Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:20 AM UTC

PDB ID	:	6UZV / pdb_00006uzv
EMDB ID	:	EMD-20963
Title	:	The structure of a red shifted photosystem I complex
Authors	:	Toporik, H.; Williams, D.; Chiu, P.L.; Mazor, Y.
Deposited on	:	2019-11-15
Resolution	:	3.10 Å(reported)
Based on initial models	:	5OY0, 6KIG

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:

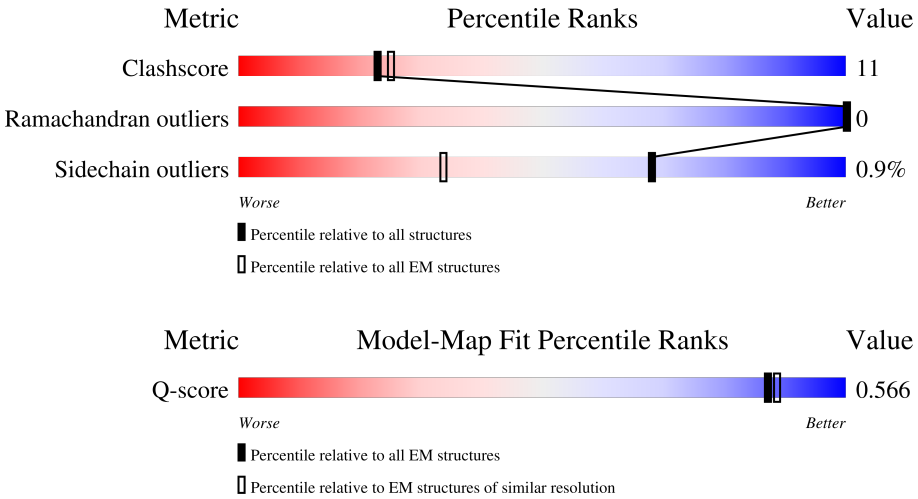
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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	751	81% 17%
1	A	751	5% 81% 17%
1	a	751	81% 17%
2	2	735	80% 19%

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Mol	Chain	Length	Quality of chain
2	B	735	79% 20%
2	b	735	80% 20%
3	3	81	78% 20%
3	C	81	77% 21%
3	c	81	75% 22%
4	4	141	13% 70% 26%
4	D	141	15% 67% 28%
4	d	141	14% 70% 26%
5	5	74	16% 74% 16% 8%
5	E	74	18% 78% 12% 8%
5	e	74	16% 74% 16% 8%
6	6	165	13% 70% 15% 15%
6	F	165	11% 76% 10% 15%
6	f	165	13% 76% 10% 15%
7	I	40	68% 25% 8%
7	h	40	62% 30% 8%
7	i	40	70% 22% 8%
8	7	40	5% 65% 32%
8	J	40	8% 75% 22%
8	j	40	8% 70% 28%
9	0	157	8% 75% 22%
9	L	157	9% 77% 20%
9	l	157	9% 76% 20%
10	9	31	10% 77% 19%
10	M	31	10% 68% 29%

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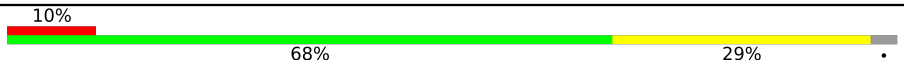
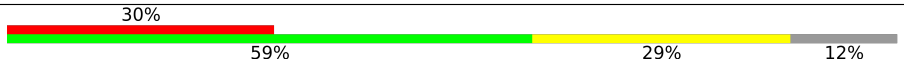
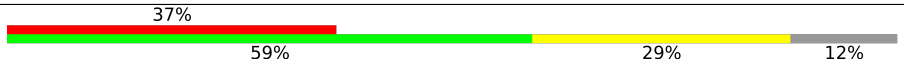
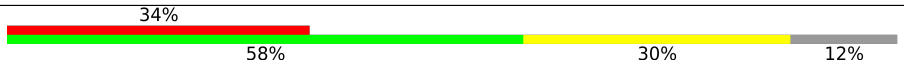
Mol	Chain	Length	Quality of chain
10	m	31	
11	8	90	
11	K	90	
11	k	90	

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
13	CL0	1	803	X	-	-	-
13	CL0	A	803	X	-	-	-
13	CL0	a	803	X	-	-	-
14	CLA	0	202	X	-	-	-
14	CLA	0	206	X	-	-	-
14	CLA	0	207	X	-	-	-
14	CLA	0	208	X	-	-	-
14	CLA	1	804	X	-	-	-
14	CLA	1	805	X	-	-	-
14	CLA	1	806	X	-	-	-
14	CLA	1	807	X	-	-	-
14	CLA	1	808	X	-	-	-
14	CLA	1	809	X	-	-	-
14	CLA	1	810	X	-	-	-
14	CLA	1	811	X	-	-	-
14	CLA	1	812	X	-	-	-
14	CLA	1	813	X	-	-	-
14	CLA	1	814	X	-	-	-
14	CLA	1	815	X	-	-	-
14	CLA	1	817	X	-	-	-
14	CLA	1	818	X	-	-	-
14	CLA	1	819	X	-	-	-
14	CLA	1	820	X	-	-	-
14	CLA	1	821	X	-	-	-
14	CLA	1	822	X	-	-	-
14	CLA	1	823	X	-	-	-
14	CLA	1	824	X	-	-	-
14	CLA	1	825	X	-	-	-
14	CLA	1	826	X	-	-	-
14	CLA	1	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	828	X	-	-	-
14	CLA	1	829	X	-	-	-
14	CLA	1	830	X	-	-	-
14	CLA	1	831	X	-	-	-
14	CLA	1	832	X	-	-	-
14	CLA	1	833	X	-	-	-
14	CLA	1	834	X	-	-	-
14	CLA	1	835	X	-	-	-
14	CLA	1	836	X	-	-	-
14	CLA	1	837	X	-	-	-
14	CLA	1	838	X	-	-	-
14	CLA	1	839	X	-	-	-
14	CLA	1	840	X	-	-	-
14	CLA	1	841	X	-	-	-
14	CLA	1	843	X	-	-	-
14	CLA	1	844	X	-	-	-
14	CLA	2	801	X	-	-	-
14	CLA	2	803	X	-	-	-
14	CLA	2	804	X	-	-	-
14	CLA	2	805	X	-	-	-
14	CLA	2	806	X	-	-	-
14	CLA	2	808	X	-	-	-
14	CLA	2	809	X	-	-	-
14	CLA	2	810	X	-	-	-
14	CLA	2	811	X	-	-	-
14	CLA	2	812	X	-	-	-
14	CLA	2	813	X	-	-	-
14	CLA	2	814	X	-	-	-
14	CLA	2	815	X	-	-	-
14	CLA	2	816	X	-	-	-
14	CLA	2	817	X	-	-	-
14	CLA	2	818	X	-	-	-
14	CLA	2	820	X	-	-	-
14	CLA	2	821	X	-	-	-
14	CLA	2	824	X	-	-	-
14	CLA	2	826	X	-	-	-
14	CLA	2	827	X	-	-	-
14	CLA	2	828	X	-	-	-
14	CLA	2	829	X	-	-	-
14	CLA	2	830	X	-	-	-
14	CLA	2	831	X	-	-	-
14	CLA	2	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	2	833	X	-	-	-
14	CLA	2	834	X	-	-	-
14	CLA	2	835	X	-	-	-
14	CLA	2	836	X	-	-	-
14	CLA	2	837	X	-	-	-
14	CLA	2	838	X	-	-	-
14	CLA	2	839	X	-	-	-
14	CLA	2	840	X	-	-	-
14	CLA	2	841	X	-	-	-
14	CLA	2	842	X	-	-	-
14	CLA	2	844	X	-	-	-
14	CLA	6	4403	X	-	-	-
14	CLA	6	4404	X	-	-	-
14	CLA	7	1101	X	-	-	-
14	CLA	7	1102	X	-	-	-
14	CLA	7	1103	X	-	-	-
14	CLA	8	4003	X	-	-	-
14	CLA	8	4004	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	B	843	X	-	-	-
14	CLA	B	845	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	F	205	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	4003	X	-	-	-
14	CLA	K	4004	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-
14	CLA	a	808	X	-	-	-
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	826	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	a	843	X	-	-	-
14	CLA	a	844	X	-	-	-
14	CLA	a	854	X	-	-	-
14	CLA	b	801	X	-	-	-
14	CLA	b	802	X	-	-	-
14	CLA	b	804	X	-	-	-
14	CLA	b	805	X	-	-	-
14	CLA	b	806	X	-	-	-
14	CLA	b	807	X	-	-	-
14	CLA	b	809	X	-	-	-
14	CLA	b	810	X	-	-	-
14	CLA	b	811	X	-	-	-
14	CLA	b	812	X	-	-	-
14	CLA	b	813	X	-	-	-
14	CLA	b	814	X	-	-	-
14	CLA	b	815	X	-	-	-
14	CLA	b	816	X	-	-	-
14	CLA	b	817	X	-	-	-
14	CLA	b	818	X	-	-	-
14	CLA	b	820	X	-	-	-
14	CLA	b	821	X	-	-	-
14	CLA	b	824	X	-	-	-
14	CLA	b	826	X	-	-	-
14	CLA	b	827	X	-	-	-
14	CLA	b	828	X	-	-	-
14	CLA	b	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	830	X	-	-	-
14	CLA	b	831	X	-	-	-
14	CLA	b	832	X	-	-	-
14	CLA	b	833	X	-	-	-
14	CLA	b	834	X	-	-	-
14	CLA	b	835	X	-	-	-
14	CLA	b	836	X	-	-	-
14	CLA	b	837	X	-	-	-
14	CLA	b	838	X	-	-	-
14	CLA	b	839	X	-	-	-
14	CLA	b	840	X	-	-	-
14	CLA	b	841	X	-	-	-
14	CLA	b	842	X	-	-	-
14	CLA	b	844	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	204	X	-	-	-
14	CLA	f	205	X	-	-	-
14	CLA	j	101	X	-	-	-
14	CLA	j	102	X	-	-	-
14	CLA	k	4003	X	-	-	-
14	CLA	l	4203	X	-	-	-
14	CLA	l	4204	X	-	-	-
14	CLA	l	4205	X	-	-	-
14	CLA	l	4206	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 72606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	1	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5806	3824	973	994	15		
2	b	733	Total	C	N	O	S	0	0
			5806	3824	973	994	15		
2	2	733	Total	C	N	O	S	0	0
			5806	3824	973	994	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		
4	4	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			537	337	95	105		
5	e	68	Total	C	N	O	0	0
			537	337	95	105		
5	5	68	Total	C	N	O	0	0
			537	337	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1086	702	180	200	4		
6	f	141	Total	C	N	O	S	0	0
			1086	702	180	200	4		
6	6	141	Total	C	N	O	S	0	0
			1086	702	180	200	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	i	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	h	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	52	3		
8	j	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	153	Total	C	N	O	S	0	0
			1138	745	186	205	2		
9	l	153	Total	C	N	O	S	0	0
			1138	745	186	205	2		
9	0	153	Total	C	N	O	S	0	0
			1138	745	186	205	2		

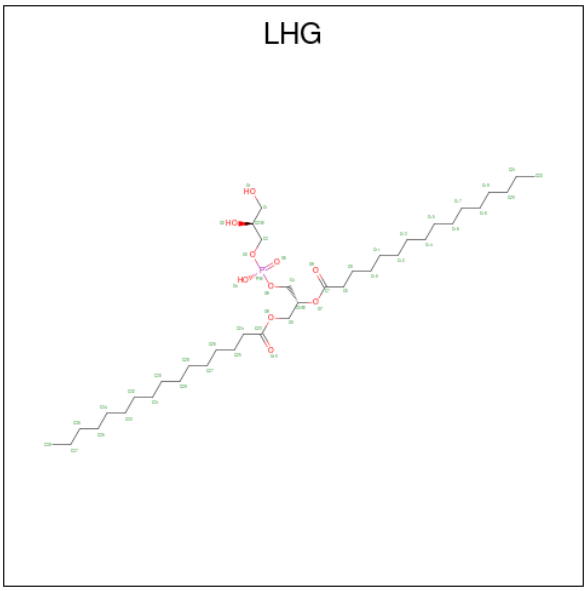
- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	30	Total	C	N	O	0	0
			230	154	35	41		
10	m	30	Total	C	N	O	0	0
			230	154	35	41		
10	9	30	Total	C	N	O	0	0
			230	154	35	41		

- Molecule 11 is a protein called Photosystem I reaction center subunit PsaK 2.

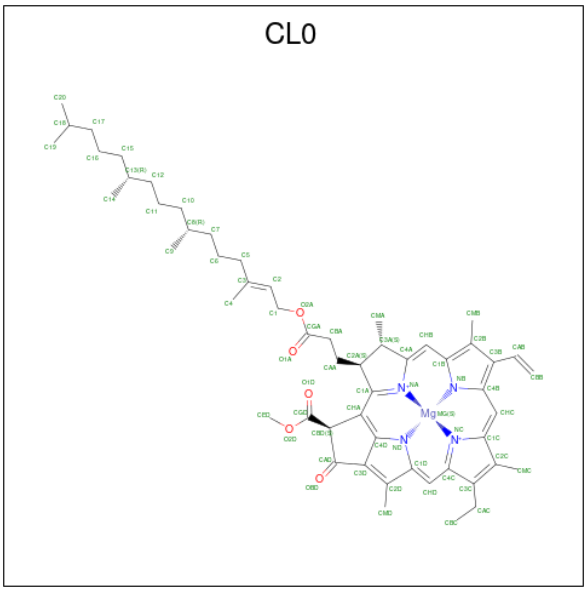
Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	79	Total	C	N	O	S	0	0
			566	373	90	98	5		
11	k	79	Total	C	N	O	S	0	0
			566	373	90	98	5		
11	8	79	Total	C	N	O	S	0	0
			566	373	90	98	5		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



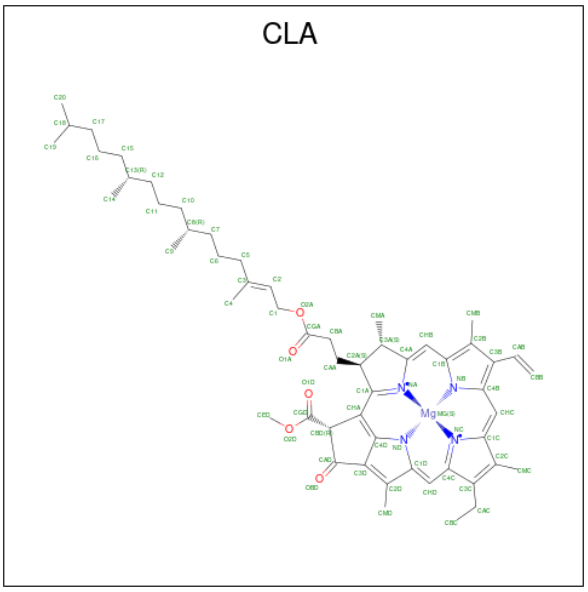
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 49	C 38	O 10	P 1	0
12	A	1	Total 33	C 22	O 10	P 1	0
12	B	1	Total 39	C 28	O 10	P 1	0
12	M	1	Total 39	C 28	O 10	P 1	0
12	a	1	Total 49	C 38	O 10	P 1	0
12	a	1	Total 33	C 22	O 10	P 1	0
12	1	1	Total 49	C 38	O 10	P 1	0
12	1	1	Total 33	C 22	O 10	P 1	0
12	b	1	Total 39	C 28	O 10	P 1	0
12	2	1	Total 39	C 28	O 10	P 1	0
12	m	1	Total 39	C 28	O 10	P 1	0
12	9	1	Total 39	C 28	O 10	P 1	0

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N		0
			27	22	1	4		

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Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N		0
			27	22	1	4		
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N		0
			27	22	1	4		
14	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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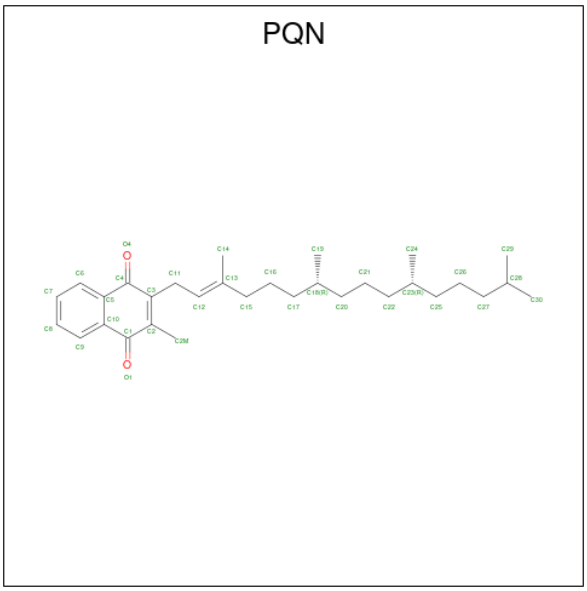
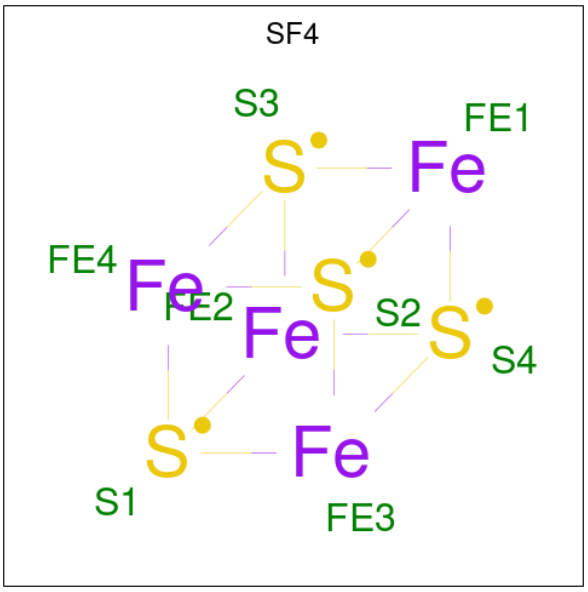
Mol	Chain	Residues	Atoms					AltConf
14	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



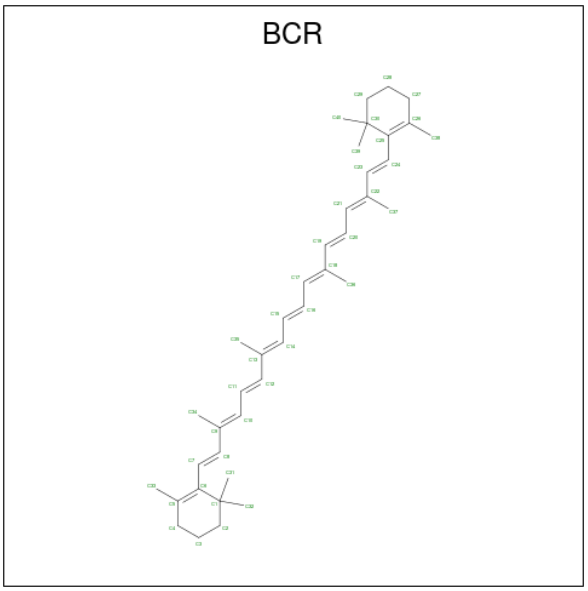
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C O 33 31 2	0
15	B	1	Total C O 33 31 2	0
15	a	1	Total C O 33 31 2	0
15	1	1	Total C O 33 31 2	0
15	b	1	Total C O 33 31 2	0
15	2	1	Total C O 33 31 2	0

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	a	1	Total Fe S 8 4 4	0
16	1	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0
16	c	1	Total Fe S 8 4 4	0
16	3	1	Total Fe S 8 4 4	0
16	3	1	Total Fe S 8 4 4	0

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 25 25	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	F	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	b	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 25 25	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	h	1	Total C 40 40	0
17	h	1	Total C 40 40	0

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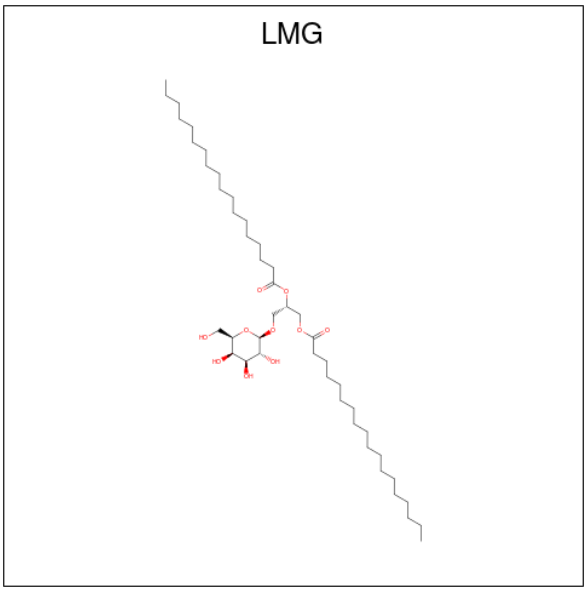
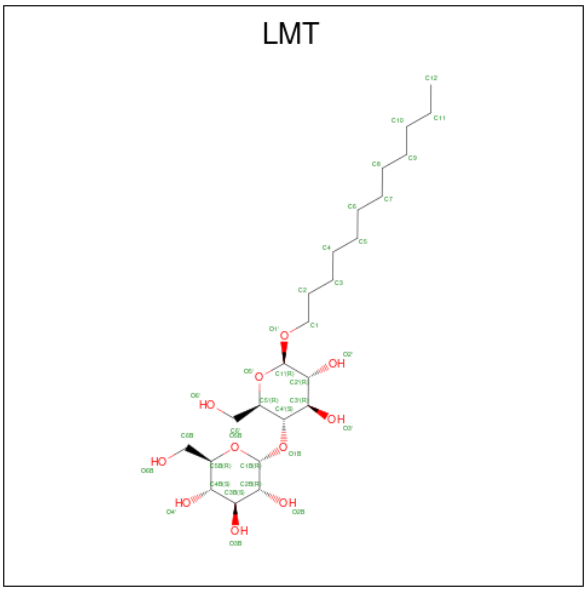
Mol	Chain	Residues	Atoms	AltConf
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	7	1	Total C 40 40	0
17	7	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	9	1	Total C 40 40	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C O 46 36 10	0
18	A	1	Total C O 32 22 10	0
18	B	1	Total C O 48 38 10	0
18	L	1	Total C O 38 28 10	0
18	a	1	Total C O 46 36 10	0
18	a	1	Total C O 32 22 10	0
18	1	1	Total C O 32 22 10	0
18	b	1	Total C O 48 38 10	0
18	2	1	Total C O 48 38 10	0
18	l	1	Total C O 38 28 10	0
18	0	1	Total C O 38 28 10	0
18	0	1	Total C O 46 36 10	0

- Molecule 19 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
19	F	1	Total C O 35 24 11	0
19	I	1	Total C O 35 24 11	0
19	f	1	Total C O 35 24 11	0
19	6	1	Total C O 35 24 11	0
19	i	1	Total C O 35 24 11	0
19	h	1	Total C O 35 24 11	0

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

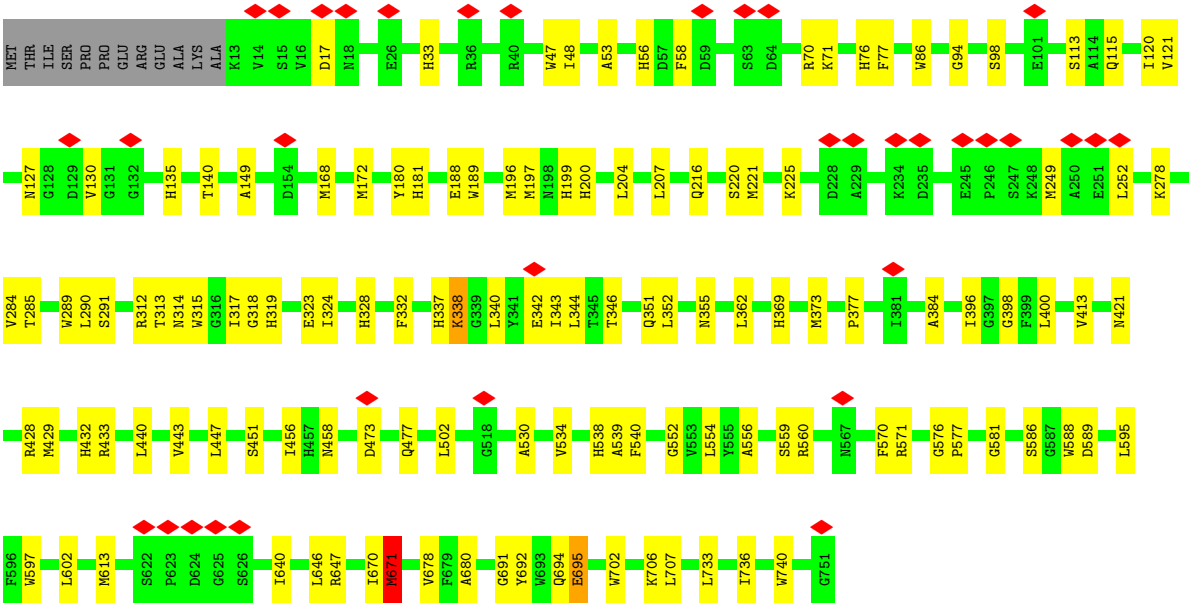
Mol	Chain	Residues	Atoms	AltConf
20	L	1	Total Ca 1 1	0
20	l	1	Total Ca 1 1	0
20	0	1	Total Ca 1 1	0

3 Residue-property plots (i)

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

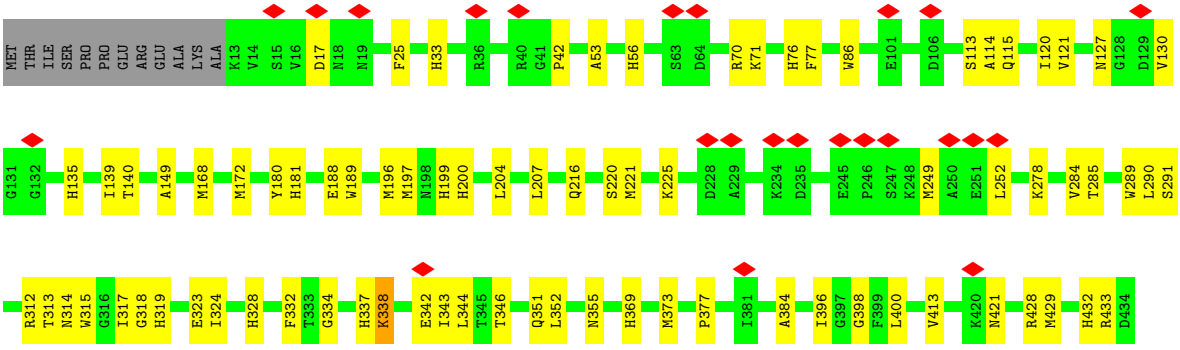
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

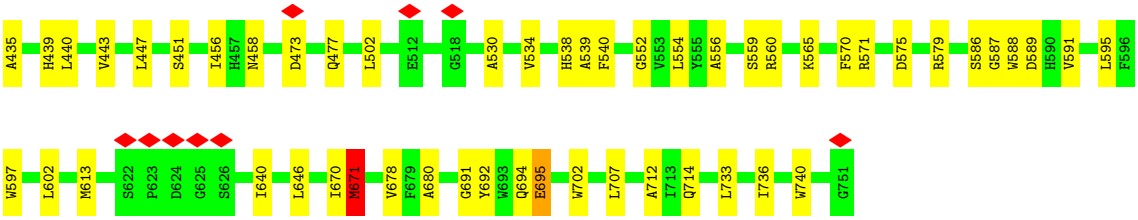
Chain A:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

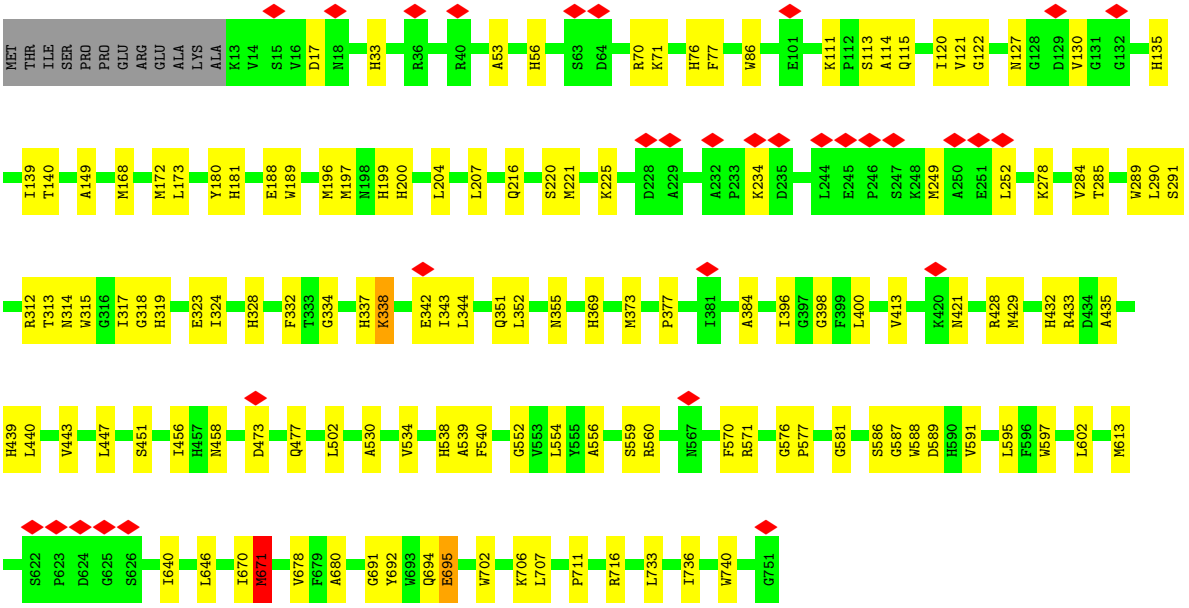
Chain a:





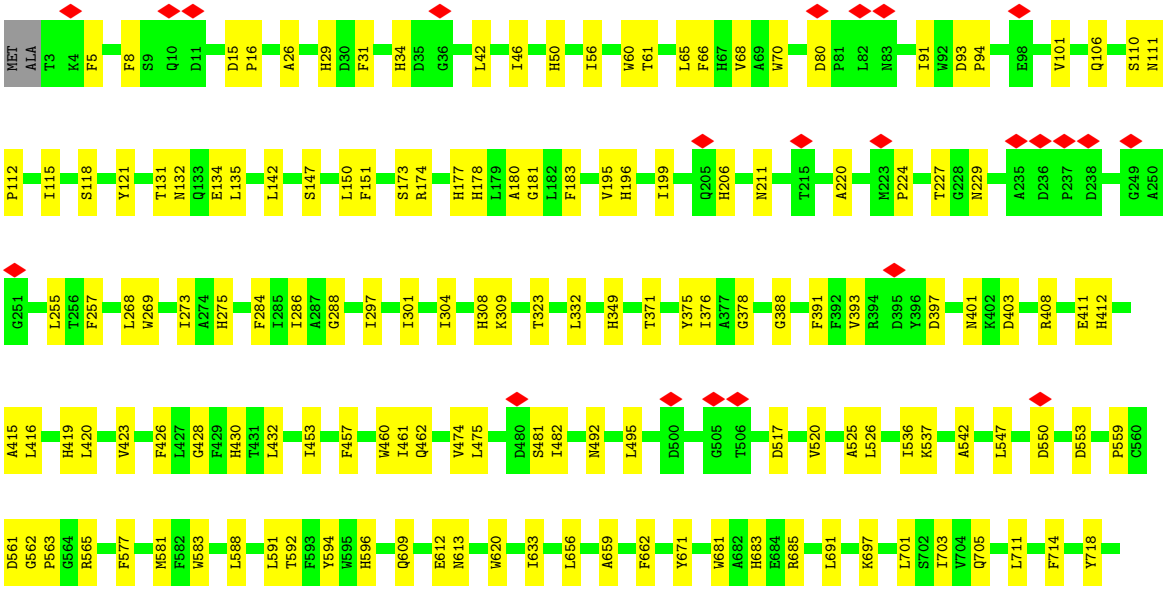
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

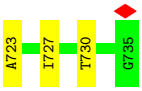
Chain 1:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

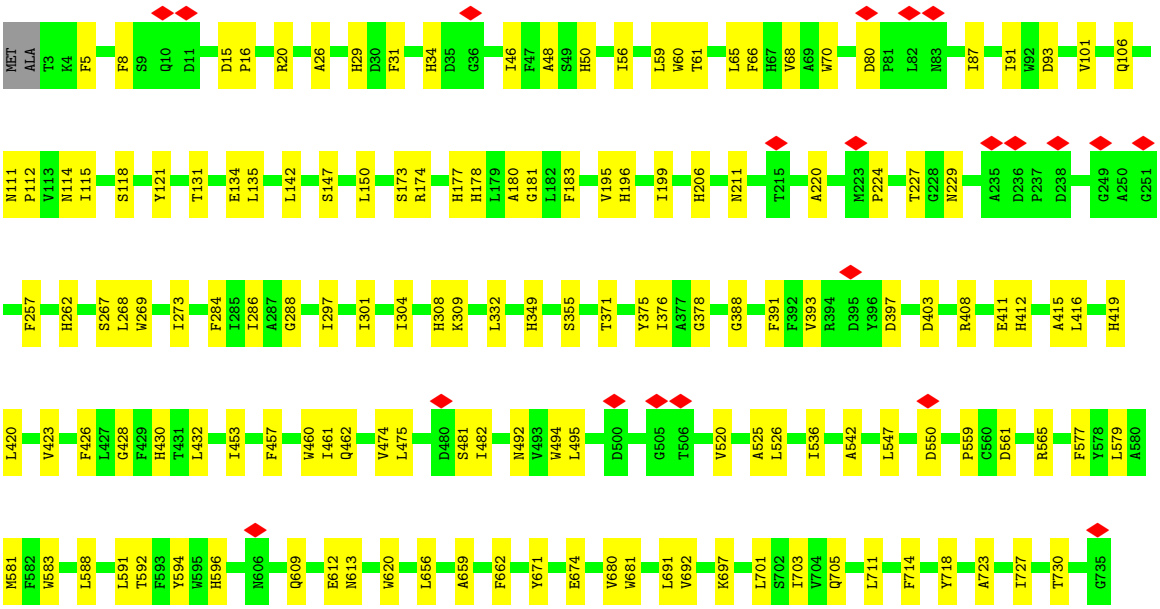
Chain B:





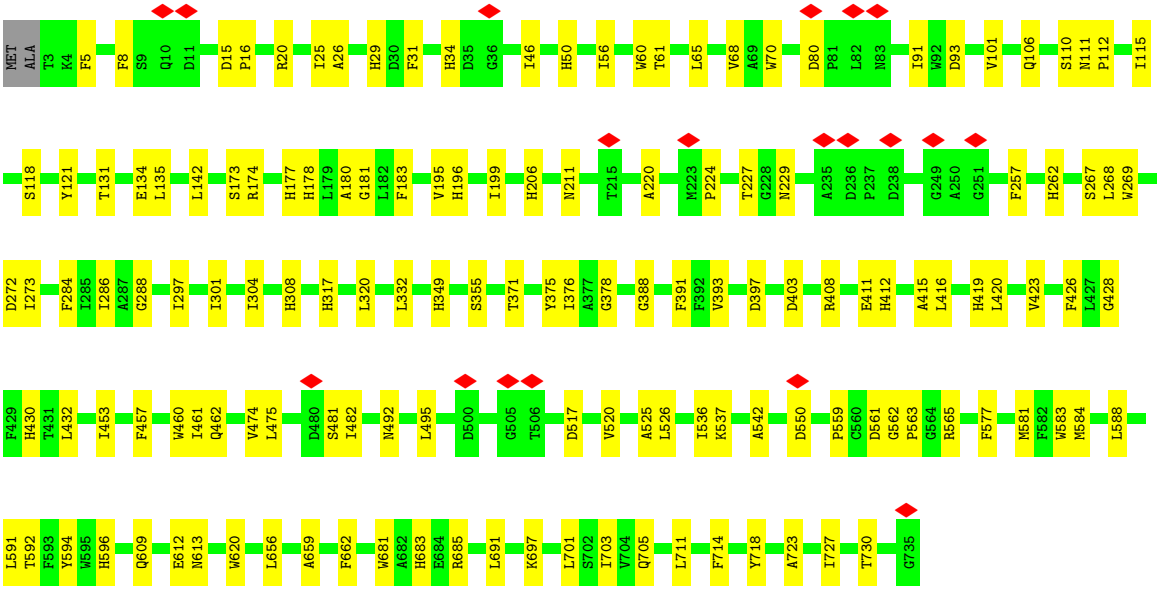
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



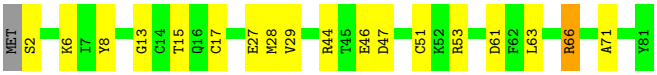
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:



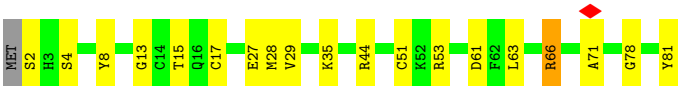
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



• Molecule 3: Photosystem I iron-sulfur center

Chain c:

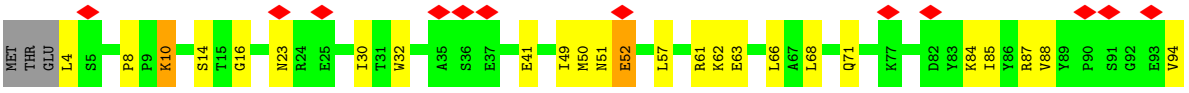


• Molecule 3: Photosystem I iron-sulfur center

Chain 3:

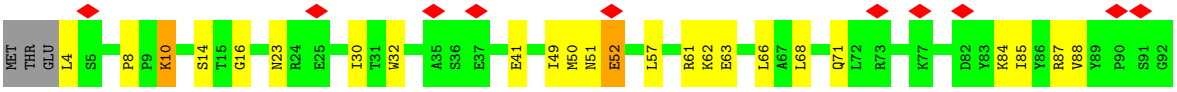
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



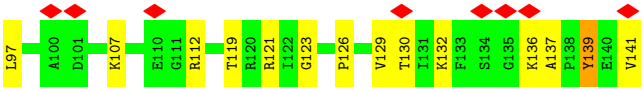
• Molecule 4: Photosystem I reaction center subunit II

Chain d:

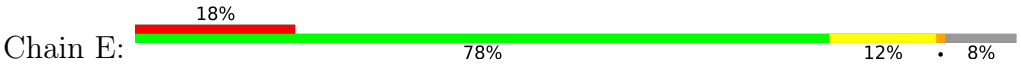


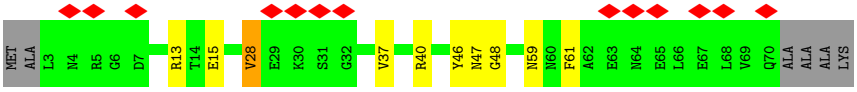
• Molecule 4: Photosystem I reaction center subunit II

Chain 4:

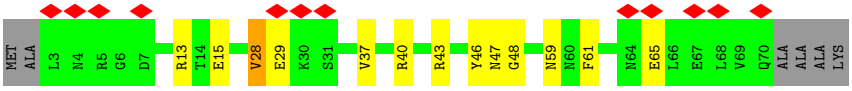


• Molecule 5: Photosystem I reaction center subunit IV

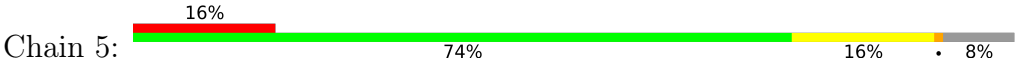


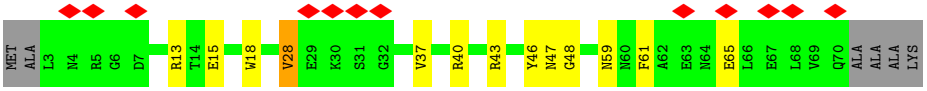


• Molecule 5: Photosystem I reaction center subunit IV

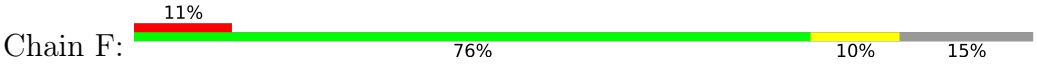


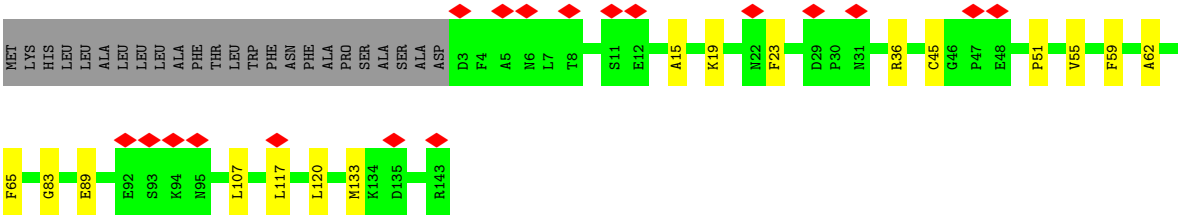
• Molecule 5: Photosystem I reaction center subunit IV



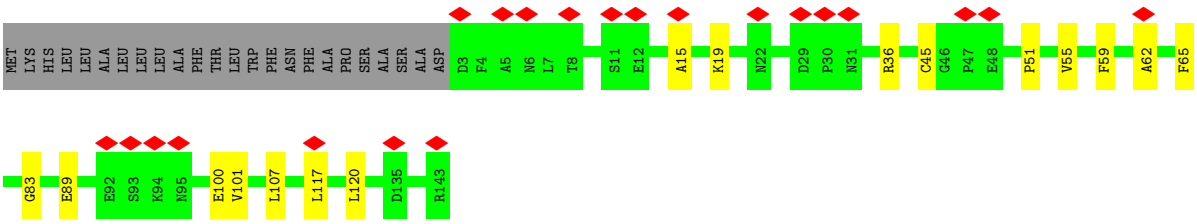


• Molecule 6: Photosystem I reaction center subunit III



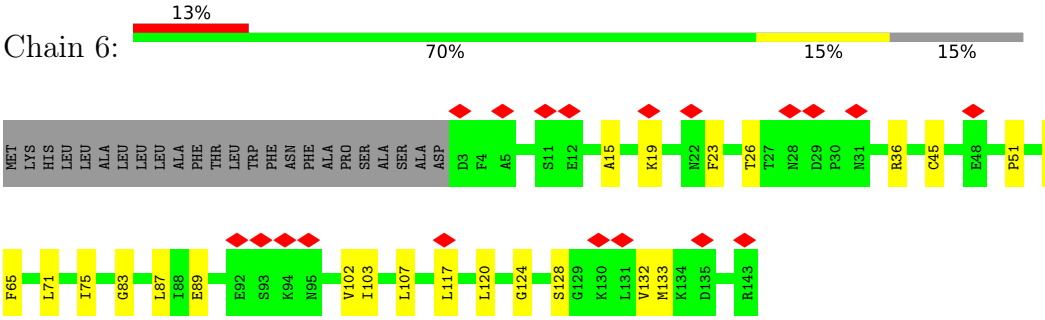


• Molecule 6: Photosystem I reaction center subunit III



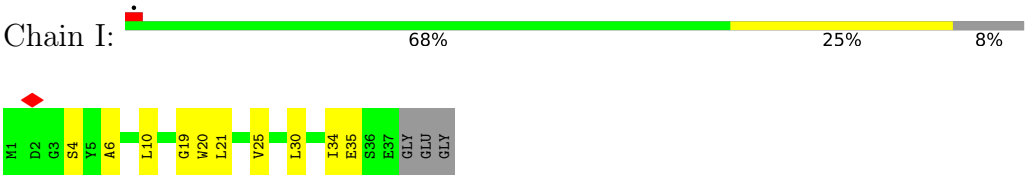
• Molecule 6: Photosystem I reaction center subunit III

Chain 6:



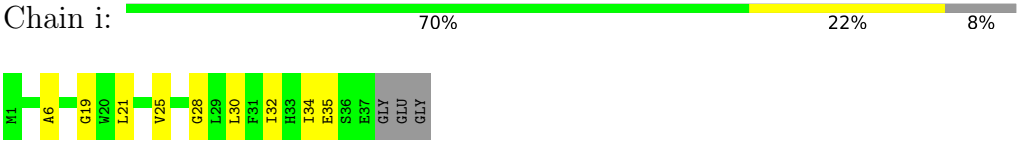
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



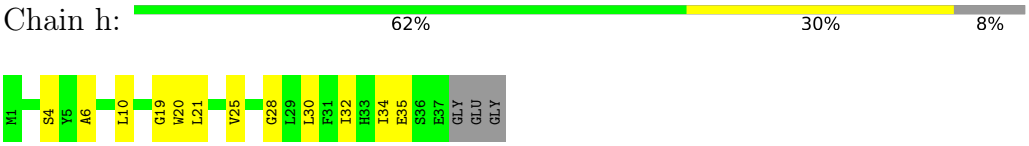
• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:



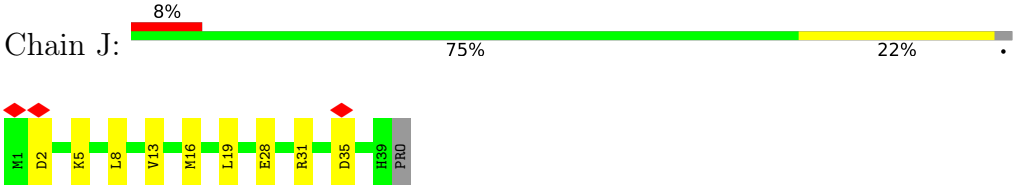
• Molecule 7: Photosystem I reaction center subunit VIII

Chain h:



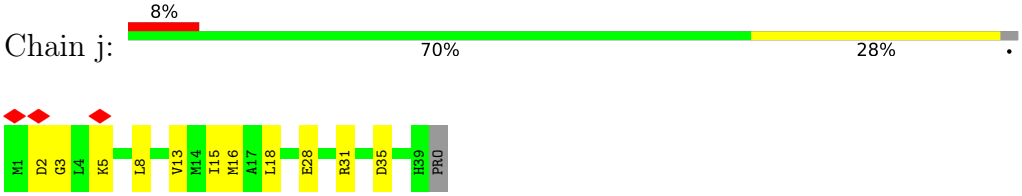
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



• Molecule 8: Photosystem I reaction center subunit IX

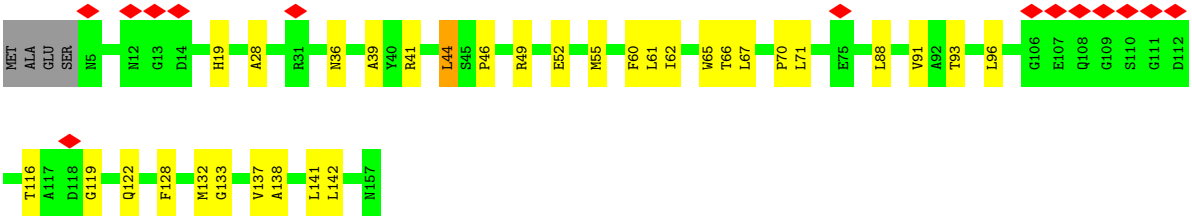
Chain j:



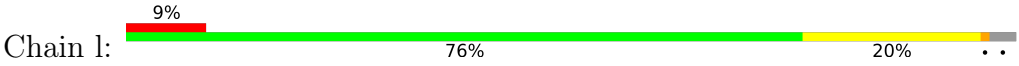
• Molecule 8: Photosystem I reaction center subunit IX

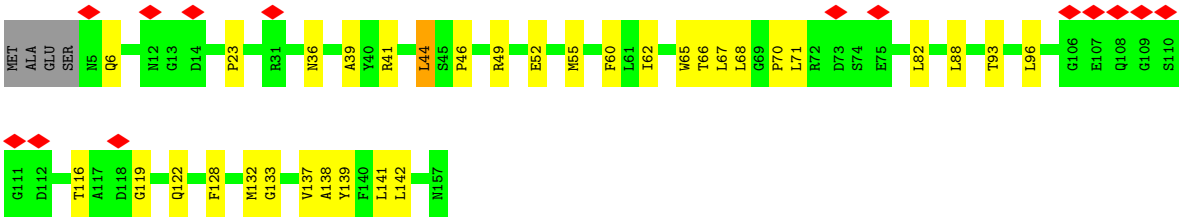
Chain 7:

• Molecule 9: Photosystem I reaction center subunit XI

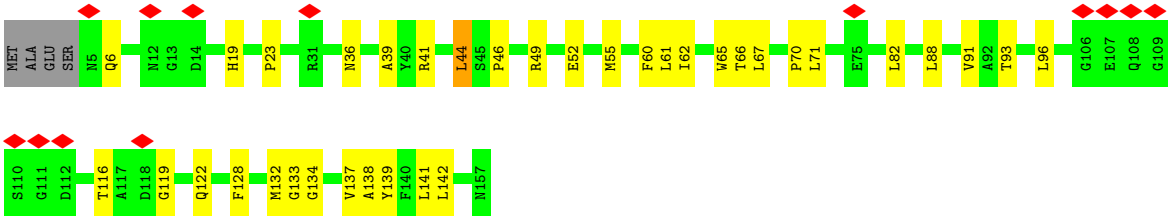


• Molecule 9: Photosystem I reaction center subunit XI

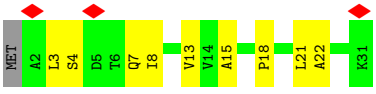




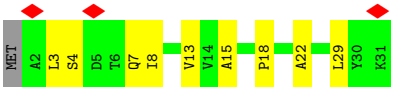
• Molecule 9: Photosystem I reaction center subunit XI



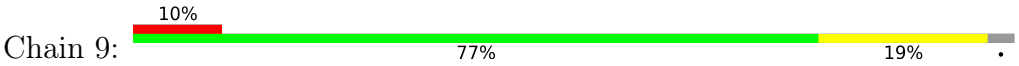
• Molecule 10: Photosystem I reaction center subunit XII

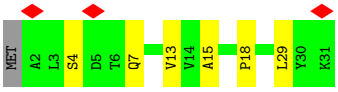


• Molecule 10: Photosystem I reaction center subunit XII

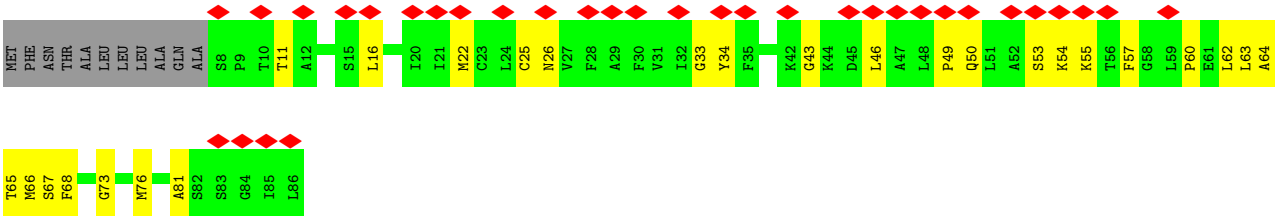


• Molecule 10: Photosystem I reaction center subunit XII

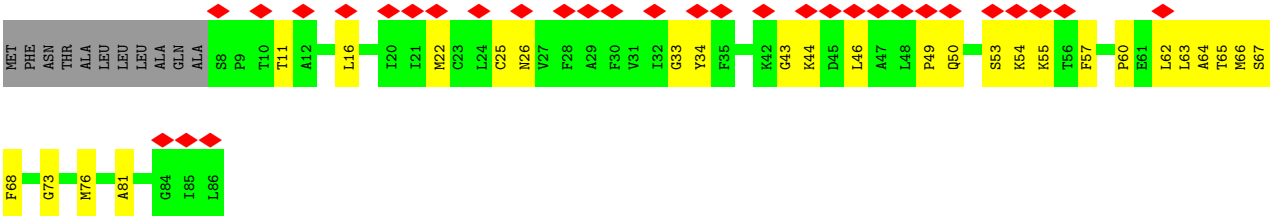




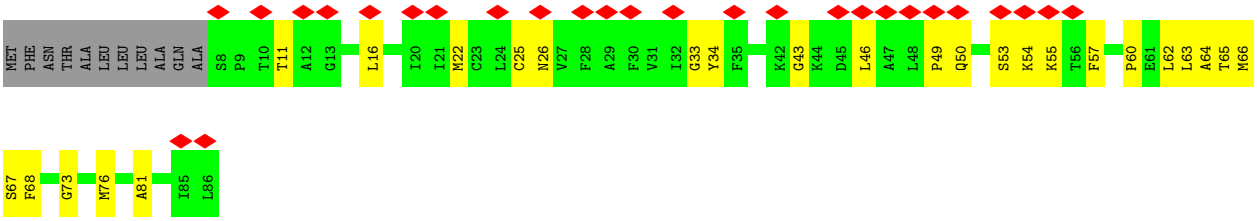
• Molecule 11: Photosystem I reaction center subunit PsaK 2



• Molecule 11: Photosystem I reaction center subunit PsaK 2



• Molecule 11: Photosystem I reaction center subunit PsaK 2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.229	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0187	Depositor
Map size (Å)	325.5, 325.5, 325.5	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: BCR, LMG, CLA, CA, LHG, PQN, SF4, CL0, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.43	0/5985	0.53	1/8158 (0.0%)
1	A	0.43	0/5985	0.53	1/8158 (0.0%)
1	a	0.43	0/5985	0.53	1/8158 (0.0%)
2	2	0.44	0/6021	0.51	0/8237
2	B	0.44	0/6021	0.51	0/8237
2	b	0.44	0/6021	0.51	0/8237
3	3	0.40	0/610	0.54	0/826
3	C	0.40	0/610	0.54	0/826
3	c	0.40	0/610	0.54	0/826
4	4	0.30	0/1102	0.57	0/1485
4	D	0.30	0/1102	0.57	0/1485
4	d	0.31	0/1102	0.57	0/1485
5	5	0.30	0/546	0.48	0/738
5	E	0.30	0/546	0.48	0/738
5	e	0.30	0/546	0.48	0/738
6	6	0.26	0/1116	0.54	0/1520
6	F	0.26	0/1116	0.54	0/1520
6	f	0.26	0/1116	0.54	0/1520
7	I	0.38	0/304	0.56	0/416
7	h	0.38	0/304	0.56	0/416
7	i	0.38	0/304	0.56	0/416
8	7	0.30	0/319	0.61	0/431
8	J	0.30	0/319	0.62	0/431
8	j	0.30	0/319	0.61	0/431
9	0	0.35	0/1168	0.47	0/1588
9	L	0.35	0/1168	0.47	0/1588
9	l	0.35	0/1168	0.47	0/1588
10	9	0.28	0/233	0.44	0/316
10	M	0.28	0/233	0.44	0/316
10	m	0.28	0/233	0.44	0/316
11	8	0.24	0/577	0.56	0/778
11	K	0.24	0/577	0.56	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	k	0.24	0/577	0.56	0/778
All	All	0.40	0/53943	0.52	3/73479 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	671	MET	CB-CG-SD	6.80	133.10	112.70
1	a	671	MET	CB-CG-SD	6.79	133.05	112.70
1	1	671	MET	CB-CG-SD	6.78	133.04	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5787	0	5646	108	0
1	A	5787	0	5646	101	0
1	a	5787	0	5646	108	0
2	2	5806	0	5567	116	0
2	B	5806	0	5567	125	0
2	b	5806	0	5567	120	0
3	3	600	0	581	12	0
3	C	600	0	581	13	0
3	c	600	0	581	16	0
4	4	1078	0	1076	29	0
4	D	1078	0	1076	31	0
4	d	1078	0	1076	29	0
5	5	537	0	520	9	0
5	E	537	0	520	8	0
5	e	537	0	520	10	0
6	6	1086	0	1063	18	0
6	F	1086	0	1063	11	0
6	f	1086	0	1063	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	293	0	292	10	0
7	h	293	0	292	12	0
7	i	293	0	292	8	0
8	7	311	0	321	13	0
8	J	311	0	321	7	0
8	j	311	0	321	8	0
9	0	1138	0	1107	32	0
9	L	1138	0	1107	27	0
9	l	1138	0	1107	29	0
10	9	230	0	248	4	0
10	M	230	0	248	9	0
10	m	230	0	248	8	0
11	8	566	0	598	22	0
11	K	566	0	598	23	0
11	k	566	0	598	25	0
12	1	82	0	110	5	0
12	2	39	0	51	2	0
12	9	39	0	48	0	0
12	A	82	0	110	5	0
12	B	39	0	51	2	0
12	M	39	0	48	0	0
12	a	82	0	110	7	0
12	b	39	0	51	2	0
12	m	39	0	48	1	0
13	1	65	0	72	0	0
13	A	65	0	72	0	0
13	a	65	0	72	3	0
14	0	260	0	288	22	0
14	1	2331	0	2248	126	0
14	2	2342	0	2160	112	0
14	6	90	0	66	5	0
14	7	147	0	130	8	0
14	8	145	0	115	4	0
14	A	2345	0	2279	131	0
14	B	2407	0	2232	123	0
14	F	141	0	107	5	0
14	J	82	0	58	2	0
14	K	145	0	115	5	0
14	L	195	0	216	15	0
14	a	2395	0	2315	131	0
14	b	2347	0	2173	112	0
14	f	141	0	107	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	j	82	0	58	2	0
14	k	90	0	66	3	0
14	l	260	0	288	30	0
15	1	33	0	46	1	0
15	2	33	0	46	6	0
15	A	33	0	46	1	0
15	B	33	0	46	9	0
15	a	33	0	46	1	0
15	b	33	0	46	8	0
16	1	8	0	0	0	0
16	3	16	0	0	1	0
16	A	8	0	0	0	0
16	C	16	0	0	1	0
16	a	8	0	0	0	0
16	c	16	0	0	1	0
17	0	120	0	168	18	0
17	1	200	0	280	16	0
17	2	225	0	313	21	0
17	6	120	0	168	10	0
17	7	80	0	112	7	0
17	8	80	0	112	5	0
17	9	40	0	56	4	0
17	A	200	0	280	17	0
17	B	265	0	369	28	0
17	F	80	0	112	4	0
17	I	80	0	112	6	0
17	J	80	0	112	5	0
17	K	80	0	112	6	0
17	L	80	0	112	10	0
17	M	40	0	56	5	0
17	a	200	0	280	16	0
17	b	305	0	425	32	0
17	f	80	0	112	5	0
17	h	80	0	112	6	0
17	i	80	0	112	5	0
17	j	80	0	112	4	0
17	k	80	0	112	5	0
17	l	40	0	56	1	0
18	0	84	0	108	3	0
18	1	32	0	34	0	0
18	2	48	0	66	3	0
18	A	78	0	96	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	48	0	66	4	0
18	L	38	0	46	1	0
18	a	78	0	96	1	0
18	b	48	0	66	3	0
18	l	38	0	46	1	0
19	6	35	0	43	0	0
19	F	35	0	43	0	0
19	I	35	0	46	1	0
19	f	35	0	44	0	0
19	h	35	0	46	1	0
19	i	35	0	46	1	0
20	0	1	0	0	0	0
20	L	1	0	0	0	0
20	l	1	0	0	0	0
All	All	72606	0	71884	1622	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 11.

