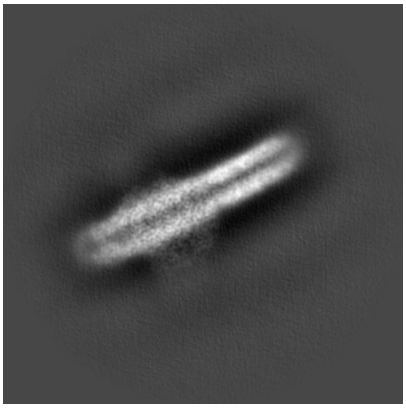
6.1.2 Raw map



X



Y

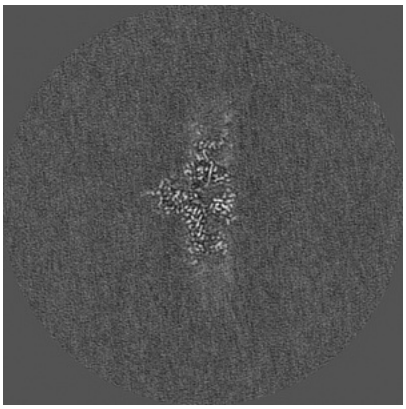


Z

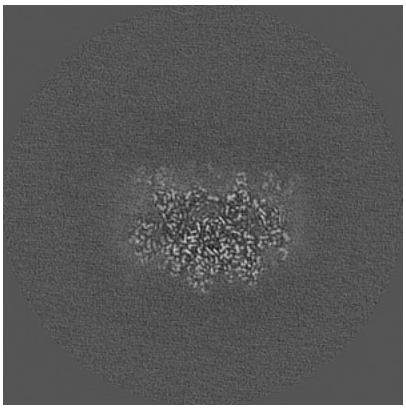
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

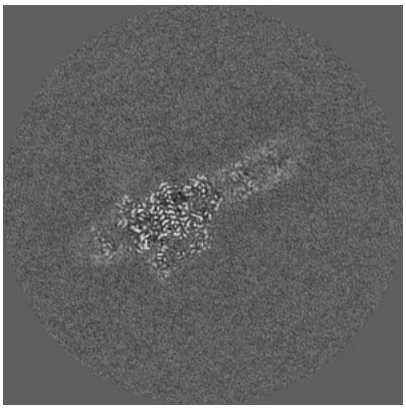
6.2.1 Primary map



X Index: 192

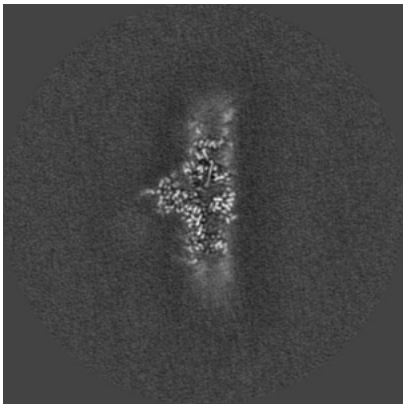


Y Index: 192

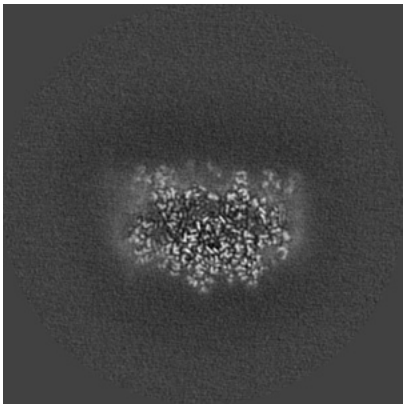


Z Index: 192

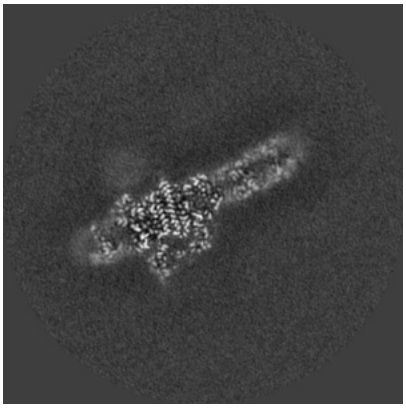
6.2.2 Raw map



X Index: 192



Y Index: 192

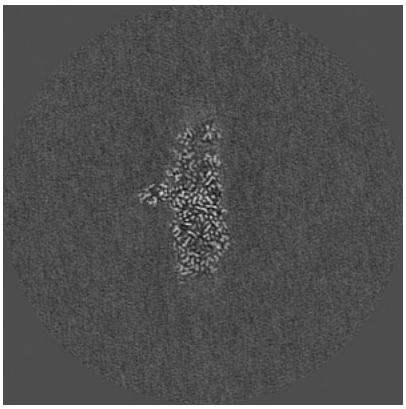


Z Index: 192

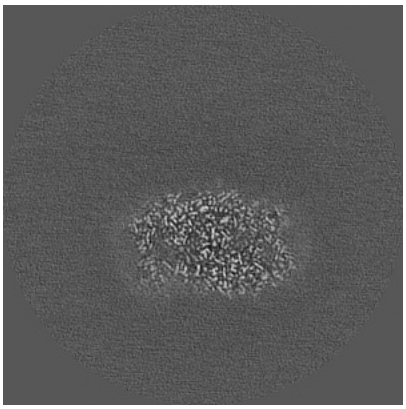
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