All (1622) 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:A:315:TRP:HB3	11:K:60:PRO:HB3	1.58	0.85
14:A:812:CLA:HBB2	14:A:815:CLA:HMA3	1.61	0.82
1:a:315:TRP:HB3	11:k:60:PRO:HB3	1.62	0.81
14:a:813:CLA:HBB2	14:a:816:CLA:HMA3	1.61	0.81
14:1:811:CLA:HBB2	14:1:814:CLA:HMA3	1.61	0.81
14:b:822:CLA:HBB1	17:b:846:BCR:H17C	1.64	0.80
14:B:823:CLA:HBB1	17:B:847:BCR:H17C	1.64	0.78
1:1:398:GLY:HA3	1:1:602:LEU:HD11	1.66	0.77
1:A:398:GLY:HA3	1:A:602:LEU:HD11	1.66	0.77
14:2:822:CLA:HBB1	17:2:846:BCR:H17C	1.64	0.77
14:b:813:CLA:HBB2	14:b:815:CLA:HMA3	1.68	0.76
1:a:398:GLY:HA3	1:a:602:LEU:HD11	1.66	0.75
14:2:813:CLA:HBB2	14:2:815:CLA:HMA3	1.68	0.75
14:B:814:CLA:HBB2	14:B:816:CLA:HMA3	1.68	0.74
1:1:71:LYS:NZ	14:1:812:CLA:OBD	2.21	0.73
1:A:71:LYS:NZ	14:A:813:CLA:OBD	2.21	0.73
1:a:71:LYS:NZ	14:a:814:CLA:OBD	2.21	0.72
17:b:853:BCR:H16C	17:f:203:BCR:HC32	1.70	0.72
14:a:805:CLA:H91	14:b:806:CLA:H112	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:PHE:HB2	7:I:34:ILE:HA	1.73	0.71
14:B:809:CLA:H162	14:B:831:CLA:HBB2	1.72	0.70
2:b:56:ILE:HD11	17:b:854:BCR:HC7	1.74	0.70
14:b:809:CLA:H162	14:b:830:CLA:HBB2	1.73	0.70
14:a:804:CLA:H3A	14:a:804:CLA:H12	1.74	0.69
14:2:801:CLA:H3A	14:2:801:CLA:H12	1.74	0.69
14:b:834:CLA:HBB1	17:f:203:BCR:H323	1.75	0.69
14:2:808:CLA:H162	14:2:830:CLA:HBB2	1.73	0.69
14:2:834:CLA:HBB1	17:6:4402:BCR:H323	1.75	0.69
14:B:828:CLA:H2	14:B:837:CLA:HBB2	1.75	0.69
14:b:827:CLA:H2	14:b:836:CLA:HBB2	1.75	0.68
14:2:827:CLA:H2	14:2:836:CLA:HBB2	1.75	0.68
14:B:801:CLA:H3A	14:B:801:CLA:H12	1.74	0.68
1:1:315:TRP:HB3	11:8:60:PRO:HB3	1.74	0.68
2:b:5:PHE:HB2	7:i:34:ILE:HA	1.75	0.68
2:2:5:PHE:HB2	7:h:34:ILE:HA	1.74	0.68
14:B:835:CLA:HBB1	17:F:203:BCR:H323	1.75	0.68
9:l:133:GLY:HA3	17:0:204:BCR:H393	1.76	0.67
9:0:133:GLY:HA3	17:0:210:BCR:H393	1.76	0.67
14:1:809:CLA:H71	17:7:1104:BCR:H372	1.75	0.67
4:D:123:GLY:N	5:E:15:GLU:OE2	2.27	0.67
11:8:49:PRO:HB2	11:8:55:LYS:HA	1.77	0.66
9:L:133:GLY:HA3	17:L:1505:BCR:H393	1.76	0.66
11:k:49:PRO:HB2	11:k:55:LYS:HA	1.77	0.66
2:B:56:ILE:HD11	17:M:102:BCR:HC7	1.77	0.66
11:K:49:PRO:HB2	11:K:55:LYS:HA	1.77	0.66
14:1:829:CLA:H18	17:7:1104:BCR:H10C	1.77	0.65
11:K:76:MET:HE2	14:K:4004:CLA:HHC	1.80	0.64
14:a:835:CLA:H122	14:b:842:CLA:H2	1.78	0.64
14:b:825:CLA:HAB	14:b:832:CLA:HMD2	1.80	0.64
11:8:76:MET:HE2	14:8:4004:CLA:HHC	1.80	0.64
14:F:205:CLA:HMB2	17:F:206:BCR:H24C	1.79	0.64
17:a:851:BCR:H373	2:b:432:LEU:HD23	1.80	0.64
14:B:826:CLA:HAB	14:B:833:CLA:HMD2	1.80	0.64
4:4:121:ARG:NH1	5:5:65:GLU:OE2	2.31	0.64
14:A:817:CLA:H2A	14:A:817:CLA:HED3	1.79	0.64
14:A:830:CLA:H18	17:J:103:BCR:H10C	1.79	0.63
14:a:854:CLA:HHC	11:k:76:MET:HE2	1.80	0.63
1:A:221:MET:HE2	1:A:291:SER:HA	1.80	0.63
1:a:221:MET:HE2	1:a:291:SER:HA	1.80	0.63
14:2:806:CLA:H3A	10:9:29:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:6:4404:CLA:HMB2	17:6:4405:BCR:H24C	1.79	0.63
14:f:205:CLA:HMB2	17:f:206:BCR:H24C	1.79	0.63
2:B:453:ILE:HD11	17:B:854:BCR:H342	1.80	0.63
1:A:355:ASN:ND2	14:A:807:CLA:OBD	2.30	0.63
11:8:50:GLN:HA	11:8:54:LYS:HA	1.81	0.63
11:k:50:GLN:HA	11:k:54:LYS:HA	1.81	0.63
14:f:201:CLA:HMC2	17:f:203:BCR:H381	1.79	0.63
3:C:61:ASP:O	5:E:59:ASN:ND2	2.30	0.63
14:2:825:CLA:HAB	14:2:832:CLA:HMD2	1.80	0.63
14:1:816:CLA:H2A	14:1:816:CLA:HED3	1.79	0.62
1:A:313:THR:HG22	1:A:314:ASN:H	1.64	0.62
11:K:50:GLN:HA	11:K:54:LYS:HA	1.81	0.62
14:1:804:CLA:H91	14:2:805:CLA:H112	1.82	0.62
6:6:103:ILE:O	8:7:9:SER:OG	2.14	0.62
1:a:76:HIS:ND1	14:a:816:CLA:OBD	2.32	0.62
1:a:313:THR:HG22	1:a:314:ASN:H	1.64	0.62
14:A:831:CLA:H121	17:A:848:BCR:H21C	1.81	0.62
17:6:4402:BCR:HC32	17:6:4406:BCR:H16C	1.82	0.62
14:a:818:CLA:HED3	14:a:818:CLA:H2A	1.79	0.62
1:1:221:MET:HE2	1:1:291:SER:HA	1.80	0.62
1:1:313:THR:HG22	1:1:314:ASN:H	1.64	0.62
2:2:20:ARG:NH2	7:h:34:ILE:O	2.26	0.62
1:a:197:MET:HE1	14:a:824:CLA:HMA1	1.82	0.62
14:a:832:CLA:H121	17:a:848:BCR:H21C	1.81	0.62
1:A:197:MET:HE1	14:A:823:CLA:HMA1	1.82	0.62
1:1:197:MET:HE1	14:1:822:CLA:HMA1	1.82	0.62
1:a:373:MET:HE2	14:a:830:CLA:HMC2	1.82	0.61
1:A:76:HIS:ND1	14:A:815:CLA:OBD	2.32	0.61
14:1:842:CLA:HMC2	14:2:801:CLA:H143	1.82	0.61
14:A:842:CLA:HMC2	14:B:801:CLA:H143	1.83	0.61
14:1:830:CLA:H121	17:1:848:BCR:H21C	1.81	0.61
1:1:373:MET:HE2	14:1:828:CLA:HMC2	1.82	0.61
8:j:28:GLU:OE1	8:j:31:ARG:NH1	2.34	0.61
2:b:286:ILE:HG22	17:b:846:BCR:H14C	1.83	0.61
2:b:453:ILE:HD11	17:b:853:BCR:H342	1.82	0.61
8:7:28:GLU:OE1	8:7:31:ARG:NH1	2.34	0.61
1:a:413:VAL:HG21	1:a:570:PHE:HB2	1.83	0.61
2:B:596:HIS:HE1	2:B:730:THR:HG23	1.66	0.60
8:J:28:GLU:OE1	8:J:31:ARG:NH1	2.34	0.60
1:1:413:VAL:HG21	1:1:570:PHE:HB2	1.83	0.60
2:b:596:HIS:HE1	2:b:730:THR:HG23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:61:ASP:O	5:5:59:ASN:ND2	2.32	0.60
17:b:850:BCR:H403	17:b:850:BCR:H371	1.84	0.60
1:A:413:VAL:HG21	1:A:570:PHE:HB2	1.83	0.60
14:a:804:CLA:H143	14:a:842:CLA:HMC2	1.83	0.60
9:0:116:THR:HG23	9:0:119:GLY:H	1.67	0.60
1:A:278:LYS:HG3	1:A:502:LEU:HD12	1.84	0.60
9:L:116:THR:HG23	9:L:119:GLY:H	1.67	0.60
14:2:812:CLA:H122	9:l:141:LEU:HD21	1.83	0.60
17:2:850:BCR:H403	17:2:850:BCR:H371	1.84	0.60
17:B:851:BCR:H403	17:B:851:BCR:H371	1.84	0.60
2:2:596:HIS:HE1	2:2:730:THR:HG23	1.66	0.60
2:B:397:ASP:HA	4:D:129:VAL:HG11	1.82	0.60
14:b:809:CLA:HBA2	14:b:831:CLA:HMB2	1.84	0.60
9:l:116:THR:HG23	9:l:119:GLY:H	1.67	0.59
1:a:278:LYS:HG3	1:a:502:LEU:HD12	1.84	0.59
9:l:36:ASN:HD21	18:l:4202:LMG:HC1	1.68	0.59
17:B:854:BCR:H16C	17:F:203:BCR:HC32	1.84	0.59
14:a:829:CLA:H2	14:a:837:CLA:HBB2	1.85	0.59
14:a:830:CLA:HMB3	14:a:837:CLA:H12	1.83	0.59
1:1:53:ALA:HB1	1:1:571:ARG:HH12	1.68	0.59
1:A:373:MET:HE2	14:A:829:CLA:HMC2	1.82	0.59
1:a:355:ASN:ND2	14:a:808:CLA:OBD	2.30	0.59
14:1:828:CLA:HMB3	14:1:835:CLA:H12	1.83	0.59
14:1:841:CLA:HMC2	17:6:4402:BCR:H381	1.84	0.59
1:A:337:HIS:NE2	12:A:802:LHG:O1	2.32	0.59
14:A:828:CLA:H2	14:A:836:CLA:HBB2	1.85	0.59
14:A:829:CLA:HMB3	14:A:836:CLA:H12	1.83	0.59
2:B:206:HIS:O	2:B:211:ASN:ND2	2.35	0.59
14:a:811:CLA:H2	14:a:831:CLA:H42	1.84	0.59
2:b:430:HIS:CG	17:b:853:BCR:H323	2.37	0.59
14:2:825:CLA:HBB2	14:2:832:CLA:HHD	1.84	0.59
14:1:809:CLA:H2	14:1:829:CLA:H42	1.84	0.59
2:2:432:LEU:HD13	14:2:803:CLA:HMB2	1.85	0.59
14:2:808:CLA:HBA2	14:2:831:CLA:HMB2	1.84	0.59
14:A:828:CLA:HAB	17:A:850:BCR:H311	1.85	0.59
2:B:286:ILE:HG22	17:B:847:BCR:H14C	1.83	0.59
2:B:432:LEU:HD13	14:B:804:CLA:HMB2	1.85	0.59
1:a:168:MET:HE2	1:a:172:MET:HE2	1.84	0.59
2:b:432:LEU:HD13	14:b:804:CLA:HMB2	1.85	0.59
2:2:426:PHE:O	2:2:430:HIS:ND1	2.36	0.59
2:B:426:PHE:O	2:B:430:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:843:CLA:HMC2	17:B:852:BCR:H381	1.85	0.58
2:2:286:ILE:HG22	17:2:846:BCR:H14C	1.83	0.58
1:A:369:HIS:ND1	14:A:820:CLA:OBD	2.35	0.58
2:b:426:PHE:O	2:b:430:HIS:ND1	2.36	0.58
1:A:53:ALA:HB1	1:A:571:ARG:HH12	1.68	0.58
1:A:168:MET:HE2	1:A:172:MET:HE2	1.85	0.58
14:A:810:CLA:H2	14:A:830:CLA:H42	1.84	0.58
14:B:826:CLA:HBB2	14:B:833:CLA:HHD	1.84	0.58
14:a:836:CLA:H8	9:l:60:PHE:HZ	1.68	0.58
14:1:838:CLA:H152	14:0:202:CLA:H193	1.85	0.58
2:b:206:HIS:O	2:b:211:ASN:ND2	2.35	0.58
2:b:349:HIS:ND1	14:b:819:CLA:OBD	2.35	0.58
9:0:62:ILE:HG13	9:0:138:ALA:HB3	1.86	0.58
1:1:76:HIS:ND1	14:1:814:CLA:OBD	2.32	0.58
1:1:369:HIS:ND1	14:1:819:CLA:OBD	2.35	0.58
2:2:561:ASP:OD2	2:2:565:ARG:NH2	2.37	0.58
14:B:809:CLA:HBA2	14:B:832:CLA:HMB2	1.84	0.58
1:1:168:MET:HE2	1:1:172:MET:HE2	1.85	0.58
14:1:827:CLA:H2	14:1:835:CLA:HBB2	1.85	0.58
4:d:123:GLY:N	5:e:15:GLU:OE2	2.36	0.58
2:B:220:ALA:HB1	2:B:224:PRO:HG2	1.86	0.58
2:2:397:ASP:HB2	4:4:129:VAL:HG21	1.85	0.58
8:7:15:ILE:HG21	14:7:1101:CLA:HED1	1.85	0.58
2:B:110:SER:HB3	7:I:4:SER:HB3	1.86	0.58
1:1:332:PHE:O	1:1:428:ARG:NH1	2.37	0.58
1:1:694:GLN:NE2	5:5:46:TYR:OH	2.37	0.58
14:1:834:CLA:H152	17:h:102:BCR:H372	1.85	0.58
14:1:842:CLA:H102	8:7:16:MET:HE1	1.84	0.58
2:2:691:LEU:HD11	9:0:39:ALA:HB1	1.86	0.58
14:A:842:CLA:H102	8:J:16:MET:HE1	1.85	0.58
2:B:561:ASP:OD2	2:B:565:ARG:NH2	2.37	0.58
9:l:62:ILE:HG13	9:l:138:ALA:HB3	1.86	0.58
3:c:17:CYS:HB3	16:c:102:SF4:S4	2.44	0.57
9:L:62:ILE:HG13	9:L:138:ALA:HB3	1.86	0.57
1:a:53:ALA:HB1	1:a:571:ARG:HH12	1.68	0.57
1:a:400:LEU:HD21	14:a:809:CLA:H142	1.86	0.57
14:a:829:CLA:HAB	17:a:850:BCR:H311	1.85	0.57
1:a:586:SER:OG	1:a:589:ASP:OD1	2.22	0.57
1:1:586:SER:OG	1:1:589:ASP:OD1	2.22	0.57
14:1:827:CLA:HAB	17:1:850:BCR:H311	1.85	0.57
14:a:831:CLA:H18	17:j:103:BCR:H10C	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:278:LYS:HG3	1:1:502:LEU:HD12	1.84	0.57
2:b:561:ASP:OD2	2:b:565:ARG:NH2	2.37	0.57
2:2:206:HIS:O	2:2:211:ASN:ND2	2.35	0.57
1:A:113:SER:HB2	1:A:130:VAL:HG21	1.87	0.57
14:B:801:CLA:HMB2	14:B:804:CLA:HBB1	1.86	0.57
14:B:813:CLA:HAB	7:I:19:GLY:HA3	1.86	0.57
17:1:851:BCR:H24C	14:2:835:CLA:HMC2	1.86	0.57
14:b:825:CLA:HBB2	14:b:832:CLA:HHD	1.84	0.57
14:b:842:CLA:HMC2	17:b:851:BCR:H381	1.85	0.57
14:A:810:CLA:HAB	14:A:830:CLA:H112	1.87	0.57
3:C:17:CYS:HB3	16:C:102:SF4:S4	2.45	0.57
1:a:332:PHE:O	1:a:428:ARG:NH1	2.37	0.57
2:b:220:ALA:HB1	2:b:224:PRO:HG2	1.86	0.57
2:b:403:ASP:OD2	2:b:408:ARG:NH2	2.38	0.57
2:b:581:MET:HG3	2:b:711:LEU:HD21	1.87	0.57
14:2:842:CLA:HMC2	17:2:851:BCR:H381	1.85	0.57
1:A:220:SER:HB3	1:A:290:LEU:HD23	1.87	0.57
1:a:86:TRP:HA	14:a:810:CLA:HBB2	1.87	0.57
14:a:811:CLA:HAB	14:a:831:CLA:H112	1.87	0.57
3:3:17:CYS:HB3	16:3:102:SF4:S4	2.44	0.57
1:A:332:PHE:O	1:A:428:ARG:NH1	2.37	0.57
1:A:586:SER:OG	1:A:589:ASP:OD1	2.22	0.57
1:1:355:ASN:ND2	14:1:806:CLA:OBD	2.30	0.57
2:B:581:MET:HG3	2:B:711:LEU:HD21	1.87	0.57
1:a:220:SER:HB3	1:a:290:LEU:HD23	1.87	0.57
5:e:28:VAL:HG13	5:e:37:VAL:HG22	1.87	0.57
14:a:840:CLA:H152	14:b:801:CLA:H193	1.85	0.56
14:1:809:CLA:HAB	14:1:829:CLA:H112	1.87	0.56
2:2:403:ASP:OD2	2:2:408:ARG:NH2	2.38	0.56
14:A:839:CLA:H152	14:B:802:CLA:H193	1.85	0.56
14:A:843:CLA:HBC1	15:B:846:PQN:H191	1.87	0.56
1:a:337:HIS:NE2	12:a:802:LHG:O1	2.32	0.56
1:1:220:SER:HB3	1:1:290:LEU:HD23	1.87	0.56
14:2:809:CLA:HMB3	14:2:810:CLA:HHB	1.87	0.56
1:A:86:TRP:HA	14:A:809:CLA:HBB2	1.87	0.56
2:B:403:ASP:OD2	2:B:408:ARG:NH2	2.38	0.56
14:F:201:CLA:HMC2	17:F:203:BCR:H381	1.86	0.56
1:1:400:LEU:HD21	14:1:807:CLA:H142	1.86	0.56
5:5:28:VAL:HG13	5:5:37:VAL:HG22	1.87	0.56
3:C:29:VAL:HG12	4:D:112:ARG:HB2	1.87	0.56
9:L:36:ASN:HD21	18:L:1506:LMG:HC1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:613:MET:HE2	14:a:839:CLA:HBC1	1.88	0.56
4:D:30:ILE:HD13	4:D:68:LEU:HD23	1.88	0.56
14:0:206:CLA:H43	17:0:210:BCR:H12C	1.88	0.56
1:A:671:MET:HG3	1:A:740:TRP:HZ3	1.71	0.56
1:a:369:HIS:ND1	14:a:821:CLA:OBD	2.35	0.56
1:a:671:MET:HG3	1:a:740:TRP:HZ3	1.71	0.56
1:1:86:TRP:HA	14:1:808:CLA:HBB2	1.87	0.56
1:1:113:SER:HB2	1:1:130:VAL:HG21	1.87	0.56
1:1:473:ASP:O	1:1:477:GLN:NE2	2.38	0.56
2:b:671:TYR:OH	14:b:806:CLA:OBD	2.21	0.56
1:A:400:LEU:HD21	14:A:808:CLA:H142	1.86	0.56
2:B:66:PHE:HZ	10:M:8:ILE:HG23	1.70	0.56
1:a:113:SER:HB2	1:a:130:VAL:HG21	1.87	0.56
1:1:671:MET:HG3	1:1:740:TRP:HZ3	1.71	0.56
14:b:810:CLA:HMB3	14:b:811:CLA:HHB	1.87	0.56
2:2:50:HIS:ND1	14:2:815:CLA:OBD	2.38	0.56
2:2:220:ALA:HB1	2:2:224:PRO:HG2	1.86	0.56
2:2:349:HIS:ND1	14:2:819:CLA:OBD	2.35	0.56
1:A:473:ASP:O	1:A:477:GLN:NE2	2.38	0.56
14:A:804:CLA:H91	14:B:806:CLA:H112	1.87	0.56
14:L:1503:CLA:H151	14:l:4203:CLA:H112	1.88	0.56
1:A:319:HIS:NE2	14:A:825:CLA:OBD	2.32	0.55
10:M:4:SER:HB3	10:M:7:GLN:HG3	1.88	0.55
1:a:473:ASP:O	1:a:477:GLN:NE2	2.38	0.55
2:b:426:PHE:CZ	17:b:853:BCR:HC21	2.41	0.55
1:A:694:GLN:NE2	5:E:46:TYR:OH	2.39	0.55
2:2:61:THR:HG23	2:2:142:LEU:HD13	1.89	0.55
4:4:41:GLU:O	4:4:71:GLN:NE2	2.40	0.55
14:a:806:CLA:HMB3	14:a:842:CLA:H43	1.89	0.55
4:4:30:ILE:HD13	4:4:68:LEU:HD23	1.88	0.55
14:B:810:CLA:HMB3	14:B:811:CLA:HHB	1.87	0.55
2:2:492:ASN:HD22	2:2:495:LEU:HD22	1.72	0.55
10:m:4:SER:HB3	10:m:7:GLN:HG3	1.88	0.55
14:A:834:CLA:H193	15:B:846:PQN:H293	1.88	0.55
2:B:520:VAL:HG11	2:B:594:TYR:HB2	1.89	0.55
14:B:826:CLA:HBB1	12:B:853:LHG:HC92	1.89	0.55
4:D:41:GLU:O	4:D:71:GLN:NE2	2.40	0.55
4:d:41:GLU:O	4:d:71:GLN:NE2	2.40	0.55
14:L:1501:CLA:H43	17:L:1505:BCR:H12C	1.88	0.55
1:a:560:ARG:HH12	2:b:681:TRP:HB2	1.71	0.55
1:1:337:HIS:NE2	12:1:802:LHG:O1	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:842:CLA:H43	14:7:1101:CLA:HMB3	1.89	0.55
4:d:30:ILE:HD13	4:d:68:LEU:HD23	1.88	0.55
14:A:805:CLA:HMB3	14:A:842:CLA:H43	1.89	0.55
14:A:821:CLA:H93	14:A:831:CLA:H171	1.89	0.55
2:B:691:LEU:HD11	9:L:39:ALA:HB1	1.88	0.55
2:b:520:VAL:HG11	2:b:594:TYR:HB2	1.89	0.55
17:6:4406:BCR:H403	17:6:4406:BCR:H371	1.89	0.55
2:B:492:ASN:HD22	2:B:495:LEU:HD22	1.72	0.55
2:2:581:MET:HG3	2:2:711:LEU:HD21	1.87	0.55
17:B:854:BCR:H403	17:B:854:BCR:H371	1.89	0.55
9:L:93:THR:HG21	9:L:128:PHE:HB2	1.89	0.55
1:a:315:TRP:HE1	11:k:44:LYS:HD2	1.72	0.55
14:2:801:CLA:HMB2	14:2:803:CLA:HBB1	1.89	0.55
14:l:4204:CLA:H43	17:0:204:BCR:H12C	1.88	0.55
14:B:813:CLA:H122	9:0:141:LEU:HD21	1.89	0.55
1:1:577:PRO:HD3	2:2:562:GLY:HA2	1.89	0.55
2:b:147:SER:HB2	10:m:18:PRO:HG3	1.89	0.55
14:b:828:CLA:H2	17:b:850:BCR:H353	1.89	0.55
5:E:28:VAL:HG13	5:E:37:VAL:HG22	1.87	0.54
1:a:429:MET:HG2	14:a:824:CLA:H202	1.89	0.54
14:1:834:CLA:H8	9:0:60:PHE:HZ	1.71	0.54
2:b:492:ASN:HD22	2:b:495:LEU:HD22	1.72	0.54
2:2:378:GLY:HA3	2:2:588:LEU:HD11	1.89	0.54
1:A:702:TRP:HH2	14:B:834:CLA:HED3	1.71	0.54
14:A:841:CLA:HBB2	6:F:83:GLY:HA3	1.88	0.54
17:A:851:BCR:H24C	14:B:836:CLA:HMC2	1.88	0.54
4:D:4:LEU:HD11	4:D:88:VAL:HG11	1.89	0.54
17:b:853:BCR:H403	17:b:853:BCR:H371	1.89	0.54
2:2:520:VAL:HG11	2:2:594:TYR:HB2	1.88	0.54
14:2:828:CLA:H2	17:2:850:BCR:H353	1.89	0.54
1:1:613:MET:HE2	14:1:837:CLA:HBC1	1.88	0.54
2:b:61:THR:HG23	2:b:142:LEU:HD13	1.89	0.54
14:2:825:CLA:HBB1	12:2:852:LHG:HC92	1.88	0.54
14:A:835:CLA:H152	17:I:102:BCR:H372	1.90	0.54
4:D:8:PRO:O	4:D:51:ASN:ND2	2.41	0.54
14:a:822:CLA:H93	14:a:832:CLA:H171	1.89	0.54
14:1:819:CLA:HAC1	14:1:835:CLA:H42	1.90	0.54
14:1:820:CLA:H93	14:1:830:CLA:H171	1.89	0.54
10:9:4:SER:HB3	10:9:7:GLN:HG3	1.88	0.54
1:A:317:ILE:HD13	11:K:64:ALA:HB2	1.88	0.54
14:A:842:CLA:H11	15:A:845:PQN:H302	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:829:CLA:H2	17:B:851:BCR:H353	1.89	0.54
1:1:736:ILE:HG23	14:1:829:CLA:HAB	1.88	0.54
14:1:842:CLA:H11	15:1:845:PQN:H302	1.90	0.54
1:a:736:ILE:HG23	14:a:831:CLA:HAB	1.89	0.54
14:a:804:CLA:HMD2	2:b:579:LEU:HB3	1.89	0.54
2:B:378:GLY:HA3	2:B:588:LEU:HD11	1.89	0.54
11:K:62:LEU:HD22	14:K:4003:CLA:HBC2	1.89	0.54
1:a:319:HIS:NE2	14:a:826:CLA:OBD	2.32	0.54
1:1:429:MET:HG2	14:1:822:CLA:H202	1.89	0.54
4:d:107:LYS:O	4:d:112:ARG:NH1	2.41	0.54
9:0:93:THR:HG21	9:0:128:PHE:HB2	1.89	0.54
1:1:342:GLU:N	1:1:342:GLU:OE2	2.41	0.54
4:d:4:LEU:HD11	4:d:88:VAL:HG11	1.89	0.54
11:k:22:MET:O	11:k:26:ASN:ND2	2.41	0.54
1:A:613:MET:HE2	14:A:838:CLA:HBC1	1.88	0.54
1:1:352:LEU:HD11	14:1:831:CLA:HBB1	1.90	0.54
14:1:838:CLA:H93	14:1:838:CLA:HBB1	1.90	0.54
2:b:378:GLY:HA3	2:b:588:LEU:HD11	1.89	0.54
11:k:62:LEU:HD22	14:k:4003:CLA:HBC2	1.89	0.54
14:A:835:CLA:H172	14:L:1502:CLA:HMB2	1.88	0.54
2:B:61:THR:HG23	2:B:142:LEU:HD13	1.89	0.54
4:D:32:TRP:HE1	4:D:50:MET:HE3	1.73	0.54
1:A:429:MET:HG2	14:A:823:CLA:H202	1.89	0.53
17:A:850:BCR:H403	17:A:850:BCR:H371	1.90	0.53
11:K:22:MET:O	11:K:26:ASN:ND2	2.41	0.53
14:a:842:CLA:H11	15:a:845:PQN:H302	1.90	0.53
2:b:131:THR:HG23	2:b:134:GLU:H	1.73	0.53
15:2:845:PQN:H242	17:2:851:BCR:H15C	1.90	0.53
1:A:342:GLU:OE2	1:A:342:GLU:N	2.41	0.53
14:a:821:CLA:HAC1	14:a:837:CLA:H42	1.90	0.53
1:1:702:TRP:HH2	14:2:833:CLA:HED3	1.73	0.53
15:b:845:PQN:H242	17:b:851:BCR:H15C	1.90	0.53
4:d:8:PRO:O	4:d:51:ASN:ND2	2.41	0.53
1:A:736:ILE:HG23	14:A:830:CLA:HAB	1.89	0.53
14:A:820:CLA:HAC1	14:A:836:CLA:H42	1.90	0.53
2:b:29:HIS:ND1	14:b:809:CLA:O1A	2.42	0.53
2:2:131:THR:HG23	2:2:134:GLU:H	1.73	0.53
4:4:4:LEU:HD11	4:4:88:VAL:HG11	1.89	0.53
9:0:36:ASN:HD21	18:0:201:LMG:HC1	1.74	0.53
2:B:671:TYR:OH	14:B:806:CLA:OBD	2.21	0.53
4:D:107:LYS:O	4:D:112:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:342:GLU:N	1:a:342:GLU:OE2	2.41	0.53
14:a:840:CLA:H93	14:a:840:CLA:HBB1	1.90	0.53
14:b:825:CLA:HBB1	12:b:852:LHG:HC92	1.88	0.53
11:8:62:LEU:HD22	14:8:4003:CLA:HBC2	1.89	0.53
1:A:670:ILE:HG23	14:B:804:CLA:H52	1.91	0.53
2:B:29:HIS:ND1	14:B:809:CLA:O1A	2.42	0.53
1:1:225:LYS:HB3	1:1:252:LEU:HD21	1.90	0.53
2:2:56:ILE:HD11	17:9:102:BCR:HC7	1.89	0.53
17:a:850:BCR:H403	17:a:850:BCR:H371	1.90	0.53
2:2:29:HIS:ND1	14:2:808:CLA:O1A	2.42	0.53
9:l:36:ASN:HB3	14:l:4204:CLA:HAC1	1.91	0.53
9:l:93:THR:HG21	9:l:128:PHE:HB2	1.89	0.53
11:K:53:SER:OG	11:K:57:PHE:HB2	2.09	0.53
14:1:807:CLA:HAA1	14:1:831:CLA:HMB2	1.91	0.53
4:4:8:PRO:O	4:4:51:ASN:ND2	2.41	0.53
4:4:107:LYS:O	4:4:112:ARG:NH1	2.41	0.53
11:8:22:MET:O	11:8:26:ASN:ND2	2.41	0.53
2:B:50:HIS:ND1	14:B:816:CLA:OBD	2.38	0.53
3:C:2:SER:N	3:C:71:ALA:O	2.42	0.53
1:a:225:LYS:HB3	1:a:252:LEU:HD21	1.90	0.53
1:a:352:LEU:HD11	14:a:833:CLA:HBB1	1.90	0.53
2:b:50:HIS:ND1	14:b:815:CLA:OBD	2.38	0.53
2:2:453:ILE:HD11	17:6:4406:BCR:H342	1.91	0.53
1:A:225:LYS:HB3	1:A:252:LEU:HD21	1.90	0.53
14:a:843:CLA:HAB	2:b:692:VAL:HG11	1.91	0.53
3:3:2:SER:N	3:3:71:ALA:O	2.42	0.53
9:0:36:ASN:HB3	14:0:206:CLA:HAC1	1.91	0.53
1:A:447:LEU:HB3	1:A:540:PHE:HB2	1.91	0.53
14:A:839:CLA:H93	14:A:839:CLA:HBB1	1.90	0.53
2:B:131:THR:HG23	2:B:134:GLU:H	1.73	0.53
4:D:61:ARG:NH1	4:D:63:GLU:OE2	2.42	0.53
6:F:36:ARG:NH1	8:J:35:ASP:OD2	2.35	0.53
17:b:854:BCR:H24C	10:m:13:VAL:HG12	1.91	0.53
4:4:32:TRP:HE1	4:4:50:MET:HE3	1.73	0.53
4:4:87:ARG:HB2	4:4:97:LEU:HD11	1.91	0.53
1:A:352:LEU:HD11	14:A:832:CLA:HBB1	1.90	0.52
10:M:13:VAL:HG12	17:M:102:BCR:H24C	1.91	0.52
14:a:804:CLA:HMB2	14:b:804:CLA:HBB1	1.91	0.52
17:1:850:BCR:H403	17:1:850:BCR:H371	1.90	0.52
4:d:87:ARG:HB2	4:d:97:LEU:HD11	1.91	0.52
4:4:123:GLY:N	5:5:15:GLU:OE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:63:LEU:O	11:k:67:SER:CB	2.57	0.52
15:B:846:PQN:H242	17:B:852:BCR:H15C	1.90	0.52
11:K:63:LEU:O	11:K:67:SER:CB	2.57	0.52
14:a:809:CLA:HAA1	14:a:833:CLA:HMB2	1.91	0.52
1:A:204:LEU:HD11	14:A:815:CLA:H42	1.92	0.52
4:D:87:ARG:HB2	4:D:97:LEU:HD11	1.91	0.52
1:a:204:LEU:HD11	14:a:816:CLA:H42	1.92	0.52
1:1:447:LEU:HB3	1:1:540:PHE:HB2	1.91	0.52
14:2:840:CLA:H93	14:2:841:CLA:HBC1	1.92	0.52
11:k:53:SER:OG	11:k:57:PHE:HB2	2.09	0.52
11:8:57:PHE:HE2	11:8:62:LEU:HD23	1.75	0.52
1:a:140:THR:HG22	1:a:384:ALA:HB1	1.92	0.52
1:a:343:ILE:HD11	1:a:421:ASN:HD22	1.74	0.52
1:1:140:THR:HG22	1:1:384:ALA:HB1	1.92	0.52
4:4:84:LYS:HB3	4:4:96:TYR:HE1	1.75	0.52
1:A:343:ILE:HD11	1:A:421:ASN:HD22	1.74	0.52
14:A:828:CLA:H11	14:A:839:CLA:HBA1	1.92	0.52
4:D:84:LYS:HB3	4:D:96:TYR:HE1	1.75	0.52
1:a:447:LEU:HB3	1:a:540:PHE:HB2	1.90	0.52
3:c:2:SER:N	3:c:71:ALA:O	2.42	0.52
11:8:53:SER:OG	11:8:57:PHE:HB2	2.09	0.52
10:9:13:VAL:HG12	17:9:102:BCR:H24C	1.91	0.52
1:1:204:LEU:HD11	14:1:814:CLA:H42	1.92	0.52
14:2:803:CLA:H201	17:7:1104:BCR:H362	1.92	0.52
11:k:57:PHE:HE2	11:k:62:LEU:HD23	1.75	0.52
14:A:835:CLA:H8	9:L:60:PHE:HZ	1.74	0.52
11:K:68:PHE:HB2	17:K:4001:BCR:H23C	1.90	0.52
1:a:694:GLN:NE2	5:e:46:TYR:OH	2.42	0.52
14:1:827:CLA:H11	14:1:838:CLA:HBA1	1.92	0.52
4:d:84:LYS:HB3	4:d:96:TYR:HE1	1.75	0.52
2:B:349:HIS:ND1	14:B:820:CLA:OBD	2.35	0.52
9:0:96:LEU:HD21	17:0:209:BCR:H383	1.92	0.52
14:A:808:CLA:HAA1	14:A:832:CLA:HMB2	1.91	0.52
2:2:462:GLN:NE2	14:2:839:CLA:OBD	2.43	0.52
4:4:61:ARG:NH1	4:4:63:GLU:OE2	2.42	0.52
6:f:59:PHE:HA	6:f:62:ALA:HB2	1.92	0.52
14:B:841:CLA:H93	14:B:842:CLA:HBC1	1.92	0.51
1:a:312:ARG:HA	1:a:318:GLY:HA3	1.93	0.51
1:a:579:ARG:HG2	3:c:78:GLY:HA3	1.91	0.51
14:1:804:CLA:H2	2:2:656:LEU:HD22	1.92	0.51
4:d:32:TRP:HE1	4:d:50:MET:HE3	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:804:CLA:H161	17:B:852:BCR:H321	1.92	0.51
2:B:415:ALA:O	2:B:419:HIS:ND1	2.37	0.51
9:L:96:LEU:HD21	17:L:1504:BCR:H383	1.92	0.51
1:a:670:ILE:HG23	14:b:804:CLA:H52	1.92	0.51
1:1:319:HIS:NE2	14:1:824:CLA:OBD	2.32	0.51
1:1:343:ILE:HD11	1:1:421:ASN:HD22	1.74	0.51
14:b:840:CLA:H93	14:b:841:CLA:HBC1	1.92	0.51
4:d:61:ARG:NH1	4:d:63:GLU:OE2	2.42	0.51
2:B:150:LEU:HD22	10:M:22:ALA:HA	1.93	0.51
2:B:462:GLN:NE2	14:B:840:CLA:OBD	2.43	0.51
1:a:595:LEU:HD21	14:a:833:CLA:HBC1	1.92	0.51
1:1:312:ARG:HA	1:1:318:GLY:HA3	1.93	0.51
11:8:63:LEU:O	11:8:67:SER:CB	2.57	0.51
9:L:36:ASN:HB3	14:L:1501:CLA:HAC1	1.91	0.51
2:b:178:HIS:HB3	14:b:826:CLA:HED3	1.93	0.51
2:b:462:GLN:NE2	14:b:839:CLA:OBD	2.43	0.51
2:b:492:ASN:HB3	2:b:495:LEU:HB2	1.93	0.51
9:l:96:LEU:HD21	17:l:4207:BCR:H383	1.92	0.51
1:A:312:ARG:HA	1:A:318:GLY:HA3	1.93	0.51
11:K:57:PHE:HE2	11:K:62:LEU:HD23	1.75	0.51
1:a:692:TYR:OH	14:a:804:CLA:OBD	2.27	0.51
17:1:851:BCR:H373	2:2:432:LEU:HD23	1.93	0.51
14:2:812:CLA:HAB	7:h:19:GLY:HA3	1.92	0.51
14:A:843:CLA:H71	14:B:843:CLA:H62	1.92	0.51
3:c:81:TYR:CG	2:b:680:VAL:HG11	2.46	0.51
2:2:415:ALA:O	2:2:419:HIS:ND1	2.37	0.51
7:h:34:ILE:HG13	7:h:35:GLU:HG2	1.93	0.51
1:A:577:PRO:HD3	2:B:562:GLY:HA2	1.93	0.51
4:D:62:LYS:HG2	4:D:66:LEU:HD23	1.93	0.51
6:6:103:ILE:N	8:7:9:SER:O	2.39	0.51
6:6:36:ARG:NH1	8:7:35:ASP:OD2	2.40	0.51
14:a:829:CLA:H11	14:a:840:CLA:HBA1	1.92	0.51
2:2:61:THR:HG21	14:2:830:CLA:H42	1.93	0.51
1:A:140:THR:HG22	1:A:384:ALA:HB1	1.92	0.51
6:F:59:PHE:HA	6:F:62:ALA:HB2	1.92	0.51
1:a:115:GLN:NE2	14:a:812:CLA:OBD	2.43	0.51
18:a:852:LMG:H141	14:l:4206:CLA:HMB2	1.93	0.51
1:1:595:LEU:HD21	14:1:831:CLA:HBC1	1.92	0.51
1:1:670:ILE:HG23	14:2:803:CLA:H52	1.93	0.51
2:b:174:ARG:HB2	14:b:815:CLA:HBC2	1.93	0.51
2:2:301:ILE:HG23	14:2:821:CLA:HED2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:LEU:HD21	14:A:832:CLA:HBC1	1.93	0.50
17:a:851:BCR:H24C	14:b:835:CLA:HMC2	1.91	0.50
1:1:678:VAL:HG11	1:1:733:LEU:HD23	1.93	0.50
2:b:61:THR:HG21	14:b:830:CLA:H42	1.93	0.50
2:B:492:ASN:HB3	2:B:495:LEU:HB2	1.93	0.50
14:1:843:CLA:H172	14:0:207:CLA:HBB1	1.93	0.50
2:B:408:ARG:O	2:B:412:HIS:ND1	2.42	0.50
17:B:854:BCR:H372	14:J:102:CLA:HBC3	1.94	0.50
1:a:678:VAL:HG11	1:a:733:LEU:HD23	1.93	0.50
14:a:811:CLA:H42	14:a:831:CLA:HMD2	1.94	0.50
17:h:102:BCR:H352	17:h:102:BCR:H341	1.94	0.50
1:A:447:LEU:O	1:A:451:SER:OG	2.28	0.50
2:B:301:ILE:HG23	14:B:822:CLA:HED2	1.93	0.50
1:a:597:TRP:CH2	14:a:805:CLA:HAB	2.47	0.50
14:a:808:CLA:H142	17:a:848:BCR:H372	1.94	0.50
2:2:492:ASN:HB3	2:2:495:LEU:HB2	1.93	0.50
2:2:111:ASN:N	2:2:111:ASN:OD1	2.44	0.50
1:A:678:VAL:HG11	1:A:733:LEU:HD23	1.93	0.50
2:B:178:HIS:HB3	14:B:827:CLA:HED3	1.93	0.50
14:1:833:CLA:H122	14:2:842:CLA:H2	1.93	0.50
1:A:597:TRP:CH2	14:A:804:CLA:HAB	2.47	0.50
9:0:41:ARG:NH2	9:0:52:GLU:OE1	2.45	0.50
14:A:843:CLA:HAA2	14:B:802:CLA:HMB1	1.94	0.50
11:K:63:LEU:O	11:K:67:SER:HB3	2.12	0.50
2:b:408:ARG:O	2:b:412:HIS:ND1	2.42	0.50
2:2:178:HIS:HB3	14:2:826:CLA:HED3	1.93	0.50
4:4:62:LYS:HG2	4:4:66:LEU:HD23	1.93	0.50
6:6:59:PHE:HA	6:6:62:ALA:HB2	1.92	0.50
1:A:692:TYR:OH	14:B:801:CLA:OBD	2.27	0.50
17:A:851:BCR:H373	2:B:432:LEU:HD23	1.94	0.50
2:B:80:ASP:N	2:B:80:ASP:OD1	2.44	0.50
14:1:840:CLA:HBB2	6:6:83:GLY:HA3	1.94	0.50
2:2:80:ASP:OD1	2:2:80:ASP:N	2.44	0.50
14:2:812:CLA:H112	14:l:4206:CLA:H151	1.94	0.50
17:6:4406:BCR:H372	14:7:1103:CLA:HBC3	1.94	0.50
9:0:132:MET:HG3	17:0:204:BCR:H24C	1.94	0.50
14:A:804:CLA:H2	2:B:656:LEU:HD22	1.93	0.49
14:A:842:CLA:H203	8:J:19:LEU:HD22	1.94	0.49
14:1:809:CLA:H42	14:1:829:CLA:HMD2	1.94	0.49
11:k:63:LEU:O	11:k:67:SER:HB3	2.12	0.49
2:B:147:SER:HB2	10:M:18:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:843:CLA:HAA2	14:b:801:CLA:HMB1	1.94	0.49
1:1:597:TRP:CH2	14:1:804:CLA:HAB	2.47	0.49
4:d:62:LYS:HG2	4:d:66:LEU:HD23	1.93	0.49
1:a:440:LEU:HA	1:a:443:VAL:HG12	1.94	0.49
2:b:181:GLY:HA3	14:b:815:CLA:HBB1	1.95	0.49
2:2:174:ARG:HB2	14:2:815:CLA:HBC2	1.93	0.49
14:1:806:CLA:H142	17:1:848:BCR:H372	1.94	0.49
11:k:46:LEU:HD11	11:k:62:LEU:HD11	1.94	0.49
1:A:680:ALA:HB3	14:B:801:CLA:HBB2	1.94	0.49
14:A:810:CLA:H42	14:A:830:CLA:HMD2	1.94	0.49
2:B:547:LEU:HA	5:E:46:TYR:HD1	1.77	0.49
14:a:842:CLA:H102	8:j:16:MET:HE1	1.92	0.49
14:1:843:CLA:HAA2	14:0:202:CLA:HMB1	1.94	0.49
2:b:301:ILE:HG23	14:b:821:CLA:HED2	1.93	0.49
2:b:332:LEU:HD11	14:b:831:CLA:HBB1	1.94	0.49
2:2:181:GLY:HA3	14:2:815:CLA:HBB1	1.95	0.49
7:i:34:ILE:HG13	7:i:35:GLU:HG2	1.93	0.49
11:8:46:LEU:HD11	11:8:62:LEU:HD11	1.94	0.49
2:B:61:THR:HG21	14:B:831:CLA:H42	1.93	0.49
14:b:802:CLA:HBB2	6:f:83:GLY:HA3	1.95	0.49
18:A:852:LMG:H141	14:L:1503:CLA:HMB2	1.95	0.49
2:B:174:ARG:HB2	14:B:816:CLA:HBC2	1.93	0.49
7:I:34:ILE:HG13	7:I:35:GLU:HG2	1.93	0.49
11:K:46:LEU:HD11	11:K:62:LEU:HD11	1.94	0.49
14:a:843:CLA:H172	14:l:4205:CLA:HBB1	1.95	0.49
2:2:26:ALA:HA	14:2:831:CLA:H43	1.95	0.49
4:d:10:LYS:HB2	4:d:49:ILE:HB	1.95	0.49
1:A:342:GLU:O	1:A:346:THR:OG1	2.28	0.49
1:A:692:TYR:CE1	2:B:537:LYS:HD2	2.48	0.49
14:A:843:CLA:H203	9:L:61:LEU:HD11	1.93	0.49
17:I:102:BCR:H341	17:I:102:BCR:H352	1.94	0.49
11:8:43:GLY:HA3	11:8:60:PRO:HG3	1.94	0.49
14:A:807:CLA:H142	17:A:848:BCR:H372	1.93	0.49
14:1:841:CLA:H51	8:7:18:LEU:HD22	1.94	0.49
2:2:332:LEU:HD11	14:2:831:CLA:HBB1	1.94	0.49
4:4:10:LYS:HB2	4:4:49:ILE:HB	1.95	0.49
11:k:43:GLY:HA3	11:k:60:PRO:HG3	1.95	0.49
11:8:63:LEU:O	11:8:67:SER:HB3	2.12	0.49
1:A:340:LEU:HD23	14:A:826:CLA:HMD3	1.94	0.49
2:B:26:ALA:HA	14:B:832:CLA:H43	1.95	0.49
2:B:181:GLY:HA3	14:B:816:CLA:HBB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:TYR:HA	2:B:588:LEU:HD13	1.95	0.49
17:L:1505:BCR:H362	14:l:4203:CLA:H151	1.95	0.49
1:a:733:LEU:HD12	12:a:801:LHG:H382	1.95	0.49
1:1:149:ALA:HB2	1:1:377:PRO:HD2	1.95	0.49
1:1:680:ALA:HB3	14:2:801:CLA:HBB2	1.95	0.49
17:i:4103:BCR:H352	17:i:4103:BCR:H341	1.94	0.49
1:A:149:ALA:HB2	1:A:377:PRO:HD2	1.95	0.48
1:A:560:ARG:HH12	2:B:681:TRP:HB2	1.78	0.48
14:A:808:CLA:HMA2	14:A:808:CLA:H2	1.95	0.48
2:B:15:ASP:OD1	2:B:15:ASP:N	2.46	0.48
2:B:609:GLN:O	2:B:613:ASN:HB2	2.13	0.48
14:B:813:CLA:H112	14:0:208:CLA:H151	1.94	0.48
1:a:317:ILE:HD11	14:a:823:CLA:H2A	1.95	0.48
1:1:733:LEU:HD12	12:1:801:LHG:H382	1.95	0.48
2:2:609:GLN:O	2:2:613:ASN:HB2	2.13	0.48
14:2:842:CLA:H141	9:0:91:VAL:HG21	1.95	0.48
2:B:111:ASN:OD1	2:B:111:ASN:N	2.44	0.48
14:B:812:CLA:H61	17:I:101:BCR:H12C	1.93	0.48
9:L:41:ARG:NH2	9:L:52:GLU:OE1	2.45	0.48
17:L:1505:BCR:H24C	9:l:132:MET:HG3	1.95	0.48
1:a:680:ALA:HB3	14:a:804:CLA:HBB2	1.95	0.48
14:a:805:CLA:H162	14:b:812:CLA:HMB2	1.94	0.48
1:1:317:ILE:HD11	14:1:821:CLA:H2A	1.95	0.48
14:1:813:CLA:HBA2	14:1:813:CLA:H3A	1.58	0.48
2:2:375:TYR:HA	2:2:588:LEU:HD13	1.95	0.48
4:d:121:ARG:NH1	5:e:65:GLU:OE2	2.46	0.48
1:A:538:HIS:HB3	14:A:838:CLA:HBB1	1.95	0.48
1:1:692:TYR:OH	14:2:801:CLA:OBD	2.27	0.48
3:c:61:ASP:O	5:e:59:ASN:ND2	2.40	0.48
2:b:180:ALA:HB2	2:b:288:GLY:HA3	1.96	0.48
2:2:180:ALA:HB2	2:2:288:GLY:HA3	1.96	0.48
14:B:810:CLA:HHB	14:B:811:CLA:HMB3	1.95	0.48
14:B:816:CLA:H192	17:B:848:BCR:H281	1.95	0.48
14:1:832:CLA:HAB	14:1:839:CLA:HBB2	1.96	0.48
2:b:26:ALA:HA	14:b:831:CLA:H43	1.95	0.48
2:b:609:GLN:O	2:b:613:ASN:HB2	2.13	0.48
14:b:810:CLA:HHB	14:b:811:CLA:HMB3	1.95	0.48
2:2:15:ASP:N	2:2:15:ASP:OD1	2.46	0.48
2:2:408:ARG:O	2:2:412:HIS:ND1	2.42	0.48
1:A:440:LEU:HA	1:A:443:VAL:HG12	1.94	0.48
14:B:801:CLA:H62	14:B:801:CLA:H41	1.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:199:HIS:CG	14:1:814:CLA:HMC2	2.49	0.48
1:1:440:LEU:HA	1:1:443:VAL:HG12	1.94	0.48
17:b:853:BCR:H372	14:j:102:CLA:HBC3	1.94	0.48
11:k:22:MET:HG3	11:k:73:GLY:HA3	1.95	0.48
1:A:733:LEU:HD12	12:A:801:LHG:H382	1.95	0.48
14:A:833:CLA:HAB	14:A:840:CLA:HBB2	1.96	0.48
14:a:834:CLA:HAB	14:a:841:CLA:HBB2	1.96	0.48
1:1:538:HIS:HB3	14:1:837:CLA:HBB1	1.95	0.48
1:A:559:SER:OG	1:A:560:ARG:N	2.47	0.48
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.95	0.48
2:B:227:THR:HG23	2:B:229:ASN:H	1.79	0.48
2:B:332:LEU:HD11	14:B:832:CLA:HBB1	1.95	0.48
1:1:539:ALA:HB2	14:1:838:CLA:HMA1	1.96	0.48
4:d:23:ASN:OD1	4:d:23:ASN:N	2.46	0.48
11:K:43:GLY:HA3	11:K:60:PRO:HG3	1.94	0.48
1:A:539:ALA:HB2	14:A:839:CLA:HMA1	1.96	0.48
2:B:550:ASP:OD1	2:B:550:ASP:N	2.46	0.48
14:B:813:CLA:H41	14:B:813:CLA:H62	1.64	0.48
4:D:10:LYS:HB2	4:D:49:ILE:HB	1.95	0.48
4:D:23:ASN:OD1	4:D:23:ASN:N	2.46	0.48
14:a:809:CLA:H2	14:a:809:CLA:HMA2	1.95	0.48
2:b:80:ASP:N	2:b:80:ASP:OD1	2.44	0.48
2:b:482:ILE:HG13	14:b:837:CLA:HMD3	1.95	0.48
14:2:809:CLA:HHB	14:2:810:CLA:HMB3	1.95	0.48
14:A:834:CLA:H122	14:B:843:CLA:H2	1.96	0.48
14:B:840:CLA:HMB1	14:B:840:CLA:HBB1	1.96	0.48
1:a:447:LEU:O	1:a:451:SER:OG	2.28	0.48
14:1:834:CLA:H172	14:0:207:CLA:HMB2	1.96	0.48
2:2:482:ILE:HG13	14:2:837:CLA:HMD3	1.96	0.48
6:6:55:VAL:HG12	6:6:65:PHE:HB2	1.96	0.48
11:8:68:PHE:HB2	17:8:4001:BCR:H23C	1.96	0.48
14:A:821:CLA:HBA2	14:A:821:CLA:H3A	1.59	0.47
14:A:841:CLA:HBB2	14:A:841:CLA:H152	1.96	0.47
14:a:814:CLA:H62	14:a:814:CLA:H102	1.59	0.47
14:a:821:CLA:H3A	14:a:821:CLA:HBA2	1.49	0.47
1:1:216:GLN:HA	1:1:220:SER:HB2	1.96	0.47
2:b:416:LEU:HB2	14:b:841:CLA:HBB2	1.96	0.47
2:b:550:ASP:OD1	2:b:550:ASP:N	2.46	0.47
14:b:802:CLA:HBB2	14:b:802:CLA:H152	1.96	0.47
14:2:815:CLA:H192	17:2:847:BCR:H281	1.95	0.47
1:A:120:ILE:HG23	1:A:121:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:482:ILE:HG13	14:B:838:CLA:HMD3	1.96	0.47
1:a:342:GLU:O	1:a:346:THR:OG1	2.28	0.47
2:b:475:LEU:O	2:b:481:SER:OG	2.30	0.47
14:b:839:CLA:HBB1	14:b:839:CLA:HMB1	1.96	0.47
2:2:91:ILE:HB	2:2:112:PRO:HB2	1.95	0.47
2:2:517:ASP:OD1	2:2:594:TYR:OH	2.29	0.47
14:8:4002:CLA:HMB2	17:8:4005:BCR:H16C	1.96	0.47
1:A:317:ILE:HD11	14:A:822:CLA:H2A	1.95	0.47
1:A:706:LYS:O	6:F:133:MET:N	2.48	0.47
14:A:822:CLA:HBB1	17:K:4005:BCR:H342	1.97	0.47
2:B:42:LEU:HD22	4:D:133:PHE:CE1	2.49	0.47
1:a:149:ALA:HB2	1:a:377:PRO:HD2	1.95	0.47
1:1:559:SER:OG	1:1:560:ARG:N	2.47	0.47
14:1:826:CLA:H143	14:1:826:CLA:H111	1.76	0.47
14:1:829:CLA:H143	14:1:829:CLA:H111	1.76	0.47
14:1:833:CLA:H171	14:2:842:CLA:HMB2	1.96	0.47
2:b:375:TYR:HA	2:b:588:LEU:HD13	1.95	0.47
2:b:393:VAL:HG23	2:b:542:ALA:HB1	1.97	0.47
4:4:57:LEU:HD23	4:4:68:LEU:HD22	1.96	0.47
9:l:41:ARG:NH2	9:l:52:GLU:OE1	2.45	0.47
1:A:199:HIS:CG	14:A:815:CLA:HMC2	2.49	0.47
12:A:801:LHG:H252	14:A:808:CLA:H41	1.97	0.47
6:F:55:VAL:HG12	6:F:65:PHE:HB2	1.96	0.47
11:K:22:MET:HG3	11:K:73:GLY:HA3	1.95	0.47
14:1:807:CLA:HMA2	14:1:807:CLA:H2	1.95	0.47
2:b:91:ILE:HB	2:b:112:PRO:HB2	1.95	0.47
14:2:812:CLA:H151	17:0:204:BCR:H362	1.95	0.47
14:2:818:CLA:H3A	14:2:818:CLA:HBA2	1.56	0.47
14:B:818:CLA:HED3	14:B:818:CLA:H2A	1.97	0.47
1:a:538:HIS:HB3	14:a:839:CLA:HBB1	1.95	0.47
14:a:805:CLA:H2	2:b:656:LEU:HD22	1.96	0.47
1:1:447:LEU:O	1:1:451:SER:OG	2.28	0.47
12:1:801:LHG:H252	14:1:807:CLA:H41	1.96	0.47
14:1:833:CLA:H193	15:2:845:PQN:H293	1.96	0.47
14:b:815:CLA:H192	17:b:847:BCR:H281	1.95	0.47
2:2:227:THR:HG23	2:2:229:ASN:H	1.79	0.47
2:2:388:GLY:HA2	17:2:850:BCR:H272	1.97	0.47
1:A:180:TYR:HB3	1:A:181:HIS:HD2	1.79	0.47
1:A:351:GLN:HG3	14:A:827:CLA:H151	1.97	0.47
14:L:1501:CLA:H122	14:L:1501:CLA:H162	1.69	0.47
14:a:836:CLA:H172	14:l:4205:CLA:HMB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:70:TRP:NE1	7:i:6:ALA:O	2.42	0.47
2:b:701:LEU:HD21	15:b:845:PQN:H152	1.97	0.47
14:2:815:CLA:H62	14:2:815:CLA:H2	1.69	0.47
4:d:57:LEU:HD23	4:d:68:LEU:HD22	1.96	0.47
1:A:115:GLN:NE2	14:A:811:CLA:OBD	2.43	0.47
14:A:824:CLA:H3A	14:A:824:CLA:HBA2	1.38	0.47
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.95	0.47
2:B:388:GLY:HA2	17:B:851:BCR:H272	1.97	0.47
1:a:199:HIS:CG	14:a:816:CLA:HMC2	2.49	0.47
12:a:801:LHG:H252	14:a:809:CLA:H41	1.96	0.47
1:1:707:LEU:HA	6:6:132:VAL:HA	1.97	0.47
14:1:809:CLA:H162	14:1:809:CLA:H141	1.75	0.47
2:b:227:THR:HG23	2:b:229:ASN:H	1.79	0.47
14:2:820:CLA:H62	14:2:820:CLA:H41	1.62	0.47
14:2:839:CLA:HBB1	14:2:839:CLA:HMB1	1.96	0.47
11:8:22:MET:HG3	11:8:73:GLY:HA3	1.95	0.47
14:l:4204:CLA:H162	14:l:4204:CLA:H122	1.69	0.47
2:B:393:VAL:HG23	2:B:542:ALA:HB1	1.96	0.47
2:B:559:PRO:HB3	2:B:703:ILE:HB	1.97	0.47
1:a:120:ILE:HG23	1:a:121:VAL:HG22	1.96	0.47
14:a:825:CLA:H3A	14:a:825:CLA:HBA2	1.37	0.47
14:1:829:CLA:H161	17:7:1104:BCR:H14C	1.97	0.47
2:b:15:ASP:OD1	2:b:15:ASP:N	2.46	0.47
2:b:20:ARG:NH2	7:i:34:ILE:O	2.38	0.47
2:b:111:ASN:OD1	2:b:111:ASN:N	2.44	0.47
2:b:388:GLY:HA2	17:b:850:BCR:H272	1.97	0.47
2:b:457:PHE:O	2:b:461:ILE:HG12	2.15	0.47
2:b:691:LEU:HD11	9:l:39:ALA:HB1	1.96	0.47
6:f:55:VAL:HG12	6:f:65:PHE:HB2	1.96	0.47
14:A:808:CLA:H152	14:A:808:CLA:H112	1.64	0.47
2:B:60:TRP:NE1	14:B:830:CLA:OBD	2.47	0.47
2:2:70:TRP:NE1	7:h:6:ALA:O	2.41	0.47
2:2:177:HIS:CG	14:2:815:CLA:HMC2	2.50	0.47
2:2:685:ARG:HD2	9:0:19:HIS:CD2	2.49	0.47
2:2:701:LEU:HD21	15:2:845:PQN:H152	1.97	0.47
6:f:36:ARG:NH1	8:j:35:ASP:OD2	2.42	0.47
14:j:101:CLA:H3A	14:j:101:CLA:HBA2	1.49	0.47
1:a:216:GLN:HA	1:a:220:SER:HB2	1.96	0.47
1:1:576:GLY:HA2	2:2:563:PRO:HD3	1.97	0.47
14:1:831:CLA:H192	14:1:831:CLA:H162	1.80	0.47
2:b:397:ASP:HB2	4:d:129:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:415:ALA:O	2:b:419:HIS:ND1	2.37	0.47
14:b:843:CLA:HMB2	17:b:851:BCR:H12C	1.97	0.47
14:l:4203:CLA:H62	14:l:4203:CLA:H41	1.64	0.47
1:A:216:GLN:HA	1:A:220:SER:HB2	1.96	0.46
1:A:284:VAL:HG23	1:A:285:THR:HG23	1.97	0.46
6:F:89:GLU:HG2	6:F:107:LEU:HD11	1.98	0.46
9:L:141:LEU:HD21	14:l:4203:CLA:H122	1.97	0.46
14:a:824:CLA:HMB2	14:a:828:CLA:HMA3	1.97	0.46
1:1:338:LYS:HE3	1:1:338:LYS:HB3	1.58	0.46
2:b:559:PRO:HB3	2:b:703:ILE:HB	1.97	0.46
14:B:809:CLA:H72	14:B:809:CLA:H111	1.48	0.46
14:K:4002:CLA:HMB2	17:K:4005:BCR:H16C	1.96	0.46
1:a:317:ILE:HG23	11:k:60:PRO:HB2	1.96	0.46
14:a:811:CLA:H3A	14:a:811:CLA:HBA2	1.67	0.46
1:1:120:ILE:HG23	1:1:121:VAL:HG22	1.96	0.46
1:1:351:GLN:HG3	14:1:826:CLA:H151	1.97	0.46
14:1:822:CLA:H42	14:1:828:CLA:H93	1.98	0.46
2:b:60:TRP:NE1	14:b:829:CLA:OBD	2.47	0.46
14:2:801:CLA:HBB1	14:2:801:CLA:HMB1	1.98	0.46
14:2:842:CLA:H93	14:2:842:CLA:H111	1.82	0.46
6:6:89:GLU:HG2	6:6:107:LEU:HD11	1.98	0.46
14:A:823:CLA:H42	14:A:829:CLA:H93	1.98	0.46
2:B:416:LEU:HB2	14:B:842:CLA:HBB2	1.96	0.46
11:K:46:LEU:HD21	11:K:62:LEU:HD21	1.97	0.46
1:a:539:ALA:HB2	14:a:840:CLA:HMA1	1.96	0.46
14:a:804:CLA:HBB1	14:a:804:CLA:HMB1	1.98	0.46
14:1:840:CLA:HBB2	14:1:840:CLA:H152	1.96	0.46
14:1:843:CLA:HBC1	15:2:845:PQN:H191	1.97	0.46
2:b:662:PHE:HB3	14:b:806:CLA:HMC2	1.98	0.46
4:4:23:ASN:OD1	4:4:23:ASN:N	2.46	0.46
11:k:46:LEU:HD21	11:k:62:LEU:HD21	1.97	0.46
11:k:68:PHE:HB2	17:k:4001:BCR:H23C	1.97	0.46
14:l:4203:CLA:H93	14:l:4203:CLA:H111	1.77	0.46
4:D:88:VAL:HG12	4:D:94:VAL:HG13	1.98	0.46
14:a:827:CLA:H42	17:a:850:BCR:H363	1.97	0.46
2:2:393:VAL:HG23	2:2:542:ALA:HB1	1.96	0.46
17:A:851:BCR:H19C	14:B:804:CLA:H143	1.96	0.46
2:B:177:HIS:CG	14:B:816:CLA:HMC2	2.50	0.46
1:a:180:TYR:HB3	1:a:181:HIS:HD2	1.79	0.46
1:a:351:GLN:HG3	14:a:828:CLA:H151	1.96	0.46
1:1:180:TYR:HB3	1:1:181:HIS:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:802:LMG:H422	14:2:831:CLA:H91	1.98	0.46
6:6:117:LEU:HD12	6:6:120:LEU:HD22	1.98	0.46
11:8:46:LEU:HD21	11:8:62:LEU:HD21	1.97	0.46
14:A:836:CLA:H61	14:A:836:CLA:H41	1.64	0.46
2:B:151:PHE:HB2	10:M:21:LEU:HD13	1.98	0.46
14:B:816:CLA:H3A	14:B:816:CLA:HBA1	1.47	0.46
4:D:57:LEU:HD23	4:D:68:LEU:HD22	1.96	0.46
7:I:21:LEU:O	7:I:25:VAL:HB	2.16	0.46
1:a:284:VAL:HG23	1:a:285:THR:HG23	1.97	0.46
14:a:830:CLA:HBA1	17:a:850:BCR:H19C	1.98	0.46
14:1:822:CLA:HMB2	14:1:826:CLA:HMA3	1.97	0.46
14:1:838:CLA:H93	14:1:838:CLA:H112	1.74	0.46
17:b:847:BCR:H15C	17:b:847:BCR:H351	1.83	0.46
14:2:817:CLA:HED3	14:2:817:CLA:H2A	1.97	0.46
6:f:117:LEU:HD12	6:f:120:LEU:HD22	1.98	0.46
7:i:21:LEU:O	7:i:25:VAL:HB	2.16	0.46
1:A:428:ARG:O	1:A:432:HIS:ND1	2.48	0.46
1:A:581:GLY:HA3	2:B:703:ILE:HD11	1.98	0.46
2:B:553:ASP:HA	4:D:138:PRO:HG2	1.98	0.46
2:B:662:PHE:HB3	14:B:806:CLA:HMC2	1.98	0.46
15:B:846:PQN:H212	15:B:846:PQN:H251	1.74	0.46
12:a:801:LHG:H241	12:a:801:LHG:HC62	1.74	0.46
14:a:824:CLA:H42	14:a:830:CLA:H93	1.98	0.46
14:a:833:CLA:H41	14:a:833:CLA:H62	1.78	0.46
14:1:828:CLA:HBA1	17:1:850:BCR:H19C	1.98	0.46
14:b:810:CLA:H13	17:i:4102:BCR:HC42	1.97	0.46
14:b:812:CLA:HBA1	14:b:812:CLA:H3A	1.37	0.46
2:2:559:PRO:HB3	2:2:703:ILE:HB	1.97	0.46
14:0:206:CLA:H162	14:0:206:CLA:H122	1.69	0.46
1:a:559:SER:OG	1:a:560:ARG:N	2.47	0.46
14:a:831:CLA:H192	14:b:804:CLA:H13	1.98	0.46
1:1:343:ILE:HG22	1:1:344:LEU:HD12	1.98	0.46
1:1:433:ARG:HE	1:1:433:ARG:HB2	1.54	0.46
14:1:825:CLA:H42	17:1:850:BCR:H363	1.97	0.46
14:b:808:CLA:H142	14:b:808:CLA:H111	1.74	0.46
17:2:849:BCR:H403	17:2:850:BCR:H391	1.98	0.46
7:h:21:LEU:O	7:h:25:VAL:HB	2.16	0.46
9:0:65:TRP:HH2	9:0:88:LEU:HD22	1.81	0.46
14:A:805:CLA:H62	14:A:841:CLA:HBC3	1.98	0.46
14:A:829:CLA:HBA1	17:A:850:BCR:H19C	1.98	0.46
14:B:801:CLA:HBB1	14:B:801:CLA:HMB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:196:MET:HE1	14:a:828:CLA:H142	1.98	0.46
1:a:646:LEU:HD12	1:a:646:LEU:HA	1.76	0.46
14:a:822:CLA:H3A	14:a:822:CLA:HBA2	1.59	0.46
1:1:196:MET:HE1	14:1:826:CLA:H142	1.98	0.46
1:1:428:ARG:O	1:1:432:HIS:ND1	2.48	0.46
2:b:177:HIS:CG	14:b:815:CLA:HMC2	2.50	0.46
2:b:371:THR:HG23	2:b:592:THR:HG21	1.98	0.46
2:b:397:ASP:HA	4:d:129:VAL:HG11	1.97	0.46
1:A:196:MET:HE1	14:A:827:CLA:H142	1.98	0.46
14:A:823:CLA:HMB2	14:A:827:CLA:HMA3	1.97	0.46
2:B:224:PRO:HA	2:B:227:THR:HG22	1.97	0.46
3:C:6:LYS:HD2	4:D:118:LYS:HE3	1.97	0.46
14:L:1503:CLA:HBA1	14:L:1503:CLA:H3A	1.67	0.46
14:a:836:CLA:H152	17:i:4103:BCR:H372	1.98	0.46
1:1:207:LEU:HD22	17:1:847:BCR:H361	1.98	0.46
14:1:840:CLA:HBC3	14:7:1101:CLA:H62	1.98	0.46
17:1:851:BCR:H19C	14:2:803:CLA:H143	1.97	0.46
2:b:150:LEU:HD22	10:m:22:ALA:HA	1.98	0.46
14:b:817:CLA:H2A	14:b:817:CLA:HED3	1.97	0.46
14:b:820:CLA:H41	14:b:820:CLA:H62	1.62	0.46
2:2:662:PHE:HB3	14:2:805:CLA:HMC2	1.98	0.46
9:l:65:TRP:HH2	9:l:88:LEU:HD22	1.81	0.46
1:a:332:PHE:HE1	9:l:23:PRO:HG2	1.81	0.45
14:a:804:CLA:H41	14:a:804:CLA:H62	1.50	0.45
14:a:843:CLA:H2	14:a:843:CLA:H61	1.69	0.45
1:1:115:GLN:NE2	14:1:810:CLA:OBD	2.43	0.45
1:1:692:TYR:CE1	2:2:537:LYS:HD2	2.51	0.45
14:1:820:CLA:H3A	14:1:820:CLA:HBA2	1.59	0.45
14:1:820:CLA:H143	14:1:820:CLA:H162	1.82	0.45
3:3:4:SER:HB2	4:4:139:TYR:HE2	1.81	0.45
2:2:269:TRP:O	2:2:273:ILE:HG12	2.17	0.45
2:2:416:LEU:HB2	14:2:841:CLA:HBB2	1.96	0.45
4:4:136:LYS:HD2	4:4:141:VAL:HG12	1.99	0.45
14:k:4002:CLA:HMB2	17:k:4004:BCR:H16C	1.96	0.45
1:A:315:TRP:HD1	11:K:60:PRO:HD3	1.81	0.45
2:B:323:THR:OG1	2:B:401:ASN:OD1	2.31	0.45
2:B:525:ALA:HB2	14:B:841:CLA:HMA1	1.98	0.45
2:B:701:LEU:HD21	15:B:846:PQN:H152	1.97	0.45
14:B:810:CLA:H93	17:M:102:BCR:H353	1.97	0.45
14:B:813:CLA:H93	14:B:813:CLA:H111	1.77	0.45
15:B:846:PQN:H212	15:B:846:PQN:H172	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:334:GLY:HA2	9:l:6:GLN:NE2	2.31	0.45
14:a:811:CLA:H162	14:a:811:CLA:H141	1.75	0.45
3:3:27:GLU:HB3	3:3:44:ARG:HH22	1.81	0.45
2:b:66:PHE:HZ	10:m:8:ILE:HG23	1.80	0.45
17:b:849:BCR:H403	17:b:850:BCR:H391	1.98	0.45
14:2:808:CLA:H11	14:2:808:CLA:HBA1	1.69	0.45
4:d:88:VAL:HG12	4:d:94:VAL:HG13	1.98	0.45
6:f:89:GLU:HG2	6:f:107:LEU:HD11	1.98	0.45
14:A:808:CLA:H2	14:A:808:CLA:H61	1.70	0.45
14:A:826:CLA:H42	17:A:850:BCR:H363	1.97	0.45
14:B:812:CLA:H43	17:I:101:BCR:HC8	1.98	0.45
17:B:850:BCR:H403	17:B:851:BCR:H391	1.98	0.45
3:C:27:GLU:HB3	3:C:44:ARG:HH22	1.81	0.45
6:F:117:LEU:HD12	6:F:120:LEU:HD22	1.98	0.45
1:a:77:PHE:CZ	14:a:813:CLA:HBB1	2.52	0.45
14:a:820:CLA:H41	14:a:820:CLA:H61	1.61	0.45
3:c:8:TYR:HE2	3:c:66:ARG:HB2	1.82	0.45
3:c:27:GLU:HB3	3:c:44:ARG:HH22	1.80	0.45
2:b:581:MET:HB3	2:b:711:LEU:HD11	1.99	0.45
14:2:843:CLA:HMB2	17:2:851:BCR:H12C	1.97	0.45
4:d:136:LYS:HD2	4:d:141:VAL:HG12	1.99	0.45
14:6:4403:CLA:CHD	8:7:18:LEU:HD21	2.47	0.45
2:B:101:VAL:HG13	2:B:112:PRO:HG3	1.99	0.45
2:B:397:ASP:HB2	4:D:129:VAL:HG21	1.98	0.45
4:D:52:GLU:H	4:D:52:GLU:HG3	1.42	0.45
17:M:102:BCR:H20C	17:M:102:BCR:H361	1.82	0.45
11:K:57:PHE:CE2	11:K:62:LEU:HD23	2.52	0.45
1:a:207:LEU:HD22	17:a:847:BCR:H361	1.98	0.45
3:c:29:VAL:HG12	4:d:112:ARG:HB2	1.98	0.45
2:b:224:PRO:HA	2:b:227:THR:HG22	1.98	0.45
2:b:525:ALA:HB2	14:b:840:CLA:HMA1	1.98	0.45
2:2:659:ALA:HB3	14:2:805:CLA:HBB2	1.99	0.45
2:B:457:PHE:O	2:B:461:ILE:HG12	2.15	0.45
2:B:517:ASP:OD1	2:B:594:TYR:OH	2.29	0.45
14:b:809:CLA:H11	14:b:809:CLA:HBA1	1.69	0.45
4:4:139:TYR:HD1	4:4:139:TYR:H	1.65	0.45
1:A:33:HIS:NE2	14:A:813:CLA:O1A	2.50	0.45
1:A:343:ILE:HG22	1:A:344:LEU:HD12	1.98	0.45
2:B:106:GLN:HG3	2:B:115:ILE:HD11	1.99	0.45
2:B:269:TRP:O	2:B:273:ILE:HG12	2.16	0.45
2:B:371:THR:HG23	2:B:592:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:315:TRP:HD1	11:k:60:PRO:HD3	1.82	0.45
2:2:60:TRP:NE1	14:2:829:CLA:OBD	2.47	0.45
2:2:581:MET:HB3	2:2:711:LEU:HD11	1.99	0.45
14:2:812:CLA:H62	14:2:812:CLA:H41	1.64	0.45
14:2:815:CLA:H111	14:2:815:CLA:H142	1.74	0.45
14:k:4002:CLA:C2B	17:k:4004:BCR:H14C	2.47	0.45
14:l:4206:CLA:H141	14:l:4206:CLA:H161	1.73	0.45
17:9:102:BCR:H20C	17:9:102:BCR:H361	1.82	0.45
1:A:77:PHE:CZ	14:A:812:CLA:HBB1	2.52	0.45
1:A:456:ILE:HD13	14:A:804:CLA:H92	1.99	0.45
14:A:839:CLA:H93	14:A:839:CLA:H112	1.74	0.45
2:B:581:MET:HB3	2:B:711:LEU:HD11	1.99	0.45
14:B:802:CLA:H41	14:B:802:CLA:H61	1.81	0.45
14:B:810:CLA:H2A	14:B:812:CLA:HED1	1.99	0.45
9:L:65:TRP:HH2	9:L:88:LEU:HD22	1.81	0.45
1:a:33:HIS:NE2	14:a:814:CLA:O1A	2.50	0.45
14:1:835:CLA:H61	14:1:835:CLA:H41	1.64	0.45
2:b:304:ILE:O	2:b:308:HIS:ND1	2.41	0.45
2:2:224:PRO:HA	2:2:227:THR:HG22	1.98	0.45
2:2:457:PHE:O	2:2:461:ILE:HG12	2.15	0.45
14:2:809:CLA:H2A	14:2:811:CLA:HED1	1.99	0.45
14:8:4002:CLA:C2B	17:8:4005:BCR:H14C	2.47	0.45
2:B:659:ALA:HB3	14:B:806:CLA:HBB2	1.99	0.45
6:F:15:ALA:O	6:F:19:LYS:HG2	2.17	0.45
17:I:102:BCR:H20C	17:I:102:BCR:H361	1.85	0.45
1:1:456:ILE:HD13	14:1:804:CLA:H92	1.99	0.45
2:b:269:TRP:O	2:b:273:ILE:HG12	2.17	0.45
2:b:659:ALA:HB3	14:b:806:CLA:HBB2	1.99	0.45
4:d:126:PRO:HG2	4:d:141:VAL:HG23	1.99	0.45
4:4:126:PRO:HG2	4:4:141:VAL:HG23	1.99	0.45
6:6:102:VAL:HG12	8:7:10:THR:HG22	1.99	0.45
2:B:460:TRP:HE1	2:B:474:VAL:HG11	1.82	0.45
18:B:803:LMG:H422	14:B:832:CLA:H91	1.98	0.45
14:B:812:CLA:H3A	14:B:812:CLA:HBA1	1.37	0.45
14:K:4002:CLA:C2B	17:K:4005:BCR:H14C	2.47	0.45
1:1:77:PHE:CZ	14:1:811:CLA:HBB1	2.52	0.45
1:1:284:VAL:HG23	1:1:285:THR:HG23	1.97	0.45
1:1:560:ARG:HH12	2:2:681:TRP:HB2	1.81	0.45
2:b:173:SER:O	2:b:177:HIS:ND1	2.37	0.45
2:b:547:LEU:HA	5:e:46:TYR:HD1	1.81	0.45
2:2:475:LEU:O	2:2:481:SER:OG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:588:LEU:HA	2:2:591:LEU:HG	1.99	0.45
4:d:139:TYR:HD1	4:d:139:TYR:H	1.65	0.45
4:4:88:VAL:HG12	4:4:94:VAL:HG13	1.98	0.45
5:e:47:ASN:OD1	5:e:48:GLY:N	2.50	0.45
5:5:47:ASN:OD1	5:5:48:GLY:N	2.50	0.45
9:0:142:LEU:HG	14:0:208:CLA:HED3	1.99	0.45
14:A:820:CLA:HBA2	14:A:820:CLA:H3A	1.49	0.45
2:B:297:ILE:HD11	14:B:823:CLA:HMA2	1.99	0.45
1:1:588:TRP:CD1	14:1:831:CLA:HMD1	2.52	0.45
1:1:646:LEU:HD12	1:1:646:LEU:HA	1.76	0.45
2:b:101:VAL:HG13	2:b:112:PRO:HG3	1.99	0.45
18:b:803:LMG:H422	14:b:831:CLA:H91	1.97	0.45
2:2:106:GLN:HG3	2:2:115:ILE:HD11	1.99	0.45
2:2:371:THR:HG23	2:2:592:THR:HG21	1.98	0.45
2:2:536:ILE:HG21	17:2:849:BCR:H281	1.99	0.45
4:d:52:GLU:H	4:d:52:GLU:HG3	1.43	0.45
9:0:55:MET:HE3	14:0:206:CLA:HMA2	1.99	0.45
9:0:133:GLY:HA2	17:0:210:BCR:H281	2.00	0.45
14:B:825:CLA:H3A	14:B:825:CLA:HBA2	1.73	0.44
4:D:136:LYS:HD2	4:D:141:VAL:HG12	1.99	0.44
19:I:103:LMT:H6E	14:0:208:CLA:H12	1.99	0.44
9:L:44:LEU:HB2	9:L:49:ARG:HH21	1.82	0.44
9:L:55:MET:HE3	14:L:1501:CLA:HMA2	1.99	0.44
1:a:343:ILE:HG22	1:a:344:LEU:HD12	1.98	0.44
1:a:456:ILE:HD13	14:a:805:CLA:H92	1.99	0.44
14:1:804:CLA:H161	17:2:851:BCR:H321	1.99	0.44
2:b:430:HIS:HB2	17:b:853:BCR:HC31	1.99	0.44
14:b:808:CLA:H162	14:b:808:CLA:H141	1.74	0.44
2:2:183:PHE:HB3	2:2:284:PHE:CD2	2.53	0.44
2:2:460:TRP:HE1	2:2:474:VAL:HG11	1.82	0.44
14:2:807:CLA:H142	14:2:807:CLA:H111	1.74	0.44
7:h:20:TRP:HB3	14:l:4206:CLA:H202	1.99	0.44
9:l:142:LEU:HG	14:l:4206:CLA:HED3	1.99	0.44
14:B:809:CLA:HBA1	14:B:809:CLA:H11	1.69	0.44
17:B:850:BCR:H24C	17:B:851:BCR:H373	1.99	0.44
3:C:8:TYR:HE2	3:C:66:ARG:HB2	1.82	0.44
4:D:137:ALA:HB3	4:D:139:TYR:HE1	1.82	0.44
4:D:139:TYR:HD1	4:D:139:TYR:H	1.65	0.44
14:a:831:CLA:H93	14:a:831:CLA:H111	1.83	0.44
1:1:317:ILE:HD13	11:8:64:ALA:HB2	1.99	0.44
14:1:807:CLA:H152	14:1:807:CLA:H112	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:843:CLA:HMB3	2:2:683:HIS:HE1	1.82	0.44
14:b:820:CLA:H3A	14:b:820:CLA:HBA2	1.63	0.44
2:2:142:LEU:HD23	2:2:142:LEU:HA	1.82	0.44
2:2:257:PHE:CE2	14:2:819:CLA:HBB1	2.53	0.44
4:d:137:ALA:HB3	4:d:139:TYR:HE1	1.82	0.44
1:A:324:ILE:O	1:A:328:HIS:ND1	2.50	0.44
14:B:844:CLA:HMB2	17:B:852:BCR:H12C	1.97	0.44
9:L:28:ALA:HB1	12:m:101:LHG:HC42	2.00	0.44
9:L:46:PRO:HA	9:L:49:ARG:HG2	1.99	0.44
9:L:142:LEU:HG	14:L:1503:CLA:HED3	1.99	0.44
14:a:822:CLA:H143	14:a:822:CLA:H162	1.81	0.44
1:1:33:HIS:NE2	14:1:812:CLA:O1A	2.50	0.44
14:1:809:CLA:H62	14:1:809:CLA:H41	1.75	0.44
2:2:297:ILE:HD11	14:2:822:CLA:HMA2	1.99	0.44
2:2:525:ALA:HB2	14:2:840:CLA:HMA1	1.98	0.44
9:l:133:GLY:HA2	17:0:204:BCR:H281	2.00	0.44
5:E:47:ASN:OD1	5:E:48:GLY:N	2.50	0.44
9:L:70:PRO:HG2	9:L:71:LEU:HD12	1.99	0.44
1:a:334:GLY:HA2	9:l:6:GLN:HE22	1.82	0.44
14:a:814:CLA:H142	14:a:814:CLA:H111	1.84	0.44
14:a:837:CLA:H71	17:a:850:BCR:H20C	1.99	0.44
14:1:819:CLA:H3A	14:1:819:CLA:HBA2	1.49	0.44
3:c:66:ARG:HD3	3:c:66:ARG:HA	1.79	0.44
2:b:257:PHE:CE2	14:b:819:CLA:HBB1	2.53	0.44
14:2:834:CLA:H92	14:2:834:CLA:H61	1.78	0.44
6:f:15:ALA:O	6:f:19:LYS:HG2	2.17	0.44
14:0:206:CLA:H201	14:0:208:CLA:H172	2.00	0.44
1:A:207:LEU:HD22	17:A:847:BCR:H361	1.98	0.44
1:A:588:TRP:CD1	14:A:832:CLA:HMD1	2.52	0.44
14:B:811:CLA:H143	14:B:811:CLA:H161	1.87	0.44
17:B:852:BCR:H20C	17:B:852:BCR:H361	1.78	0.44
1:a:121:VAL:HB	14:b:835:CLA:HMD1	1.99	0.44
1:a:588:TRP:CD1	14:a:833:CLA:HMD1	2.52	0.44
1:a:694:GLN:HB3	2:b:547:LEU:HD22	1.99	0.44
3:3:8:TYR:HE2	3:3:66:ARG:HB2	1.81	0.44
2:b:87:ILE:O	2:b:121:TYR:OH	2.28	0.44
14:2:811:CLA:H152	17:h:101:BCR:H341	1.99	0.44
14:A:805:CLA:H203	14:A:842:CLA:H152	2.00	0.44
14:A:832:CLA:H92	14:A:832:CLA:H61	1.82	0.44
2:B:594:TYR:HA	2:B:620:TRP:HH2	1.82	0.44
9:L:133:GLY:HA2	17:L:1505:BCR:H281	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:806:CLA:H62	14:b:802:CLA:HBC3	1.98	0.44
1:1:334:GLY:HA2	9:0:6:GLN:NE2	2.32	0.44
14:b:810:CLA:H61	14:b:810:CLA:H2	1.75	0.44
17:b:853:BCR:H15C	17:b:853:BCR:H351	1.82	0.44
2:2:101:VAL:HG13	2:2:112:PRO:HG3	1.99	0.44
2:2:397:ASP:HA	4:4:129:VAL:HG11	2.00	0.44
14:2:815:CLA:H3A	14:2:815:CLA:HBA1	1.47	0.44
6:6:15:ALA:O	6:6:19:LYS:HG2	2.17	0.44
17:i:4103:BCR:H20C	17:i:4103:BCR:H361	1.85	0.44
11:k:25:CYS:SG	11:k:76:MET:HG3	2.58	0.44
9:l:46:PRO:HA	9:l:49:ARG:HG2	1.99	0.44
2:B:588:LEU:HA	2:B:591:LEU:HG	1.99	0.44
14:B:843:CLA:H141	9:L:91:VAL:HG21	2.00	0.44
14:L:1501:CLA:HBB1	17:L:1505:BCR:HC7	2.00	0.44
17:L:1505:BCR:H15C	17:L:1505:BCR:H351	1.86	0.44
1:a:396:ILE:HG23	14:a:809:CLA:H143	1.99	0.44
14:a:811:CLA:H91	14:a:811:CLA:H112	1.76	0.44
1:1:56:HIS:CE1	14:1:806:CLA:HBB2	2.53	0.44
1:1:200:HIS:ND1	14:1:826:CLA:OBD	2.44	0.44
1:1:691:GLY:O	1:1:695:GLU:HG3	2.18	0.44
14:1:804:CLA:H162	14:2:811:CLA:HMB2	2.00	0.44
14:1:830:CLA:H202	14:1:830:CLA:H161	1.72	0.44
2:b:536:ILE:HG21	17:b:849:BCR:H281	1.99	0.44
14:b:810:CLA:H2A	14:b:812:CLA:HED1	1.99	0.44
4:d:132:LYS:HA	4:d:132:LYS:HD2	1.76	0.44
4:4:137:ALA:HB3	4:4:139:TYR:HE1	1.82	0.44
7:i:19:GLY:HA3	14:l:4203:CLA:HAB	2.00	0.44
14:0:206:CLA:HBB1	17:0:210:BCR:HC7	2.00	0.44
1:A:646:LEU:HA	1:A:646:LEU:HD12	1.76	0.44
2:B:536:ILE:HG21	17:B:850:BCR:H281	1.99	0.44
14:B:843:CLA:H3A	14:B:843:CLA:HBA2	1.78	0.44
9:L:66:THR:HG21	9:L:142:LEU:HD13	2.00	0.44
1:a:317:ILE:HD13	11:k:64:ALA:HB2	2.00	0.44
14:a:837:CLA:H61	14:a:837:CLA:H41	1.64	0.44
1:1:396:ILE:HG23	14:1:807:CLA:H143	1.99	0.44
14:1:825:CLA:H41	14:1:825:CLA:H62	1.75	0.44
14:1:835:CLA:H71	17:1:850:BCR:H20C	1.99	0.44
3:3:29:VAL:HG12	4:4:112:ARG:HB2	2.00	0.44
2:b:588:LEU:HA	2:b:591:LEU:HG	1.99	0.44
2:2:173:SER:O	2:2:177:HIS:ND1	2.37	0.44
17:6:4406:BCR:H15C	17:6:4406:BCR:H351	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:836:CLA:H71	17:A:850:BCR:H20C	1.99	0.44
8:J:8:LEU:HD13	8:J:13:VAL:HG11	2.00	0.44
17:M:102:BCR:H15C	17:M:102:BCR:H351	1.83	0.44
11:K:25:CYS:SG	11:K:76:MET:HG3	2.58	0.44
1:a:56:HIS:CE1	14:a:808:CLA:HBB2	2.53	0.44
12:a:801:LHG:H282	12:a:801:LHG:H251	1.84	0.44
2:b:183:PHE:HB3	2:b:284:PHE:CD2	2.53	0.44
15:b:845:PQN:H212	15:b:845:PQN:H251	1.74	0.44
8:7:8:LEU:HD13	8:7:13:VAL:HG11	2.00	0.44
9:l:70:PRO:HG2	9:l:71:LEU:HD12	1.99	0.44
14:l:4204:CLA:H201	14:l:4206:CLA:H172	2.00	0.44
1:A:576:GLY:HA2	2:B:563:PRO:HD3	2.00	0.43
1:A:647:ARG:HA	2:B:633:ILE:HD12	1.99	0.43
14:A:839:CLA:H193	17:I:102:BCR:H371	1.99	0.43
2:B:183:PHE:HB3	2:B:284:PHE:CD2	2.53	0.43
14:L:1503:CLA:H12	19:i:4101:LMT:H6E	1.99	0.43
14:a:832:CLA:H91	14:a:832:CLA:H111	1.80	0.43
1:1:332:PHE:HE1	9:0:23:PRO:HG2	1.83	0.43
11:8:11:THR:HA	11:8:81:ALA:HB1	2.00	0.43
9:l:55:MET:HE3	14:l:4204:CLA:HMA2	1.99	0.43
9:0:66:THR:HG21	9:0:142:LEU:HD13	2.00	0.43
1:A:17:ASP:OD2	1:A:70:ARG:NH2	2.51	0.43
17:A:851:BCR:H15C	17:A:851:BCR:H351	1.88	0.43
3:C:66:ARG:HD3	3:C:66:ARG:HA	1.79	0.43
1:1:17:ASP:OD2	1:1:70:ARG:NH2	2.51	0.43
2:b:46:ILE:HG21	14:b:808:CLA:H201	2.00	0.43
2:b:106:GLN:HG3	2:b:115:ILE:HD11	1.99	0.43
2:b:268:LEU:HB2	2:b:273:ILE:HD11	2.00	0.43
14:b:825:CLA:CBB	14:b:832:CLA:HHD	2.48	0.43
2:2:550:ASP:OD1	2:2:550:ASP:N	2.46	0.43
17:f:203:BCR:H20C	17:f:203:BCR:H361	1.88	0.43
11:8:57:PHE:CE2	11:8:62:LEU:HD23	2.52	0.43
9:l:44:LEU:HB2	9:l:49:ARG:HH21	1.82	0.43
9:0:46:PRO:HA	9:0:49:ARG:HG2	1.99	0.43
14:A:830:CLA:H143	14:A:830:CLA:H111	1.76	0.43
2:B:195:VAL:HA	2:B:199:ILE:HD12	2.01	0.43
17:B:850:BCR:H20C	17:B:850:BCR:H361	1.74	0.43
14:a:806:CLA:H42	14:f:201:CLA:HAA1	2.01	0.43
14:b:810:CLA:H93	17:b:854:BCR:H353	2.00	0.43
14:b:842:CLA:HBA2	14:b:842:CLA:H3A	1.78	0.43
1:A:338:LYS:HB3	1:A:338:LYS:HE3	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HG23	14:A:808:CLA:H143	1.99	0.43
1:A:691:GLY:O	1:A:695:GLU:HG3	2.18	0.43
14:A:821:CLA:H143	14:A:821:CLA:H162	1.81	0.43
14:A:827:CLA:H111	14:A:827:CLA:H143	1.76	0.43
2:B:257:PHE:CE2	14:B:820:CLA:HBB1	2.53	0.43
17:B:851:BCR:H15C	17:B:851:BCR:H351	1.81	0.43
14:a:828:CLA:H143	14:a:828:CLA:H111	1.77	0.43
14:1:842:CLA:H152	14:7:1101:CLA:H203	2.00	0.43
2:b:460:TRP:HE1	2:b:474:VAL:HG11	1.82	0.43
2:2:268:LEU:HB2	2:2:273:ILE:HD11	2.00	0.43
14:2:843:CLA:H41	14:2:843:CLA:H62	1.76	0.43
14:2:843:CLA:H11	15:2:845:PQN:H261	2.01	0.43
5:5:13:ARG:HD2	5:5:61:PHE:HE1	1.83	0.43
14:0:208:CLA:H61	14:0:208:CLA:H41	1.69	0.43
14:A:843:CLA:H172	14:L:1502:CLA:HBB1	1.99	0.43
2:B:195:VAL:HG23	2:B:196:HIS:CD2	2.54	0.43
14:B:844:CLA:H62	14:B:844:CLA:H41	1.76	0.43
4:D:66:LEU:HD22	4:D:85:ILE:HD13	2.01	0.43
14:L:1503:CLA:H161	14:L:1503:CLA:H141	1.73	0.43
14:a:806:CLA:H203	14:a:842:CLA:H152	2.00	0.43
2:b:297:ILE:HD11	14:b:822:CLA:HMA2	1.99	0.43
2:2:195:VAL:HA	2:2:199:ILE:HD12	2.01	0.43
2:2:594:TYR:HA	2:2:620:TRP:HH2	1.82	0.43
18:2:802:LMG:H332	14:2:808:CLA:H41	2.00	0.43
6:f:45:CYS:HB3	6:f:51:PRO:HA	2.00	0.43
19:h:103:LMT:H6E	14:l:4206:CLA:H12	1.99	0.43
11:k:57:PHE:CE2	11:k:62:LEU:HD23	2.52	0.43
11:8:25:CYS:SG	11:8:76:MET:HG3	2.58	0.43
9:0:70:PRO:HG2	9:0:71:LEU:HD12	1.99	0.43
10:9:15:ALA:HA	10:9:18:PRO:HD2	2.00	0.43
18:B:803:LMG:H332	14:B:809:CLA:H41	2.00	0.43
4:D:126:PRO:HG2	4:D:141:VAL:HG23	1.99	0.43
5:E:13:ARG:HD2	5:E:61:PHE:HE1	1.83	0.43
14:L:1501:CLA:H201	14:L:1503:CLA:H172	2.00	0.43
1:1:571:ARG:HH11	12:1:801:LHG:HC41	1.84	0.43
14:1:841:CLA:HAA1	14:7:1101:CLA:H42	2.01	0.43
14:1:843:CLA:H203	9:0:61:LEU:HD11	1.99	0.43
17:1:849:BCR:H11C	17:1:849:BCR:H341	1.87	0.43
17:b:849:BCR:H20C	17:b:849:BCR:H361	1.74	0.43
14:l:4206:CLA:HBA1	14:l:4206:CLA:H3A	1.67	0.43
14:A:830:CLA:H161	17:J:103:BCR:H14C	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:LEU:HB2	2:B:273:ILE:HD11	2.00	0.43
2:B:430:HIS:CG	17:B:854:BCR:H323	2.52	0.43
14:B:813:CLA:H2	14:B:813:CLA:HED2	2.00	0.43
14:B:822:CLA:HMB2	14:B:827:CLA:HMA2	2.01	0.43
11:K:11:THR:HA	11:K:81:ALA:HB1	2.00	0.43
1:1:323:GLU:N	1:1:323:GLU:OE2	2.52	0.43
2:b:48:ALA:HB3	10:m:29:LEU:HD21	1.99	0.43
14:b:821:CLA:HMB2	14:b:826:CLA:HMA2	2.01	0.43
14:b:843:CLA:HBA1	17:b:851:BCR:H352	2.00	0.43
17:b:849:BCR:H24C	17:b:850:BCR:H373	1.99	0.43
17:b:854:BCR:H15C	17:b:854:BCR:H351	1.83	0.43
2:2:46:ILE:HG21	14:2:807:CLA:H201	2.00	0.43
2:2:262:HIS:N	2:2:267:SER:O	2.42	0.43
14:2:812:CLA:H2	14:2:812:CLA:HED2	2.00	0.43
14:2:843:CLA:HBA1	17:2:851:BCR:H352	2.00	0.43
4:d:66:LEU:HD22	4:d:85:ILE:HD13	2.01	0.43
9:0:46:PRO:HB2	9:0:122:GLN:HB2	2.01	0.43
14:A:810:CLA:H141	14:A:810:CLA:H162	1.75	0.43
18:B:803:LMG:H332	14:B:809:CLA:H51	2.01	0.43
14:B:808:CLA:H142	14:B:808:CLA:H111	1.74	0.43
17:J:103:BCR:H331	17:J:103:BCR:H342	2.01	0.43
14:K:4004:CLA:H11	14:K:4004:CLA:H51	1.75	0.43
17:a:847:BCR:H15C	17:a:847:BCR:H351	1.91	0.43
2:b:8:PHE:HB2	2:b:34:HIS:CG	2.54	0.43
2:b:118:SER:HA	14:b:829:CLA:HMA2	2.00	0.43
14:b:843:CLA:H11	15:b:845:PQN:H261	2.01	0.43
2:2:195:VAL:HG23	2:2:196:HIS:CD2	2.54	0.43
2:2:376:ILE:HD12	14:2:808:CLA:H143	2.01	0.43
5:e:13:ARG:HD2	5:e:61:PHE:HE1	1.83	0.43
8:j:8:LEU:HD13	8:j:13:VAL:HG11	2.00	0.43
11:k:11:THR:HA	11:k:81:ALA:HB1	2.00	0.43
9:l:67:LEU:HD12	14:l:4206:CLA:HHB	2.01	0.43
9:0:44:LEU:HB2	9:0:49:ARG:HH21	1.82	0.43
18:0:203:LMG:H141	14:0:208:CLA:HMB2	2.00	0.43
14:0:208:CLA:H112	14:0:208:CLA:H142	1.73	0.43
1:A:278:LYS:HD2	1:A:289:TRP:CE2	2.54	0.43
2:B:475:LEU:O	2:B:481:SER:OG	2.30	0.43
14:B:808:CLA:H162	14:B:808:CLA:H141	1.74	0.43
14:B:813:CLA:O2A	14:B:813:CLA:H2A	2.18	0.43
14:B:844:CLA:H11	15:B:846:PQN:H261	2.01	0.43
1:a:435:ALA:O	1:a:439:HIS:ND1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:309:LYS:HB2	2:b:309:LYS:HE2	1.85	0.43
2:b:594:TYR:HA	2:b:620:TRP:HH2	1.82	0.43
2:2:118:SER:HA	14:2:829:CLA:HMA2	2.00	0.43
7:i:30:LEU:HD23	7:i:30:LEU:HA	1.90	0.43
17:j:103:BCR:H331	17:j:103:BCR:H342	2.01	0.43
17:9:102:BCR:H15C	17:9:102:BCR:H351	1.83	0.43
1:A:189:TRP:CZ2	14:A:815:CLA:HAC2	2.54	0.43
1:A:323:GLU:OE2	1:A:323:GLU:N	2.52	0.43
7:I:30:LEU:HD23	7:I:30:LEU:HA	1.91	0.43
14:a:824:CLA:H2	14:a:824:CLA:H62	1.72	0.43
14:a:835:CLA:H171	14:b:842:CLA:HMB2	2.00	0.43
1:1:127:ASN:HB3	1:1:135:HIS:HB3	2.01	0.43
1:1:189:TRP:CZ2	14:1:814:CLA:HAC2	2.54	0.43
1:1:278:LYS:HD2	1:1:289:TRP:CE2	2.54	0.43
2:b:16:PRO:HB2	2:b:697:LYS:HZ3	1.83	0.43
2:b:195:VAL:HG23	2:b:196:HIS:CD2	2.54	0.43
18:2:802:LMG:H332	14:2:808:CLA:H51	2.01	0.43
14:2:821:CLA:HMB2	14:2:826:CLA:HMA2	2.01	0.43
14:f:204:CLA:HBB2	17:j:103:BCR:H312	2.01	0.43
6:6:124:GLY:O	6:6:128:SER:OG	2.27	0.43
1:A:56:HIS:CE1	14:A:807:CLA:HBB2	2.53	0.42
1:A:127:ASN:HB3	1:A:135:HIS:HB3	2.01	0.42
14:A:819:CLA:H61	14:A:819:CLA:H41	1.61	0.42
2:B:701:LEU:HD22	2:B:705:GLN:NE2	2.34	0.42
6:F:45:CYS:HB3	6:F:51:PRO:HA	2.00	0.42
9:L:46:PRO:HB2	9:L:122:GLN:HB2	2.01	0.42
1:a:17:ASP:OD2	1:a:70:ARG:NH2	2.51	0.42
1:a:691:GLY:O	1:a:695:GLU:HG3	2.18	0.42
14:a:832:CLA:H202	14:a:832:CLA:H161	1.72	0.42
3:c:4:SER:HB2	4:d:139:TYR:HE2	1.84	0.42
14:b:843:CLA:H41	14:b:843:CLA:H62	1.76	0.42
15:b:845:PQN:H212	15:b:845:PQN:H172	1.71	0.42
4:4:132:LYS:HD2	4:4:132:LYS:HA	1.76	0.42
14:0:208:CLA:H152	14:0:208:CLA:H18	1.88	0.42
1:A:571:ARG:HH11	12:A:801:LHG:HC41	1.84	0.42
14:A:842:CLA:HMC2	14:B:801:CLA:H112	2.01	0.42
2:B:428:GLY:HA2	2:B:526:LEU:HD22	2.00	0.42
14:B:844:CLA:HBA1	17:B:852:BCR:H352	2.00	0.42
1:1:122:GLY:HA2	6:6:26:THR:HA	2.01	0.42
2:b:701:LEU:HD22	2:b:705:GLN:NE2	2.35	0.42
14:b:818:CLA:HBA2	14:b:818:CLA:H3A	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:16:PRO:HB2	2:2:697:LYS:HZ3	1.84	0.42
2:2:31:PHE:HE1	14:2:806:CLA:HED1	1.84	0.42
14:2:825:CLA:HMB3	12:2:852:LHG:HC12	2.01	0.42
4:d:32:TRP:NE1	4:d:50:MET:HE3	2.35	0.42
14:B:805:CLA:H161	14:B:805:CLA:H122	1.80	0.42
4:D:121:ARG:NH1	5:E:13:ARG:HG3	2.33	0.42
7:I:10:LEU:HD12	7:I:10:LEU:HA	1.92	0.42
1:a:278:LYS:HD2	1:a:289:TRP:CE2	2.54	0.42
14:a:831:CLA:H203	14:b:804:CLA:H101	2.02	0.42
1:1:324:ILE:O	1:1:328:HIS:ND1	2.50	0.42
1:1:711:PRO:HA	6:6:87:LEU:HD21	2.00	0.42
2:b:428:GLY:HA2	2:b:526:LEU:HD22	2.00	0.42
14:b:815:CLA:H3A	14:b:815:CLA:HBA1	1.47	0.42
14:2:812:CLA:O2A	14:2:812:CLA:H2A	2.18	0.42
4:4:52:GLU:H	4:4:52:GLU:HG3	1.43	0.42
14:6:4403:CLA:HBB2	17:7:1104:BCR:H312	2.01	0.42
9:l:46:PRO:HB2	9:l:122:GLN:HB2	2.01	0.42
9:l:66:THR:HG21	9:l:142:LEU:HD13	2.00	0.42
9:l:137:VAL:HG21	17:0:204:BCR:H372	2.00	0.42
14:l:4204:CLA:HBB1	17:0:204:BCR:HC7	2.00	0.42
14:0:208:CLA:H141	14:0:208:CLA:H161	1.72	0.42
14:A:830:CLA:H93	14:B:804:CLA:H18	2.00	0.42
2:B:70:TRP:NE1	7:I:6:ALA:O	2.43	0.42
14:B:811:CLA:H2	14:B:811:CLA:H71	2.02	0.42
14:B:826:CLA:CBB	14:B:833:CLA:HHD	2.48	0.42
14:B:829:CLA:H111	14:B:829:CLA:H72	1.65	0.42
14:B:838:CLA:HMB1	17:B:851:BCR:HC32	2.02	0.42
17:L:1505:BCR:H20C	17:L:1505:BCR:H361	1.83	0.42
10:M:15:ALA:HA	10:M:18:PRO:HD2	2.01	0.42
14:a:806:CLA:O1D	14:f:201:CLA:H3A	2.20	0.42
14:a:840:CLA:H122	14:l:4205:CLA:H203	2.00	0.42
14:a:842:CLA:H142	14:a:842:CLA:H111	1.92	0.42
14:1:829:CLA:H93	14:2:803:CLA:H18	2.02	0.42
18:b:803:LMG:H332	14:b:809:CLA:H41	2.00	0.42
14:b:809:CLA:H72	14:b:809:CLA:H111	1.48	0.42
14:b:816:CLA:HAB	14:b:830:CLA:H162	2.01	0.42
17:2:849:BCR:H24C	17:2:850:BCR:H373	1.99	0.42
8:7:2:ASP:HA	8:7:5:LYS:HB2	2.02	0.42
14:A:814:CLA:H41	14:A:822:CLA:H42	2.02	0.42
14:A:831:CLA:H111	14:A:831:CLA:H91	1.80	0.42
2:B:8:PHE:HB2	2:B:34:HIS:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ILE:HG21	14:B:808:CLA:H201	2.00	0.42
14:B:826:CLA:HMB3	12:B:853:LHG:HC12	2.01	0.42
7:I:20:TRP:HB3	14:0:208:CLA:H202	2.01	0.42
14:J:101:CLA:H3A	14:J:101:CLA:HBA2	1.49	0.42
14:a:804:CLA:H112	14:a:842:CLA:HMC2	2.01	0.42
14:a:841:CLA:O2D	14:a:841:CLA:H2A	2.20	0.42
17:a:847:BCR:H361	17:a:847:BCR:H20C	1.89	0.42
3:c:35:LYS:HD3	5:e:29:GLU:HG2	2.01	0.42
2:b:408:ARG:HA	2:b:411:GLU:HB2	2.02	0.42
2:2:304:ILE:O	2:2:308:HIS:ND1	2.41	0.42
2:2:584:MET:HE3	2:2:584:MET:HB3	1.96	0.42
2:2:701:LEU:HD22	2:2:705:GLN:NE2	2.34	0.42
17:2:847:BCR:H20C	17:2:847:BCR:H361	1.87	0.42
4:4:66:LEU:HD22	4:4:85:ILE:HD13	2.01	0.42
6:6:45:CYS:HB3	6:6:51:PRO:HA	2.00	0.42
17:6:4402:BCR:H20C	17:6:4402:BCR:H361	1.87	0.42
7:h:21:LEU:HD21	14:l:4206:CLA:H141	2.01	0.42
14:A:805:CLA:H92	14:A:805:CLA:H61	1.69	0.42
14:A:807:CLA:H93	17:A:848:BCR:H23C	2.01	0.42
14:A:832:CLA:H41	14:A:832:CLA:H62	1.78	0.42
2:B:376:ILE:HD12	14:B:809:CLA:H143	2.01	0.42
2:B:412:HIS:NE2	2:B:416:LEU:HD23	2.35	0.42
14:B:820:CLA:H93	14:B:820:CLA:H62	1.75	0.42
8:J:2:ASP:HA	8:J:5:LYS:HB2	2.02	0.42
1:a:200:HIS:ND1	14:a:828:CLA:OBD	2.44	0.42
1:1:173:LEU:HD23	1:1:173:LEU:HA	1.91	0.42
1:1:716:ARG:CZ	5:5:46:TYR:HE2	2.33	0.42
14:1:812:CLA:H62	14:1:812:CLA:H102	1.59	0.42
3:3:13:GLY:HA2	3:3:28:MET:HE1	2.02	0.42
14:b:837:CLA:HMB1	17:b:850:BCR:HC32	2.02	0.42
2:2:428:GLY:HA2	2:2:526:LEU:HD22	2.00	0.42
14:f:201:CLA:H51	8:j:18:LEU:HD22	2.00	0.42
14:A:805:CLA:H42	14:F:201:CLA:HAA1	2.01	0.42
17:A:850:BCR:H11C	17:A:850:BCR:H341	1.90	0.42
2:B:408:ARG:HA	2:B:411:GLU:HB2	2.02	0.42
14:B:801:CLA:H143	14:B:801:CLA:H112	1.84	0.42
14:B:817:CLA:HAB	14:B:831:CLA:H162	2.01	0.42
14:B:819:CLA:H2	14:B:819:CLA:H62	1.74	0.42
1:a:42:PRO:HG3	6:f:101:VAL:HG21	2.01	0.42
1:a:323:GLU:OE2	1:a:323:GLU:N	2.52	0.42
1:a:714:GLN:NE2	5:e:43:ARG:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:803:CL0:H11	14:b:805:CLA:HAA1	2.00	0.42
14:a:827:CLA:H62	14:a:827:CLA:H41	1.75	0.42
14:a:831:CLA:H201	14:b:835:CLA:HBC1	2.01	0.42
1:1:111:LYS:HE3	1:1:111:LYS:HB2	1.96	0.42
2:b:591:LEU:HD22	14:b:839:CLA:HBB2	2.02	0.42
14:b:815:CLA:H142	14:b:815:CLA:H111	1.74	0.42
2:2:8:PHE:HB2	2:2:34:HIS:CG	2.54	0.42
14:2:811:CLA:H61	17:h:101:BCR:H12C	2.02	0.42
10:m:15:ALA:HA	10:m:18:PRO:HD2	2.01	0.42
14:A:807:CLA:CGA	14:A:807:CLA:H3A	2.49	0.42
14:A:823:CLA:H102	14:A:823:CLA:H61	1.84	0.42
14:A:836:CLA:HMD2	14:A:837:CLA:HBB1	2.02	0.42
2:B:132:ASN:HB3	10:M:3:LEU:HD13	2.02	0.42
14:B:813:CLA:H151	17:0:210:BCR:H362	2.01	0.42
14:B:821:CLA:H62	14:B:821:CLA:H41	1.62	0.42
14:B:821:CLA:HBA2	14:B:821:CLA:H3A	1.63	0.42
4:D:132:LYS:HD2	4:D:132:LYS:HA	1.76	0.42
1:a:127:ASN:HB3	1:a:135:HIS:HB3	2.01	0.42
1:a:338:LYS:HB3	1:a:338:LYS:HE3	1.58	0.42
1:a:428:ARG:O	1:a:432:HIS:ND1	2.48	0.42
1:a:530:ALA:O	1:a:534:VAL:HG23	2.20	0.42
14:1:806:CLA:CGA	14:1:806:CLA:H3A	2.49	0.42
18:b:803:LMG:H332	14:b:809:CLA:H51	2.01	0.42
14:b:811:CLA:H2	14:b:811:CLA:H71	2.02	0.42
2:2:591:LEU:HD22	14:2:839:CLA:HBB2	2.02	0.42
14:2:809:CLA:H13	17:h:101:BCR:HC42	2.01	0.42
14:2:811:CLA:H122	14:2:811:CLA:H8	1.96	0.42
7:h:10:LEU:HD12	7:h:10:LEU:HA	1.92	0.42
14:l:4203:CLA:H2A	14:l:4203:CLA:O2A	2.18	0.42
1:A:433:ARG:HE	1:A:433:ARG:HB2	1.54	0.42
1:A:530:ALA:O	1:A:534:VAL:HG23	2.20	0.42
14:A:827:CLA:HBA1	14:A:831:CLA:H201	2.02	0.42
14:A:842:CLA:H142	14:A:842:CLA:H111	1.92	0.42
14:A:843:CLA:HMB3	2:B:683:HIS:HE1	1.85	0.42
2:B:553:ASP:OD1	2:B:553:ASP:N	2.49	0.42
1:a:712:ALA:N	6:f:100:GLU:OE2	2.51	0.42
12:a:801:LHG:H331	12:a:801:LHG:H362	1.81	0.42
1:1:86:TRP:NE1	14:1:829:CLA:OBD	2.53	0.42
14:1:826:CLA:H2	14:1:826:CLA:H62	1.85	0.42
14:1:842:CLA:HMC2	14:2:801:CLA:H112	2.01	0.42
9:0:137:VAL:HG21	17:0:210:BCR:H372	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASN:HD22	1:A:640:ILE:HB	1.85	0.42
14:A:820:CLA:HBC1	14:A:829:CLA:H192	2.02	0.42
2:B:118:SER:HA	14:B:830:CLA:HMA2	2.00	0.42
2:B:309:LYS:HE2	2:B:309:LYS:HB2	1.85	0.42
14:B:819:CLA:H3A	14:B:819:CLA:HBA2	1.57	0.42
14:B:841:CLA:H92	14:B:841:CLA:H61	1.91	0.42
14:B:843:CLA:H93	14:B:843:CLA:H111	1.82	0.42
1:a:189:TRP:CZ2	14:a:816:CLA:HAC2	2.54	0.42
17:a:849:BCR:H20C	17:a:849:BCR:H361	1.85	0.42
1:1:458:ASN:HD22	1:1:640:ILE:HB	1.85	0.42
2:b:376:ILE:HD12	14:b:809:CLA:H143	2.01	0.42
14:b:842:CLA:H93	14:b:842:CLA:H111	1.82	0.42
14:b:843:CLA:HBA2	15:b:845:PQN:H241	2.02	0.42
15:2:845:PQN:H212	15:2:845:PQN:H251	1.74	0.42
17:7:1104:BCR:H342	17:7:1104:BCR:H331	2.01	0.42
1:A:433:ARG:HG2	1:A:554:LEU:HB3	2.02	0.41
14:B:816:CLA:H62	14:B:816:CLA:H2	1.69	0.41
14:B:831:CLA:H61	14:B:831:CLA:H41	1.90	0.41
14:B:844:CLA:HBA2	15:B:846:PQN:H241	2.02	0.41
7:I:21:LEU:HD21	14:0:208:CLA:H141	2.01	0.41
9:L:132:MET:HG3	17:0:210:BCR:H24C	2.02	0.41
1:a:433:ARG:HG2	1:a:554:LEU:HB3	2.02	0.41
1:a:575:ASP:OD1	3:c:53:ARG:NE	2.52	0.41
1:a:707:LEU:HD11	14:b:802:CLA:HMA1	2.02	0.41
14:a:833:CLA:H111	14:a:833:CLA:H152	1.77	0.41
14:a:835:CLA:H193	15:b:845:PQN:H293	2.02	0.41
14:a:837:CLA:HMD2	14:a:838:CLA:HBB1	2.02	0.41
1:1:433:ARG:HG2	1:1:554:LEU:HB3	2.02	0.41
12:1:801:LHG:H282	12:1:801:LHG:H251	1.84	0.41
14:1:819:CLA:HBC1	14:1:828:CLA:H192	2.02	0.41
14:1:841:CLA:H3A	14:7:1101:CLA:O1D	2.20	0.41
3:c:13:GLY:HA2	3:c:28:MET:HE1	2.02	0.41
3:3:66:ARG:HH12	2:2:561:ASP:CG	2.27	0.41
2:2:408:ARG:HA	2:2:411:GLU:HB2	2.02	0.41
17:2:849:BCR:H361	17:2:849:BCR:H20C	1.74	0.41
5:5:18:TRP:NE1	5:5:43:ARG:O	2.43	0.41
1:A:200:HIS:ND1	14:A:827:CLA:OBD	2.44	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.84	0.41
14:A:805:CLA:O1D	14:F:201:CLA:H3A	2.20	0.41
14:A:822:CLA:H143	17:A:847:BCR:H24C	2.02	0.41
2:B:723:ALA:O	2:B:727:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:804:CLA:HMB3	14:B:805:CLA:H18	2.02	0.41
14:B:807:CLA:H51	18:0:201:LMG:H342	2.02	0.41
9:L:67:LEU:HD12	14:L:1503:CLA:HHB	2.01	0.41
1:a:200:HIS:HB3	14:a:828:CLA:HED3	2.01	0.41
1:a:324:ILE:O	1:a:328:HIS:ND1	2.50	0.41
13:a:803:CL0:H7	14:b:805:CLA:HMB3	2.02	0.41
14:a:806:CLA:HED1	8:j:15:ILE:HG21	2.02	0.41
14:a:828:CLA:HBA1	14:a:832:CLA:H201	2.02	0.41
1:1:197:MET:HE3	1:1:197:MET:HB2	1.90	0.41
1:1:552:GLY:O	1:1:556:ALA:HB2	2.20	0.41
1:1:581:GLY:HA3	2:2:703:ILE:HD11	2.02	0.41
14:1:818:CLA:H61	14:1:818:CLA:H41	1.61	0.41
14:1:829:CLA:H201	14:2:835:CLA:HBC1	2.02	0.41
14:b:825:CLA:HMB3	12:b:852:LHG:HC12	2.01	0.41
2:2:723:ALA:O	2:2:727:ILE:HB	2.21	0.41
14:2:811:CLA:H3A	14:2:811:CLA:HBA1	1.37	0.41
14:2:825:CLA:CBB	14:2:832:CLA:HHD	2.48	0.41
4:4:32:TRP:NE1	4:4:50:MET:HE3	2.35	0.41
9:0:67:LEU:HD12	14:0:208:CLA:HHB	2.01	0.41
1:A:47:TRP:HE3	1:A:48:ILE:HD13	1.85	0.41
1:A:200:HIS:HB3	14:A:827:CLA:HED3	2.01	0.41
6:F:36:ARG:HD3	8:J:35:ASP:OD2	2.20	0.41
17:J:104:BCR:H15C	17:J:104:BCR:H351	1.89	0.41
9:L:137:VAL:HG21	17:L:1505:BCR:H372	2.00	0.41
11:K:33:GLY:HA3	11:K:65:THR:HG22	2.02	0.41
14:a:808:CLA:H93	17:a:848:BCR:H23C	2.01	0.41
14:a:823:CLA:H143	17:a:847:BCR:H24C	2.02	0.41
1:1:707:LEU:HD11	14:1:840:CLA:HMA1	2.02	0.41
14:1:823:CLA:HBA2	14:1:823:CLA:H3A	1.38	0.41
14:1:826:CLA:HBA1	14:1:830:CLA:H201	2.02	0.41
8:j:2:ASP:HA	8:j:5:LYS:HB2	2.02	0.41
11:k:66:MET:HE3	17:k:4004:BCR:H351	2.02	0.41
17:0:204:BCR:H15C	17:0:204:BCR:H351	1.86	0.41
12:A:801:LHG:H282	12:A:801:LHG:H251	1.83	0.41
14:A:832:CLA:H111	14:A:832:CLA:H152	1.77	0.41
17:A:848:BCR:H361	17:A:848:BCR:H20C	1.75	0.41
2:B:31:PHE:HE1	14:B:807:CLA:HED1	1.84	0.41
2:B:391:PHE:CD2	17:B:851:BCR:H282	2.56	0.41
14:B:809:CLA:HHB	14:B:832:CLA:HAB	2.03	0.41
14:B:813:CLA:H111	14:B:813:CLA:H143	1.88	0.41
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:32:TRP:NE1	4:D:50:MET:HE3	2.35	0.41
11:K:66:MET:HE3	17:K:4005:BCR:H351	2.02	0.41
14:a:804:CLA:O1A	14:b:804:CLA:HBB2	2.19	0.41
14:a:836:CLA:HMA2	9:l:68:LEU:HB3	2.01	0.41
14:1:806:CLA:H93	17:1:848:BCR:H23C	2.01	0.41
14:1:821:CLA:H143	17:1:847:BCR:H24C	2.02	0.41
14:1:843:CLA:H2	14:1:843:CLA:H61	1.69	0.41
3:c:63:LEU:HD23	3:c:63:LEU:HA	1.93	0.41
2:b:59:LEU:HD12	17:b:854:BCR:H341	2.02	0.41
2:b:195:VAL:HA	2:b:199:ILE:HD12	2.01	0.41
2:b:412:HIS:NE2	2:b:416:LEU:HD23	2.35	0.41
14:b:804:CLA:HMB3	14:b:805:CLA:H18	2.01	0.41
14:b:811:CLA:H143	14:b:811:CLA:H161	1.86	0.41
2:2:65:LEU:HD23	2:2:135:LEU:HD23	2.02	0.41
14:2:808:CLA:H111	14:2:808:CLA:H72	1.48	0.41
14:l:4206:CLA:H142	14:l:4206:CLA:H112	1.73	0.41
14:A:813:CLA:H62	14:A:813:CLA:H102	1.59	0.41
14:A:822:CLA:H52	14:A:822:CLA:H8	1.95	0.41
14:A:840:CLA:H2A	14:A:840:CLA:O2D	2.20	0.41
17:B:848:BCR:H15C	17:B:848:BCR:H351	1.82	0.41
3:C:51:CYS:SG	3:C:53:ARG:HG3	2.61	0.41
1:1:334:GLY:HA2	9:0:6:GLN:HE22	1.85	0.41
2:b:420:LEU:HA	2:b:423:VAL:HG12	2.03	0.41
14:b:812:CLA:H61	17:i:4102:BCR:H12C	2.03	0.41
14:b:815:CLA:H121	14:b:815:CLA:H161	1.77	0.41
14:b:818:CLA:H2	14:b:818:CLA:H62	1.74	0.41
14:2:816:CLA:HAB	14:2:830:CLA:H162	2.00	0.41
14:2:837:CLA:HMB1	17:2:850:BCR:HC32	2.02	0.41
14:6:4403:CLA:HBC3	8:7:18:LEU:HD23	2.02	0.41
7:h:30:LEU:HD23	7:h:30:LEU:HA	1.90	0.41
17:k:4001:BCR:H351	17:k:4001:BCR:H15C	1.79	0.41
11:8:33:GLY:HA3	11:8:65:THR:HG22	2.02	0.41
14:l:4203:CLA:HED2	14:l:4203:CLA:H2	2.00	0.41
14:l:4205:CLA:H91	14:l:4205:CLA:H112	1.93	0.41
17:K:4001:BCR:H351	17:K:4001:BCR:H15C	1.79	0.41
1:a:552:GLY:O	1:a:556:ALA:HB2	2.20	0.41
14:a:808:CLA:CGA	14:a:808:CLA:H3A	2.49	0.41
14:a:831:CLA:H161	17:j:103:BCR:H14C	2.02	0.41
1:1:200:HIS:HB3	14:1:826:CLA:HED3	2.01	0.41
2:b:268:LEU:HD12	2:b:355:SER:HB3	2.03	0.41
14:b:802:CLA:H93	14:b:802:CLA:H61	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:834:CLA:H61	14:b:834:CLA:H92	1.78	0.41
17:b:850:BCR:H351	17:b:850:BCR:H15C	1.81	0.41
2:2:474:VAL:HG23	2:2:475:LEU:H	1.86	0.41
14:l:4206:CLA:H152	14:l:4206:CLA:H18	1.88	0.41
2:B:65:LEU:HD23	2:B:135:LEU:HD23	2.03	0.41
2:B:173:SER:O	2:B:177:HIS:ND1	2.37	0.41
2:B:304:ILE:O	2:B:308:HIS:ND1	2.41	0.41
14:B:810:CLA:HMB3	14:B:811:CLA:H3A	2.03	0.41
1:a:565:LYS:NZ	2:b:674:GLU:OE1	2.47	0.41
14:a:815:CLA:H3A	14:a:815:CLA:HBA2	1.58	0.41
1:1:530:ALA:O	1:1:534:VAL:HG23	2.20	0.41
2:b:68:VAL:HG13	2:b:121:TYR:CZ	2.56	0.41
11:k:33:GLY:HA3	11:k:65:THR:HG22	2.02	0.41
14:A:805:CLA:H192	14:A:842:CLA:H101	2.03	0.41
14:A:810:CLA:H91	14:A:810:CLA:H112	1.76	0.41
14:A:834:CLA:HAB	14:A:835:CLA:HHB	2.02	0.41
14:A:843:CLA:H2	14:A:843:CLA:H61	1.69	0.41
3:C:13:GLY:HA2	3:C:28:MET:HE1	2.02	0.41
1:a:114:ALA:H	1:a:139:ILE:HG23	1.86	0.41
1:a:571:ARG:HH11	12:a:801:LHG:HC41	1.84	0.41
1:a:702:TRP:HH2	14:b:833:CLA:HED3	1.84	0.41
14:a:835:CLA:HAB	14:a:836:CLA:HHB	2.02	0.41
14:a:854:CLA:H51	14:a:854:CLA:H11	1.75	0.41
1:1:435:ALA:O	1:1:439:HIS:ND1	2.42	0.41
14:1:813:CLA:H41	14:1:821:CLA:H42	2.02	0.41
14:1:839:CLA:O2D	14:1:839:CLA:H2A	2.20	0.41
14:1:842:CLA:H101	14:7:1101:CLA:H192	2.03	0.41
2:b:714:PHE:O	2:b:718:TYR:HB2	2.21	0.41
17:b:851:BCR:H20C	17:b:851:BCR:H361	1.78	0.41
2:2:420:LEU:HA	2:2:423:VAL:HG12	2.03	0.41
2:2:714:PHE:O	2:2:718:TYR:HB2	2.21	0.41
14:2:803:CLA:H162	14:2:803:CLA:H202	1.81	0.41
9:0:82:LEU:HD13	9:0:139:TYR:HB2	2.02	0.41
1:A:552:GLY:O	1:A:556:ALA:HB2	2.20	0.41
14:A:814:CLA:H3A	14:A:814:CLA:HBA2	1.58	0.41
14:A:827:CLA:H2	14:A:827:CLA:H62	1.85	0.41
14:A:828:CLA:H93	14:A:828:CLA:H62	1.79	0.41
2:B:93:ASP:HA	2:B:94:PRO:HD3	1.94	0.41
2:B:420:LEU:HD23	2:B:420:LEU:HA	1.79	0.41
2:B:577:PHE:HE1	14:B:832:CLA:HAC2	1.86	0.41
2:B:583:TRP:CH2	14:B:804:CLA:HAB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:LEU:HD22	14:B:840:CLA:HBB2	2.02	0.41
2:B:714:PHE:O	2:B:718:TYR:HB2	2.21	0.41
14:B:808:CLA:H202	14:B:808:CLA:H161	1.87	0.41
14:B:840:CLA:HMB2	14:B:842:CLA:HED1	2.03	0.41
17:J:104:BCR:H11C	17:J:104:BCR:H341	1.93	0.41
11:K:34:TYR:HE1	11:K:53:SER:HB2	1.85	0.41
14:a:815:CLA:H41	14:a:823:CLA:H42	2.02	0.41
14:a:821:CLA:HBC1	14:a:830:CLA:H192	2.02	0.41
1:1:114:ALA:H	1:1:139:ILE:HG23	1.86	0.41
3:3:5:VAL:HG11	3:3:26:LEU:HD21	2.03	0.41
2:b:114:ASN:ND2	14:b:812:CLA:OBD	2.53	0.41
14:b:808:CLA:H161	14:b:808:CLA:H202	1.86	0.41
14:b:824:CLA:HBA2	14:b:824:CLA:H3A	1.73	0.41
14:b:837:CLA:HBA1	14:b:837:CLA:H3A	1.85	0.41
2:2:268:LEU:HD12	2:2:355:SER:HB3	2.03	0.41
2:2:412:HIS:NE2	2:2:416:LEU:HD23	2.35	0.41
2:2:577:PHE:HE1	14:2:831:CLA:HAC2	1.86	0.41
11:8:66:MET:HE3	17:8:4005:BCR:H351	2.02	0.41
14:l:4203:CLA:H111	14:l:4203:CLA:H143	1.88	0.41
14:0:207:CLA:H91	14:0:207:CLA:H112	1.93	0.41
2:B:65:LEU:HD11	17:B:849:BCR:H281	2.03	0.41
1:a:458:ASN:HD22	1:a:640:ILE:HB	1.85	0.41
14:a:811:CLA:HBB1	14:a:812:CLA:O1A	2.21	0.41
14:1:842:CLA:H203	8:7:19:LEU:HD22	2.03	0.41
17:1:850:BCR:H11C	17:1:850:BCR:H341	1.91	0.41
3:c:51:CYS:SG	3:c:53:ARG:HG3	2.61	0.41
3:3:15:THR:HA	3:3:28:MET:HE2	2.03	0.41
3:3:51:CYS:SG	3:3:53:ARG:HG3	2.61	0.41
2:b:577:PHE:HE1	14:b:831:CLA:HAC2	1.86	0.41
2:b:723:ALA:O	2:b:727:ILE:HB	2.21	0.41
2:2:25:ILE:HG12	17:0:209:BCR:HC41	2.03	0.41
2:2:68:VAL:HG13	2:2:121:TYR:CZ	2.56	0.41
14:2:817:CLA:H2A	14:2:817:CLA:CED	2.51	0.41
14:2:830:CLA:H3A	14:2:830:CLA:HBA2	1.85	0.41
6:6:23:PHE:HB3	6:6:36:ARG:HH21	1.86	0.41
7:i:28:GLY:O	7:i:32:ILE:HG12	2.21	0.41
14:A:810:CLA:HBB1	14:A:811:CLA:O1A	2.21	0.40
2:B:685:ARG:HD2	9:L:19:HIS:CD2	2.55	0.40
17:B:852:BCR:H15C	17:B:852:BCR:H351	1.89	0.40
3:C:15:THR:HA	3:C:28:MET:HE2	2.03	0.40
6:F:23:PHE:HB3	6:F:36:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:831:CLA:H162	14:a:831:CLA:H202	1.70	0.40
1:1:587:GLY:O	1:1:591:VAL:HG23	2.22	0.40
1:1:706:LYS:O	6:6:133:MET:N	2.52	0.40
2:2:391:PHE:CD2	17:2:850:BCR:H282	2.56	0.40
14:2:810:CLA:H2	14:2:810:CLA:H71	2.02	0.40
14:2:812:CLA:H93	14:2:812:CLA:H111	1.77	0.40
17:2:847:BCR:H15C	17:2:847:BCR:H351	1.83	0.40
9:0:134:GLY:HA2	9:0:137:VAL:HG12	2.03	0.40
14:A:830:CLA:H201	14:B:836:CLA:HBC1	2.03	0.40
17:A:849:BCR:HC31	17:A:849:BCR:H323	1.92	0.40
14:1:807:CLA:H2	14:1:807:CLA:H61	1.70	0.40
2:b:31:PHE:HE1	14:b:807:CLA:HED1	1.84	0.40
2:b:93:ASP:OD1	2:b:93:ASP:N	2.54	0.40
2:2:93:ASP:OD1	2:2:93:ASP:N	2.54	0.40
17:2:846:BCR:H15C	17:2:846:BCR:H351	1.86	0.40
6:6:71:LEU:O	6:6:75:ILE:HG12	2.21	0.40
7:h:28:GLY:O	7:h:32:ILE:HG12	2.21	0.40
9:l:41:ARG:HB3	9:l:44:LEU:HD13	2.03	0.40
1:A:707:LEU:HD11	14:A:841:CLA:HMA1	2.02	0.40
14:A:813:CLA:H192	14:A:813:CLA:H161	1.90	0.40
14:A:831:CLA:H202	14:A:831:CLA:H161	1.72	0.40
2:B:93:ASP:N	2:B:93:ASP:OD1	2.54	0.40
2:B:255:LEU:HB3	2:B:275:HIS:HD2	1.87	0.40
18:B:803:LMG:H191	15:B:846:PQN:H301	2.04	0.40
14:B:818:CLA:H2A	14:B:818:CLA:CED	2.51	0.40
10:M:3:LEU:HD23	10:M:8:ILE:HD11	2.03	0.40
1:a:25:PHE:HB3	8:j:3:GLY:HA3	2.03	0.40
1:a:671:MET:HG3	1:a:740:TRP:CZ3	2.55	0.40
1:1:234:LYS:HA	1:1:234:LYS:HD3	1.90	0.40
14:1:809:CLA:HBA2	14:1:809:CLA:H3A	1.66	0.40
14:1:809:CLA:HBB1	14:1:810:CLA:O1A	2.21	0.40
17:1:848:BCR:H20C	17:1:848:BCR:H361	1.75	0.40
2:b:583:TRP:CH2	14:b:804:CLA:HAB	2.56	0.40
14:b:817:CLA:H2A	14:b:817:CLA:CED	2.51	0.40
2:2:272:ASP:OD1	14:2:819:CLA:HHB	2.22	0.40
14:2:808:CLA:HED1	14:2:831:CLA:H2	2.04	0.40
14:2:840:CLA:H92	14:2:840:CLA:H61	1.91	0.40
17:2:848:BCR:H15C	17:2:848:BCR:H351	1.89	0.40
4:4:14:SER:OG	4:4:16:GLY:O	2.39	0.40
17:6:4406:BCR:H20C	17:6:4406:BCR:H361	1.92	0.40
17:0:210:BCR:H15C	17:0:210:BCR:H351	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:810:CLA:H3A	14:A:810:CLA:HBA2	1.66	0.40
2:B:16:PRO:HB2	2:B:697:LYS:HZ3	1.85	0.40
2:B:68:VAL:HG13	2:B:121:TYR:CZ	2.56	0.40
2:B:420:LEU:HA	2:B:423:VAL:HG12	2.03	0.40
14:a:833:CLA:H61	14:a:833:CLA:H92	1.82	0.40
17:a:850:BCR:H11C	17:a:850:BCR:H341	1.91	0.40
14:1:835:CLA:HMD2	14:1:836:CLA:HBB1	2.02	0.40
3:c:15:THR:HA	3:c:28:MET:HE2	2.03	0.40
2:b:391:PHE:CD2	17:b:850:BCR:H282	2.55	0.40
2:2:583:TRP:CH2	14:2:803:CLA:HAB	2.56	0.40
14:2:803:CLA:HMB3	14:2:804:CLA:H18	2.02	0.40
14:2:808:CLA:HHB	14:2:831:CLA:HAB	2.03	0.40
14:f:205:CLA:CGD	14:f:205:CLA:HAA2	2.52	0.40
14:6:4404:CLA:HAA2	14:6:4404:CLA:CGD	2.51	0.40
11:k:34:TYR:HE1	11:k:53:SER:HB2	1.85	0.40
11:8:34:TYR:HE1	11:8:53:SER:HB2	1.85	0.40
9:l:82:LEU:HD13	9:l:139:TYR:HB2	2.02	0.40
9:0:41:ARG:HH22	9:0:52:GLU:CD	2.30	0.40
1:A:58:PHE:CD2	14:A:807:CLA:HMC2	2.57	0.40
1:A:94:GLY:O	1:A:98:SER:OG	2.40	0.40
2:B:426:PHE:CZ	17:B:854:BCR:HC21	2.56	0.40
14:B:809:CLA:HED1	14:B:832:CLA:H2	2.04	0.40
3:C:46:GLU:HG2	3:C:47:ASP:OD2	2.22	0.40
4:D:14:SER:OG	4:D:16:GLY:O	2.39	0.40
14:F:205:CLA:HMA3	14:F:205:CLA:HHB	1.91	0.40
1:a:86:TRP:NE1	14:a:831:CLA:OBD	2.53	0.40
1:a:587:GLY:O	1:a:591:VAL:HG23	2.22	0.40
13:a:803:CL0:H57	13:a:803:CL0:H60	1.92	0.40
14:a:843:CLA:HBC1	15:b:845:PQN:H191	2.04	0.40
14:1:821:CLA:H52	14:1:821:CLA:H8	1.95	0.40
14:1:829:CLA:H161	17:7:1104:BCR:H12C	2.03	0.40
14:1:833:CLA:HAB	14:1:834:CLA:HHB	2.02	0.40
2:b:65:LEU:HD23	2:b:135:LEU:HD23	2.02	0.40
2:b:262:HIS:N	2:b:267:SER:O	2.42	0.40
2:b:494:TRP:NE1	14:b:836:CLA:HED1	2.37	0.40
14:b:810:CLA:HMB3	14:b:811:CLA:H3A	2.03	0.40
14:b:825:CLA:HED3	14:b:825:CLA:H2A	2.04	0.40
2:2:110:SER:HB3	7:h:4:SER:HB3	2.04	0.40
2:2:317:HIS:HB3	2:2:320:LEU:HD12	2.04	0.40
14:2:801:CLA:H143	14:2:801:CLA:H112	1.84	0.40
14:2:831:CLA:H61	14:2:831:CLA:H41	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:14:SER:OG	4:d:16:GLY:O	2.39	0.40
17:h:102:BCR:H20C	17:h:102:BCR:H361	1.85	0.40
17:8:4001:BCR:H20C	17:8:4001:BCR:H361	1.87	0.40
10:m:3:LEU:HD23	10:m:8:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	A	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	a	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
2	2	731/735 (100%)	700 (96%)	31 (4%)	0	100	100
2	B	731/735 (100%)	700 (96%)	31 (4%)	0	100	100
2	b	731/735 (100%)	700 (96%)	31 (4%)	0	100	100
3	3	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	127 (93%)	9 (7%)	0	100	100
4	D	136/141 (96%)	127 (93%)	9 (7%)	0	100	100
4	d	136/141 (96%)	127 (93%)	9 (7%)	0	100	100
5	5	66/74 (89%)	63 (96%)	3 (4%)	0	100	100
5	E	66/74 (89%)	63 (96%)	3 (4%)	0	100	100
5	e	66/74 (89%)	63 (96%)	3 (4%)	0	100	100
6	6	139/165 (84%)	131 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	139/165 (84%)	131 (94%)	8 (6%)	0	100	100
6	f	139/165 (84%)	131 (94%)	8 (6%)	0	100	100
7	I	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
7	h	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
7	i	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
8	7	37/40 (92%)	34 (92%)	3 (8%)	0	100	100
8	J	37/40 (92%)	34 (92%)	3 (8%)	0	100	100
8	j	37/40 (92%)	34 (92%)	3 (8%)	0	100	100
9	0	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
9	L	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
9	l	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
10	9	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
10	M	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
10	m	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
11	8	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
11	K	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
11	k	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
All	All	6645/6915 (96%)	6366 (96%)	279 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	593/603 (98%)	588 (99%)	5 (1%)	73	81
1	A	593/603 (98%)	588 (99%)	5 (1%)	73	81
1	a	539/603 (89%)	534 (99%)	5 (1%)	70	80
2	2	585/588 (100%)	584 (100%)	1 (0%)	87	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	585/588 (100%)	584 (100%)	1 (0%)	87	89
2	b	585/588 (100%)	584 (100%)	1 (0%)	87	89
3	3	68/69 (99%)	67 (98%)	1 (2%)	57	75
3	C	68/69 (99%)	67 (98%)	1 (2%)	57	75
3	c	68/69 (99%)	67 (98%)	1 (2%)	57	75
4	4	113/116 (97%)	108 (96%)	5 (4%)	25	56
4	D	113/116 (97%)	108 (96%)	5 (4%)	25	56
4	d	113/116 (97%)	108 (96%)	5 (4%)	25	56
5	5	58/60 (97%)	56 (97%)	2 (3%)	32	63
5	E	58/60 (97%)	56 (97%)	2 (3%)	32	63
5	e	58/60 (97%)	56 (97%)	2 (3%)	32	63
6	6	114/137 (83%)	114 (100%)	0	100	100
6	F	114/137 (83%)	114 (100%)	0	100	100
6	f	114/137 (83%)	114 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
7	h	31/32 (97%)	31 (100%)	0	100	100
7	i	31/32 (97%)	31 (100%)	0	100	100
8	7	34/35 (97%)	34 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
8	j	34/35 (97%)	34 (100%)	0	100	100
9	0	111/118 (94%)	110 (99%)	1 (1%)	70	80
9	L	111/118 (94%)	110 (99%)	1 (1%)	70	80
9	l	111/118 (94%)	110 (99%)	1 (1%)	70	80
10	9	24/25 (96%)	24 (100%)	0	100	100
10	M	24/25 (96%)	24 (100%)	0	100	100
10	m	24/25 (96%)	24 (100%)	0	100	100
11	8	59/68 (87%)	58 (98%)	1 (2%)	53	74
11	K	59/68 (87%)	58 (98%)	1 (2%)	53	74
11	k	59/68 (87%)	58 (98%)	1 (2%)	53	74
All	All	5316/5553 (96%)	5268 (99%)	48 (1%)	68	80