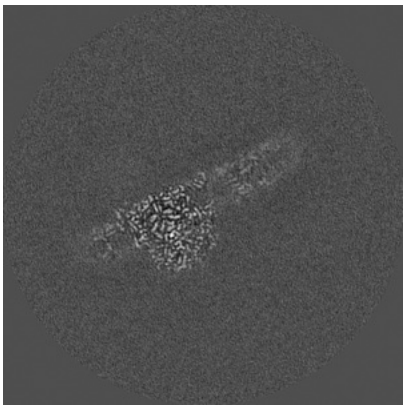
6.3.1 Primary map



X Index: 169

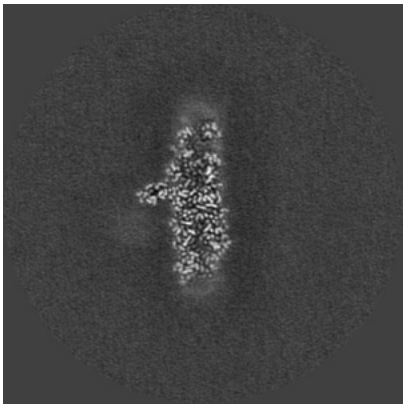


Y Index: 180

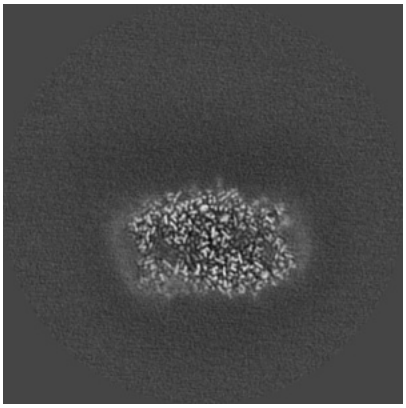


Z Index: 201

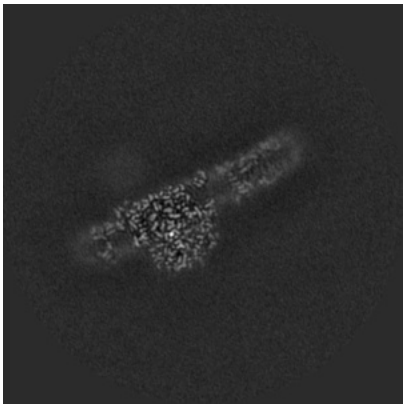
6.3.2 Raw map



X Index: 168



Y Index: 180

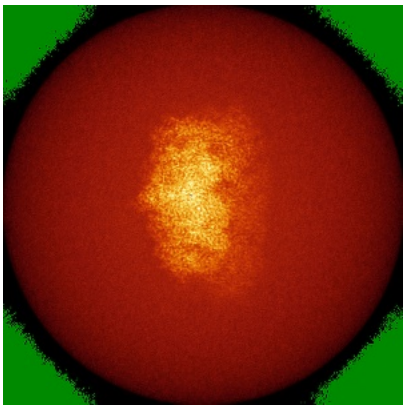


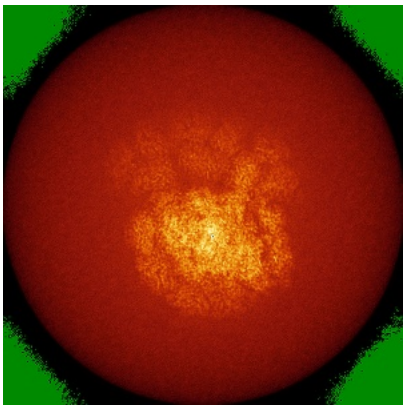
Z Index: 201

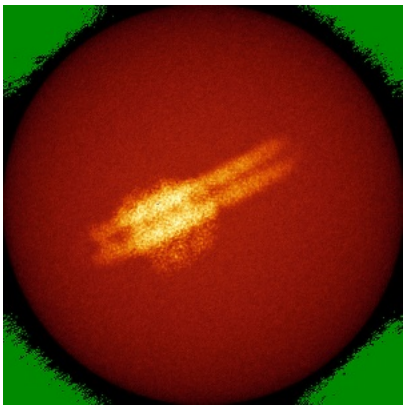
The images above show the largest variance slices of the map in three orthogonal directions.

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

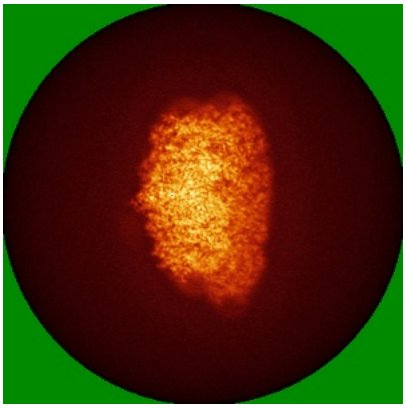
6.4.1 Primary map

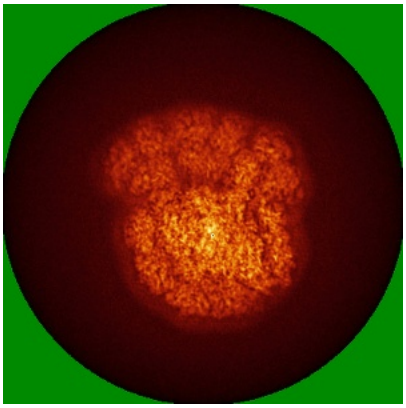

X

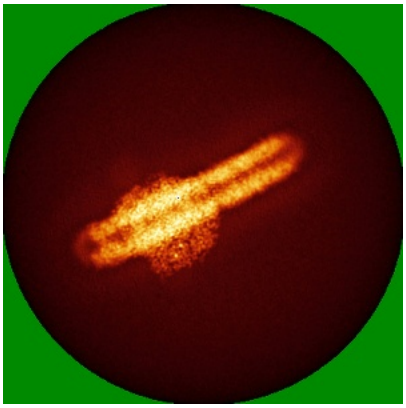

Y


Z

6.4.2 Raw map


X

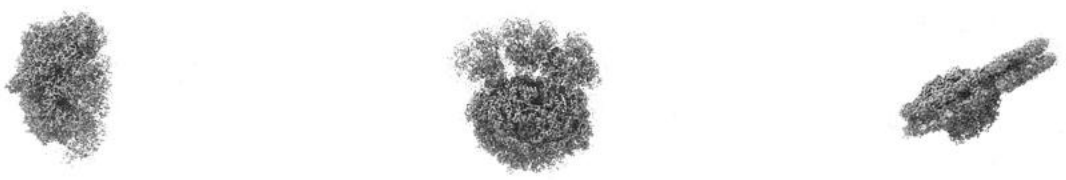

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

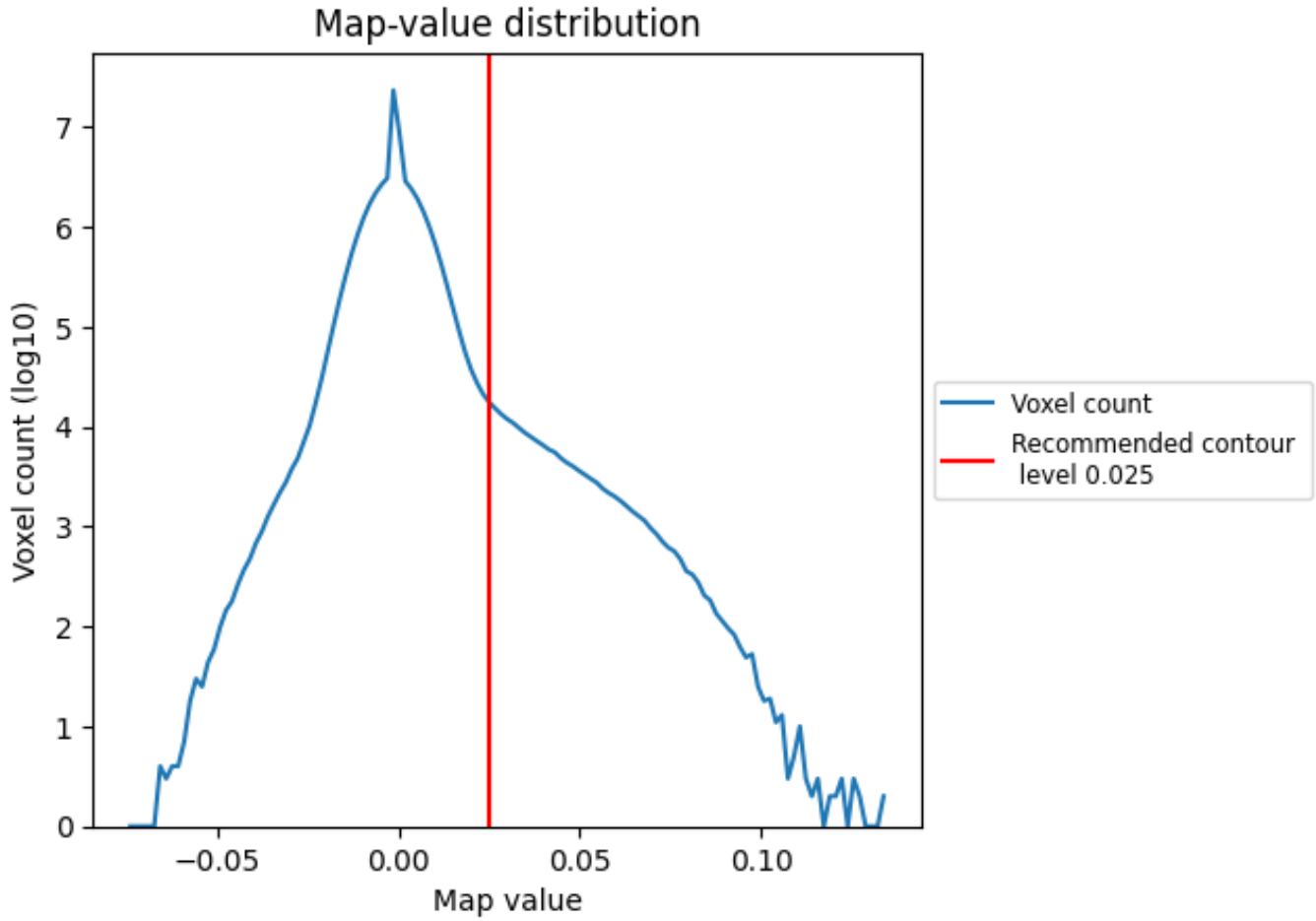
6.6 Mask visualisation (i)