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	A	249	MET
1	A	338	LYS
1	A	671	MET
1	A	695	GLU
2	B	612	GLU
3	C	66	ARG
4	D	10	LYS
4	D	52	GLU
4	D	119	THR
4	D	130	THR
4	D	139	TYR
5	E	28	VAL
5	E	40	ARG
9	L	44	LEU
11	K	16	LEU
1	a	188	GLU
1	a	249	MET
1	a	338	LYS
1	a	671	MET
1	a	695	GLU
1	1	188	GLU
1	1	249	MET
1	1	338	LYS
1	1	671	MET
1	1	695	GLU
3	c	66	ARG
3	3	66	ARG
2	b	612	GLU
2	2	612	GLU
4	d	10	LYS
4	d	52	GLU
4	d	119	THR
4	d	130	THR
4	d	139	TYR
4	4	10	LYS
4	4	52	GLU
4	4	119	THR
4	4	130	THR
4	4	139	TYR
5	e	28	VAL
5	e	40	ARG
5	5	28	VAL

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Mol	Chain	Res	Type
5	5	40	ARG
11	k	16	LEU
11	8	16	LEU
9	l	44	LEU
9	0	44	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	393	HIS
1	A	694	GLN
1	A	714	GLN
2	B	14	GLN
2	B	133	GLN
2	B	158	GLN
2	B	264	GLN
2	B	326	ASN
2	B	478	ASN
2	B	599	HIS
2	B	705	GLN
3	C	38	GLN
6	F	22	ASN
9	L	6	GLN
9	L	36	ASN
10	M	7	GLN
1	a	224	ASN
1	a	393	HIS
1	a	637	GLN
1	a	694	GLN
1	1	224	ASN
1	1	393	HIS
1	1	694	GLN
1	1	714	GLN
3	c	38	GLN
3	3	38	GLN
2	b	14	GLN
2	b	133	GLN
2	b	158	GLN
2	b	264	GLN
2	b	326	ASN
2	b	478	ASN

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Mol	Chain	Res	Type
2	b	705	GLN
2	2	14	GLN
2	2	133	GLN
2	2	158	GLN
2	2	264	GLN
2	2	326	ASN
2	2	478	ASN
2	2	599	HIS
2	2	705	GLN
6	f	22	ASN
6	6	22	ASN
9	l	6	GLN
9	l	36	ASN
9	0	6	GLN
9	0	36	ASN
10	m	7	GLN
10	9	7	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 408 ligands modelled in this entry, 3 are monoatomic - leaving 405 for Mogul analysis.

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	$\#\|Z\|>2$
14	CLA	1	821	-	64,68,73	1.18	9 (14%)	76,107,113	1.24	7 (9%)
14	CLA	2	805	-	69,73,73	1.16	11 (15%)	82,113,113	1.46	7 (8%)
17	BCR	i	4103	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	8 (14%)
14	CLA	b	843	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	9 (10%)
14	CLA	A	832	-	69,73,73	1.20	9 (13%)	82,113,113	1.42	7 (8%)
17	BCR	1	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.41	9 (16%)
17	BCR	b	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	1	829	-	69,73,73	1.13	11 (15%)	82,113,113	1.47	11 (13%)
14	CLA	1	826	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	8 (9%)
14	CLA	F	204	-	49,53,73	1.35	8 (16%)	58,89,113	1.59	6 (10%)
14	CLA	2	819	-	59,63,73	1.26	9 (15%)	70,101,113	1.53	7 (10%)
14	CLA	A	820	-	58,62,73	1.27	9 (15%)	68,99,113	1.44	7 (10%)
14	CLA	A	828	-	59,63,73	1.23	9 (15%)	70,101,113	1.22	5 (7%)
14	CLA	b	816	-	50,54,73	1.32	9 (18%)	59,90,113	1.45	4 (6%)
14	CLA	b	833	-	59,63,73	1.22	9 (15%)	70,101,113	1.37	6 (8%)
14	CLA	a	829	-	59,63,73	1.23	9 (15%)	70,101,113	1.22	5 (7%)
17	BCR	J	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	A	844	12	49,53,73	1.36	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	B	822	-	51,55,73	1.36	8 (15%)	60,91,113	1.45	8 (13%)
14	CLA	B	830	-	64,68,73	1.19	9 (14%)	76,107,113	1.37	6 (7%)
14	CLA	2	823	-	49,53,73	1.35	9 (18%)	58,89,113	1.51	5 (8%)
14	CLA	A	810	1	69,73,73	1.13	10 (14%)	82,113,113	1.20	8 (9%)
19	LMT	I	103	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)
14	CLA	B	804	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	9 (10%)
17	BCR	B	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	B	817	-	50,54,73	1.32	9 (18%)	59,90,113	1.46	4 (6%)
14	CLA	B	835	-	62,66,73	1.23	10 (16%)	73,104,113	1.37	6 (8%)
14	CLA	a	843	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	7 (8%)
14	CLA	a	842	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	1	823	-	53,57,73	1.27	8 (15%)	61,93,113	1.53	7 (11%)
19	LMT	f	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
14	CLA	a	813	-	49,53,73	1.37	10 (20%)	58,89,113	1.41	5 (8%)
14	CLA	l	4205	-	69,73,73	1.14	10 (14%)	82,113,113	1.38	8 (9%)
17	BCR	l	4207	-	41,41,41	1.21	2 (4%)	56,56,56	1.41	10 (17%)
17	BCR	I	102	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LMT	h	103	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)
16	SF4	A	846	2,1	0,12,12	-	-	-		
17	BCR	6	4402	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	7 (12%)
17	BCR	i	4102	-	41,41,41	1.23	2 (4%)	56,56,56	1.37	5 (8%)
13	CL0	A	803	-	58,73,73	2.14	15 (25%)	60,113,113	1.80	16 (26%)
17	BCR	9	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	A	804	-	69,73,73	1.22	9 (13%)	82,113,113	1.14	5 (6%)
14	CLA	a	814	-	69,73,73	1.17	11 (15%)	82,113,113	1.37	8 (9%)
14	CLA	b	835	-	49,53,73	1.40	10 (20%)	58,89,113	1.60	7 (12%)
14	CLA	A	837	1	49,53,73	1.38	9 (18%)	58,89,113	1.55	5 (8%)
14	CLA	2	825	-	49,53,73	1.37	10 (20%)	58,89,113	1.51	4 (6%)
12	LHG	M	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	2	824	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	4 (6%)
14	CLA	2	844	-	27,35,73	1.81	6 (22%)	32,60,113	1.72	5 (15%)
14	CLA	A	817	-	49,53,73	1.36	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	2	831	-	64,68,73	1.28	8 (12%)	76,107,113	1.57	7 (9%)
14	CLA	7	1101	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	6 (7%)
14	CLA	A	818	-	50,54,73	1.34	8 (16%)	59,90,113	1.33	5 (8%)
14	CLA	1	830	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
14	CLA	2	803	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	8 (9%)
14	CLA	B	844	-	69,73,73	1.15	7 (10%)	82,113,113	1.37	9 (10%)
14	CLA	1	817	-	50,54,73	1.34	8 (16%)	59,90,113	1.33	5 (8%)
14	CLA	1	835	-	58,62,73	1.28	10 (17%)	68,99,113	1.39	6 (8%)
16	SF4	3	102	3	0,12,12	-	-	-		
14	CLA	a	820	-	58,62,73	1.22	8 (13%)	68,99,113	1.41	6 (8%)
14	CLA	2	817	-	49,53,73	1.36	9 (18%)	58,89,113	1.47	5 (8%)
14	CLA	b	820	-	64,68,73	1.18	9 (14%)	76,107,113	1.37	9 (11%)
17	BCR	A	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	10 (17%)
17	BCR	J	103	-	41,41,41	1.23	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	b	804	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	8 (9%)
14	CLA	b	844	-	27,35,73	1.80	6 (22%)	32,60,113	1.72	5 (15%)
17	BCR	b	848	-	25,25,41	1.18	2 (8%)	33,33,56	1.35	7 (21%)
14	CLA	L	1502	-	69,73,73	1.15	11 (15%)	82,113,113	1.38	8 (9%)
14	CLA	J	101	-	49,53,73	1.36	9 (18%)	58,89,113	1.52	6 (10%)
17	BCR	2	851	-	41,41,41	1.22	3 (7%)	56,56,56	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	825	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	A	821	-	69,73,73	1.15	11 (15%)	82,113,113	1.31	8 (9%)
17	BCR	M	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	8	4003	-	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
14	CLA	A	825	-	55,59,73	1.29	8 (14%)	64,96,113	1.54	4 (6%)
17	BCR	h	102	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	9 (16%)
14	CLA	6	4403	-	49,53,73	1.35	8 (16%)	58,89,113	1.58	6 (10%)
14	CLA	a	840	-	69,73,73	1.17	11 (15%)	82,113,113	1.31	6 (7%)
14	CLA	2	827	-	54,58,73	1.28	10 (18%)	64,95,113	1.27	9 (14%)
12	LHG	b	852	-	38,38,48	0.71	1 (2%)	41,44,54	1.22	3 (7%)
14	CLA	2	821	-	51,55,73	1.35	9 (17%)	60,91,113	1.44	7 (11%)
15	PQN	a	845	-	34,34,34	0.41	0	43,45,45	1.23	4 (9%)
14	CLA	B	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.48	11 (13%)
14	CLA	A	836	-	58,62,73	1.27	9 (15%)	68,99,113	1.39	6 (8%)
14	CLA	1	822	-	69,73,73	1.18	10 (14%)	82,113,113	1.35	8 (9%)
14	CLA	k	4003	-	49,53,73	1.39	8 (16%)	58,89,113	1.54	6 (10%)
17	BCR	1	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	F	205	-	49,53,73	1.37	11 (22%)	58,89,113	1.46	9 (15%)
14	CLA	2	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.16	5 (6%)
16	SF4	a	846	2,1	0,12,12	-	-	-		
14	CLA	a	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.21	6 (7%)
13	CL0	a	803	-	58,73,73	2.13	14 (24%)	60,113,113	1.81	16 (26%)
14	CLA	B	818	-	49,53,73	1.35	9 (18%)	58,89,113	1.46	4 (6%)
14	CLA	f	204	-	49,53,73	1.36	8 (16%)	58,89,113	1.59	6 (10%)
14	CLA	2	813	-	49,53,73	1.36	9 (18%)	58,89,113	1.40	6 (10%)
14	CLA	a	804	-	64,68,73	1.23	11 (17%)	76,107,113	1.46	10 (13%)
14	CLA	k	4002	-	49,53,73	1.39	9 (18%)	58,89,113	1.50	6 (10%)
14	CLA	B	836	-	49,53,73	1.40	10 (20%)	58,89,113	1.61	7 (12%)
14	CLA	A	808	-	69,73,73	1.17	9 (13%)	82,113,113	1.41	7 (8%)
14	CLA	a	834	-	54,58,73	1.30	8 (14%)	64,95,113	1.69	10 (15%)
14	CLA	a	837	-	58,62,73	1.27	10 (17%)	68,99,113	1.39	6 (8%)
14	CLA	J	102	-	41,45,73	1.46	9 (21%)	50,78,113	1.35	5 (10%)
14	CLA	B	808	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	8 (9%)
17	BCR	7	1104	-	41,41,41	1.23	3 (7%)	56,56,56	1.32	5 (8%)
15	PQN	A	845	-	34,34,34	0.42	0	43,45,45	1.23	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	827	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	8 (9%)
14	CLA	2	807	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	8 (9%)
14	CLA	2	833	-	59,63,73	1.23	9 (15%)	70,101,113	1.38	6 (8%)
17	BCR	B	854	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	8 (14%)
15	PQN	1	845	-	34,34,34	0.42	0	43,45,45	1.23	4 (9%)
14	CLA	2	841	-	50,54,73	1.30	11 (22%)	59,90,113	1.57	8 (13%)
18	LMG	L	1506	-	38,38,55	0.86	0	46,46,63	1.29	5 (10%)
18	LMG	a	852	-	46,46,55	0.85	1 (2%)	54,54,63	1.30	6 (11%)
19	LMT	6	4401	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
14	CLA	A	842	-	69,73,73	1.14	8 (11%)	82,113,113	1.32	5 (6%)
17	BCR	a	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.31	9 (16%)
17	BCR	b	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.30	6 (10%)
14	CLA	2	811	-	65,69,73	1.19	9 (13%)	77,108,113	1.48	8 (10%)
14	CLA	7	1103	-	41,45,73	1.46	9 (21%)	50,78,113	1.36	5 (10%)
14	CLA	a	812	1	54,58,73	1.31	9 (16%)	64,95,113	1.53	8 (12%)
14	CLA	b	826	-	59,63,73	1.27	10 (16%)	70,101,113	1.45	9 (12%)
14	CLA	1	805	-	54,58,73	1.27	10 (18%)	64,95,113	1.51	8 (12%)
14	CLA	1	813	-	58,62,73	1.26	11 (18%)	68,99,113	1.45	7 (10%)
17	BCR	7	1105	-	41,41,41	1.18	3 (7%)	56,56,56	1.32	7 (12%)
17	BCR	j	104	-	41,41,41	1.19	3 (7%)	56,56,56	1.31	6 (10%)
14	CLA	1	836	1	49,53,73	1.38	9 (18%)	58,89,113	1.55	6 (10%)
14	CLA	a	818	-	49,53,73	1.34	8 (16%)	58,89,113	1.43	4 (6%)
17	BCR	8	4005	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
12	LHG	m	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	a	839	-	55,59,73	1.27	8 (14%)	64,96,113	1.40	9 (14%)
14	CLA	b	822	-	49,53,73	1.35	9 (18%)	58,89,113	1.51	4 (6%)
14	CLA	b	802	-	69,73,73	1.13	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	b	828	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	B	843	-	69,73,73	1.16	9 (13%)	82,113,113	1.16	4 (4%)
14	CLA	A	841	-	69,73,73	1.14	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	b	806	-	69,73,73	1.15	10 (14%)	82,113,113	1.47	7 (8%)
14	CLA	A	834	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	f	205	-	49,53,73	1.37	11 (22%)	58,89,113	1.45	9 (15%)
14	CLA	b	834	-	62,66,73	1.23	10 (16%)	73,104,113	1.37	6 (8%)
14	CLA	A	805	-	69,73,73	1.16	9 (13%)	82,113,113	1.21	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	1	843	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	7 (8%)
14	CLA	1	842	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	A	813	-	69,73,73	1.16	11 (15%)	82,113,113	1.37	8 (9%)
14	CLA	a	808	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	B	813	-	69,73,73	1.16	11 (15%)	82,113,113	1.38	8 (9%)
14	CLA	1	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.30	5 (6%)
14	CLA	b	808	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	8 (9%)
14	CLA	2	809	-	64,68,73	1.19	8 (12%)	76,107,113	1.25	6 (7%)
14	CLA	B	828	-	54,58,73	1.28	10 (18%)	64,95,113	1.27	9 (14%)
14	CLA	B	841	-	66,70,73	1.17	9 (13%)	78,109,113	1.25	6 (7%)
16	SF4	C	101	3	0,12,12	-	-	-		
14	CLA	a	827	-	63,67,73	1.20	8 (12%)	74,105,113	1.47	8 (10%)
15	PQN	b	845	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
14	CLA	A	833	-	54,58,73	1.30	8 (14%)	64,95,113	1.68	10 (15%)
14	CLA	1	837	-	55,59,73	1.26	9 (16%)	64,96,113	1.39	9 (14%)
18	LMG	l	4202	-	38,38,55	0.86	0	46,46,63	1.30	5 (10%)
17	BCR	b	854	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
17	BCR	A	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
14	CLA	2	837	-	49,53,73	1.38	10 (20%)	58,89,113	1.49	4 (6%)
14	CLA	L	1503	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	7 (8%)
14	CLA	B	833	-	49,53,73	1.37	11 (22%)	58,89,113	1.65	7 (12%)
17	BCR	1	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	5 (8%)
14	CLA	b	841	-	50,54,73	1.31	11 (22%)	59,90,113	1.58	8 (13%)
14	CLA	b	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.16	5 (6%)
14	CLA	0	202	-	69,73,73	1.14	10 (14%)	82,113,113	1.26	8 (9%)
14	CLA	1	808	-	50,54,73	1.32	10 (20%)	59,90,113	1.48	6 (10%)
14	CLA	B	811	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	6 (7%)
17	BCR	B	852	-	41,41,41	1.23	3 (7%)	56,56,56	1.33	8 (14%)
14	CLA	l	4203	-	69,73,73	1.16	11 (15%)	82,113,113	1.36	8 (9%)
18	LMG	A	853	-	32,32,55	0.91	1 (3%)	40,40,63	1.21	4 (10%)
14	CLA	A	830	-	69,73,73	1.12	11 (15%)	82,113,113	1.47	11 (13%)
14	CLA	A	811	1	54,58,73	1.31	9 (16%)	64,95,113	1.52	8 (12%)
14	CLA	1	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.45	11 (13%)
17	BCR	B	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	a	838	1	49,53,73	1.39	9 (18%)	58,89,113	1.55	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	L	1501	9	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
14	CLA	2	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.35	6 (7%)
14	CLA	j	102	-	41,45,73	1.46	9 (21%)	50,78,113	1.36	5 (10%)
14	CLA	a	841	-	51,55,73	1.31	10 (19%)	60,91,113	1.46	5 (8%)
14	CLA	2	812	-	69,73,73	1.16	11 (15%)	82,113,113	1.37	8 (9%)
14	CLA	1	841	-	55,59,73	1.29	10 (18%)	64,96,113	1.39	6 (9%)
17	BCR	a	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	1	804	-	69,73,73	1.22	10 (14%)	82,113,113	1.14	5 (6%)
14	CLA	A	829	-	69,73,73	1.15	8 (11%)	82,113,113	1.45	6 (7%)
16	SF4	c	101	3	0,12,12	-	-	-		
14	CLA	B	809	-	69,73,73	1.20	12 (17%)	82,113,113	1.40	6 (7%)
17	BCR	b	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.40	10 (17%)
14	CLA	A	838	-	55,59,73	1.27	9 (16%)	64,96,113	1.40	9 (14%)
14	CLA	b	813	-	49,53,73	1.35	8 (16%)	58,89,113	1.40	6 (10%)
14	CLA	B	845	-	27,35,73	1.80	6 (22%)	32,60,113	1.71	5 (15%)
14	CLA	A	822	-	64,68,73	1.19	9 (14%)	76,107,113	1.24	7 (9%)
14	CLA	1	820	-	69,73,73	1.15	10 (14%)	82,113,113	1.31	8 (9%)
14	CLA	a	816	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	7 (10%)
14	CLA	B	812	-	65,69,73	1.19	9 (13%)	77,108,113	1.48	8 (10%)
14	CLA	a	833	-	69,73,73	1.20	9 (13%)	82,113,113	1.43	8 (9%)
14	CLA	1	811	-	49,53,73	1.37	10 (20%)	58,89,113	1.41	5 (8%)
14	CLA	B	824	-	49,53,73	1.36	9 (18%)	58,89,113	1.52	5 (8%)
17	BCR	k	4004	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	5 (8%)
14	CLA	b	814	-	49,53,73	1.35	10 (20%)	58,89,113	1.49	6 (10%)
14	CLA	2	806	-	58,62,73	1.21	9 (15%)	68,99,113	1.37	8 (11%)
14	CLA	1	844	12	49,53,73	1.35	9 (18%)	58,89,113	1.46	5 (8%)
17	BCR	K	4005	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
14	CLA	1	825	-	63,67,73	1.20	8 (12%)	74,105,113	1.46	8 (10%)
14	CLA	a	825	-	53,57,73	1.27	8 (15%)	61,93,113	1.53	7 (11%)
14	CLA	a	830	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	6 (7%)
14	CLA	a	811	1	69,73,73	1.13	9 (13%)	82,113,113	1.19	7 (8%)
14	CLA	1	831	-	69,73,73	1.19	8 (11%)	82,113,113	1.42	8 (9%)
14	CLA	a	819	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
14	CLA	a	844	12	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	b	824	-	49,53,73	1.36	9 (18%)	58,89,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.44	11 (13%)
14	CLA	a	810	-	50,54,73	1.32	10 (20%)	59,90,113	1.47	6 (10%)
18	LMG	A	852	-	46,46,55	0.86	1 (2%)	54,54,63	1.30	6 (11%)
14	CLA	l	4204	9	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
14	CLA	1	840	-	69,73,73	1.13	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	A	831	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	b	830	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
17	BCR	B	851	-	41,41,41	1.25	5 (12%)	56,56,56	1.56	10 (17%)
14	CLA	b	817	-	49,53,73	1.36	10 (20%)	58,89,113	1.47	4 (6%)
13	CL0	1	803	-	58,73,73	2.13	15 (25%)	60,113,113	1.81	16 (26%)
12	LHG	1	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	K	4003	-	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
14	CLA	b	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.48	11 (13%)
14	CLA	1	812	-	69,73,73	1.17	11 (15%)	82,113,113	1.37	9 (10%)
14	CLA	a	854	-	59,63,73	1.25	9 (15%)	70,101,113	1.26	8 (11%)
17	BCR	A	848	-	41,41,41	1.19	2 (4%)	56,56,56	1.21	5 (8%)
14	CLA	2	834	-	62,66,73	1.23	10 (16%)	73,104,113	1.37	6 (8%)
14	CLA	1	824	-	55,59,73	1.29	9 (16%)	64,96,113	1.55	4 (6%)
14	CLA	B	819	-	59,63,73	1.22	10 (16%)	70,101,113	1.45	7 (10%)
18	LMG	a	853	-	32,32,55	0.91	1 (3%)	40,40,63	1.21	4 (10%)
14	CLA	a	832	-	69,73,73	1.16	10 (14%)	82,113,113	1.35	8 (9%)
17	BCR	b	851	-	41,41,41	1.22	3 (7%)	56,56,56	1.34	8 (14%)
17	BCR	2	846	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	7 (12%)
17	BCR	I	101	-	41,41,41	1.24	2 (4%)	56,56,56	1.37	5 (8%)
14	CLA	1	818	-	58,62,73	1.23	7 (12%)	68,99,113	1.42	6 (8%)
14	CLA	A	823	-	69,73,73	1.18	10 (14%)	82,113,113	1.36	8 (9%)
14	CLA	a	822	-	69,73,73	1.15	11 (15%)	82,113,113	1.31	8 (9%)
17	BCR	2	848	-	25,25,41	1.18	2 (8%)	33,33,56	1.34	5 (15%)
17	BCR	F	203	-	41,41,41	1.26	2 (4%)	56,56,56	1.38	7 (12%)
17	BCR	6	4406	-	41,41,41	1.25	3 (7%)	56,56,56	1.39	8 (14%)
14	CLA	2	843	-	69,73,73	1.15	8 (11%)	82,113,113	1.38	9 (10%)
14	CLA	b	819	-	59,63,73	1.27	9 (15%)	70,101,113	1.52	8 (11%)
14	CLA	a	821	-	58,62,73	1.27	9 (15%)	68,99,113	1.44	7 (10%)
14	CLA	b	823	-	49,53,73	1.35	9 (18%)	58,89,113	1.52	5 (8%)
17	BCR	K	4001	-	41,41,41	1.25	3 (7%)	56,56,56	1.43	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	839	-	54,58,73	1.28	8 (14%)	64,95,113	1.52	10 (15%)
17	BCR	j	103	-	41,41,41	1.23	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	K	4004	-	59,63,73	1.25	9 (15%)	70,101,113	1.26	8 (11%)
17	BCR	1	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
14	CLA	2	801	-	64,68,73	1.23	10 (15%)	76,107,113	1.46	10 (13%)
14	CLA	B	831	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
14	CLA	2	822	-	49,53,73	1.35	9 (18%)	58,89,113	1.51	5 (8%)
14	CLA	B	840	-	54,58,73	1.28	9 (16%)	64,95,113	1.52	10 (15%)
12	LHG	9	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	a	835	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	9 (10%)
16	SF4	c	102	3	0,12,12	-	-	-		
14	CLA	K	4002	-	49,53,73	1.39	9 (18%)	58,89,113	1.49	6 (10%)
17	BCR	0	209	-	41,41,41	1.20	2 (4%)	56,56,56	1.41	9 (16%)
12	LHG	1	802	14	32,32,48	0.87	1 (3%)	35,38,54	1.30	3 (8%)
14	CLA	7	1102	-	49,53,73	1.36	9 (18%)	58,89,113	1.53	6 (10%)
14	CLA	1	819	-	58,62,73	1.26	8 (13%)	68,99,113	1.44	7 (10%)
12	LHG	a	802	14	32,32,48	0.88	1 (3%)	35,38,54	1.30	3 (8%)
14	CLA	b	831	-	64,68,73	1.29	8 (12%)	76,107,113	1.56	7 (9%)
17	BCR	6	4405	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	7 (12%)
17	BCR	2	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	b	825	-	49,53,73	1.37	9 (18%)	58,89,113	1.49	4 (6%)
14	CLA	B	827	-	59,63,73	1.27	10 (16%)	70,101,113	1.45	9 (12%)
14	CLA	A	809	-	50,54,73	1.32	10 (20%)	59,90,113	1.47	6 (10%)
17	BCR	h	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.36	5 (8%)
14	CLA	2	835	-	49,53,73	1.40	10 (20%)	58,89,113	1.60	7 (12%)
14	CLA	2	829	-	64,68,73	1.18	9 (14%)	76,107,113	1.38	6 (7%)
14	CLA	b	821	-	51,55,73	1.36	8 (15%)	60,91,113	1.44	8 (13%)
14	CLA	2	815	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	8 (9%)
14	CLA	2	826	-	59,63,73	1.27	10 (16%)	70,101,113	1.46	9 (12%)
14	CLA	0	208	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	7 (8%)
14	CLA	A	816	-	49,53,73	1.37	10 (20%)	58,89,113	1.48	6 (10%)
14	CLA	b	829	-	64,68,73	1.19	9 (14%)	76,107,113	1.37	6 (7%)
14	CLA	8	4004	-	59,63,73	1.25	9 (15%)	70,101,113	1.26	8 (11%)
14	CLA	0	206	9	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	0	207	-	69,73,73	1.14	11 (15%)	82,113,113	1.39	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	831	-	69,73,73	1.13	11 (15%)	82,113,113	1.47	11 (13%)
14	CLA	A	843	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	7 (8%)
14	CLA	A	839	-	69,73,73	1.17	10 (14%)	82,113,113	1.31	6 (7%)
14	CLA	2	832	-	49,53,73	1.36	11 (22%)	58,89,113	1.65	7 (12%)
17	BCR	A	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	F	201	-	55,59,73	1.29	10 (18%)	64,96,113	1.39	6 (9%)
17	BCR	B	849	-	25,25,41	1.17	2 (8%)	33,33,56	1.34	6 (18%)
14	CLA	B	842	-	50,54,73	1.31	11 (22%)	59,90,113	1.56	7 (11%)
14	CLA	B	810	-	64,68,73	1.19	9 (14%)	76,107,113	1.26	7 (9%)
14	CLA	1	809	1	69,73,73	1.13	9 (13%)	82,113,113	1.19	6 (7%)
17	BCR	2	850	-	41,41,41	1.25	5 (12%)	56,56,56	1.55	10 (17%)
14	CLA	1	816	-	49,53,73	1.35	8 (16%)	58,89,113	1.42	3 (5%)
14	CLA	a	809	-	69,73,73	1.17	9 (13%)	82,113,113	1.41	7 (8%)
14	CLA	2	816	-	50,54,73	1.33	9 (18%)	59,90,113	1.46	4 (6%)
14	CLA	1	838	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	2	838	-	50,54,73	1.35	9 (18%)	59,90,113	1.44	7 (11%)
14	CLA	b	810	-	64,68,73	1.19	8 (12%)	76,107,113	1.25	6 (7%)
14	CLA	8	4002	-	49,53,73	1.39	9 (18%)	58,89,113	1.50	6 (10%)
16	SF4	C	102	3	0,12,12	-	-	-		
14	CLA	A	806	-	54,58,73	1.27	10 (18%)	64,95,113	1.53	8 (12%)
12	LHG	2	852	-	38,38,48	0.71	1 (2%)	41,44,54	1.22	3 (7%)
14	CLA	6	4404	-	49,53,73	1.37	11 (22%)	58,89,113	1.45	9 (15%)
14	CLA	b	827	-	54,58,73	1.28	10 (18%)	64,95,113	1.27	9 (14%)
14	CLA	B	832	-	64,68,73	1.29	8 (12%)	76,107,113	1.57	7 (9%)
14	CLA	B	807	-	58,62,73	1.21	9 (15%)	68,99,113	1.38	9 (13%)
14	CLA	b	809	-	69,73,73	1.19	11 (15%)	82,113,113	1.40	6 (7%)
14	CLA	B	839	-	50,54,73	1.34	9 (18%)	59,90,113	1.44	7 (11%)
17	BCR	8	4001	-	41,41,41	1.26	3 (7%)	56,56,56	1.42	7 (12%)
14	CLA	b	832	-	49,53,73	1.37	11 (22%)	58,89,113	1.66	7 (12%)
14	CLA	B	837	-	49,53,73	1.35	10 (20%)	58,89,113	1.45	9 (15%)
14	CLA	b	807	-	58,62,73	1.21	9 (15%)	68,99,113	1.38	8 (11%)
14	CLA	1	827	-	59,63,73	1.23	10 (16%)	70,101,113	1.23	5 (7%)
14	CLA	2	814	-	49,53,73	1.35	10 (20%)	58,89,113	1.49	6 (10%)
14	CLA	b	811	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	6 (7%)
17	BCR	a	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.42	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	a	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.41	9 (16%)
14	CLA	f	201	-	55,59,73	1.29	10 (18%)	64,96,113	1.40	6 (9%)
14	CLA	A	812	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	1	807	-	69,73,73	1.17	9 (13%)	82,113,113	1.42	7 (8%)
14	CLA	B	801	-	64,68,73	1.23	10 (15%)	76,107,113	1.47	10 (13%)
14	CLA	A	840	-	51,55,73	1.31	10 (19%)	60,91,113	1.46	5 (8%)
14	CLA	1	810	1	54,58,73	1.31	9 (16%)	64,95,113	1.53	8 (12%)
14	CLA	1	832	-	54,58,73	1.31	8 (14%)	64,95,113	1.69	10 (15%)
14	CLA	A	824	-	53,57,73	1.28	9 (16%)	61,93,113	1.53	7 (11%)
14	CLA	2	820	-	64,68,73	1.19	9 (14%)	76,107,113	1.36	9 (11%)
14	CLA	B	816	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	8 (9%)
17	BCR	F	206	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	7 (12%)
16	SF4	3	101	3	0,12,12	-	-	-		
14	CLA	a	823	-	64,68,73	1.19	9 (14%)	76,107,113	1.24	7 (9%)
17	BCR	L	1504	-	41,41,41	1.21	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	b	837	-	49,53,73	1.38	10 (20%)	58,89,113	1.50	4 (6%)
14	CLA	A	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	B	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.53	7 (10%)
14	CLA	a	817	-	49,53,73	1.36	10 (20%)	58,89,113	1.48	6 (10%)
14	CLA	1	814	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	7 (10%)
14	CLA	2	840	-	66,70,73	1.17	8 (12%)	78,109,113	1.25	5 (6%)
15	PQN	2	845	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
17	BCR	L	1505	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	8 (14%)
12	LHG	B	853	-	38,38,48	0.72	1 (2%)	41,44,54	1.22	3 (7%)
17	BCR	b	853	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	8 (14%)
19	LMT	i	4101	-	36,36,36	1.20	6 (16%)	47,47,47	1.19	3 (6%)
14	CLA	A	814	-	58,62,73	1.25	11 (18%)	68,99,113	1.44	7 (10%)
14	CLA	B	806	-	69,73,73	1.16	11 (15%)	82,113,113	1.47	7 (8%)
14	CLA	B	814	-	49,53,73	1.35	7 (14%)	58,89,113	1.39	6 (10%)
14	CLA	B	821	-	64,68,73	1.18	9 (14%)	76,107,113	1.36	9 (11%)
14	CLA	l	4206	-	69,73,73	1.14	9 (13%)	82,113,113	1.24	7 (8%)
14	CLA	b	812	-	65,69,73	1.19	9 (13%)	77,108,113	1.48	8 (10%)
12	LHG	a	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	A	815	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	7 (10%)
14	CLA	A	826	-	63,67,73	1.20	8 (12%)	74,105,113	1.47	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	840	-	66,70,73	1.17	8 (12%)	78,109,113	1.25	5 (6%)
14	CLA	a	805	-	69,73,73	1.21	9 (13%)	82,113,113	1.14	5 (6%)
14	CLA	2	836	-	49,53,73	1.35	10 (20%)	58,89,113	1.46	9 (15%)
14	CLA	1	833	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	a	824	-	69,73,73	1.17	10 (14%)	82,113,113	1.35	8 (9%)
14	CLA	b	818	-	59,63,73	1.21	10 (16%)	70,101,113	1.44	7 (10%)
14	CLA	b	801	-	69,73,73	1.14	10 (14%)	82,113,113	1.27	8 (9%)
18	LMG	0	203	-	46,46,55	0.85	1 (2%)	54,54,63	1.30	6 (11%)
14	CLA	B	838	-	49,53,73	1.38	10 (20%)	58,89,113	1.50	4 (6%)
14	CLA	j	101	-	49,53,73	1.36	9 (18%)	58,89,113	1.52	6 (10%)
17	BCR	k	4001	-	41,41,41	1.25	3 (7%)	56,56,56	1.42	7 (12%)
19	LMT	F	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
18	LMG	0	201	-	38,38,55	0.86	0	46,46,63	1.30	5 (10%)
17	BCR	2	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	B	815	-	49,53,73	1.35	10 (20%)	58,89,113	1.49	6 (10%)
17	BCR	f	206	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	7 (12%)
14	CLA	B	802	-	69,73,73	1.14	10 (14%)	82,113,113	1.26	8 (9%)
16	SF4	1	846	2,1	0,12,12	-	-	-		
17	BCR	1	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.31	9 (16%)
17	BCR	a	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
17	BCR	0	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	9 (16%)
14	CLA	1	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.44	6 (7%)
14	CLA	B	834	-	59,63,73	1.23	9 (15%)	70,101,113	1.37	6 (8%)
14	CLA	b	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	8 (9%)
14	CLA	a	807	-	54,58,73	1.28	10 (18%)	64,95,113	1.52	8 (12%)
14	CLA	2	818	-	59,63,73	1.22	10 (16%)	70,101,113	1.45	7 (10%)
14	CLA	2	828	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	2	839	-	54,58,73	1.28	8 (14%)	64,95,113	1.51	10 (15%)
17	BCR	A	850	-	41,41,41	1.29	3 (7%)	56,56,56	1.41	9 (16%)
14	CLA	2	830	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	8 (9%)
14	CLA	a	828	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	8 (9%)
14	CLA	1	839	-	51,55,73	1.31	10 (19%)	60,91,113	1.47	5 (8%)
17	BCR	B	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.41	10 (17%)
18	LMG	1	852	-	32,32,55	0.90	1 (3%)	40,40,63	1.21	4 (10%)
17	BCR	f	203	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	829	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	B	826	-	49,53,73	1.36	10 (20%)	58,89,113	1.49	4 (6%)
12	LHG	A	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	2	808	-	69,73,73	1.19	11 (15%)	82,113,113	1.40	6 (7%)
12	LHG	A	802	14	32,32,48	0.87	1 (3%)	35,38,54	1.30	3 (8%)
18	LMG	B	803	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
14	CLA	A	819	-	58,62,73	1.22	7 (12%)	68,99,113	1.42	6 (8%)
14	CLA	1	815	-	49,53,73	1.36	10 (20%)	58,89,113	1.49	6 (10%)
17	BCR	b	850	-	41,41,41	1.25	5 (12%)	56,56,56	1.55	10 (17%)
17	BCR	0	210	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	9 (16%)
14	CLA	a	815	-	58,62,73	1.26	11 (18%)	68,99,113	1.45	7 (10%)
14	CLA	a	826	-	55,59,73	1.29	10 (18%)	64,96,113	1.54	4 (6%)
15	PQN	B	846	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
18	LMG	2	802	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
14	CLA	a	836	-	69,73,73	1.14	7 (10%)	82,113,113	1.45	11 (13%)
14	CLA	b	836	-	49,53,73	1.35	10 (20%)	58,89,113	1.46	9 (15%)
14	CLA	b	838	-	50,54,73	1.35	9 (18%)	59,90,113	1.45	7 (11%)
18	LMG	b	803	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
14	CLA	B	823	-	49,53,73	1.35	9 (18%)	58,89,113	1.50	4 (6%)
14	CLA	2	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.48	11 (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
14	CLA	1	821	-	1/1/14/20	8/33/109/115	-
14	CLA	2	805	-	1/1/15/20	14/39/115/115	-
17	BCR	i	4103	-	-	20/29/63/63	0/2/2/2
14	CLA	b	843	-	-	20/39/115/115	-
14	CLA	A	832	-	1/1/15/20	20/39/115/115	-
17	BCR	1	850	-	-	19/29/63/63	0/2/2/2
17	BCR	b	846	-	-	12/29/63/63	0/2/2/2
14	CLA	1	829	-	1/1/15/20	10/39/115/115	-
14	CLA	1	826	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	F	204	-	1/1/11/20	6/15/91/115	-
14	CLA	2	819	-	-	8/27/103/115	-
14	CLA	A	820	-	1/1/12/20	6/26/102/115	-
14	CLA	A	828	-	1/1/13/20	6/27/103/115	-
14	CLA	b	816	-	1/1/11/20	7/17/93/115	-
14	CLA	b	833	-	1/1/13/20	14/27/103/115	-
14	CLA	a	829	-	1/1/13/20	6/27/103/115	-
17	BCR	J	104	-	-	10/29/63/63	0/2/2/2
14	CLA	A	844	12	1/1/11/20	6/15/91/115	-
14	CLA	B	822	-	1/1/11/20	5/18/94/115	-
14	CLA	B	830	-	1/1/14/20	7/33/109/115	-
14	CLA	2	823	-	-	8/15/91/115	-
14	CLA	A	810	1	1/1/15/20	23/39/115/115	-
19	LMT	I	103	-	-	8/21/61/61	0/2/2/2
14	CLA	B	804	-	1/1/15/20	13/39/115/115	-
17	BCR	B	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	817	-	1/1/11/20	7/17/93/115	-
14	CLA	B	835	-	1/1/13/20	15/31/107/115	-
14	CLA	a	843	-	1/1/15/20	18/39/115/115	-
14	CLA	a	842	-	-	13/39/115/115	-
14	CLA	1	823	-	1/1/11/20	13/20/96/115	-
19	LMT	f	202	-	-	3/21/61/61	0/2/2/2
14	CLA	a	813	-	1/1/11/20	8/15/91/115	-
14	CLA	l	4205	-	1/1/15/20	11/39/115/115	-
17	BCR	l	4207	-	-	14/29/63/63	0/2/2/2
17	BCR	I	102	-	-	20/29/63/63	0/2/2/2
19	LMT	h	103	-	-	8/21/61/61	0/2/2/2
16	SF4	A	846	2,1	-	-	0/6/5/5
17	BCR	6	4402	-	-	13/29/63/63	0/2/2/2
17	BCR	i	4102	-	-	16/29/63/63	0/2/2/2
13	CL0	A	803	-	3/3/20/25	13/37/135/135	-
17	BCR	9	102	-	-	15/29/63/63	0/2/2/2
14	CLA	A	804	-	1/1/15/20	10/39/115/115	-
14	CLA	a	814	-	1/1/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	835	-	1/1/11/20	4/15/91/115	-
14	CLA	A	837	1	1/1/11/20	6/15/91/115	-
14	CLA	2	825	-	-	6/15/91/115	-
12	LHG	M	101	-	-	20/43/43/53	-
14	CLA	2	824	-	1/1/11/20	7/15/91/115	-
14	CLA	2	844	-	1/1/5/20	-	-
14	CLA	A	817	-	-	3/15/91/115	-
14	CLA	2	831	-	1/1/14/20	12/33/109/115	-
14	CLA	7	1101	-	1/1/15/20	16/39/115/115	-
14	CLA	A	818	-	1/1/11/20	7/17/93/115	-
14	CLA	1	830	-	1/1/15/20	7/39/115/115	-
14	CLA	2	803	-	1/1/15/20	13/39/115/115	-
14	CLA	B	844	-	-	20/39/115/115	-
14	CLA	1	817	-	1/1/11/20	7/17/93/115	-
14	CLA	1	835	-	1/1/12/20	10/26/102/115	-
16	SF4	3	102	3	-	-	0/6/5/5
14	CLA	a	820	-	1/1/12/20	7/26/102/115	-
14	CLA	2	817	-	1/1/11/20	3/15/91/115	-
14	CLA	b	820	-	1/1/14/20	15/33/109/115	-
17	BCR	A	847	-	-	11/29/63/63	0/2/2/2
17	BCR	J	103	-	-	13/29/63/63	0/2/2/2
14	CLA	b	804	-	1/1/15/20	13/39/115/115	-
14	CLA	b	844	-	1/1/5/20	-	-
17	BCR	b	848	-	-	4/18/35/63	0/1/1/2
14	CLA	L	1502	-	1/1/15/20	11/39/115/115	-
14	CLA	J	101	-	1/1/11/20	8/15/91/115	-
17	BCR	2	851	-	-	10/29/63/63	0/2/2/2
14	CLA	B	825	-	1/1/11/20	7/15/91/115	-
14	CLA	A	821	-	1/1/15/20	19/39/115/115	-
17	BCR	M	102	-	-	15/29/63/63	0/2/2/2
14	CLA	8	4003	-	1/1/11/20	10/15/91/115	-
14	CLA	A	825	-	1/1/12/20	10/23/99/115	-
17	BCR	h	102	-	-	20/29/63/63	0/2/2/2
14	CLA	6	4403	-	1/1/11/20	6/15/91/115	-
14	CLA	a	840	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LHG	b	852	-	-	22/43/43/53	-
14	CLA	2	827	-	1/1/12/20	2/21/97/115	-
14	CLA	2	821	-	1/1/11/20	5/18/94/115	-
15	PQN	a	845	-	-	4/23/43/43	0/2/2/2
14	CLA	B	805	-	1/1/15/20	13/39/115/115	-
14	CLA	A	836	-	1/1/12/20	10/26/102/115	-
14	CLA	1	822	-	1/1/15/20	13/39/115/115	-
14	CLA	k	4003	-	1/1/11/20	10/15/91/115	-
17	BCR	1	849	-	-	7/29/63/63	0/2/2/2
14	CLA	F	205	-	1/1/11/20	7/15/91/115	-
14	CLA	2	842	-	1/1/15/20	13/39/115/115	-
16	SF4	a	846	2,1	-	-	0/6/5/5
14	CLA	a	806	-	1/1/15/20	16/39/115/115	-
13	CL0	a	803	-	3/3/20/25	13/37/135/135	-
14	CLA	B	818	-	1/1/11/20	3/15/91/115	-
14	CLA	f	204	-	1/1/11/20	7/15/91/115	-
14	CLA	2	813	-	1/1/11/20	5/15/91/115	-
14	CLA	a	804	-	1/1/14/20	11/33/109/115	-
14	CLA	k	4002	-	-	8/15/91/115	-
14	CLA	B	836	-	1/1/11/20	4/15/91/115	-
14	CLA	A	808	-	1/1/15/20	14/39/115/115	-
14	CLA	a	834	-	1/1/12/20	3/21/97/115	-
14	CLA	a	837	-	1/1/12/20	10/26/102/115	-
14	CLA	J	102	-	1/1/8/20	3/4/76/115	-
14	CLA	B	808	-	-	11/39/115/115	-
17	BCR	7	1104	-	-	13/29/63/63	0/2/2/2
15	PQN	A	845	-	-	4/23/43/43	0/2/2/2
14	CLA	A	827	-	1/1/15/20	14/39/115/115	-
14	CLA	2	807	-	-	11/39/115/115	-
14	CLA	2	833	-	1/1/13/20	14/27/103/115	-
17	BCR	B	854	-	-	13/29/63/63	0/2/2/2
15	PQN	1	845	-	-	4/23/43/43	0/2/2/2
14	CLA	2	841	-	1/1/11/20	4/17/93/115	-
18	LMG	L	1506	-	-	20/33/53/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMG	a	852	-	-	21/41/61/70	0/1/1/1
19	LMT	6	4401	-	-	3/21/61/61	0/2/2/2
14	CLA	A	842	-	-	13/39/115/115	-
17	BCR	a	847	-	-	11/29/63/63	0/2/2/2
17	BCR	b	847	-	-	7/29/63/63	0/2/2/2
14	CLA	2	811	-	1/1/14/20	13/35/111/115	-
14	CLA	7	1103	-	1/1/8/20	3/4/76/115	-
14	CLA	a	812	1	1/1/12/20	8/21/97/115	-
14	CLA	b	826	-	1/1/13/20	4/27/103/115	-
14	CLA	1	805	-	1/1/12/20	3/21/97/115	-
14	CLA	1	813	-	1/1/12/20	11/26/102/115	-
17	BCR	7	1105	-	-	10/29/63/63	0/2/2/2
17	BCR	j	104	-	-	10/29/63/63	0/2/2/2
14	CLA	1	836	1	1/1/11/20	6/15/91/115	-
14	CLA	a	818	-	-	3/15/91/115	-
17	BCR	8	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	a	839	-	1/1/12/20	8/23/99/115	-
12	LHG	m	101	-	-	20/43/43/53	-
14	CLA	b	822	-	-	7/15/91/115	-
14	CLA	b	802	-	1/1/15/20	9/39/115/115	-
14	CLA	b	828	-	1/1/15/20	9/39/115/115	-
14	CLA	B	843	-	1/1/15/20	13/39/115/115	-
14	CLA	A	841	-	1/1/15/20	9/39/115/115	-
14	CLA	b	806	-	1/1/15/20	14/39/115/115	-
14	CLA	A	834	-	1/1/15/20	16/39/115/115	-
14	CLA	f	205	-	1/1/11/20	7/15/91/115	-
14	CLA	b	834	-	1/1/13/20	15/31/107/115	-
14	CLA	A	805	-	1/1/15/20	16/39/115/115	-
14	CLA	1	843	-	1/1/15/20	18/39/115/115	-
14	CLA	1	842	-	-	13/39/115/115	-
14	CLA	A	813	-	1/1/15/20	19/39/115/115	-
14	CLA	a	808	-	1/1/15/20	17/39/115/115	-
14	CLA	B	813	-	1/1/15/20	8/39/115/115	-
14	CLA	1	806	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	808	-	-	11/39/115/115	-
14	CLA	2	809	-	1/1/14/20	9/33/109/115	-
14	CLA	B	828	-	1/1/12/20	2/21/97/115	-
14	CLA	B	841	-	1/1/14/20	8/36/112/115	-
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	a	827	-	1/1/13/20	15/32/108/115	-
15	PQN	b	845	-	-	10/23/43/43	0/2/2/2
14	CLA	A	833	-	1/1/12/20	3/21/97/115	-
14	CLA	1	837	-	1/1/12/20	8/23/99/115	-
18	LMG	l	4202	-	-	20/33/53/70	0/1/1/1
17	BCR	b	854	-	-	15/29/63/63	0/2/2/2
17	BCR	A	851	-	-	21/29/63/63	0/2/2/2
14	CLA	2	837	-	1/1/11/20	4/15/91/115	-
14	CLA	L	1503	-	1/1/15/20	14/39/115/115	-
14	CLA	B	833	-	1/1/11/20	6/15/91/115	-
17	BCR	1	848	-	-	11/29/63/63	0/2/2/2
14	CLA	b	841	-	1/1/11/20	4/17/93/115	-
14	CLA	b	842	-	1/1/15/20	13/39/115/115	-
14	CLA	0	202	-	1/1/15/20	11/39/115/115	-
14	CLA	1	808	-	1/1/11/20	6/17/93/115	-
14	CLA	B	811	-	1/1/15/20	16/39/115/115	-
17	BCR	B	852	-	-	10/29/63/63	0/2/2/2
14	CLA	l	4203	-	1/1/15/20	8/39/115/115	-
18	LMG	A	853	-	-	8/27/47/70	0/1/1/1
14	CLA	A	830	-	1/1/15/20	10/39/115/115	-
14	CLA	A	811	1	1/1/12/20	8/21/97/115	-
14	CLA	1	834	-	1/1/15/20	7/39/115/115	-
17	BCR	B	847	-	-	12/29/63/63	0/2/2/2
14	CLA	a	838	1	1/1/11/20	6/15/91/115	-
14	CLA	L	1501	9	1/1/15/20	14/39/115/115	-
14	CLA	2	810	-	1/1/15/20	17/39/115/115	-
14	CLA	j	102	-	1/1/8/20	3/4/76/115	-
14	CLA	a	841	-	1/1/11/20	3/18/94/115	-
14	CLA	2	812	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	841	-	1/1/12/20	11/23/99/115	-
17	BCR	a	848	-	-	10/29/63/63	0/2/2/2
14	CLA	1	804	-	1/1/15/20	10/39/115/115	-
14	CLA	A	829	-	1/1/15/20	11/39/115/115	-
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	B	809	-	1/1/15/20	24/39/115/115	-
17	BCR	b	849	-	-	15/29/63/63	0/2/2/2
14	CLA	A	838	-	1/1/12/20	8/23/99/115	-
14	CLA	b	813	-	1/1/11/20	5/15/91/115	-
14	CLA	B	845	-	1/1/5/20	-	-
14	CLA	A	822	-	1/1/14/20	8/33/109/115	-
14	CLA	1	820	-	1/1/15/20	19/39/115/115	-
14	CLA	a	816	-	1/1/13/20	10/27/103/115	-
14	CLA	B	812	-	1/1/14/20	13/35/111/115	-
14	CLA	a	833	-	1/1/15/20	20/39/115/115	-
14	CLA	1	811	-	1/1/11/20	8/15/91/115	-
14	CLA	B	824	-	-	8/15/91/115	-
17	BCR	k	4004	-	-	10/29/63/63	0/2/2/2
14	CLA	b	814	-	1/1/11/20	11/15/91/115	-
14	CLA	2	806	-	1/1/12/20	10/26/102/115	-
14	CLA	1	844	12	1/1/11/20	6/15/91/115	-
17	BCR	K	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	1	825	-	1/1/13/20	15/32/108/115	-
14	CLA	a	825	-	1/1/11/20	13/20/96/115	-
14	CLA	a	830	-	1/1/15/20	11/39/115/115	-
14	CLA	a	811	1	1/1/15/20	23/39/115/115	-
14	CLA	1	831	-	1/1/15/20	20/39/115/115	-
14	CLA	a	819	-	1/1/11/20	7/17/93/115	-
14	CLA	a	844	12	1/1/11/20	6/15/91/115	-
14	CLA	b	824	-	1/1/11/20	7/15/91/115	-
14	CLA	A	835	-	1/1/15/20	7/39/115/115	-
14	CLA	a	810	-	1/1/11/20	6/17/93/115	-
18	LMG	A	852	-	-	21/41/61/70	0/1/1/1
14	CLA	l	4204	9	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	840	-	1/1/15/20	9/39/115/115	-
14	CLA	A	831	-	1/1/15/20	7/39/115/115	-
14	CLA	b	830	-	1/1/15/20	8/39/115/115	-
17	BCR	B	851	-	-	19/29/63/63	0/2/2/2
14	CLA	b	817	-	1/1/11/20	3/15/91/115	-
13	CL0	1	803	-	3/3/20/25	13/37/135/135	-
12	LHG	1	801	-	-	22/53/53/53	-
14	CLA	K	4003	-	1/1/11/20	10/15/91/115	-
14	CLA	b	805	-	1/1/15/20	13/39/115/115	-
14	CLA	1	812	-	1/1/15/20	19/39/115/115	-
14	CLA	a	854	-	1/1/13/20	7/27/103/115	-
17	BCR	A	848	-	-	11/29/63/63	0/2/2/2
14	CLA	2	834	-	1/1/13/20	15/31/107/115	-
14	CLA	1	824	-	1/1/12/20	10/23/99/115	-
14	CLA	B	819	-	1/1/13/20	10/27/103/115	-
18	LMG	a	853	-	-	8/27/47/70	0/1/1/1
14	CLA	a	832	-	1/1/15/20	7/39/115/115	-
17	BCR	b	851	-	-	10/29/63/63	0/2/2/2
17	BCR	2	846	-	-	12/29/63/63	0/2/2/2
17	BCR	I	101	-	-	16/29/63/63	0/2/2/2
14	CLA	1	818	-	1/1/12/20	7/26/102/115	-
14	CLA	A	823	-	1/1/15/20	13/39/115/115	-
14	CLA	a	822	-	1/1/15/20	19/39/115/115	-
17	BCR	2	848	-	-	4/18/35/63	0/1/1/2
17	BCR	F	203	-	-	13/29/63/63	0/2/2/2
17	BCR	6	4406	-	-	13/29/63/63	0/2/2/2
14	CLA	2	843	-	-	20/39/115/115	-
14	CLA	b	819	-	-	8/27/103/115	-
14	CLA	a	821	-	1/1/12/20	6/26/102/115	-
14	CLA	b	823	-	-	8/15/91/115	-
17	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	b	839	-	1/1/12/20	7/21/97/115	-
17	BCR	j	103	-	-	13/29/63/63	0/2/2/2
14	CLA	K	4004	-	1/1/13/20	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	1	851	-	-	21/29/63/63	0/2/2/2
14	CLA	2	801	-	1/1/14/20	11/33/109/115	-
14	CLA	B	831	-	1/1/15/20	8/39/115/115	-
14	CLA	2	822	-	-	7/15/91/115	-
14	CLA	B	840	-	1/1/12/20	7/21/97/115	-
12	LHG	9	101	-	-	20/43/43/53	-
14	CLA	a	835	-	1/1/15/20	16/39/115/115	-
16	SF4	c	102	3	-	-	0/6/5/5
14	CLA	K	4002	-	-	8/15/91/115	-
17	BCR	0	209	-	-	14/29/63/63	0/2/2/2
14	CLA	7	1102	-	1/1/11/20	8/15/91/115	-
12	LHG	1	802	14	-	13/37/37/53	-
14	CLA	1	819	-	1/1/12/20	6/26/102/115	-
12	LHG	a	802	14	-	13/37/37/53	-
14	CLA	b	831	-	1/1/14/20	12/33/109/115	-
17	BCR	6	4405	-	-	13/29/63/63	0/2/2/2
17	BCR	2	849	-	-	15/29/63/63	0/2/2/2
14	CLA	b	825	-	-	6/15/91/115	-
14	CLA	B	827	-	1/1/13/20	4/27/103/115	-
14	CLA	A	809	-	1/1/11/20	6/17/93/115	-
17	BCR	h	101	-	-	16/29/63/63	0/2/2/2
14	CLA	2	835	-	1/1/11/20	4/15/91/115	-
14	CLA	2	829	-	1/1/14/20	7/33/109/115	-
14	CLA	b	821	-	1/1/11/20	5/18/94/115	-
14	CLA	2	815	-	1/1/15/20	22/39/115/115	-
14	CLA	2	826	-	1/1/13/20	4/27/103/115	-
14	CLA	0	208	-	1/1/15/20	14/39/115/115	-
14	CLA	A	816	-	1/1/11/20	4/15/91/115	-
14	CLA	b	829	-	1/1/14/20	7/33/109/115	-
14	CLA	8	4004	-	1/1/13/20	7/27/103/115	-
14	CLA	0	206	9	1/1/15/20	14/39/115/115	-
14	CLA	0	207	-	1/1/15/20	11/39/115/115	-
14	CLA	a	831	-	1/1/15/20	10/39/115/115	-
14	CLA	A	843	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	839	-	1/1/15/20	11/39/115/115	-
14	CLA	2	832	-	1/1/11/20	6/15/91/115	-
17	BCR	A	849	-	-	7/29/63/63	0/2/2/2
14	CLA	F	201	-	1/1/12/20	11/23/99/115	-
17	BCR	B	849	-	-	4/18/35/63	0/1/1/2
14	CLA	B	842	-	1/1/11/20	4/17/93/115	-
14	CLA	B	810	-	1/1/14/20	9/33/109/115	-
14	CLA	1	809	1	1/1/15/20	23/39/115/115	-
17	BCR	2	850	-	-	19/29/63/63	0/2/2/2
14	CLA	1	816	-	-	3/15/91/115	-
14	CLA	a	809	-	1/1/15/20	14/39/115/115	-
14	CLA	2	816	-	1/1/11/20	7/17/93/115	-
14	CLA	1	838	-	1/1/15/20	11/39/115/115	-
14	CLA	2	838	-	1/1/11/20	5/17/93/115	-
14	CLA	b	810	-	1/1/14/20	9/33/109/115	-
14	CLA	8	4002	-	-	8/15/91/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	806	-	1/1/12/20	3/21/97/115	-
12	LHG	2	852	-	-	22/43/43/53	-
14	CLA	6	4404	-	1/1/11/20	7/15/91/115	-
14	CLA	b	827	-	1/1/12/20	2/21/97/115	-
14	CLA	B	832	-	1/1/14/20	12/33/109/115	-
14	CLA	B	807	-	1/1/12/20	10/26/102/115	-
14	CLA	b	809	-	1/1/15/20	24/39/115/115	-
14	CLA	B	839	-	1/1/11/20	5/17/93/115	-
17	BCR	8	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	b	832	-	1/1/11/20	6/15/91/115	-
14	CLA	B	837	-	1/1/11/20	4/15/91/115	-
14	CLA	b	807	-	1/1/12/20	10/26/102/115	-
14	CLA	1	827	-	1/1/13/20	6/27/103/115	-
14	CLA	2	814	-	1/1/11/20	11/15/91/115	-
14	CLA	b	811	-	1/1/15/20	16/39/115/115	-
17	BCR	a	849	-	-	7/29/63/63	0/2/2/2
17	BCR	a	850	-	-	19/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	f	201	-	1/1/12/20	11/23/99/115	-
14	CLA	A	812	-	1/1/11/20	8/15/91/115	-
14	CLA	1	807	-	1/1/15/20	14/39/115/115	-
14	CLA	B	801	-	1/1/14/20	11/33/109/115	-
14	CLA	A	840	-	1/1/11/20	3/18/94/115	-
14	CLA	1	810	1	1/1/12/20	8/21/97/115	-
14	CLA	1	832	-	1/1/12/20	3/21/97/115	-
14	CLA	A	824	-	1/1/11/20	13/20/96/115	-
14	CLA	2	820	-	1/1/14/20	15/33/109/115	-
14	CLA	B	816	-	1/1/15/20	22/39/115/115	-
17	BCR	F	206	-	-	14/29/63/63	0/2/2/2
16	SF4	3	101	3	-	-	0/6/5/5
14	CLA	a	823	-	1/1/14/20	8/33/109/115	-
17	BCR	L	1504	-	-	14/29/63/63	0/2/2/2
14	CLA	b	837	-	1/1/11/20	4/15/91/115	-
14	CLA	A	807	-	1/1/15/20	17/39/115/115	-
14	CLA	B	820	-	-	8/27/103/115	-
14	CLA	a	817	-	1/1/11/20	4/15/91/115	-
14	CLA	1	814	-	1/1/13/20	10/27/103/115	-
14	CLA	2	840	-	1/1/14/20	8/36/112/115	-
15	PQN	2	845	-	-	10/23/43/43	0/2/2/2
17	BCR	L	1505	-	-	13/29/63/63	0/2/2/2
12	LHG	B	853	-	-	22/43/43/53	-
17	BCR	b	853	-	-	13/29/63/63	0/2/2/2
19	LMT	i	4101	-	-	8/21/61/61	0/2/2/2
14	CLA	A	814	-	1/1/12/20	11/26/102/115	-
14	CLA	B	806	-	1/1/15/20	14/39/115/115	-
14	CLA	B	814	-	1/1/11/20	5/15/91/115	-
14	CLA	B	821	-	1/1/14/20	15/33/109/115	-
14	CLA	l	4206	-	1/1/15/20	14/39/115/115	-
14	CLA	b	812	-	1/1/14/20	13/35/111/115	-
12	LHG	a	801	-	-	22/53/53/53	-
14	CLA	A	815	-	1/1/13/20	10/27/103/115	-
14	CLA	A	826	-	1/1/13/20	15/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	840	-	1/1/14/20	8/36/112/115	-
14	CLA	a	805	-	1/1/15/20	10/39/115/115	-
14	CLA	2	836	-	1/1/11/20	4/15/91/115	-
14	CLA	1	833	-	1/1/15/20	16/39/115/115	-
14	CLA	a	824	-	1/1/15/20	13/39/115/115	-
14	CLA	b	818	-	1/1/13/20	10/27/103/115	-
14	CLA	b	801	-	1/1/15/20	11/39/115/115	-
18	LMG	0	203	-	-	21/41/61/70	0/1/1/1
14	CLA	B	838	-	1/1/11/20	4/15/91/115	-
14	CLA	j	101	-	1/1/11/20	8/15/91/115	-
17	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
19	LMT	F	202	-	-	3/21/61/61	0/2/2/2
18	LMG	0	201	-	-	20/33/53/70	0/1/1/1
17	BCR	2	847	-	-	7/29/63/63	0/2/2/2
14	CLA	B	815	-	1/1/11/20	11/15/91/115	-
17	BCR	f	206	-	-	13/29/63/63	0/2/2/2
14	CLA	B	802	-	1/1/15/20	11/39/115/115	-
16	SF4	1	846	2,1	-	-	0/6/5/5
17	BCR	1	847	-	-	11/29/63/63	0/2/2/2
17	BCR	a	851	-	-	21/29/63/63	0/2/2/2
17	BCR	0	204	-	-	13/29/63/63	0/2/2/2
14	CLA	1	828	-	1/1/15/20	11/39/115/115	-
14	CLA	B	834	-	1/1/13/20	14/27/103/115	-
14	CLA	b	815	-	1/1/15/20	22/39/115/115	-
14	CLA	a	807	-	1/1/12/20	3/21/97/115	-
14	CLA	2	818	-	1/1/13/20	10/27/103/115	-
14	CLA	2	828	-	1/1/15/20	9/39/115/115	-
14	CLA	2	839	-	1/1/12/20	7/21/97/115	-
17	BCR	A	850	-	-	19/29/63/63	0/2/2/2
14	CLA	2	830	-	1/1/15/20	8/39/115/115	-
14	CLA	a	828	-	1/1/15/20	14/39/115/115	-
14	CLA	1	839	-	1/1/11/20	3/18/94/115	-
17	BCR	B	850	-	-	15/29/63/63	0/2/2/2
18	LMG	1	852	-	-	8/27/47/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	f	203	-	-	13/29/63/63	0/2/2/2
14	CLA	B	829	-	1/1/15/20	9/39/115/115	-
14	CLA	B	826	-	-	6/15/91/115	-
12	LHG	A	801	-	-	22/53/53/53	-
14	CLA	2	808	-	1/1/15/20	24/39/115/115	-
12	LHG	A	802	14	-	13/37/37/53	-
18	LMG	B	803	-	-	20/43/63/70	0/1/1/1
14	CLA	A	819	-	1/1/12/20	7/26/102/115	-
14	CLA	1	815	-	1/1/11/20	4/15/91/115	-
17	BCR	b	850	-	-	19/29/63/63	0/2/2/2
17	BCR	0	210	-	-	13/29/63/63	0/2/2/2
14	CLA	a	815	-	1/1/12/20	11/26/102/115	-
14	CLA	a	826	-	1/1/12/20	10/23/99/115	-
15	PQN	B	846	-	-	10/23/43/43	0/2/2/2
18	LMG	2	802	-	-	20/43/63/70	0/1/1/1
14	CLA	a	836	-	1/1/15/20	7/39/115/115	-
14	CLA	b	836	-	1/1/11/20	4/15/91/115	-
14	CLA	b	838	-	1/1/11/20	5/17/93/115	-
18	LMG	b	803	-	-	20/43/63/70	0/1/1/1
14	CLA	B	823	-	-	7/15/91/115	-
14	CLA	2	804	-	1/1/15/20	13/39/115/115	-