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

7 Map analysis

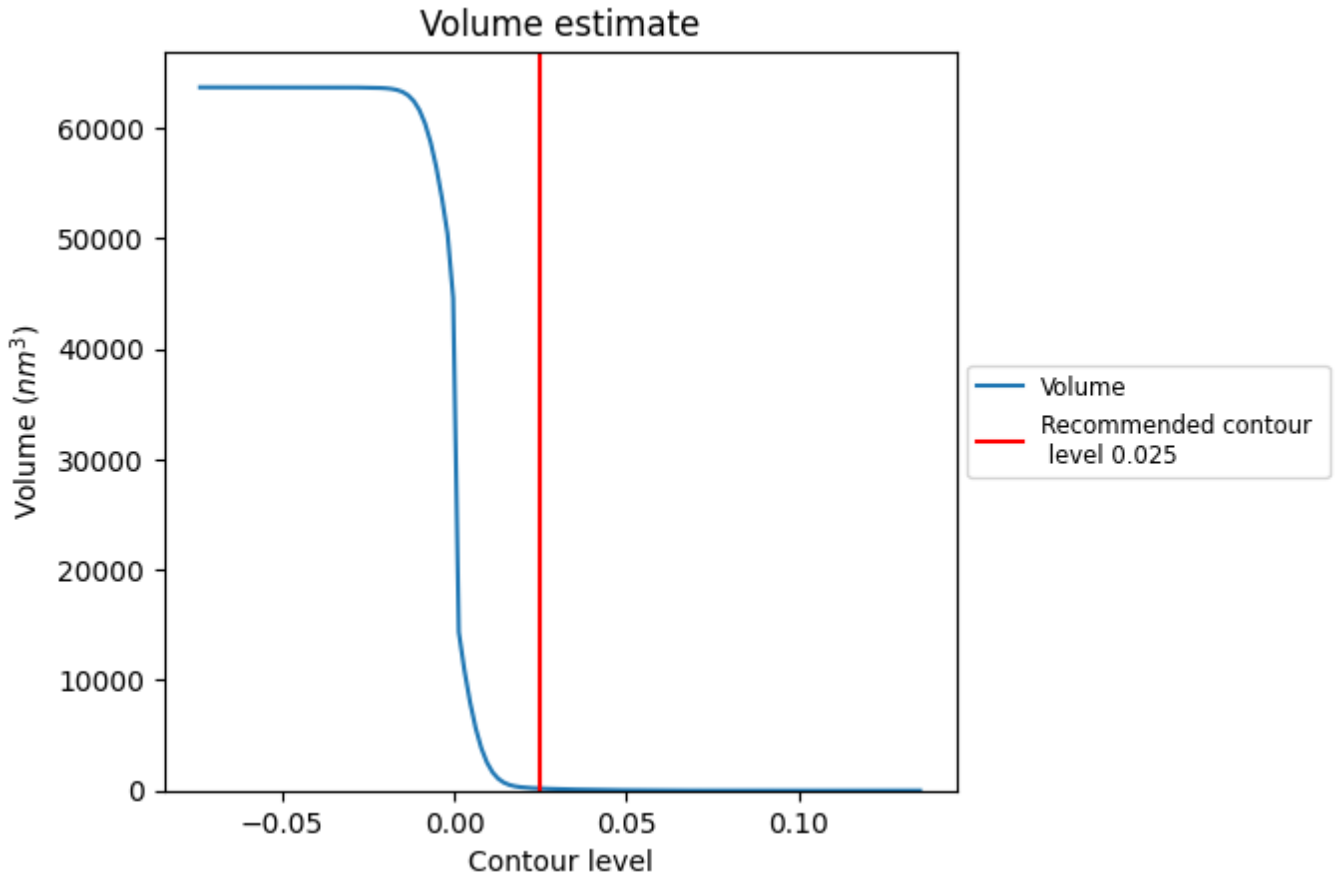
This section contains the results of statistical analysis of the map.

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.

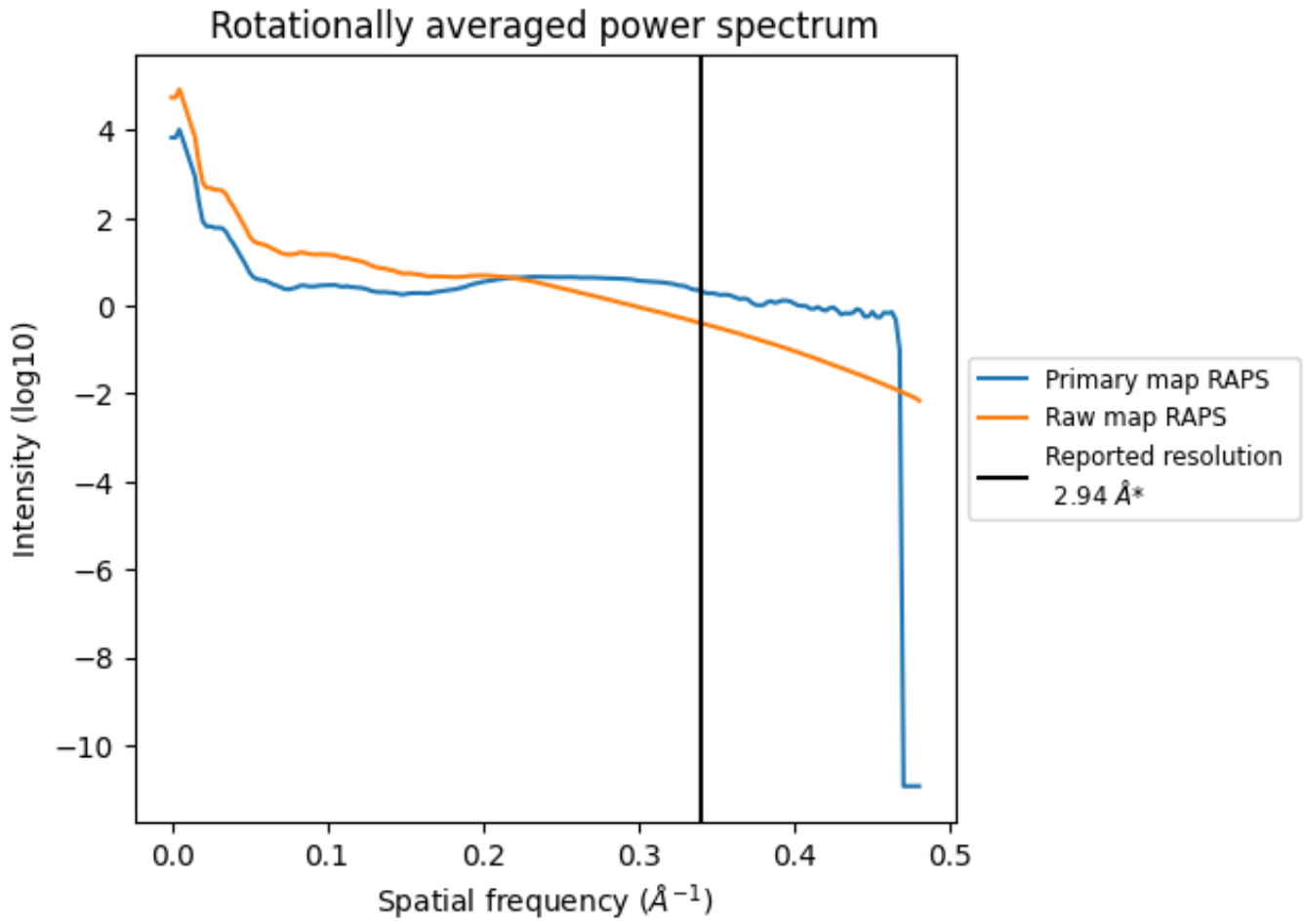
7.2 Volume estimate



The volume at the recommended contour level is 188 nm^3; this corresponds to an approximate mass of 169 kDa.