All (2926) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	803	CL0	C1B-C2B	8.20	1.48	1.39
13	1	803	CL0	C1B-C2B	8.13	1.48	1.39
13	a	803	CL0	C1B-C2B	8.09	1.48	1.39
13	a	803	CL0	C3B-C4B	6.64	1.47	1.41
13	A	803	CL0	C3B-C4B	6.63	1.47	1.41
13	1	803	CL0	C3B-C4B	6.60	1.47	1.41
13	a	803	CL0	C1D-C2D	6.34	1.46	1.39
13	A	803	CL0	C1D-C2D	6.33	1.46	1.39
13	1	803	CL0	C1D-C2D	6.29	1.46	1.39
17	a	849	BCR	C1-C6	-4.26	1.48	1.53
14	B	845	CLA	C2B-C1B	4.25	1.49	1.40
14	b	844	CLA	C2B-C1B	4.23	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	844	CLA	C3B-C4B	4.23	1.49	1.40
14	2	844	CLA	C2B-C1B	4.22	1.49	1.40
14	b	844	CLA	C3B-C4B	4.22	1.49	1.40
14	B	845	CLA	C3B-C4B	4.21	1.49	1.40
17	A	849	BCR	C1-C6	-4.21	1.48	1.53
17	1	849	BCR	C1-C6	-4.16	1.48	1.53
17	J	103	BCR	C1-C6	-4.04	1.48	1.53
17	1	850	BCR	C1-C6	-4.03	1.48	1.53
17	j	103	BCR	C1-C6	-4.02	1.48	1.53
17	8	4001	BCR	C1-C6	-4.01	1.48	1.53
17	A	850	BCR	C1-C6	-4.00	1.48	1.53
17	a	850	BCR	C1-C6	-4.00	1.48	1.53
17	7	1104	BCR	C1-C6	-3.99	1.48	1.53
17	K	4001	BCR	C1-C6	-3.98	1.48	1.53
17	k	4001	BCR	C1-C6	-3.98	1.48	1.53
17	i	4103	BCR	C1-C6	-3.93	1.48	1.53
17	h	102	BCR	C1-C6	-3.88	1.48	1.53
17	I	102	BCR	C1-C6	-3.88	1.48	1.53
17	I	101	BCR	C1-C6	-3.86	1.48	1.53
14	b	831	CLA	CMB-C2B	-3.84	1.42	1.50
14	2	831	CLA	CMB-C2B	-3.82	1.42	1.50
14	B	832	CLA	CMB-C2B	-3.81	1.43	1.50
17	i	4102	BCR	C1-C6	-3.81	1.48	1.53
17	h	101	BCR	C1-C6	-3.78	1.48	1.53
17	6	4406	BCR	C1-C6	-3.72	1.49	1.53
17	b	853	BCR	C1-C6	-3.72	1.49	1.53
17	1	847	BCR	C30-C25	-3.71	1.49	1.53
17	B	854	BCR	C1-C6	-3.71	1.49	1.53
17	a	847	BCR	C30-C25	-3.70	1.49	1.53
17	A	847	BCR	C30-C25	-3.70	1.49	1.53
17	a	847	BCR	C1-C6	-3.66	1.49	1.53
13	a	803	CL0	C3D-C4D	3.65	1.47	1.41
13	A	803	CL0	C3D-C4D	3.64	1.47	1.41
17	0	204	BCR	C1-C6	-3.64	1.49	1.53
17	L	1505	BCR	C1-C6	-3.62	1.49	1.53
17	A	847	BCR	C1-C6	-3.61	1.49	1.53
17	0	210	BCR	C1-C6	-3.61	1.49	1.53
13	1	803	CL0	C3D-C4D	3.60	1.47	1.41
17	6	4402	BCR	C30-C25	-3.60	1.49	1.53
17	F	203	BCR	C30-C25	-3.59	1.49	1.53
17	1	847	BCR	C1-C6	-3.58	1.49	1.53
17	f	203	BCR	C1-C6	-3.57	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	203	BCR	C1-C6	-3.57	1.49	1.53
17	f	203	BCR	C30-C25	-3.56	1.49	1.53
17	2	849	BCR	C1-C6	-3.56	1.49	1.53
17	6	4402	BCR	C1-C6	-3.55	1.49	1.53
14	A	832	CLA	CMB-C2B	-3.54	1.43	1.50
17	b	849	BCR	C1-C6	-3.54	1.49	1.53
14	1	831	CLA	CMB-C2B	-3.53	1.43	1.50
17	B	850	BCR	C1-C6	-3.53	1.49	1.53
14	a	833	CLA	CMB-C2B	-3.52	1.43	1.50
17	b	846	BCR	C30-C25	-3.51	1.49	1.53
17	L	1504	BCR	C30-C25	-3.50	1.49	1.53
17	2	848	BCR	C30-C25	-3.49	1.49	1.53
17	6	4405	BCR	C1-C6	-3.49	1.49	1.53
17	a	848	BCR	C30-C25	-3.48	1.49	1.53
14	7	1103	CLA	C1D-ND	3.48	1.42	1.37
17	2	851	BCR	C30-C25	-3.48	1.49	1.53
17	7	1105	BCR	C30-C25	-3.48	1.49	1.53
17	j	104	BCR	C30-C25	-3.47	1.49	1.53
17	l	4207	BCR	C30-C25	-3.47	1.49	1.53
17	M	102	BCR	C1-C6	-3.46	1.49	1.53
17	b	848	BCR	C30-C25	-3.46	1.49	1.53
17	A	848	BCR	C1-C6	-3.46	1.49	1.53
17	2	846	BCR	C30-C25	-3.45	1.49	1.53
17	h	102	BCR	C30-C25	-3.45	1.49	1.53
17	B	847	BCR	C30-C25	-3.44	1.49	1.53
14	J	102	CLA	C1D-ND	3.44	1.42	1.37
17	B	852	BCR	C30-C25	-3.44	1.49	1.53
17	b	851	BCR	C30-C25	-3.43	1.49	1.53
14	2	838	CLA	C1D-ND	3.43	1.42	1.37
17	J	104	BCR	C30-C25	-3.43	1.49	1.53
17	1	848	BCR	C1-C6	-3.43	1.49	1.53
17	9	102	BCR	C1-C6	-3.43	1.49	1.53
14	j	102	CLA	C1D-ND	3.43	1.42	1.37
17	B	849	BCR	C30-C25	-3.43	1.49	1.53
14	K	4003	CLA	C1D-ND	3.43	1.42	1.37
17	a	848	BCR	C1-C6	-3.42	1.49	1.53
17	0	209	BCR	C30-C25	-3.42	1.49	1.53
17	A	848	BCR	C30-C25	-3.42	1.49	1.53
17	I	102	BCR	C30-C25	-3.42	1.49	1.53
14	b	838	CLA	C1D-ND	3.42	1.42	1.37
14	k	4003	CLA	C1D-ND	3.41	1.42	1.37
17	b	854	BCR	C1-C6	-3.41	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	f	206	BCR	C1-C6	-3.40	1.49	1.53
17	i	4103	BCR	C30-C25	-3.40	1.49	1.53
17	F	206	BCR	C1-C6	-3.39	1.49	1.53
17	1	848	BCR	C30-C25	-3.39	1.49	1.53
14	B	839	CLA	C1D-ND	3.39	1.42	1.37
17	B	851	BCR	C1-C6	-3.37	1.49	1.53
14	A	818	CLA	C1D-ND	3.36	1.42	1.37
17	b	850	BCR	C1-C6	-3.36	1.49	1.53
17	2	850	BCR	C1-C6	-3.36	1.49	1.53
17	7	1105	BCR	C1-C6	-3.35	1.49	1.53
17	2	846	BCR	C1-C6	-3.35	1.49	1.53
14	8	4003	CLA	C1D-ND	3.35	1.42	1.37
17	0	209	BCR	C1-C6	-3.34	1.49	1.53
17	j	104	BCR	C1-C6	-3.34	1.49	1.53
17	l	4207	BCR	C1-C6	-3.34	1.49	1.53
17	b	846	BCR	C1-C6	-3.33	1.49	1.53
14	1	817	CLA	C1D-ND	3.32	1.42	1.37
17	2	850	BCR	C30-C25	-3.32	1.49	1.53
17	B	847	BCR	C1-C6	-3.32	1.49	1.53
17	b	851	BCR	C1-C6	-3.31	1.49	1.53
17	B	852	BCR	C1-C6	-3.31	1.49	1.53
14	a	819	CLA	C1D-ND	3.31	1.42	1.37
14	2	844	CLA	C2D-C1D	3.31	1.48	1.42
17	2	849	BCR	C30-C25	-3.30	1.49	1.53
17	1	850	BCR	C30-C25	-3.30	1.49	1.53
17	b	849	BCR	C30-C25	-3.30	1.49	1.53
17	B	850	BCR	C30-C25	-3.30	1.49	1.53
17	a	850	BCR	C30-C25	-3.29	1.49	1.53
17	L	1504	BCR	C1-C6	-3.29	1.49	1.53
14	b	844	CLA	C2D-C1D	3.28	1.48	1.42
17	A	850	BCR	C30-C25	-3.28	1.49	1.53
14	B	845	CLA	C2D-C1D	3.28	1.48	1.42
17	B	851	BCR	C30-C25	-3.28	1.49	1.53
17	J	104	BCR	C1-C6	-3.27	1.49	1.53
17	K	4005	BCR	C1-C6	-3.27	1.49	1.53
17	A	851	BCR	C1-C6	-3.27	1.49	1.53
17	I	101	BCR	C30-C25	-3.27	1.49	1.53
17	B	854	BCR	C30-C25	-3.27	1.49	1.53
17	8	4005	BCR	C1-C6	-3.26	1.49	1.53
14	k	4002	CLA	C1D-ND	3.25	1.42	1.37
17	1	851	BCR	C1-C6	-3.25	1.49	1.53
17	b	850	BCR	C30-C25	-3.24	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	851	BCR	C1-C6	-3.24	1.49	1.53
17	b	853	BCR	C30-C25	-3.24	1.49	1.53
14	8	4002	CLA	C1D-ND	3.24	1.42	1.37
17	k	4004	BCR	C1-C6	-3.22	1.49	1.53
17	6	4406	BCR	C30-C25	-3.22	1.49	1.53
14	K	4002	CLA	C1D-ND	3.22	1.42	1.37
17	h	101	BCR	C30-C25	-3.20	1.49	1.53
17	i	4102	BCR	C30-C25	-3.19	1.49	1.53
17	2	851	BCR	C1-C6	-3.19	1.49	1.53
17	b	847	BCR	C1-C6	-3.19	1.49	1.53
14	a	838	CLA	C1D-ND	3.18	1.42	1.37
14	2	833	CLA	C1D-ND	3.18	1.42	1.37
14	J	101	CLA	C1D-ND	3.17	1.42	1.37
14	7	1102	CLA	C1D-ND	3.16	1.42	1.37
17	a	851	BCR	C30-C25	-3.16	1.49	1.53
14	j	101	CLA	C1D-ND	3.15	1.42	1.37
14	A	837	CLA	C1D-ND	3.15	1.42	1.37
17	b	854	BCR	C30-C25	-3.14	1.49	1.53
14	B	834	CLA	C1D-ND	3.14	1.42	1.37
17	2	847	BCR	C1-C6	-3.13	1.49	1.53
17	7	1104	BCR	C30-C25	-3.13	1.49	1.53
17	A	851	BCR	C30-C25	-3.13	1.49	1.53
17	j	103	BCR	C30-C25	-3.13	1.49	1.53
17	8	4001	BCR	C30-C25	-3.12	1.49	1.53
14	A	836	CLA	CMB-C2B	-3.12	1.44	1.50
14	a	837	CLA	CMB-C2B	-3.12	1.44	1.50
14	b	833	CLA	C1D-ND	3.12	1.42	1.37
17	9	102	BCR	C30-C25	-3.12	1.49	1.53
14	F	205	CLA	C1D-ND	3.11	1.41	1.37
14	1	835	CLA	CMB-C2B	-3.11	1.44	1.50
14	f	205	CLA	C1D-ND	3.11	1.41	1.37
17	1	851	BCR	C30-C25	-3.10	1.49	1.53
14	L	1503	CLA	C1D-ND	3.10	1.41	1.37
14	0	208	CLA	C1D-ND	3.10	1.41	1.37
14	K	4004	CLA	C1D-ND	3.10	1.41	1.37
17	J	103	BCR	C30-C25	-3.09	1.49	1.53
14	1	836	CLA	C1D-ND	3.09	1.41	1.37
14	b	817	CLA	C1D-ND	3.09	1.41	1.37
17	K	4001	BCR	C30-C25	-3.09	1.49	1.53
14	8	4004	CLA	C1D-ND	3.09	1.41	1.37
17	B	848	BCR	C1-C6	-3.09	1.49	1.53
14	A	817	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	4206	CLA	C1D-ND	3.09	1.41	1.37
17	M	102	BCR	C30-C25	-3.08	1.49	1.53
14	2	817	CLA	C1D-ND	3.08	1.41	1.37
14	6	4404	CLA	C1D-ND	3.06	1.41	1.37
13	a	803	CL0	CMD-C2D	-3.06	1.45	1.51
17	2	847	BCR	C30-C25	-3.06	1.49	1.53
13	1	803	CL0	CMD-C2D	-3.05	1.45	1.51
14	a	823	CLA	C1D-ND	3.05	1.41	1.37
14	1	816	CLA	C1D-ND	3.05	1.41	1.37
14	a	854	CLA	C1D-ND	3.04	1.41	1.37
14	B	818	CLA	C1D-ND	3.04	1.41	1.37
13	a	803	CL0	CAC-C3C	-3.04	1.46	1.51
13	A	803	CL0	CMD-C2D	-3.04	1.45	1.51
17	k	4001	BCR	C30-C25	-3.04	1.49	1.53
14	B	844	CLA	CMB-C2B	-3.03	1.44	1.50
14	A	827	CLA	C1D-ND	3.03	1.41	1.37
13	1	803	CL0	CAC-C3C	-3.03	1.46	1.51
14	A	822	CLA	C1D-ND	3.03	1.41	1.37
17	b	847	BCR	C30-C25	-3.03	1.49	1.53
14	b	843	CLA	CMB-C2B	-3.03	1.44	1.50
14	2	823	CLA	C1D-ND	3.03	1.41	1.37
14	0	206	CLA	C1D-ND	3.03	1.41	1.37
14	l	4204	CLA	C1D-ND	3.02	1.41	1.37
14	2	828	CLA	C1D-ND	3.02	1.41	1.37
17	B	848	BCR	C30-C25	-3.02	1.49	1.53
14	B	829	CLA	C1D-ND	3.02	1.41	1.37
14	2	843	CLA	CMB-C2B	-3.02	1.44	1.50
14	b	837	CLA	C1D-ND	3.01	1.41	1.37
14	B	822	CLA	CMB-C2B	-3.01	1.44	1.50
13	A	803	CL0	CAC-C3C	-3.01	1.46	1.51
14	a	830	CLA	CMC-C2C	-3.01	1.44	1.50
14	f	204	CLA	C1D-ND	3.01	1.41	1.37
14	B	824	CLA	C1D-ND	3.00	1.41	1.37
14	a	828	CLA	C1D-ND	3.00	1.41	1.37
14	B	838	CLA	C1D-ND	3.00	1.41	1.37
14	F	204	CLA	C1D-ND	3.00	1.41	1.37
14	L	1501	CLA	C1D-ND	2.99	1.41	1.37
14	1	810	CLA	CMD-C2D	-2.99	1.44	1.50
14	6	4403	CLA	C1D-ND	2.99	1.41	1.37
14	b	828	CLA	C1D-ND	2.99	1.41	1.37
14	b	830	CLA	CMD-C2D	-2.98	1.44	1.50
14	1	821	CLA	C1D-ND	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	828	CLA	CMC-C2C	-2.98	1.44	1.50
14	2	837	CLA	C1D-ND	2.98	1.41	1.37
14	a	812	CLA	CMD-C2D	-2.98	1.44	1.50
14	A	811	CLA	CMD-C2D	-2.97	1.44	1.50
14	2	821	CLA	CMB-C2B	-2.97	1.44	1.50
14	B	812	CLA	CMB-C2B	-2.97	1.44	1.50
14	b	821	CLA	CMB-C2B	-2.97	1.44	1.50
14	1	843	CLA	CMB-C2B	-2.97	1.44	1.50
14	2	830	CLA	CMD-C2D	-2.97	1.44	1.50
14	a	818	CLA	C1D-ND	2.97	1.41	1.37
14	A	829	CLA	CMC-C2C	-2.97	1.44	1.50
14	b	823	CLA	C1D-ND	2.97	1.41	1.37
14	1	826	CLA	C1D-ND	2.97	1.41	1.37
14	B	823	CLA	C4B-NB	2.97	1.41	1.37
14	b	822	CLA	C4B-NB	2.97	1.41	1.37
14	1	812	CLA	C1D-ND	2.96	1.41	1.37
14	B	831	CLA	CMD-C2D	-2.96	1.44	1.50
14	2	844	CLA	CAD-C3D	-2.95	1.45	1.50
14	a	834	CLA	CMD-C2D	-2.95	1.44	1.50
14	B	817	CLA	C1D-ND	2.95	1.41	1.37
14	A	833	CLA	CMD-C2D	-2.95	1.44	1.50
14	A	843	CLA	CMB-C2B	-2.95	1.44	1.50
14	b	844	CLA	CAD-C3D	-2.95	1.45	1.50
13	1	803	CL0	CMB-C2B	-2.94	1.45	1.51
14	A	804	CLA	C1D-ND	2.94	1.41	1.37
14	1	832	CLA	MG-NB	-2.94	2.00	2.05
14	B	832	CLA	CMD-C2D	-2.94	1.44	1.50
14	a	843	CLA	CMB-C2B	-2.94	1.44	1.50
14	1	832	CLA	CMD-C2D	-2.94	1.44	1.50
14	b	812	CLA	CMB-C2B	-2.94	1.44	1.50
13	A	803	CL0	CMB-C2B	-2.94	1.45	1.51
17	k	4004	BCR	C30-C25	-2.94	1.50	1.53
14	2	822	CLA	C4B-NB	2.93	1.41	1.37
14	B	845	CLA	CAD-C3D	-2.93	1.45	1.50
17	8	4005	BCR	C30-C25	-2.93	1.50	1.53
14	a	805	CLA	C1D-ND	2.93	1.41	1.37
14	b	815	CLA	C1D-ND	2.93	1.41	1.37
14	2	811	CLA	CMB-C2B	-2.93	1.44	1.50
14	b	816	CLA	C1D-ND	2.93	1.41	1.37
14	2	831	CLA	CMD-C2D	-2.93	1.44	1.50
17	K	4005	BCR	C30-C25	-2.93	1.50	1.53
14	a	813	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	k	4003	CLA	C4B-NB	2.93	1.41	1.37
14	A	833	CLA	MG-NB	-2.93	2.00	2.05
14	B	822	CLA	C4B-NB	2.92	1.41	1.37
14	A	816	CLA	C1D-ND	2.92	1.41	1.37
14	b	831	CLA	CMD-C2D	-2.92	1.44	1.50
14	2	816	CLA	C1D-ND	2.92	1.41	1.37
14	2	814	CLA	C1D-ND	2.91	1.41	1.37
14	8	4003	CLA	C4B-NB	2.91	1.41	1.37
14	1	811	CLA	C1D-ND	2.91	1.41	1.37
14	a	814	CLA	C1D-ND	2.91	1.41	1.37
14	b	814	CLA	C1D-ND	2.91	1.41	1.37
14	2	815	CLA	C1D-ND	2.91	1.41	1.37
13	a	803	CL0	CMB-C2B	-2.91	1.45	1.51
14	b	821	CLA	C4B-NB	2.90	1.41	1.37
14	B	822	CLA	C1D-ND	2.90	1.41	1.37
14	a	817	CLA	C1D-ND	2.90	1.41	1.37
14	2	803	CLA	C1D-ND	2.90	1.41	1.37
14	B	815	CLA	C1D-ND	2.90	1.41	1.37
14	1	815	CLA	C1D-ND	2.90	1.41	1.37
14	2	822	CLA	C1D-ND	2.90	1.41	1.37
14	a	834	CLA	MG-NB	-2.89	2.00	2.05
14	A	812	CLA	C1D-ND	2.89	1.41	1.37
14	1	804	CLA	C1D-ND	2.89	1.41	1.37
14	b	822	CLA	C1D-ND	2.89	1.41	1.37
14	1	805	CLA	C1D-ND	2.89	1.41	1.37
14	B	823	CLA	C1D-ND	2.89	1.41	1.37
14	B	816	CLA	C1D-ND	2.88	1.41	1.37
14	b	835	CLA	C1D-ND	2.88	1.41	1.37
17	6	4405	BCR	C30-C25	-2.88	1.50	1.53
14	2	805	CLA	CMC-C2C	-2.88	1.44	1.50
14	B	806	CLA	CMC-C2C	-2.88	1.44	1.50
14	b	806	CLA	CMC-C2C	-2.88	1.44	1.50
14	A	806	CLA	C1D-ND	2.88	1.41	1.37
14	B	826	CLA	CMD-C2D	-2.87	1.44	1.50
14	A	824	CLA	C1D-ND	2.87	1.41	1.37
14	a	838	CLA	C4B-NB	2.87	1.41	1.37
14	B	836	CLA	CMB-C2B	-2.86	1.44	1.50
14	a	826	CLA	CMD-C2D	-2.86	1.44	1.50
14	A	813	CLA	C1D-ND	2.86	1.41	1.37
14	B	802	CLA	C1D-ND	2.86	1.41	1.37
14	K	4003	CLA	C4B-NB	2.86	1.41	1.37
14	J	102	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	843	CLA	C1D-ND	2.85	1.41	1.37
14	2	818	CLA	C1D-ND	2.85	1.41	1.37
17	F	206	BCR	C30-C25	-2.85	1.50	1.53
14	b	842	CLA	C1D-ND	2.85	1.41	1.37
14	2	835	CLA	C1D-ND	2.85	1.41	1.37
14	A	837	CLA	C4B-NB	2.85	1.41	1.37
14	a	807	CLA	C1D-ND	2.85	1.41	1.37
14	2	821	CLA	C4B-NB	2.85	1.41	1.37
17	f	206	BCR	C30-C25	-2.85	1.50	1.53
14	2	820	CLA	C1D-ND	2.85	1.41	1.37
14	b	801	CLA	C1D-ND	2.85	1.41	1.37
14	B	837	CLA	C1D-ND	2.84	1.41	1.37
14	k	4002	CLA	C4B-NB	2.84	1.41	1.37
14	2	825	CLA	CMD-C2D	-2.84	1.44	1.50
14	1	836	CLA	C4B-NB	2.84	1.41	1.37
14	1	823	CLA	C1D-ND	2.84	1.41	1.37
14	2	835	CLA	CMB-C2B	-2.84	1.44	1.50
14	b	835	CLA	CMB-C2B	-2.84	1.45	1.50
14	b	819	CLA	C1D-ND	2.84	1.41	1.37
14	2	821	CLA	C1D-ND	2.84	1.41	1.37
14	B	801	CLA	CMC-C2C	-2.83	1.45	1.50
14	b	804	CLA	C1D-ND	2.83	1.41	1.37
14	b	825	CLA	CMD-C2D	-2.83	1.45	1.50
14	1	825	CLA	C1D-ND	2.83	1.41	1.37
14	A	825	CLA	CMD-C2D	-2.83	1.45	1.50
14	b	836	CLA	C1D-ND	2.83	1.41	1.37
14	a	805	CLA	CMB-C2B	-2.83	1.45	1.50
14	2	801	CLA	CMC-C2C	-2.83	1.45	1.50
14	B	804	CLA	C1D-ND	2.83	1.41	1.37
14	b	813	CLA	C1D-ND	2.83	1.41	1.37
14	a	827	CLA	C1D-ND	2.83	1.41	1.37
14	b	819	CLA	CMB-C2B	-2.83	1.45	1.50
14	B	836	CLA	C1D-ND	2.83	1.41	1.37
14	j	102	CLA	C4B-NB	2.83	1.41	1.37
14	K	4002	CLA	C4B-NB	2.82	1.41	1.37
14	A	815	CLA	C1D-ND	2.82	1.41	1.37
14	B	814	CLA	C1D-ND	2.82	1.41	1.37
14	2	813	CLA	C1D-ND	2.82	1.41	1.37
14	a	809	CLA	C1D-ND	2.82	1.41	1.37
14	2	836	CLA	C1D-ND	2.82	1.41	1.37
14	0	202	CLA	C1D-ND	2.82	1.41	1.37
14	B	820	CLA	C1D-ND	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	841	CLA	C1D-ND	2.82	1.41	1.37
14	b	821	CLA	C1D-ND	2.82	1.41	1.37
14	2	826	CLA	C1D-ND	2.81	1.41	1.37
14	2	826	CLA	CMD-C2D	-2.81	1.45	1.50
14	B	827	CLA	CMD-C2D	-2.81	1.45	1.50
14	A	826	CLA	C1D-ND	2.81	1.41	1.37
14	1	814	CLA	C1D-ND	2.81	1.41	1.37
14	B	824	CLA	C4B-NB	2.81	1.41	1.37
14	2	839	CLA	MG-NB	-2.81	2.00	2.05
14	1	835	CLA	C1D-ND	2.81	1.41	1.37
14	2	828	CLA	C4B-NB	2.81	1.41	1.37
17	1	849	BCR	C30-C25	-2.81	1.50	1.53
14	1	804	CLA	CMB-C2B	-2.81	1.45	1.50
14	2	810	CLA	C1D-ND	2.81	1.41	1.37
14	A	804	CLA	MG-NB	-2.80	2.00	2.05
14	B	820	CLA	CMB-C2B	-2.80	1.45	1.50
14	b	839	CLA	MG-NB	-2.80	2.00	2.05
14	2	840	CLA	C1D-ND	2.80	1.41	1.37
14	1	824	CLA	CMD-C2D	-2.80	1.45	1.50
14	2	842	CLA	C1D-ND	2.80	1.41	1.37
14	A	844	CLA	C1D-ND	2.80	1.41	1.37
14	A	804	CLA	CMB-C2B	-2.80	1.45	1.50
14	B	819	CLA	C1D-ND	2.80	1.41	1.37
14	1	807	CLA	C1D-ND	2.80	1.41	1.37
14	8	4002	CLA	C4B-NB	2.80	1.41	1.37
14	a	825	CLA	C1D-ND	2.80	1.41	1.37
17	A	849	BCR	C30-C25	-2.80	1.50	1.53
14	b	820	CLA	C1D-ND	2.79	1.41	1.37
14	A	842	CLA	C1D-ND	2.79	1.41	1.37
14	A	810	CLA	C1D-ND	2.79	1.41	1.37
14	b	826	CLA	C1D-ND	2.79	1.41	1.37
13	1	803	CL0	CMC-C2C	-2.79	1.46	1.50
14	A	820	CLA	C1D-ND	2.79	1.41	1.37
14	a	844	CLA	C1D-ND	2.79	1.41	1.37
14	A	808	CLA	C1D-ND	2.78	1.41	1.37
14	2	819	CLA	CMB-C2B	-2.78	1.45	1.50
14	b	828	CLA	C4B-NB	2.78	1.41	1.37
14	b	811	CLA	C1D-ND	2.78	1.41	1.37
14	B	840	CLA	MG-NB	-2.78	2.00	2.05
14	A	805	CLA	C1D-ND	2.78	1.41	1.37
14	B	827	CLA	C1D-ND	2.78	1.41	1.37
14	2	819	CLA	C1D-ND	2.78	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	826	CLA	CMD-C2D	-2.78	1.45	1.50
14	a	842	CLA	C1D-ND	2.78	1.41	1.37
14	a	821	CLA	C1D-ND	2.77	1.41	1.37
14	a	843	CLA	CMC-C2C	-2.77	1.45	1.50
14	a	816	CLA	C1D-ND	2.77	1.41	1.37
14	b	818	CLA	C1D-ND	2.77	1.41	1.37
14	b	829	CLA	C1D-ND	2.77	1.41	1.37
14	2	806	CLA	C1D-ND	2.77	1.41	1.37
14	a	804	CLA	CMC-C2C	-2.77	1.45	1.50
14	7	1102	CLA	C4B-NB	2.77	1.41	1.37
14	a	805	CLA	MG-NB	-2.77	2.00	2.05
17	a	849	BCR	C30-C25	-2.77	1.50	1.53
14	1	819	CLA	C1D-ND	2.77	1.41	1.37
14	B	809	CLA	C1D-ND	2.77	1.41	1.37
14	b	824	CLA	C1D-ND	2.77	1.41	1.37
14	B	808	CLA	C1D-ND	2.77	1.41	1.37
14	1	842	CLA	C1D-ND	2.77	1.41	1.37
14	b	840	CLA	C1D-ND	2.77	1.41	1.37
14	1	843	CLA	CMC-C2C	-2.77	1.45	1.50
14	a	804	CLA	CMD-C2D	-2.76	1.45	1.50
14	2	824	CLA	C1D-ND	2.76	1.41	1.37
14	A	839	CLA	C1D-ND	2.76	1.41	1.37
14	7	1103	CLA	C4B-NB	2.76	1.41	1.37
14	7	1101	CLA	C1D-ND	2.76	1.41	1.37
13	a	803	CL0	CMC-C2C	-2.76	1.46	1.50
14	B	801	CLA	CMD-C2D	-2.76	1.45	1.50
14	b	808	CLA	C1D-ND	2.76	1.41	1.37
14	2	834	CLA	C1D-ND	2.76	1.41	1.37
14	b	811	CLA	CMC-C2C	-2.76	1.45	1.50
14	b	843	CLA	C1D-ND	2.76	1.41	1.37
14	A	843	CLA	CMC-C2C	-2.76	1.45	1.50
14	B	821	CLA	C1D-ND	2.76	1.41	1.37
14	a	840	CLA	C1D-ND	2.76	1.41	1.37
14	B	825	CLA	C1D-ND	2.75	1.41	1.37
14	b	809	CLA	C1D-ND	2.75	1.41	1.37
13	A	803	CL0	CMC-C2C	-2.75	1.46	1.50
14	a	822	CLA	C1D-ND	2.75	1.41	1.37
14	2	801	CLA	CMD-C2D	-2.75	1.45	1.50
14	1	817	CLA	C4B-NB	2.75	1.41	1.37
14	b	834	CLA	C1D-ND	2.75	1.41	1.37
14	2	831	CLA	MG-NB	-2.75	2.00	2.05
14	A	821	CLA	C1D-ND	2.75	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	832	CLA	MG-NB	-2.75	2.00	2.05
14	a	806	CLA	C1D-ND	2.74	1.41	1.37
14	b	825	CLA	C1D-ND	2.74	1.41	1.37
14	1	804	CLA	MG-NB	-2.74	2.00	2.05
14	b	823	CLA	C4B-NB	2.74	1.41	1.37
14	2	823	CLA	C4B-NB	2.74	1.41	1.37
14	2	810	CLA	CMC-C2C	-2.74	1.45	1.50
14	b	831	CLA	MG-NB	-2.74	2.00	2.05
14	a	837	CLA	C1D-ND	2.74	1.41	1.37
14	J	101	CLA	C4B-NB	2.73	1.41	1.37
14	1	820	CLA	C1D-ND	2.73	1.41	1.37
14	1	844	CLA	C1D-ND	2.73	1.41	1.37
14	B	828	CLA	C1D-ND	2.73	1.41	1.37
14	B	831	CLA	C1D-ND	2.73	1.41	1.37
14	1	809	CLA	C1D-ND	2.73	1.41	1.37
14	a	815	CLA	C1D-ND	2.73	1.41	1.37
14	2	825	CLA	C1D-ND	2.73	1.41	1.37
14	B	807	CLA	C1D-ND	2.72	1.41	1.37
14	B	826	CLA	C1D-ND	2.72	1.41	1.37
14	K	4003	CLA	C1B-C2B	2.72	1.49	1.43
14	a	831	CLA	C1D-ND	2.72	1.41	1.37
14	1	835	CLA	C4B-NB	2.72	1.41	1.37
14	b	807	CLA	C1D-ND	2.72	1.41	1.37
14	B	811	CLA	CMC-C2C	-2.72	1.45	1.50
14	B	810	CLA	C1D-ND	2.72	1.41	1.37
14	A	835	CLA	C1D-ND	2.72	1.41	1.37
14	1	808	CLA	C1D-ND	2.72	1.41	1.37
14	2	807	CLA	C1D-ND	2.72	1.41	1.37
13	1	803	CL0	C1A-CHA	-2.72	1.36	1.40
14	K	4004	CLA	C1B-C2B	2.72	1.49	1.43
14	B	811	CLA	C1D-ND	2.72	1.41	1.37
14	B	829	CLA	C4B-NB	2.72	1.41	1.37
14	a	811	CLA	C1D-ND	2.72	1.41	1.37
14	2	843	CLA	C1D-ND	2.72	1.41	1.37
14	A	836	CLA	C1D-ND	2.72	1.41	1.37
13	A	803	CL0	C1A-CHA	-2.71	1.36	1.40
14	1	830	CLA	CMD-C2D	-2.71	1.45	1.50
14	2	808	CLA	C1D-ND	2.71	1.41	1.37
14	2	827	CLA	C1D-ND	2.71	1.41	1.37
14	j	101	CLA	C4B-NB	2.71	1.41	1.37
13	a	803	CL0	C1A-CHA	-2.71	1.36	1.40
14	7	1103	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	827	CLA	C1D-ND	2.71	1.41	1.37
14	1	822	CLA	C1D-ND	2.71	1.41	1.37
14	B	832	CLA	C1D-ND	2.71	1.41	1.37
14	b	824	CLA	C4B-NB	2.71	1.41	1.37
14	B	844	CLA	C1D-ND	2.71	1.41	1.37
14	a	829	CLA	C1D-ND	2.70	1.41	1.37
14	1	829	CLA	C1D-ND	2.70	1.41	1.37
14	B	830	CLA	C1D-ND	2.70	1.41	1.37
14	k	4003	CLA	C1B-C2B	2.70	1.49	1.43
14	1	813	CLA	C1D-ND	2.70	1.41	1.37
14	b	804	CLA	MG-NB	-2.70	2.00	2.05
14	A	843	CLA	C1D-ND	2.70	1.41	1.37
14	2	830	CLA	C1D-ND	2.70	1.41	1.37
14	j	102	CLA	C1B-C2B	2.70	1.49	1.43
14	a	832	CLA	CMD-C2D	-2.70	1.45	1.50
14	1	828	CLA	C1D-ND	2.70	1.41	1.37
14	B	805	CLA	MG-NB	-2.70	2.00	2.05
14	B	835	CLA	C1D-ND	2.70	1.41	1.37
14	b	805	CLA	CMD-C2D	-2.70	1.45	1.50
14	b	831	CLA	C1D-ND	2.69	1.41	1.37
14	B	833	CLA	C4B-NB	2.69	1.41	1.37
14	b	810	CLA	C1D-ND	2.69	1.41	1.37
14	b	836	CLA	C4B-NB	2.69	1.41	1.37
14	2	838	CLA	C4B-NB	2.69	1.41	1.37
14	l	4203	CLA	C1D-ND	2.69	1.41	1.37
14	A	831	CLA	MG-NB	-2.69	2.00	2.05
14	a	810	CLA	C1D-ND	2.69	1.41	1.37
14	a	833	CLA	C1D-ND	2.69	1.41	1.37
14	B	804	CLA	MG-NB	-2.69	2.00	2.05
14	8	4004	CLA	C1B-C2B	2.69	1.49	1.43
14	a	828	CLA	CMD-C2D	-2.69	1.45	1.50
14	A	818	CLA	C4B-NB	2.69	1.41	1.37
14	1	827	CLA	C1D-ND	2.69	1.41	1.37
14	A	831	CLA	CMD-C2D	-2.69	1.45	1.50
14	2	812	CLA	C1D-ND	2.69	1.41	1.37
14	1	826	CLA	CMD-C2D	-2.69	1.45	1.50
14	1	841	CLA	CMD-C2D	-2.69	1.45	1.50
14	A	823	CLA	C1D-ND	2.69	1.41	1.37
14	8	4003	CLA	C1B-C2B	2.69	1.49	1.43
14	a	824	CLA	C1D-ND	2.69	1.41	1.37
14	A	840	CLA	C1D-ND	2.69	1.41	1.37
14	b	832	CLA	C4B-NB	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	841	CLA	C1D-ND	2.68	1.41	1.37
14	B	825	CLA	C4B-NB	2.68	1.41	1.37
14	a	819	CLA	C4B-NB	2.68	1.41	1.37
14	1	832	CLA	CMB-C2B	-2.68	1.45	1.50
14	2	832	CLA	C4B-NB	2.68	1.41	1.37
14	1	838	CLA	C1D-ND	2.68	1.41	1.37
14	a	854	CLA	C1B-C2B	2.68	1.49	1.43
14	2	842	CLA	CMD-C2D	-2.68	1.45	1.50
14	1	840	CLA	C1D-ND	2.68	1.41	1.37
14	2	803	CLA	MG-NB	-2.68	2.00	2.05
14	F	205	CLA	C4B-NB	2.68	1.41	1.37
14	f	205	CLA	C4B-NB	2.68	1.41	1.37
14	A	828	CLA	C1D-ND	2.68	1.41	1.37
14	B	805	CLA	CMD-C2D	-2.68	1.45	1.50
14	A	809	CLA	C1D-ND	2.68	1.41	1.37
14	1	834	CLA	C1D-ND	2.68	1.41	1.37
14	b	842	CLA	CMD-C2D	-2.68	1.45	1.50
14	6	4404	CLA	C4B-NB	2.68	1.41	1.37
14	b	841	CLA	MG-NB	-2.67	2.00	2.05
14	a	837	CLA	C4B-NB	2.67	1.41	1.37
14	2	804	CLA	MG-NB	-2.67	2.00	2.05
14	A	811	CLA	C1D-ND	2.67	1.41	1.37
14	1	831	CLA	C1D-ND	2.67	1.41	1.37
14	a	812	CLA	MG-NB	-2.67	2.00	2.05
14	B	811	CLA	CMD-C2D	-2.67	1.45	1.50
14	2	836	CLA	C4B-NB	2.67	1.41	1.37
14	B	813	CLA	C1D-ND	2.67	1.41	1.37
14	A	836	CLA	C4B-NB	2.67	1.41	1.37
14	2	841	CLA	MG-NB	-2.67	2.00	2.05
14	2	804	CLA	CMD-C2D	-2.67	1.45	1.50
14	8	4004	CLA	C4B-NB	2.67	1.41	1.37
14	0	207	CLA	C1D-ND	2.67	1.41	1.37
14	A	822	CLA	C4B-NB	2.67	1.41	1.37
14	B	838	CLA	C4B-NB	2.67	1.41	1.37
14	A	829	CLA	C1D-ND	2.67	1.41	1.37
14	2	829	CLA	C1D-ND	2.67	1.41	1.37
14	a	834	CLA	CMB-C2B	-2.66	1.45	1.50
12	a	802	LHG	O7-C5	-2.66	1.40	1.46
14	a	839	CLA	MG-NB	-2.66	2.00	2.05
14	b	837	CLA	C4B-NB	2.66	1.41	1.37
14	1	830	CLA	MG-NB	-2.66	2.00	2.05
14	A	823	CLA	MG-NB	-2.66	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	837	CLA	C4B-NB	2.66	1.41	1.37
14	b	805	CLA	MG-NB	-2.66	2.00	2.05
14	1	810	CLA	C1D-ND	2.66	1.41	1.37
14	2	831	CLA	C1D-ND	2.66	1.41	1.37
14	A	838	CLA	MG-NB	-2.66	2.00	2.05
14	F	201	CLA	CMD-C2D	-2.66	1.45	1.50
14	b	811	CLA	CMD-C2D	-2.66	1.45	1.50
14	b	802	CLA	C1D-ND	2.66	1.41	1.37
14	A	830	CLA	C1D-ND	2.65	1.41	1.37
14	a	824	CLA	C4B-NB	2.65	1.41	1.37
14	1	843	CLA	C1D-ND	2.65	1.41	1.37
14	1	822	CLA	MG-NB	-2.65	2.00	2.05
14	J	102	CLA	C1B-C2B	2.65	1.49	1.43
14	A	832	CLA	MG-NB	-2.65	2.00	2.05
14	1	831	CLA	MG-NB	-2.65	2.00	2.05
14	F	201	CLA	C1D-ND	2.65	1.41	1.37
14	2	809	CLA	C1D-ND	2.65	1.41	1.37
14	b	830	CLA	C1D-ND	2.65	1.41	1.37
14	b	838	CLA	C4B-NB	2.65	1.41	1.37
14	1	824	CLA	MG-NB	-2.65	2.00	2.05
14	B	842	CLA	MG-NB	-2.65	2.00	2.05
14	A	827	CLA	CMD-C2D	-2.65	1.45	1.50
14	a	826	CLA	MG-NB	-2.65	2.00	2.05
14	f	201	CLA	CMD-C2D	-2.65	1.45	1.50
14	f	201	CLA	C1D-ND	2.64	1.41	1.37
14	A	805	CLA	CMD-C2D	-2.64	1.45	1.50
14	A	833	CLA	CMB-C2B	-2.64	1.45	1.50
14	A	832	CLA	C1D-ND	2.64	1.41	1.37
14	a	806	CLA	CMD-C2D	-2.64	1.45	1.50
14	2	810	CLA	CMD-C2D	-2.64	1.45	1.50
14	B	837	CLA	C4B-NB	2.64	1.41	1.37
14	a	843	CLA	C1D-ND	2.64	1.41	1.37
14	B	843	CLA	CMD-C2D	-2.64	1.45	1.50
14	A	814	CLA	C1D-ND	2.64	1.41	1.37
14	1	837	CLA	MG-NB	-2.63	2.00	2.05
14	a	823	CLA	C4B-NB	2.63	1.41	1.37
14	7	1101	CLA	CMD-C2D	-2.63	1.45	1.50
14	a	812	CLA	C1D-ND	2.63	1.41	1.37
14	A	823	CLA	C4B-NB	2.63	1.41	1.37
14	7	1101	CLA	C4B-NB	2.63	1.41	1.37
14	a	832	CLA	MG-NB	-2.63	2.00	2.05
14	a	832	CLA	CMB-C2B	-2.63	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	839	CLA	C4B-NB	2.63	1.41	1.37
14	2	824	CLA	C4B-NB	2.63	1.41	1.37
14	a	833	CLA	MG-NB	-2.63	2.00	2.05
14	b	832	CLA	CMB-C2B	-2.63	1.45	1.50
14	L	1502	CLA	C1D-ND	2.63	1.41	1.37
14	B	829	CLA	CMC-C2C	-2.63	1.45	1.50
14	1	817	CLA	C1B-C2B	2.63	1.49	1.43
14	A	827	CLA	C4B-NB	2.62	1.41	1.37
14	A	811	CLA	MG-NB	-2.62	2.00	2.05
14	B	833	CLA	CMB-C2B	-2.62	1.45	1.50
14	2	814	CLA	C4B-NB	2.62	1.41	1.37
14	A	805	CLA	C4B-NB	2.62	1.41	1.37
14	0	206	CLA	MG-NB	-2.62	2.00	2.05
14	a	839	CLA	C1D-ND	2.62	1.41	1.37
14	a	830	CLA	C1D-ND	2.62	1.41	1.37
14	2	832	CLA	CMB-C2B	-2.62	1.45	1.50
14	B	812	CLA	MG-NB	-2.62	2.00	2.05
14	1	821	CLA	C4B-NB	2.62	1.41	1.37
14	b	828	CLA	CMC-C2C	-2.62	1.45	1.50
14	1	822	CLA	CMB-C2B	-2.62	1.45	1.50
14	1	839	CLA	C1D-ND	2.62	1.41	1.37
14	B	801	CLA	MG-NB	-2.62	2.00	2.05
14	2	811	CLA	MG-NB	-2.61	2.00	2.05
14	K	4004	CLA	C4B-NB	2.61	1.41	1.37
14	1	810	CLA	MG-NB	-2.61	2.00	2.05
14	a	836	CLA	C1D-ND	2.61	1.41	1.37
14	a	824	CLA	MG-NB	-2.61	2.00	2.05
19	F	202	LMT	O2'-C2'	-2.61	1.36	1.43
14	b	801	CLA	C4B-NB	2.61	1.41	1.37
14	b	840	CLA	CMD-C2D	-2.61	1.45	1.50
14	B	841	CLA	CMD-C2D	-2.61	1.45	1.50
14	L	1501	CLA	MG-NB	-2.61	2.00	2.05
14	a	804	CLA	MG-NB	-2.61	2.00	2.05
14	l	4205	CLA	C1D-ND	2.61	1.41	1.37
12	A	802	LHG	O7-C5	-2.60	1.40	1.46
12	1	802	LHG	O7-C5	-2.60	1.40	1.46
14	1	812	CLA	MG-NB	-2.60	2.00	2.05
14	A	831	CLA	CMB-C2B	-2.60	1.45	1.50
14	A	825	CLA	MG-NB	-2.60	2.00	2.05
14	a	822	CLA	MG-NB	-2.60	2.00	2.05
14	2	824	CLA	CMD-C2D	-2.60	1.45	1.50
14	B	815	CLA	C4B-NB	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	841	CLA	C1D-ND	2.60	1.41	1.37
14	l	4204	CLA	MG-NB	-2.60	2.00	2.05
14	1	806	CLA	CMD-C2D	-2.60	1.45	1.50
14	a	820	CLA	C1D-ND	2.60	1.41	1.37
14	A	834	CLA	MG-NB	-2.60	2.00	2.05
14	1	818	CLA	C1D-ND	2.60	1.41	1.37
14	b	832	CLA	MG-NB	-2.60	2.00	2.05
14	2	801	CLA	MG-NB	-2.60	2.00	2.05
14	A	841	CLA	MG-NB	-2.60	2.00	2.05
14	b	817	CLA	CMC-C2C	-2.60	1.45	1.50
14	a	835	CLA	C1D-ND	2.60	1.41	1.37
19	6	4401	LMT	O2'-C2'	-2.60	1.36	1.43
14	a	806	CLA	C4B-NB	2.59	1.41	1.37
14	2	834	CLA	C3B-C4B	2.59	1.50	1.42
14	b	812	CLA	MG-NB	-2.59	2.00	2.05
14	2	832	CLA	MG-NB	-2.59	2.00	2.05
14	b	812	CLA	C1D-ND	2.59	1.41	1.37
14	a	821	CLA	CMB-C2B	-2.59	1.45	1.50
14	1	822	CLA	C4B-NB	2.59	1.41	1.37
14	A	812	CLA	C4B-NB	2.59	1.41	1.37
14	1	819	CLA	CMB-C2B	-2.59	1.45	1.50
14	2	817	CLA	CMC-C2C	-2.59	1.45	1.50
14	2	828	CLA	CMC-C2C	-2.59	1.45	1.50
14	k	4002	CLA	C1B-C2B	2.59	1.49	1.43
14	2	840	CLA	CMD-C2D	-2.59	1.45	1.50
14	b	834	CLA	C3B-C4B	2.58	1.50	1.42
14	b	824	CLA	CMD-C2D	-2.58	1.45	1.50
14	1	837	CLA	C1D-ND	2.58	1.41	1.37
14	A	820	CLA	CMB-C2B	-2.58	1.45	1.50
14	K	4002	CLA	C1B-C2B	2.58	1.49	1.43
14	A	821	CLA	MG-NB	-2.58	2.00	2.05
14	B	835	CLA	C3B-C4B	2.58	1.50	1.42
14	a	814	CLA	MG-NB	-2.58	2.00	2.05
13	1	803	CL0	CHC-C4B	-2.58	1.35	1.39
19	f	202	LMT	O2'-C2'	-2.58	1.36	1.43
14	B	831	CLA	MG-NB	-2.58	2.00	2.05
14	A	823	CLA	CMC-C2C	-2.58	1.45	1.50
14	a	804	CLA	C1B-NB	-2.58	1.34	1.37
14	A	818	CLA	C1B-C2B	2.58	1.49	1.43
14	B	812	CLA	C1D-ND	2.58	1.41	1.37
14	b	814	CLA	C4B-NB	2.58	1.41	1.37
14	a	824	CLA	CMB-C2B	-2.57	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	830	CLA	CMB-C2B	-2.57	1.45	1.50
14	A	838	CLA	C1D-ND	2.57	1.41	1.37
14	B	834	CLA	C4B-NB	2.57	1.41	1.37
14	L	1503	CLA	C4B-NB	2.57	1.41	1.37
14	1	840	CLA	MG-NB	-2.57	2.00	2.05
14	a	835	CLA	MG-NB	-2.57	2.00	2.05
14	1	843	CLA	CMD-C2D	-2.57	1.45	1.50
14	b	833	CLA	C4B-NB	2.57	1.41	1.37
14	1	820	CLA	MG-NB	-2.57	2.00	2.05
14	1	811	CLA	C4B-NB	2.57	1.41	1.37
14	a	819	CLA	C1B-C2B	2.57	1.49	1.43
14	A	807	CLA	CMD-C2D	-2.57	1.45	1.50
14	a	842	CLA	CMC-C2C	-2.57	1.45	1.50
14	a	812	CLA	C4B-NB	2.57	1.41	1.37
14	B	833	CLA	MG-NB	-2.57	2.00	2.05
14	A	823	CLA	CMB-C2B	-2.57	1.45	1.50
14	2	811	CLA	C1D-ND	2.57	1.41	1.37
14	b	809	CLA	MG-NB	-2.57	2.00	2.05
14	b	834	CLA	MG-NB	-2.57	2.00	2.05
14	2	830	CLA	MG-NB	-2.57	2.00	2.05
14	A	819	CLA	C1D-ND	2.57	1.41	1.37
14	b	824	CLA	C1B-C2B	2.56	1.49	1.43
14	A	843	CLA	CMD-C2D	-2.56	1.45	1.50
14	B	825	CLA	CMD-C2D	-2.56	1.45	1.50
14	b	838	CLA	C1B-C2B	2.56	1.49	1.43
14	2	838	CLA	C1B-C2B	2.56	1.49	1.43
14	a	813	CLA	CMB-C2B	-2.56	1.45	1.50
14	A	813	CLA	CMB-C2B	-2.56	1.45	1.50
14	A	807	CLA	CMC-C2C	-2.56	1.45	1.50
14	A	813	CLA	MG-NB	-2.56	2.00	2.05
13	a	803	CL0	CHC-C4B	-2.56	1.35	1.39
14	2	833	CLA	C4B-NB	2.56	1.41	1.37
14	a	828	CLA	C4B-NB	2.56	1.41	1.37
14	b	826	CLA	MG-NB	-2.56	2.00	2.05
14	a	854	CLA	C4B-NB	2.56	1.41	1.37
14	B	818	CLA	CMC-C2C	-2.56	1.45	1.50
14	A	811	CLA	C4B-NB	2.56	1.41	1.37
14	a	843	CLA	CMD-C2D	-2.56	1.45	1.50
14	a	824	CLA	CMC-C2C	-2.56	1.45	1.50
14	B	835	CLA	MG-NB	-2.56	2.00	2.05
14	b	830	CLA	MG-NB	-2.55	2.00	2.05
14	a	811	CLA	MG-NB	-2.55	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	826	CLA	C4B-NB	2.55	1.41	1.37
14	1	830	CLA	C1D-ND	2.55	1.41	1.37
14	B	839	CLA	C1B-C2B	2.55	1.49	1.43
14	2	809	CLA	CMD-C2D	-2.55	1.45	1.50
14	1	822	CLA	CMC-C2C	-2.55	1.45	1.50
14	a	808	CLA	CMD-C2D	-2.55	1.45	1.50
14	1	826	CLA	C4B-NB	2.55	1.41	1.37
14	1	838	CLA	CMB-C2B	-2.55	1.45	1.50
14	1	841	CLA	C1D-ND	2.55	1.41	1.37
17	A	849	BCR	C33-C5	-2.55	1.46	1.50
14	b	825	CLA	C4B-NB	2.55	1.41	1.37
14	a	831	CLA	MG-NB	-2.55	2.00	2.05
14	A	842	CLA	CMC-C2C	-2.55	1.45	1.50
17	b	853	BCR	C33-C5	-2.55	1.46	1.50
14	a	808	CLA	MG-NB	-2.55	2.00	2.05
14	b	821	CLA	MG-NB	-2.55	2.00	2.05
14	2	834	CLA	MG-NB	-2.55	2.00	2.05
14	1	806	CLA	CMB-C2B	-2.55	1.45	1.50
14	B	809	CLA	MG-NB	-2.55	2.00	2.05
14	a	840	CLA	CMB-C2B	-2.55	1.45	1.50
14	A	807	CLA	MG-NB	-2.54	2.00	2.05
14	2	821	CLA	MG-NB	-2.54	2.00	2.05
17	6	4406	BCR	C33-C5	-2.54	1.46	1.50
14	A	820	CLA	MG-NB	-2.54	2.00	2.05
14	B	836	CLA	C4B-NB	2.54	1.41	1.37
14	8	4002	CLA	C1B-C2B	2.54	1.49	1.43
14	1	825	CLA	MG-NB	-2.54	2.00	2.05
14	1	812	CLA	CMB-C2B	-2.54	1.45	1.50
14	b	835	CLA	C4B-NB	2.54	1.41	1.37
14	a	827	CLA	MG-NB	-2.54	2.00	2.05
14	a	814	CLA	CMB-C2B	-2.54	1.45	1.50
14	a	844	CLA	C1B-C2B	2.54	1.49	1.43
14	2	839	CLA	C1D-ND	2.54	1.41	1.37
14	A	807	CLA	CMB-C2B	-2.54	1.45	1.50
14	1	829	CLA	MG-NB	-2.54	2.00	2.05
14	B	822	CLA	MG-NB	-2.54	2.00	2.05
14	A	830	CLA	MG-NB	-2.54	2.00	2.05
14	A	831	CLA	C1D-ND	2.54	1.41	1.37
14	1	806	CLA	CMC-C2C	-2.54	1.45	1.50
14	1	806	CLA	MG-NB	-2.54	2.00	2.05
14	1	833	CLA	MG-NB	-2.53	2.00	2.05
14	0	208	CLA	C4B-NB	2.53	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	819	CLA	MG-NB	-2.53	2.00	2.05
14	2	826	CLA	MG-NB	-2.53	2.00	2.05
14	0	207	CLA	MG-NB	-2.53	2.00	2.05
14	2	803	CLA	CMB-C2B	-2.53	1.45	1.50
14	B	802	CLA	C4B-NB	2.53	1.41	1.37
14	b	802	CLA	MG-NB	-2.53	2.00	2.05
17	a	849	BCR	C33-C5	-2.53	1.46	1.50
14	2	810	CLA	MG-NB	-2.53	2.00	2.05
14	1	811	CLA	CMB-C2B	-2.53	1.45	1.50
14	1	842	CLA	CMC-C2C	-2.53	1.45	1.50
19	f	202	LMT	O3'-C3'	-2.53	1.36	1.43
14	B	805	CLA	C1B-C2B	2.53	1.49	1.43
14	a	830	CLA	MG-NB	-2.53	2.00	2.05
14	a	804	CLA	CMB-C2B	-2.53	1.45	1.50
19	F	202	LMT	O3'-C3'	-2.53	1.36	1.43
14	B	806	CLA	CMD-C2D	-2.53	1.45	1.50
14	1	842	CLA	C4B-NB	2.53	1.41	1.37
14	B	811	CLA	MG-NB	-2.53	2.00	2.05
14	1	810	CLA	C4B-NB	2.53	1.41	1.37
14	l	4206	CLA	C4B-NB	2.53	1.41	1.37
14	1	831	CLA	CMD-C2D	-2.53	1.45	1.50
14	2	824	CLA	C1B-C2B	2.53	1.49	1.43
14	B	810	CLA	MG-NB	-2.53	2.00	2.05
14	a	808	CLA	CMC-C2C	-2.53	1.45	1.50
14	b	804	CLA	CMB-C2B	-2.52	1.45	1.50
14	B	821	CLA	MG-NB	-2.52	2.00	2.05
14	1	824	CLA	C1B-C2B	2.52	1.49	1.43
14	b	805	CLA	C1B-C2B	2.52	1.49	1.43
14	b	811	CLA	MG-NB	-2.52	2.00	2.05
14	B	838	CLA	MG-NB	-2.52	2.00	2.05
14	1	807	CLA	MG-NB	-2.52	2.00	2.05
14	2	825	CLA	C4B-NB	2.52	1.41	1.37
17	B	854	BCR	C33-C5	-2.52	1.46	1.50
14	a	826	CLA	C1B-C2B	2.52	1.49	1.43
14	2	819	CLA	MG-NB	-2.52	2.00	2.05
14	0	202	CLA	C4B-NB	2.52	1.41	1.37
14	A	839	CLA	CMB-C2B	-2.52	1.45	1.50
14	B	813	CLA	C4B-NB	2.52	1.41	1.37
14	2	834	CLA	C4B-NB	2.52	1.41	1.37
14	A	834	CLA	C1D-ND	2.52	1.41	1.37
14	a	813	CLA	C4B-NB	2.52	1.41	1.37
14	A	832	CLA	CMD-C2D	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	816	CLA	CMC-C2C	-2.52	1.45	1.50
14	L	1502	CLA	MG-NB	-2.52	2.00	2.05
14	a	821	CLA	MG-NB	-2.52	2.00	2.05
14	2	808	CLA	MG-NB	-2.52	2.00	2.05
14	a	822	CLA	CMB-C2B	-2.52	1.45	1.50
14	2	801	CLA	CMB-C2B	-2.52	1.45	1.50
14	A	835	CLA	MG-NB	-2.52	2.00	2.05
14	A	807	CLA	C1D-ND	2.52	1.41	1.37
14	2	812	CLA	C4B-NB	2.52	1.41	1.37
14	A	844	CLA	C1B-C2B	2.51	1.49	1.43
14	1	834	CLA	MG-NB	-2.51	2.00	2.05
14	a	808	CLA	CMB-C2B	-2.51	1.45	1.50
14	B	836	CLA	MG-NB	-2.51	2.00	2.05
14	a	809	CLA	MG-NB	-2.51	2.00	2.05
14	B	804	CLA	CMB-C2B	-2.51	1.45	1.50
14	b	819	CLA	MG-NB	-2.51	2.00	2.05
14	b	820	CLA	MG-NB	-2.51	2.00	2.05
14	2	803	CLA	CMD-C2D	-2.51	1.45	1.50
13	A	803	CL0	CHC-C4B	-2.51	1.35	1.39
14	B	804	CLA	CMD-C2D	-2.51	1.45	1.50
14	b	804	CLA	CMD-C2D	-2.51	1.45	1.50
14	b	835	CLA	CMD-C2D	-2.51	1.45	1.50
14	A	814	CLA	C4B-NB	2.51	1.41	1.37
14	a	842	CLA	C4B-NB	2.51	1.41	1.37
14	l	4203	CLA	C4B-NB	2.51	1.41	1.37
14	B	827	CLA	MG-NB	-2.51	2.00	2.05
14	a	841	CLA	MG-NB	-2.51	2.00	2.05
14	1	809	CLA	MG-NB	-2.51	2.00	2.05
14	B	825	CLA	C1B-C2B	2.51	1.49	1.43
14	A	825	CLA	C1B-C2B	2.51	1.49	1.43
14	2	809	CLA	MG-NB	-2.51	2.00	2.05
14	B	801	CLA	C1B-NB	-2.51	1.34	1.37
14	1	834	CLA	CMC-C2C	-2.51	1.45	1.50
14	b	806	CLA	CMD-C2D	-2.51	1.45	1.50
14	l	4205	CLA	MG-NB	-2.51	2.00	2.05
14	1	806	CLA	C1B-C2B	2.51	1.49	1.43
14	A	829	CLA	MG-NB	-2.51	2.00	2.05
14	1	828	CLA	MG-NB	-2.51	2.00	2.05
14	2	808	CLA	CMC-C2C	-2.51	1.45	1.50
14	b	805	CLA	MG-ND	-2.51	2.00	2.05
14	A	834	CLA	C1B-NB	-2.51	1.34	1.37
13	a	803	CL0	CMA-C3A	-2.50	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	836	CLA	CMC-C2C	-2.50	1.45	1.50
14	a	840	CLA	MG-NB	-2.50	2.00	2.05
14	1	804	CLA	CMC-C2C	-2.50	1.45	1.50
14	a	815	CLA	C4B-NB	2.50	1.41	1.37
14	A	812	CLA	CMB-C2B	-2.50	1.45	1.50
14	B	809	CLA	CMC-C2C	-2.50	1.45	1.50
14	a	836	CLA	MG-NB	-2.50	2.00	2.05
14	A	810	CLA	CMC-C2C	-2.50	1.45	1.50
14	A	815	CLA	CMC-C2C	-2.50	1.45	1.50
14	B	826	CLA	C4B-NB	2.50	1.41	1.37
14	B	807	CLA	C4B-NB	2.50	1.41	1.37
14	2	801	CLA	C1B-NB	-2.50	1.34	1.37
14	A	835	CLA	CMC-C2C	-2.50	1.45	1.50
14	1	813	CLA	C4B-NB	2.50	1.41	1.37
14	2	806	CLA	C4B-NB	2.50	1.41	1.37
14	1	838	CLA	MG-NB	-2.50	2.00	2.05
14	1	820	CLA	CMB-C2B	-2.50	1.45	1.50
14	A	825	CLA	C1D-ND	2.50	1.41	1.37
14	B	810	CLA	CMD-C2D	-2.50	1.45	1.50
14	B	823	CLA	C1B-C2B	2.50	1.49	1.43
14	2	805	CLA	CMD-C2D	-2.50	1.45	1.50
14	b	822	CLA	C1B-C2B	2.50	1.49	1.43
18	A	852	LMG	O7-C8	-2.50	1.40	1.46
14	b	810	CLA	MG-NB	-2.50	2.00	2.05
14	a	832	CLA	C1D-ND	2.50	1.41	1.37
14	2	820	CLA	MG-NB	-2.50	2.00	2.05
14	2	840	CLA	CMB-C2B	-2.50	1.45	1.50
14	1	844	CLA	C1B-C2B	2.50	1.49	1.43
14	F	201	CLA	C4B-NB	2.50	1.41	1.37
14	A	826	CLA	MG-NB	-2.50	2.00	2.05
14	B	812	CLA	CMD-C2D	-2.50	1.45	1.50
14	B	827	CLA	C4B-NB	2.50	1.41	1.37
14	B	835	CLA	C4B-NB	2.50	1.41	1.37
19	6	4401	LMT	O3'-C3'	-2.50	1.36	1.43
14	a	825	CLA	MG-NB	-2.49	2.00	2.05
14	B	837	CLA	CMD-C2D	-2.49	1.45	1.50
14	a	842	CLA	CMD-C2D	-2.49	1.45	1.50
14	1	809	CLA	CMC-C2C	-2.49	1.45	1.50
14	1	833	CLA	C1D-ND	2.49	1.41	1.37
14	b	841	CLA	C1D-ND	2.49	1.41	1.37
14	2	835	CLA	C4B-NB	2.49	1.41	1.37
14	A	844	CLA	CMC-C2C	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	810	CLA	CMD-C2D	-2.49	1.45	1.50
14	B	842	CLA	C1D-ND	2.49	1.41	1.37
14	A	824	CLA	C1B-C2B	2.49	1.49	1.43
13	1	803	CL0	CMA-C3A	-2.49	1.49	1.53
14	B	840	CLA	C1D-ND	2.49	1.41	1.37
14	2	816	CLA	C4B-NB	2.49	1.41	1.37
14	2	804	CLA	C1B-C2B	2.49	1.49	1.43
14	b	809	CLA	CMC-C2C	-2.49	1.45	1.50
14	2	818	CLA	MG-NB	-2.49	2.00	2.05
14	2	822	CLA	C1B-C2B	2.49	1.49	1.43
14	2	813	CLA	CMB-C2B	-2.49	1.45	1.50
14	1	823	CLA	MG-NB	-2.49	2.00	2.05
14	A	817	CLA	C4B-NB	2.49	1.41	1.37
17	1	849	BCR	C33-C5	-2.49	1.47	1.50
14	1	816	CLA	C1B-C2B	2.49	1.49	1.43
14	1	808	CLA	C4B-NB	2.49	1.41	1.37
14	b	839	CLA	C1D-ND	2.49	1.41	1.37
14	2	805	CLA	MG-NB	-2.49	2.00	2.05
14	A	808	CLA	MG-NB	-2.49	2.00	2.05
14	A	807	CLA	C1B-C2B	2.49	1.49	1.43
14	1	809	CLA	CMD-C2D	-2.49	1.45	1.50
14	l	4203	CLA	CMC-C2C	-2.49	1.45	1.50
14	L	1502	CLA	C4B-NB	2.49	1.41	1.37
14	1	832	CLA	C1B-NB	-2.49	1.34	1.37
14	A	839	CLA	MG-NB	-2.49	2.00	2.05
14	2	813	CLA	C4B-NB	2.49	1.41	1.37
14	A	810	CLA	MG-NB	-2.49	2.00	2.05
14	1	835	CLA	MG-NB	-2.49	2.00	2.05
14	a	839	CLA	CMB-C2B	-2.49	1.45	1.50
14	b	805	CLA	CMC-C2C	-2.49	1.45	1.50
14	a	811	CLA	CMC-C2C	-2.49	1.45	1.50
14	2	807	CLA	CMB-C2B	-2.49	1.45	1.50
14	1	833	CLA	C1B-NB	-2.48	1.34	1.37
14	2	803	CLA	CMC-C2C	-2.48	1.45	1.50
14	2	835	CLA	CMD-C2D	-2.48	1.45	1.50
14	2	836	CLA	CMD-C2D	-2.48	1.45	1.50
14	A	836	CLA	MG-NB	-2.48	2.00	2.05
14	1	841	CLA	C4B-NB	2.48	1.41	1.37
14	2	818	CLA	C4B-NB	2.48	1.41	1.37
14	A	833	CLA	C1B-NB	-2.48	1.34	1.37
14	a	833	CLA	CMD-C2D	-2.48	1.45	1.50
14	f	205	CLA	C1B-C2B	2.48	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	817	CLA	C1B-C2B	2.48	1.49	1.43
14	b	804	CLA	CMC-C2C	-2.48	1.45	1.50
14	b	826	CLA	CMB-C2B	-2.48	1.45	1.50
14	A	844	CLA	C4B-NB	2.48	1.41	1.37
18	a	852	LMG	O7-C8	-2.48	1.40	1.46
14	b	808	CLA	CMD-C2D	-2.48	1.45	1.50
19	f	202	LMT	O1'-C1'	-2.48	1.36	1.40
14	a	818	CLA	C4B-NB	2.48	1.41	1.37
14	B	805	CLA	CMC-C2C	-2.48	1.45	1.50
14	b	806	CLA	MG-NB	-2.48	2.00	2.05
14	B	820	CLA	MG-NB	-2.48	2.00	2.05
14	f	201	CLA	C4B-NB	2.48	1.41	1.37
14	A	840	CLA	MG-NB	-2.48	2.00	2.05
14	1	823	CLA	C1B-C2B	2.48	1.48	1.43
14	b	829	CLA	MG-NB	-2.48	2.00	2.05
14	a	825	CLA	C1B-C2B	2.48	1.48	1.43
14	A	810	CLA	CMD-C2D	-2.48	1.45	1.50
14	b	808	CLA	CMB-C2B	-2.48	1.45	1.50
14	A	824	CLA	MG-NB	-2.48	2.00	2.05
14	A	829	CLA	CMB-C2B	-2.48	1.45	1.50
14	1	824	CLA	C4B-NB	2.48	1.41	1.37
18	0	203	LMG	O7-C8	-2.48	1.40	1.46
14	A	842	CLA	MG-NB	-2.48	2.00	2.05
14	1	839	CLA	MG-NB	-2.48	2.00	2.05
14	b	818	CLA	MG-NB	-2.48	2.00	2.05
14	6	4404	CLA	C1B-C2B	2.48	1.48	1.43
14	A	821	CLA	CMB-C2B	-2.47	1.45	1.50
14	A	825	CLA	C4B-NB	2.47	1.41	1.37
14	1	806	CLA	C1D-ND	2.47	1.41	1.37
14	1	824	CLA	C1D-ND	2.47	1.41	1.37
14	B	836	CLA	CMD-C2D	-2.47	1.45	1.50
14	2	815	CLA	CMC-C2C	-2.47	1.45	1.50
14	A	842	CLA	CMD-C2D	-2.47	1.45	1.50
14	B	804	CLA	CMC-C2C	-2.47	1.45	1.50
14	b	836	CLA	CMD-C2D	-2.47	1.45	1.50
14	a	842	CLA	MG-NB	-2.47	2.00	2.05
14	B	819	CLA	C4B-NB	2.47	1.41	1.37
14	b	807	CLA	C4B-NB	2.47	1.41	1.37
14	F	204	CLA	MG-NB	-2.47	2.00	2.05
14	2	812	CLA	CMC-C2C	-2.47	1.45	1.50
14	A	838	CLA	CMB-C2B	-2.47	1.45	1.50
14	B	830	CLA	MG-NB	-2.47	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	204	CLA	C4B-NB	2.47	1.41	1.37
13	A	803	CL0	CMA-C3A	-2.47	1.49	1.53
14	2	837	CLA	MG-NB	-2.47	2.00	2.05
14	a	839	CLA	CMD-C2D	-2.47	1.45	1.50
14	1	818	CLA	MG-NB	-2.47	2.00	2.05
14	A	834	CLA	CMD-C2D	-2.47	1.45	1.50
14	2	809	CLA	C1B-C2B	2.47	1.48	1.43
14	1	822	CLA	CMD-C2D	-2.47	1.45	1.50
14	F	204	CLA	C4B-NB	2.47	1.41	1.37
14	b	834	CLA	C4B-NB	2.47	1.41	1.37
14	B	827	CLA	CMB-C2B	-2.47	1.45	1.50
14	B	828	CLA	CMD-C2D	-2.47	1.45	1.50
14	a	826	CLA	C1D-ND	2.47	1.41	1.37
14	A	819	CLA	MG-NB	-2.47	2.00	2.05
14	a	811	CLA	CMD-C2D	-2.47	1.45	1.50
14	b	843	CLA	CMD-C2D	-2.47	1.45	1.50
14	2	826	CLA	CMB-C2B	-2.47	1.45	1.50
14	1	826	CLA	MG-NB	-2.47	2.00	2.05
14	B	805	CLA	MG-ND	-2.46	2.00	2.05
14	B	814	CLA	MG-NB	-2.46	2.00	2.05
14	b	837	CLA	MG-NB	-2.46	2.00	2.05
14	1	828	CLA	CMB-C2B	-2.46	1.45	1.50
14	b	815	CLA	CMC-C2C	-2.46	1.45	1.50
14	1	814	CLA	CMC-C2C	-2.46	1.45	1.50
14	2	825	CLA	CMC-C2C	-2.46	1.45	1.50
14	B	836	CLA	CMC-C2C	-2.46	1.45	1.50
14	B	819	CLA	MG-NB	-2.46	2.00	2.05
14	b	831	CLA	CMC-C2C	-2.46	1.45	1.50
14	B	817	CLA	C4B-NB	2.46	1.41	1.37
14	B	810	CLA	C1B-C2B	2.46	1.48	1.43
14	1	842	CLA	MG-NB	-2.46	2.00	2.05
14	a	835	CLA	C1B-NB	-2.46	1.34	1.37
14	2	804	CLA	MG-ND	-2.46	2.00	2.05
14	B	820	CLA	CMC-C2C	-2.46	1.45	1.50
14	a	834	CLA	C1B-NB	-2.46	1.34	1.37
14	f	204	CLA	MG-NB	-2.46	2.00	2.05
14	B	801	CLA	CMB-C2B	-2.46	1.45	1.50
14	6	4403	CLA	C4B-NB	2.46	1.41	1.37
14	0	207	CLA	C4B-NB	2.46	1.41	1.37
18	B	803	LMG	O7-C8	-2.46	1.40	1.46
13	1	803	CL0	MG-NB	-2.46	2.00	2.05
14	b	813	CLA	CMB-C2B	-2.46	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	839	CLA	CMD-C2D	-2.46	1.45	1.50
14	2	811	CLA	CMD-C2D	-2.46	1.45	1.50
14	b	818	CLA	C4B-NB	2.46	1.41	1.37
14	A	804	CLA	CMC-C2C	-2.46	1.45	1.50
14	2	829	CLA	CMD-C2D	-2.46	1.45	1.50
14	a	833	CLA	CMC-C2C	-2.46	1.45	1.50
14	b	812	CLA	CMD-C2D	-2.46	1.45	1.50
14	2	843	CLA	CMD-C2D	-2.46	1.45	1.50
14	a	815	CLA	CMD-C2D	-2.46	1.45	1.50
14	a	821	CLA	CMD-C2D	-2.46	1.45	1.50
14	A	827	CLA	MG-NB	-2.46	2.00	2.05
14	A	838	CLA	CMD-C2D	-2.46	1.45	1.50
14	2	829	CLA	MG-NB	-2.46	2.00	2.05
14	a	824	CLA	CMD-C2D	-2.45	1.45	1.50
14	b	835	CLA	MG-NB	-2.45	2.00	2.05
14	a	805	CLA	CMC-C2C	-2.45	1.45	1.50
14	A	812	CLA	MG-NB	-2.45	2.00	2.05
14	2	827	CLA	MG-NB	-2.45	2.00	2.05
14	2	804	CLA	CMC-C2C	-2.45	1.45	1.50
18	b	803	LMG	O7-C8	-2.45	1.40	1.46
14	2	835	CLA	MG-NB	-2.45	2.00	2.05
14	2	831	CLA	CMC-C2C	-2.45	1.45	1.50
14	B	814	CLA	C4B-NB	2.45	1.41	1.37
14	1	818	CLA	CMC-C2C	-2.45	1.45	1.50
14	2	839	CLA	CMD-C2D	-2.45	1.45	1.50
14	b	840	CLA	CMB-C2B	-2.45	1.45	1.50
14	b	812	CLA	CMC-C2C	-2.45	1.45	1.50
14	2	837	CLA	CMD-C2D	-2.45	1.45	1.50
14	B	830	CLA	CMD-C2D	-2.45	1.45	1.50
14	b	819	CLA	CMC-C2C	-2.45	1.45	1.50
14	A	805	CLA	MG-NB	-2.45	2.00	2.05
14	l	4204	CLA	C4B-NB	2.45	1.41	1.37
14	A	814	CLA	CMD-C2D	-2.45	1.45	1.50
14	b	825	CLA	MG-NB	-2.45	2.00	2.05
14	a	835	CLA	CMD-C2D	-2.45	1.45	1.50
14	B	828	CLA	MG-NB	-2.45	2.00	2.05
13	a	803	CL0	MG-NB	-2.45	2.00	2.05
14	L	1502	CLA	CMB-C2B	-2.45	1.45	1.50
14	2	827	CLA	CMD-C2D	-2.45	1.45	1.50
14	A	832	CLA	CMC-C2C	-2.45	1.45	1.50
14	b	827	CLA	CMD-C2D	-2.45	1.45	1.50
14	a	830	CLA	CMB-C2B	-2.45	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	806	CLA	MG-NB	-2.45	2.00	2.05
14	F	205	CLA	C1B-C2B	2.45	1.48	1.43
14	a	810	CLA	C4B-NB	2.45	1.41	1.37
14	b	831	CLA	C1B-NB	-2.45	1.34	1.37
14	2	819	CLA	CMC-C2C	-2.45	1.45	1.50
14	J	101	CLA	C1B-C2B	2.45	1.48	1.43
14	l	4205	CLA	C4B-NB	2.45	1.41	1.37
14	A	826	CLA	CMC-C2C	-2.45	1.45	1.50
14	6	4403	CLA	C1B-C2B	2.44	1.48	1.43
14	A	836	CLA	CMD-C2D	-2.44	1.45	1.50
14	B	816	CLA	CMC-C2C	-2.44	1.45	1.50
14	B	821	CLA	CMB-C2B	-2.44	1.45	1.50
14	a	808	CLA	C1D-ND	2.44	1.41	1.37
14	a	837	CLA	MG-NB	-2.44	2.00	2.05
14	2	825	CLA	MG-NB	-2.44	2.00	2.05
14	b	835	CLA	CMC-C2C	-2.44	1.45	1.50
17	B	851	BCR	C38-C26	-2.44	1.47	1.50
14	a	814	CLA	C4B-NB	2.44	1.41	1.37
14	B	814	CLA	CMB-C2B	-2.44	1.45	1.50
14	B	844	CLA	CMD-C2D	-2.44	1.45	1.50
14	b	829	CLA	CMD-C2D	-2.44	1.45	1.50
14	b	810	CLA	C1B-C2B	2.44	1.48	1.43
14	a	806	CLA	MG-NB	-2.44	2.00	2.05
14	A	843	CLA	C4B-NB	2.44	1.41	1.37
14	A	804	CLA	CMD-C2D	-2.44	1.45	1.50
14	a	808	CLA	C1B-C2B	2.44	1.48	1.43
14	A	827	CLA	CMB-C2B	-2.44	1.45	1.50
14	a	844	CLA	CMC-C2C	-2.44	1.45	1.50
14	1	826	CLA	CMB-C2B	-2.44	1.45	1.50
14	1	844	CLA	CMC-C2C	-2.44	1.45	1.50
14	1	812	CLA	C4B-NB	2.44	1.41	1.37
14	B	838	CLA	C1B-C2B	2.44	1.48	1.43
14	7	1101	CLA	CMB-C2B	-2.44	1.45	1.50
14	b	837	CLA	C1B-C2B	2.44	1.48	1.43
14	A	829	CLA	CMD-C2D	-2.44	1.45	1.50
19	i	4101	LMT	O3'-C3'	-2.44	1.36	1.43
13	A	803	CL0	MG-NB	-2.44	2.01	2.05
14	1	813	CLA	CMD-C2D	-2.44	1.45	1.50
14	b	825	CLA	CMC-C2C	-2.44	1.45	1.50
14	b	843	CLA	C1B-C2B	2.44	1.48	1.43
14	f	204	CLA	C1B-C2B	2.44	1.48	1.43
14	7	1102	CLA	C1B-C2B	2.44	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	833	CLA	CMD-C2D	-2.44	1.45	1.50
14	1	842	CLA	CMD-C2D	-2.44	1.45	1.50
14	2	826	CLA	C4B-NB	2.44	1.41	1.37
14	1	837	CLA	CMB-C2B	-2.44	1.45	1.50
14	A	820	CLA	CMD-C2D	-2.43	1.45	1.50
14	2	835	CLA	CMC-C2C	-2.43	1.45	1.50
14	2	807	CLA	MG-NB	-2.43	2.01	2.05
14	B	818	CLA	MG-NB	-2.43	2.01	2.05
14	a	813	CLA	MG-NB	-2.43	2.01	2.05
14	a	818	CLA	C1B-C2B	2.43	1.48	1.43
14	B	826	CLA	MG-NB	-2.43	2.01	2.05
17	b	850	BCR	C38-C26	-2.43	1.47	1.50
14	B	808	CLA	CMD-C2D	-2.43	1.45	1.50
14	b	826	CLA	C4B-NB	2.43	1.41	1.37
14	B	808	CLA	CMB-C2B	-2.43	1.45	1.50
14	B	832	CLA	CMC-C2C	-2.43	1.45	1.50
14	a	837	CLA	CMD-C2D	-2.43	1.45	1.50
14	a	828	CLA	MG-NB	-2.43	2.01	2.05
14	A	805	CLA	C1B-C2B	2.43	1.48	1.43
14	A	842	CLA	C4B-NB	2.43	1.41	1.37
14	7	1101	CLA	C1B-C2B	2.43	1.48	1.43
14	1	837	CLA	CMD-C2D	-2.43	1.45	1.50
14	B	813	CLA	CMC-C2C	-2.43	1.45	1.50
14	B	841	CLA	CMB-C2B	-2.43	1.45	1.50
14	B	832	CLA	C1B-NB	-2.43	1.34	1.37
14	2	817	CLA	MG-NB	-2.43	2.01	2.05
14	2	843	CLA	C1B-C2B	2.43	1.48	1.43
14	2	823	CLA	C1B-C2B	2.43	1.48	1.43
14	L	1503	CLA	MG-NB	-2.43	2.01	2.05
14	2	841	CLA	C1D-ND	2.43	1.41	1.37
14	a	830	CLA	CMD-C2D	-2.43	1.45	1.50
14	b	827	CLA	MG-NB	-2.43	2.01	2.05
14	A	823	CLA	CMD-C2D	-2.43	1.45	1.50
14	b	813	CLA	C4B-NB	2.43	1.41	1.37
14	a	806	CLA	C1B-C2B	2.43	1.48	1.43
14	B	826	CLA	CMC-C2C	-2.43	1.45	1.50
14	2	831	CLA	C1B-NB	-2.43	1.34	1.37
14	B	838	CLA	CMD-C2D	-2.43	1.45	1.50
14	2	807	CLA	CMC-C2C	-2.43	1.45	1.50
14	B	844	CLA	C1B-C2B	2.43	1.48	1.43
14	L	1501	CLA	C4B-NB	2.42	1.41	1.37
18	2	802	LMG	O7-C8	-2.42	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	812	CLA	CMC-C2C	-2.42	1.45	1.50
14	a	828	CLA	CMB-C2B	-2.42	1.45	1.50
19	I	103	LMT	O3'-C3'	-2.42	1.37	1.43
14	A	819	CLA	CMD-C2D	-2.42	1.45	1.50
14	b	817	CLA	MG-NB	-2.42	2.01	2.05
14	B	840	CLA	CMD-C2D	-2.42	1.45	1.50
14	a	820	CLA	CMC-C2C	-2.42	1.45	1.50
14	a	841	CLA	CMD-C2D	-2.42	1.45	1.50
14	6	4403	CLA	MG-NB	-2.42	2.01	2.05
14	0	207	CLA	CMB-C2B	-2.42	1.45	1.50
14	b	820	CLA	CMB-C2B	-2.42	1.45	1.50
14	1	843	CLA	C4B-NB	2.42	1.41	1.37
14	1	820	CLA	CMD-C2D	-2.42	1.45	1.50
14	a	827	CLA	CMC-C2C	-2.42	1.45	1.50
14	1	836	CLA	CMB-C2B	-2.42	1.45	1.50
14	2	807	CLA	CMD-C2D	-2.42	1.45	1.50
14	a	820	CLA	MG-NB	-2.42	2.01	2.05
14	1	811	CLA	MG-NB	-2.42	2.01	2.05
14	a	820	CLA	CMD-C2D	-2.42	1.45	1.50
14	2	820	CLA	CMB-C2B	-2.42	1.45	1.50
14	1	821	CLA	CMD-C2D	-2.42	1.45	1.50
14	1	818	CLA	C1B-C2B	2.42	1.48	1.43
14	a	820	CLA	C1B-C2B	2.42	1.48	1.43
14	B	844	CLA	C4B-NB	2.42	1.41	1.37
14	a	823	CLA	CMD-C2D	-2.42	1.45	1.50
14	1	828	CLA	CMD-C2D	-2.42	1.45	1.50
14	A	841	CLA	CMD-C2D	-2.42	1.45	1.50
14	1	804	CLA	CMD-C2D	-2.42	1.45	1.50
14	1	831	CLA	CMC-C2C	-2.42	1.45	1.50
14	b	837	CLA	CMD-C2D	-2.42	1.45	1.50
14	2	811	CLA	CMC-C2C	-2.42	1.45	1.50
14	B	824	CLA	C1B-C2B	2.42	1.48	1.43
14	a	829	CLA	CMD-C2D	-2.41	1.45	1.50
14	A	809	CLA	C4B-NB	2.41	1.41	1.37
14	b	823	CLA	C1B-C2B	2.41	1.48	1.43
14	1	825	CLA	CMC-C2C	-2.41	1.45	1.50
14	2	842	CLA	CMB-C2B	-2.41	1.45	1.50
14	2	837	CLA	C1B-C2B	2.41	1.48	1.43
14	B	809	CLA	CMD-C2D	-2.41	1.45	1.50
14	2	843	CLA	C4B-NB	2.41	1.41	1.37
14	a	831	CLA	CMD-C2D	-2.41	1.45	1.50
14	b	825	CLA	CMB-C2B	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	204	CLA	C1B-C2B	2.41	1.48	1.43
19	F	202	LMT	O1'-C1'	-2.41	1.36	1.40
14	a	810	CLA	CMB-C2B	-2.41	1.45	1.50
14	b	828	CLA	CMD-C2D	-2.41	1.45	1.50
14	A	830	CLA	CMD-C2D	-2.41	1.45	1.50
14	0	208	CLA	CMD-C2D	-2.41	1.45	1.50
14	B	843	CLA	C4B-NB	2.41	1.41	1.37
14	a	806	CLA	CMB-C2B	-2.41	1.45	1.50
14	j	101	CLA	C1B-C2B	2.41	1.48	1.43
14	b	815	CLA	MG-NB	-2.41	2.01	2.05
14	1	840	CLA	CMD-C2D	-2.41	1.45	1.50
14	2	815	CLA	MG-NB	-2.41	2.01	2.05
14	b	813	CLA	MG-NB	-2.41	2.01	2.05
14	7	1101	CLA	MG-NB	-2.41	2.01	2.05
14	a	817	CLA	CMC-C2C	-2.41	1.45	1.50
17	2	850	BCR	C38-C26	-2.41	1.47	1.50
12	a	801	LHG	O7-C5	-2.41	1.40	1.46
14	A	805	CLA	CMB-C2B	-2.41	1.45	1.50
14	2	816	CLA	C1B-C2B	2.41	1.48	1.43
14	b	842	CLA	CMB-C2B	-2.41	1.45	1.50
14	1	839	CLA	CMD-C2D	-2.40	1.45	1.50
14	2	828	CLA	CMD-C2D	-2.40	1.45	1.50
19	h	103	LMT	O3'-C3'	-2.40	1.37	1.43
14	1	818	CLA	CMD-C2D	-2.40	1.45	1.50
14	1	827	CLA	CMD-C2D	-2.40	1.45	1.50
14	b	831	CLA	MG-ND	-2.40	2.01	2.05
19	6	4401	LMT	O1'-C1'	-2.40	1.36	1.40
14	A	819	CLA	CMC-C2C	-2.40	1.45	1.50
14	A	821	CLA	CMD-C2D	-2.40	1.45	1.50
14	1	819	CLA	CMD-C2D	-2.40	1.45	1.50
14	A	819	CLA	C1B-C2B	2.40	1.48	1.43
14	A	828	CLA	CMD-C2D	-2.40	1.45	1.50
14	b	808	CLA	MG-NB	-2.40	2.01	2.05
14	1	835	CLA	CMD-C2D	-2.40	1.45	1.50
14	b	837	CLA	CMB-C2B	-2.40	1.45	1.50
14	B	816	CLA	MG-NB	-2.40	2.01	2.05
14	1	844	CLA	C4B-NB	2.40	1.41	1.37
14	A	808	CLA	C1B-NB	-2.40	1.34	1.37
14	a	822	CLA	CMD-C2D	-2.40	1.45	1.50
14	2	803	CLA	MG-ND	-2.40	2.01	2.05
14	A	809	CLA	CMB-C2B	-2.40	1.45	1.50
14	a	809	CLA	C1B-NB	-2.40	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	0	206	CLA	C4B-NB	2.40	1.41	1.37
14	1	808	CLA	MG-NB	-2.40	2.01	2.05
14	b	814	CLA	CMB-C2B	-2.40	1.45	1.50
14	a	817	CLA	C4B-NB	2.40	1.41	1.37
14	1	816	CLA	C4B-NB	2.40	1.41	1.37
14	1	838	CLA	C4B-NB	2.40	1.41	1.37
14	A	840	CLA	CMD-C2D	-2.39	1.45	1.50
14	1	842	CLA	CMB-C2B	-2.39	1.45	1.50
12	1	801	LHG	O7-C5	-2.39	1.41	1.46
14	B	808	CLA	CMC-C2C	-2.39	1.45	1.50
14	a	807	CLA	CMC-C2C	-2.39	1.45	1.50
14	1	821	CLA	C1B-C2B	2.39	1.48	1.43
14	A	816	CLA	CMC-C2C	-2.39	1.45	1.50
14	b	809	CLA	CMD-C2D	-2.39	1.45	1.50
14	1	827	CLA	MG-NB	-2.39	2.01	2.05
14	2	813	CLA	MG-NB	-2.39	2.01	2.05
14	F	204	CLA	CMD-C2D	-2.39	1.45	1.50
14	A	828	CLA	MG-NB	-2.39	2.01	2.05
14	b	816	CLA	C4B-NB	2.39	1.41	1.37
14	b	843	CLA	C4B-NB	2.39	1.41	1.37
14	B	826	CLA	CMB-C2B	-2.39	1.45	1.50
14	b	839	CLA	CMB-C2B	-2.39	1.45	1.50
14	b	828	CLA	C1B-C2B	2.39	1.48	1.43
14	b	809	CLA	CMB-C2B	-2.39	1.45	1.50
14	A	822	CLA	C1B-C2B	2.39	1.48	1.43
14	2	828	CLA	C1B-C2B	2.39	1.48	1.43
14	B	843	CLA	CMB-C2B	-2.39	1.45	1.50
14	0	206	CLA	CMB-C2B	-2.39	1.45	1.50
14	1	829	CLA	CMD-C2D	-2.39	1.45	1.50
14	A	813	CLA	CMC-C2C	-2.39	1.45	1.50
14	B	811	CLA	CMB-C2B	-2.39	1.45	1.50
14	1	808	CLA	CMB-C2B	-2.39	1.45	1.50
14	1	815	CLA	CMD-C2D	-2.39	1.45	1.50
14	1	834	CLA	CMB-C2B	-2.39	1.45	1.50
14	2	814	CLA	CMB-C2B	-2.39	1.45	1.50
14	2	832	CLA	CMD-C2D	-2.39	1.45	1.50
14	A	835	CLA	CMD-C2D	-2.39	1.45	1.50
14	B	838	CLA	CMB-C2B	-2.39	1.45	1.50
14	L	1503	CLA	CMD-C2D	-2.39	1.45	1.50
14	2	809	CLA	CMB-C2B	-2.39	1.45	1.50
14	0	202	CLA	CMB-C2B	-2.39	1.45	1.50
14	B	816	CLA	CMB-C2B	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	805	CLA	CMC-C2C	-2.38	1.45	1.50
14	F	201	CLA	MG-NB	-2.38	2.01	2.05
14	b	812	CLA	C1B-NB	-2.38	1.34	1.37
14	B	829	CLA	C1B-C2B	2.38	1.48	1.43
14	a	831	CLA	CMC-C2C	-2.38	1.45	1.50
14	a	838	CLA	CMB-C2B	-2.38	1.45	1.50
14	b	811	CLA	C1B-C2B	2.38	1.48	1.43
14	a	805	CLA	CMD-C2D	-2.38	1.45	1.50
14	a	836	CLA	CMB-C2B	-2.38	1.45	1.50
14	B	805	CLA	CMB-C2B	-2.38	1.45	1.50
14	b	842	CLA	C4B-NB	2.38	1.41	1.37
14	b	802	CLA	CMD-C2D	-2.38	1.45	1.50
14	1	820	CLA	C4B-NB	2.38	1.41	1.37
14	A	816	CLA	CMD-C2D	-2.38	1.45	1.50
14	A	842	CLA	CMB-C2B	-2.38	1.45	1.50
14	B	829	CLA	CMD-C2D	-2.38	1.45	1.50
14	B	808	CLA	MG-NB	-2.38	2.01	2.05
14	B	833	CLA	CMD-C2D	-2.38	1.45	1.50
14	j	101	CLA	MG-NB	-2.38	2.01	2.05
14	0	208	CLA	MG-NB	-2.38	2.01	2.05
14	B	840	CLA	CMB-C2B	-2.38	1.45	1.50
14	a	825	CLA	CMD-C2D	-2.38	1.45	1.50
14	A	837	CLA	C3B-C4B	2.38	1.49	1.42
14	b	820	CLA	C1B-C2B	2.38	1.48	1.43
14	K	4004	CLA	MG-NB	-2.38	2.01	2.05
14	B	827	CLA	C1B-NB	-2.38	1.34	1.37
14	l	4206	CLA	MG-NB	-2.38	2.01	2.05
14	A	813	CLA	C4B-NB	2.38	1.41	1.37
14	a	827	CLA	CMD-C2D	-2.38	1.45	1.50
14	A	839	CLA	C4B-NB	2.38	1.41	1.37
14	2	812	CLA	MG-NB	-2.37	2.01	2.05
14	l	4203	CLA	MG-NB	-2.37	2.01	2.05
14	A	814	CLA	C1B-C2B	2.37	1.48	1.43
14	B	813	CLA	CMB-C2B	-2.37	1.45	1.50
14	1	829	CLA	CMC-C2C	-2.37	1.45	1.50
14	2	808	CLA	CMD-C2D	-2.37	1.45	1.50
14	a	829	CLA	MG-NB	-2.37	2.01	2.05
14	a	830	CLA	C1B-C2B	2.37	1.48	1.43
14	B	832	CLA	MG-ND	-2.37	2.01	2.05
14	B	821	CLA	C1B-C2B	2.37	1.48	1.43
14	b	816	CLA	C1B-C2B	2.37	1.48	1.43
14	a	827	CLA	CMB-C2B	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	807	CLA	C4B-NB	2.37	1.41	1.37
14	2	820	CLA	C1B-C2B	2.37	1.48	1.43
14	J	101	CLA	MG-NB	-2.37	2.01	2.05
14	A	829	CLA	C1B-C2B	2.37	1.48	1.43
14	A	837	CLA	CMB-C2B	-2.37	1.45	1.50
14	a	808	CLA	C4B-NB	2.37	1.41	1.37
14	a	844	CLA	C4B-NB	2.37	1.41	1.37
14	b	811	CLA	CMB-C2B	-2.37	1.45	1.50
14	A	816	CLA	C4B-NB	2.37	1.41	1.37
14	1	825	CLA	CMB-C2B	-2.37	1.45	1.50
14	1	812	CLA	CMC-C2C	-2.37	1.45	1.50
14	2	825	CLA	CMB-C2B	-2.37	1.45	1.50
14	a	810	CLA	MG-NB	-2.37	2.01	2.05
14	B	809	CLA	CMB-C2B	-2.37	1.45	1.50
14	1	807	CLA	C1B-NB	-2.37	1.34	1.37
14	B	817	CLA	C1B-C2B	2.37	1.48	1.43
14	1	815	CLA	CMC-C2C	-2.37	1.45	1.50
14	b	805	CLA	CMB-C2B	-2.37	1.45	1.50
14	b	830	CLA	CMB-C2B	-2.37	1.45	1.50
14	2	839	CLA	CMB-C2B	-2.37	1.45	1.50
14	l	4205	CLA	CMB-C2B	-2.37	1.45	1.50
14	b	808	CLA	CMC-C2C	-2.37	1.45	1.50
14	l	4206	CLA	CMD-C2D	-2.37	1.45	1.50
14	a	840	CLA	C4B-NB	2.37	1.41	1.37
14	A	822	CLA	CMD-C2D	-2.37	1.45	1.50
14	1	838	CLA	CMD-C2D	-2.37	1.45	1.50
14	a	809	CLA	CMD-C2D	-2.36	1.45	1.50
14	B	832	CLA	C4B-NB	2.36	1.41	1.37
14	B	841	CLA	MG-NB	-2.36	2.01	2.05
14	b	832	CLA	CMD-C2D	-2.36	1.45	1.50
14	a	842	CLA	CMB-C2B	-2.36	1.45	1.50
14	2	842	CLA	C4B-NB	2.36	1.41	1.37
14	A	808	CLA	C4B-NB	2.36	1.41	1.37
14	B	815	CLA	MG-NB	-2.36	2.01	2.05
14	b	807	CLA	CMD-C2D	-2.36	1.45	1.50
14	b	821	CLA	CMC-C2C	-2.36	1.45	1.50
14	b	821	CLA	CMD-C2D	-2.36	1.45	1.50
14	2	808	CLA	CMB-C2B	-2.36	1.45	1.50
14	A	824	CLA	CMD-C2D	-2.36	1.45	1.50
14	b	827	CLA	CMC-C2C	-2.36	1.45	1.50
14	2	830	CLA	CMB-C2B	-2.36	1.45	1.50
14	A	835	CLA	CMB-C2B	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	802	CLA	CMB-C2B	-2.36	1.45	1.50
14	A	806	CLA	CMC-C2C	-2.36	1.45	1.50
14	B	828	CLA	CMC-C2C	-2.36	1.45	1.50
14	1	818	CLA	C4B-NB	2.36	1.41	1.37
14	A	816	CLA	C1B-C2B	2.36	1.48	1.43
14	B	811	CLA	C1B-C2B	2.36	1.48	1.43
14	B	822	CLA	CMD-C2D	-2.36	1.45	1.50
14	b	815	CLA	CMD-C2D	-2.36	1.45	1.50
14	2	812	CLA	CMD-C2D	-2.36	1.45	1.50
14	7	1101	CLA	CMC-C2C	-2.36	1.45	1.50
14	A	826	CLA	CMB-C2B	-2.36	1.45	1.50
14	l	4204	CLA	CMD-C2D	-2.36	1.45	1.50
14	B	810	CLA	CMB-C2B	-2.36	1.45	1.50
12	A	801	LHG	O7-C5	-2.36	1.41	1.46
14	A	827	CLA	C1B-NB	-2.36	1.34	1.37
14	a	815	CLA	C1B-C2B	2.36	1.48	1.43
14	a	812	CLA	CMB-C2B	-2.36	1.45	1.50
14	0	208	CLA	C1B-C2B	2.36	1.48	1.43
14	A	808	CLA	CMC-C2C	-2.36	1.45	1.50
14	B	815	CLA	CMB-C2B	-2.36	1.45	1.50
14	2	815	CLA	CMB-C2B	-2.36	1.45	1.50
14	b	804	CLA	MG-ND	-2.36	2.01	2.05
14	2	814	CLA	MG-NB	-2.36	2.01	2.05
14	2	831	CLA	MG-ND	-2.36	2.01	2.05
14	8	4004	CLA	MG-NB	-2.36	2.01	2.05
14	B	833	CLA	C1D-ND	2.36	1.41	1.37
14	a	843	CLA	C4B-NB	2.36	1.41	1.37
14	1	825	CLA	CMD-C2D	-2.36	1.45	1.50
14	a	814	CLA	CMC-C2C	-2.35	1.45	1.50
14	f	204	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	832	CLA	C1D-ND	2.35	1.41	1.37
14	1	836	CLA	C3B-C4B	2.35	1.49	1.42
14	1	828	CLA	C1B-C2B	2.35	1.48	1.43
14	B	830	CLA	CMB-C2B	-2.35	1.45	1.50
14	a	817	CLA	CMD-C2D	-2.35	1.45	1.50
14	2	827	CLA	CMC-C2C	-2.35	1.45	1.50
14	b	815	CLA	CMB-C2B	-2.35	1.45	1.50
14	2	841	CLA	CMD-C2D	-2.35	1.45	1.50
14	A	840	CLA	C4B-NB	2.35	1.41	1.37
14	1	805	CLA	C4B-NB	2.35	1.41	1.37
14	2	812	CLA	CMB-C2B	-2.35	1.45	1.50
14	b	840	CLA	MG-NB	-2.35	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	815	CLA	C4B-NB	2.35	1.41	1.37
14	B	842	CLA	CMD-C2D	-2.35	1.46	1.50
14	a	810	CLA	CMD-C2D	-2.35	1.46	1.50
14	a	844	CLA	CMB-C2B	-2.35	1.46	1.50
14	2	804	CLA	CMB-C2B	-2.35	1.46	1.50
14	2	806	CLA	CMD-C2D	-2.35	1.46	1.50
14	1	839	CLA	C4B-NB	2.35	1.40	1.37
14	2	840	CLA	MG-NB	-2.35	2.01	2.05
14	L	1501	CLA	CMD-C2D	-2.35	1.46	1.50
14	1	841	CLA	MG-NB	-2.35	2.01	2.05
14	A	806	CLA	C1B-C2B	2.35	1.48	1.43
14	A	830	CLA	CMC-C2C	-2.35	1.46	1.50
14	B	831	CLA	CMB-C2B	-2.35	1.46	1.50
14	2	818	CLA	C1B-C2B	2.35	1.48	1.43
14	1	807	CLA	C4B-NB	2.35	1.40	1.37
14	1	806	CLA	C4B-NB	2.35	1.40	1.37
14	2	811	CLA	C1B-NB	-2.35	1.34	1.37
14	B	812	CLA	C1B-NB	-2.35	1.34	1.37
14	A	840	CLA	CMB-C2B	-2.35	1.46	1.50
14	B	807	CLA	CMD-C2D	-2.35	1.46	1.50
14	b	810	CLA	CMB-C2B	-2.35	1.46	1.50
14	L	1503	CLA	C1B-C2B	2.35	1.48	1.43
14	B	813	CLA	MG-NB	-2.35	2.01	2.05
14	A	809	CLA	MG-NB	-2.35	2.01	2.05
14	B	827	CLA	MG-ND	-2.35	2.01	2.05
14	2	840	CLA	C4B-NB	2.35	1.40	1.37
14	1	807	CLA	CMC-C2C	-2.35	1.46	1.50
14	2	803	CLA	C4B-NB	2.35	1.40	1.37
14	A	828	CLA	C1B-C2B	2.35	1.48	1.43
14	1	833	CLA	CMB-C2B	-2.35	1.46	1.50
14	2	810	CLA	CMB-C2B	-2.35	1.46	1.50
14	A	815	CLA	MG-NB	-2.35	2.01	2.05
14	2	812	CLA	C3B-C4B	2.35	1.49	1.42
14	B	819	CLA	C1B-C2B	2.35	1.48	1.43
14	1	823	CLA	CMD-C2D	-2.34	1.46	1.50
14	2	810	CLA	C1B-C2B	2.34	1.48	1.43
14	B	841	CLA	C4B-NB	2.34	1.40	1.37
14	B	822	CLA	CMC-C2C	-2.34	1.46	1.50
14	a	807	CLA	C1B-C2B	2.34	1.48	1.43
14	1	815	CLA	C1B-C2B	2.34	1.48	1.43
14	A	826	CLA	CMD-C2D	-2.34	1.46	1.50
14	1	807	CLA	CMD-C2D	-2.34	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	841	CLA	CMC-C2C	-2.34	1.46	1.50
14	a	840	CLA	CMD-C2D	-2.34	1.46	1.50
14	A	806	CLA	C4B-NB	2.34	1.40	1.37
14	B	813	CLA	C3B-C4B	2.34	1.49	1.42
14	a	838	CLA	C3B-C4B	2.34	1.49	1.42
14	B	827	CLA	CMC-C2C	-2.34	1.46	1.50
14	b	801	CLA	CMB-C2B	-2.34	1.46	1.50
14	b	816	CLA	CMD-C2D	-2.34	1.46	1.50
14	7	1102	CLA	MG-NB	-2.34	2.01	2.05
14	2	821	CLA	CMC-C2C	-2.34	1.46	1.50
14	l	4205	CLA	CMD-C2D	-2.34	1.46	1.50
14	b	838	CLA	MG-NB	-2.34	2.01	2.05
14	b	814	CLA	MG-NB	-2.34	2.01	2.05
14	1	827	CLA	C1B-C2B	2.34	1.48	1.43
14	l	4203	CLA	CMB-C2B	-2.34	1.46	1.50
14	a	833	CLA	C4B-NB	2.34	1.40	1.37
14	2	832	CLA	C1D-ND	2.34	1.40	1.37
14	2	842	CLA	CMC-C2C	-2.34	1.46	1.50
14	f	201	CLA	MG-NB	-2.34	2.01	2.05
14	L	1501	CLA	CMB-C2B	-2.34	1.46	1.50
14	B	845	CLA	CHC-C1C	2.34	1.43	1.38
14	a	854	CLA	MG-NB	-2.34	2.01	2.05
14	k	4002	CLA	C3B-C4B	2.34	1.49	1.42
14	2	842	CLA	MG-NB	-2.34	2.01	2.05
14	a	823	CLA	C1B-C2B	2.34	1.48	1.43
14	A	808	CLA	CMD-C2D	-2.34	1.46	1.50
14	a	809	CLA	C4B-NB	2.34	1.40	1.37
14	8	4002	CLA	C3B-C4B	2.34	1.49	1.42
14	2	839	CLA	C1B-NB	-2.34	1.34	1.37