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

7.3 Rotationally averaged power spectrum (i)

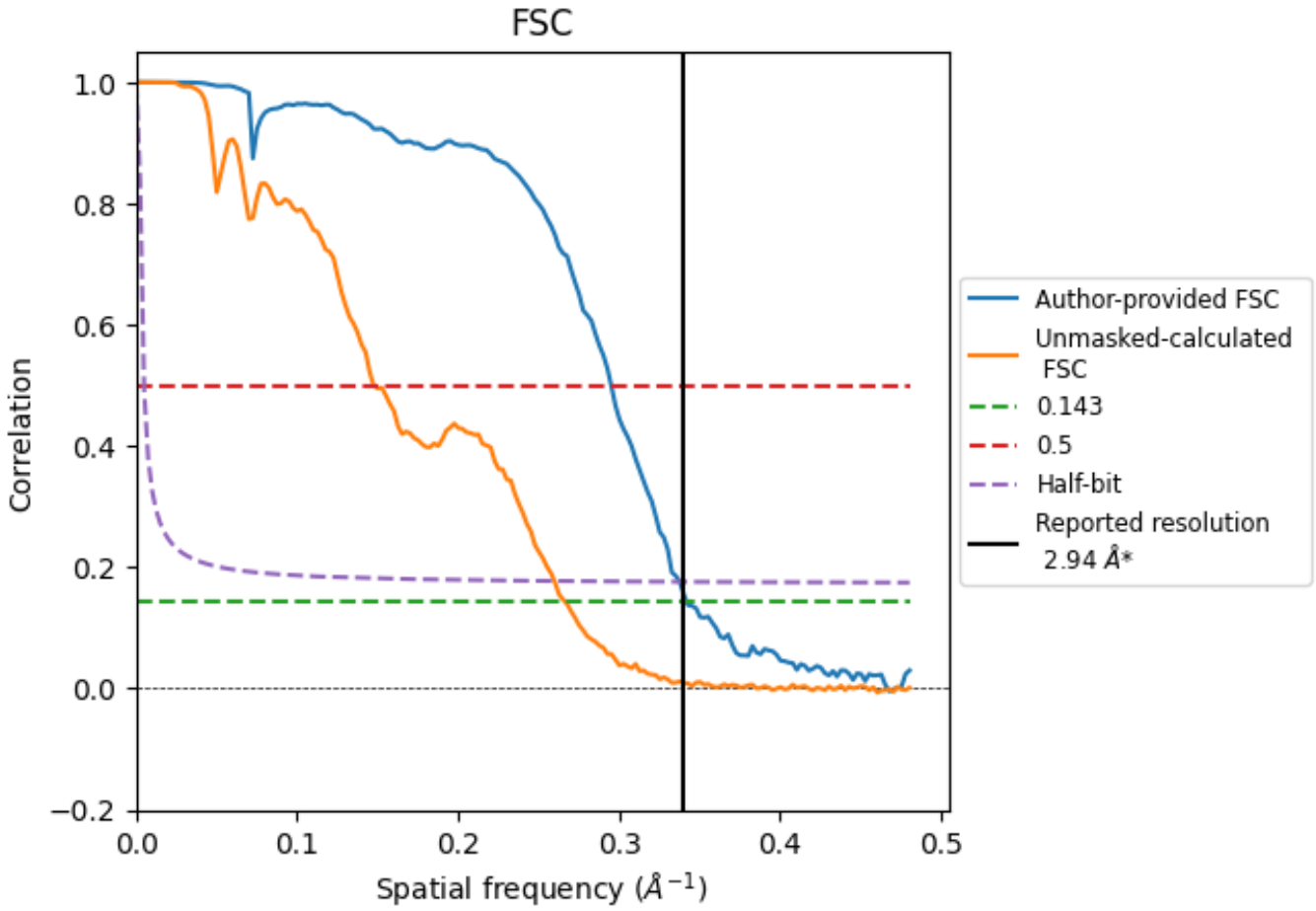


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

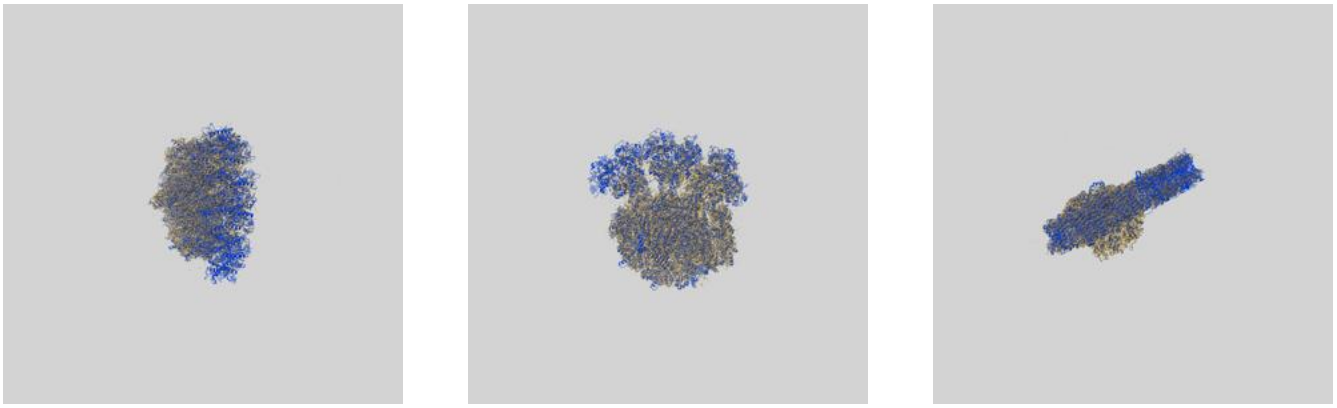
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.39	2.96
Unmasked-calculated*	3.75	6.77	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 2.94 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33737 and PDB model 7YCA. Per-residue inclusion information can be found in section 3 on page 45.

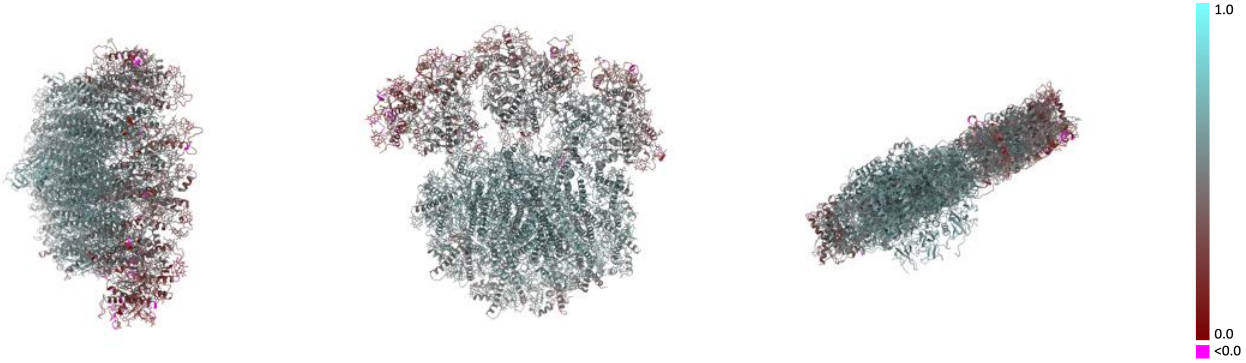
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

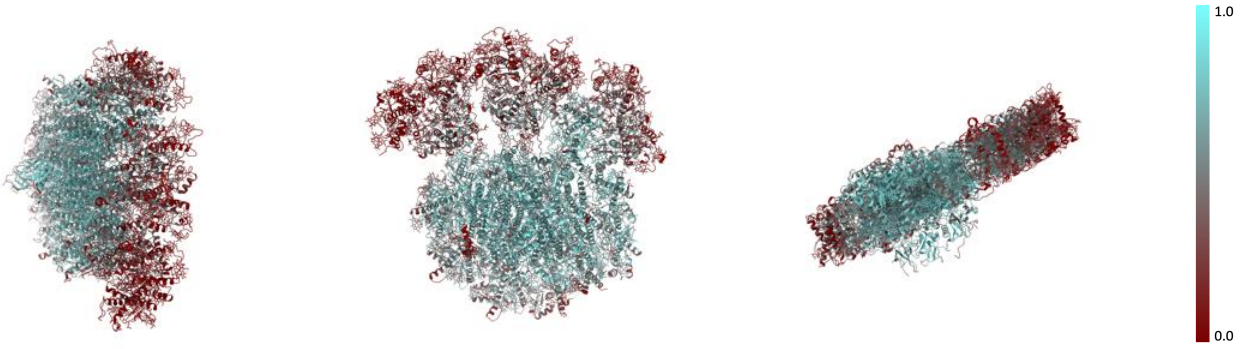
9.2 Q-score mapped to coordinate model



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.