14	2	837	CLA	CMB-C2B	-2.34	1.46	1.50
14	b	844	CLA	CHC-C1C	2.34	1.43	1.38
14	0	207	CLA	CMD-C2D	-2.33	1.46	1.50
14	b	807	CLA	C1B-C2B	2.33	1.48	1.43
14	A	839	CLA	CMD-C2D	-2.33	1.46	1.50
14	a	833	CLA	MG-ND	-2.33	2.01	2.05
14	b	818	CLA	C1B-C2B	2.33	1.48	1.43
14	2	821	CLA	CMD-C2D	-2.33	1.46	1.50
14	B	816	CLA	CMD-C2D	-2.33	1.46	1.50
14	2	821	CLA	C3B-C4B	2.33	1.49	1.42
14	1	805	CLA	C1B-C2B	2.33	1.48	1.43
14	L	1502	CLA	CMD-C2D	-2.33	1.46	1.50
14	0	202	CLA	CMD-C2D	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	823	CLA	MG-NB	-2.33	2.01	2.05
14	l	4206	CLA	C1B-C2B	2.33	1.48	1.43
14	b	814	CLA	C1B-C2B	2.33	1.48	1.43
14	b	801	CLA	CMD-C2D	-2.33	1.46	1.50
14	1	843	CLA	MG-NB	-2.33	2.01	2.05
14	1	813	CLA	C1B-C2B	2.33	1.48	1.43
14	A	841	CLA	CMB-C2B	-2.33	1.46	1.50
14	b	820	CLA	CMD-C2D	-2.33	1.46	1.50
14	6	4403	CLA	CMD-C2D	-2.33	1.46	1.50
14	a	809	CLA	CMC-C2C	-2.33	1.46	1.50
14	B	828	CLA	C4B-NB	2.33	1.40	1.37
14	B	821	CLA	CMC-C2C	-2.33	1.46	1.50
14	l	4204	CLA	CMB-C2B	-2.33	1.46	1.50
14	B	815	CLA	C1B-C2B	2.33	1.48	1.43
14	a	836	CLA	CMD-C2D	-2.33	1.46	1.50
14	B	840	CLA	C1B-NB	-2.33	1.34	1.37
14	2	827	CLA	C4B-NB	2.33	1.40	1.37
14	A	809	CLA	CMD-C2D	-2.33	1.46	1.50
14	B	817	CLA	CMD-C2D	-2.33	1.46	1.50
14	1	834	CLA	CMD-C2D	-2.33	1.46	1.50
14	2	829	CLA	CMB-C2B	-2.33	1.46	1.50
14	b	821	CLA	C3B-C4B	2.33	1.49	1.42
14	A	837	CLA	MG-NB	-2.33	2.01	2.05
14	1	810	CLA	CMB-C2B	-2.33	1.46	1.50
14	1	844	CLA	CMB-C2B	-2.33	1.46	1.50
14	a	817	CLA	MG-NB	-2.33	2.01	2.05
14	a	840	CLA	CMC-C2C	-2.33	1.46	1.50
14	b	841	CLA	CMD-C2D	-2.33	1.46	1.50
14	B	813	CLA	CMD-C2D	-2.32	1.46	1.50
14	a	829	CLA	C1B-C2B	2.32	1.48	1.43
14	A	819	CLA	C4B-NB	2.32	1.40	1.37
14	b	831	CLA	C4B-NB	2.32	1.40	1.37
14	A	811	CLA	CMB-C2B	-2.32	1.46	1.50
14	2	805	CLA	C1B-NB	-2.32	1.34	1.37
14	A	832	CLA	MG-ND	-2.32	2.01	2.05
14	A	839	CLA	CMC-C2C	-2.32	1.46	1.50
14	B	802	CLA	CMD-C2D	-2.32	1.46	1.50
14	b	840	CLA	CMC-C2C	-2.32	1.46	1.50
14	2	820	CLA	CMD-C2D	-2.32	1.46	1.50
14	2	810	CLA	C4B-NB	2.32	1.40	1.37
14	b	807	CLA	CMC-C2C	-2.32	1.46	1.50
14	2	840	CLA	CMC-C2C	-2.32	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	826	CLA	CMC-C2C	-2.32	1.46	1.50
14	2	826	CLA	CMC-C2C	-2.32	1.46	1.50
14	B	809	CLA	C4B-NB	2.32	1.40	1.37
14	a	806	CLA	CMC-C2C	-2.32	1.46	1.50
14	b	820	CLA	CMC-C2C	-2.32	1.46	1.50
14	2	820	CLA	CMC-C2C	-2.32	1.46	1.50
14	f	201	CLA	CMB-C2B	-2.32	1.46	1.50
14	B	821	CLA	CMD-C2D	-2.32	1.46	1.50
14	1	840	CLA	CMC-C2C	-2.32	1.46	1.50
14	a	838	CLA	MG-NB	-2.32	2.01	2.05
14	B	807	CLA	CMC-C2C	-2.32	1.46	1.50
14	1	820	CLA	CMC-C2C	-2.32	1.46	1.50
14	l	4203	CLA	CMD-C2D	-2.32	1.46	1.50
14	B	804	CLA	MG-ND	-2.32	2.01	2.05
14	b	829	CLA	CMB-C2B	-2.32	1.46	1.50
14	1	808	CLA	CMD-C2D	-2.32	1.46	1.50
14	B	804	CLA	C4B-NB	2.32	1.40	1.37
14	b	802	CLA	CMC-C2C	-2.31	1.46	1.50
19	i	4101	LMT	O2B-C2B	-2.31	1.37	1.43
14	a	817	CLA	C1B-C2B	2.31	1.48	1.43
14	B	822	CLA	C3B-C4B	2.31	1.49	1.42
14	a	835	CLA	CMB-C2B	-2.31	1.46	1.50
14	b	804	CLA	C4B-NB	2.31	1.40	1.37
14	2	831	CLA	C4B-NB	2.31	1.40	1.37
14	1	827	CLA	CMC-C2C	-2.31	1.46	1.50
14	2	806	CLA	C1B-C2B	2.31	1.48	1.43
14	B	839	CLA	MG-NB	-2.31	2.01	2.05
14	2	808	CLA	C1B-NB	-2.31	1.34	1.37
14	2	838	CLA	MG-NB	-2.31	2.01	2.05
14	2	807	CLA	C4B-NB	2.31	1.40	1.37
14	a	829	CLA	CMC-C2C	-2.31	1.46	1.50
14	2	826	CLA	MG-ND	-2.31	2.01	2.05
14	b	806	CLA	C1B-NB	-2.31	1.34	1.37
14	K	4002	CLA	C3B-C4B	2.31	1.49	1.42
14	2	816	CLA	MG-NB	-2.31	2.01	2.05
14	1	809	CLA	CMB-C2B	-2.31	1.46	1.50
14	1	812	CLA	CMD-C2D	-2.31	1.46	1.50
14	1	839	CLA	CMB-C2B	-2.31	1.46	1.50
14	A	816	CLA	MG-NB	-2.31	2.01	2.05
14	1	819	CLA	MG-ND	-2.31	2.01	2.05
14	2	814	CLA	CMD-C2D	-2.31	1.46	1.50
14	b	814	CLA	CMD-C2D	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	825	CLA	C4B-NB	2.31	1.40	1.37
14	A	834	CLA	CMB-C2B	-2.31	1.46	1.50
14	b	817	CLA	C4B-NB	2.31	1.40	1.37
14	B	806	CLA	C1B-NB	-2.31	1.34	1.37
14	1	826	CLA	C1B-NB	-2.31	1.34	1.37
19	I	103	LMT	O3B-C3B	-2.31	1.37	1.43
14	2	815	CLA	CMD-C2D	-2.31	1.46	1.50
14	B	824	CLA	MG-NB	-2.31	2.01	2.05
14	1	836	CLA	MG-NB	-2.31	2.01	2.05
14	A	828	CLA	CMC-C2C	-2.31	1.46	1.50
14	b	842	CLA	CMC-C2C	-2.31	1.46	1.50
14	B	825	CLA	MG-NB	-2.31	2.01	2.05
14	0	206	CLA	CMD-C2D	-2.31	1.46	1.50
14	2	823	CLA	MG-NB	-2.31	2.01	2.05
14	l	4203	CLA	C3B-C4B	2.31	1.49	1.42
14	B	843	CLA	MG-NB	-2.31	2.01	2.05
14	a	821	CLA	MG-ND	-2.31	2.01	2.05
19	h	103	LMT	O3B-C3B	-2.31	1.37	1.43
14	1	822	CLA	C1B-C2B	2.31	1.48	1.43
14	b	824	CLA	MG-NB	-2.31	2.01	2.05
14	2	824	CLA	MG-NB	-2.30	2.01	2.05
14	A	806	CLA	CMB-C2B	-2.30	1.46	1.50
14	A	844	CLA	CMB-C2B	-2.30	1.46	1.50
14	B	808	CLA	C4B-NB	2.30	1.40	1.37
19	I	103	LMT	O2B-C2B	-2.30	1.37	1.43
14	a	820	CLA	C4B-NB	2.30	1.40	1.37
14	b	819	CLA	CMD-C2D	-2.30	1.46	1.50
14	a	831	CLA	C4B-NB	2.30	1.40	1.37
14	b	808	CLA	C4B-NB	2.30	1.40	1.37
14	2	814	CLA	C1B-C2B	2.30	1.48	1.43
14	B	817	CLA	MG-NB	-2.30	2.01	2.05
14	b	842	CLA	MG-NB	-2.30	2.01	2.05
14	a	823	CLA	CMC-C2C	-2.30	1.46	1.50
14	1	841	CLA	CMB-C2B	-2.30	1.46	1.50
14	A	805	CLA	CMC-C2C	-2.30	1.46	1.50
14	B	843	CLA	CMC-C2C	-2.30	1.46	1.50
14	B	807	CLA	C1B-C2B	2.30	1.48	1.43
14	a	841	CLA	C4B-NB	2.30	1.40	1.37
14	1	840	CLA	CMB-C2B	-2.30	1.46	1.50
14	A	843	CLA	MG-NB	-2.30	2.01	2.05
19	i	4101	LMT	O2'-C2'	-2.30	1.37	1.43
14	2	807	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	816	CLA	C4B-NB	2.30	1.40	1.37
14	b	840	CLA	C4B-NB	2.30	1.40	1.37
14	f	201	CLA	C1B-C2B	2.30	1.48	1.43
14	2	822	CLA	CMD-C2D	-2.30	1.46	1.50
14	1	814	CLA	MG-NB	-2.30	2.01	2.05
14	A	814	CLA	MG-NB	-2.30	2.01	2.05
14	1	831	CLA	MG-ND	-2.30	2.01	2.05
14	2	844	CLA	CHC-C1C	2.30	1.43	1.38
14	A	806	CLA	CMD-C2D	-2.30	1.46	1.50
14	A	841	CLA	CMC-C2C	-2.30	1.46	1.50
14	1	815	CLA	MG-NB	-2.30	2.01	2.05
14	A	832	CLA	C4B-NB	2.30	1.40	1.37
14	A	813	CLA	CMD-C2D	-2.30	1.46	1.50
14	1	838	CLA	CMC-C2C	-2.30	1.46	1.50
19	h	103	LMT	O2'-C2'	-2.30	1.37	1.43
14	b	816	CLA	MG-NB	-2.30	2.01	2.05
14	A	807	CLA	C4B-NB	2.29	1.40	1.37
14	b	809	CLA	C4B-NB	2.29	1.40	1.37
14	B	842	CLA	CMB-C2B	-2.29	1.46	1.50
14	1	810	CLA	MG-ND	-2.29	2.01	2.05
14	b	822	CLA	CMD-C2D	-2.29	1.46	1.50
14	a	815	CLA	C3B-C4B	2.29	1.49	1.42
14	B	815	CLA	CMD-C2D	-2.29	1.46	1.50
14	b	827	CLA	C1B-C2B	2.29	1.48	1.43
14	2	829	CLA	C1B-C2B	2.29	1.48	1.43
14	a	822	CLA	CMC-C2C	-2.29	1.46	1.50
14	2	806	CLA	CMC-C2C	-2.29	1.46	1.50
14	A	808	CLA	CMB-C2B	-2.29	1.46	1.50
14	A	824	CLA	C4B-NB	2.29	1.40	1.37
14	b	826	CLA	C1B-NB	-2.29	1.34	1.37
14	B	820	CLA	CMD-C2D	-2.29	1.46	1.50
14	f	205	CLA	MG-NB	-2.29	2.01	2.05
14	b	841	CLA	CMB-C2B	-2.29	1.46	1.50
14	2	839	CLA	CMC-C2C	-2.29	1.46	1.50
14	2	817	CLA	C4B-NB	2.29	1.40	1.37
14	A	820	CLA	MG-ND	-2.29	2.01	2.05
14	2	841	CLA	CMB-C2B	-2.29	1.46	1.50
14	1	814	CLA	C4B-NB	2.29	1.40	1.37
19	I	103	LMT	O2'-C2'	-2.29	1.37	1.43
14	a	843	CLA	MG-NB	-2.29	2.01	2.05
14	1	831	CLA	C4B-NB	2.29	1.40	1.37
14	2	826	CLA	C1B-NB	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	816	CLA	MG-NB	-2.29	2.01	2.05
14	a	816	CLA	C3B-C4B	2.29	1.49	1.42
14	b	808	CLA	C1B-C2B	2.29	1.48	1.43
19	h	103	LMT	O2B-C2B	-2.29	1.37	1.43
14	A	815	CLA	C4B-NB	2.29	1.40	1.37
14	B	835	CLA	CHC-C1C	2.29	1.43	1.38
14	A	831	CLA	CMC-C2C	-2.29	1.46	1.50
14	B	837	CLA	MG-NB	-2.29	2.01	2.05
14	6	4404	CLA	MG-NB	-2.29	2.01	2.05
14	a	807	CLA	CMD-C2D	-2.29	1.46	1.50
14	a	814	CLA	CMD-C2D	-2.29	1.46	1.50
14	A	820	CLA	C4B-NB	2.29	1.40	1.37
14	a	822	CLA	C4B-NB	2.29	1.40	1.37
14	B	840	CLA	MG-ND	-2.29	2.01	2.05
14	2	836	CLA	C1B-C2B	2.28	1.48	1.43
14	a	807	CLA	CMB-C2B	-2.28	1.46	1.50
14	b	805	CLA	C1D-ND	2.28	1.40	1.37
14	a	828	CLA	C1B-NB	-2.28	1.34	1.37
14	B	830	CLA	C1B-C2B	2.28	1.48	1.43
14	b	839	CLA	CMC-C2C	-2.28	1.46	1.50
14	a	841	CLA	CMB-C2B	-2.28	1.46	1.50
14	2	816	CLA	CMD-C2D	-2.28	1.46	1.50
14	A	826	CLA	C1B-C2B	2.28	1.48	1.43
14	2	828	CLA	MG-NB	-2.28	2.01	2.05
14	b	836	CLA	C1B-C2B	2.28	1.48	1.43
14	b	827	CLA	C4B-NB	2.28	1.40	1.37
14	B	834	CLA	C1B-C2B	2.28	1.48	1.43
14	1	841	CLA	C1B-C2B	2.28	1.48	1.43
14	a	805	CLA	MG-ND	-2.28	2.01	2.05
14	2	818	CLA	CMC-C2C	-2.28	1.46	1.50
14	B	837	CLA	C1B-C2B	2.28	1.48	1.43
14	A	821	CLA	C4B-NB	2.28	1.40	1.37
14	1	819	CLA	C4B-NB	2.28	1.40	1.37
14	2	815	CLA	C1B-C2B	2.28	1.48	1.43
14	K	4004	CLA	CMD-C2D	-2.28	1.46	1.50
14	1	838	CLA	C1B-NB	-2.28	1.34	1.37
19	i	4101	LMT	O3B-C3B	-2.28	1.37	1.43
14	A	821	CLA	CMC-C2C	-2.28	1.46	1.50
14	1	821	CLA	CMC-C2C	-2.28	1.46	1.50
14	b	839	CLA	MG-ND	-2.28	2.01	2.05
14	2	834	CLA	CHC-C1C	2.28	1.43	1.38
14	B	808	CLA	C1B-C2B	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	833	CLA	MG-ND	-2.28	2.01	2.05
14	a	821	CLA	C4B-NB	2.28	1.40	1.37
14	2	839	CLA	MG-ND	-2.28	2.01	2.05
14	B	823	CLA	CMD-C2D	-2.28	1.46	1.50
14	1	813	CLA	C3B-C4B	2.28	1.49	1.42
14	b	834	CLA	CHC-C1C	2.28	1.43	1.38
14	2	833	CLA	C1B-C2B	2.28	1.48	1.43
14	B	816	CLA	C1B-C2B	2.28	1.48	1.43
14	b	834	CLA	CMB-C2B	-2.28	1.46	1.50
14	a	824	CLA	C1B-C2B	2.28	1.48	1.43
14	b	815	CLA	C1B-C2B	2.27	1.48	1.43
14	F	201	CLA	CMB-C2B	-2.27	1.46	1.50
14	F	201	CLA	C1B-C2B	2.27	1.48	1.43
14	A	830	CLA	C4B-NB	2.27	1.40	1.37
14	2	819	CLA	CMD-C2D	-2.27	1.46	1.50
14	8	4004	CLA	CMD-C2D	-2.27	1.46	1.50
14	A	811	CLA	MG-ND	-2.27	2.01	2.05
14	B	818	CLA	CMD-C2D	-2.27	1.46	1.50
14	B	840	CLA	CMC-C2C	-2.27	1.46	1.50
14	a	818	CLA	CMC-C2C	-2.27	1.46	1.50
14	b	802	CLA	CMB-C2B	-2.27	1.46	1.50
14	A	810	CLA	CMB-C2B	-2.27	1.46	1.50
14	B	829	CLA	CMB-C2B	-2.27	1.46	1.50
14	b	824	CLA	CMB-C2B	-2.27	1.46	1.50
14	b	830	CLA	CMC-C2C	-2.27	1.46	1.50
14	a	811	CLA	C4B-NB	2.27	1.40	1.37
14	b	818	CLA	CMC-C2C	-2.27	1.46	1.50
14	1	823	CLA	C4B-NB	2.27	1.40	1.37
14	B	835	CLA	CMB-C2B	-2.27	1.46	1.50
14	1	804	CLA	MG-ND	-2.27	2.01	2.05
14	k	4003	CLA	MG-NB	-2.27	2.01	2.05
14	b	811	CLA	C4B-NB	2.27	1.40	1.37
14	2	808	CLA	C4B-NB	2.27	1.40	1.37
14	1	829	CLA	C4B-NB	2.27	1.40	1.37
14	a	818	CLA	MG-NB	-2.27	2.01	2.05
14	2	801	CLA	MG-ND	-2.27	2.01	2.05
14	B	835	CLA	CMD-C2D	-2.27	1.46	1.50
14	A	839	CLA	C1B-NB	-2.27	1.34	1.37
14	B	809	CLA	C1B-NB	-2.27	1.34	1.37
14	A	822	CLA	CMC-C2C	-2.27	1.46	1.50
14	a	811	CLA	CMB-C2B	-2.27	1.46	1.50
14	2	806	CLA	CMB-C2B	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	819	CLA	CMC-C2C	-2.27	1.46	1.50
14	b	834	CLA	CMD-C2D	-2.27	1.46	1.50
14	6	4404	CLA	CMD-C2D	-2.27	1.46	1.50
14	B	818	CLA	C4B-NB	2.27	1.40	1.37
14	a	854	CLA	CMD-C2D	-2.27	1.46	1.50
14	1	807	CLA	CMB-C2B	-2.27	1.46	1.50
14	2	834	CLA	CMB-C2B	-2.27	1.46	1.50
14	2	836	CLA	CMB-C2B	-2.27	1.46	1.50
14	A	815	CLA	C3B-C4B	2.26	1.49	1.42
14	2	801	CLA	C1D-ND	2.26	1.40	1.37
14	b	817	CLA	CMD-C2D	-2.26	1.46	1.50
17	i	4103	BCR	C33-C5	-2.26	1.47	1.50
14	b	826	CLA	MG-ND	-2.26	2.01	2.05
14	a	826	CLA	CMC-C2C	-2.26	1.46	1.50
14	A	822	CLA	MG-NB	-2.26	2.01	2.05
14	B	802	CLA	MG-NB	-2.26	2.01	2.05
14	b	841	CLA	MG-ND	-2.26	2.01	2.05
14	2	836	CLA	MG-NB	-2.26	2.01	2.05
14	B	837	CLA	CMB-C2B	-2.26	1.46	1.50
14	1	805	CLA	CMB-C2B	-2.26	1.46	1.50
14	1	819	CLA	CMC-C2C	-2.26	1.46	1.50
14	6	4404	CLA	C3B-C4B	2.26	1.49	1.42
14	a	815	CLA	MG-NB	-2.26	2.01	2.05
17	I	102	BCR	C33-C5	-2.26	1.47	1.50
14	B	842	CLA	MG-ND	-2.26	2.01	2.05
14	a	827	CLA	C1B-C2B	2.26	1.48	1.43
14	2	827	CLA	C1B-C2B	2.26	1.48	1.43
14	0	202	CLA	MG-NB	-2.26	2.01	2.05
17	h	102	BCR	C33-C5	-2.26	1.47	1.50
14	F	204	CLA	CMB-C2B	-2.26	1.46	1.50
14	F	205	CLA	MG-NB	-2.26	2.01	2.05
14	2	816	CLA	CMC-C2C	-2.26	1.46	1.50
14	2	840	CLA	C1B-C2B	2.26	1.48	1.43
14	a	840	CLA	C1B-NB	-2.26	1.34	1.37
14	B	834	CLA	MG-NB	-2.26	2.01	2.05
14	a	832	CLA	CMC-C2C	-2.26	1.46	1.50
14	b	836	CLA	CMB-C2B	-2.26	1.46	1.50
14	B	828	CLA	C1B-C2B	2.26	1.48	1.43
14	b	836	CLA	MG-NB	-2.26	2.01	2.05
14	B	834	CLA	CMB-C2B	-2.26	1.46	1.50
14	b	816	CLA	CMC-C2C	-2.26	1.46	1.50
14	b	841	CLA	CMC-C2C	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	824	CLA	CMC-C2C	-2.26	1.46	1.50
14	b	834	CLA	CMC-C2C	-2.26	1.46	1.50
14	A	823	CLA	C1B-C2B	2.26	1.48	1.43
14	2	832	CLA	CMC-C2C	-2.26	1.46	1.50
14	6	4403	CLA	CMB-C2B	-2.26	1.46	1.50
14	a	811	CLA	C1B-C2B	2.26	1.48	1.43
14	1	811	CLA	C1B-C2B	2.26	1.48	1.43
14	B	842	CLA	CMC-C2C	-2.26	1.46	1.50
14	a	834	CLA	MG-ND	-2.26	2.01	2.05
14	1	805	CLA	CMD-C2D	-2.26	1.46	1.50
14	2	817	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	804	CLA	C4B-NB	2.26	1.40	1.37
14	b	839	CLA	C1B-NB	-2.26	1.34	1.37
14	1	814	CLA	C3B-C4B	2.26	1.49	1.42
14	1	829	CLA	CMB-C2B	-2.26	1.46	1.50
14	2	838	CLA	CMB-C2B	-2.25	1.46	1.50
14	b	801	CLA	MG-NB	-2.25	2.01	2.05
14	a	838	CLA	C1B-C2B	2.25	1.48	1.43
14	2	835	CLA	C1B-C2B	2.25	1.48	1.43
14	F	205	CLA	C3B-C4B	2.25	1.49	1.42
14	B	815	CLA	CMC-C2C	-2.25	1.46	1.50
14	B	835	CLA	CMC-C2C	-2.25	1.46	1.50
14	B	819	CLA	CMD-C2D	-2.25	1.46	1.50
14	a	809	CLA	CMB-C2B	-2.25	1.46	1.50
14	1	812	CLA	C1B-NB	-2.25	1.34	1.37
14	A	810	CLA	C1B-C2B	2.25	1.48	1.43
14	b	833	CLA	C1B-C2B	2.25	1.48	1.43
14	B	805	CLA	C1D-ND	2.25	1.40	1.37
14	A	811	CLA	C1B-NB	-2.25	1.34	1.37
14	f	205	CLA	CMD-C2D	-2.25	1.46	1.50
14	a	813	CLA	C1B-C2B	2.25	1.48	1.43
14	1	810	CLA	C1B-NB	-2.25	1.34	1.37
14	2	820	CLA	C1B-NB	-2.25	1.34	1.37
14	a	819	CLA	CMB-C2B	-2.25	1.46	1.50
14	2	818	CLA	CMD-C2D	-2.25	1.46	1.50
14	F	201	CLA	CMC-C2C	-2.25	1.46	1.50
14	F	205	CLA	CMD-C2D	-2.25	1.46	1.50
14	b	829	CLA	C1B-C2B	2.25	1.48	1.43
14	B	831	CLA	C1B-NB	-2.25	1.34	1.37
14	a	832	CLA	MG-ND	-2.25	2.01	2.05
14	A	814	CLA	CMB-C2B	-2.25	1.46	1.50
14	A	816	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	828	CLA	MG-NB	-2.25	2.01	2.05
14	b	833	CLA	MG-NB	-2.25	2.01	2.05
14	A	828	CLA	CMB-C2B	-2.25	1.46	1.50
14	1	813	CLA	CMC-C2C	-2.25	1.46	1.50
14	b	813	CLA	C1B-C2B	2.25	1.48	1.43
14	B	814	CLA	C1B-C2B	2.25	1.48	1.43
14	8	4002	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	832	CLA	MG-ND	-2.25	2.01	2.05
14	2	813	CLA	C1B-C2B	2.25	1.48	1.43
14	B	831	CLA	CMC-C2C	-2.25	1.46	1.50
14	L	1502	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	832	CLA	CMC-C2C	-2.25	1.46	1.50
14	b	833	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	842	CLA	C4B-NB	2.25	1.40	1.37
14	2	833	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	810	CLA	CMC-C2C	-2.25	1.46	1.50
14	2	817	CLA	C1B-C2B	2.25	1.48	1.43
14	a	839	CLA	CMC-C2C	-2.25	1.46	1.50
14	B	811	CLA	C4B-NB	2.25	1.40	1.37
14	A	821	CLA	C1B-NB	-2.25	1.34	1.37
14	a	812	CLA	MG-ND	-2.25	2.01	2.05
14	1	830	CLA	MG-ND	-2.25	2.01	2.05
14	A	812	CLA	C1B-C2B	2.25	1.48	1.43
14	a	817	CLA	CMB-C2B	-2.25	1.46	1.50
14	2	834	CLA	CMC-C2C	-2.25	1.46	1.50
14	f	201	CLA	CMC-C2C	-2.25	1.46	1.50
14	A	814	CLA	C3B-C4B	2.25	1.49	1.42
14	b	807	CLA	CMB-C2B	-2.25	1.46	1.50
14	1	827	CLA	CMB-C2B	-2.24	1.46	1.50
14	A	831	CLA	MG-ND	-2.24	2.01	2.05
14	a	821	CLA	C1B-C2B	2.24	1.48	1.43
14	a	831	CLA	C1B-C2B	2.24	1.48	1.43
14	1	816	CLA	CMC-C2C	-2.24	1.46	1.50
14	2	828	CLA	CMB-C2B	-2.24	1.46	1.50
14	a	804	CLA	MG-ND	-2.24	2.01	2.05
14	a	810	CLA	C1B-C2B	2.24	1.48	1.43
14	1	821	CLA	MG-NB	-2.24	2.01	2.05
14	1	844	CLA	MG-NB	-2.24	2.01	2.05
14	1	809	CLA	C1B-C2B	2.24	1.48	1.43
14	1	835	CLA	C1B-C2B	2.24	1.48	1.43
14	A	820	CLA	CMC-C2C	-2.24	1.46	1.50
14	1	830	CLA	CMC-C2C	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	834	CLA	CMD-C2D	-2.24	1.46	1.50
14	8	4002	CLA	CMD-C2D	-2.24	1.46	1.50
14	2	843	CLA	CMC-C2C	-2.24	1.46	1.50
14	2	805	CLA	CMB-C2B	-2.24	1.46	1.50
14	2	841	CLA	CMC-C2C	-2.24	1.46	1.50
14	B	841	CLA	C1B-C2B	2.24	1.48	1.43
14	1	836	CLA	CMD-C2D	-2.24	1.46	1.50
14	k	4002	CLA	CMD-C2D	-2.24	1.46	1.50
14	B	806	CLA	C1D-ND	2.24	1.40	1.37
14	A	844	CLA	MG-NB	-2.24	2.01	2.05
14	K	4003	CLA	MG-NB	-2.24	2.01	2.05
14	b	810	CLA	CMC-C2C	-2.24	1.46	1.50
14	a	841	CLA	C3B-C4B	2.24	1.49	1.42
14	2	842	CLA	C1B-C2B	2.24	1.48	1.43
14	A	815	CLA	C1B-C2B	2.24	1.48	1.43
14	a	829	CLA	C4B-NB	2.24	1.40	1.37
14	B	806	CLA	MG-ND	-2.24	2.01	2.05
14	B	820	CLA	MG-ND	-2.24	2.01	2.05
14	2	843	CLA	MG-NB	-2.24	2.01	2.05
14	A	837	CLA	C1B-C2B	2.24	1.48	1.43
14	b	818	CLA	CMD-C2D	-2.24	1.46	1.50
14	a	814	CLA	C1B-NB	-2.24	1.34	1.37
14	b	814	CLA	CMC-C2C	-2.24	1.46	1.50
14	b	832	CLA	CMC-C2C	-2.24	1.46	1.50
14	b	806	CLA	C1D-ND	2.24	1.40	1.37
14	1	836	CLA	C1B-C2B	2.24	1.48	1.43
14	b	829	CLA	CMC-C2C	-2.23	1.46	1.50
14	B	836	CLA	C1B-C2B	2.23	1.48	1.43
14	B	807	CLA	CMB-C2B	-2.23	1.46	1.50
14	2	830	CLA	CMC-C2C	-2.23	1.46	1.50
14	b	832	CLA	C1B-C2B	2.23	1.48	1.43
14	J	101	CLA	C3B-C4B	2.23	1.49	1.42
14	a	823	CLA	MG-NB	-2.23	2.01	2.05
14	1	816	CLA	MG-NB	-2.23	2.01	2.05
14	a	834	CLA	CMC-C2C	-2.23	1.46	1.50
14	B	825	CLA	CMB-C2B	-2.23	1.46	1.50
14	a	831	CLA	CMB-C2B	-2.23	1.46	1.50
14	k	4002	CLA	MG-NB	-2.23	2.01	2.05
14	b	822	CLA	C3B-C4B	2.23	1.49	1.42
14	b	817	CLA	C1B-C2B	2.23	1.48	1.43
14	B	817	CLA	CMC-C2C	-2.23	1.46	1.50
14	a	821	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	817	CLA	CMB-C2B	-2.23	1.46	1.50
14	a	815	CLA	CMB-C2B	-2.23	1.46	1.50
14	l	4205	CLA	CMC-C2C	-2.23	1.46	1.50
13	A	803	CL0	MG-ND	-2.23	2.01	2.05
14	1	819	CLA	C1B-C2B	2.23	1.48	1.43
14	2	841	CLA	MG-ND	-2.23	2.01	2.05
14	1	809	CLA	C4B-NB	2.23	1.40	1.37
14	2	805	CLA	C1D-ND	2.23	1.40	1.37
14	2	824	CLA	CMB-C2B	-2.23	1.46	1.50
14	2	833	CLA	CMD-C2D	-2.23	1.46	1.50
14	B	844	CLA	MG-NB	-2.23	2.01	2.05
14	A	812	CLA	CMD-C2D	-2.23	1.46	1.50
14	2	813	CLA	CMD-C2D	-2.23	1.46	1.50
14	2	814	CLA	CMC-C2C	-2.23	1.46	1.50
14	j	101	CLA	C3B-C4B	2.23	1.49	1.42
14	a	813	CLA	CMD-C2D	-2.23	1.46	1.50
14	2	829	CLA	CMC-C2C	-2.23	1.46	1.50
14	a	844	CLA	MG-NB	-2.23	2.01	2.05
14	A	841	CLA	C4B-NB	2.23	1.40	1.37
14	b	823	CLA	C3B-C4B	2.23	1.49	1.42
17	a	850	BCR	C33-C5	-2.23	1.47	1.50
14	A	817	CLA	CMC-C2C	-2.23	1.46	1.50
14	B	812	CLA	C4B-NB	2.23	1.40	1.37
14	b	809	CLA	C1B-NB	-2.23	1.34	1.37
14	a	813	CLA	C3B-C4B	2.23	1.49	1.42
14	7	1102	CLA	C3B-C4B	2.23	1.49	1.42
14	K	4002	CLA	MG-NB	-2.23	2.01	2.05
14	1	824	CLA	CMB-C2B	-2.23	1.46	1.50
14	b	840	CLA	C1B-C2B	2.23	1.48	1.43
14	a	812	CLA	C1B-NB	-2.23	1.34	1.37
14	A	817	CLA	CMB-C2B	-2.23	1.46	1.50
14	B	830	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	825	CLA	C1B-C2B	2.23	1.48	1.43
14	1	838	CLA	C1B-C2B	2.23	1.48	1.43
14	A	840	CLA	C3B-C4B	2.23	1.49	1.42
14	A	818	CLA	CMB-C2B	-2.23	1.46	1.50
14	B	814	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	820	CLA	C1B-NB	-2.23	1.34	1.37
14	B	833	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	814	CLA	C1B-C2B	2.23	1.48	1.43
14	1	816	CLA	CMB-C2B	-2.23	1.46	1.50
14	f	205	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	813	CLA	CMB-C2B	-2.22	1.46	1.50
14	B	820	CLA	C1B-NB	-2.22	1.34	1.37
17	A	850	BCR	C33-C5	-2.22	1.47	1.50
14	B	829	CLA	MG-NB	-2.22	2.01	2.05
14	1	810	CLA	CMC-C2C	-2.22	1.46	1.50
14	B	801	CLA	C1D-ND	2.22	1.40	1.37
14	2	822	CLA	C3B-C4B	2.22	1.49	1.42
14	B	839	CLA	CMB-C2B	-2.22	1.46	1.50
14	1	839	CLA	C3B-C4B	2.22	1.49	1.42
14	b	843	CLA	CMC-C2C	-2.22	1.46	1.50
14	a	839	CLA	C1B-C2B	2.22	1.48	1.43
14	K	4002	CLA	CMD-C2D	-2.22	1.46	1.50
14	b	843	CLA	MG-NB	-2.22	2.01	2.05
14	A	838	CLA	C1B-C2B	2.22	1.48	1.43
14	a	809	CLA	C1B-C2B	2.22	1.48	1.43
14	b	835	CLA	C1B-C2B	2.22	1.48	1.43
14	1	811	CLA	CMD-C2D	-2.22	1.46	1.50
14	1	837	CLA	CMC-C2C	-2.22	1.46	1.50
14	A	840	CLA	C1B-NB	-2.22	1.34	1.37
14	2	830	CLA	C1B-NB	-2.22	1.34	1.37
14	1	809	CLA	CHC-C1C	2.22	1.42	1.38
14	B	833	CLA	C1B-C2B	2.22	1.48	1.43
14	b	842	CLA	C1B-C2B	2.22	1.48	1.43
14	B	801	CLA	MG-ND	-2.22	2.01	2.05
14	B	824	CLA	CMD-C2D	-2.22	1.46	1.50
14	b	836	CLA	C3B-C4B	2.22	1.49	1.42
14	b	841	CLA	C4B-NB	2.22	1.40	1.37
14	1	837	CLA	C1B-NB	-2.22	1.34	1.37
14	b	838	CLA	CMB-C2B	-2.22	1.46	1.50
14	0	207	CLA	CMC-C2C	-2.22	1.46	1.50
14	1	823	CLA	CMC-C2C	-2.22	1.46	1.50
14	A	809	CLA	C1B-C2B	2.22	1.48	1.43
14	B	813	CLA	C1B-NB	-2.22	1.34	1.37
14	2	836	CLA	C3B-C4B	2.22	1.49	1.42
14	L	1502	CLA	C1B-C2B	2.22	1.48	1.43
14	a	826	CLA	CMB-C2B	-2.22	1.46	1.50
14	b	822	CLA	MG-NB	-2.22	2.01	2.05
14	2	833	CLA	MG-NB	-2.22	2.01	2.05
14	1	827	CLA	C4B-NB	2.22	1.40	1.37
14	1	814	CLA	CMD-C2D	-2.22	1.46	1.50
14	A	812	CLA	C3B-C4B	2.22	1.49	1.42
14	A	817	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	811	CLA	C4B-NB	2.22	1.40	1.37
14	a	833	CLA	C1B-NB	-2.22	1.34	1.37
14	A	819	CLA	CMB-C2B	-2.22	1.46	1.50
14	A	838	CLA	CMC-C2C	-2.22	1.46	1.50
14	B	823	CLA	C3B-C4B	2.22	1.49	1.42
14	K	4002	CLA	CMC-C2C	-2.22	1.46	1.50
14	b	833	CLA	CMD-C2D	-2.22	1.46	1.50
14	2	817	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	804	CLA	C1D-ND	2.22	1.40	1.37
14	A	842	CLA	C1B-C2B	2.22	1.48	1.43
14	a	837	CLA	C1B-C2B	2.22	1.48	1.43
14	b	817	CLA	CMB-C2B	-2.22	1.46	1.50
14	1	829	CLA	C1B-C2B	2.22	1.48	1.43
14	1	811	CLA	C3B-C4B	2.22	1.49	1.42
14	2	823	CLA	C3B-C4B	2.22	1.49	1.42
14	b	812	CLA	C4B-NB	2.22	1.40	1.37
14	k	4002	CLA	CMB-C2B	-2.22	1.46	1.50
14	K	4004	CLA	CHC-C1C	2.22	1.42	1.38
14	1	815	CLA	CMB-C2B	-2.22	1.46	1.50
14	A	825	CLA	CMC-C2C	-2.21	1.46	1.50
14	B	844	CLA	CMC-C2C	-2.21	1.46	1.50
14	B	818	CLA	CMB-C2B	-2.21	1.46	1.50
14	A	836	CLA	C1B-C2B	2.21	1.48	1.43
14	A	841	CLA	C1B-C2B	2.21	1.48	1.43
14	A	817	CLA	CMD-C2D	-2.21	1.46	1.50
14	A	830	CLA	CMB-C2B	-2.21	1.46	1.50
14	1	808	CLA	C1B-C2B	2.21	1.48	1.43
14	1	814	CLA	CMB-C2B	-2.21	1.46	1.50
14	2	813	CLA	CMC-C2C	-2.21	1.46	1.50
14	8	4003	CLA	MG-NB	-2.21	2.01	2.05
14	2	817	CLA	C3B-C4B	2.21	1.49	1.42
14	A	815	CLA	CMB-C2B	-2.21	1.46	1.50
14	k	4002	CLA	CMC-C2C	-2.21	1.46	1.50
14	A	820	CLA	C1B-C2B	2.21	1.48	1.43
14	b	828	CLA	CMB-C2B	-2.21	1.46	1.50
14	a	818	CLA	C3B-C4B	2.21	1.49	1.42
14	A	824	CLA	CMC-C2C	-2.21	1.46	1.50
14	b	833	CLA	CMC-C2C	-2.21	1.46	1.50
14	A	811	CLA	C1B-C2B	2.21	1.48	1.43
12	2	852	LHG	O7-C5	-2.21	1.41	1.46
14	a	815	CLA	CMC-C2C	-2.21	1.46	1.50
14	b	823	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	833	CLA	CMC-C2C	-2.21	1.46	1.50
14	b	801	CLA	CMC-C2C	-2.21	1.46	1.50
14	1	813	CLA	MG-NB	-2.21	2.01	2.05
14	b	802	CLA	C1B-C2B	2.21	1.48	1.43
14	F	205	CLA	CMC-C2C	-2.21	1.46	1.50
14	f	204	CLA	CMB-C2B	-2.21	1.46	1.50
14	a	854	CLA	CHC-C1C	2.21	1.42	1.38
14	A	837	CLA	CMD-C2D	-2.21	1.46	1.50
14	b	813	CLA	CMD-C2D	-2.21	1.46	1.50
14	1	820	CLA	MG-ND	-2.21	2.01	2.05
14	a	812	CLA	CMC-C2C	-2.21	1.46	1.50
14	b	830	CLA	C1B-NB	-2.21	1.35	1.37
14	A	829	CLA	MG-ND	-2.21	2.01	2.05
14	a	818	CLA	CMD-C2D	-2.21	1.46	1.50
17	k	4001	BCR	C33-C5	-2.21	1.47	1.50
14	B	837	CLA	C3B-C4B	2.21	1.49	1.42
14	1	840	CLA	C4B-NB	2.21	1.40	1.37
14	a	838	CLA	CMD-C2D	-2.21	1.46	1.50
14	a	816	CLA	C1B-C2B	2.21	1.48	1.43
14	1	826	CLA	CMC-C2C	-2.21	1.46	1.50
14	f	205	CLA	CMC-C2C	-2.21	1.46	1.50
14	a	842	CLA	C1B-C2B	2.21	1.48	1.43
14	A	830	CLA	C1B-C2B	2.20	1.48	1.43
14	1	833	CLA	CMC-C2C	-2.20	1.46	1.50
14	B	818	CLA	C1B-C2B	2.20	1.48	1.43
14	a	816	CLA	CMB-C2B	-2.20	1.46	1.50
14	a	829	CLA	CMB-C2B	-2.20	1.46	1.50
14	1	842	CLA	C1B-C2B	2.20	1.48	1.43
14	1	807	CLA	C1B-C2B	2.20	1.48	1.43
14	l	4205	CLA	C1B-C2B	2.20	1.48	1.43
14	A	833	CLA	CMC-C2C	-2.20	1.46	1.50
14	7	1102	CLA	CMD-C2D	-2.20	1.46	1.50
14	A	843	CLA	C1B-C2B	2.20	1.48	1.43
14	b	802	CLA	C4B-NB	2.20	1.40	1.37
14	B	823	CLA	MG-NB	-2.20	2.01	2.05
14	A	804	CLA	MG-ND	-2.20	2.01	2.05
14	B	833	CLA	C1B-NB	-2.20	1.35	1.37
14	a	832	CLA	C1B-NB	-2.20	1.35	1.37
14	2	812	CLA	C1B-NB	-2.20	1.35	1.37
14	1	816	CLA	C3B-C4B	2.20	1.49	1.42
14	b	819	CLA	MG-ND	-2.20	2.01	2.05
14	l	4206	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	4001	BCR	C33-C5	-2.20	1.47	1.50
14	1	828	CLA	MG-ND	-2.20	2.01	2.05
14	2	827	CLA	CMB-C2B	-2.20	1.46	1.50
14	2	819	CLA	MG-ND	-2.20	2.01	2.05
14	B	834	CLA	CMC-C2C	-2.20	1.46	1.50
14	L	1503	CLA	CMB-C2B	-2.20	1.46	1.50
14	A	831	CLA	C1B-NB	-2.20	1.35	1.37
14	A	817	CLA	MG-NB	-2.20	2.01	2.05
14	B	821	CLA	C4B-NB	2.20	1.40	1.37
14	l	4203	CLA	C1B-NB	-2.20	1.35	1.37
14	a	830	CLA	MG-ND	-2.20	2.01	2.05
14	A	814	CLA	CMC-C2C	-2.20	1.46	1.50
14	2	838	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	821	CLA	C1B-NB	-2.20	1.35	1.37
14	L	1501	CLA	CHC-C1C	2.20	1.42	1.38
14	0	208	CLA	CMB-C2B	-2.20	1.46	1.50
14	A	816	CLA	C1B-NB	-2.20	1.35	1.37
14	A	827	CLA	CMC-C2C	-2.20	1.46	1.50
14	a	844	CLA	CMD-C2D	-2.20	1.46	1.50
14	8	4002	CLA	MG-NB	-2.20	2.01	2.05
14	B	802	CLA	CMC-C2C	-2.20	1.46	1.50
14	A	813	CLA	C1B-NB	-2.20	1.35	1.37
14	1	839	CLA	C1B-NB	-2.20	1.35	1.37
14	2	841	CLA	C1B-C2B	2.20	1.48	1.43
14	A	834	CLA	CMC-C2C	-2.20	1.46	1.50
14	b	832	CLA	MG-ND	-2.19	2.01	2.05
14	0	207	CLA	C1B-C2B	2.19	1.48	1.43
18	A	853	LMG	O7-C8	-2.19	1.41	1.46
14	L	1502	CLA	C1B-NB	-2.19	1.35	1.37
14	b	822	CLA	CMB-C2B	-2.19	1.46	1.50
14	A	810	CLA	CHC-C1C	2.19	1.42	1.38
14	a	812	CLA	C1B-C2B	2.19	1.48	1.43
14	a	818	CLA	CMB-C2B	-2.19	1.46	1.50
14	1	840	CLA	C1B-C2B	2.19	1.48	1.43
14	a	807	CLA	MG-NB	-2.19	2.01	2.05
12	B	853	LHG	O7-C5	-2.19	1.41	1.46
14	A	840	CLA	CMC-C2C	-2.19	1.46	1.50
14	b	806	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	822	CLA	MG-NB	-2.19	2.01	2.05
14	b	838	CLA	CMD-C2D	-2.19	1.46	1.50
14	1	837	CLA	C1B-C2B	2.19	1.48	1.43
14	1	816	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	843	CLA	C1B-C2B	2.19	1.48	1.43
14	j	101	CLA	CMD-C2D	-2.19	1.46	1.50
14	1	815	CLA	C1B-NB	-2.19	1.35	1.37
14	2	841	CLA	C4B-NB	2.19	1.40	1.37
14	B	818	CLA	C3B-C4B	2.19	1.49	1.42
14	B	833	CLA	MG-ND	-2.19	2.01	2.05
14	a	816	CLA	CMD-C2D	-2.19	1.46	1.50
14	a	837	CLA	CMC-C2C	-2.19	1.46	1.50
14	1	844	CLA	CMD-C2D	-2.19	1.46	1.50
14	b	838	CLA	CMC-C2C	-2.19	1.46	1.50
14	A	810	CLA	C4B-NB	2.19	1.40	1.37
14	b	829	CLA	C1B-NB	-2.19	1.35	1.37
14	K	4002	CLA	CMB-C2B	-2.19	1.46	1.50
14	1	841	CLA	CMC-C2C	-2.19	1.46	1.50
17	0	210	BCR	C30-C25	-2.19	1.51	1.53
14	1	843	CLA	C1B-C2B	2.19	1.48	1.43
14	l	4204	CLA	CHC-C1C	2.19	1.42	1.38
14	B	834	CLA	CMD-C2D	-2.19	1.46	1.50
14	2	822	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	823	CLA	CMD-C2D	-2.19	1.46	1.50
14	b	812	CLA	MG-ND	-2.19	2.01	2.05
14	B	842	CLA	C1B-NB	-2.19	1.35	1.37
14	b	835	CLA	C1B-NB	-2.19	1.35	1.37
18	a	853	LMG	O7-C8	-2.19	1.41	1.46
14	A	827	CLA	C1B-C2B	2.19	1.48	1.43
14	A	812	CLA	CMC-C2C	-2.19	1.46	1.50
14	a	835	CLA	CMC-C2C	-2.19	1.46	1.50
14	B	807	CLA	CHC-C1C	2.19	1.42	1.38
14	2	809	CLA	CMC-C2C	-2.19	1.46	1.50
14	8	4004	CLA	CHC-C1C	2.19	1.42	1.38
14	2	829	CLA	C1B-NB	-2.19	1.35	1.37
14	a	825	CLA	CMC-C2C	-2.19	1.46	1.50
14	7	1103	CLA	C3B-C4B	2.19	1.49	1.42
14	2	823	CLA	CMB-C2B	-2.19	1.46	1.50
14	a	840	CLA	C1B-C2B	2.19	1.48	1.43
12	b	852	LHG	O7-C5	-2.19	1.41	1.46
14	A	828	CLA	C4B-NB	2.19	1.40	1.37
14	b	817	CLA	CHC-C1C	2.19	1.42	1.38
14	A	815	CLA	CMD-C2D	-2.19	1.46	1.50
14	2	817	CLA	CHC-C1C	2.19	1.42	1.38
14	a	828	CLA	CMC-C2C	-2.19	1.46	1.50
14	B	824	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	822	CLA	C1B-NB	-2.18	1.35	1.37
14	b	819	CLA	C1B-NB	-2.18	1.35	1.37
14	b	827	CLA	CMB-C2B	-2.18	1.46	1.50
14	a	820	CLA	CMB-C2B	-2.18	1.46	1.50
14	1	817	CLA	MG-NB	-2.18	2.01	2.05
14	1	826	CLA	C1B-C2B	2.18	1.48	1.43
14	b	823	CLA	CMB-C2B	-2.18	1.46	1.50
18	1	852	LMG	O7-C8	-2.18	1.41	1.46
14	a	835	CLA	MG-ND	-2.18	2.01	2.05
14	a	804	CLA	C1D-ND	2.18	1.40	1.37
14	b	813	CLA	CMC-C2C	-2.18	1.46	1.50
14	2	805	CLA	CHC-C1C	2.18	1.42	1.38
14	b	816	CLA	CMB-C2B	-2.18	1.46	1.50
14	A	806	CLA	CHC-C1C	2.18	1.42	1.38
14	b	820	CLA	C1B-NB	-2.18	1.35	1.37
14	A	811	CLA	CMC-C2C	-2.18	1.46	1.50
14	2	820	CLA	C4B-NB	2.18	1.40	1.37
14	a	819	CLA	CMD-C2D	-2.18	1.46	1.50
13	1	803	CL0	MG-ND	-2.18	2.01	2.05
14	b	819	CLA	C4B-NB	2.18	1.40	1.37
14	B	806	CLA	CMB-C2B	-2.18	1.46	1.50
14	2	819	CLA	C4B-NB	2.18	1.40	1.37
13	a	803	CL0	MG-ND	-2.18	2.01	2.05
14	2	805	CLA	MG-ND	-2.18	2.01	2.05
14	1	817	CLA	CMD-C2D	-2.18	1.46	1.50
14	2	806	CLA	C3B-C4B	2.18	1.49	1.42
14	8	4003	CLA	C3B-C4B	2.18	1.49	1.42
14	b	807	CLA	CHC-C1C	2.18	1.42	1.38
14	B	842	CLA	C1B-C2B	2.18	1.48	1.43
14	2	837	CLA	C3B-C4B	2.18	1.49	1.42
14	B	824	CLA	CMB-C2B	-2.18	1.46	1.50
14	0	202	CLA	CMC-C2C	-2.18	1.46	1.50
19	F	202	LMT	O3B-C3B	-2.18	1.37	1.43
17	0	204	BCR	C30-C25	-2.18	1.51	1.53
14	a	807	CLA	CHC-C1C	2.18	1.42	1.38
14	1	822	CLA	CHC-C1C	2.18	1.42	1.38
14	1	836	CLA	CHC-C1C	2.18	1.42	1.38
14	a	804	CLA	CAA-C2A	-2.18	1.50	1.54
14	B	820	CLA	C4B-NB	2.18	1.40	1.37
14	0	208	CLA	C3B-C4B	2.18	1.49	1.42
14	J	101	CLA	CMD-C2D	-2.17	1.46	1.50
14	A	836	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	823	CLA	CMB-C2B	-2.17	1.46	1.50
14	B	829	CLA	C3B-C4B	2.17	1.49	1.42
14	B	806	CLA	CHC-C1C	2.17	1.42	1.38
14	A	840	CLA	C1B-C2B	2.17	1.48	1.43
14	f	204	CLA	CMC-C2C	-2.17	1.46	1.50
14	A	838	CLA	C1B-NB	-2.17	1.35	1.37
14	1	831	CLA	C1B-NB	-2.17	1.35	1.37
14	B	843	CLA	C1B-C2B	2.17	1.48	1.43
14	A	821	CLA	MG-ND	-2.17	2.01	2.05
14	B	839	CLA	CMC-C2C	-2.17	1.46	1.50
14	a	822	CLA	MG-ND	-2.17	2.01	2.05
14	B	814	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	828	CLA	CMB-C2B	-2.17	1.46	1.50
14	b	806	CLA	MG-ND	-2.17	2.01	2.05
14	B	817	CLA	CMB-C2B	-2.17	1.46	1.50
14	B	837	CLA	CHC-C1C	2.17	1.42	1.38
14	1	833	CLA	MG-ND	-2.17	2.01	2.05
14	f	204	CLA	MG-ND	-2.17	2.01	2.05
14	1	818	CLA	CMB-C2B	-2.17	1.46	1.50
14	A	839	CLA	C1B-C2B	2.17	1.48	1.43
14	B	830	CLA	C1B-NB	-2.17	1.35	1.37
14	A	825	CLA	CMB-C2B	-2.17	1.46	1.50
14	1	805	CLA	MG-NB	-2.17	2.01	2.05
19	f	202	LMT	O3B-C3B	-2.17	1.37	1.43
14	2	832	CLA	C1B-C2B	2.17	1.48	1.43
14	l	4206	CLA	C3B-C4B	2.17	1.49	1.42
14	1	835	CLA	CMC-C2C	-2.17	1.46	1.50
14	l	4205	CLA	C1B-NB	-2.17	1.35	1.37
14	A	815	CLA	CHC-C1C	2.17	1.42	1.38
14	A	832	CLA	C1B-NB	-2.17	1.35	1.37
14	a	813	CLA	CMC-C2C	-2.17	1.46	1.50
14	B	813	CLA	CHC-C1C	2.17	1.42	1.38
14	8	4002	CLA	CMB-C2B	-2.17	1.46	1.50
14	b	807	CLA	C3B-C4B	2.17	1.49	1.42
14	b	828	CLA	C3B-C4B	2.17	1.49	1.42
14	b	820	CLA	C4B-NB	2.17	1.40	1.37
14	A	823	CLA	CHC-C1C	2.17	1.42	1.38
14	L	1502	CLA	CHC-C1C	2.17	1.42	1.38
14	2	828	CLA	C3B-C4B	2.17	1.49	1.42
14	k	4003	CLA	C3B-C4B	2.17	1.49	1.42
14	B	818	CLA	CHC-C1C	2.17	1.42	1.38
14	L	1503	CLA	C3B-C4B	2.17	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	j	102	CLA	C3B-C4B	2.17	1.49	1.42
14	6	4404	CLA	CMC-C2C	-2.17	1.46	1.50
14	b	841	CLA	C1B-C2B	2.16	1.48	1.43
14	6	4404	CLA	C1B-NB	-2.16	1.35	1.37
14	B	809	CLA	MG-ND	-2.16	2.01	2.05
14	2	811	CLA	MG-ND	-2.16	2.01	2.05
14	b	832	CLA	C1B-NB	-2.16	1.35	1.37
14	a	828	CLA	C1B-C2B	2.16	1.48	1.43
14	A	808	CLA	C1B-C2B	2.16	1.48	1.43
14	A	835	CLA	C1B-C2B	2.16	1.48	1.43
14	2	808	CLA	MG-ND	-2.16	2.01	2.05
14	2	834	CLA	C1B-NB	-2.16	1.35	1.37
14	2	822	CLA	CMC-C2C	-2.16	1.46	1.50
14	b	841	CLA	C1B-NB	-2.16	1.35	1.37
14	1	810	CLA	C1B-C2B	2.16	1.48	1.43
14	B	838	CLA	C3B-C4B	2.16	1.49	1.42
14	2	837	CLA	CMC-C2C	-2.16	1.46	1.50
14	A	833	CLA	C1D-ND	2.16	1.40	1.37
14	a	817	CLA	C1B-NB	-2.16	1.35	1.37
14	b	817	CLA	C3B-C4B	2.16	1.49	1.42
14	0	206	CLA	C3B-C4B	2.16	1.49	1.42
14	1	839	CLA	C1B-C2B	2.16	1.48	1.43
14	B	804	CLA	CHC-C1C	2.16	1.42	1.38
14	1	832	CLA	C1D-ND	2.16	1.40	1.37
14	1	830	CLA	C1B-NB	-2.16	1.35	1.37
14	1	811	CLA	CMC-C2C	-2.16	1.46	1.50
14	a	811	CLA	CHC-C1C	2.16	1.42	1.38
14	0	206	CLA	CHC-C1C	2.16	1.42	1.38
19	6	4401	LMT	O3B-C3B	-2.16	1.37	1.43
14	6	4403	CLA	CMC-C2C	-2.16	1.46	1.50
14	1	814	CLA	CHC-C1C	2.16	1.42	1.38
14	2	816	CLA	CMB-C2B	-2.16	1.46	1.50
14	2	841	CLA	C1B-NB	-2.16	1.35	1.37
14	b	830	CLA	MG-ND	-2.16	2.01	2.05
14	2	830	CLA	MG-ND	-2.16	2.01	2.05
14	A	818	CLA	MG-NB	-2.16	2.01	2.05
14	B	812	CLA	MG-ND	-2.16	2.01	2.05
14	b	837	CLA	C3B-C4B	2.16	1.49	1.42
14	1	805	CLA	CHC-C1C	2.16	1.42	1.38
14	B	801	CLA	C4B-NB	2.16	1.40	1.37
14	7	1103	CLA	MG-NB	-2.16	2.01	2.05
14	2	816	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	823	CLA	CHC-C1C	2.15	1.42	1.38
14	l	4204	CLA	C3B-C4B	2.15	1.49	1.42
17	8	4001	BCR	C33-C5	-2.15	1.47	1.50
14	a	827	CLA	C4B-NB	2.15	1.40	1.37
14	0	207	CLA	C1B-NB	-2.15	1.35	1.37
14	A	807	CLA	MG-ND	-2.15	2.01	2.05
14	J	101	CLA	CHC-C1C	2.15	1.42	1.38
17	L	1505	BCR	C30-C25	-2.15	1.51	1.53
14	2	815	CLA	C4B-NB	2.15	1.40	1.37
14	a	808	CLA	MG-ND	-2.15	2.01	2.05
14	a	816	CLA	CHC-C1C	2.15	1.42	1.38
14	a	841	CLA	C1B-C2B	2.15	1.48	1.43
14	b	804	CLA	CHC-C1C	2.15	1.42	1.38
14	B	836	CLA	C1B-NB	-2.15	1.35	1.37
14	2	835	CLA	C1B-NB	-2.15	1.35	1.37
14	b	816	CLA	CHC-C1C	2.15	1.42	1.38
14	b	814	CLA	C3B-C4B	2.15	1.49	1.42
19	i	4101	LMT	O4'-C4B	-2.15	1.37	1.43
14	b	823	CLA	CHC-C1C	2.15	1.42	1.38
14	2	819	CLA	C1B-NB	-2.15	1.35	1.37
14	j	101	CLA	CMB-C2B	-2.15	1.46	1.50
14	2	832	CLA	MG-ND	-2.15	2.01	2.05
14	l	4203	CLA	MG-ND	-2.15	2.01	2.05
14	2	812	CLA	CHC-C1C	2.15	1.42	1.38
17	1	850	BCR	C33-C5	-2.15	1.47	1.50
14	B	831	CLA	MG-ND	-2.15	2.01	2.05
14	b	825	CLA	C3B-C4B	2.15	1.49	1.42
14	A	806	CLA	MG-NB	-2.15	2.01	2.05
14	L	1501	CLA	C3B-C4B	2.15	1.49	1.42
14	A	818	CLA	CMD-C2D	-2.15	1.46	1.50
14	a	814	CLA	CHC-C1C	2.15	1.42	1.38
14	2	812	CLA	MG-ND	-2.15	2.01	2.05
14	a	839	CLA	C1B-NB	-2.15	1.35	1.37
14	A	824	CLA	CMB-C2B	-2.15	1.46	1.50
14	2	838	CLA	CMC-C2C	-2.15	1.46	1.50
14	K	4003	CLA	C3B-C4B	2.15	1.49	1.42
14	F	204	CLA	MG-ND	-2.15	2.01	2.05
14	2	836	CLA	CMC-C2C	-2.15	1.46	1.50
14	B	835	CLA	C1B-NB	-2.15	1.35	1.37
14	j	102	CLA	CBD-CAD	2.15	1.56	1.51
14	b	806	CLA	CHC-C1C	2.15	1.42	1.38
14	b	836	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	810	CLA	C4B-NB	2.15	1.40	1.37
14	a	841	CLA	C1B-NB	-2.15	1.35	1.37
14	l	4204	CLA	C1B-C2B	2.15	1.48	1.43
14	2	801	CLA	C4B-NB	2.15	1.40	1.37
14	J	102	CLA	CMB-C2B	-2.15	1.46	1.50
14	B	817	CLA	CHC-C1C	2.14	1.42	1.38
14	a	814	CLA	MG-ND	-2.14	2.01	2.05
14	A	833	CLA	C4B-NB	2.14	1.40	1.37
14	B	837	CLA	CMC-C2C	-2.14	1.46	1.50
14	J	102	CLA	C3B-C4B	2.14	1.49	1.42
14	A	844	CLA	CMD-C2D	-2.14	1.46	1.50
14	1	808	CLA	CMC-C2C	-2.14	1.46	1.50
14	b	824	CLA	CMC-C2C	-2.14	1.46	1.50
14	b	844	CLA	MG-NB	-2.14	2.01	2.05
14	b	837	CLA	CMC-C2C	-2.14	1.46	1.50
14	a	819	CLA	MG-NB	-2.14	2.01	2.05
14	1	832	CLA	C4B-NB	2.14	1.40	1.37
17	2	848	BCR	C12-C13	-2.14	1.44	1.50
14	L	1501	CLA	C1B-C2B	2.14	1.48	1.43
14	1	834	CLA	C1B-C2B	2.14	1.48	1.43
14	2	801	CLA	C3B-C4B	2.14	1.49	1.42
14	f	205	CLA	CMB-C2B	-2.14	1.46	1.50
14	1	825	CLA	C4B-NB	2.14	1.40	1.37
14	b	836	CLA	CMC-C2C	-2.14	1.46	1.50
14	1	806	CLA	MG-ND	-2.14	2.01	2.05
14	b	827	CLA	C3B-C4B	2.14	1.49	1.42
14	A	838	CLA	MG-ND	-2.14	2.01	2.05
14	6	4403	CLA	MG-ND	-2.14	2.01	2.05
14	1	837	CLA	MG-ND	-2.14	2.01	2.05
14	2	825	CLA	C3B-C4B	2.14	1.49	1.42
13	A	803	CL0	CBD-CGD	-2.14	1.49	1.52
14	B	807	CLA	C3B-C4B	2.14	1.49	1.42
14	B	825	CLA	CMC-C2C	-2.14	1.46	1.50
14	a	837	CLA	MG-ND	-2.14	2.01	2.05
14	2	844	CLA	MG-NB	-2.14	2.01	2.05
14	j	102	CLA	MG-NB	-2.14	2.01	2.05
14	A	816	CLA	C3B-C4B	2.14	1.49	1.42
14	2	814	CLA	C3B-C4B	2.14	1.49	1.42
14	a	838	CLA	CHC-C1C	2.14	1.42	1.38
14	J	102	CLA	MG-NB	-2.14	2.01	2.05
14	j	101	CLA	CHC-C1C	2.14	1.42	1.38
14	a	836	CLA	C1B-C2B	2.14	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	836	CLA	CHC-C1C	2.14	1.42	1.38
14	1	815	CLA	C3B-C4B	2.14	1.49	1.42
14	B	813	CLA	MG-ND	-2.13	2.01	2.05
14	F	204	CLA	CMC-C2C	-2.13	1.46	1.50
14	1	836	CLA	CMC-C2C	-2.13	1.46	1.50
14	a	810	CLA	CMC-C2C	-2.13	1.46	1.50
14	2	806	CLA	CHC-C1C	2.13	1.42	1.38
14	A	804	CLA	C4B-NB	2.13	1.40	1.37
14	B	819	CLA	C1B-NB	-2.13	1.35	1.37
14	b	834	CLA	C1B-NB	-2.13	1.35	1.37
14	2	832	CLA	C1B-NB	-2.13	1.35	1.37
14	F	205	CLA	CMB-C2B	-2.13	1.46	1.50
14	2	823	CLA	CMC-C2C	-2.13	1.46	1.50
14	a	805	CLA	CAB-C3B	-2.13	1.41	1.47
14	a	822	CLA	C1B-C2B	2.13	1.48	1.43
14	2	827	CLA	C3B-C4B	2.13	1.48	1.42
14	A	834	CLA	MG-ND	-2.13	2.01	2.05
14	7	1102	CLA	CMB-C2B	-2.13	1.46	1.50
14	B	828	CLA	C3B-C4B	2.13	1.48	1.42
14	1	835	CLA	MG-ND	-2.13	2.01	2.05
14	b	838	CLA	C3B-C4B	2.13	1.48	1.42
14	2	824	CLA	CMC-C2C	-2.13	1.46	1.50
14	b	819	CLA	C1B-C2B	2.13	1.48	1.43
14	b	822	CLA	CMC-C2C	-2.13	1.46	1.50
14	0	202	CLA	C3B-C4B	2.13	1.48	1.42
14	B	823	CLA	CMC-C2C	-2.13	1.46	1.50
14	B	815	CLA	C3B-C4B	2.13	1.48	1.42
14	a	824	CLA	MG-ND	-2.13	2.01	2.05
14	2	820	CLA	MG-ND	-2.13	2.01	2.05
14	B	820	CLA	C1B-C2B	2.13	1.48	1.43
14	7	1103	CLA	CBD-CAD	2.13	1.56	1.51
14	A	826	CLA	C4B-NB	2.13	1.40	1.37
14	a	824	CLA	CHC-C1C	2.12	1.42	1.38
14	0	207	CLA	CHC-C1C	2.12	1.42	1.38
14	F	205	CLA	C1B-NB	-2.12	1.35	1.37
14	0	206	CLA	C1B-C2B	2.12	1.48	1.43
14	B	839	CLA	CMD-C2D	-2.12	1.46	1.50
14	J	101	CLA	CMB-C2B	-2.12	1.46	1.50
14	7	1103	CLA	CMB-C2B	-2.12	1.46	1.50
14	a	834	CLA	C4B-NB	2.12	1.40	1.37
14	b	810	CLA	C1B-NB	-2.12	1.35	1.37
14	B	839	CLA	C3B-C4B	2.12	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	809	CLA	CMC-C2C	-2.12	1.46	1.50
14	1	821	CLA	CMB-C2B	-2.12	1.46	1.50
14	b	837	CLA	MG-ND	-2.12	2.01	2.05
14	B	801	CLA	CAA-C2A	-2.12	1.50	1.54
14	a	841	CLA	CMC-C2C	-2.12	1.46	1.50
14	A	826	CLA	C1B-NB	-2.12	1.35	1.37
17	b	848	BCR	C12-C13	-2.12	1.44	1.50
14	1	822	CLA	MG-ND	-2.12	2.01	2.05
14	b	820	CLA	MG-ND	-2.12	2.01	2.05
14	b	815	CLA	C4B-NB	2.12	1.40	1.37
17	B	852	BCR	C38-C26	-2.12	1.47	1.50
14	6	4404	CLA	CHC-C1C	2.12	1.42	1.38
14	l	4203	CLA	CHC-C1C	2.12	1.42	1.38
14	1	817	CLA	C3B-C4B	2.12	1.48	1.42
14	b	809	CLA	MG-ND	-2.12	2.01	2.05
19	I	103	LMT	O4'-C4B	-2.12	1.37	1.43
14	1	812	CLA	CHC-C1C	2.12	1.42	1.38
14	b	809	CLA	C1B-C2B	2.12	1.48	1.43
14	L	1503	CLA	CMC-C2C	-2.12	1.46	1.50
14	A	823	CLA	MG-ND	-2.12	2.01	2.05
14	b	832	CLA	CHC-C1C	2.12	1.42	1.38
14	f	205	CLA	CHC-C1C	2.12	1.42	1.38
14	7	1102	CLA	CHC-C1C	2.12	1.42	1.38
14	B	806	CLA	C3B-C4B	2.12	1.48	1.42
14	A	821	CLA	C1B-C2B	2.12	1.48	1.43
14	A	813	CLA	CHC-C1C	2.12	1.42	1.38
14	1	804	CLA	CAB-C3B	-2.12	1.41	1.47
14	B	816	CLA	C4B-NB	2.12	1.40	1.37
14	F	201	CLA	MG-ND	-2.12	2.01	2.05
14	A	822	CLA	CMB-C2B	-2.12	1.46	1.50
17	i	4103	BCR	C38-C26	-2.12	1.47	1.50
14	a	810	CLA	C3B-C4B	2.12	1.48	1.42
14	2	838	CLA	CHC-C1C	2.12	1.42	1.38
14	a	838	CLA	CMC-C2C	-2.12	1.46	1.50
14	2	819	CLA	C1B-C2B	2.12	1.48	1.43
14	A	809	CLA	C3B-C4B	2.12	1.48	1.42
14	l	4205	CLA	CHC-C1C	2.12	1.42	1.38
14	B	838	CLA	CMC-C2C	-2.12	1.46	1.50
14	b	806	CLA	C3B-C4B	2.12	1.48	1.42
14	A	825	CLA	MG-ND	-2.12	2.01	2.05
14	F	205	CLA	CHC-C1C	2.12	1.42	1.38
14	K	4004	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	821	CLA	MG-ND	-2.12	2.01	2.05
14	2	826	CLA	CHC-C1C	2.11	1.42	1.38
14	1	804	CLA	C4B-NB	2.11	1.40	1.37
14	1	839	CLA	CMC-C2C	-2.11	1.46	1.50
19	h	103	LMT	O4'-C4B	-2.11	1.37	1.43
14	B	824	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	837	CLA	CHC-C1C	2.11	1.42	1.38
14	2	818	CLA	C1B-NB	-2.11	1.35	1.37
14	B	819	CLA	CMB-C2B	-2.11	1.46	1.50
14	1	823	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	840	CLA	MG-ND	-2.11	2.01	2.05
14	2	835	CLA	MG-ND	-2.11	2.01	2.05
14	a	825	CLA	CMB-C2B	-2.11	1.46	1.50
14	0	208	CLA	CMC-C2C	-2.11	1.46	1.50
14	1	827	CLA	C3B-C4B	2.11	1.48	1.42
14	A	818	CLA	C3B-C4B	2.11	1.48	1.42
14	a	826	CLA	MG-ND	-2.11	2.01	2.05
14	f	201	CLA	MG-ND	-2.11	2.01	2.05
14	1	833	CLA	C1B-C2B	2.11	1.48	1.43
14	b	829	CLA	MG-ND	-2.11	2.01	2.05
14	k	4003	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	809	CLA	MG-ND	-2.11	2.01	2.05
14	F	205	CLA	MG-ND	-2.11	2.01	2.05
14	a	810	CLA	MG-ND	-2.11	2.01	2.05
14	2	803	CLA	CHC-C1C	2.11	1.42	1.38
14	B	802	CLA	C3B-C4B	2.11	1.48	1.42
14	j	102	CLA	CMD-C2D	-2.11	1.46	1.50
14	2	838	CLA	C3B-C4B	2.11	1.48	1.42
14	a	835	CLA	C1B-C2B	2.11	1.48	1.43
14	b	801	CLA	C3B-C4B	2.11	1.48	1.42
14	J	102	CLA	CBD-CAD	2.11	1.56	1.51
14	b	835	CLA	MG-ND	-2.11	2.01	2.05
14	0	202	CLA	CHC-C1C	2.11	1.42	1.38
14	a	834	CLA	C1D-ND	2.11	1.40	1.37
14	1	841	CLA	MG-ND	-2.11	2.01	2.05
14	b	822	CLA	CHC-C1C	2.11	1.42	1.38
14	2	805	CLA	C3B-C4B	2.11	1.48	1.42
14	0	202	CLA	C1B-C2B	2.11	1.48	1.43
14	B	845	CLA	MG-NB	-2.11	2.01	2.05
14	b	821	CLA	MG-ND	-2.11	2.01	2.05
14	B	826	CLA	C3B-C4B	2.11	1.48	1.42
14	B	810	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	825	CLA	C1B-NB	-2.11	1.35	1.37
14	A	809	CLA	CHC-C1C	2.11	1.42	1.38
14	1	812	CLA	MG-ND	-2.11	2.01	2.05
14	2	833	CLA	CHC-C1C	2.11	1.42	1.38
17	B	849	BCR	C12-C13	-2.11	1.44	1.50
13	1	803	CL0	C3A-C2A	-2.11	1.52	1.54
14	b	826	CLA	CHC-C1C	2.11	1.42	1.38
14	2	841	CLA	CHC-C1C	2.11	1.42	1.38
14	2	818	CLA	C3B-C4B	2.11	1.48	1.42
14	K	4003	CLA	CHC-C1C	2.10	1.42	1.38
14	A	813	CLA	MG-ND	-2.10	2.01	2.05
14	B	826	CLA	C1B-C2B	2.10	1.48	1.43
14	2	825	CLA	C1B-C2B	2.10	1.48	1.43
14	1	820	CLA	C3B-C4B	2.10	1.48	1.42
14	1	820	CLA	C1B-C2B	2.10	1.48	1.43
14	B	824	CLA	CHC-C1C	2.10	1.42	1.38
14	j	102	CLA	CMB-C2B	-2.10	1.46	1.50
14	B	801	CLA	C3B-C4B	2.10	1.48	1.42
14	B	830	CLA	MG-ND	-2.10	2.01	2.05
14	b	805	CLA	C1B-NB	-2.10	1.35	1.37
14	2	804	CLA	C1B-NB	-2.10	1.35	1.37
14	a	854	CLA	CMB-C2B	-2.10	1.46	1.50
14	0	208	CLA	CHC-C1C	2.10	1.42	1.38
14	2	801	CLA	CAA-C2A	-2.10	1.50	1.54
14	2	806	CLA	MG-NB	-2.10	2.01	2.05
14	2	837	CLA	MG-ND	-2.10	2.01	2.05
14	a	823	CLA	CMB-C2B	-2.10	1.46	1.50
14	J	102	CLA	CMD-C2D	-2.10	1.46	1.50
14	a	817	CLA	C3B-C4B	2.10	1.48	1.42
14	F	201	CLA	C3B-C4B	2.10	1.48	1.42
14	b	825	CLA	MG-ND	-2.10	2.01	2.05
14	B	830	CLA	C4B-NB	2.10	1.40	1.37
14	b	829	CLA	C4B-NB	2.10	1.40	1.37
14	2	808	CLA	C1B-C2B	2.10	1.48	1.43
17	I	102	BCR	C38-C26	-2.10	1.47	1.50
14	b	801	CLA	C1B-C2B	2.10	1.48	1.43
14	A	836	CLA	MG-ND	-2.10	2.01	2.05
14	B	822	CLA	MG-ND	-2.10	2.01	2.05
14	A	837	CLA	CMC-C2C	-2.10	1.46	1.50
14	8	4003	CLA	CMD-C2D	-2.10	1.46	1.50
14	b	818	CLA	C3B-C4B	2.10	1.48	1.42
14	B	819	CLA	C3B-C4B	2.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	823	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	810	CLA	CHC-C1C	2.10	1.42	1.38
14	1	829	CLA	CHC-C1C	2.10	1.42	1.38
14	2	822	CLA	CHC-C1C	2.10	1.42	1.38
14	1	808	CLA	MG-ND	-2.10	2.01	2.05
14	A	834	CLA	C1B-C2B	2.10	1.48	1.43
14	a	804	CLA	C3B-C4B	2.10	1.48	1.42
14	A	830	CLA	CHC-C1C	2.10	1.42	1.38
14	b	841	CLA	CHC-C1C	2.10	1.42	1.38
14	b	818	CLA	CMB-C2B	-2.10	1.46	1.50
14	B	812	CLA	C1B-C2B	2.10	1.48	1.43
13	a	803	CL0	CBD-CGD	-2.10	1.49	1.52
14	2	809	CLA	C1B-NB	-2.10	1.35	1.37
14	8	4003	CLA	CMB-C2B	-2.09	1.46	1.50
14	b	802	CLA	MG-ND	-2.09	2.01	2.05
14	f	205	CLA	MG-ND	-2.09	2.01	2.05
14	f	201	CLA	C3B-C4B	2.09	1.48	1.42
14	a	854	CLA	CMC-C2C	-2.09	1.46	1.50
14	B	827	CLA	CHC-C1C	2.09	1.42	1.38
14	2	829	CLA	MG-ND	-2.09	2.01	2.05
14	K	4003	CLA	CMB-C2B	-2.09	1.46	1.50
14	a	828	CLA	MG-ND	-2.09	2.01	2.05
14	a	805	CLA	C4B-NB	2.09	1.40	1.37
14	a	829	CLA	C3B-C4B	2.09	1.48	1.42
14	1	808	CLA	C3B-C4B	2.09	1.48	1.42
14	6	4404	CLA	CMB-C2B	-2.09	1.46	1.50
14	f	205	CLA	C1B-NB	-2.09	1.35	1.37
14	A	804	CLA	CAB-C3B	-2.09	1.41	1.47
14	a	841	CLA	MG-ND	-2.09	2.01	2.05
14	2	808	CLA	CHC-C1C	2.09	1.42	1.38
14	b	833	CLA	CHC-C1C	2.09	1.42	1.38
14	1	841	CLA	C3B-C4B	2.09	1.48	1.42
14	B	802	CLA	C1B-C2B	2.09	1.48	1.43
14	B	823	CLA	CHC-C1C	2.09	1.42	1.38
14	A	831	CLA	C4B-NB	2.09	1.40	1.37
14	B	807	CLA	MG-NB	-2.09	2.01	2.05
14	B	825	CLA	C3B-C4B	2.09	1.48	1.42
14	B	809	CLA	C1B-C2B	2.09	1.48	1.43
14	1	805	CLA	C3B-C4B	2.09	1.48	1.42
14	a	807	CLA	C3B-C4B	2.09	1.48	1.42
14	a	823	CLA	C3B-C4B	2.09	1.48	1.42
14	B	808	CLA	MG-ND	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	839	CLA	MG-ND	-2.09	2.01	2.05
14	K	4003	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	821	CLA	C3B-C4B	2.09	1.48	1.42
14	A	843	CLA	MG-ND	-2.09	2.01	2.05
14	1	826	CLA	MG-ND	-2.09	2.01	2.05
14	2	825	CLA	MG-ND	-2.09	2.01	2.05
14	k	4003	CLA	CHC-C1C	2.08	1.42	1.38
14	A	823	CLA	C3B-C4B	2.08	1.48	1.42
17	2	851	BCR	C38-C26	-2.08	1.47	1.50
14	A	806	CLA	C3B-C4B	2.08	1.48	1.42
14	1	824	CLA	MG-ND	-2.08	2.01	2.05
14	b	842	CLA	MG-ND	-2.08	2.01	2.05
14	L	1502	CLA	C3B-C4B	2.08	1.48	1.42
14	8	4004	CLA	C3B-C4B	2.08	1.48	1.42
14	l	4206	CLA	CMC-C2C	-2.08	1.46	1.50
17	h	102	BCR	C38-C26	-2.08	1.47	1.50
14	K	4004	CLA	CMC-C2C	-2.08	1.46	1.50
14	a	819	CLA	C3B-C4B	2.08	1.48	1.42
14	b	825	CLA	C1B-C2B	2.08	1.48	1.43
14	8	4004	CLA	CMB-C2B	-2.08	1.46	1.50
14	2	818	CLA	CMB-C2B	-2.08	1.46	1.50
14	L	1501	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	839	CLA	C3B-C4B	2.08	1.48	1.42
14	a	843	CLA	C3B-C4B	2.08	1.48	1.42
14	A	814	CLA	CHC-C1C	2.08	1.42	1.38
14	B	841	CLA	C3B-C4B	2.08	1.48	1.42
14	b	818	CLA	C1B-NB	-2.08	1.35	1.37
14	a	854	CLA	C3B-C4B	2.08	1.48	1.42
14	2	837	CLA	CHC-C1C	2.08	1.42	1.38
14	A	822	CLA	C3B-C4B	2.08	1.48	1.42
14	A	827	CLA	MG-ND	-2.08	2.01	2.05
14	2	840	CLA	C3B-C4B	2.08	1.48	1.42
14	b	838	CLA	CHC-C1C	2.08	1.42	1.38
14	1	838	CLA	C3B-C4B	2.08	1.48	1.42
14	B	834	CLA	CHC-C1C	2.08	1.42	1.38
14	1	843	CLA	C3B-C4B	2.08	1.48	1.42
13	1	803	CL0	CBD-CGD	-2.08	1.49	1.52
14	b	808	CLA	MG-ND	-2.07	2.01	2.05
14	L	1503	CLA	CHC-C1C	2.07	1.42	1.38
14	b	833	CLA	C3B-C4B	2.07	1.48	1.42
14	B	842	CLA	CHC-C1C	2.07	1.42	1.38
14	b	824	CLA	C3B-C4B	2.07	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	826	CLA	C3B-C4B	2.07	1.48	1.42
14	b	816	CLA	C3B-C4B	2.07	1.48	1.42
14	6	4404	CLA	MG-ND	-2.07	2.01	2.05
14	B	833	CLA	CHC-C1C	2.07	1.42	1.38
14	B	839	CLA	CHC-C1C	2.07	1.42	1.38
14	b	840	CLA	C3B-C4B	2.07	1.48	1.42
14	8	4004	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	813	CLA	C1B-C2B	2.07	1.48	1.43
14	A	828	CLA	C3B-C4B	2.07	1.48	1.42
14	2	832	CLA	CHC-C1C	2.07	1.42	1.38
18	B	803	LMG	O1-C7	-2.07	1.40	1.43
14	a	806	CLA	MG-ND	-2.07	2.01	2.05
14	2	824	CLA	C3B-C4B	2.07	1.48	1.42
14	a	822	CLA	C3B-C4B	2.07	1.48	1.42
14	A	843	CLA	C3B-C4B	2.07	1.48	1.42
14	l	4205	CLA	C3B-C4B	2.07	1.48	1.42
14	k	4003	CLA	CMB-C2B	-2.07	1.46	1.50
14	l	4206	CLA	CHC-C1C	2.07	1.42	1.38
14	a	830	CLA	C1B-NB	-2.07	1.35	1.37
14	B	829	CLA	MG-ND	-2.07	2.01	2.05
14	7	1103	CLA	CMD-C2D	-2.07	1.46	1.50
14	1	808	CLA	CHC-C1C	2.07	1.42	1.38
14	1	828	CLA	C1B-NB	-2.07	1.35	1.37
14	a	827	CLA	C1B-NB	-2.07	1.35	1.37
14	7	1101	CLA	MG-ND	-2.07	2.01	2.05
14	K	4004	CLA	C3B-C4B	2.07	1.48	1.42
14	A	829	CLA	C1B-NB	-2.07	1.35	1.37
14	f	201	CLA	C1B-NB	-2.07	1.35	1.37
14	l	4204	CLA	CMC-C2C	-2.07	1.46	1.50
14	1	829	CLA	C3B-C4B	2.07	1.48	1.42
14	a	831	CLA	MG-ND	-2.07	2.01	2.05
14	a	831	CLA	CHC-C1C	2.07	1.42	1.38
14	B	810	CLA	C4B-NB	2.07	1.40	1.37
14	1	830	CLA	C4B-NB	2.07	1.40	1.37
14	B	802	CLA	CHC-C1C	2.07	1.42	1.38
14	A	806	CLA	MG-ND	-2.07	2.01	2.05
14	A	844	CLA	MG-ND	-2.07	2.01	2.05
14	K	4002	CLA	CHC-C1C	2.07	1.42	1.38
14	0	207	CLA	C3B-C4B	2.07	1.48	1.42
17	b	851	BCR	C38-C26	-2.06	1.47	1.50
14	B	836	CLA	MG-ND	-2.06	2.01	2.05
14	B	809	CLA	C3B-C4B	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	809	CLA	C3B-C4B	2.06	1.48	1.42
14	1	829	CLA	MG-ND	-2.06	2.01	2.05
17	b	854	BCR	C33-C5	-2.06	1.47	1.50
14	b	809	CLA	C3B-C4B	2.06	1.48	1.42
14	2	808	CLA	C3B-C4B	2.06	1.48	1.42
14	B	826	CLA	MG-ND	-2.06	2.01	2.05
14	a	842	CLA	MG-ND	-2.06	2.01	2.05
14	b	830	CLA	C4B-NB	2.06	1.40	1.37
14	2	829	CLA	C4B-NB	2.06	1.40	1.37
14	A	816	CLA	MG-ND	-2.06	2.01	2.05
14	b	807	CLA	MG-NB	-2.06	2.01	2.05
14	b	802	CLA	C3B-C4B	2.06	1.48	1.42
14	2	833	CLA	C3B-C4B	2.06	1.48	1.42
19	6	4401	LMT	O2B-C2B	-2.06	1.37	1.43
14	b	801	CLA	C1B-NB	-2.06	1.35	1.37
14	A	841	CLA	MG-ND	-2.06	2.01	2.05
14	1	813	CLA	CMA-C3A	-2.06	1.48	1.53
14	1	821	CLA	C3B-C4B	2.06	1.48	1.42
14	A	822	CLA	CHC-C1C	2.06	1.42	1.38
14	B	804	CLA	C1B-NB	-2.06	1.35	1.37
14	A	830	CLA	C3B-C4B	2.06	1.48	1.42
14	2	826	CLA	C3B-C4B	2.06	1.48	1.42
14	B	843	CLA	MG-ND	-2.06	2.01	2.05
14	1	842	CLA	MG-ND	-2.06	2.01	2.05
14	2	811	CLA	C1B-C2B	2.06	1.48	1.43
14	a	840	CLA	C3B-C4B	2.06	1.48	1.42
14	2	816	CLA	C3B-C4B	2.06	1.48	1.42
14	2	842	CLA	C3B-C4B	2.06	1.48	1.42
14	b	817	CLA	C1B-NB	-2.06	1.35	1.37
14	a	843	CLA	MG-ND	-2.06	2.01	2.05
14	1	843	CLA	MG-ND	-2.06	2.01	2.05
14	A	805	CLA	MG-ND	-2.06	2.01	2.05
14	a	829	CLA	MG-ND	-2.06	2.01	2.05
14	b	814	CLA	MG-ND	-2.06	2.01	2.05
14	b	801	CLA	CHC-C1C	2.06	1.42	1.38
14	0	202	CLA	C1B-NB	-2.06	1.35	1.37
14	A	808	CLA	MG-ND	-2.06	2.01	2.05
14	1	839	CLA	MG-ND	-2.06	2.01	2.05
14	b	841	CLA	C3B-C4B	2.06	1.48	1.42
14	2	842	CLA	MG-ND	-2.06	2.01	2.05
14	8	4003	CLA	CHC-C1C	2.06	1.42	1.38
14	1	840	CLA	C3B-C4B	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	821	CLA	MG-ND	-2.06	2.01	2.05
14	B	809	CLA	CHC-C1C	2.05	1.42	1.38
14	B	838	CLA	MG-ND	-2.05	2.01	2.05
14	A	804	CLA	C1B-NB	-2.05	1.35	1.37
14	1	811	CLA	C1B-NB	-2.05	1.35	1.37
19	I	103	LMT	O1'-C1'	-2.05	1.36	1.40
14	A	810	CLA	C3B-C4B	2.05	1.48	1.42
14	1	840	CLA	MG-ND	-2.05	2.01	2.05
14	2	827	CLA	MG-ND	-2.05	2.01	2.05
14	A	841	CLA	C3B-C4B	2.05	1.48	1.42
14	B	827	CLA	C3B-C4B	2.05	1.48	1.42
14	B	834	CLA	C3B-C4B	2.05	1.48	1.42
14	1	835	CLA	C3B-C4B	2.05	1.48	1.42
14	B	828	CLA	MG-ND	-2.05	2.01	2.05
14	b	814	CLA	CHC-C1C	2.05	1.42	1.38
19	6	4401	LMT	O4'-C4B	-2.05	1.37	1.43
14	j	101	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	838	CLA	CHC-C1C	2.05	1.42	1.38
14	0	206	CLA	CMC-C2C	-2.05	1.46	1.50
14	A	830	CLA	MG-ND	-2.05	2.01	2.05
14	a	817	CLA	MG-ND	-2.05	2.01	2.05
14	b	818	CLA	MG-ND	-2.05	2.01	2.05
14	a	815	CLA	CHC-C1C	2.05	1.42	1.38
14	a	832	CLA	C1B-C2B	2.05	1.47	1.43
14	b	827	CLA	MG-ND	-2.05	2.01	2.05
14	A	836	CLA	C3B-C4B	2.05	1.48	1.42
19	f	202	LMT	O4'-C4B	-2.05	1.37	1.43
14	B	817	CLA	C3B-C4B	2.05	1.48	1.42
14	a	831	CLA	C3B-C4B	2.05	1.48	1.42
14	b	809	CLA	CHC-C1C	2.05	1.42	1.38
14	B	836	CLA	C3B-C4B	2.05	1.48	1.42
14	b	842	CLA	C3B-C4B	2.05	1.48	1.42
14	a	831	CLA	C1B-NB	-2.05	1.35	1.37
14	2	805	CLA	C4B-NB	2.05	1.40	1.37
14	2	836	CLA	MG-ND	-2.05	2.01	2.05
14	2	814	CLA	CHC-C1C	2.05	1.42	1.38
14	1	806	CLA	C1B-NB	-2.05	1.35	1.37
14	2	803	CLA	C1B-NB	-2.05	1.35	1.37
14	1	805	CLA	MG-ND	-2.05	2.01	2.05
14	B	843	CLA	C3B-C4B	2.05	1.48	1.42
14	A	830	CLA	C1B-NB	-2.05	1.35	1.37
14	J	102	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	832	CLA	C3B-C4B	2.05	1.48	1.42
14	A	831	CLA	C1B-C2B	2.05	1.47	1.43
14	1	813	CLA	CHC-C1C	2.05	1.42	1.38
19	i	4101	LMT	O1'-C1'	-2.04	1.36	1.40
14	A	838	CLA	C4B-NB	2.04	1.40	1.37
17	j	104	BCR	C33-C5	-2.04	1.47	1.50
13	A	803	CL0	C3A-C2A	-2.04	1.53	1.54
14	1	812	CLA	C1B-C2B	2.04	1.47	1.43
14	a	811	CLA	C3B-C4B	2.04	1.48	1.42
17	f	203	BCR	C38-C26	-2.04	1.47	1.50
14	A	842	CLA	MG-ND	-2.04	2.01	2.05
14	2	807	CLA	MG-ND	-2.04	2.01	2.05
14	A	818	CLA	CMC-C2C	-2.04	1.46	1.50
14	b	804	CLA	C1B-NB	-2.04	1.35	1.37
14	2	809	CLA	C4B-NB	2.04	1.40	1.37
14	B	841	CLA	CHC-C1C	2.04	1.42	1.38
14	1	815	CLA	MG-ND	-2.04	2.01	2.05
14	J	101	CLA	CMC-C2C	-2.04	1.46	1.50
19	h	103	LMT	O1'-C1'	-2.04	1.36	1.40
14	B	825	CLA	MG-ND	-2.04	2.01	2.05
14	1	822	CLA	C3B-C4B	2.04	1.48	1.42
14	B	828	CLA	C1B-NB	-2.04	1.35	1.37
14	b	811	CLA	MG-ND	-2.04	2.01	2.05
14	a	814	CLA	C3B-C4B	2.04	1.48	1.42
17	2	850	BCR	C33-C5	-2.04	1.47	1.50
19	f	202	LMT	O2B-C2B	-2.04	1.37	1.43
14	B	837	CLA	MG-ND	-2.04	2.01	2.05
14	b	839	CLA	C1B-C2B	2.04	1.47	1.43
17	B	851	BCR	C36-C18	-2.04	1.46	1.50
14	2	830	CLA	C4B-NB	2.04	1.40	1.37
14	2	818	CLA	MG-ND	-2.04	2.01	2.05
14	a	823	CLA	CHC-C1C	2.04	1.42	1.38
14	B	815	CLA	MG-ND	-2.04	2.01	2.05
14	B	811	CLA	C1B-NB	-2.04	1.35	1.37
14	b	836	CLA	MG-ND	-2.04	2.01	2.05
14	1	841	CLA	C1B-NB	-2.04	1.35	1.37
14	1	812	CLA	C3B-C4B	2.04	1.48	1.42
14	2	814	CLA	MG-ND	-2.04	2.01	2.05
14	a	819	CLA	CMC-C2C	-2.04	1.46	1.50
14	A	824	CLA	C3B-C4B	2.04	1.48	1.42
14	1	804	CLA	C1B-NB	-2.03	1.35	1.37
14	l	4204	CLA	MG-ND	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	4203	CLA	C1B-C2B	2.03	1.47	1.43
14	1	813	CLA	MG-ND	-2.03	2.01	2.05
14	1	844	CLA	MG-ND	-2.03	2.01	2.05
14	2	839	CLA	C1B-C2B	2.03	1.47	1.43
14	a	804	CLA	CHC-C1C	2.03	1.42	1.38
14	1	821	CLA	CHC-C1C	2.03	1.42	1.38
14	2	812	CLA	C1B-C2B	2.03	1.47	1.43
17	2	850	BCR	C36-C18	-2.03	1.46	1.50
14	a	809	CLA	MG-ND	-2.03	2.01	2.05
14	b	837	CLA	CHC-C1C	2.03	1.42	1.38
14	B	819	CLA	MG-ND	-2.03	2.01	2.05
14	2	827	CLA	C1B-NB	-2.03	1.35	1.37
17	b	850	BCR	C36-C18	-2.03	1.46	1.50
14	A	813	CLA	C3B-C4B	2.03	1.48	1.42
14	a	840	CLA	MG-ND	-2.03	2.01	2.05
14	b	827	CLA	C1B-NB	-2.03	1.35	1.37
14	2	834	CLA	C1B-C2B	2.03	1.47	1.43
14	a	824	CLA	C3B-C4B	2.03	1.48	1.42
14	a	844	CLA	C3B-C4B	2.03	1.48	1.42
14	2	810	CLA	MG-ND	-2.03	2.01	2.05
14	7	1102	CLA	CMC-C2C	-2.03	1.46	1.50
14	8	4002	CLA	CHC-C1C	2.03	1.42	1.38
14	a	844	CLA	MG-ND	-2.03	2.01	2.05
14	1	837	CLA	C4B-NB	2.03	1.40	1.37
14	2	813	CLA	C3B-C4B	2.03	1.48	1.42
14	B	831	CLA	C4B-NB	2.03	1.40	1.37
14	2	843	CLA	MG-ND	-2.03	2.01	2.05
14	B	840	CLA	C1B-C2B	2.03	1.47	1.43
14	a	807	CLA	MG-ND	-2.03	2.01	2.05
14	1	844	CLA	C3B-C4B	2.03	1.48	1.42
19	F	202	LMT	O4'-C4B	-2.03	1.37	1.43
14	b	828	CLA	MG-ND	-2.03	2.01	2.05
14	a	832	CLA	C4B-NB	2.03	1.40	1.37
14	a	833	CLA	C1B-C2B	2.03	1.47	1.43
17	J	104	BCR	C33-C5	-2.03	1.47	1.50
14	a	826	CLA	CHC-C1C	2.03	1.42	1.38
19	F	202	LMT	O2B-C2B	-2.03	1.37	1.43
14	k	4002	CLA	CHC-C1C	2.03	1.42	1.38
17	7	1104	BCR	C33-C5	-2.03	1.47	1.50
14	2	821	CLA	CHC-C1C	2.03	1.42	1.38
17	M	102	BCR	C33-C5	-2.03	1.47	1.50
14	b	812	CLA	C1B-C2B	2.03	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	829	CLA	C1B-NB	-2.03	1.35	1.37
14	a	822	CLA	CHC-C1C	2.03	1.42	1.38
14	a	837	CLA	C3B-C4B	2.02	1.48	1.42
14	A	828	CLA	MG-ND	-2.02	2.01	2.05
14	b	834	CLA	C1B-C2B	2.02	1.47	1.43
14	7	1103	CLA	CHC-C1C	2.02	1.42	1.38
14	1	830	CLA	C3B-C4B	2.02	1.48	1.42
14	B	805	CLA	C1B-NB	-2.02	1.35	1.37
17	2	846	BCR	C38-C26	-2.02	1.47	1.50
14	B	831	CLA	C1B-C2B	2.02	1.47	1.43
14	2	824	CLA	MG-ND	-2.02	2.01	2.05
17	b	850	BCR	C33-C5	-2.02	1.47	1.50
14	2	832	CLA	C3B-C4B	2.02	1.48	1.42
14	A	832	CLA	C1B-C2B	2.02	1.47	1.43
14	2	828	CLA	CHC-C1C	2.02	1.42	1.38
14	2	813	CLA	MG-ND	-2.02	2.01	2.05
14	2	815	CLA	MG-ND	-2.02	2.01	2.05
14	2	810	CLA	C1B-NB	-2.02	1.35	1.37
14	b	835	CLA	C3B-C4B	2.02	1.48	1.42
14	A	844	CLA	C3B-C4B	2.02	1.48	1.42
14	1	830	CLA	C1B-C2B	2.02	1.47	1.43
14	A	820	CLA	CHC-C1C	2.02	1.42	1.38
14	2	841	CLA	C3B-C4B	2.02	1.48	1.42
14	1	811	CLA	MG-ND	-2.02	2.01	2.05
14	b	813	CLA	MG-ND	-2.02	2.01	2.05
14	1	806	CLA	CMA-C3A	-2.02	1.48	1.53
14	B	802	CLA	C1B-NB	-2.02	1.35	1.37
14	F	201	CLA	C1B-NB	-2.02	1.35	1.37
14	1	835	CLA	C1B-NB	-2.02	1.35	1.37
14	A	824	CLA	MG-ND	-2.02	2.01	2.05
14	L	1501	CLA	MG-ND	-2.02	2.01	2.05
14	L	1502	CLA	MG-ND	-2.02	2.01	2.05
14	a	837	CLA	C1B-NB	-2.02	1.35	1.37
14	1	827	CLA	C1B-NB	-2.02	1.35	1.37
14	2	835	CLA	C3B-C4B	2.02	1.48	1.42
14	a	815	CLA	MG-ND	-2.02	2.01	2.05
14	b	843	CLA	MG-ND	-2.02	2.01	2.05
14	a	825	CLA	C3B-C4B	2.02	1.48	1.42
14	1	823	CLA	C3B-C4B	2.02	1.48	1.42
14	2	805	CLA	C1B-C2B	2.02	1.47	1.43
14	B	811	CLA	MG-ND	-2.02	2.01	2.05
14	1	834	CLA	C1B-NB	-2.02	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	842	CLA	C3B-C4B	2.01	1.48	1.42
14	a	805	CLA	C1B-C2B	2.01	1.47	1.43
14	A	807	CLA	C1B-NB	-2.01	1.35	1.37
14	B	842	CLA	C3B-C4B	2.01	1.48	1.42
17	6	4402	BCR	C38-C26	-2.01	1.47	1.50
14	B	826	CLA	CHC-C1C	2.01	1.42	1.38
14	B	833	CLA	C3B-C4B	2.01	1.48	1.42
14	B	809	CLA	CAC-C3C	-2.01	1.45	1.51
14	A	821	CLA	CHC-C1C	2.01	1.42	1.38
14	j	102	CLA	CHC-C1C	2.01	1.42	1.38
18	b	803	LMG	O1-C7	-2.01	1.40	1.43
14	b	824	CLA	MG-ND	-2.01	2.01	2.05
14	2	825	CLA	CHC-C1C	2.01	1.42	1.38
17	a	850	BCR	C38-C26	-2.01	1.47	1.50
14	a	821	CLA	CHC-C1C	2.01	1.42	1.38
14	A	813	CLA	C1B-C2B	2.01	1.47	1.43
14	B	816	CLA	MG-ND	-2.01	2.01	2.05
14	B	806	CLA	C4B-NB	2.01	1.40	1.37
14	1	827	CLA	MG-ND	-2.01	2.01	2.05
14	a	814	CLA	C1B-C2B	2.01	1.47	1.43
14	a	815	CLA	CMA-C3A	-2.01	1.48	1.53
14	a	832	CLA	C3B-C4B	2.01	1.48	1.42
14	b	815	CLA	C3B-C4B	2.01	1.48	1.42
14	a	826	CLA	C3B-C4B	2.01	1.48	1.42
14	B	806	CLA	C1B-C2B	2.01	1.47	1.43
14	B	835	CLA	C1B-C2B	2.01	1.47	1.43
14	a	842	CLA	C3B-C4B	2.01	1.48	1.42
14	a	813	CLA	C1B-NB	-2.01	1.35	1.37
14	a	836	CLA	CHC-C1C	2.01	1.42	1.38
14	b	830	CLA	C1B-C2B	2.01	1.47	1.43
14	A	805	CLA	C3B-C4B	2.01	1.48	1.42
14	a	806	CLA	C3B-C4B	2.01	1.48	1.42
14	a	840	CLA	CHC-C1C	2.01	1.42	1.38
14	A	810	CLA	MG-ND	-2.01	2.01	2.05
14	a	813	CLA	MG-ND	-2.01	2.01	2.05
14	a	820	CLA	MG-ND	-2.01	2.01	2.05
17	B	851	BCR	C33-C5	-2.01	1.47	1.50
14	A	839	CLA	MG-ND	-2.01	2.01	2.05
14	0	207	CLA	MG-ND	-2.01	2.01	2.05
14	1	804	CLA	C1B-C2B	2.01	1.47	1.43
14	A	835	CLA	C1B-NB	-2.01	1.35	1.37
14	2	810	CLA	C3B-C4B	2.00	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	1101	CLA	C3B-C4B	2.00	1.48	1.42
17	1	850	BCR	C38-C26	-2.00	1.47	1.50
18	2	802	LMG	O1-C7	-2.00	1.40	1.43
14	A	814	CLA	C1B-NB	-2.00	1.35	1.37
14	b	815	CLA	MG-ND	-2.00	2.01	2.05
14	B	815	CLA	CHC-C1C	2.00	1.42	1.38
14	B	840	CLA	C4B-NB	2.00	1.40	1.37
14	b	806	CLA	C4B-NB	2.00	1.40	1.37
14	1	807	CLA	MG-ND	-2.00	2.01	2.05
17	7	1105	BCR	C33-C5	-2.00	1.47	1.50
14	B	816	CLA	C3B-C4B	2.00	1.48	1.42
14	A	814	CLA	CMA-C3A	-2.00	1.49	1.53
14	a	808	CLA	C1B-NB	-2.00	1.35	1.37
14	1	817	CLA	CMC-C2C	-2.00	1.46	1.50
14	1	824	CLA	C3B-C4B	2.00	1.48	1.42
14	B	810	CLA	MG-ND	-2.00	2.01	2.05

All (2695) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	829	CLA	C4A-NA-C1A	8.22	110.43	106.68
14	a	830	CLA	C4A-NA-C1A	8.19	110.42	106.68
14	1	828	CLA	C4A-NA-C1A	8.17	110.41	106.68
14	A	825	CLA	C4A-NA-C1A	7.96	110.31	106.68
14	1	824	CLA	C4A-NA-C1A	7.94	110.30	106.68
14	a	826	CLA	C4A-NA-C1A	7.88	110.27	106.68
14	f	204	CLA	C4A-NA-C1A	7.74	110.21	106.68
14	F	204	CLA	C4A-NA-C1A	7.69	110.19	106.68
14	A	830	CLA	C4A-NA-C1A	7.60	110.15	106.68
14	6	4403	CLA	C4A-NA-C1A	7.57	110.13	106.68
14	a	831	CLA	C4A-NA-C1A	7.54	110.12	106.68
14	B	824	CLA	C4A-NA-C1A	7.53	110.12	106.68
14	1	829	CLA	C4A-NA-C1A	7.52	110.11	106.68
14	b	823	CLA	C4A-NA-C1A	7.50	110.10	106.68
14	K	4003	CLA	C4A-NA-C1A	7.49	110.09	106.68
14	J	101	CLA	C4A-NA-C1A	7.47	110.09	106.68
14	7	1102	CLA	C4A-NA-C1A	7.47	110.09	106.68
14	8	4003	CLA	C4A-NA-C1A	7.47	110.08	106.68
14	2	823	CLA	C4A-NA-C1A	7.45	110.08	106.68
14	j	101	CLA	C4A-NA-C1A	7.44	110.07	106.68
14	2	804	CLA	C4A-NA-C1A	7.43	110.07	106.68
14	b	805	CLA	C4A-NA-C1A	7.43	110.07	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	810	CLA	C4A-NA-C1A	7.43	110.07	106.68
14	a	825	CLA	C4A-NA-C1A	7.43	110.07	106.68
14	b	811	CLA	C4A-NA-C1A	7.43	110.07	106.68
14	A	807	CLA	C4A-NA-C1A	7.41	110.06	106.68
14	B	811	CLA	C4A-NA-C1A	7.41	110.06	106.68
14	k	4003	CLA	C4A-NA-C1A	7.41	110.06	106.68
14	A	824	CLA	C4A-NA-C1A	7.40	110.06	106.68
14	a	808	CLA	C4A-NA-C1A	7.40	110.06	106.68
14	b	812	CLA	C4A-NA-C1A	7.38	110.05	106.68
14	2	811	CLA	C4A-NA-C1A	7.38	110.05	106.68
14	B	812	CLA	C4A-NA-C1A	7.38	110.04	106.68
14	1	823	CLA	C4A-NA-C1A	7.37	110.04	106.68
14	B	805	CLA	C4A-NA-C1A	7.35	110.03	106.68
14	B	836	CLA	C4A-NA-C1A	7.35	110.03	106.68
14	b	822	CLA	C4A-NA-C1A	7.34	110.03	106.68
14	B	820	CLA	C4A-NA-C1A	7.34	110.03	106.68
14	2	819	CLA	C4A-NA-C1A	7.34	110.03	106.68
14	2	835	CLA	C4A-NA-C1A	7.33	110.02	106.68
14	B	813	CLA	C4A-NA-C1A	7.32	110.02	106.68
14	1	806	CLA	C4A-NA-C1A	7.32	110.02	106.68
14	2	831	CLA	C4A-NA-C1A	7.31	110.01	106.68
14	b	819	CLA	C4A-NA-C1A	7.30	110.01	106.68
14	2	822	CLA	C4A-NA-C1A	7.28	110.00	106.68
14	1	810	CLA	C4A-NA-C1A	7.28	110.00	106.68
14	B	832	CLA	C4A-NA-C1A	7.28	110.00	106.68
14	B	809	CLA	C4A-NA-C1A	7.27	110.00	106.68
14	b	835	CLA	C4A-NA-C1A	7.27	110.00	106.68
14	a	812	CLA	C4A-NA-C1A	7.27	109.99	106.68
14	2	812	CLA	C4A-NA-C1A	7.26	109.99	106.68
14	B	823	CLA	C4A-NA-C1A	7.25	109.99	106.68
14	B	838	CLA	C4A-NA-C1A	7.25	109.99	106.68
14	b	809	CLA	C4A-NA-C1A	7.24	109.98	106.68
14	2	808	CLA	C4A-NA-C1A	7.24	109.98	106.68
14	b	837	CLA	C4A-NA-C1A	7.24	109.98	106.68
14	A	806	CLA	C4A-NA-C1A	7.23	109.98	106.68
14	b	831	CLA	C4A-NA-C1A	7.22	109.97	106.68
14	a	807	CLA	C4A-NA-C1A	7.21	109.97	106.68
14	2	824	CLA	C4A-NA-C1A	7.21	109.97	106.68
14	a	827	CLA	C4A-NA-C1A	7.20	109.97	106.68
14	b	824	CLA	C4A-NA-C1A	7.20	109.96	106.68
14	A	837	CLA	C4A-NA-C1A	7.19	109.96	106.68
14	B	825	CLA	C4A-NA-C1A	7.19	109.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	806	CLA	C4A-NA-C1A	7.19	109.96	106.68
14	a	838	CLA	C4A-NA-C1A	7.19	109.96	106.68
14	2	837	CLA	C4A-NA-C1A	7.19	109.96	106.68
14	A	811	CLA	C4A-NA-C1A	7.16	109.94	106.68
14	1	805	CLA	C4A-NA-C1A	7.15	109.94	106.68
14	1	836	CLA	C4A-NA-C1A	7.14	109.94	106.68
14	A	826	CLA	C4A-NA-C1A	7.13	109.93	106.68
14	B	806	CLA	C4A-NA-C1A	7.13	109.93	106.68
14	l	4203	CLA	C4A-NA-C1A	7.12	109.93	106.68
14	a	809	CLA	C4A-NA-C1A	7.11	109.92	106.68
14	1	825	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	1	807	CLA	C4A-NA-C1A	7.09	109.91	106.68
14	2	805	CLA	C4A-NA-C1A	7.09	109.91	106.68
14	2	818	CLA	C4A-NA-C1A	7.07	109.91	106.68
14	A	808	CLA	C4A-NA-C1A	7.06	109.90	106.68
14	B	819	CLA	C4A-NA-C1A	7.03	109.89	106.68
14	A	842	CLA	C4A-NA-C1A	7.02	109.88	106.68
14	a	836	CLA	C4A-NA-C1A	6.92	109.84	106.68
14	a	842	CLA	C4A-NA-C1A	6.92	109.84	106.68
14	1	834	CLA	C4A-NA-C1A	6.92	109.84	106.68
14	1	842	CLA	C4A-NA-C1A	6.89	109.82	106.68
14	b	818	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	a	803	CL0	C1B-CHB-C4A	6.84	125.72	121.32
14	a	841	CLA	C4A-NA-C1A	6.84	109.80	106.68
14	1	815	CLA	C4A-NA-C1A	6.83	109.80	106.68
14	b	841	CLA	C4A-NA-C1A	6.81	109.79	106.68
14	1	839	CLA	C4A-NA-C1A	6.81	109.79	106.68
14	a	817	CLA	C4A-NA-C1A	6.80	109.78	106.68
13	A	803	CL0	C1B-CHB-C4A	6.80	125.70	121.32
14	1	844	CLA	C4A-NA-C1A	6.80	109.78	106.68
14	2	841	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	A	835	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	k	4002	CLA	C4A-NA-C1A	6.78	109.77	106.68
13	1	803	CL0	C1B-CHB-C4A	6.78	125.69	121.32
14	A	840	CLA	C4A-NA-C1A	6.77	109.77	106.68
14	A	816	CLA	C4A-NA-C1A	6.76	109.76	106.68
14	a	834	CLA	C4A-NA-C1A	6.75	109.76	106.68
14	1	832	CLA	C4A-NA-C1A	6.75	109.76	106.68
14	A	841	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	8	4002	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	1	813	CLA	C4A-NA-C1A	6.73	109.75	106.68
14	B	842	CLA	C4A-NA-C1A	6.72	109.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	K	4002	CLA	C4A-NA-C1A	6.72	109.74	106.68
14	a	815	CLA	C4A-NA-C1A	6.72	109.74	106.68
14	1	840	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	b	802	CLA	C4A-NA-C1A	6.69	109.73	106.68
14	2	844	CLA	C4A-NA-C1A	6.69	109.73	106.68
14	A	844	CLA	C4A-NA-C1A	6.68	109.73	106.68
14	b	844	CLA	C4A-NA-C1A	6.68	109.73	106.68
14	b	832	CLA	C4A-NA-C1A	6.68	109.73	106.68
14	a	844	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	A	833	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	2	832	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	A	814	CLA	C4A-NA-C1A	6.64	109.71	106.68
14	2	843	CLA	C4A-NA-C1A	6.64	109.71	106.68
14	B	808	CLA	C4A-NA-C1A	6.63	109.70	106.68
14	b	843	CLA	C4A-NA-C1A	6.63	109.70	106.68
14	a	840	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	B	845	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	1	808	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	B	833	CLA	C4A-NA-C1A	6.61	109.70	106.68
14	B	844	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	2	816	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	A	819	CLA	C4A-NA-C1A	6.59	109.69	106.68
14	a	818	CLA	C4A-NA-C1A	6.58	109.68	106.68
14	A	817	CLA	C4A-NA-C1A	6.57	109.68	106.68
14	a	810	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	b	808	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	1	838	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	2	829	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	A	839	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	2	807	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	1	818	CLA	C4A-NA-C1A	6.54	109.66	106.68
14	a	820	CLA	C4A-NA-C1A	6.52	109.66	106.68
14	b	817	CLA	C4A-NA-C1A	6.52	109.66	106.68
14	A	809	CLA	C4A-NA-C1A	6.52	109.65	106.68
14	B	817	CLA	C4A-NA-C1A	6.52	109.65	106.68
14	1	816	CLA	C4A-NA-C1A	6.51	109.65	106.68
14	b	816	CLA	C4A-NA-C1A	6.50	109.64	106.68
14	B	830	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	b	838	CLA	C4A-NA-C1A	6.44	109.62	106.68
14	2	817	CLA	C4A-NA-C1A	6.44	109.62	106.68
14	0	207	CLA	C4A-NA-C1A	6.41	109.60	106.68
14	b	829	CLA	C4A-NA-C1A	6.40	109.60	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	826	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	B	818	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	a	833	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	B	839	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	2	838	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	A	832	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	L	1502	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	l	4205	CLA	C4A-NA-C1A	6.30	109.55	106.68
14	B	827	CLA	C4A-NA-C1A	6.26	109.53	106.68
14	1	819	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	b	826	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	L	1501	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	b	820	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	2	833	CLA	C4A-NA-C1A	6.24	109.52	106.68
14	1	811	CLA	C4A-NA-C1A	6.23	109.52	106.68
14	1	831	CLA	C4A-NA-C1A	6.23	109.52	106.68
14	l	4204	CLA	C4A-NA-C1A	6.23	109.52	106.68
14	a	813	CLA	C4A-NA-C1A	6.20	109.51	106.68
14	0	206	CLA	C4A-NA-C1A	6.20	109.51	106.68
14	a	837	CLA	C4A-NA-C1A	6.19	109.50	106.68
14	A	820	CLA	C4A-NA-C1A	6.18	109.50	106.68
14	2	820	CLA	C4A-NA-C1A	6.18	109.50	106.68
14	a	821	CLA	C4A-NA-C1A	6.17	109.50	106.68
14	1	835	CLA	C4A-NA-C1A	6.17	109.49	106.68
14	A	812	CLA	C4A-NA-C1A	6.15	109.49	106.68
14	B	834	CLA	C4A-NA-C1A	6.15	109.48	106.68
14	1	833	CLA	C4A-NA-C1A	6.14	109.48	106.68
14	B	821	CLA	C4A-NA-C1A	6.10	109.46	106.68
14	a	835	CLA	C4A-NA-C1A	6.10	109.46	106.68
14	A	834	CLA	C4A-NA-C1A	6.09	109.46	106.68
14	A	836	CLA	C4A-NA-C1A	6.09	109.46	106.68
14	B	815	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	B	807	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	b	814	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	2	825	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	b	833	CLA	C4A-NA-C1A	6.04	109.44	106.68
14	2	814	CLA	C4A-NA-C1A	6.00	109.42	106.68
14	b	807	CLA	C4A-NA-C1A	5.95	109.39	106.68
14	B	810	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	b	815	CLA	C4A-NA-C1A	5.91	109.38	106.68
14	B	816	CLA	C4A-NA-C1A	5.90	109.37	106.68
14	B	826	CLA	C4A-NA-C1A	5.89	109.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	825	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	A	815	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	2	809	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	b	810	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	2	806	CLA	C4A-NA-C1A	5.79	109.32	106.68
14	2	836	CLA	C4A-NA-C1A	5.78	109.32	106.68
14	1	814	CLA	C4A-NA-C1A	5.77	109.31	106.68
14	2	815	CLA	C4A-NA-C1A	5.76	109.31	106.68
14	a	816	CLA	C4A-NA-C1A	5.75	109.30	106.68
14	A	818	CLA	C4A-NA-C1A	5.74	109.30	106.68
14	a	819	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	a	832	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	1	817	CLA	C4A-NA-C1A	5.71	109.28	106.68
14	B	837	CLA	C4A-NA-C1A	5.70	109.28	106.68
14	b	836	CLA	C4A-NA-C1A	5.70	109.28	106.68
14	f	201	CLA	C4A-NA-C1A	5.69	109.28	106.68
14	1	841	CLA	C4A-NA-C1A	5.67	109.27	106.68
14	F	201	CLA	C4A-NA-C1A	5.61	109.24	106.68
14	7	1103	CLA	C4A-NA-C1A	5.61	109.24	106.68
14	A	831	CLA	C4A-NA-C1A	5.61	109.24	106.68
14	1	830	CLA	C4A-NA-C1A	5.61	109.24	106.68
14	l	4206	CLA	C4A-NA-C1A	5.60	109.23	106.68
14	j	102	CLA	C4A-NA-C1A	5.59	109.23	106.68
14	b	821	CLA	C4A-NA-C1A	5.56	109.22	106.68
14	J	102	CLA	C4A-NA-C1A	5.56	109.22	106.68
14	L	1503	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	B	822	CLA	C4A-NA-C1A	5.53	109.20	106.68
14	a	806	CLA	C4A-NA-C1A	5.53	109.20	106.68
14	A	805	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	1	812	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	A	813	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	7	1101	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	2	821	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	0	208	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	a	814	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	b	801	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	A	823	CLA	C4A-NA-C1A	5.38	109.13	106.68
14	0	202	CLA	C4A-NA-C1A	5.34	109.11	106.68
14	a	824	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	1	822	CLA	C4A-NA-C1A	5.29	109.09	106.68
14	B	802	CLA	C4A-NA-C1A	5.29	109.09	106.68
14	b	834	CLA	C4A-NA-C1A	5.26	109.08	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	835	CLA	C4A-NA-C1A	5.23	109.06	106.68
14	A	821	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	a	822	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	b	830	CLA	C4A-NA-C1A	5.18	109.04	106.68
14	B	831	CLA	C4A-NA-C1A	5.16	109.03	106.68
14	B	801	CLA	C4A-NA-C1A	5.15	109.03	106.68
14	2	834	CLA	C4A-NA-C1A	5.15	109.03	106.68
14	b	813	CLA	C4A-NA-C1A	5.15	109.03	106.68
14	1	820	CLA	C4A-NA-C1A	5.12	109.02	106.68
14	B	829	CLA	C4A-NA-C1A	5.12	109.01	106.68
14	2	813	CLA	C4A-NA-C1A	5.11	109.01	106.68
14	2	828	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	B	812	CLA	CMB-C2B-C1B	-5.07	117.70	125.42
14	2	811	CLA	CMB-C2B-C1B	-5.06	117.72	125.42
14	2	830	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	a	804	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	b	812	CLA	CMB-C2B-C1B	-5.05	117.73	125.42
14	a	828	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	b	828	CLA	C4A-NA-C1A	5.04	108.98	106.68
14	1	826	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	2	801	CLA	C4A-NA-C1A	4.99	108.96	106.68
14	B	832	CLA	CMB-C2B-C1B	-4.98	117.83	125.42
14	B	814	CLA	C4A-NA-C1A	4.96	108.94	106.68
14	2	831	CLA	CMB-C2B-C1B	-4.96	117.87	125.42
14	A	827	CLA	C4A-NA-C1A	4.95	108.94	106.68
14	a	854	CLA	C4A-NA-C1A	4.94	108.93	106.68
14	b	831	CLA	CMB-C2B-C1B	-4.94	117.90	125.42
14	B	840	CLA	CMB-C2B-C1B	-4.92	117.93	125.42
14	b	839	CLA	CMB-C2B-C1B	-4.91	117.94	125.42
14	K	4004	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	2	839	CLA	CMB-C2B-C1B	-4.87	118.01	125.42
14	8	4004	CLA	C4A-NA-C1A	4.85	108.89	106.68
14	B	804	CLA	C3B-C4B-NB	-4.76	106.28	110.53
14	1	821	CLA	C4A-NA-C1A	4.75	108.84	106.68
14	b	804	CLA	C3B-C4B-NB	-4.74	106.30	110.53
14	1	827	CLA	C4A-NA-C1A	4.73	108.84	106.68
14	a	823	CLA	C4A-NA-C1A	4.72	108.83	106.68
14	A	822	CLA	C4A-NA-C1A	4.71	108.83	106.68
14	2	803	CLA	C3B-C4B-NB	-4.70	106.33	110.53
14	1	833	CLA	C3B-C4B-NB	-4.67	106.36	110.53
14	A	828	CLA	C4A-NA-C1A	4.66	108.81	106.68
14	a	829	CLA	C4A-NA-C1A	4.65	108.80	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	834	CLA	C3B-C4B-NB	-4.65	106.38	110.53
14	A	843	CLA	C4A-NA-C1A	4.62	108.78	106.68
14	a	835	CLA	C3B-C4B-NB	-4.60	106.42	110.53
14	a	827	CLA	C3B-C4B-NB	-4.60	106.43	110.53
14	a	811	CLA	C4A-NA-C1A	4.59	108.78	106.68
14	A	826	CLA	C3B-C4B-NB	-4.59	106.43	110.53
14	A	810	CLA	C4A-NA-C1A	4.58	108.77	106.68
14	1	825	CLA	C3B-C4B-NB	-4.58	106.44	110.53
14	1	843	CLA	C4A-NA-C1A	4.57	108.77	106.68
14	a	843	CLA	C4A-NA-C1A	4.56	108.76	106.68
14	2	834	CLA	C3B-C4B-NB	-4.56	106.46	110.53
14	B	843	CLA	C3B-C4B-NB	-4.55	106.47	110.53
14	b	842	CLA	C3B-C4B-NB	-4.54	106.47	110.53
14	2	842	CLA	C3B-C4B-NB	-4.53	106.49	110.53
14	B	835	CLA	C3B-C4B-NB	-4.49	106.52	110.53
14	b	834	CLA	C3B-C4B-NB	-4.49	106.52	110.53
14	1	809	CLA	C4A-NA-C1A	4.47	108.72	106.68
12	a	801	LHG	O4-P-O5	4.46	133.18	112.44
12	A	801	LHG	O4-P-O5	4.45	133.14	112.44
12	1	801	LHG	O4-P-O5	4.45	133.13	112.44
14	2	839	CLA	C3B-C4B-NB	-4.44	106.57	110.53
12	9	101	LHG	O4-P-O5	4.44	133.09	112.44
12	M	101	LHG	O4-P-O5	4.44	133.08	112.44
12	m	101	LHG	O4-P-O5	4.43	133.04	112.44
14	b	839	CLA	C3B-C4B-NB	-4.42	106.58	110.53
14	b	806	CLA	C3B-C4B-NB	-4.41	106.59	110.53
14	B	806	CLA	C3B-C4B-NB	-4.41	106.59	110.53
12	b	852	LHG	O4-P-O5	4.41	132.97	112.44
14	B	840	CLA	C3B-C4B-NB	-4.41	106.59	110.53
12	1	802	LHG	O4-P-O5	4.41	132.95	112.44
12	2	852	LHG	O4-P-O5	4.40	132.93	112.44
12	a	802	LHG	O4-P-O5	4.40	132.92	112.44
12	B	853	LHG	O4-P-O5	4.40	132.91	112.44
12	A	802	LHG	O4-P-O5	4.40	132.91	112.44
14	1	831	CLA	CMB-C2B-C1B	-4.40	118.72	125.42
14	2	805	CLA	C3B-C4B-NB	-4.39	106.61	110.53
14	A	832	CLA	CMB-C2B-C1B	-4.39	118.74	125.42
14	a	833	CLA	CMB-C2B-C1B	-4.39	118.74	125.42
14	a	834	CLA	C3B-C4B-NB	-4.36	106.64	110.53
14	1	832	CLA	C3B-C4B-NB	-4.35	106.64	110.53
14	A	833	CLA	C3B-C4B-NB	-4.33	106.67	110.53
14	L	1502	CLA	C3B-C4B-NB	-4.31	106.69	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	205	CLA	C4A-NA-C1A	4.29	108.64	106.68
14	l	4205	CLA	C3B-C4B-NB	-4.29	106.70	110.53
14	0	207	CLA	C3B-C4B-NB	-4.27	106.71	110.53
14	B	801	CLA	CMB-C2B-C1B	-4.25	118.95	125.42
14	a	839	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	B	840	CLA	C4A-NA-C1A	4.24	108.61	106.68
14	a	804	CLA	CMB-C2B-C1B	-4.23	118.98	125.42
14	A	838	CLA	C4A-NA-C1A	4.22	108.61	106.68
14	f	205	CLA	C4A-NA-C1A	4.22	108.61	106.68
14	b	839	CLA	C4A-NA-C1A	4.22	108.60	106.68
14	6	4404	CLA	C4A-NA-C1A	4.21	108.60	106.68
14	2	801	CLA	CMB-C2B-C1B	-4.21	119.01	125.42
14	1	837	CLA	C4A-NA-C1A	4.21	108.60	106.68
14	1	830	CLA	CMB-C2B-C1B	-4.20	119.02	125.42
14	2	839	CLA	C4A-NA-C1A	4.20	108.59	106.68
14	a	832	CLA	CMB-C2B-C1B	-4.19	119.04	125.42
14	A	831	CLA	CMB-C2B-C1B	-4.19	119.04	125.42
14	B	831	CLA	CMB-C2B-C1B	-4.17	119.06	125.42
13	1	803	CL0	C4D-CHA-CBD	-4.17	104.76	108.97
17	0	209	BCR	C24-C23-C22	-4.17	120.06	126.23
14	b	830	CLA	CMB-C2B-C1B	-4.15	119.10	125.42
13	A	803	CL0	C4D-CHA-CBD	-4.15	104.78	108.97
17	L	1504	BCR	C24-C23-C22	-4.15	120.10	126.23
17	l	4207	BCR	C24-C23-C22	-4.15	120.10	126.23
14	2	830	CLA	CMB-C2B-C1B	-4.14	119.12	125.42
13	a	803	CL0	C4D-CHA-CBD	-4.13	104.80	108.97
14	a	824	CLA	C3B-C4B-NB	-4.12	106.86	110.53
14	A	823	CLA	C3B-C4B-NB	-4.11	106.86	110.53
14	1	822	CLA	C3B-C4B-NB	-4.09	106.88	110.53
14	B	841	CLA	C4A-NA-C1A	4.07	108.53	106.68
14	b	831	CLA	C3B-C4B-NB	-4.05	106.92	110.53
14	B	832	CLA	C3B-C4B-NB	-4.02	106.94	110.53
17	I	101	BCR	C15-C16-C17	-4.02	115.29	123.52
14	a	810	CLA	C3B-C4B-NB	-4.02	106.94	110.53
17	h	101	BCR	C15-C16-C17	-4.01	115.32	123.52
14	2	831	CLA	C3B-C4B-NB	-4.00	106.95	110.53
15	2	845	PQN	C11-C12-C13	-4.00	119.93	126.83
14	2	840	CLA	C4A-NA-C1A	4.00	108.50	106.68
17	i	4102	BCR	C15-C16-C17	-4.00	115.34	123.52
17	b	850	BCR	C24-C23-C22	-4.00	120.32	126.23
14	A	809	CLA	C3B-C4B-NB	-4.00	106.96	110.53
17	8	4005	BCR	C2-C1-C6	4.00	116.24	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	851	BCR	C24-C23-C22	-3.99	120.33	126.23
15	B	846	PQN	C11-C12-C13	-3.99	119.96	126.83
17	k	4004	BCR	C2-C1-C6	3.99	116.23	110.44
14	1	808	CLA	C3B-C4B-NB	-3.98	106.97	110.53
14	0	206	CLA	C3B-C4B-NB	-3.98	106.98	110.53
17	2	849	BCR	C15-C16-C17	-3.98	115.38	123.52
17	b	849	BCR	C15-C16-C17	-3.97	115.39	123.52
15	b	845	PQN	C11-C12-C13	-3.97	119.99	126.83
17	K	4005	BCR	C2-C1-C6	3.97	116.21	110.44
14	l	4204	CLA	C3B-C4B-NB	-3.96	106.99	110.53
17	B	850	BCR	C15-C16-C17	-3.96	115.42	123.52
14	B	815	CLA	O2D-CGD-O1D	-3.96	116.14	123.85
14	L	1501	CLA	C3B-C4B-NB	-3.95	107.00	110.53
14	b	840	CLA	C4A-NA-C1A	3.94	108.47	106.68
17	2	850	BCR	C24-C23-C22	-3.93	120.42	126.23
14	b	814	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
14	2	814	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
14	a	834	CLA	CMB-C2B-C1B	-3.92	119.45	125.42
14	A	833	CLA	CMB-C2B-C1B	-3.89	119.50	125.42
14	b	826	CLA	CMB-C2B-C1B	-3.88	119.51	125.42
14	A	820	CLA	C3B-C4B-NB	-3.88	107.07	110.53
14	a	831	CLA	C3B-C4B-NB	-3.88	107.07	110.53
14	1	819	CLA	C3B-C4B-NB	-3.88	107.07	110.53
14	2	826	CLA	CMB-C2B-C1B	-3.88	119.52	125.42
14	A	830	CLA	C3B-C4B-NB	-3.87	107.07	110.53
14	1	832	CLA	CMB-C2B-C1B	-3.87	119.53	125.42
14	B	827	CLA	CMB-C2B-C1B	-3.86	119.54	125.42
14	a	821	CLA	C3B-C4B-NB	-3.86	107.09	110.53
14	f	201	CLA	C3B-C4B-NB	-3.85	107.09	110.53
14	b	841	CLA	C3B-C4B-NB	-3.85	107.09	110.53
14	1	818	CLA	C3B-C4B-NB	-3.84	107.10	110.53
14	1	829	CLA	C3B-C4B-NB	-3.83	107.11	110.53
14	B	805	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
14	2	804	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
14	B	842	CLA	C3B-C4B-NB	-3.83	107.11	110.53
14	1	841	CLA	C3B-C4B-NB	-3.83	107.11	110.53
14	A	819	CLA	C3B-C4B-NB	-3.83	107.11	110.53
14	f	205	CLA	C2A-C3A-C4A	-3.82	95.69	101.87
14	F	201	CLA	C3B-C4B-NB	-3.82	107.12	110.53
14	2	841	CLA	C3B-C4B-NB	-3.82	107.12	110.53
14	b	805	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
14	a	820	CLA	C3B-C4B-NB	-3.81	107.13	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	834	CLA	C3B-C4B-NB	-3.80	107.13	110.53
14	6	4404	CLA	C2A-C3A-C4A	-3.80	95.73	101.87
14	A	808	CLA	C3B-C4B-NB	-3.80	107.14	110.53
14	F	205	CLA	C2A-C3A-C4A	-3.80	95.73	101.87
14	2	843	CLA	C3B-C4B-NB	-3.79	107.14	110.53
14	1	807	CLA	C3B-C4B-NB	-3.78	107.15	110.53
14	A	835	CLA	C3B-C4B-NB	-3.77	107.16	110.53
14	a	836	CLA	C3B-C4B-NB	-3.76	107.17	110.53
14	b	819	CLA	CMB-C2B-C1B	-3.76	119.70	125.42
14	1	842	CLA	C3B-C4B-NB	-3.76	107.18	110.53
14	b	841	CLA	CMB-C2B-C1B	-3.75	119.71	125.42
17	h	102	BCR	C15-C16-C17	-3.75	115.85	123.52
14	a	809	CLA	C3B-C4B-NB	-3.75	107.19	110.53
14	B	820	CLA	CMB-C2B-C1B	-3.75	119.72	125.42
14	B	842	CLA	CMB-C2B-C1B	-3.75	119.72	125.42
14	b	843	CLA	C3B-C4B-NB	-3.75	107.19	110.53
14	b	802	CLA	C3B-C4B-NB	-3.74	107.19	110.53
14	2	819	CLA	CMB-C2B-C1B	-3.74	119.72	125.42
14	2	841	CLA	CMB-C2B-C1B	-3.74	119.73	125.42
14	b	825	CLA	C3B-C4B-NB	-3.74	107.19	110.53
17	I	102	BCR	C15-C16-C17	-3.74	115.88	123.52
14	2	825	CLA	C3B-C4B-NB	-3.73	107.20	110.53
14	B	844	CLA	C3B-C4B-NB	-3.72	107.21	110.53
14	B	826	CLA	C3B-C4B-NB	-3.72	107.21	110.53
14	A	813	CLA	CMB-C2B-C1B	-3.72	119.75	125.42
17	i	4103	BCR	C15-C16-C17	-3.72	115.91	123.52
14	a	814	CLA	CMB-C2B-C1B	-3.72	119.76	125.42
14	1	812	CLA	CMB-C2B-C1B	-3.71	119.77	125.42
14	1	840	CLA	C3B-C4B-NB	-3.71	107.22	110.53
14	a	816	CLA	C3B-C4B-NB	-3.70	107.22	110.53
14	A	811	CLA	C3B-C4B-NB	-3.70	107.23	110.53
14	a	842	CLA	C3B-C4B-NB	-3.69	107.23	110.53
14	1	814	CLA	C3B-C4B-NB	-3.69	107.23	110.53
14	b	833	CLA	C3B-C4B-NB	-3.68	107.24	110.53
14	A	841	CLA	C3B-C4B-NB	-3.68	107.24	110.53
14	A	842	CLA	C3B-C4B-NB	-3.68	107.25	110.53
14	2	833	CLA	C3B-C4B-NB	-3.67	107.25	110.53
14	1	810	CLA	C3B-C4B-NB	-3.67	107.26	110.53
14	a	812	CLA	C3B-C4B-NB	-3.67	107.26	110.53
14	A	838	CLA	C3B-C4B-NB	-3.66	107.26	110.53
14	a	839	CLA	C3B-C4B-NB	-3.65	107.27	110.53
14	1	831	CLA	O2D-CGD-O1D	-3.65	116.75	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	834	CLA	C3B-C4B-NB	-3.64	107.28	110.53
14	A	832	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
14	B	830	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
17	7	1104	BCR	C7-C8-C9	-3.64	120.85	126.23
17	j	103	BCR	C7-C8-C9	-3.63	120.86	126.23
14	A	815	CLA	C3B-C4B-NB	-3.63	107.29	110.53
14	a	833	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
14	b	829	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
14	2	829	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
14	B	833	CLA	C3B-C4B-NB	-3.62	107.30	110.53
14	2	832	CLA	C3B-C4B-NB	-3.62	107.30	110.53
14	b	832	CLA	C3B-C4B-NB	-3.61	107.31	110.53
17	J	103	BCR	C7-C8-C9	-3.61	120.89	126.23
14	1	833	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
17	k	4001	BCR	C15-C14-C13	-3.61	122.22	127.28
14	6	4403	CLA	C3B-C4B-NB	-3.59	107.32	110.53
14	A	834	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
14	2	813	CLA	C3B-C4B-NB	-3.59	107.33	110.53
14	b	832	CLA	CHD-C1D-ND	-3.59	119.76	124.80
14	1	837	CLA	C3B-C4B-NB	-3.59	107.33	110.53
14	2	818	CLA	C3B-C4B-NB	-3.58	107.33	110.53
14	a	835	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
17	K	4001	BCR	C15-C14-C13	-3.58	122.26	127.28
14	1	809	CLA	C3B-C4B-NB	-3.57	107.34	110.53
14	B	833	CLA	CHD-C1D-ND	-3.57	119.78	124.80
14	B	819	CLA	C3B-C4B-NB	-3.57	107.34	110.53
17	1	849	BCR	C15-C16-C17	-3.57	116.22	123.52
17	a	849	BCR	C15-C16-C17	-3.56	116.23	123.52
17	A	849	BCR	C15-C16-C17	-3.56	116.23	123.52
14	2	810	CLA	C3B-C4B-NB	-3.56	107.35	110.53
14	A	806	CLA	C3B-C4B-NB	-3.56	107.36	110.53
14	b	811	CLA	C3B-C4B-NB	-3.56	107.36	110.53
14	f	204	CLA	C3B-C4B-NB	-3.56	107.36	110.53
14	A	810	CLA	C3B-C4B-NB	-3.55	107.36	110.53
14	B	811	CLA	C3B-C4B-NB	-3.55	107.36	110.53
17	8	4001	BCR	C15-C14-C13	-3.55	122.30	127.28
14	2	832	CLA	CHD-C1D-ND	-3.55	119.81	124.80
14	a	807	CLA	C3B-C4B-NB	-3.55	107.36	110.53
14	a	804	CLA	C3B-C4B-NB	-3.55	107.36	110.53
14	2	808	CLA	C3B-C4B-NB	-3.55	107.36	110.53
14	b	809	CLA	C3B-C4B-NB	-3.54	107.37	110.53
14	B	814	CLA	C3B-C4B-NB	-3.54	107.37	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	845	PQN	C14-C13-C15	3.54	121.38	115.23
14	B	809	CLA	C3B-C4B-NB	-3.54	107.37	110.53
17	i	4103	BCR	C11-C10-C9	-3.54	122.31	127.28
15	a	845	PQN	C14-C13-C15	3.54	121.37	115.23
14	F	204	CLA	C3B-C4B-NB	-3.53	107.38	110.53
14	b	818	CLA	C3B-C4B-NB	-3.52	107.38	110.53
17	I	102	BCR	C15-C14-C13	-3.52	122.34	127.28
14	2	801	CLA	C3B-C4B-NB	-3.52	107.39	110.53
15	1	845	PQN	C14-C13-C15	3.52	121.33	115.23
14	B	822	CLA	C3B-C4B-NB	-3.52	107.39	110.53
17	h	102	BCR	C11-C10-C9	-3.51	122.35	127.28
14	a	811	CLA	C3B-C4B-NB	-3.51	107.40	110.53
14	1	805	CLA	C3B-C4B-NB	-3.51	107.40	110.53
14	8	4003	CLA	C3B-C4B-NB	-3.50	107.41	110.53
14	b	813	CLA	C3B-C4B-NB	-3.50	107.41	110.53
14	B	801	CLA	C3B-C4B-NB	-3.50	107.41	110.53
14	l	4205	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
17	i	4103	BCR	C15-C14-C13	-3.49	122.38	127.28
14	A	821	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
14	L	1502	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
14	A	838	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
14	1	837	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
14	b	837	CLA	C3B-C4B-NB	-3.49	107.42	110.53
14	a	822	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
14	2	821	CLA	C3B-C4B-NB	-3.48	107.42	110.53
14	1	820	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
14	0	207	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
14	1	820	CLA	CMB-C2B-C1B	-3.48	120.12	125.42
14	a	839	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
14	1	813	CLA	C3B-C4B-NB	-3.48	107.43	110.53
13	1	803	CL0	O2D-CGD-CBD	3.48	114.77	110.95
14	2	837	CLA	C3B-C4B-NB	-3.47	107.43	110.53
14	b	810	CLA	O2D-CGD-O1D	-3.47	117.08	123.85
14	A	821	CLA	CMB-C2B-C1B	-3.47	120.13	125.42
14	B	810	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
14	b	808	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
14	2	809	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
14	b	821	CLA	C3B-C4B-NB	-3.47	107.43	110.53
13	a	803	CL0	O2D-CGD-CBD	3.47	114.76	110.95
14	2	807	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
14	a	815	CLA	C3B-C4B-NB	-3.47	107.44	110.53
14	K	4003	CLA	C3B-C4B-NB	-3.47	107.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	k	4003	CLA	C3B-C4B-NB	-3.47	107.44	110.53
14	B	808	CLA	O2D-CGD-O1D	-3.46	117.10	123.85
14	A	823	CLA	CMB-C2B-C1B	-3.46	120.15	125.42
17	I	102	BCR	C11-C10-C9	-3.46	122.42	127.28
17	2	851	BCR	C24-C23-C22	-3.45	121.13	126.23
14	a	822	CLA	CMB-C2B-C1B	-3.45	120.17	125.42
14	A	805	CLA	C3B-C4B-NB	-3.45	107.45	110.53
17	L	1505	BCR	C28-C27-C26	-3.45	107.91	114.06
14	1	812	CLA	C3B-C4B-NB	-3.44	107.45	110.53
13	A	803	CL0	O2D-CGD-CBD	3.44	114.73	110.95
17	h	102	BCR	C15-C14-C13	-3.44	122.45	127.28
17	b	851	BCR	C24-C23-C22	-3.44	121.14	126.23
14	a	834	CLA	CHD-C1D-ND	-3.44	119.97	124.80
14	2	840	CLA	C3B-C4B-NB	-3.44	107.46	110.53
14	b	840	CLA	C3B-C4B-NB	-3.44	107.46	110.53
17	0	204	BCR	C28-C27-C26	-3.43	107.93	114.06
17	0	210	BCR	C28-C27-C26	-3.43	107.94	114.06
14	1	822	CLA	CMB-C2B-C1B	-3.43	120.19	125.42
14	B	841	CLA	C3B-C4B-NB	-3.43	107.47	110.53
14	1	832	CLA	CHD-C1D-ND	-3.43	119.98	124.80
17	B	852	BCR	C24-C23-C22	-3.43	121.16	126.23
14	a	806	CLA	C3B-C4B-NB	-3.43	107.47	110.53
14	a	824	CLA	CMB-C2B-C1B	-3.42	120.21	125.42
14	a	815	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
14	1	834	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
14	B	838	CLA	C3B-C4B-NB	-3.42	107.48	110.53
14	7	1101	CLA	C3B-C4B-NB	-3.42	107.48	110.53
14	A	814	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
17	B	854	BCR	C15-C14-C13	-3.41	122.49	127.28
14	1	813	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
17	i	4102	BCR	C15-C14-C13	-3.41	122.50	127.28
17	I	101	BCR	C15-C14-C13	-3.40	122.51	127.28
17	b	853	BCR	C15-C14-C13	-3.40	122.51	127.28
14	A	833	CLA	CHD-C1D-ND	-3.40	120.02	124.80
14	a	836	CLA	O2D-CGD-O1D	-3.40	117.24	123.85
14	b	827	CLA	C4A-NA-C1A	3.39	108.23	106.68
17	a	850	BCR	C15-C16-C17	-3.39	116.58	123.52
17	h	101	BCR	C15-C14-C13	-3.39	122.53	127.28
14	A	814	CLA	C3B-C4B-NB	-3.39	107.51	110.53
14	8	4004	CLA	C3B-C4B-NB	-3.39	107.51	110.53
14	A	835	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
17	L	1505	BCR	C15-C16-C17	-3.38	116.60	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	813	CLA	C3B-C4B-NB	-3.38	107.51	110.53
17	A	850	BCR	C15-C16-C17	-3.38	116.60	123.52
14	a	825	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
17	0	210	BCR	C15-C16-C17	-3.37	116.62	123.52
14	a	814	CLA	C3B-C4B-NB	-3.37	107.52	110.53
14	1	823	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
14	A	824	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
14	B	813	CLA	C3B-C4B-NB	-3.37	107.53	110.53
17	6	4406	BCR	C15-C14-C13	-3.36	122.56	127.28
17	0	204	BCR	C15-C16-C17	-3.36	116.65	123.52
17	k	4001	BCR	C15-C16-C17	-3.36	116.65	123.52
17	8	4001	BCR	C15-C16-C17	-3.35	116.66	123.52
14	2	812	CLA	C3B-C4B-NB	-3.35	107.54	110.53
14	1	839	CLA	C3B-C4B-NB	-3.34	107.55	110.53
14	1	823	CLA	C3B-C4B-NB	-3.34	107.55	110.53
14	B	828	CLA	C4A-NA-C1A	3.34	108.20	106.68
14	A	824	CLA	C3B-C4B-NB	-3.34	107.55	110.53
17	1	850	BCR	C15-C16-C17	-3.33	116.70	123.52
17	K	4001	BCR	C15-C16-C17	-3.33	116.70	123.52
14	b	822	CLA	C3B-C4B-NB	-3.33	107.56	110.53
14	2	827	CLA	C4A-NA-C1A	3.33	108.20	106.68
14	2	822	CLA	C3B-C4B-NB	-3.33	107.56	110.53
14	l	4203	CLA	C3B-C4B-NB	-3.32	107.56	110.53
14	L	1501	CLA	CMB-C2B-C1B	-3.32	120.37	125.42
14	a	825	CLA	C3B-C4B-NB	-3.32	107.57	110.53
14	a	854	CLA	C3B-C4B-NB	-3.31	107.57	110.53
14	1	840	CLA	C1-C2-C3	-3.31	120.77	126.20
14	b	801	CLA	C3B-C4B-NB	-3.31	107.57	110.53
14	0	202	CLA	C3B-C4B-NB	-3.31	107.58	110.53
14	b	818	CLA	CMB-C2B-C1B	-3.30	120.39	125.42
14	K	4004	CLA	C3B-C4B-NB	-3.30	107.58	110.53
19	i	4101	LMT	O5B-C5B-C4B	3.30	115.64	109.70
14	B	823	CLA	C3B-C4B-NB	-3.30	107.58	110.53
14	A	840	CLA	C3B-C4B-NB	-3.30	107.59	110.53
14	A	841	CLA	C1-C2-C3	-3.30	120.80	126.20
14	b	802	CLA	C1-C2-C3	-3.29	120.80	126.20
14	l	4204	CLA	CMB-C2B-C1B	-3.29	120.41	125.42
14	1	838	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
14	1	804	CLA	C3B-C4B-NB	-3.29	107.59	110.53
13	1	803	CL0	O2D-CGD-O1D	-3.29	117.44	123.85
14	B	827	CLA	C3B-C4B-NB	-3.29	107.60	110.53
14	B	802	CLA	C3B-C4B-NB	-3.29	107.60	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	803	CL0	O2D-CGD-O1D	-3.28	117.46	123.85
14	2	826	CLA	C3B-C4B-NB	-3.28	107.60	110.53
14	A	804	CLA	C3B-C4B-NB	-3.28	107.60	110.53
14	1	824	CLA	C3B-C4B-NB	-3.28	107.60	110.53
14	B	827	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
14	0	206	CLA	CMB-C2B-C1B	-3.28	120.42	125.42
14	2	826	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
14	A	839	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
14	2	818	CLA	CMB-C2B-C1B	-3.28	120.43	125.42
14	A	843	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
14	b	826	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
13	A	803	CL0	O2D-CGD-O1D	-3.28	117.47	123.85
14	B	841	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
14	b	840	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
14	a	840	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
14	a	842	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
14	B	833	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
19	h	103	LMT	O5B-C5B-C4B	3.27	115.59	109.70
14	2	840	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
14	a	843	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
14	b	842	CLA	C4A-NA-C1A	3.27	108.17	106.68
14	a	841	CLA	C3B-C4B-NB	-3.27	107.61	110.53
14	2	842	CLA	C4A-NA-C1A	3.27	108.17	106.68
14	a	826	CLA	C3B-C4B-NB	-3.27	107.61	110.53
14	B	819	CLA	CMB-C2B-C1B	-3.27	120.45	125.42
14	1	843	CLA	O2D-CGD-O1D	-3.26	117.49	123.85
14	1	815	CLA	C3B-C4B-NB	-3.26	107.62	110.53
14	b	816	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
14	1	842	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
14	B	817	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
14	a	805	CLA	C3B-C4B-NB	-3.26	107.62	110.53
14	B	818	CLA	C3B-C4B-NB	-3.25	107.62	110.53
19	I	103	LMT	O5B-C5B-C4B	3.25	115.56	109.70
14	2	832	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
17	B	851	BCR	C15-C14-C13	-3.25	122.72	127.28
14	a	837	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
14	A	825	CLA	C3B-C4B-NB	-3.25	107.63	110.53
14	1	804	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
14	b	817	CLA	C3B-C4B-NB	-3.25	107.63	110.53
14	A	842	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
14	a	823	CLA	C3B-C4B-NB	-3.24	107.64	110.53
14	a	805	CLA	O2D-CGD-O1D	-3.24	117.55	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	826	CLA	C3B-C4B-NB	-3.24	107.64	110.53
14	2	817	CLA	C3B-C4B-NB	-3.24	107.64	110.53
14	A	836	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
14	B	843	CLA	C4A-NA-C1A	3.23	108.15	106.68
17	2	850	BCR	C15-C14-C13	-3.23	122.75	127.28
14	A	816	CLA	C3B-C4B-NB	-3.23	107.65	110.53
14	b	832	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
14	1	835	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
14	2	834	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
17	j	103	BCR	C15-C16-C17	-3.23	116.92	123.52
14	A	804	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	b	834	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	2	816	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
17	b	846	BCR	C15-C16-C17	-3.22	116.94	123.52
17	b	850	BCR	C15-C14-C13	-3.21	122.77	127.28
17	7	1104	BCR	C15-C16-C17	-3.21	116.94	123.52
14	b	838	CLA	C3B-C4B-NB	-3.21	107.66	110.53
14	B	835	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
14	2	844	CLA	C3A-C4A-CHB	-3.21	119.98	123.91
14	b	804	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
14	2	835	CLA	C2B-C1B-NB	-3.21	107.00	110.33
17	B	847	BCR	C15-C16-C17	-3.20	116.96	123.52
14	2	838	CLA	C3B-C4B-NB	-3.20	107.67	110.53
17	J	103	BCR	C15-C16-C17	-3.20	116.97	123.52
14	0	208	CLA	C3B-C4B-NB	-3.20	107.67	110.53
14	a	817	CLA	C3B-C4B-NB	-3.20	107.68	110.53
14	1	821	CLA	C3B-C4B-NB	-3.20	107.68	110.53
14	8	4002	CLA	C3B-C4B-NB	-3.20	107.68	110.53
14	B	830	CLA	C3B-C4B-NB	-3.19	107.68	110.53
14	1	822	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
13	a	803	CL0	C1-C2-C3	-3.19	120.97	126.20
14	a	807	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	1	806	CLA	C3B-C4B-NB	-3.19	107.68	110.53
14	B	804	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
17	2	846	BCR	C15-C16-C17	-3.19	117.00	123.52
14	1	840	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	B	821	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	B	839	CLA	C3B-C4B-NB	-3.19	107.69	110.53
14	L	1503	CLA	C3B-C4B-NB	-3.19	107.69	110.53
14	a	808	CLA	C3B-C4B-NB	-3.19	107.69	110.53
17	9	102	BCR	C15-C16-C17	-3.19	117.00	123.52
14	b	802	CLA	O2D-CGD-O1D	-3.18	117.65	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	806	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
14	b	836	CLA	C3B-C4B-NB	-3.18	107.69	110.53
14	b	844	CLA	C3A-C4A-CHB	-3.18	120.02	123.91
14	k	4002	CLA	C3B-C4B-NB	-3.18	107.69	110.53
14	l	4206	CLA	C3B-C4B-NB	-3.18	107.69	110.53
17	a	851	BCR	C24-C23-C22	-3.18	121.53	126.23
14	A	822	CLA	C3B-C4B-NB	-3.18	107.69	110.53
14	2	803	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
14	1	830	CLA	C3B-C4B-NB	-3.17	107.70	110.53
14	B	806	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
14	A	823	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	a	824	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
13	1	803	CL0	C1-C2-C3	-3.17	121.01	126.20
14	A	841	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	a	832	CLA	C3B-C4B-NB	-3.17	107.70	110.53
14	b	820	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
17	b	854	BCR	C15-C16-C17	-3.17	117.04	123.52
17	A	851	BCR	C24-C23-C22	-3.17	121.55	126.23
14	B	845	CLA	C3A-C4A-CHB	-3.17	120.03	123.91
14	2	829	CLA	C3B-C4B-NB	-3.17	107.70	110.53
14	b	801	CLA	CMB-C2B-C1B	-3.17	120.60	125.42
17	M	102	BCR	C15-C16-C17	-3.16	117.04	123.52
14	1	805	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
17	1	851	BCR	C24-C23-C22	-3.16	121.56	126.23
14	b	815	CLA	C3B-C4B-NB	-3.16	107.71	110.53
14	1	828	CLA	C3B-C4B-NB	-3.16	107.71	110.53
14	2	815	CLA	C3B-C4B-NB	-3.16	107.71	110.53
14	B	802	CLA	CMB-C2B-C1B	-3.16	120.61	125.42
17	2	850	BCR	C15-C16-C17	-3.16	117.06	123.52
14	2	820	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
14	A	837	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
14	2	814	CLA	C3B-C4B-NB	-3.15	107.72	110.53
14	b	839	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
17	b	850	BCR	C15-C16-C17	-3.15	117.07	123.52
14	K	4002	CLA	C3B-C4B-NB	-3.15	107.72	110.53
14	b	811	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
14	B	840	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
14	a	807	CLA	CMB-C2B-C1B	-3.15	120.62	125.42
14	A	829	CLA	C3B-C4B-NB	-3.15	107.72	110.53
14	2	818	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
14	2	805	CLA	CMB-C2B-C1B	-3.15	120.62	125.42
14	B	819	CLA	O2D-CGD-O1D	-3.15	117.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	829	CLA	C3B-C4B-NB	-3.15	107.72	110.53
14	b	835	CLA	C2B-C1B-NB	-3.14	107.06	110.33
14	1	836	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
17	2	849	BCR	C27-C26-C25	3.14	126.95	122.70
14	b	814	CLA	C3B-C4B-NB	-3.14	107.72	110.53
14	b	806	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
14	b	819	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
14	A	806	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
14	0	202	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
14	2	810	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
14	B	815	CLA	C3B-C4B-NB	-3.14	107.73	110.53
14	a	838	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
14	B	816	CLA	C3B-C4B-NB	-3.14	107.73	110.53
17	B	851	BCR	C15-C16-C17	-3.13	117.11	123.52
17	1	851	BCR	C15-C16-C17	-3.13	117.11	123.52
14	1	805	CLA	CMB-C2B-C1B	-3.13	120.65	125.42
13	A	803	CL0	C1-C2-C3	-3.13	121.07	126.20
14	A	807	CLA	C3B-C4B-NB	-3.13	107.74	110.53
14	B	836	CLA	C2B-C1B-NB	-3.13	107.08	110.33
14	b	818	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	B	834	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	2	801	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	2	836	CLA	C3B-C4B-NB	-3.12	107.74	110.53
14	B	820	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	1	808	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	b	833	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	2	833	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	2	825	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
17	A	851	BCR	C15-C16-C17	-3.12	117.14	123.52
14	2	839	CLA	O2D-CGD-O1D	-3.11	117.78	123.85
14	A	817	CLA	C3B-C4B-NB	-3.11	107.75	110.53
14	1	832	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	A	833	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	1	824	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	A	809	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	a	823	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	a	826	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	B	836	CLA	C3B-C4B-NB	-3.11	107.75	110.53
14	B	801	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	B	837	CLA	C3B-C4B-NB	-3.11	107.75	110.53
14	B	826	CLA	CMB-C2B-C1B	-3.11	120.69	125.42
14	7	1102	CLA	C3B-C4B-NB	-3.11	107.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	825	CLA	CMB-C2B-C1B	-3.11	120.69	125.42
14	a	834	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
14	A	825	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	A	831	CLA	C3B-C4B-NB	-3.10	107.76	110.53
14	b	835	CLA	C3B-C4B-NB	-3.10	107.76	110.53
14	B	811	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	2	807	CLA	C3B-C4B-NB	-3.10	107.76	110.53
17	a	851	BCR	C15-C16-C17	-3.10	117.18	123.52
14	a	830	CLA	C3B-C4B-NB	-3.10	107.77	110.53
14	F	205	CLA	C2A-C1A-CHA	3.10	129.24	123.87
14	B	808	CLA	C3B-C4B-NB	-3.10	107.77	110.53
17	A	849	BCR	C11-C10-C9	-3.09	122.94	127.28
14	B	845	CLA	C1B-NB-C4B	3.09	108.48	106.31
14	a	804	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	a	810	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	1	821	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	2	819	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	f	205	CLA	C2A-C1A-CHA	3.09	129.23	123.87
14	6	4404	CLA	C2A-C1A-CHA	3.09	129.23	123.87
17	B	850	BCR	C27-C26-C25	3.09	126.88	122.70
14	A	810	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	a	830	CLA	CMB-C2B-C1B	-3.09	120.72	125.42
12	1	802	LHG	O8-C23-C24	3.09	120.52	111.15
14	A	822	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	2	814	CLA	O2D-CGD-CBD	3.08	116.62	111.23
14	A	829	CLA	CMB-C2B-C1B	-3.08	120.72	125.42
14	2	822	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
14	1	828	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
14	B	815	CLA	O2D-CGD-CBD	3.08	116.61	111.23
14	2	824	CLA	C3B-C4B-NB	-3.08	107.78	110.53
14	1	839	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	b	824	CLA	C3B-C4B-NB	-3.07	107.79	110.53
14	1	818	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
14	2	813	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
14	b	813	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
17	b	849	BCR	C27-C26-C25	3.07	126.85	122.70
14	b	844	CLA	C1B-NB-C4B	3.07	108.46	106.31
12	A	802	LHG	O8-C23-C24	3.07	120.45	111.15
14	A	840	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
12	a	802	LHG	O8-C23-C24	3.06	120.44	111.15
14	1	838	CLA	C3B-C4B-NB	-3.06	107.80	110.53
14	B	814	CLA	O2D-CGD-O1D	-3.06	117.89	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	205	CLA	C3B-C4B-NB	-3.06	107.80	110.53
14	a	841	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	1	809	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	a	831	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	b	814	CLA	O2D-CGD-CBD	3.06	116.58	111.23
14	b	808	CLA	C3B-C4B-NB	-3.06	107.80	110.53
14	A	819	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
17	1	849	BCR	C11-C10-C9	-3.06	122.99	127.28
14	b	828	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	B	829	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	a	811	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	1	829	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	a	818	CLA	C3B-C4B-NB	-3.05	107.80	110.53
14	2	844	CLA	C1B-NB-C4B	3.05	108.45	106.31
14	a	838	CLA	C3B-C4B-NB	-3.05	107.81	110.53
14	2	828	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
14	A	830	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
14	2	835	CLA	C3B-C4B-NB	-3.05	107.81	110.53
17	B	854	BCR	C11-C10-C9	-3.05	123.01	127.28
14	a	820	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
14	2	816	CLA	C3B-C4B-NB	-3.04	107.81	110.53
14	A	839	CLA	C3B-C4B-NB	-3.04	107.81	110.53
14	a	804	CLA	CMB-C2B-C3B	3.04	133.71	126.55
14	B	823	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	b	807	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	2	806	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	2	805	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	a	806	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
17	7	1104	BCR	C11-C10-C9	-3.04	123.02	127.28
17	K	4001	BCR	C24-C23-C22	-3.04	121.74	126.23
17	a	849	BCR	C11-C10-C9	-3.03	123.02	127.28
14	B	801	CLA	CMB-C2B-C3B	3.03	133.68	126.55
14	A	805	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
19	h	103	LMT	C1'-O5'-C5'	-3.03	107.80	113.72
19	i	4101	LMT	C1'-O5'-C5'	-3.03	107.81	113.72
14	b	843	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	7	1101	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	B	807	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	B	806	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
14	B	842	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
14	1	828	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
14	A	837	CLA	C3B-C4B-NB	-3.03	107.83	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	k	4001	BCR	C24-C23-C22	-3.02	121.76	126.23
17	B	851	BCR	C11-C10-C9	-3.02	123.04	127.28
14	b	806	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
14	1	816	CLA	C3B-C4B-NB	-3.02	107.83	110.53
19	I	103	LMT	C1'-O5'-C5'	-3.02	107.82	113.72
17	6	4406	BCR	C11-C10-C9	-3.02	123.04	127.28
14	1	807	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	B	825	CLA	C3B-C4B-NB	-3.02	107.83	110.53
14	b	841	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
17	J	103	BCR	C11-C10-C9	-3.02	123.05	127.28
14	2	843	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
17	8	4001	BCR	C24-C23-C22	-3.02	121.77	126.23
17	2	850	BCR	C11-C10-C9	-3.02	123.05	127.28
14	2	801	CLA	CMB-C2B-C3B	3.02	133.64	126.55
14	b	807	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	b	822	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	1	836	CLA	C3B-C4B-NB	-3.01	107.84	110.53
17	b	853	BCR	C11-C10-C9	-3.01	123.06	127.28
14	6	4404	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	2	831	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
14	J	101	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	1	831	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	K	4004	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
17	j	103	BCR	C11-C10-C9	-3.01	123.06	127.28
14	b	830	CLA	C3B-C4B-NB	-3.01	107.85	110.53
14	a	833	CLA	C3B-C4B-NB	-3.01	107.85	110.53
14	2	830	CLA	C3B-C4B-NB	-3.01	107.85	110.53
14	A	829	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
14	1	825	CLA	CHD-C1D-ND	-3.00	120.58	124.80
14	1	826	CLA	CHD-C1D-ND	-3.00	120.58	124.80
14	2	841	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	b	831	CLA	C2D-C1D-ND	-3.00	107.16	110.13
14	a	840	CLA	C3B-C4B-NB	-3.00	107.85	110.53
14	a	854	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
14	B	844	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
14	1	819	CLA	CMB-C2B-C1B	-3.00	120.86	125.42
17	b	850	BCR	C11-C10-C9	-3.00	123.08	127.28
14	B	807	CLA	C3B-C4B-NB	-3.00	107.86	110.53
14	2	825	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
14	b	816	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	B	826	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
14	j	101	CLA	C3B-C4B-NB	-2.99	107.86	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	832	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	1	820	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	1	841	CLA	C1-C2-C3	-2.98	121.31	126.20
14	b	825	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
14	B	832	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
14	2	806	CLA	C3B-C4B-NB	-2.98	107.87	110.53
14	8	4004	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
17	2	849	BCR	C30-C25-C26	-2.98	118.56	122.64
14	B	833	CLA	CMB-C2B-C1B	-2.98	120.88	125.42
17	6	4402	BCR	C15-C16-C17	-2.98	117.43	123.52
14	b	836	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	A	808	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	F	201	CLA	C1-C2-C3	-2.98	121.32	126.20
14	b	831	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	B	832	CLA	C2D-C1D-ND	-2.98	107.18	110.13
14	a	821	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
14	A	826	CLA	CHD-C1D-ND	-2.97	120.62	124.80
14	A	820	CLA	CMB-C2B-C1B	-2.97	120.89	125.42
14	a	809	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
17	1	847	BCR	C24-C23-C22	-2.97	121.84	126.23
17	a	847	BCR	C24-C23-C22	-2.97	121.84	126.23
17	A	850	BCR	C15-C14-C13	-2.97	123.11	127.28
14	a	827	CLA	CHD-C1D-ND	-2.97	120.63	124.80
14	f	205	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	a	830	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
14	2	827	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
14	2	831	CLA	C2D-C1D-ND	-2.97	107.19	110.13
14	B	828	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
14	a	813	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	a	828	CLA	CHD-C1D-ND	-2.96	120.63	124.80
14	b	827	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
14	B	831	CLA	C3B-C4B-NB	-2.96	107.89	110.53
14	B	812	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
14	2	811	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
14	A	827	CLA	CHD-C1D-ND	-2.96	120.64	124.80
14	B	837	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	0	202	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	b	812	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	B	817	CLA	C3B-C4B-NB	-2.96	107.89	110.53
14	B	809	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
17	7	1105	BCR	C15-C16-C17	-2.96	117.47	123.52
17	f	203	BCR	C15-C16-C17	-2.96	117.47	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	201	CLA	C1-C2-C3	-2.95	121.36	126.20
14	2	836	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
17	a	850	BCR	C15-C14-C13	-2.95	123.14	127.28
17	6	4406	BCR	C7-C8-C9	-2.95	121.87	126.23
14	A	821	CLA	C3B-C4B-NB	-2.95	107.90	110.53
17	F	203	BCR	C15-C16-C17	-2.95	117.49	123.52
17	A	847	BCR	C24-C23-C22	-2.95	121.88	126.23
14	A	812	CLA	C3B-C4B-NB	-2.95	107.90	110.53
14	b	809	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
14	2	808	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
14	B	802	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
14	b	832	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
14	1	810	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
14	2	832	CLA	CMB-C2B-C1B	-2.94	120.95	125.42
14	1	811	CLA	C3B-C4B-NB	-2.93	107.91	110.53
14	f	201	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	A	811	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	a	812	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	B	822	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
14	b	821	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
14	b	801	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	j	101	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	F	201	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
17	B	850	BCR	C30-C25-C26	-2.93	118.64	122.64
17	1	850	BCR	C15-C14-C13	-2.92	123.18	127.28
14	7	1102	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
17	B	854	BCR	C7-C8-C9	-2.92	121.91	126.23
17	j	104	BCR	C15-C16-C17	-2.92	117.54	123.52
14	2	823	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	J	104	BCR	C15-C16-C17	-2.91	117.56	123.52
14	1	841	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	b	853	BCR	C7-C8-C9	-2.91	121.93	126.23
14	2	821	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
14	J	101	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
14	j	102	CLA	C3B-C4B-NB	-2.90	107.94	110.53
14	B	824	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	A	849	BCR	C15-C14-C13	-2.90	123.21	127.28
14	A	827	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	l	4203	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
17	b	849	BCR	C30-C25-C26	-2.90	118.67	122.64
14	a	808	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	a	844	CLA	O2D-CGD-O1D	-2.90	118.21	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	844	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	A	807	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
17	1	849	BCR	C15-C14-C13	-2.89	123.22	127.28
17	b	848	BCR	C27-C26-C25	2.89	126.61	122.70
13	A	803	CL0	CHA-C1A-C2A	-2.89	126.52	133.31
13	a	803	CL0	CHA-C1A-C2A	-2.89	126.52	133.31
14	6	4404	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	f	205	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	J	102	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	A	844	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
17	a	849	BCR	C15-C14-C13	-2.89	123.23	127.28
14	1	826	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
14	1	830	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
14	2	812	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
14	a	832	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	1	803	CL0	CHA-C1A-C2A	-2.88	126.54	133.31
18	A	853	LMG	O6-C1-O1	-2.88	103.23	110.04
14	B	820	CLA	C3B-C4B-NB	-2.88	107.96	110.53
14	7	1103	CLA	C3B-C4B-NB	-2.88	107.96	110.53
14	b	823	CLA	C3B-C4B-NB	-2.88	107.96	110.53
18	1	852	LMG	O6-C1-O1	-2.88	103.24	110.04
14	F	205	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
14	L	1503	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
14	A	831	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	a	828	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	M	102	BCR	C24-C23-C22	-2.87	121.98	126.23
14	a	809	CLA	C1-C2-C3	-2.87	121.49	126.20
14	2	817	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	9	102	BCR	C24-C23-C22	-2.87	121.99	126.23
14	B	818	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
14	1	806	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	b	819	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	0	208	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	b	854	BCR	C24-C23-C22	-2.87	122.00	126.23
14	b	828	CLA	C3B-C4B-NB	-2.87	107.97	110.53
18	a	853	LMG	O6-C1-O1	-2.86	103.27	110.04
17	B	849	BCR	C27-C26-C25	2.86	126.58	122.70
14	B	818	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
14	b	805	CLA	C1-C2-C3	-2.86	121.51	126.20
14	1	827	CLA	C3B-C4B-NB	-2.86	107.97	110.53
14	2	828	CLA	C3B-C4B-NB	-2.86	107.97	110.53
17	B	851	BCR	C37-C22-C21	-2.86	118.19	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	822	CLA	C3B-C4B-NB	-2.86	107.98	110.53
14	2	816	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
14	b	823	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
14	2	819	CLA	C3B-C4B-NB	-2.85	107.98	110.53
14	B	817	CLA	CMB-C2B-C1B	-2.85	121.07	125.42
14	2	823	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
14	a	829	CLA	C3B-C4B-NB	-2.85	107.99	110.53
14	B	829	CLA	C3B-C4B-NB	-2.85	107.99	110.53
14	b	817	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
17	2	848	BCR	C27-C26-C25	2.84	126.55	122.70
14	B	813	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	1	812	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	A	844	CLA	C3B-C4B-NB	-2.84	107.99	110.53
14	b	817	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	l	4206	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	1	807	CLA	C1-C2-C3	-2.84	121.54	126.20
14	2	817	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
14	2	842	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	2	850	BCR	C37-C22-C21	-2.84	118.22	122.82
14	b	805	CLA	C3B-C4B-NB	-2.84	108.00	110.53
14	2	805	CLA	CHD-C1D-ND	-2.84	120.81	124.80
14	B	824	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
13	1	803	CL0	C3C-C4C-NC	-2.83	107.73	114.65
17	6	4405	BCR	C15-C14-C13	-2.83	123.31	127.28
14	1	843	CLA	CHB-C4A-NA	2.83	128.49	124.40
13	a	803	CL0	C3C-C4C-NC	-2.83	107.74	114.65
14	b	842	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	2	804	CLA	C1-C2-C3	-2.83	121.56	126.20
17	b	850	BCR	C37-C22-C21	-2.83	118.24	122.82
14	A	813	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
14	1	827	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	2	827	CLA	C3B-C4B-NB	-2.82	108.01	110.53
17	f	206	BCR	C15-C14-C13	-2.82	123.32	127.28
14	a	814	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	a	843	CLA	CHB-C4A-NA	2.82	128.47	124.40
14	A	808	CLA	C1-C2-C3	-2.82	121.58	126.20
17	7	1105	BCR	C27-C26-C25	2.82	126.51	122.70
14	1	844	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	A	803	CL0	C3C-C4C-NC	-2.81	107.77	114.65
14	B	806	CLA	CHD-C1D-ND	-2.81	120.84	124.80
14	f	201	CLA	CAA-CBA-CGA	-2.81	105.22	113.21
14	A	828	CLA	O2D-CGD-O1D	-2.81	118.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	805	CLA	C1-C2-C3	-2.81	121.59	126.20
14	A	828	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	M	102	BCR	C15-C14-C13	-2.81	123.34	127.28
14	B	805	CLA	C3B-C4B-NB	-2.81	108.02	110.53
14	2	804	CLA	C3B-C4B-NB	-2.81	108.02	110.53
14	a	844	CLA	C3B-C4B-NB	-2.81	108.02	110.53
14	a	809	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
14	b	816	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
18	B	803	LMG	O6-C1-O1	-2.81	103.41	110.04
14	B	843	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
14	b	806	CLA	CHD-C1D-ND	-2.80	120.86	124.80
17	F	206	BCR	C15-C14-C13	-2.80	123.35	127.28
17	b	854	BCR	C15-C14-C13	-2.80	123.35	127.28
14	1	841	CLA	CAA-CBA-CGA	-2.80	105.25	113.21
14	A	843	CLA	CHB-C4A-NA	2.80	128.44	124.40
14	a	829	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
17	0	209	BCR	C27-C26-C25	2.80	126.49	122.70
14	A	830	CLA	C1-C2-C3	-2.80	121.61	126.20
14	F	201	CLA	CAA-CBA-CGA	-2.80	105.26	113.21
17	L	1504	BCR	C27-C26-C25	2.80	126.48	122.70
18	b	803	LMG	O6-C1-O1	-2.80	103.43	110.04
14	b	827	CLA	C3B-C4B-NB	-2.80	108.03	110.53
14	1	807	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
17	F	203	BCR	C11-C10-C9	-2.80	123.36	127.28
17	f	206	BCR	C27-C26-C25	2.80	126.48	122.70
17	l	4207	BCR	C27-C26-C25	2.79	126.48	122.70
18	2	802	LMG	O6-C1-O1	-2.79	103.44	110.04
17	9	102	BCR	C15-C14-C13	-2.79	123.36	127.28
14	b	809	CLA	C1-C2-C3	-2.79	121.62	126.20
14	B	807	CLA	CHB-C4A-NA	2.79	128.43	124.40
14	A	836	CLA	C3B-C4B-NB	-2.79	108.04	110.53
14	2	808	CLA	C1-C2-C3	-2.79	121.63	126.20
14	2	830	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
14	a	831	CLA	C1-C2-C3	-2.79	121.63	126.20
14	B	822	CLA	C2B-C1B-NB	-2.79	107.44	110.33
14	b	810	CLA	C3B-C4B-NB	-2.78	108.04	110.53
17	f	203	BCR	C11-C10-C9	-2.78	123.37	127.28
17	6	4405	BCR	C27-C26-C25	2.78	126.46	122.70
17	B	850	BCR	C7-C8-C9	-2.78	122.12	126.23
14	b	807	CLA	CHB-C4A-NA	2.78	128.41	124.40
14	B	821	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
14	B	809	CLA	C1-C2-C3	-2.78	121.64	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	829	CLA	C1-C2-C3	-2.78	121.64	126.20
17	F	206	BCR	C27-C26-C25	2.78	126.46	122.70
14	a	834	CLA	C2B-C1B-NB	-2.77	107.45	110.33
14	2	821	CLA	C2B-C1B-NB	-2.77	107.45	110.33
14	b	832	CLA	CHD-C1D-C2D	2.77	131.26	125.49
14	b	820	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
14	B	828	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	B	833	CLA	CHD-C1D-C2D	2.77	131.25	125.49
14	1	835	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	b	838	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
14	2	832	CLA	CHD-C1D-C2D	2.77	131.25	125.49
14	1	817	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
14	A	816	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
14	A	808	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
14	B	831	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	1	815	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
17	b	847	BCR	C15-C16-C17	-2.76	117.87	123.52
14	b	821	CLA	C2B-C1B-NB	-2.76	107.46	110.33
14	K	4003	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	a	839	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
17	A	848	BCR	C27-C26-C25	2.76	126.43	122.70
17	B	848	BCR	C28-C27-C26	-2.76	109.13	114.06
17	B	848	BCR	C15-C16-C17	-2.76	117.87	123.52
14	2	820	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
14	B	839	CLA	CHD-C1D-ND	-2.76	120.92	124.80
14	B	837	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
14	2	838	CLA	CHD-C1D-ND	-2.76	120.92	124.80
14	k	4003	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	8	4003	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	a	837	CLA	C3B-C4B-NB	-2.75	108.07	110.53
14	b	836	CLA	CMB-C2B-C1B	-2.75	121.22	125.42
14	a	819	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
14	A	838	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
14	b	808	CLA	O2D-CGD-CBD	2.75	116.04	111.23
14	B	839	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
17	1	848	BCR	C27-C26-C25	2.75	126.42	122.70
17	b	847	BCR	C28-C27-C26	-2.75	109.15	114.06
17	2	847	BCR	C28-C27-C26	-2.75	109.15	114.06
14	A	818	CLA	CHB-C4A-NA	2.75	128.37	124.40
17	b	849	BCR	C7-C8-C9	-2.75	122.17	126.23
14	2	807	CLA	O2D-CGD-CBD	2.75	116.04	111.23
14	A	814	CLA	C1-C2-C3	-2.75	121.69	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	j	104	BCR	C27-C26-C25	2.75	126.42	122.70
14	B	828	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
17	2	847	BCR	C15-C16-C17	-2.75	117.90	123.52
17	J	104	BCR	C27-C26-C25	2.75	126.42	122.70
14	B	808	CLA	O2D-CGD-CBD	2.75	116.03	111.23
14	2	836	CLA	CMB-C2B-C1B	-2.75	121.24	125.42
17	B	847	BCR	C27-C26-C25	2.75	126.41	122.70
14	A	818	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	1	813	CLA	C1-C2-C3	-2.75	121.70	126.20
14	A	836	CLA	O2A-CGA-O1A	-2.74	116.76	123.63
14	B	810	CLA	C3B-C4B-NB	-2.74	108.08	110.53
14	a	837	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
14	b	815	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
14	b	827	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
14	a	817	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
17	A	851	BCR	C28-C27-C26	-2.74	109.17	114.06
14	2	838	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	2	827	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
14	B	816	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	1	835	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
14	2	806	CLA	CHB-C4A-NA	2.73	128.35	124.40
17	a	851	BCR	C28-C27-C26	-2.73	109.18	114.06
17	a	848	BCR	C27-C26-C25	2.73	126.39	122.70
17	6	4402	BCR	C11-C10-C9	-2.73	123.45	127.28
14	b	838	CLA	CHD-C1D-ND	-2.73	120.96	124.80
14	2	815	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
14	A	833	CLA	C2B-C1B-NB	-2.73	107.50	110.33
14	B	836	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
14	6	4403	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	a	815	CLA	C1-C2-C3	-2.72	121.74	126.20
17	1	851	BCR	C28-C27-C26	-2.72	109.20	114.06
14	F	204	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
14	b	830	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
14	2	811	CLA	C3B-C4B-NB	-2.72	108.10	110.53
17	2	849	BCR	C7-C8-C9	-2.72	122.22	126.23
17	b	846	BCR	C15-C14-C13	-2.72	123.47	127.28
14	B	809	CLA	CHD-C1D-ND	-2.71	120.98	124.80
14	b	812	CLA	C3B-C4B-NB	-2.71	108.11	110.53
14	1	837	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
14	b	835	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
14	1	817	CLA	CHB-C4A-NA	2.71	128.31	124.40
14	f	204	CLA	O2D-CGD-O1D	-2.71	118.57	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	812	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	a	850	BCR	C11-C10-C9	-2.71	123.48	127.28
14	1	816	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
14	a	818	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
17	A	850	BCR	C11-C10-C9	-2.71	123.48	127.28
14	1	811	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
14	1	819	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
17	K	4001	BCR	C28-C27-C26	-2.71	109.23	114.06
14	a	819	CLA	CHB-C4A-NA	2.70	128.30	124.40
14	2	835	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
17	b	846	BCR	C27-C26-C25	2.70	126.35	122.70
14	A	817	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	a	821	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
17	k	4001	BCR	C28-C27-C26	-2.70	109.25	114.06
14	2	809	CLA	C3B-C4B-NB	-2.70	108.12	110.53
12	1	801	LHG	C11-C10-C9	-2.70	100.74	114.37
17	i	4103	BCR	C24-C23-C22	-2.70	122.25	126.23
13	A	803	CL0	C1C-CHC-C4B	2.70	125.71	116.07
17	6	4406	BCR	C33-C5-C6	-2.69	121.54	124.48
13	1	803	CL0	C1C-CHC-C4B	2.69	125.71	116.07
17	I	102	BCR	C24-C23-C22	-2.69	122.25	126.23
17	b	853	BCR	C33-C5-C6	-2.69	121.55	124.48
14	f	204	CLA	CMB-C2B-C1B	-2.69	121.32	125.42
14	a	813	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
14	1	832	CLA	C2B-C1B-NB	-2.69	107.54	110.33
17	8	4001	BCR	C28-C27-C26	-2.69	109.26	114.06
14	2	808	CLA	CHD-C1D-ND	-2.69	121.02	124.80
12	a	801	LHG	C11-C10-C9	-2.69	100.78	114.37
17	2	846	BCR	C27-C26-C25	2.69	126.34	122.70
13	a	803	CL0	C1C-CHC-C4B	2.69	125.69	116.07
17	b	847	BCR	C15-C14-C13	-2.69	123.51	127.28
14	b	830	CLA	CHB-C4A-NA	2.69	128.28	124.40
14	b	809	CLA	CHD-C1D-ND	-2.69	121.02	124.80
14	B	805	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
14	k	4002	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
12	B	853	LHG	O8-C23-C24	2.68	120.02	111.83
14	A	810	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
14	A	820	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
17	B	854	BCR	C33-C5-C6	-2.68	121.56	124.48
14	A	812	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
17	1	850	BCR	C11-C10-C9	-2.68	123.52	127.28
12	A	801	LHG	C11-C10-C9	-2.68	100.82	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	846	BCR	C15-C14-C13	-2.68	123.52	127.28
14	A	815	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
14	1	821	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
14	a	825	CLA	O2D-CGD-CBD	2.68	115.91	111.23
14	8	4002	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	a	831	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
14	K	4002	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	a	811	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
14	A	830	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
17	8	4005	BCR	C3-C4-C5	-2.67	109.29	114.06
12	b	852	LHG	O8-C23-C24	2.67	119.99	111.83
14	b	805	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
14	B	831	CLA	CHB-C4A-NA	2.67	128.25	124.40
17	2	849	BCR	C11-C10-C9	-2.67	123.53	127.28
14	2	830	CLA	CHB-C4A-NA	2.67	128.25	124.40
17	2	847	BCR	C15-C14-C13	-2.67	123.53	127.28
17	K	4005	BCR	C3-C4-C5	-2.67	109.29	114.06
17	6	4406	BCR	C27-C26-C25	2.67	126.31	122.70
14	B	822	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
14	a	816	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
17	b	849	BCR	C11-C10-C9	-2.67	123.54	127.28
12	2	852	LHG	O8-C23-C24	2.67	119.97	111.83
14	b	829	CLA	O2D-CGD-CBD	2.67	115.89	111.23
17	B	847	BCR	C15-C14-C13	-2.67	123.54	127.28
17	h	102	BCR	C24-C23-C22	-2.66	122.29	126.23
14	6	4403	CLA	CMB-C2B-C1B	-2.66	121.36	125.42
14	2	829	CLA	O2D-CGD-CBD	2.66	115.88	111.23
17	k	4004	BCR	C3-C4-C5	-2.66	109.31	114.06
14	2	821	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	L	1502	CLA	O2D-CGD-CBD	2.66	115.88	111.23
14	B	830	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
14	F	204	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
14	1	829	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
14	l	4205	CLA	O2D-CGD-CBD	2.66	115.87	111.23
14	A	822	CLA	CMB-C2B-C1B	-2.66	121.38	125.42
14	A	843	CLA	C1-C2-C3	-2.66	121.85	126.20
14	b	821	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
14	2	808	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
14	2	843	CLA	CHD-C1D-ND	-2.65	121.07	124.80
14	a	823	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
14	a	843	CLA	C1-C2-C3	-2.65	121.85	126.20
14	0	207	CLA	O2D-CGD-CBD	2.65	115.86	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	825	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	B	830	CLA	O2D-CGD-CBD	2.65	115.86	111.23
14	2	829	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
14	b	843	CLA	CHD-C1D-ND	-2.65	121.08	124.80
14	B	809	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
14	1	814	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
17	B	854	BCR	C27-C26-C25	2.64	126.28	122.70
14	1	825	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
14	B	844	CLA	CHD-C1D-ND	-2.64	121.08	124.80
14	A	816	CLA	CMB-C2B-C1B	-2.64	121.39	125.42
14	1	815	CLA	CMB-C2B-C1B	-2.64	121.39	125.42
14	1	823	CLA	O2D-CGD-CBD	2.64	115.85	111.23
14	b	809	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
17	B	850	BCR	C11-C10-C9	-2.64	123.58	127.28
17	2	850	BCR	C28-C27-C26	-2.64	109.35	114.06
14	2	804	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
14	1	843	CLA	C1-C2-C3	-2.64	121.88	126.20
14	A	815	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
14	a	816	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
17	b	853	BCR	C27-C26-C25	2.63	126.26	122.70
17	b	853	BCR	C15-C16-C17	-2.63	118.13	123.52
14	A	826	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
17	B	848	BCR	C15-C14-C13	-2.63	123.59	127.28
17	b	854	BCR	C27-C26-C25	2.63	126.26	122.70
17	B	851	BCR	C28-C27-C26	-2.63	109.37	114.06
17	M	102	BCR	C27-C26-C25	2.63	126.26	122.70
17	6	4406	BCR	C15-C16-C17	-2.63	118.14	123.52
17	F	203	BCR	C15-C14-C13	-2.63	123.59	127.28
17	b	850	BCR	C28-C27-C26	-2.63	109.37	114.06
14	A	804	CLA	CHA-C1A-NA	-2.63	120.45	126.39
12	1	802	LHG	C11-C10-C9	-2.62	101.10	114.37
14	1	809	CLA	CMB-C2B-C1B	-2.62	121.42	125.42
14	a	827	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
14	a	817	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
14	b	829	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
14	b	841	CLA	O2D-CGD-CBD	2.62	115.81	111.23
12	a	802	LHG	C11-C10-C9	-2.62	101.13	114.37
17	f	203	BCR	C15-C14-C13	-2.62	123.61	127.28
14	a	805	CLA	CHA-C1A-NA	-2.62	120.46	126.39
17	0	204	BCR	C11-C10-C9	-2.62	123.61	127.28
14	b	824	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
14	A	824	CLA	O2D-CGD-CBD	2.62	115.80	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	854	BCR	C15-C16-C17	-2.62	118.17	123.52
14	2	841	CLA	O2D-CGD-CBD	2.62	115.80	111.23
12	A	802	LHG	C11-C10-C9	-2.61	101.15	114.37
17	6	4402	BCR	C15-C14-C13	-2.61	123.61	127.28
14	a	836	CLA	C2D-C1D-ND	-2.61	107.54	110.13
14	1	822	CLA	CHA-C1A-NA	-2.61	120.47	126.39
14	A	823	CLA	CHA-C1A-NA	-2.61	120.48	126.39
14	a	824	CLA	CHA-C1A-NA	-2.61	120.48	126.39
14	b	815	CLA	C2D-C1D-ND	-2.61	107.54	110.13
17	F	203	BCR	C24-C23-C22	-2.61	122.38	126.23
14	1	814	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
14	1	804	CLA	CHA-C1A-NA	-2.61	120.49	126.39
17	f	203	BCR	C24-C23-C22	-2.60	122.38	126.23
14	B	842	CLA	O2D-CGD-CBD	2.60	115.78	111.23
14	1	834	CLA	C2D-C1D-ND	-2.60	107.55	110.13
14	2	824	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
17	1	850	BCR	C33-C5-C6	-2.60	121.65	124.48
14	1	834	CLA	CHB-C4A-NA	2.60	128.15	124.40
14	L	1502	CLA	CHD-C1D-ND	-2.60	121.15	124.80
17	a	850	BCR	C33-C5-C6	-2.60	121.65	124.48
14	b	819	CLA	CMC-C2C-C1C	-2.60	120.98	125.03
14	A	811	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
14	A	835	CLA	C2D-C1D-ND	-2.59	107.56	110.13
17	6	4402	BCR	C24-C23-C22	-2.59	122.40	126.23
17	9	102	BCR	C27-C26-C25	2.59	126.20	122.70
14	B	820	CLA	CMC-C2C-C1C	-2.59	120.99	125.03
17	l	4207	BCR	C11-C10-C9	-2.59	123.65	127.28
12	m	101	LHG	O8-C23-C24	2.59	119.72	111.83
14	0	206	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
17	0	210	BCR	C11-C10-C9	-2.58	123.66	127.28
14	b	837	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
17	A	850	BCR	C20-C21-C22	-2.58	123.66	127.28
14	2	837	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
14	a	836	CLA	C1-C2-C3	-2.58	121.97	126.20
17	A	847	BCR	C27-C26-C25	2.58	126.19	122.70
17	a	847	BCR	C27-C26-C25	2.58	126.19	122.70
18	A	853	LMG	C1-C2-C3	-2.58	104.58	110.01
14	a	812	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
17	L	1504	BCR	C11-C10-C9	-2.58	123.66	127.28
14	2	819	CLA	CMC-C2C-C1C	-2.58	121.01	125.03
17	1	847	BCR	C27-C26-C25	2.58	126.19	122.70
17	f	203	BCR	C16-C15-C14	-2.58	118.25	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	810	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
12	M	101	LHG	O8-C23-C24	2.57	119.69	111.83
14	B	825	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	6	4402	BCR	C16-C15-C14	-2.57	118.25	123.52
17	L	1505	BCR	C11-C10-C9	-2.57	123.67	127.28
18	1	852	LMG	C1-C2-C3	-2.57	104.60	110.01
17	0	209	BCR	C11-C10-C9	-2.57	123.67	127.28
17	A	851	BCR	C7-C8-C9	-2.57	122.43	126.23
14	b	811	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
17	F	203	BCR	C16-C15-C14	-2.57	118.26	123.52
14	a	809	CLA	CHD-C1D-ND	-2.57	121.19	124.80
14	a	836	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	9	101	LHG	O8-C23-C24	2.57	119.67	111.83
14	1	807	CLA	CHD-C1D-ND	-2.57	121.19	124.80
14	a	832	CLA	CHB-C4A-NA	2.57	128.11	124.40
18	a	853	LMG	C1-C2-C3	-2.57	104.61	110.01
17	A	849	BCR	C33-C5-C6	-2.57	121.68	124.48
14	A	827	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
17	J	103	BCR	C27-C26-C25	2.57	126.17	122.70
14	a	828	CLA	C3B-C4B-NB	-2.56	108.24	110.53
14	0	207	CLA	CHD-C1D-ND	-2.56	121.19	124.80
14	A	827	CLA	C3B-C4B-NB	-2.56	108.24	110.53
14	a	828	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
14	2	810	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
14	L	1501	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
14	1	826	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
17	1	850	BCR	C20-C21-C22	-2.56	123.69	127.28
14	K	4004	CLA	CHB-C4A-NA	2.56	128.09	124.40
14	8	4004	CLA	CHB-C4A-NA	2.56	128.09	124.40
14	L	1503	CLA	CMB-C2B-C1B	-2.56	121.53	125.42
14	l	4204	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
14	B	811	CLA	O2A-CGA-O1A	-2.56	117.24	123.63
14	b	823	CLA	CHA-C1A-NA	-2.56	120.61	126.39
14	2	823	CLA	CHA-C1A-NA	-2.56	120.61	126.39
14	A	839	CLA	C1-C2-C3	-2.55	122.01	126.20
14	A	808	CLA	CHD-C1D-ND	-2.55	121.21	124.80
14	B	816	CLA	C2D-C1D-ND	-2.55	107.60	110.13
14	b	833	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
14	a	822	CLA	O2D-CGD-CBD	2.55	115.69	111.23
17	A	850	BCR	C33-C5-C6	-2.55	121.70	124.48
17	f	206	BCR	C15-C16-C17	-2.55	118.31	123.52
14	B	838	CLA	O2D-CGD-O1D	-2.55	118.89	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	835	CLA	C1-C2-C3	-2.55	122.02	126.20
14	0	208	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
14	1	838	CLA	C1-C2-C3	-2.55	122.03	126.20
14	b	834	CLA	CHD-C1D-ND	-2.55	121.22	124.80
14	B	824	CLA	CHA-C1A-NA	-2.55	120.62	126.39
17	8	4005	BCR	C27-C26-C25	2.55	126.14	122.70
14	1	834	CLA	C1-C2-C3	-2.55	122.03	126.20
14	b	835	CLA	CHA-C1A-NA	-2.54	120.63	126.39
14	a	854	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	b	824	CLA	CHB-C4A-NA	2.54	128.07	124.40
17	j	104	BCR	C24-C23-C22	-2.54	122.47	126.23
14	1	820	CLA	O2D-CGD-CBD	2.54	115.67	111.23
14	A	821	CLA	O2D-CGD-CBD	2.54	115.67	111.23
17	1	851	BCR	C7-C8-C9	-2.54	122.47	126.23
17	6	4405	BCR	C15-C16-C17	-2.54	118.32	123.52
17	K	4005	BCR	C27-C26-C25	2.54	126.14	122.70
17	j	103	BCR	C27-C26-C25	2.54	126.14	122.70
14	A	831	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	2	824	CLA	CHB-C4A-NA	2.54	128.07	124.40
18	B	803	LMG	O2-C2-C1	-2.54	104.02	110.08
17	7	1104	BCR	C27-C26-C25	2.54	126.13	122.70
14	a	840	CLA	C1-C2-C3	-2.54	122.04	126.20
18	2	802	LMG	C40-C39-C38	-2.54	101.54	114.37
14	2	833	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
14	A	835	CLA	CHB-C4A-NA	2.54	128.06	124.40
14	B	835	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
14	b	827	CLA	O1D-CGD-CBD	2.54	129.52	124.52
14	2	827	CLA	O1D-CGD-CBD	2.54	129.52	124.52
14	l	4205	CLA	CHD-C1D-ND	-2.54	121.23	124.80
18	B	803	LMG	C40-C39-C38	-2.54	101.55	114.37
14	l	4206	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
14	b	818	CLA	CMB-C2B-C3B	2.54	132.51	126.55
14	1	826	CLA	C3B-C4B-NB	-2.54	108.27	110.53
14	B	834	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
14	2	815	CLA	C2D-C1D-ND	-2.53	107.62	110.13
14	2	834	CLA	CHD-C1D-ND	-2.53	121.24	124.80
14	b	834	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
14	B	836	CLA	CHA-C1A-NA	-2.53	120.66	126.39
17	F	206	BCR	C15-C16-C17	-2.53	118.34	123.52
14	B	828	CLA	O1D-CGD-CBD	2.53	129.51	124.52
14	2	834	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
17	J	104	BCR	C24-C23-C22	-2.53	122.49	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a	851	BCR	C7-C8-C9	-2.53	122.49	126.23
18	b	803	LMG	C40-C39-C38	-2.53	101.57	114.37
17	6	4405	BCR	C11-C10-C9	-2.53	123.73	127.28
14	B	819	CLA	CMB-C2B-C3B	2.53	132.50	126.55
17	a	850	BCR	C20-C21-C22	-2.53	123.73	127.28
17	a	847	BCR	C15-C16-C17	-2.53	118.34	123.52
17	1	849	BCR	C33-C5-C6	-2.53	121.72	124.48
18	b	803	LMG	O2-C2-C1	-2.53	104.05	110.08
14	2	835	CLA	CHA-C1A-NA	-2.53	120.67	126.39
17	A	847	BCR	C7-C8-C9	-2.53	122.50	126.23
17	k	4004	BCR	C27-C26-C25	2.53	126.12	122.70
14	2	818	CLA	CMB-C2B-C3B	2.53	132.49	126.55
14	a	809	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
18	2	802	LMG	O2-C2-C1	-2.52	104.06	110.08
17	A	847	BCR	C15-C16-C17	-2.52	118.36	123.52
14	B	801	CLA	C4-C3-C5	2.52	119.60	115.23
17	1	847	BCR	C15-C16-C17	-2.52	118.36	123.52
17	f	206	BCR	C11-C10-C9	-2.52	123.75	127.28
17	0	204	BCR	C15-C14-C13	-2.51	123.75	127.28
14	k	4002	CLA	CHB-C4A-NA	2.51	128.03	124.40
17	a	847	BCR	C7-C8-C9	-2.51	122.52	126.23
17	1	847	BCR	C7-C8-C9	-2.51	122.52	126.23
17	F	206	BCR	C11-C10-C9	-2.51	123.75	127.28
14	b	804	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
17	i	4102	BCR	C27-C26-C25	2.51	126.10	122.70
14	8	4002	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	a	824	CLA	CMA-C3A-C2A	-2.51	104.27	113.98
14	B	840	CLA	CMB-C2B-C3B	2.51	132.46	126.55
14	b	839	CLA	CMB-C2B-C3B	2.51	132.45	126.55
13	A	803	CL0	CMD-C2D-C3D	2.51	129.69	124.68
17	L	1505	BCR	C15-C14-C13	-2.51	123.76	127.28
14	A	808	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
14	a	829	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
14	A	823	CLA	CMA-C3A-C2A	-2.51	104.29	113.98
13	a	803	CL0	CMD-C2D-C3D	2.51	129.69	124.68
14	1	822	CLA	CMA-C3A-C2A	-2.50	104.30	113.98
14	A	841	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
14	1	807	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
14	l	4203	CLA	C2D-C1D-ND	-2.50	107.65	110.13
14	2	807	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	b	802	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
17	7	1105	BCR	C24-C23-C22	-2.50	122.53	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	843	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
17	I	101	BCR	C27-C26-C25	2.50	126.08	122.70
14	2	839	CLA	CHD-C1D-ND	-2.50	121.28	124.80
14	2	811	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	B	804	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
14	1	830	CLA	CHB-C4A-NA	2.50	128.00	124.40
14	B	835	CLA	CHD-C1D-ND	-2.50	121.29	124.80
17	h	101	BCR	C27-C26-C25	2.50	126.08	122.70
14	2	822	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	0	210	BCR	C15-C14-C13	-2.49	123.78	127.28
14	2	820	CLA	C3B-C4B-NB	-2.49	108.30	110.53
14	B	840	CLA	CHD-C1D-ND	-2.49	121.29	124.80
14	2	839	CLA	CMB-C2B-C3B	2.49	132.41	126.55
14	1	840	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
17	0	209	BCR	C15-C16-C17	-2.49	118.43	123.52
14	2	803	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
14	2	844	CLA	CHB-C4A-NA	2.49	127.97	124.43
17	0	209	BCR	C15-C14-C13	-2.49	123.79	127.28
14	K	4002	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	0	209	BCR	C20-C21-C22	-2.49	123.79	127.28
13	1	803	CL0	CMD-C2D-C3D	2.49	129.65	124.68
14	a	841	CLA	CHA-C1A-NA	-2.48	120.76	126.39
17	a	849	BCR	C33-C5-C6	-2.48	121.77	124.48
14	1	839	CLA	CHA-C1A-NA	-2.48	120.77	126.39
17	b	849	BCR	C40-C30-C25	2.48	114.14	110.24
14	B	813	CLA	C2D-C1D-ND	-2.48	107.67	110.13
14	2	801	CLA	C4-C3-C5	2.48	119.54	115.23
14	K	4003	CLA	CHB-C4A-NA	2.48	127.98	124.40
17	2	849	BCR	C40-C30-C25	2.48	114.13	110.24
14	a	804	CLA	C4-C3-C5	2.48	119.53	115.23
17	9	102	BCR	C33-C5-C6	-2.48	121.78	124.48
17	l	4207	BCR	C15-C16-C17	-2.48	118.44	123.52
14	b	812	CLA	CHB-C4A-NA	2.48	127.98	124.40
17	2	848	BCR	C15-C16-C17	-2.48	118.45	123.52
14	b	839	CLA	CHD-C1D-ND	-2.48	121.32	124.80
14	8	4003	CLA	CHB-C4A-NA	2.48	127.97	124.40
17	L	1504	BCR	C15-C16-C17	-2.48	118.45	123.52
13	a	803	CL0	C4C-CHD-C1D	2.48	124.93	116.07
14	A	828	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
17	B	850	BCR	C40-C30-C25	2.47	114.12	110.24
14	a	815	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
14	B	812	CLA	CHB-C4A-NA	2.47	127.97	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	6	4405	BCR	C2-C1-C6	2.47	114.03	110.44
14	b	802	CLA	CAA-CBA-CGA	-2.47	106.19	113.21
17	B	849	BCR	C15-C16-C17	-2.47	118.46	123.52
14	b	843	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
14	b	844	CLA	CHB-C4A-NA	2.47	127.94	124.43
14	1	840	CLA	CAA-CBA-CGA	-2.47	106.20	113.21
14	A	840	CLA	CHA-C1A-NA	-2.47	120.80	126.39
14	B	823	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	b	808	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	k	4003	CLA	CHB-C4A-NA	2.47	127.96	124.40
17	2	847	BCR	C7-C8-C9	-2.47	122.59	126.23
13	1	803	CL0	C4C-CHD-C1D	2.47	124.89	116.07
17	l	4207	BCR	C20-C21-C22	-2.47	123.82	127.28
15	B	846	PQN	C16-C15-C13	-2.46	107.47	113.47
15	2	845	PQN	C16-C15-C13	-2.46	107.47	113.47
17	a	847	BCR	C16-C15-C14	-2.46	118.48	123.52
13	A	803	CL0	C4C-CHD-C1D	2.46	124.87	116.07
14	1	813	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
14	A	814	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
14	1	827	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
14	B	808	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	a	839	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
17	b	848	BCR	C15-C16-C17	-2.46	118.49	123.52
17	A	847	BCR	C16-C15-C14	-2.46	118.49	123.52
14	2	831	CLA	C3C-C4C-NC	-2.46	107.28	110.43
17	L	1504	BCR	C20-C21-C22	-2.45	123.84	127.28
14	A	841	CLA	CAA-CBA-CGA	-2.45	106.24	113.21
14	a	839	CLA	C2D-C1D-ND	-2.45	107.70	110.13
14	B	813	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	b	845	PQN	C16-C15-C13	-2.45	107.50	113.47
17	1	847	BCR	C16-C15-C14	-2.45	118.50	123.52
17	2	848	BCR	C35-C13-C12	2.45	120.23	114.59
14	b	822	CLA	CHB-C4A-NA	2.45	127.94	124.40
14	B	835	CLA	CAA-CBA-CGA	-2.45	106.25	113.21
17	b	847	BCR	C7-C8-C9	-2.45	122.61	126.23
17	b	848	BCR	C35-C13-C12	2.45	120.22	114.59
14	b	820	CLA	C3B-C4B-NB	-2.45	108.34	110.53
14	B	845	CLA	CHB-C4A-NA	2.45	127.91	124.43
14	a	824	CLA	C1-C2-C3	-2.45	122.19	126.20
14	2	843	CLA	CHB-C4A-NA	2.45	127.93	124.40
14	b	834	CLA	CAA-CBA-CGA	-2.44	106.27	113.21
14	B	814	CLA	CMB-C2B-C1B	-2.44	121.70	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	834	CLA	O2D-CGD-CBD	2.44	115.50	111.23
14	b	807	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
17	L	1504	BCR	C15-C14-C13	-2.44	123.86	127.28
14	2	813	CLA	CHB-C4A-NA	2.44	127.92	124.40
17	f	206	BCR	C2-C1-C6	2.44	113.98	110.44
17	B	848	BCR	C7-C8-C9	-2.44	122.62	126.23
14	B	832	CLA	C3C-C4C-NC	-2.44	107.30	110.43
14	1	822	CLA	C1-C2-C3	-2.44	122.20	126.20
17	2	850	BCR	C20-C21-C22	-2.44	123.86	127.28
14	A	838	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
14	2	812	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	A	838	CLA	C2D-C1D-ND	-2.44	107.71	110.13
17	F	206	BCR	C2-C1-C6	2.44	113.98	110.44
17	l	4207	BCR	C15-C14-C13	-2.44	123.86	127.28
14	A	823	CLA	C1-C2-C3	-2.44	122.20	126.20
14	B	844	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	2	812	CLA	C2D-C1D-ND	-2.44	107.71	110.13
14	2	806	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
17	B	849	BCR	C35-C13-C12	2.44	120.19	114.59
14	2	834	CLA	CAA-CBA-CGA	-2.44	106.29	113.21
17	b	850	BCR	C20-C21-C22	-2.43	123.87	127.28
14	a	836	CLA	O2D-CGD-CBD	2.43	115.48	111.23
14	B	844	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
14	b	831	CLA	C3C-C4C-NC	-2.43	107.32	110.43
18	0	201	LMG	O7-C10-O9	-2.43	118.02	123.70
17	b	854	BCR	C33-C5-C6	-2.43	121.83	124.48
14	b	836	CLA	CHA-C1A-NA	-2.43	120.89	126.39
14	B	807	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
13	1	803	CL0	CMB-C2B-C3B	2.43	129.53	124.68
14	1	837	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
14	B	821	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	1	837	CLA	O2D-CGD-CBD	2.43	115.47	111.23
17	L	1505	BCR	C39-C30-C25	2.42	114.04	110.24
14	b	813	CLA	CHB-C4A-NA	2.42	127.90	124.40
17	M	102	BCR	C33-C5-C6	-2.42	121.84	124.48
14	1	835	CLA	C1-C2-C3	-2.42	122.23	126.20
14	B	836	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	m	101	LHG	C11-C10-C9	-2.42	102.13	114.37
12	M	101	LHG	C11-C10-C9	-2.42	102.14	114.37
12	9	101	LHG	C11-C10-C9	-2.42	102.14	114.37
14	b	833	CLA	CHB-C4A-NA	2.42	127.89	124.40
13	a	803	CL0	CMB-C2B-C3B	2.42	129.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	1506	LMG	O7-C10-O9	-2.42	118.05	123.70
14	2	827	CLA	CHD-C1D-ND	-2.42	121.40	124.80
18	l	4202	LMG	O7-C10-O9	-2.42	118.06	123.70
14	A	835	CLA	O2D-CGD-CBD	2.42	115.45	111.23
17	B	851	BCR	C20-C21-C22	-2.42	123.89	127.28
13	1	803	CL0	C3D-C4D-CHA	2.41	112.21	108.54
17	2	851	BCR	C10-C11-C12	-2.41	116.20	123.20
17	j	104	BCR	C15-C14-C13	-2.41	123.89	127.28
14	A	805	CLA	O2D-CGD-CBD	2.41	115.45	111.23
17	0	204	BCR	C39-C30-C25	2.41	114.03	110.24
15	1	845	PQN	C11-C12-C13	-2.41	122.67	126.83
17	h	102	BCR	C35-C13-C14	-2.41	118.91	122.82
14	7	1101	CLA	O2D-CGD-CBD	2.41	115.44	111.23
14	b	835	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	1	851	BCR	C15-C14-C13	-2.41	123.90	127.28
14	A	836	CLA	C1-C2-C3	-2.41	122.25	126.20
15	a	845	PQN	C11-C12-C13	-2.41	122.68	126.83
14	b	827	CLA	CHD-C1D-ND	-2.41	121.41	124.80
14	2	833	CLA	CHB-C4A-NA	2.41	127.87	124.40
17	B	852	BCR	C10-C11-C12	-2.41	116.23	123.20
17	8	4001	BCR	C29-C30-C25	2.41	113.93	110.44
14	2	835	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	1	818	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
13	A	803	CL0	CMB-C2B-C3B	2.40	129.49	124.68
14	a	837	CLA	C1-C2-C3	-2.40	122.26	126.20
14	2	836	CLA	CHA-C1A-NA	-2.40	120.95	126.39
14	1	837	CLA	C2D-C1D-ND	-2.40	107.75	110.13
17	2	847	BCR	C29-C30-C25	2.40	113.93	110.44
14	B	828	CLA	CHD-C1D-ND	-2.40	121.42	124.80
14	b	843	CLA	CHB-C4A-NA	2.40	127.86	124.40
17	0	210	BCR	C39-C30-C25	2.40	114.01	110.24
14	A	806	CLA	C1-C2-C3	-2.40	122.88	126.76
14	a	806	CLA	O2D-CGD-CBD	2.40	115.42	111.23
17	b	846	BCR	C24-C23-C22	-2.40	122.69	126.23
17	a	851	BCR	C15-C14-C13	-2.40	123.91	127.28
14	a	820	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
14	B	837	CLA	CHA-C1A-NA	-2.40	120.96	126.39
14	B	814	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	b	840	CLA	C1-C2-C3	-2.40	122.27	126.20
14	B	841	CLA	C1-C2-C3	-2.40	122.27	126.20
14	b	813	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
14	l	4203	CLA	CHB-C4A-NA	2.40	127.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	102	BCR	C27-C26-C25	2.40	125.94	122.70
14	a	807	CLA	C1-C2-C3	-2.40	122.89	126.76
14	A	819	CLA	CMB-C2B-C1B	-2.39	121.77	125.42
14	B	834	CLA	CHB-C4A-NA	2.39	127.86	124.40
14	a	831	CLA	O2D-CGD-CBD	2.39	115.42	111.23
17	b	851	BCR	C10-C11-C12	-2.39	116.26	123.20
18	a	852	LMG	C38-C37-C36	-2.39	102.27	114.37
14	A	824	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
14	A	830	CLA	CMB-C2B-C3B	2.39	132.18	126.55
14	1	829	CLA	CMB-C2B-C3B	2.39	132.17	126.55
17	0	209	BCR	C39-C30-C25	2.39	113.99	110.24
17	B	847	BCR	C24-C23-C22	-2.39	122.70	126.23
14	2	813	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
14	a	831	CLA	CMB-C2B-C3B	2.39	132.17	126.55
18	0	203	LMG	C38-C37-C36	-2.39	102.30	114.37
18	A	852	LMG	C38-C37-C36	-2.39	102.30	114.37
14	a	839	CLA	C1-C2-C3	-2.39	122.29	126.20
17	b	847	BCR	C29-C30-C25	2.39	113.91	110.44
17	7	1105	BCR	C15-C14-C13	-2.39	123.93	127.28
14	a	827	CLA	C4-C3-C5	2.39	119.37	115.23
17	h	102	BCR	C27-C26-C25	2.38	125.92	122.70
17	2	848	BCR	C40-C30-C25	2.38	113.98	110.24
14	A	827	CLA	C2A-C1A-CHA	2.38	128.00	123.87
17	A	851	BCR	C15-C14-C13	-2.38	123.94	127.28
14	a	839	CLA	O2D-CGD-CBD	2.38	115.39	111.23
15	A	845	PQN	C11-C12-C13	-2.38	122.73	126.83
14	1	825	CLA	C4-C3-C5	2.38	119.36	115.23
13	A	803	CL0	C3D-C4D-CHA	2.38	112.16	108.54
14	l	4205	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
18	a	852	LMG	O6-C1-O1	-2.38	104.42	110.04
14	1	829	CLA	O2D-CGD-CBD	2.38	115.39	111.23
14	0	207	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
17	I	102	BCR	C35-C13-C14	-2.38	118.96	122.82
14	a	825	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
17	l	4207	BCR	C39-C30-C25	2.38	113.97	110.24
14	b	838	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
17	k	4001	BCR	C29-C30-C25	2.38	113.89	110.44
14	a	811	CLA	O2D-CGD-CBD	2.38	115.39	111.23
18	0	203	LMG	O6-C1-O1	-2.38	104.43	110.04
14	a	822	CLA	CMB-C2B-C3B	2.38	132.14	126.55
14	a	829	CLA	CHD-C1D-ND	-2.38	121.46	124.80
14	A	821	CLA	CMB-C2B-C3B	2.38	132.14	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	i	4103	BCR	C27-C26-C25	2.38	125.91	122.70
17	L	1504	BCR	C39-C30-C25	2.38	113.97	110.24
17	i	4103	BCR	C35-C13-C14	-2.38	118.97	122.82
14	B	813	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
14	A	838	CLA	O2D-CGD-CBD	2.37	115.38	111.23
14	1	819	CLA	C1-C2-C3	-2.37	122.31	126.20
13	a	803	CL0	C3D-C4D-CHA	2.37	112.15	108.54
14	A	826	CLA	C4-C3-C5	2.37	119.35	115.23
14	1	823	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
14	2	840	CLA	C1-C2-C3	-2.37	122.31	126.20
17	K	4001	BCR	C29-C30-C25	2.37	113.88	110.44
14	a	804	CLA	CAA-CBA-CGA	-2.37	106.48	113.21
17	b	850	BCR	C7-C8-C9	-2.37	122.73	126.23
17	k	4004	BCR	C7-C8-C9	-2.37	122.73	126.23
14	A	820	CLA	C1-C2-C3	-2.37	122.31	126.20
14	1	837	CLA	C1-C2-C3	-2.37	122.32	126.20
14	1	820	CLA	CMB-C2B-C3B	2.37	132.12	126.55
17	B	848	BCR	C29-C30-C25	2.37	113.88	110.44
14	A	838	CLA	C1-C2-C3	-2.37	122.32	126.20
14	a	828	CLA	C2A-C1A-CHA	2.36	127.97	123.87
14	1	826	CLA	C2A-C1A-CHA	2.36	127.97	123.87
17	2	846	BCR	C24-C23-C22	-2.36	122.74	126.23
14	B	839	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
14	l	4203	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
18	A	852	LMG	O6-C1-O1	-2.36	104.46	110.04
14	1	809	CLA	O2D-CGD-CBD	2.36	115.36	111.23
14	1	805	CLA	C1-C2-C3	-2.36	122.94	126.76
17	8	4005	BCR	C7-C8-C9	-2.36	122.74	126.23
14	2	838	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
14	b	827	CLA	CMB-C2B-C3B	2.36	132.10	126.55
14	B	828	CLA	CMB-C2B-C3B	2.36	132.10	126.55
14	A	830	CLA	O2D-CGD-CBD	2.36	115.35	111.23
14	2	801	CLA	CAA-CBA-CGA	-2.36	106.51	113.21
17	A	847	BCR	C15-C14-C13	-2.36	123.97	127.28
14	2	827	CLA	CMB-C2B-C3B	2.36	132.10	126.55
14	A	828	CLA	CHD-C1D-ND	-2.36	121.48	124.80
18	0	201	LMG	C38-C37-C36	-2.36	102.45	114.37
14	2	812	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
14	A	810	CLA	O2D-CGD-CBD	2.36	115.35	111.23
17	1	847	BCR	C15-C14-C13	-2.36	123.97	127.28
17	K	4005	BCR	C7-C8-C9	-2.36	122.75	126.23
13	1	803	CL0	C4D-ND-C1D	2.36	107.01	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	1506	LMG	C38-C37-C36	-2.36	102.46	114.37
17	a	847	BCR	C15-C14-C13	-2.36	123.97	127.28
14	1	827	CLA	CHD-C1D-ND	-2.36	121.49	124.80
18	l	4202	LMG	C38-C37-C36	-2.35	102.47	114.37
17	K	4001	BCR	C33-C5-C6	-2.35	121.92	124.48
17	F	203	BCR	C27-C26-C25	2.35	125.88	122.70
14	L	1502	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
14	B	801	CLA	CAA-CBA-CGA	-2.35	106.53	113.21
13	a	803	CL0	C4D-ND-C1D	2.35	107.00	105.22
18	b	803	LMG	O7-C10-O9	-2.35	118.22	123.70
17	B	847	BCR	C33-C5-C6	-2.35	121.92	124.48
17	J	104	BCR	C15-C14-C13	-2.35	123.99	127.28
17	B	849	BCR	C40-C30-C25	2.35	113.92	110.24
17	f	203	BCR	C27-C26-C25	2.34	125.87	122.70
17	B	851	BCR	C7-C8-C9	-2.34	122.77	126.23
17	2	850	BCR	C7-C8-C9	-2.34	122.77	126.23
14	a	805	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
14	a	821	CLA	C1-C2-C3	-2.34	122.37	126.20
18	b	803	LMG	C38-C37-C36	-2.34	102.55	114.37
14	B	810	CLA	CHB-C4A-NA	2.34	127.77	124.40
14	2	829	CLA	CHB-C4A-NA	2.34	127.77	124.40
14	l	4203	CLA	CHA-C1A-NA	-2.34	121.10	126.39
14	A	831	CLA	CHA-C1A-NA	-2.34	121.10	126.39
14	2	843	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
17	6	4402	BCR	C27-C26-C25	2.33	125.86	122.70
14	a	837	CLA	CMB-C2B-C1B	-2.33	121.86	125.42
18	2	802	LMG	C38-C37-C36	-2.33	102.58	114.37
14	a	832	CLA	CHA-C1A-NA	-2.33	121.11	126.39
17	b	848	BCR	C40-C30-C25	2.33	113.90	110.24
18	B	803	LMG	O7-C10-O9	-2.33	118.26	123.70
14	A	836	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
14	B	831	CLA	C2D-C1D-ND	-2.33	107.82	110.13
14	a	834	CLA	O2D-CGD-CBD	2.33	115.30	111.23
14	1	830	CLA	C1-C2-C3	-2.33	122.38	126.20
14	1	804	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
17	A	850	BCR	C27-C26-C25	2.33	125.85	122.70
12	M	101	LHG	C27-C26-C25	-2.33	102.60	114.37
14	a	841	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
14	1	839	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
18	B	803	LMG	C38-C37-C36	-2.33	102.60	114.37
14	1	832	CLA	O2D-CGD-CBD	2.33	115.30	111.23
14	1	835	CLA	CMB-C2B-C1B	-2.33	121.88	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	830	CLA	C2D-C1D-ND	-2.33	107.82	110.13
17	1	849	BCR	C24-C23-C22	-2.33	122.79	126.23
12	9	101	LHG	C27-C26-C25	-2.33	102.61	114.37
17	a	849	BCR	C27-C26-C25	2.32	125.84	122.70
14	A	833	CLA	O2D-CGD-CBD	2.32	115.29	111.23
14	1	830	CLA	CHA-C1A-NA	-2.32	121.13	126.39
12	m	101	LHG	C27-C26-C25	-2.32	102.63	114.37
18	2	802	LMG	O7-C10-O9	-2.32	118.28	123.70
14	b	843	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
14	2	812	CLA	CHA-C1A-NA	-2.32	121.14	126.39
14	A	821	CLA	C1-C2-C3	-2.32	122.40	126.20
14	a	807	CLA	O2D-CGD-CBD	2.32	115.28	111.23
14	B	837	CLA	CMB-C2B-C3B	2.32	132.00	126.55
14	1	814	CLA	CHB-C4A-NA	2.32	127.74	124.40
17	2	846	BCR	C33-C5-C6	-2.32	121.96	124.48
14	B	844	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
14	2	811	CLA	CHA-C1A-NA	-2.31	121.16	126.39
14	2	806	CLA	C3C-C4C-NC	-2.31	107.47	110.43
14	1	834	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
14	B	806	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	A	804	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
17	a	849	BCR	C24-C23-C22	-2.31	122.82	126.23
14	2	836	CLA	CMB-C2B-C3B	2.31	131.98	126.55
19	6	4401	LMT	C1'-O5'-C5'	-2.31	109.21	113.72
14	A	831	CLA	C1-C2-C3	-2.31	122.42	126.20
14	A	815	CLA	CHB-C4A-NA	2.31	127.73	124.40
12	A	801	LHG	C20-C19-C18	-2.31	102.70	114.37
14	b	836	CLA	CMB-C2B-C3B	2.31	131.98	126.55
17	8	4001	BCR	C33-C5-C6	-2.31	121.97	124.48
14	2	809	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	b	826	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
14	a	816	CLA	CHB-C4A-NA	2.31	127.73	124.40
12	1	801	LHG	C20-C19-C18	-2.31	102.71	114.37
14	A	840	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
14	B	827	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
14	b	804	CLA	CHA-C1A-NA	-2.30	121.17	126.39
19	I	103	LMT	C2'-C3'-C4'	2.30	114.91	109.68
14	b	826	CLA	CHA-C1A-NA	-2.30	121.17	126.39
14	A	835	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
14	B	807	CLA	C3C-C4C-NC	-2.30	107.48	110.43
17	1	848	BCR	C30-C25-C26	-2.30	119.49	122.64
14	b	806	CLA	CHB-C4A-NA	2.30	127.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	846	BCR	C33-C5-C6	-2.30	121.97	124.48
17	2	847	BCR	C33-C5-C6	-2.30	121.97	124.48
14	B	804	CLA	CHA-C1A-NA	-2.30	121.18	126.39
19	F	202	LMT	C1'-O5'-C5'	-2.30	109.23	113.72
14	b	807	CLA	C3C-C4C-NC	-2.30	107.48	110.43
14	B	813	CLA	CHA-C1A-NA	-2.30	121.18	126.39
14	6	4403	CLA	CHA-C1A-NA	-2.30	121.19	126.39
17	1	850	BCR	C27-C26-C25	2.30	125.81	122.70
12	a	801	LHG	C20-C19-C18	-2.30	102.76	114.37
14	1	820	CLA	C1-C2-C3	-2.30	122.44	126.20
14	b	810	CLA	CHB-C4A-NA	2.30	127.71	124.40
14	B	812	CLA	CHA-C1A-NA	-2.30	121.19	126.39
14	A	806	CLA	O2D-CGD-CBD	2.29	115.24	111.23
14	a	832	CLA	C1-C2-C3	-2.29	122.44	126.20
17	a	850	BCR	C27-C26-C25	2.29	125.81	122.70
17	1	849	BCR	C27-C26-C25	2.29	125.81	122.70
14	2	826	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
14	A	805	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
14	B	827	CLA	CHA-C1A-NA	-2.29	121.20	126.39
17	A	848	BCR	C30-C25-C26	-2.29	119.50	122.64
17	A	849	BCR	C24-C23-C22	-2.29	122.85	126.23
14	a	822	CLA	C1-C2-C3	-2.29	122.44	126.20
19	h	103	LMT	C2'-C3'-C4'	2.29	114.88	109.68
14	B	804	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
14	a	806	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
14	1	819	CLA	CHB-C4A-NA	2.29	127.70	124.40
17	A	848	BCR	C40-C30-C25	2.29	113.83	110.24
17	A	849	BCR	C27-C26-C25	2.29	125.80	122.70
17	k	4001	BCR	C33-C5-C6	-2.29	121.99	124.48
14	F	204	CLA	CHA-C1A-NA	-2.29	121.21	126.39
17	1	847	BCR	C11-C10-C9	-2.29	124.07	127.28
14	7	1101	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
14	b	812	CLA	CHA-C1A-NA	-2.29	121.21	126.39
14	b	830	CLA	C2D-C1D-ND	-2.29	107.86	110.13
14	1	828	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	2	805	CLA	CMB-C2B-C3B	2.28	131.92	126.55
14	B	830	CLA	CHB-C4A-NA	2.28	127.70	124.40
14	1	810	CLA	CHA-C1A-NA	-2.28	121.22	126.39
14	2	803	CLA	CHA-C1A-NA	-2.28	121.22	126.39
14	2	803	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
14	2	805	CLA	CHB-C4A-NA	2.28	127.69	124.40
19	f	202	LMT	C1'-O5'-C5'	-2.28	109.26	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	841	CLA	CHD-C1D-ND	-2.28	121.59	124.80
14	2	826	CLA	CHA-C1A-NA	-2.28	121.22	126.39
19	i	4101	LMT	C2'-C3'-C4'	2.28	114.86	109.68
14	f	204	CLA	CHA-C1A-NA	-2.28	121.23	126.39
14	b	804	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
17	a	850	BCR	C24-C23-C22	-2.28	122.86	126.23
17	a	851	BCR	C10-C11-C12	-2.28	116.60	123.20
14	A	811	CLA	CHA-C1A-NA	-2.28	121.23	126.39
17	1	851	BCR	C29-C30-C25	2.28	113.75	110.44
14	1	805	CLA	O2D-CGD-CBD	2.28	115.21	111.23
17	a	848	BCR	C40-C30-C25	2.28	113.81	110.24
14	b	820	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	a	839	CLA	CHA-C1A-NA	-2.27	121.24	126.39
14	7	1103	CLA	CAA-C2A-C3A	-2.27	111.01	116.23
14	2	841	CLA	CHD-C1D-ND	-2.27	121.60	124.80
17	1	848	BCR	C40-C30-C25	2.27	113.81	110.24
17	K	4001	BCR	C11-C10-C9	-2.27	124.09	127.28
14	1	838	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
14	2	815	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
17	a	848	BCR	C30-C25-C26	-2.27	119.53	122.64
14	B	806	CLA	CMB-C2B-C3B	2.27	131.90	126.55
14	a	836	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
14	b	829	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	2	820	CLA	CHB-C4A-NA	2.27	127.68	124.40
17	1	851	BCR	C10-C11-C12	-2.27	116.61	123.20
14	f	205	CLA	O2A-CGA-O1A	-2.27	117.49	123.33
14	a	830	CLA	CHB-C4A-NA	2.27	127.68	124.40
17	A	851	BCR	C10-C11-C12	-2.27	116.62	123.20
14	a	838	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	A	838	CLA	CHA-C1A-NA	-2.27	121.25	126.39
17	a	851	BCR	C29-C30-C25	2.27	113.73	110.44
12	1	801	LHG	C18-C17-C16	-2.27	102.90	114.37
14	J	102	CLA	CAA-C2A-C3A	-2.27	111.03	116.23
17	1	850	BCR	C24-C23-C22	-2.27	122.88	126.23
14	6	4404	CLA	O2A-CGA-O1A	-2.27	117.50	123.33
14	b	806	CLA	CMB-C2B-C3B	2.27	131.88	126.55
14	b	805	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	B	844	CLA	C1-C2-C3	-2.27	122.48	126.20
12	A	801	LHG	C18-C17-C16	-2.27	102.91	114.37
17	b	847	BCR	C33-C5-C6	-2.27	122.01	124.48
17	b	848	BCR	C24-C23-C22	-2.27	122.88	126.23
14	2	818	CLA	CHB-C4A-NA	2.26	127.67	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	842	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
12	a	801	LHG	C18-C17-C16	-2.26	102.93	114.37
14	B	821	CLA	CMB-C2B-C3B	2.26	131.87	126.55
14	a	831	CLA	C2D-C1D-ND	-2.26	107.89	110.13
17	B	848	BCR	C33-C5-C6	-2.26	122.02	124.48
14	b	838	CLA	C2D-C1D-ND	-2.26	107.89	110.13
17	a	847	BCR	C11-C10-C9	-2.26	124.11	127.28
17	2	850	BCR	C29-C30-C25	2.26	113.72	110.44
14	1	817	CLA	C3B-C4B-NB	-2.26	108.51	110.53
14	j	102	CLA	CAA-C2A-C3A	-2.26	111.05	116.23
14	a	812	CLA	CHA-C1A-NA	-2.26	121.27	126.39
14	1	810	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
14	F	205	CLA	O2A-CGA-O1A	-2.26	117.52	123.33
14	A	818	CLA	C3B-C4B-NB	-2.26	108.51	110.53
14	a	821	CLA	CHB-C4A-NA	2.26	127.66	124.40
17	2	849	BCR	C15-C14-C13	-2.26	124.11	127.28
14	2	843	CLA	C1-C2-C3	-2.26	122.50	126.20
14	1	837	CLA	CHA-C1A-NA	-2.26	121.28	126.39
17	L	1505	BCR	C33-C5-C6	-2.26	122.02	124.48
14	A	820	CLA	CHB-C4A-NA	2.26	127.66	124.40
17	A	851	BCR	C29-C30-C25	2.26	113.72	110.44
14	a	812	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
14	L	1502	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
17	A	847	BCR	C11-C10-C9	-2.25	124.12	127.28
14	j	102	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	b	826	CLA	C2D-C1D-ND	-2.25	107.90	110.13
14	A	829	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	1	829	CLA	C2D-C1D-ND	-2.25	107.90	110.13
17	b	850	BCR	C29-C30-C25	2.25	113.71	110.44
14	B	842	CLA	CHD-C1D-ND	-2.25	121.64	124.80
17	A	850	BCR	C24-C23-C22	-2.25	122.91	126.23
14	B	839	CLA	C2D-C1D-ND	-2.25	107.90	110.13
17	b	851	BCR	C16-C15-C14	-2.25	118.92	123.52
14	2	842	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
14	A	811	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
14	1	821	CLA	CMB-C2B-C3B	2.25	131.84	126.55
14	J	101	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
14	A	830	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
14	a	831	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
17	2	848	BCR	C24-C23-C22	-2.25	122.91	126.23
14	b	820	CLA	CMB-C2B-C3B	2.25	131.83	126.55
17	2	851	BCR	C16-C15-C14	-2.25	118.92	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	829	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
14	2	804	CLA	CHB-C4A-NA	2.24	127.64	124.40
14	b	843	CLA	C1-C2-C3	-2.24	122.52	126.20
14	J	102	CLA	CHB-C4A-NA	2.24	127.64	124.40
17	8	4001	BCR	C11-C10-C9	-2.24	124.13	127.28
14	b	823	CLA	CHB-C4A-NA	2.24	127.64	124.40
14	a	819	CLA	C3B-C4B-NB	-2.24	108.53	110.53
14	K	4004	CLA	C1-C2-C3	-2.24	122.53	126.20
14	B	822	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	A	839	CLA	O2D-CGD-CBD	2.24	115.15	111.23
18	b	803	LMG	O1-C1-C2	-2.24	104.87	108.27
14	a	835	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
17	B	851	BCR	C29-C30-C25	2.24	113.69	110.44
14	B	824	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	A	843	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
14	A	837	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	B	821	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	1	826	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	a	840	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
14	B	819	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	b	815	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
18	2	802	LMG	O1-C1-C2	-2.23	104.88	108.27
14	b	837	CLA	CHA-C1A-NA	-2.23	121.33	126.39
14	2	821	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
14	b	828	CLA	CAA-CBA-CGA	-2.23	106.86	113.21
14	j	101	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
17	8	4005	BCR	C24-C23-C22	-2.23	122.93	126.23
14	l	4205	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
17	0	210	BCR	C33-C5-C6	-2.23	122.05	124.48
14	2	820	CLA	CMB-C2B-C3B	2.23	131.80	126.55
14	1	836	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	a	840	CLA	O2D-CGD-CBD	2.23	115.13	111.23
17	1	851	BCR	C31-C1-C6	2.23	113.74	110.24
14	B	816	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
17	B	849	BCR	C24-C23-C22	-2.23	122.93	126.23
18	A	852	LMG	O3-C3-C2	-2.23	105.12	110.38
14	2	837	CLA	CHA-C1A-NA	-2.23	121.34	126.39
14	7	1102	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
14	b	821	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
18	0	203	LMG	O3-C3-C2	-2.23	105.12	110.38
14	A	827	CLA	CHB-C4A-NA	2.23	127.62	124.40
17	k	4001	BCR	C11-C10-C9	-2.23	124.15	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	850	BCR	C27-C26-C25	2.23	125.71	122.70
14	1	838	CLA	O2D-CGD-CBD	2.23	115.12	111.23
14	B	805	CLA	CHB-C4A-NA	2.23	127.61	124.40
14	B	829	CLA	CAA-CBA-CGA	-2.23	106.89	113.21
14	j	102	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
14	1	834	CLA	CAA-CBA-CGA	-2.23	106.89	113.21
17	B	852	BCR	C16-C15-C14	-2.23	118.96	123.52
14	a	828	CLA	CHB-C4A-NA	2.23	127.61	124.40
14	B	838	CLA	CHA-C1A-NA	-2.23	121.35	126.39
14	b	821	CLA	CHB-C1B-NB	2.22	127.39	124.05
14	B	843	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
17	K	4005	BCR	C24-C23-C22	-2.22	122.95	126.23
14	2	823	CLA	CHB-C4A-NA	2.22	127.61	124.40
17	B	850	BCR	C15-C14-C13	-2.22	124.16	127.28
14	a	836	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
14	2	828	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
14	7	1103	CLA	CHB-C4A-NA	2.22	127.61	124.40
13	A	803	CL0	C4D-ND-C1D	2.22	106.91	105.22
14	A	822	CLA	CMB-C2B-C3B	2.22	131.77	126.55
14	2	810	CLA	O2D-CGD-CBD	2.22	115.11	111.23
14	A	839	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
14	a	854	CLA	C1-C2-C3	-2.22	122.56	126.20
17	k	4004	BCR	C24-C23-C22	-2.22	122.95	126.23
14	2	838	CLA	C2D-C1D-ND	-2.22	107.93	110.13
14	0	207	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	a	810	CLA	CMB-C2B-C1B	-2.22	122.05	125.42
14	1	833	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
17	b	849	BCR	C33-C5-C6	-2.21	122.07	124.48
14	7	1103	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
14	B	827	CLA	O2D-CGD-CBD	2.21	115.10	111.23
17	A	851	BCR	C31-C1-C6	2.21	113.71	110.24
14	b	818	CLA	CHB-C4A-NA	2.21	127.59	124.40
14	2	826	CLA	O2D-CGD-CBD	2.21	115.10	111.23
14	b	830	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
14	a	843	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
14	A	811	CLA	C2D-C1D-ND	-2.21	107.94	110.13
17	j	104	BCR	C31-C1-C6	2.21	113.71	110.24
14	A	826	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
17	i	4102	BCR	C11-C10-C9	-2.21	124.18	127.28
18	a	852	LMG	O3-C3-C2	-2.21	105.17	110.38
14	a	823	CLA	CMB-C2B-C3B	2.21	131.75	126.55
14	2	826	CLA	C2D-C1D-ND	-2.21	107.94	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	831	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
14	1	808	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
14	2	821	CLA	CHB-C1B-NB	2.21	127.36	124.05
14	2	830	CLA	CHA-C1A-NA	-2.21	121.39	126.39
17	b	850	BCR	C27-C26-C25	2.21	125.69	122.70
14	2	830	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
17	1	849	BCR	C7-C8-C9	-2.21	122.97	126.23
14	1	820	CLA	C3C-C4C-NC	-2.21	107.60	110.43
14	1	843	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
14	A	827	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	2	826	CLA	CHB-C4A-NA	2.21	127.58	124.40
14	a	828	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
17	a	851	BCR	C31-C1-C6	2.21	113.70	110.24
14	8	4004	CLA	C1-C2-C3	-2.20	122.59	126.20
14	b	811	CLA	O2D-CGD-CBD	2.20	115.08	111.23
14	B	821	CLA	C3C-C4C-NC	-2.20	107.61	110.43
14	b	826	CLA	O2D-CGD-CBD	2.20	115.08	111.23
14	b	808	CLA	C1-C2-C3	-2.20	122.59	126.20
17	A	849	BCR	C7-C8-C9	-2.20	122.98	126.23
14	A	834	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
14	0	206	CLA	CHD-C1D-ND	-2.20	121.71	124.80
17	B	851	BCR	C27-C26-C25	2.20	125.67	122.70
14	J	102	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
14	A	812	CLA	C2D-C1D-ND	-2.20	107.95	110.13
14	B	822	CLA	CHB-C1B-NB	2.20	127.34	124.05
17	J	104	BCR	C31-C1-C6	2.19	113.68	110.24
14	1	831	CLA	O1D-CGD-CBD	2.19	128.84	124.52
14	a	812	CLA	C2D-C1D-ND	-2.19	107.95	110.13
14	A	835	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
14	b	830	CLA	CHA-C1A-NA	-2.19	121.42	126.39
14	L	1501	CLA	CHB-C4A-NA	2.19	127.56	124.40
14	a	835	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
14	1	826	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
14	b	838	CLA	CHB-C4A-NA	2.19	127.56	124.40
14	A	830	CLA	C2D-C1D-ND	-2.19	107.96	110.13
14	a	813	CLA	C2D-C1D-ND	-2.19	107.96	110.13
17	B	850	BCR	C24-C23-C22	-2.19	122.99	126.23
14	2	803	CLA	C6-C7-C8	-2.19	108.68	115.97
14	a	827	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
14	1	810	CLA	C2D-C1D-ND	-2.19	107.96	110.13
14	B	811	CLA	C6-C5-C3	2.19	118.80	113.47
17	a	849	BCR	C7-C8-C9	-2.19	123.00	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	803	LMG	O1-C1-C2	-2.19	104.95	108.27
14	l	4206	CLA	CHB-C4A-NA	2.19	127.56	124.40
14	B	811	CLA	O2D-CGD-CBD	2.19	115.06	111.23
14	B	808	CLA	C1-C2-C3	-2.19	122.61	126.20
17	b	849	BCR	C15-C14-C13	-2.19	124.21	127.28
14	B	831	CLA	CHA-C1A-NA	-2.19	121.43	126.39
12	A	801	LHG	O8-C23-C24	2.19	118.51	111.83
12	a	801	LHG	O8-C23-C24	2.19	118.51	111.83
14	b	804	CLA	C6-C7-C8	-2.19	108.69	115.97
14	1	811	CLA	C2D-C1D-ND	-2.19	107.96	110.13
14	b	839	CLA	C2D-C1D-ND	-2.19	107.96	110.13
17	0	204	BCR	C33-C5-C6	-2.19	122.10	124.48
17	B	852	BCR	C2-C1-C6	2.19	113.61	110.44
14	A	832	CLA	O1D-CGD-CBD	2.19	128.83	124.52
14	B	827	CLA	C2D-C1D-ND	-2.19	107.96	110.13
17	b	853	BCR	C24-C23-C22	-2.19	123.00	126.23
14	A	834	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
17	h	101	BCR	C11-C10-C9	-2.18	124.22	127.28
14	B	829	CLA	C1-C2-C3	-2.18	122.62	126.20
13	a	803	CL0	O2A-CGA-O1A	-2.18	118.17	123.63
17	b	849	BCR	C24-C23-C22	-2.18	123.01	126.23
14	l	4204	CLA	CHD-C1D-ND	-2.18	121.73	124.80
14	B	807	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	b	819	CLA	C2D-C1D-ND	-2.18	107.97	110.13
12	1	801	LHG	O8-C23-C24	2.18	118.49	111.83
14	L	1501	CLA	CHD-C1D-ND	-2.18	121.73	124.80
18	0	203	LMG	O2-C2-C1	-2.18	104.88	110.08
14	2	807	CLA	C1-C2-C3	-2.18	122.62	126.20
14	A	809	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
14	2	820	CLA	C3C-C4C-NC	-2.18	107.64	110.43
14	B	804	CLA	C6-C7-C8	-2.18	108.72	115.97
14	b	820	CLA	C3C-C4C-NC	-2.18	107.64	110.43
14	0	206	CLA	CHB-C4A-NA	2.18	127.54	124.40
14	A	821	CLA	C3C-C4C-NC	-2.18	107.64	110.43
14	2	810	CLA	C6-C5-C3	2.18	118.77	113.47
14	a	833	CLA	O1D-CGD-CBD	2.18	128.81	124.52
14	0	208	CLA	CHB-C4A-NA	2.18	127.54	124.40
17	2	849	BCR	C24-C23-C22	-2.18	123.02	126.23
14	L	1503	CLA	CHB-C4A-NA	2.18	127.54	124.40
15	1	845	PQN	C12-C11-C3	-2.17	106.72	112.08
17	j	104	BCR	C11-C10-C9	-2.17	124.23	127.28
17	B	850	BCR	C33-C5-C6	-2.17	122.11	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a	848	BCR	C33-C5-C6	-2.17	122.11	124.48
17	1	848	BCR	C33-C5-C6	-2.17	122.11	124.48
17	2	851	BCR	C2-C1-C6	2.17	113.60	110.44
14	1	833	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
12	1	801	LHG	O8-C23-O10	-2.17	118.19	123.63
14	2	828	CLA	C1-C2-C3	-2.17	122.64	126.20
14	A	819	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
17	b	851	BCR	C2-C1-C6	2.17	113.59	110.44
14	B	842	CLA	C4D-C3D-CAD	-2.17	105.75	108.11
12	a	801	LHG	O8-C23-O10	-2.17	118.20	123.63
14	b	826	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	B	820	CLA	C2D-C1D-ND	-2.17	107.98	110.13
17	2	849	BCR	C33-C5-C6	-2.17	122.12	124.48
14	B	841	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	l	4204	CLA	CHB-C4A-NA	2.17	127.53	124.40
17	7	1105	BCR	C31-C1-C6	2.17	113.64	110.24
15	a	845	PQN	C12-C11-C3	-2.17	106.74	112.08
17	F	206	BCR	C40-C30-C25	2.17	113.64	110.24
14	2	838	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	B	840	CLA	C2D-C1D-ND	-2.17	107.98	110.13
14	2	841	CLA	C4D-C3D-CAD	-2.16	105.75	108.11
17	6	4406	BCR	C24-C23-C22	-2.16	123.03	126.23
14	b	828	CLA	C1-C2-C3	-2.16	122.65	126.20
14	2	839	CLA	C2D-C1D-ND	-2.16	107.98	110.13
18	0	201	LMG	O2-C2-C1	-2.16	104.92	110.08
17	6	4405	BCR	C40-C30-C25	2.16	113.64	110.24
14	A	805	CLA	C1-C2-C3	-2.16	122.65	126.20
14	A	835	CLA	CHD-C1D-ND	-2.16	121.76	124.80
17	J	104	BCR	C11-C10-C9	-2.16	124.25	127.28
18	A	852	LMG	O2-C2-C1	-2.16	104.92	110.08
13	1	803	CL0	O2A-CGA-O1A	-2.16	118.22	123.63
17	9	102	BCR	C7-C8-C9	-2.16	123.04	126.23
14	1	805	CLA	C2D-C1D-ND	-2.16	107.99	110.13
14	b	811	CLA	C6-C5-C3	2.16	118.73	113.47
17	I	102	BCR	C33-C5-C6	-2.16	122.13	124.48
17	M	102	BCR	C7-C8-C9	-2.16	123.04	126.23
12	A	801	LHG	O8-C23-O10	-2.16	118.23	123.63
14	b	807	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	a	822	CLA	C3C-C4C-NC	-2.16	107.66	110.43
17	I	101	BCR	C11-C10-C9	-2.16	124.25	127.28
18	l	4202	LMG	O2-C2-C1	-2.16	104.93	110.08
17	B	852	BCR	C28-C27-C26	-2.16	110.21	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	801	CLA	CHB-C4A-NA	2.16	127.51	124.40
14	b	841	CLA	C4D-C3D-CAD	-2.16	105.76	108.11
14	B	808	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
17	2	851	BCR	C28-C27-C26	-2.16	110.21	114.06
17	B	850	BCR	C20-C21-C22	-2.16	124.25	127.28
14	2	806	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	1	834	CLA	CHD-C1D-ND	-2.16	121.77	124.80
17	a	850	BCR	C35-C13-C14	-2.16	119.32	122.82
15	A	845	PQN	C12-C11-C3	-2.16	106.77	112.08
18	a	852	LMG	O2-C2-C1	-2.15	104.94	110.08
14	A	831	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
17	7	1105	BCR	C11-C10-C9	-2.15	124.26	127.28
14	B	821	CLA	CAA-CBA-CGA	-2.15	107.09	113.21
14	1	833	CLA	O1D-CGD-CBD	2.15	128.76	124.52
17	b	851	BCR	C28-C27-C26	-2.15	110.22	114.06
14	B	839	CLA	CHB-C4A-NA	2.15	127.51	124.40
17	a	850	BCR	C16-C15-C14	-2.15	119.11	123.52
17	B	854	BCR	C24-C23-C22	-2.15	123.05	126.23
14	2	820	CLA	CAA-CBA-CGA	-2.15	107.10	113.21
14	a	806	CLA	C1-C2-C3	-2.15	122.67	126.20
14	b	810	CLA	O2D-CGD-CBD	2.15	114.99	111.23
14	1	812	CLA	CHB-C1B-NB	2.15	127.28	124.05
14	j	101	CLA	CHB-C4A-NA	2.15	127.50	124.40
14	A	813	CLA	CHB-C1B-NB	2.15	127.27	124.05
14	b	820	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
14	b	808	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
14	2	819	CLA	C2D-C1D-ND	-2.15	108.00	110.13
12	A	801	LHG	C27-C26-C25	-2.15	103.51	114.37
17	J	103	BCR	C15-C14-C13	-2.15	124.27	127.28
14	J	101	CLA	CHB-C4A-NA	2.15	127.50	124.40
17	A	850	BCR	C35-C13-C14	-2.15	119.34	122.82
14	A	816	CLA	CHA-C1A-NA	-2.15	121.53	126.39
14	A	806	CLA	CHA-C1A-NA	-2.15	121.53	126.39
18	L	1506	LMG	O2-C2-C1	-2.15	104.96	110.08
17	A	850	BCR	C16-C15-C14	-2.15	119.13	123.52
14	1	818	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
14	a	833	CLA	C2D-C1D-ND	-2.15	108.00	110.13
14	8	4004	CLA	C2D-C1D-ND	-2.15	108.00	110.13
14	B	812	CLA	C3A-C2A-C1A	2.15	104.55	101.34
14	1	805	CLA	CHA-C1A-NA	-2.14	121.53	126.39
14	2	811	CLA	C3A-C2A-C1A	2.14	104.55	101.34
14	2	804	CLA	O2D-CGD-CBD	2.14	114.98	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	206	BCR	C40-C30-C25	2.14	113.60	110.24
17	1	850	BCR	C35-C13-C14	-2.14	119.34	122.82
17	7	1104	BCR	C15-C14-C13	-2.14	124.27	127.28
14	B	827	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	1	825	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
14	1	830	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	a	817	CLA	CHA-C1A-NA	-2.14	121.54	126.39
17	b	854	BCR	C7-C8-C9	-2.14	123.07	126.23
14	2	807	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
12	a	801	LHG	C27-C26-C25	-2.14	103.55	114.37
13	A	803	CL0	O2A-CGA-O1A	-2.14	118.28	123.63
14	a	832	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	a	814	CLA	CHB-C4A-NA	2.14	127.48	124.40
12	2	852	LHG	C27-C26-C25	-2.14	103.57	114.37
12	b	852	LHG	C27-C26-C25	-2.14	103.57	114.37
14	2	836	CLA	CHB-C4A-NA	2.14	127.48	124.40
12	1	801	LHG	C27-C26-C25	-2.14	103.57	114.37
17	1	848	BCR	C16-C15-C14	-2.13	119.15	123.52
17	j	103	BCR	C15-C14-C13	-2.13	124.28	127.28
14	A	834	CLA	O1D-CGD-CBD	2.13	128.73	124.52
14	B	813	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
14	F	201	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
14	b	805	CLA	O2D-CGD-CBD	2.13	114.96	111.23
14	2	807	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
14	j	101	CLA	CHA-C1A-NA	-2.13	121.56	126.39
14	A	813	CLA	CHB-C4A-NA	2.13	127.48	124.40
14	A	819	CLA	CHB-C4A-NA	2.13	127.48	124.40
18	2	802	LMG	O3-C3-C2	-2.13	105.35	110.38
14	7	1102	CLA	CHA-C1A-NA	-2.13	121.57	126.39
18	b	803	LMG	O3-C3-C2	-2.13	105.35	110.38
14	2	840	CLA	CHB-C4A-NA	2.13	127.47	124.40
14	a	820	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
14	a	814	CLA	CHB-C1B-NB	2.13	127.24	124.05
14	b	840	CLA	CHB-C4A-NA	2.13	127.47	124.40
17	a	848	BCR	C16-C15-C14	-2.13	119.16	123.52
14	2	809	CLA	O2D-CGD-CBD	2.13	114.95	111.23
14	a	854	CLA	C2D-C1D-ND	-2.13	108.02	110.13
14	a	820	CLA	CHB-C4A-NA	2.13	127.47	124.40
14	1	812	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
14	1	815	CLA	CHA-C1A-NA	-2.13	121.58	126.39
12	B	853	LHG	C27-C26-C25	-2.13	103.62	114.37
14	A	807	CLA	CHD-C1D-ND	-2.13	121.81	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	l	4202	LMG	O3-C3-C2	-2.13	105.37	110.38
18	0	201	LMG	O3-C3-C2	-2.13	105.37	110.38
14	7	1101	CLA	C1-C2-C3	-2.13	122.72	126.20
14	a	815	CLA	O2D-CGD-CBD	2.13	114.94	111.23
14	A	843	CLA	C3B-C4B-NB	-2.13	108.63	110.53
18	B	803	LMG	O3-C3-C2	-2.12	105.37	110.38
14	7	1102	CLA	CHB-C4A-NA	2.12	127.47	124.40
14	B	844	CLA	C2D-C1D-ND	-2.12	108.02	110.13
14	1	844	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	b	815	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	B	808	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
14	B	805	CLA	O2D-CGD-CBD	2.12	114.94	111.23
14	A	814	CLA	O2D-CGD-CBD	2.12	114.94	111.23
14	b	808	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
14	b	843	CLA	C2D-C1D-ND	-2.12	108.03	110.13
14	2	833	CLA	O1D-CGD-CBD	2.12	128.70	124.52
14	B	816	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	f	205	CLA	CAA-C2A-C1A	2.12	118.93	111.97
14	a	807	CLA	CHA-C1A-NA	-2.12	121.59	126.39
14	b	820	CLA	C4-C3-C5	2.12	118.91	115.23
14	1	843	CLA	C2D-C1D-ND	-2.12	108.03	110.13
14	a	835	CLA	O1D-CGD-CBD	2.12	128.70	124.52
14	b	812	CLA	C3A-C2A-C1A	2.12	104.51	101.34
14	1	812	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	1	818	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	A	844	CLA	CHB-C4A-NA	2.12	127.45	124.40
14	2	832	CLA	CHD-C4C-C3C	2.12	127.86	124.77
17	b	851	BCR	C27-C26-C25	2.12	125.56	122.70
14	a	843	CLA	C2D-C1D-ND	-2.12	108.03	110.13
17	2	849	BCR	C20-C21-C22	-2.12	124.31	127.28
14	a	824	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
18	a	852	LMG	O7-C10-O9	-2.12	118.76	123.70
14	a	836	CLA	CHD-C1D-ND	-2.12	121.83	124.80
14	2	803	CLA	CAA-CBA-CGA	-2.11	107.20	113.21
14	1	829	CLA	C6-C7-C8	-2.11	108.94	115.97
14	l	4203	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
14	a	811	CLA	CMB-C2B-C3B	2.11	131.52	126.55
14	J	101	CLA	CHA-C1A-NA	-2.11	121.60	126.39
14	B	821	CLA	C4-C3-C5	2.11	118.90	115.23
14	1	813	CLA	O2D-CGD-CBD	2.11	114.93	111.23
14	A	830	CLA	C6-C7-C8	-2.11	108.94	115.97
14	F	205	CLA	CAA-C2A-C1A	2.11	118.90	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	802	CLA	CHB-C4A-NA	2.11	127.45	124.40
14	b	810	CLA	C2D-C1D-ND	-2.11	108.03	110.13
17	h	102	BCR	C33-C5-C6	-2.11	122.18	124.48
17	A	848	BCR	C16-C15-C14	-2.11	119.20	123.52
14	6	4404	CLA	CAA-C2A-C1A	2.11	118.89	111.97
14	b	836	CLA	CHB-C4A-NA	2.11	127.45	124.40
17	0	204	BCR	C21-C20-C19	-2.11	117.08	123.20
18	L	1506	LMG	O3-C3-C2	-2.11	105.40	110.38
14	A	841	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
17	1	850	BCR	C16-C15-C14	-2.11	119.20	123.52
14	8	4004	CLA	CHA-C1A-NA	-2.11	121.61	126.39
14	A	810	CLA	CMB-C2B-C3B	2.11	131.51	126.55
14	b	804	CLA	CAA-CBA-CGA	-2.11	107.22	113.21
14	1	825	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	0	202	CLA	CHB-C4A-NA	2.11	127.44	124.40
14	1	822	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	f	201	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
14	1	833	CLA	CHB-C4A-NA	2.11	127.44	124.40
14	A	816	CLA	CMB-C2B-C3B	2.11	131.51	126.55
14	A	829	CLA	C1-C2-C3	-2.11	122.74	126.20
14	6	4404	CLA	CHA-C1A-NA	-2.11	121.62	126.39
14	a	814	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	b	833	CLA	O1D-CGD-CBD	2.11	128.67	124.52
17	i	4103	BCR	C33-C5-C6	-2.11	122.19	124.48
14	a	827	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	B	845	CLA	C1C-NC-C4C	2.11	107.64	106.68
17	0	210	BCR	C21-C20-C19	-2.11	117.10	123.20
15	b	845	PQN	C2M-C2-C3	-2.11	120.99	124.45
14	a	843	CLA	C3B-C4B-NB	-2.11	108.65	110.53
14	f	205	CLA	CHA-C1A-NA	-2.11	121.62	126.39
14	2	801	CLA	CHD-C1D-ND	-2.11	121.84	124.80
14	A	837	CLA	CHA-C1A-NA	-2.11	121.62	126.39
14	a	838	CLA	CHA-C1A-NA	-2.11	121.62	126.39
17	A	848	BCR	C33-C5-C6	-2.11	122.19	124.48
14	A	843	CLA	C2D-C1D-ND	-2.10	108.04	110.13
14	a	830	CLA	C1-C2-C3	-2.10	122.75	126.20
14	B	804	CLA	CAA-CBA-CGA	-2.10	107.23	113.21
15	1	845	PQN	C2M-C2-C3	-2.10	120.99	124.45
14	a	835	CLA	CHB-C4A-NA	2.10	127.44	124.40
17	b	849	BCR	C20-C21-C22	-2.10	124.33	127.28
18	a	852	LMG	O1-C7-C8	-2.10	105.71	110.82
14	2	820	CLA	C4-C3-C5	2.10	118.88	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	831	CLA	C6-C7-C8	-2.10	108.98	115.97
14	1	808	CLA	C2D-C1D-ND	-2.10	108.05	110.13
14	A	826	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	0	207	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	f	205	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
14	F	205	CLA	CHA-C1A-NA	-2.10	121.64	126.39
17	9	102	BCR	C20-C21-C22	-2.10	124.33	127.28
14	A	834	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	a	817	CLA	CMB-C2B-C3B	2.10	131.49	126.55
14	1	836	CLA	CHA-C1A-NA	-2.10	121.64	126.39
14	A	815	CLA	CAC-C3C-C2C	-2.10	123.70	127.56
14	2	839	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
14	1	815	CLA	CMB-C2B-C3B	2.10	131.49	126.55
14	K	4004	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
14	a	854	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
18	A	852	LMG	O1-C7-C8	-2.10	105.72	110.82
14	1	841	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
14	2	812	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
14	8	4002	CLA	CHD-C1D-ND	-2.10	121.85	124.80
14	a	807	CLA	C2D-C1D-ND	-2.10	108.05	110.13
14	1	831	CLA	C2D-C1D-ND	-2.10	108.05	110.13
14	B	834	CLA	O1D-CGD-CBD	2.10	128.65	124.52
14	B	810	CLA	O2D-CGD-CBD	2.09	114.89	111.23
14	A	823	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	b	802	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	B	805	CLA	O1D-CGD-CBD	2.09	128.65	124.52
14	2	819	CLA	C3C-C4C-NC	-2.09	107.75	110.43
17	B	854	BCR	C4-C5-C6	2.09	125.53	122.70
14	A	813	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
18	0	203	LMG	O1-C7-C8	-2.09	105.73	110.82
14	1	810	CLA	C1-C2-C3	-2.09	123.38	126.76
18	0	203	LMG	O7-C10-O9	-2.09	118.81	123.70
14	K	4004	CLA	C2D-C1D-ND	-2.09	108.06	110.13
17	6	4406	BCR	C4-C5-C6	2.09	125.53	122.70
14	1	809	CLA	CMB-C2B-C3B	2.09	131.47	126.55
13	a	803	CL0	OBD-CAD-CBD	-2.09	122.75	125.82
14	A	844	CLA	CHD-C1D-ND	-2.09	121.86	124.80
17	B	852	BCR	C27-C26-C25	2.09	125.53	122.70
14	a	812	CLA	C1-C2-C3	-2.09	123.38	126.76
14	b	819	CLA	C3C-C4C-NC	-2.09	107.75	110.43
14	1	840	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	B	846	PQN	C2M-C2-C3	-2.09	121.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	832	CLA	CHD-C4C-C3C	2.09	127.82	124.77
14	a	804	CLA	CHD-C1D-ND	-2.09	121.86	124.80
14	B	837	CLA	CHB-C4A-NA	2.09	127.41	124.40
14	a	854	CLA	CHA-C1A-NA	-2.09	121.66	126.39
18	A	853	LMG	O7-C10-O9	-2.09	118.82	123.70
14	b	827	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
14	a	816	CLA	CAC-C3C-C2C	-2.09	123.72	127.56
14	1	814	CLA	CAC-C3C-C2C	-2.09	123.72	127.56
14	1	828	CLA	C1-C2-C3	-2.09	122.78	126.20
14	A	834	CLA	C1-C2-C3	-2.09	122.78	126.20
14	b	839	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
14	1	842	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
14	B	833	CLA	CHD-C4C-C3C	2.09	127.82	124.77
14	B	820	CLA	C3C-C4C-NC	-2.09	107.76	110.43
14	2	827	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
14	a	819	CLA	CHA-C1A-NA	-2.08	121.67	126.39
15	A	845	PQN	C2M-C2-C3	-2.08	121.02	124.45
15	a	845	PQN	C2M-C2-C3	-2.08	121.03	124.45
17	F	206	BCR	C33-C5-C6	-2.08	122.21	124.48
17	1	847	BCR	C33-C5-C6	-2.08	122.21	124.48
14	B	801	CLA	CHD-C1D-ND	-2.08	121.87	124.80
14	1	811	CLA	CHB-C4A-NA	2.08	127.41	124.40
18	A	852	LMG	O7-C10-O9	-2.08	118.83	123.70
17	L	1504	BCR	C2-C1-C6	2.08	113.47	110.44
14	A	812	CLA	CHB-C4A-NA	2.08	127.41	124.40
14	f	204	CLA	CHB-C4A-NA	2.08	127.41	124.40
14	A	818	CLA	CHA-C1A-NA	-2.08	121.67	126.39
17	L	1505	BCR	C21-C20-C19	-2.08	117.17	123.20
17	b	853	BCR	C4-C5-C6	2.08	125.52	122.70
17	A	847	BCR	C33-C5-C6	-2.08	122.21	124.48
14	B	840	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
14	1	817	CLA	CHA-C1A-NA	-2.08	121.68	126.39
14	a	844	CLA	CHD-C1D-ND	-2.08	121.87	124.80
14	a	842	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	A	803	CL0	OBD-CAD-CBD	-2.08	122.77	125.82
14	1	821	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	a	844	CLA	CHB-C4A-NA	2.08	127.40	124.40
14	a	823	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	L	1501	CLA	CHA-C1A-NA	-2.08	121.68	126.39
14	K	4004	CLA	CHA-C1A-NA	-2.08	121.68	126.39
14	a	825	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	b	841	CLA	CHB-C4A-NA	2.08	127.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	815	CLA	CHB-C4A-NA	2.08	127.40	124.40
14	A	842	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	a	835	CLA	C1-C2-C3	-2.08	122.79	126.20
14	1	821	CLA	C1-C2-C3	-2.08	122.80	126.20
14	A	824	CLA	CHB-C4A-NA	2.08	127.40	124.40
17	b	851	BCR	C15-C16-C17	-2.08	119.27	123.52
14	2	804	CLA	O1D-CGD-CBD	2.07	128.61	124.52
14	2	818	CLA	C1-C2-C3	-2.07	122.80	126.20
14	a	810	CLA	C2D-C1D-ND	-2.07	108.07	110.13
14	2	843	CLA	C2D-C1D-ND	-2.07	108.07	110.13
17	2	851	BCR	C27-C26-C25	2.07	125.51	122.70
14	F	205	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
14	6	4404	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
14	l	4205	CLA	CHB-C4A-NA	2.07	127.39	124.40
17	f	206	BCR	C33-C5-C6	-2.07	122.22	124.48
14	1	823	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	A	811	CLA	C1-C2-C3	-2.07	123.41	126.76
14	1	832	CLA	C1-C2-C3	-2.07	123.41	126.76
14	8	4004	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
14	2	809	CLA	C2D-C1D-ND	-2.07	108.08	110.13
14	a	805	CLA	CHB-C4A-NA	2.07	127.39	124.40
17	l	4207	BCR	C2-C1-C6	2.07	113.45	110.44
14	l	4204	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	a	808	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	0	206	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	a	825	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	A	824	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	1	814	CLA	CHD-C1D-ND	-2.07	121.89	124.80
18	a	853	LMG	O7-C10-O9	-2.07	118.87	123.70
14	1	823	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	B	801	CLA	O2D-CGD-CBD	2.07	114.84	111.23
14	B	828	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	A	822	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
17	0	209	BCR	C2-C1-C6	2.07	113.44	110.44
17	a	847	BCR	C33-C5-C6	-2.07	122.23	124.48
14	1	833	CLA	C1-C2-C3	-2.07	122.81	126.20
14	F	204	CLA	CHB-C4A-NA	2.07	127.38	124.40
14	2	841	CLA	CHB-C4A-NA	2.06	127.38	124.40
14	B	802	CLA	CMB-C2B-C3B	2.06	131.40	126.55
14	b	805	CLA	O1D-CGD-CBD	2.06	128.59	124.52
14	k	4002	CLA	CHD-C1D-ND	-2.06	121.90	124.80
14	B	840	CLA	CHA-C1A-NA	-2.06	121.72	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	0	202	CLA	CMB-C2B-C3B	2.06	131.40	126.55
15	2	845	PQN	C2M-C2-C3	-2.06	121.06	124.45
14	a	833	CLA	CHB-C4A-NA	2.06	127.38	124.40
14	A	833	CLA	C1-C2-C3	-2.06	123.43	126.76
14	b	839	CLA	CHA-C1A-NA	-2.06	121.72	126.39
14	b	818	CLA	C1-C2-C3	-2.06	122.82	126.20
14	1	806	CLA	CHD-C1D-ND	-2.06	121.90	124.80
14	a	815	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
14	1	808	CLA	CHB-C4A-NA	2.06	127.37	124.40
18	A	853	LMG	O3-C3-C2	-2.06	105.52	110.38
14	1	819	CLA	CHA-C1A-NA	-2.06	121.73	126.39
13	1	803	CL0	OBD-CAD-CBD	-2.06	122.80	125.82
14	b	801	CLA	CMB-C2B-C3B	2.06	131.39	126.55
18	1	852	LMG	O7-C10-O9	-2.06	118.89	123.70
17	B	847	BCR	C11-C10-C9	-2.06	124.39	127.28
14	K	4003	CLA	CHA-C1A-NA	-2.06	121.73	126.39
17	1	847	BCR	C10-C11-C12	-2.06	117.24	123.20
14	0	202	CLA	CHB-C1B-NB	2.06	127.13	124.05
14	1	843	CLA	C3B-C4B-NB	-2.06	108.69	110.53
17	2	851	BCR	C15-C16-C17	-2.06	119.31	123.52
14	A	822	CLA	C1-C2-C3	-2.06	122.83	126.20
14	L	1503	CLA	C1-C2-C3	-2.05	122.83	126.20
14	L	1502	CLA	CHB-C4A-NA	2.05	127.36	124.40
14	K	4002	CLA	CHD-C1D-ND	-2.05	121.91	124.80
14	a	821	CLA	CHA-C1A-NA	-2.05	121.74	126.39
14	2	839	CLA	CHA-C1A-NA	-2.05	121.74	126.39
17	B	852	BCR	C15-C16-C17	-2.05	119.32	123.52
17	B	852	BCR	C20-C21-C22	-2.05	124.40	127.28
17	b	854	BCR	C20-C21-C22	-2.05	124.40	127.28
17	l	4207	BCR	C38-C26-C25	-2.05	122.25	124.48
14	A	807	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
14	b	839	CLA	C1-C2-C3	-2.05	123.44	126.76
17	M	102	BCR	C20-C21-C22	-2.05	124.40	127.28
14	8	4003	CLA	CHA-C1A-NA	-2.05	121.75	126.39
14	a	810	CLA	CHB-C4A-NA	2.05	127.36	124.40
14	a	813	CLA	CHB-C4A-NA	2.05	127.36	124.40
14	A	820	CLA	CHA-C1A-NA	-2.05	121.75	126.39
17	0	204	BCR	C29-C30-C25	2.05	113.42	110.44
17	l	4207	BCR	C33-C5-C6	-2.05	122.25	124.48
14	A	809	CLA	C2D-C1D-ND	-2.05	108.10	110.13
14	A	832	CLA	C2D-C1D-ND	-2.05	108.10	110.13
14	b	801	CLA	CHB-C1B-NB	2.05	127.12	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	832	CLA	CHD-C1D-C2D	2.05	129.75	125.49
14	A	814	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
17	b	848	BCR	C30-C25-C26	-2.05	119.84	122.64
17	b	854	BCR	C10-C11-C12	-2.05	117.26	123.20
14	k	4003	CLA	CHA-C1A-NA	-2.05	121.75	126.39
14	B	819	CLA	C1-C2-C3	-2.05	122.84	126.20
14	A	833	CLA	CHD-C1D-C2D	2.05	129.75	125.49
14	A	806	CLA	C2D-C1D-ND	-2.05	108.10	110.13
14	B	828	CLA	C1-C2-C3	-2.05	123.45	126.76
17	9	102	BCR	C10-C11-C12	-2.05	117.27	123.20
14	b	844	CLA	C1C-NC-C4C	2.05	107.61	106.68
14	K	4003	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
14	a	823	CLA	C1-C2-C3	-2.05	122.84	126.20
14	B	805	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
17	b	846	BCR	C11-C10-C9	-2.05	124.41	127.28
14	0	208	CLA	C1-C2-C3	-2.05	122.84	126.20
14	2	801	CLA	CHB-C1B-NB	2.05	127.12	124.05
14	k	4003	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
14	a	834	CLA	C1-C2-C3	-2.05	123.45	126.76
17	h	101	BCR	C33-C5-C6	-2.04	122.25	124.48
14	1	806	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
14	B	836	CLA	O2A-CGA-O1A	-2.04	118.07	123.33
14	A	815	CLA	CHD-C1D-ND	-2.04	121.93	124.80
18	a	853	LMG	O3-C3-C2	-2.04	105.56	110.38
14	1	813	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
17	I	102	BCR	C1-C6-C5	-2.04	119.84	122.64
14	l	4204	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
14	8	4003	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
17	7	1105	BCR	C1-C6-C5	-2.04	119.84	122.64
17	I	101	BCR	C33-C5-C6	-2.04	122.26	124.48
17	0	209	BCR	C38-C26-C25	-2.04	122.26	124.48
14	B	802	CLA	CHB-C1B-NB	2.04	127.11	124.05
14	2	839	CLA	C1-C2-C3	-2.04	123.46	126.76
14	1	844	CLA	CHD-C1D-ND	-2.04	121.93	124.80
14	a	814	CLA	C4-C3-C5	2.04	118.77	115.23
14	B	802	CLA	CHA-C1A-NA	-2.04	121.77	126.39
14	l	4206	CLA	C1-C2-C3	-2.04	122.85	126.20
17	2	846	BCR	C7-C8-C9	-2.04	123.22	126.23
14	b	805	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	B	840	CLA	C1-C2-C3	-2.04	123.46	126.76
14	8	4002	CLA	CHA-C1A-NA	-2.04	121.77	126.39
14	2	835	CLA	O2A-CGA-O1A	-2.04	118.08	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	807	CLA	CMB-C2B-C3B	2.04	131.35	126.55
15	B	846	PQN	C16-C17-C18	-2.04	109.19	115.97
14	0	206	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
17	A	847	BCR	C10-C11-C12	-2.04	117.29	123.20
17	2	846	BCR	C11-C10-C9	-2.04	124.42	127.28
14	2	804	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	b	805	CLA	C3C-C4C-NC	-2.04	107.82	110.43
14	B	816	CLA	C1-C2-C3	-2.04	122.86	126.20
17	h	102	BCR	C21-C20-C19	-2.04	117.30	123.20
14	a	808	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	a	834	CLA	CHD-C1D-C2D	2.04	129.72	125.49
17	J	104	BCR	C1-C6-C5	-2.04	119.85	122.64
14	a	842	CLA	CHD-C1D-ND	-2.04	121.94	124.80
17	F	203	BCR	C10-C11-C12	-2.04	117.30	123.20
14	B	815	CLA	CHB-C4A-NA	2.04	127.34	124.40
14	2	804	CLA	C3C-C4C-NC	-2.04	107.82	110.43
14	b	801	CLA	CHA-C1A-NA	-2.04	121.78	126.39
15	b	845	PQN	C16-C17-C18	-2.04	109.20	115.97
17	B	849	BCR	C30-C25-C26	-2.04	119.85	122.64
14	a	804	CLA	O2D-CGD-CBD	2.04	114.79	111.23
14	B	807	CLA	CMB-C2B-C3B	2.04	131.34	126.55
17	a	847	BCR	C10-C11-C12	-2.03	117.31	123.20
14	2	814	CLA	O2A-CGA-O1A	-2.03	118.10	123.33
14	B	805	CLA	C3C-C4C-NC	-2.03	107.82	110.43
14	B	807	CLA	C2D-C1D-ND	-2.03	108.11	110.13
18	1	852	LMG	O3-C3-C2	-2.03	105.58	110.38
14	B	832	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
14	b	827	CLA	C1-C2-C3	-2.03	123.47	126.76
14	2	827	CLA	C1-C2-C3	-2.03	123.47	126.76
14	2	801	CLA	O2D-CGD-CBD	2.03	114.78	111.23
14	B	810	CLA	C2D-C1D-ND	-2.03	108.11	110.13
14	b	814	CLA	CHB-C4A-NA	2.03	127.33	124.40
17	0	210	BCR	C29-C30-C25	2.03	113.39	110.44
14	b	835	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
14	a	842	CLA	O2D-CGD-CBD	2.03	114.78	111.23
14	2	815	CLA	C1-C2-C3	-2.03	122.87	126.20
14	2	814	CLA	CHB-C4A-NA	2.03	127.33	124.40
14	6	4403	CLA	CHB-C4A-NA	2.03	127.33	124.40
15	2	845	PQN	C16-C17-C18	-2.03	109.22	115.97
14	B	801	CLA	CHB-C1B-NB	2.03	127.09	124.05
14	2	844	CLA	C1C-NC-C4C	2.03	107.61	106.68
14	B	814	CLA	CHA-C1A-NA	-2.03	121.80	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	815	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
14	A	809	CLA	CHB-C4A-NA	2.03	127.33	124.40
14	A	832	CLA	CHB-C4A-NA	2.03	127.33	124.40
13	A	803	CL0	O1D-CGD-CBD	2.03	127.80	124.72
14	a	811	CLA	CHB-C4A-NA	2.03	127.33	124.40
14	b	805	CLA	CBA-CAA-C2A	-2.03	107.76	113.79
17	L	1505	BCR	C29-C30-C25	2.03	113.39	110.44
18	0	201	LMG	O6-C1-O1	-2.03	105.25	110.04
14	0	202	CLA	CHA-C1A-NA	-2.03	121.80	126.39
14	b	804	CLA	CHB-C1B-NB	2.03	127.09	124.05
14	A	835	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
17	M	102	BCR	C10-C11-C12	-2.03	117.33	123.20
14	L	1501	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
17	2	851	BCR	C20-C21-C22	-2.03	124.44	127.28
17	i	4103	BCR	C21-C20-C19	-2.03	117.33	123.20
14	b	836	CLA	O2A-CGA-O1A	-2.03	118.12	123.33
14	b	812	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
17	6	4405	BCR	C33-C5-C6	-2.02	122.28	124.48
17	b	851	BCR	C20-C21-C22	-2.02	124.44	127.28
14	a	834	CLA	CHA-C1A-NA	-2.02	121.81	126.39
14	2	836	CLA	C3C-C4C-NC	-2.02	107.84	110.43
14	2	806	CLA	CMB-C2B-C3B	2.02	131.31	126.55
14	k	4002	CLA	CHA-C1A-NA	-2.02	121.81	126.39
17	0	210	BCR	C7-C8-C9	-2.02	123.24	126.23
14	1	832	CLA	CHA-C1A-NA	-2.02	121.81	126.39
14	2	803	CLA	CHB-C1B-NB	2.02	127.08	124.05
14	A	810	CLA	CHB-C4A-NA	2.02	127.32	124.40
14	b	821	CLA	CHB-C4A-NA	2.02	127.32	124.40
14	2	815	CLA	CHD-C1D-ND	-2.02	121.96	124.80
14	2	817	CLA	CHD-C1D-ND	-2.02	121.96	124.80
17	L	1504	BCR	C38-C26-C25	-2.02	122.28	124.48
14	2	813	CLA	CHA-C1A-NA	-2.02	121.81	126.39
17	b	846	BCR	C7-C8-C9	-2.02	123.24	126.23
14	K	4002	CLA	CHA-C1A-NA	-2.02	121.81	126.39
14	b	815	CLA	C1-C2-C3	-2.02	122.88	126.20
13	1	803	CL0	O1D-CGD-CBD	2.02	127.79	124.72
14	a	816	CLA	CHD-C1D-ND	-2.02	121.96	124.80
14	1	829	CLA	CHD-C1D-ND	-2.02	121.96	124.80
14	1	831	CLA	C3C-C4C-NC	-2.02	107.84	110.43
14	2	804	CLA	CBA-CAA-C2A	-2.02	107.78	113.79
17	h	102	BCR	C1-C6-C5	-2.02	119.88	122.64
17	f	203	BCR	C10-C11-C12	-2.02	117.35	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	813	CLA	CHA-C1A-NA	-2.02	121.82	126.39
14	B	825	CLA	O2D-CGD-CBD	2.02	114.76	111.23
14	b	814	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
14	B	837	CLA	C3C-C4C-NC	-2.02	107.84	110.43
14	a	833	CLA	C3C-C4C-NC	-2.02	107.84	110.43
14	b	831	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
13	a	803	CL0	O1D-CGD-CBD	2.02	127.78	124.72
14	A	804	CLA	CHB-C4A-NA	2.02	127.31	124.40
14	B	805	CLA	CBA-CAA-C2A	-2.02	107.79	113.79
14	1	834	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
17	I	102	BCR	C21-C20-C19	-2.02	117.35	123.20
14	A	825	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
14	2	811	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
14	1	804	CLA	CHB-C4A-NA	2.02	127.31	124.40
14	1	824	CLA	C1-C2-C3	-2.02	122.89	126.20
14	1	840	CLA	O2D-CGD-CBD	2.02	114.76	111.23
14	1	831	CLA	CHB-C4A-NA	2.02	127.31	124.40
17	0	204	BCR	C7-C8-C9	-2.02	123.25	126.23
14	A	813	CLA	C4-C3-C5	2.02	118.73	115.23
14	A	833	CLA	CHA-C1A-NA	-2.02	121.83	126.39
17	B	847	BCR	C7-C8-C9	-2.02	123.25	126.23
14	b	815	CLA	CHD-C1D-ND	-2.02	121.97	124.80
14	B	804	CLA	C1-C2-C3	-2.02	122.89	126.20
14	B	812	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
14	B	810	CLA	CHD-C1D-ND	-2.01	121.97	124.80
17	6	4402	BCR	C10-C11-C12	-2.01	117.36	123.20
14	2	831	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
17	i	4102	BCR	C33-C5-C6	-2.01	122.29	124.48
14	1	842	CLA	CHD-C1D-ND	-2.01	121.97	124.80
18	l	4202	LMG	O6-C1-O1	-2.01	105.29	110.04
14	A	841	CLA	O2D-CGD-CBD	2.01	114.75	111.23
14	1	812	CLA	C4-C3-C5	2.01	118.72	115.23
14	B	816	CLA	CHD-C1D-ND	-2.01	121.97	124.80
14	1	842	CLA	O2D-CGD-CBD	2.01	114.75	111.23
14	1	812	CLA	C1-C2-C3	-2.01	122.90	126.20
17	A	847	BCR	C16-C17-C18	-2.01	124.46	127.28
14	B	841	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
14	A	830	CLA	CHD-C1D-ND	-2.01	121.97	124.80
14	a	831	CLA	CHD-C1D-ND	-2.01	121.97	124.80
14	A	842	CLA	CHD-C1D-ND	-2.01	121.98	124.80
14	b	824	CLA	O2D-CGD-CBD	2.01	114.74	111.23
14	a	836	CLA	O2A-CGA-O1A	-2.01	118.61	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	1506	LMG	O6-C1-O1	-2.01	105.30	110.04
14	A	810	CLA	CHD-C1D-ND	-2.01	121.98	124.80
14	2	836	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
14	a	826	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
14	L	1503	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
14	1	836	CLA	C3A-C2A-C1A	2.01	104.34	101.34
14	1	825	CLA	C11-C10-C8	-2.01	109.30	115.97
14	a	804	CLA	CHB-C1B-NB	2.01	127.06	124.05
14	a	827	CLA	C11-C10-C8	-2.00	109.30	115.97
17	a	848	BCR	C7-C8-C9	-2.00	123.27	126.23
14	a	835	CLA	CMB-C2B-C3B	2.00	131.26	126.55
14	b	819	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
14	a	818	CLA	CHB-C4A-NA	2.00	127.29	124.40
14	0	208	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
14	B	837	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
14	b	802	CLA	O2D-CGD-CBD	2.00	114.73	111.23
14	b	842	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
14	A	817	CLA	CHB-C4A-NA	2.00	127.29	124.40
17	L	1504	BCR	C33-C5-C6	-2.00	122.30	124.48
17	a	849	BCR	C16-C15-C14	-2.00	119.42	123.52
14	l	4206	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
14	B	804	CLA	CHB-C1B-NB	2.00	127.05	124.05
14	2	822	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
14	2	842	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
14	B	822	CLA	CHB-C4A-NA	2.00	127.29	124.40
17	b	848	BCR	C15-C14-C13	-2.00	124.42	127.48
14	b	836	CLA	C3C-C4C-NC	-2.00	107.87	110.43