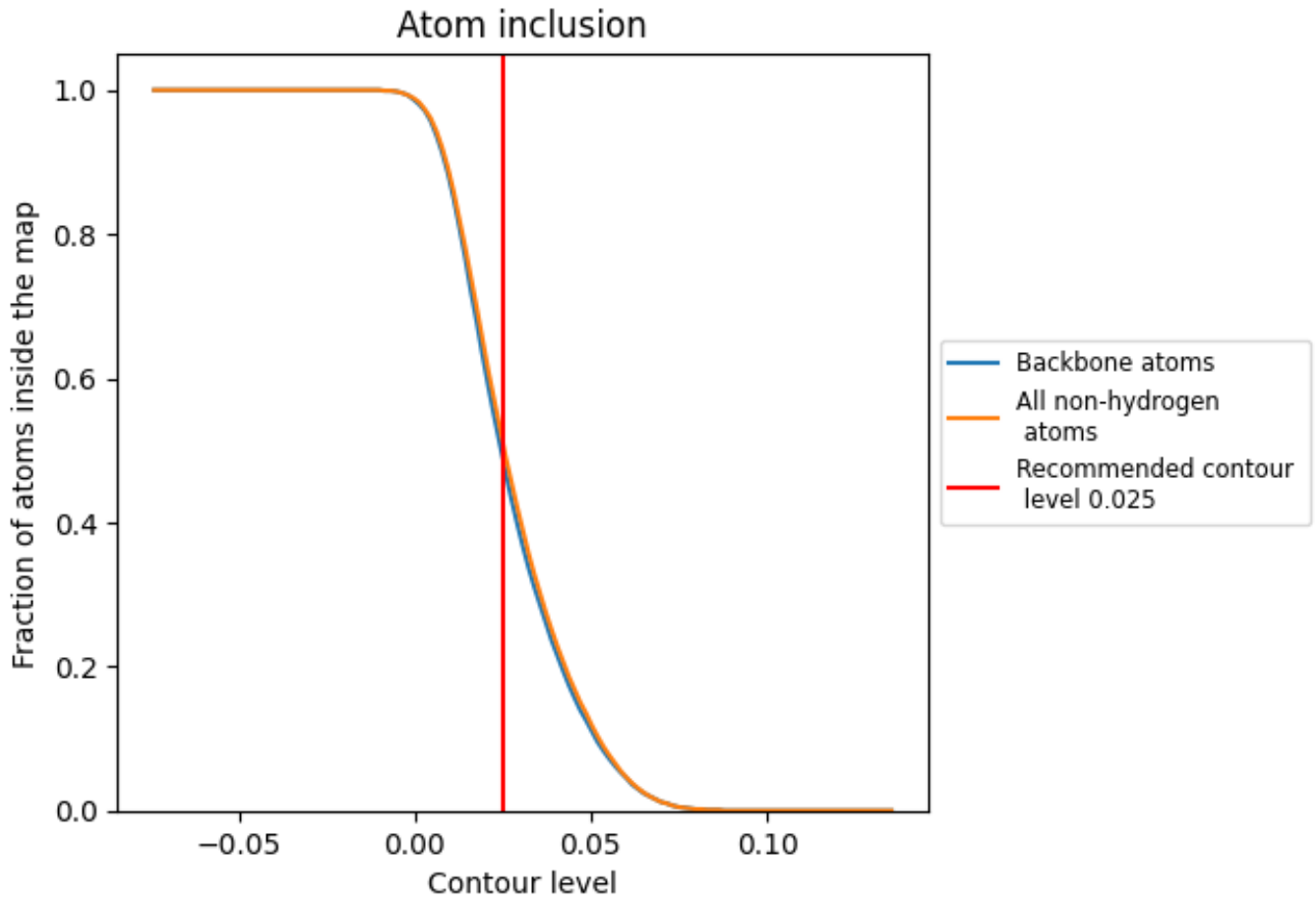
9.3 Atom inclusion mapped to coordinate model



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 51% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5110	0.5140
1	0.3170	0.4450
2	0.5160	0.5240
3	0.5610	0.5590
4	0.4200	0.4810
5	0.5730	0.5480
6	0.6330	0.5670
A	0.7720	0.6190
B	0.7600	0.6090
C	0.7780	0.6160
D	0.6260	0.5840
E	0.6110	0.5870
F	0.5970	0.5620
G	0.3990	0.4970
H	0.6320	0.5770
I	0.6670	0.5760
J	0.6620	0.5760
K	0.6500	0.5780
L	0.7290	0.6100
M	0.6490	0.5930
N	0.3080	0.4830
O	0.6920	0.5910
P	0.2520	0.3960
Q	0.5640	0.5220
R	0.3340	0.4370
S	0.2460	0.4000
T	0.3560	0.4660
U	0.1480	0.3670
V	0.1590	0.3420
W	0.3080	0.4200
X	0.0560	0.2600