All (270) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	803	CL0	NA
13	A	803	CL0	NC
13	A	803	CL0	ND
13	a	803	CL0	NA
13	a	803	CL0	NC
13	a	803	CL0	ND
13	1	803	CL0	NA
13	1	803	CL0	NC
13	1	803	CL0	ND
14	A	804	CLA	ND
14	A	805	CLA	ND

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Mol	Chain	Res	Type	Atom
14	A	806	CLA	ND
14	A	807	CLA	ND
14	A	808	CLA	ND
14	A	809	CLA	ND
14	A	810	CLA	ND
14	A	811	CLA	ND
14	A	812	CLA	ND
14	A	813	CLA	ND
14	A	814	CLA	ND
14	A	815	CLA	ND
14	A	816	CLA	ND
14	A	818	CLA	ND
14	A	819	CLA	ND
14	A	820	CLA	ND
14	A	821	CLA	ND
14	A	822	CLA	ND
14	A	823	CLA	ND
14	A	824	CLA	ND
14	A	825	CLA	ND
14	A	826	CLA	ND
14	A	827	CLA	ND
14	A	828	CLA	ND
14	A	829	CLA	ND
14	A	830	CLA	ND
14	A	831	CLA	ND
14	A	832	CLA	ND
14	A	833	CLA	ND
14	A	834	CLA	ND
14	A	835	CLA	ND
14	A	836	CLA	ND
14	A	837	CLA	ND
14	A	838	CLA	ND
14	A	839	CLA	ND
14	A	840	CLA	ND
14	A	841	CLA	ND
14	A	843	CLA	ND
14	A	844	CLA	ND
14	B	801	CLA	ND
14	B	802	CLA	ND
14	B	804	CLA	ND
14	B	805	CLA	ND
14	B	806	CLA	ND

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Mol	Chain	Res	Type	Atom
14	B	807	CLA	ND
14	B	809	CLA	ND
14	B	810	CLA	ND
14	B	811	CLA	ND
14	B	812	CLA	ND
14	B	813	CLA	ND
14	B	814	CLA	ND
14	B	815	CLA	ND
14	B	816	CLA	ND
14	B	817	CLA	ND
14	B	818	CLA	ND
14	B	819	CLA	ND
14	B	821	CLA	ND
14	B	822	CLA	ND
14	B	825	CLA	ND
14	B	827	CLA	ND
14	B	828	CLA	ND
14	B	829	CLA	ND
14	B	830	CLA	ND
14	B	831	CLA	ND
14	B	832	CLA	ND
14	B	833	CLA	ND
14	B	834	CLA	ND
14	B	835	CLA	ND
14	B	836	CLA	ND
14	B	837	CLA	ND
14	B	838	CLA	ND
14	B	839	CLA	ND
14	B	840	CLA	ND
14	B	841	CLA	ND
14	B	842	CLA	ND
14	B	843	CLA	ND
14	B	845	CLA	ND
14	F	201	CLA	ND
14	F	204	CLA	ND
14	F	205	CLA	ND
14	J	101	CLA	ND
14	J	102	CLA	ND
14	L	1501	CLA	ND
14	L	1502	CLA	ND
14	L	1503	CLA	ND
14	K	4003	CLA	ND

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Mol	Chain	Res	Type	Atom
14	K	4004	CLA	ND
14	a	804	CLA	ND
14	a	805	CLA	ND
14	a	806	CLA	ND
14	a	807	CLA	ND
14	a	808	CLA	ND
14	a	809	CLA	ND
14	a	810	CLA	ND
14	a	811	CLA	ND
14	a	812	CLA	ND
14	a	813	CLA	ND
14	a	814	CLA	ND
14	a	815	CLA	ND
14	a	816	CLA	ND
14	a	817	CLA	ND
14	a	819	CLA	ND
14	a	820	CLA	ND
14	a	821	CLA	ND
14	a	822	CLA	ND
14	a	823	CLA	ND
14	a	824	CLA	ND
14	a	825	CLA	ND
14	a	826	CLA	ND
14	a	827	CLA	ND
14	a	828	CLA	ND
14	a	829	CLA	ND
14	a	830	CLA	ND
14	a	831	CLA	ND
14	a	832	CLA	ND
14	a	833	CLA	ND
14	a	834	CLA	ND
14	a	835	CLA	ND
14	a	836	CLA	ND
14	a	837	CLA	ND
14	a	838	CLA	ND
14	a	839	CLA	ND
14	a	840	CLA	ND
14	a	841	CLA	ND
14	a	843	CLA	ND
14	a	844	CLA	ND
14	a	854	CLA	ND
14	1	804	CLA	ND

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Mol	Chain	Res	Type	Atom
14	1	805	CLA	ND
14	1	806	CLA	ND
14	1	807	CLA	ND
14	1	808	CLA	ND
14	1	809	CLA	ND
14	1	810	CLA	ND
14	1	811	CLA	ND
14	1	812	CLA	ND
14	1	813	CLA	ND
14	1	814	CLA	ND
14	1	815	CLA	ND
14	1	817	CLA	ND
14	1	818	CLA	ND
14	1	819	CLA	ND
14	1	820	CLA	ND
14	1	821	CLA	ND
14	1	822	CLA	ND
14	1	823	CLA	ND
14	1	824	CLA	ND
14	1	825	CLA	ND
14	1	826	CLA	ND
14	1	827	CLA	ND
14	1	828	CLA	ND
14	1	829	CLA	ND
14	1	830	CLA	ND
14	1	831	CLA	ND
14	1	832	CLA	ND
14	1	833	CLA	ND
14	1	834	CLA	ND
14	1	835	CLA	ND
14	1	836	CLA	ND
14	1	837	CLA	ND
14	1	838	CLA	ND
14	1	839	CLA	ND
14	1	840	CLA	ND
14	1	841	CLA	ND
14	1	843	CLA	ND
14	1	844	CLA	ND
14	b	801	CLA	ND
14	b	802	CLA	ND
14	b	804	CLA	ND
14	b	805	CLA	ND

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Mol	Chain	Res	Type	Atom
14	b	806	CLA	ND
14	b	807	CLA	ND
14	b	809	CLA	ND
14	b	810	CLA	ND
14	b	811	CLA	ND
14	b	812	CLA	ND
14	b	813	CLA	ND
14	b	814	CLA	ND
14	b	815	CLA	ND
14	b	816	CLA	ND
14	b	817	CLA	ND
14	b	818	CLA	ND
14	b	820	CLA	ND
14	b	821	CLA	ND
14	b	824	CLA	ND
14	b	826	CLA	ND
14	b	827	CLA	ND
14	b	828	CLA	ND
14	b	829	CLA	ND
14	b	830	CLA	ND
14	b	831	CLA	ND
14	b	832	CLA	ND
14	b	833	CLA	ND
14	b	834	CLA	ND
14	b	835	CLA	ND
14	b	836	CLA	ND
14	b	837	CLA	ND
14	b	838	CLA	ND
14	b	839	CLA	ND
14	b	840	CLA	ND
14	b	841	CLA	ND
14	b	842	CLA	ND
14	b	844	CLA	ND
14	2	801	CLA	ND
14	2	803	CLA	ND
14	2	804	CLA	ND
14	2	805	CLA	ND
14	2	806	CLA	ND
14	2	808	CLA	ND
14	2	809	CLA	ND
14	2	810	CLA	ND
14	2	811	CLA	ND

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Mol	Chain	Res	Type	Atom
14	2	812	CLA	ND
14	2	813	CLA	ND
14	2	814	CLA	ND
14	2	815	CLA	ND
14	2	816	CLA	ND
14	2	817	CLA	ND
14	2	818	CLA	ND
14	2	820	CLA	ND
14	2	821	CLA	ND
14	2	824	CLA	ND
14	2	826	CLA	ND
14	2	827	CLA	ND
14	2	828	CLA	ND
14	2	829	CLA	ND
14	2	830	CLA	ND
14	2	831	CLA	ND
14	2	832	CLA	ND
14	2	833	CLA	ND
14	2	834	CLA	ND
14	2	835	CLA	ND
14	2	836	CLA	ND
14	2	837	CLA	ND
14	2	838	CLA	ND
14	2	839	CLA	ND
14	2	840	CLA	ND
14	2	841	CLA	ND
14	2	842	CLA	ND
14	2	844	CLA	ND
14	f	201	CLA	ND
14	f	204	CLA	ND
14	f	205	CLA	ND
14	6	4403	CLA	ND
14	6	4404	CLA	ND
14	j	101	CLA	ND
14	j	102	CLA	ND
14	7	1101	CLA	ND
14	7	1102	CLA	ND
14	7	1103	CLA	ND
14	k	4003	CLA	ND
14	8	4003	CLA	ND
14	8	4004	CLA	ND
14	l	4203	CLA	ND

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Mol	Chain	Res	Type	Atom
14	l	4204	CLA	ND
14	l	4205	CLA	ND
14	l	4206	CLA	ND
14	0	202	CLA	ND
14	0	206	CLA	ND
14	0	207	CLA	ND
14	0	208	CLA	ND

All (4268) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	801	LHG	C3-O3-P-O4
12	A	801	LHG	O10-C23-O8-C6
12	A	802	LHG	O1-C1-C2-C3
12	A	802	LHG	C3-O3-P-O4
12	A	802	LHG	C3-O3-P-O5
12	A	802	LHG	C3-O3-P-O6
12	B	853	LHG	C4-O6-P-O3
12	B	853	LHG	C4-O6-P-O4
12	B	853	LHG	O9-C7-O7-C5
12	B	853	LHG	C8-C7-O7-C5
12	M	101	LHG	C3-O3-P-O6
12	M	101	LHG	C4-O6-P-O4
12	M	101	LHG	C4-O6-P-O5
12	a	801	LHG	C3-O3-P-O4
12	a	801	LHG	O10-C23-O8-C6
12	a	802	LHG	O1-C1-C2-C3
12	a	802	LHG	C3-O3-P-O4
12	a	802	LHG	C3-O3-P-O5
12	a	802	LHG	C3-O3-P-O6
12	1	801	LHG	C3-O3-P-O4
12	1	801	LHG	O10-C23-O8-C6
12	1	802	LHG	O1-C1-C2-C3
12	1	802	LHG	C3-O3-P-O4
12	1	802	LHG	C3-O3-P-O5
12	1	802	LHG	C3-O3-P-O6
12	b	852	LHG	C4-O6-P-O3
12	b	852	LHG	C4-O6-P-O4
12	b	852	LHG	O9-C7-O7-C5
12	b	852	LHG	C8-C7-O7-C5
12	2	852	LHG	C4-O6-P-O3
12	2	852	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
12	2	852	LHG	O9-C7-O7-C5
12	2	852	LHG	C8-C7-O7-C5
12	m	101	LHG	C3-O3-P-O6
12	m	101	LHG	C4-O6-P-O4
12	m	101	LHG	C4-O6-P-O5
12	9	101	LHG	C3-O3-P-O6
12	9	101	LHG	C4-O6-P-O4
12	9	101	LHG	C4-O6-P-O5
13	A	803	CL0	C11-C12-C13-C14
13	a	803	CL0	C11-C12-C13-C14
13	1	803	CL0	C11-C12-C13-C14
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	807	CLA	C1A-C2A-CAA-CBA
14	A	807	CLA	C3A-C2A-CAA-CBA
14	A	807	CLA	CAD-CBD-CGD-O1D
14	A	807	CLA	CAD-CBD-CGD-O2D
14	A	808	CLA	C1A-C2A-CAA-CBA
14	A	808	CLA	CBD-CGD-O2D-CED
14	A	808	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	C4B-C3B-CAB-CBB
14	A	810	CLA	C1A-C2A-CAA-CBA
14	A	810	CLA	C3A-C2A-CAA-CBA
14	A	810	CLA	CHA-CBD-CGD-O1D
14	A	810	CLA	CHA-CBD-CGD-O2D
14	A	812	CLA	C1A-C2A-CAA-CBA
14	A	812	CLA	C3A-C2A-CAA-CBA
14	A	812	CLA	C4B-C3B-CAB-CBB
14	A	813	CLA	C1A-C2A-CAA-CBA
14	A	813	CLA	CBD-CGD-O2D-CED
14	A	814	CLA	C1A-C2A-CAA-CBA
14	A	814	CLA	C3A-C2A-CAA-CBA
14	A	815	CLA	C1A-C2A-CAA-CBA
14	A	816	CLA	CBD-CGD-O2D-CED
14	A	817	CLA	C4B-C3B-CAB-CBB
14	A	817	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	C4B-C3B-CAB-CBB
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	A	821	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	C1A-C2A-CAA-CBA
14	A	824	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	CHA-CBD-CGD-O1D
14	A	824	CLA	CHA-CBD-CGD-O2D
14	A	825	CLA	CAD-CBD-CGD-O1D
14	A	825	CLA	CAD-CBD-CGD-O2D
14	A	825	CLA	C2-C3-C5-C6
14	A	825	CLA	C4-C3-C5-C6
14	A	826	CLA	C4B-C3B-CAB-CBB
14	A	827	CLA	C6-C7-C8-C9
14	A	827	CLA	C14-C13-C15-C16
14	A	834	CLA	C4B-C3B-CAB-CBB
14	A	835	CLA	C2B-C3B-CAB-CBB
14	A	836	CLA	C4B-C3B-CAB-CBB
14	A	836	CLA	C2-C3-C5-C6
14	A	836	CLA	C4-C3-C5-C6
14	A	838	CLA	C2-C3-C5-C6
14	A	839	CLA	C4B-C3B-CAB-CBB
14	A	840	CLA	C1A-C2A-CAA-CBA
14	A	840	CLA	C3A-C2A-CAA-CBA
14	A	842	CLA	C4B-C3B-CAB-CBB
14	A	843	CLA	C1A-C2A-CAA-CBA
14	A	843	CLA	C4B-C3B-CAB-CBB
14	B	802	CLA	C1A-C2A-CAA-CBA
14	B	804	CLA	CAD-CBD-CGD-O1D
14	B	804	CLA	CAD-CBD-CGD-O2D
14	B	806	CLA	C6-C7-C8-C9
14	B	807	CLA	CHA-CBD-CGD-O1D
14	B	807	CLA	CHA-CBD-CGD-O2D
14	B	808	CLA	CHA-CBD-CGD-O1D
14	B	808	CLA	CHA-CBD-CGD-O2D
14	B	809	CLA	C4B-C3B-CAB-CBB
14	B	809	CLA	C14-C13-C15-C16
14	B	811	CLA	C4B-C3B-CAB-CBB
14	B	811	CLA	CHA-CBD-CGD-O1D
14	B	811	CLA	CHA-CBD-CGD-O2D
14	B	812	CLA	C3A-C2A-CAA-CBA
14	B	815	CLA	C1A-C2A-CAA-CBA
14	B	815	CLA	C4B-C3B-CAB-CBB
14	B	815	CLA	CHA-CBD-CGD-O1D
14	B	815	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	817	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	CBA-CGA-O2A-C1
14	B	819	CLA	C1A-C2A-CAA-CBA
14	B	819	CLA	C3A-C2A-CAA-CBA
14	B	821	CLA	C3A-C2A-CAA-CBA
14	B	822	CLA	CBD-CGD-O2D-CED
14	B	823	CLA	C1A-C2A-CAA-CBA
14	B	823	CLA	C3A-C2A-CAA-CBA
14	B	823	CLA	C4B-C3B-CAB-CBB
14	B	824	CLA	C1A-C2A-CAA-CBA
14	B	824	CLA	C4B-C3B-CAB-CBB
14	B	824	CLA	CHA-CBD-CGD-O1D
14	B	824	CLA	CHA-CBD-CGD-O2D
14	B	825	CLA	C1A-C2A-CAA-CBA
14	B	825	CLA	C4B-C3B-CAB-CBB
14	B	826	CLA	CBD-CGD-O2D-CED
14	B	831	CLA	C1A-C2A-CAA-CBA
14	B	831	CLA	C3A-C2A-CAA-CBA
14	B	832	CLA	CHA-CBD-CGD-O1D
14	B	832	CLA	CHA-CBD-CGD-O2D
14	B	835	CLA	C1A-C2A-CAA-CBA
14	B	836	CLA	C1A-C2A-CAA-CBA
14	B	836	CLA	C4B-C3B-CAB-CBB
14	B	837	CLA	CBD-CGD-O2D-CED
14	B	838	CLA	C1A-C2A-CAA-CBA
14	B	838	CLA	C3A-C2A-CAA-CBA
14	B	838	CLA	C4B-C3B-CAB-CBB
14	B	839	CLA	CBA-CGA-O2A-C1
14	B	843	CLA	C1A-C2A-CAA-CBA
14	B	843	CLA	C4B-C3B-CAB-CBB
14	B	844	CLA	C4B-C3B-CAB-CBB
14	B	844	CLA	CBD-CGD-O2D-CED
14	F	201	CLA	C4B-C3B-CAB-CBB
14	F	205	CLA	C1A-C2A-CAA-CBA
14	F	205	CLA	C3A-C2A-CAA-CBA
14	J	101	CLA	C1A-C2A-CAA-CBA
14	J	101	CLA	C3A-C2A-CAA-CBA
14	J	101	CLA	C4B-C3B-CAB-CBB
14	J	101	CLA	CAD-CBD-CGD-O1D
14	J	101	CLA	CAD-CBD-CGD-O2D
14	J	101	CLA	CBD-CGD-O2D-CED
14	J	102	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	L	1501	CLA	C1A-C2A-CAA-CBA
14	L	1501	CLA	C3A-C2A-CAA-CBA
14	L	1502	CLA	C4B-C3B-CAB-CBB
14	K	4002	CLA	C4B-C3B-CAB-CBB
14	K	4003	CLA	CAD-CBD-CGD-O2D
14	K	4004	CLA	C1A-C2A-CAA-CBA
14	K	4004	CLA	C2B-C3B-CAB-CBB
14	a	806	CLA	C1A-C2A-CAA-CBA
14	a	806	CLA	CHA-CBD-CGD-O1D
14	a	806	CLA	CHA-CBD-CGD-O2D
14	a	807	CLA	C1A-C2A-CAA-CBA
14	a	808	CLA	C1A-C2A-CAA-CBA
14	a	808	CLA	C3A-C2A-CAA-CBA
14	a	808	CLA	CAD-CBD-CGD-O1D
14	a	808	CLA	CAD-CBD-CGD-O2D
14	a	809	CLA	C1A-C2A-CAA-CBA
14	a	809	CLA	CBD-CGD-O2D-CED
14	a	809	CLA	O1D-CGD-O2D-CED
14	a	810	CLA	C4B-C3B-CAB-CBB
14	a	811	CLA	C1A-C2A-CAA-CBA
14	a	811	CLA	C3A-C2A-CAA-CBA
14	a	811	CLA	CHA-CBD-CGD-O1D
14	a	811	CLA	CHA-CBD-CGD-O2D
14	a	813	CLA	C1A-C2A-CAA-CBA
14	a	813	CLA	C3A-C2A-CAA-CBA
14	a	813	CLA	C4B-C3B-CAB-CBB
14	a	814	CLA	C1A-C2A-CAA-CBA
14	a	814	CLA	CBD-CGD-O2D-CED
14	a	815	CLA	C1A-C2A-CAA-CBA
14	a	815	CLA	C3A-C2A-CAA-CBA
14	a	816	CLA	C1A-C2A-CAA-CBA
14	a	817	CLA	CBD-CGD-O2D-CED
14	a	818	CLA	C4B-C3B-CAB-CBB
14	a	818	CLA	CBD-CGD-O2D-CED
14	a	819	CLA	C4B-C3B-CAB-CBB
14	a	821	CLA	C1A-C2A-CAA-CBA
14	a	821	CLA	C3A-C2A-CAA-CBA
14	a	821	CLA	C2B-C3B-CAB-CBB
14	a	822	CLA	C3A-C2A-CAA-CBA
14	a	825	CLA	C1A-C2A-CAA-CBA
14	a	825	CLA	C3A-C2A-CAA-CBA
14	a	825	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	a	825	CLA	CHA-CBD-CGD-O2D
14	a	826	CLA	CAD-CBD-CGD-O1D
14	a	826	CLA	CAD-CBD-CGD-O2D
14	a	826	CLA	C2-C3-C5-C6
14	a	826	CLA	C4-C3-C5-C6
14	a	827	CLA	C4B-C3B-CAB-CBB
14	a	828	CLA	C6-C7-C8-C9
14	a	828	CLA	C14-C13-C15-C16
14	a	835	CLA	C4B-C3B-CAB-CBB
14	a	836	CLA	C2B-C3B-CAB-CBB
14	a	837	CLA	C4B-C3B-CAB-CBB
14	a	837	CLA	C2-C3-C5-C6
14	a	837	CLA	C4-C3-C5-C6
14	a	839	CLA	C2-C3-C5-C6
14	a	840	CLA	C4B-C3B-CAB-CBB
14	a	841	CLA	C1A-C2A-CAA-CBA
14	a	841	CLA	C3A-C2A-CAA-CBA
14	a	842	CLA	C4B-C3B-CAB-CBB
14	a	843	CLA	C1A-C2A-CAA-CBA
14	a	843	CLA	C4B-C3B-CAB-CBB
14	a	854	CLA	C1A-C2A-CAA-CBA
14	a	854	CLA	C2B-C3B-CAB-CBB
14	1	805	CLA	C1A-C2A-CAA-CBA
14	1	806	CLA	C1A-C2A-CAA-CBA
14	1	806	CLA	C3A-C2A-CAA-CBA
14	1	806	CLA	CAD-CBD-CGD-O1D
14	1	806	CLA	CAD-CBD-CGD-O2D
14	1	807	CLA	C1A-C2A-CAA-CBA
14	1	807	CLA	CBD-CGD-O2D-CED
14	1	807	CLA	O1D-CGD-O2D-CED
14	1	808	CLA	C4B-C3B-CAB-CBB
14	1	809	CLA	C1A-C2A-CAA-CBA
14	1	809	CLA	C3A-C2A-CAA-CBA
14	1	809	CLA	CHA-CBD-CGD-O1D
14	1	809	CLA	CHA-CBD-CGD-O2D
14	1	811	CLA	C1A-C2A-CAA-CBA
14	1	811	CLA	C3A-C2A-CAA-CBA
14	1	811	CLA	C4B-C3B-CAB-CBB
14	1	812	CLA	C1A-C2A-CAA-CBA
14	1	812	CLA	CBD-CGD-O2D-CED
14	1	813	CLA	C1A-C2A-CAA-CBA
14	1	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	1	814	CLA	C1A-C2A-CAA-CBA
14	1	815	CLA	CBD-CGD-O2D-CED
14	1	816	CLA	C4B-C3B-CAB-CBB
14	1	816	CLA	CBD-CGD-O2D-CED
14	1	817	CLA	C4B-C3B-CAB-CBB
14	1	819	CLA	C1A-C2A-CAA-CBA
14	1	819	CLA	C3A-C2A-CAA-CBA
14	1	819	CLA	C2B-C3B-CAB-CBB
14	1	820	CLA	C3A-C2A-CAA-CBA
14	1	823	CLA	C1A-C2A-CAA-CBA
14	1	823	CLA	C3A-C2A-CAA-CBA
14	1	823	CLA	CHA-CBD-CGD-O1D
14	1	823	CLA	CHA-CBD-CGD-O2D
14	1	824	CLA	CAD-CBD-CGD-O1D
14	1	824	CLA	CAD-CBD-CGD-O2D
14	1	824	CLA	C2-C3-C5-C6
14	1	824	CLA	C4-C3-C5-C6
14	1	825	CLA	C4B-C3B-CAB-CBB
14	1	826	CLA	C6-C7-C8-C9
14	1	826	CLA	C14-C13-C15-C16
14	1	833	CLA	C4B-C3B-CAB-CBB
14	1	834	CLA	C2B-C3B-CAB-CBB
14	1	835	CLA	C4B-C3B-CAB-CBB
14	1	835	CLA	C2-C3-C5-C6
14	1	835	CLA	C4-C3-C5-C6
14	1	837	CLA	C2-C3-C5-C6
14	1	838	CLA	C4B-C3B-CAB-CBB
14	1	839	CLA	C1A-C2A-CAA-CBA
14	1	839	CLA	C3A-C2A-CAA-CBA
14	1	841	CLA	C4B-C3B-CAB-CBB
14	1	842	CLA	C4B-C3B-CAB-CBB
14	1	843	CLA	C1A-C2A-CAA-CBA
14	1	843	CLA	C4B-C3B-CAB-CBB
14	b	801	CLA	C1A-C2A-CAA-CBA
14	b	804	CLA	CAD-CBD-CGD-O1D
14	b	804	CLA	CAD-CBD-CGD-O2D
14	b	806	CLA	C6-C7-C8-C9
14	b	807	CLA	CHA-CBD-CGD-O1D
14	b	807	CLA	CHA-CBD-CGD-O2D
14	b	808	CLA	CHA-CBD-CGD-O1D
14	b	808	CLA	CHA-CBD-CGD-O2D
14	b	809	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	809	CLA	C14-C13-C15-C16
14	b	811	CLA	C4B-C3B-CAB-CBB
14	b	811	CLA	CHA-CBD-CGD-O1D
14	b	811	CLA	CHA-CBD-CGD-O2D
14	b	812	CLA	C3A-C2A-CAA-CBA
14	b	814	CLA	C1A-C2A-CAA-CBA
14	b	814	CLA	C4B-C3B-CAB-CBB
14	b	814	CLA	CHA-CBD-CGD-O1D
14	b	814	CLA	CHA-CBD-CGD-O2D
14	b	816	CLA	C1A-C2A-CAA-CBA
14	b	816	CLA	CBA-CGA-O2A-C1
14	b	818	CLA	C1A-C2A-CAA-CBA
14	b	818	CLA	C3A-C2A-CAA-CBA
14	b	820	CLA	C3A-C2A-CAA-CBA
14	b	821	CLA	CBD-CGD-O2D-CED
14	b	822	CLA	C1A-C2A-CAA-CBA
14	b	822	CLA	C3A-C2A-CAA-CBA
14	b	822	CLA	C4B-C3B-CAB-CBB
14	b	823	CLA	C1A-C2A-CAA-CBA
14	b	823	CLA	C4B-C3B-CAB-CBB
14	b	823	CLA	CHA-CBD-CGD-O1D
14	b	823	CLA	CHA-CBD-CGD-O2D
14	b	824	CLA	C1A-C2A-CAA-CBA
14	b	824	CLA	C4B-C3B-CAB-CBB
14	b	825	CLA	CBD-CGD-O2D-CED
14	b	830	CLA	C1A-C2A-CAA-CBA
14	b	830	CLA	C3A-C2A-CAA-CBA
14	b	831	CLA	CHA-CBD-CGD-O1D
14	b	831	CLA	CHA-CBD-CGD-O2D
14	b	834	CLA	C1A-C2A-CAA-CBA
14	b	835	CLA	C1A-C2A-CAA-CBA
14	b	835	CLA	C4B-C3B-CAB-CBB
14	b	836	CLA	CBD-CGD-O2D-CED
14	b	837	CLA	C1A-C2A-CAA-CBA
14	b	837	CLA	C3A-C2A-CAA-CBA
14	b	837	CLA	C4B-C3B-CAB-CBB
14	b	838	CLA	CBA-CGA-O2A-C1
14	b	842	CLA	C1A-C2A-CAA-CBA
14	b	842	CLA	C4B-C3B-CAB-CBB
14	b	843	CLA	C4B-C3B-CAB-CBB
14	b	843	CLA	CBD-CGD-O2D-CED
14	2	803	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	2	803	CLA	CAD-CBD-CGD-O2D
14	2	805	CLA	C6-C7-C8-C9
14	2	806	CLA	CHA-CBD-CGD-O1D
14	2	806	CLA	CHA-CBD-CGD-O2D
14	2	807	CLA	CHA-CBD-CGD-O1D
14	2	807	CLA	CHA-CBD-CGD-O2D
14	2	808	CLA	C4B-C3B-CAB-CBB
14	2	808	CLA	C14-C13-C15-C16
14	2	810	CLA	C4B-C3B-CAB-CBB
14	2	810	CLA	CHA-CBD-CGD-O1D
14	2	810	CLA	CHA-CBD-CGD-O2D
14	2	811	CLA	C3A-C2A-CAA-CBA
14	2	814	CLA	C1A-C2A-CAA-CBA
14	2	814	CLA	C4B-C3B-CAB-CBB
14	2	814	CLA	CHA-CBD-CGD-O1D
14	2	814	CLA	CHA-CBD-CGD-O2D
14	2	816	CLA	C1A-C2A-CAA-CBA
14	2	816	CLA	CBA-CGA-O2A-C1
14	2	818	CLA	C1A-C2A-CAA-CBA
14	2	818	CLA	C3A-C2A-CAA-CBA
14	2	820	CLA	C3A-C2A-CAA-CBA
14	2	821	CLA	CBD-CGD-O2D-CED
14	2	822	CLA	C1A-C2A-CAA-CBA
14	2	822	CLA	C3A-C2A-CAA-CBA
14	2	822	CLA	C4B-C3B-CAB-CBB
14	2	823	CLA	C1A-C2A-CAA-CBA
14	2	823	CLA	C4B-C3B-CAB-CBB
14	2	823	CLA	CHA-CBD-CGD-O1D
14	2	823	CLA	CHA-CBD-CGD-O2D
14	2	824	CLA	C1A-C2A-CAA-CBA
14	2	824	CLA	C4B-C3B-CAB-CBB
14	2	825	CLA	CBD-CGD-O2D-CED
14	2	830	CLA	C1A-C2A-CAA-CBA
14	2	830	CLA	C3A-C2A-CAA-CBA
14	2	831	CLA	CHA-CBD-CGD-O1D
14	2	831	CLA	CHA-CBD-CGD-O2D
14	2	834	CLA	C1A-C2A-CAA-CBA
14	2	835	CLA	C1A-C2A-CAA-CBA
14	2	835	CLA	C4B-C3B-CAB-CBB
14	2	836	CLA	CBD-CGD-O2D-CED
14	2	837	CLA	C1A-C2A-CAA-CBA
14	2	837	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	2	837	CLA	C4B-C3B-CAB-CBB
14	2	838	CLA	CBA-CGA-O2A-C1
14	2	842	CLA	C1A-C2A-CAA-CBA
14	2	842	CLA	C4B-C3B-CAB-CBB
14	2	843	CLA	C4B-C3B-CAB-CBB
14	2	843	CLA	CBD-CGD-O2D-CED
14	f	201	CLA	C4B-C3B-CAB-CBB
14	f	205	CLA	C1A-C2A-CAA-CBA
14	f	205	CLA	C3A-C2A-CAA-CBA
14	6	4404	CLA	C1A-C2A-CAA-CBA
14	6	4404	CLA	C3A-C2A-CAA-CBA
14	j	101	CLA	C1A-C2A-CAA-CBA
14	j	101	CLA	C3A-C2A-CAA-CBA
14	j	101	CLA	C4B-C3B-CAB-CBB
14	j	101	CLA	CAD-CBD-CGD-O1D
14	j	101	CLA	CAD-CBD-CGD-O2D
14	j	101	CLA	CBD-CGD-O2D-CED
14	j	102	CLA	C4B-C3B-CAB-CBB
14	7	1101	CLA	C1A-C2A-CAA-CBA
14	7	1101	CLA	CHA-CBD-CGD-O1D
14	7	1101	CLA	CHA-CBD-CGD-O2D
14	7	1102	CLA	C1A-C2A-CAA-CBA
14	7	1102	CLA	C3A-C2A-CAA-CBA
14	7	1102	CLA	C4B-C3B-CAB-CBB
14	7	1102	CLA	CAD-CBD-CGD-O1D
14	7	1102	CLA	CAD-CBD-CGD-O2D
14	7	1102	CLA	CBD-CGD-O2D-CED
14	7	1103	CLA	C4B-C3B-CAB-CBB
14	k	4002	CLA	C4B-C3B-CAB-CBB
14	k	4003	CLA	CAD-CBD-CGD-O2D
14	8	4002	CLA	C4B-C3B-CAB-CBB
14	8	4003	CLA	CAD-CBD-CGD-O2D
14	8	4004	CLA	C1A-C2A-CAA-CBA
14	8	4004	CLA	C2B-C3B-CAB-CBB
14	l	4204	CLA	C1A-C2A-CAA-CBA
14	l	4204	CLA	C3A-C2A-CAA-CBA
14	l	4205	CLA	C4B-C3B-CAB-CBB
14	0	202	CLA	C1A-C2A-CAA-CBA
14	0	206	CLA	C1A-C2A-CAA-CBA
14	0	206	CLA	C3A-C2A-CAA-CBA
14	0	207	CLA	C4B-C3B-CAB-CBB
17	A	847	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	A	847	BCR	C11-C12-C13-C35
17	A	847	BCR	C20-C21-C22-C23
17	A	847	BCR	C20-C21-C22-C37
17	A	848	BCR	C21-C22-C23-C24
17	A	848	BCR	C37-C22-C23-C24
17	A	849	BCR	C22-C23-C24-C25
17	A	850	BCR	C7-C8-C9-C34
17	A	850	BCR	C11-C12-C13-C35
17	A	850	BCR	C14-C15-C16-C17
17	A	850	BCR	C16-C17-C18-C19
17	A	850	BCR	C36-C18-C19-C20
17	A	850	BCR	C18-C19-C20-C21
17	A	850	BCR	C20-C21-C22-C23
17	A	850	BCR	C20-C21-C22-C37
17	A	850	BCR	C22-C23-C24-C25
17	A	851	BCR	C7-C8-C9-C10
17	A	851	BCR	C10-C11-C12-C13
17	A	851	BCR	C11-C12-C13-C35
17	A	851	BCR	C17-C18-C19-C20
17	A	851	BCR	C18-C19-C20-C21
17	A	851	BCR	C20-C21-C22-C23
17	A	851	BCR	C20-C21-C22-C37
17	A	851	BCR	C37-C22-C23-C24
17	A	851	BCR	C22-C23-C24-C25
17	B	847	BCR	C6-C7-C8-C9
17	B	847	BCR	C18-C19-C20-C21
17	B	848	BCR	C11-C10-C9-C8
17	B	848	BCR	C37-C22-C23-C24
17	B	850	BCR	C10-C11-C12-C13
17	B	850	BCR	C11-C12-C13-C14
17	B	850	BCR	C21-C22-C23-C24
17	B	850	BCR	C37-C22-C23-C24
17	B	850	BCR	C22-C23-C24-C25
17	B	851	BCR	C11-C10-C9-C8
17	B	851	BCR	C10-C11-C12-C13
17	B	851	BCR	C14-C15-C16-C17
17	B	851	BCR	C18-C19-C20-C21
17	B	851	BCR	C37-C22-C23-C24
17	B	851	BCR	C22-C23-C24-C25
17	B	852	BCR	C21-C22-C23-C24
17	B	852	BCR	C37-C22-C23-C24
17	B	852	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
17	B	854	BCR	C20-C21-C22-C37
17	B	854	BCR	C22-C23-C24-C25
17	F	203	BCR	C7-C8-C9-C10
17	F	203	BCR	C35-C13-C14-C15
17	F	203	BCR	C21-C22-C23-C24
17	F	203	BCR	C37-C22-C23-C24
17	F	206	BCR	C6-C7-C8-C9
17	F	206	BCR	C7-C8-C9-C10
17	F	206	BCR	C10-C11-C12-C13
17	F	206	BCR	C21-C22-C23-C24
17	F	206	BCR	C37-C22-C23-C24
17	I	101	BCR	C6-C7-C8-C9
17	I	101	BCR	C7-C8-C9-C10
17	I	101	BCR	C7-C8-C9-C34
17	I	101	BCR	C11-C12-C13-C14
17	I	101	BCR	C11-C12-C13-C35
17	I	101	BCR	C37-C22-C23-C24
17	I	102	BCR	C5-C6-C7-C8
17	I	102	BCR	C6-C7-C8-C9
17	I	102	BCR	C7-C8-C9-C34
17	I	102	BCR	C10-C11-C12-C13
17	I	102	BCR	C11-C12-C13-C14
17	I	102	BCR	C12-C13-C14-C15
17	I	102	BCR	C16-C17-C18-C36
17	J	103	BCR	C6-C7-C8-C9
17	J	103	BCR	C22-C23-C24-C25
17	J	104	BCR	C20-C21-C22-C37
17	J	104	BCR	C21-C22-C23-C24
17	J	104	BCR	C37-C22-C23-C24
17	L	1504	BCR	C17-C18-C19-C20
17	L	1504	BCR	C37-C22-C23-C24
17	L	1504	BCR	C23-C24-C25-C26
17	L	1504	BCR	C23-C24-C25-C30
17	L	1505	BCR	C6-C7-C8-C9
17	L	1505	BCR	C11-C10-C9-C34
17	L	1505	BCR	C37-C22-C23-C24
17	L	1505	BCR	C22-C23-C24-C25
17	M	102	BCR	C7-C8-C9-C34
17	M	102	BCR	C20-C21-C22-C37
17	M	102	BCR	C21-C22-C23-C24
17	M	102	BCR	C22-C23-C24-C25
17	K	4001	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
17	K	4001	BCR	C21-C22-C23-C24
17	K	4005	BCR	C35-C13-C14-C15
17	K	4005	BCR	C18-C19-C20-C21
17	K	4005	BCR	C37-C22-C23-C24
17	a	847	BCR	C6-C7-C8-C9
17	a	847	BCR	C11-C12-C13-C35
17	a	847	BCR	C20-C21-C22-C23
17	a	847	BCR	C20-C21-C22-C37
17	a	848	BCR	C21-C22-C23-C24
17	a	848	BCR	C37-C22-C23-C24
17	a	849	BCR	C22-C23-C24-C25
17	a	850	BCR	C7-C8-C9-C34
17	a	850	BCR	C11-C12-C13-C35
17	a	850	BCR	C14-C15-C16-C17
17	a	850	BCR	C16-C17-C18-C19
17	a	850	BCR	C36-C18-C19-C20
17	a	850	BCR	C18-C19-C20-C21
17	a	850	BCR	C20-C21-C22-C23
17	a	850	BCR	C20-C21-C22-C37
17	a	850	BCR	C22-C23-C24-C25
17	a	851	BCR	C7-C8-C9-C10
17	a	851	BCR	C10-C11-C12-C13
17	a	851	BCR	C11-C12-C13-C35
17	a	851	BCR	C17-C18-C19-C20
17	a	851	BCR	C18-C19-C20-C21
17	a	851	BCR	C20-C21-C22-C23
17	a	851	BCR	C20-C21-C22-C37
17	a	851	BCR	C37-C22-C23-C24
17	a	851	BCR	C22-C23-C24-C25
17	1	847	BCR	C6-C7-C8-C9
17	1	847	BCR	C11-C12-C13-C35
17	1	847	BCR	C20-C21-C22-C23
17	1	847	BCR	C20-C21-C22-C37
17	1	848	BCR	C21-C22-C23-C24
17	1	848	BCR	C37-C22-C23-C24
17	1	849	BCR	C22-C23-C24-C25
17	1	850	BCR	C7-C8-C9-C34
17	1	850	BCR	C11-C12-C13-C35
17	1	850	BCR	C14-C15-C16-C17
17	1	850	BCR	C16-C17-C18-C19
17	1	850	BCR	C36-C18-C19-C20
17	1	850	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
17	1	850	BCR	C20-C21-C22-C23
17	1	850	BCR	C20-C21-C22-C37
17	1	850	BCR	C22-C23-C24-C25
17	1	851	BCR	C7-C8-C9-C10
17	1	851	BCR	C10-C11-C12-C13
17	1	851	BCR	C11-C12-C13-C35
17	1	851	BCR	C17-C18-C19-C20
17	1	851	BCR	C18-C19-C20-C21
17	1	851	BCR	C20-C21-C22-C23
17	1	851	BCR	C20-C21-C22-C37
17	1	851	BCR	C37-C22-C23-C24
17	1	851	BCR	C22-C23-C24-C25
17	b	846	BCR	C6-C7-C8-C9
17	b	846	BCR	C18-C19-C20-C21
17	b	847	BCR	C11-C10-C9-C8
17	b	847	BCR	C37-C22-C23-C24
17	b	849	BCR	C10-C11-C12-C13
17	b	849	BCR	C11-C12-C13-C14
17	b	849	BCR	C21-C22-C23-C24
17	b	849	BCR	C37-C22-C23-C24
17	b	849	BCR	C22-C23-C24-C25
17	b	850	BCR	C11-C10-C9-C8
17	b	850	BCR	C10-C11-C12-C13
17	b	850	BCR	C14-C15-C16-C17
17	b	850	BCR	C18-C19-C20-C21
17	b	850	BCR	C37-C22-C23-C24
17	b	850	BCR	C22-C23-C24-C25
17	b	851	BCR	C21-C22-C23-C24
17	b	851	BCR	C37-C22-C23-C24
17	b	851	BCR	C22-C23-C24-C25
17	b	853	BCR	C20-C21-C22-C37
17	b	853	BCR	C22-C23-C24-C25
17	b	854	BCR	C7-C8-C9-C34
17	b	854	BCR	C20-C21-C22-C37
17	b	854	BCR	C21-C22-C23-C24
17	b	854	BCR	C22-C23-C24-C25
17	2	846	BCR	C6-C7-C8-C9
17	2	846	BCR	C18-C19-C20-C21
17	2	847	BCR	C11-C10-C9-C8
17	2	847	BCR	C37-C22-C23-C24
17	2	849	BCR	C10-C11-C12-C13
17	2	849	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	2	849	BCR	C21-C22-C23-C24
17	2	849	BCR	C37-C22-C23-C24
17	2	849	BCR	C22-C23-C24-C25
17	2	850	BCR	C11-C10-C9-C8
17	2	850	BCR	C10-C11-C12-C13
17	2	850	BCR	C14-C15-C16-C17
17	2	850	BCR	C18-C19-C20-C21
17	2	850	BCR	C37-C22-C23-C24
17	2	850	BCR	C22-C23-C24-C25
17	2	851	BCR	C21-C22-C23-C24
17	2	851	BCR	C37-C22-C23-C24
17	2	851	BCR	C22-C23-C24-C25
17	f	203	BCR	C7-C8-C9-C10
17	f	203	BCR	C35-C13-C14-C15
17	f	203	BCR	C21-C22-C23-C24
17	f	203	BCR	C37-C22-C23-C24
17	f	206	BCR	C6-C7-C8-C9
17	f	206	BCR	C7-C8-C9-C10
17	f	206	BCR	C10-C11-C12-C13
17	f	206	BCR	C21-C22-C23-C24
17	f	206	BCR	C37-C22-C23-C24
17	6	4402	BCR	C7-C8-C9-C10
17	6	4402	BCR	C35-C13-C14-C15
17	6	4402	BCR	C21-C22-C23-C24
17	6	4402	BCR	C37-C22-C23-C24
17	6	4405	BCR	C6-C7-C8-C9
17	6	4405	BCR	C7-C8-C9-C10
17	6	4405	BCR	C10-C11-C12-C13
17	6	4405	BCR	C21-C22-C23-C24
17	6	4405	BCR	C37-C22-C23-C24
17	6	4406	BCR	C20-C21-C22-C37
17	6	4406	BCR	C22-C23-C24-C25
17	i	4102	BCR	C6-C7-C8-C9
17	i	4102	BCR	C7-C8-C9-C10
17	i	4102	BCR	C7-C8-C9-C34
17	i	4102	BCR	C11-C12-C13-C14
17	i	4102	BCR	C11-C12-C13-C35
17	i	4102	BCR	C37-C22-C23-C24
17	i	4103	BCR	C5-C6-C7-C8
17	i	4103	BCR	C6-C7-C8-C9
17	i	4103	BCR	C7-C8-C9-C34
17	i	4103	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	i	4103	BCR	C11-C12-C13-C14
17	i	4103	BCR	C12-C13-C14-C15
17	i	4103	BCR	C16-C17-C18-C36
17	h	101	BCR	C6-C7-C8-C9
17	h	101	BCR	C7-C8-C9-C10
17	h	101	BCR	C7-C8-C9-C34
17	h	101	BCR	C11-C12-C13-C14
17	h	101	BCR	C11-C12-C13-C35
17	h	101	BCR	C37-C22-C23-C24
17	h	102	BCR	C5-C6-C7-C8
17	h	102	BCR	C6-C7-C8-C9
17	h	102	BCR	C7-C8-C9-C34
17	h	102	BCR	C10-C11-C12-C13
17	h	102	BCR	C11-C12-C13-C14
17	h	102	BCR	C12-C13-C14-C15
17	h	102	BCR	C16-C17-C18-C36
17	j	103	BCR	C6-C7-C8-C9
17	j	103	BCR	C22-C23-C24-C25
17	j	104	BCR	C20-C21-C22-C37
17	j	104	BCR	C21-C22-C23-C24
17	j	104	BCR	C37-C22-C23-C24
17	7	1104	BCR	C6-C7-C8-C9
17	7	1104	BCR	C22-C23-C24-C25
17	7	1105	BCR	C20-C21-C22-C37
17	7	1105	BCR	C21-C22-C23-C24
17	7	1105	BCR	C37-C22-C23-C24
17	k	4001	BCR	C7-C8-C9-C34
17	k	4001	BCR	C21-C22-C23-C24
17	k	4004	BCR	C35-C13-C14-C15
17	k	4004	BCR	C18-C19-C20-C21
17	k	4004	BCR	C37-C22-C23-C24
17	8	4001	BCR	C7-C8-C9-C34
17	8	4001	BCR	C21-C22-C23-C24
17	8	4005	BCR	C35-C13-C14-C15
17	8	4005	BCR	C18-C19-C20-C21
17	8	4005	BCR	C37-C22-C23-C24
17	l	4207	BCR	C17-C18-C19-C20
17	l	4207	BCR	C37-C22-C23-C24
17	l	4207	BCR	C23-C24-C25-C26
17	l	4207	BCR	C23-C24-C25-C30
17	0	204	BCR	C6-C7-C8-C9
17	0	204	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
17	0	204	BCR	C37-C22-C23-C24
17	0	204	BCR	C22-C23-C24-C25
17	0	209	BCR	C17-C18-C19-C20
17	0	209	BCR	C37-C22-C23-C24
17	0	209	BCR	C23-C24-C25-C26
17	0	209	BCR	C23-C24-C25-C30
17	0	210	BCR	C6-C7-C8-C9
17	0	210	BCR	C11-C10-C9-C34
17	0	210	BCR	C37-C22-C23-C24
17	0	210	BCR	C22-C23-C24-C25
17	9	102	BCR	C7-C8-C9-C34
17	9	102	BCR	C20-C21-C22-C37
17	9	102	BCR	C21-C22-C23-C24
17	9	102	BCR	C22-C23-C24-C25
18	A	852	LMG	C11-C10-O7-C8
18	A	853	LMG	O6-C1-O1-C7
18	L	1506	LMG	C9-C8-O7-C10
18	L	1506	LMG	C11-C10-O7-C8
18	a	852	LMG	C11-C10-O7-C8
18	a	853	LMG	O6-C1-O1-C7
18	1	852	LMG	O6-C1-O1-C7
18	l	4202	LMG	C9-C8-O7-C10
18	l	4202	LMG	C11-C10-O7-C8
18	0	201	LMG	C9-C8-O7-C10
18	0	201	LMG	C11-C10-O7-C8
18	0	203	LMG	C11-C10-O7-C8
19	I	103	LMT	O5'-C1'-O1'-C1
19	I	103	LMT	C2-C1-O1'-C1'
19	i	4101	LMT	O5'-C1'-O1'-C1
19	i	4101	LMT	C2-C1-O1'-C1'
19	h	103	LMT	O5'-C1'-O1'-C1
19	h	103	LMT	C2-C1-O1'-C1'
14	A	818	CLA	O1D-CGD-O2D-CED
14	a	819	CLA	O1D-CGD-O2D-CED
14	1	817	CLA	O1D-CGD-O2D-CED
14	B	837	CLA	O1D-CGD-O2D-CED
14	F	201	CLA	O1D-CGD-O2D-CED
14	K	4002	CLA	O1D-CGD-O2D-CED
14	1	841	CLA	O1D-CGD-O2D-CED
14	b	836	CLA	O1D-CGD-O2D-CED
14	2	836	CLA	O1D-CGD-O2D-CED
14	f	201	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	k	4002	CLA	O1D-CGD-O2D-CED
14	8	4002	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	CBD-CGD-O2D-CED
14	A	825	CLA	CBD-CGD-O2D-CED
14	A	834	CLA	CBD-CGD-O2D-CED
14	B	805	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	CBD-CGD-O2D-CED
14	B	817	CLA	CBD-CGD-O2D-CED
14	F	201	CLA	CBD-CGD-O2D-CED
14	K	4002	CLA	CBD-CGD-O2D-CED
14	K	4003	CLA	CBD-CGD-O2D-CED
14	a	819	CLA	CBD-CGD-O2D-CED
14	a	826	CLA	CBD-CGD-O2D-CED
14	a	835	CLA	CBD-CGD-O2D-CED
14	1	817	CLA	CBD-CGD-O2D-CED
14	1	824	CLA	CBD-CGD-O2D-CED
14	1	833	CLA	CBD-CGD-O2D-CED
14	1	841	CLA	CBD-CGD-O2D-CED
14	b	805	CLA	CBD-CGD-O2D-CED
14	b	814	CLA	CBD-CGD-O2D-CED
14	b	816	CLA	CBD-CGD-O2D-CED
14	2	804	CLA	CBD-CGD-O2D-CED
14	2	814	CLA	CBD-CGD-O2D-CED
14	2	816	CLA	CBD-CGD-O2D-CED
14	f	201	CLA	CBD-CGD-O2D-CED
14	k	4002	CLA	CBD-CGD-O2D-CED
14	k	4003	CLA	CBD-CGD-O2D-CED
14	8	4002	CLA	CBD-CGD-O2D-CED
14	8	4003	CLA	CBD-CGD-O2D-CED
14	A	834	CLA	O1A-CGA-O2A-C1
14	B	809	CLA	O1A-CGA-O2A-C1
14	B	829	CLA	O1A-CGA-O2A-C1
14	B	843	CLA	O1A-CGA-O2A-C1
14	a	835	CLA	O1A-CGA-O2A-C1
14	1	833	CLA	O1A-CGA-O2A-C1
14	b	809	CLA	O1A-CGA-O2A-C1
14	b	828	CLA	O1A-CGA-O2A-C1
14	b	842	CLA	O1A-CGA-O2A-C1
14	2	808	CLA	O1A-CGA-O2A-C1
14	2	828	CLA	O1A-CGA-O2A-C1
14	2	842	CLA	O1A-CGA-O2A-C1
14	B	839	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	838	CLA	O1A-CGA-O2A-C1
14	2	838	CLA	O1A-CGA-O2A-C1
19	I	103	LMT	O5B-C1B-O1B-C4'
19	i	4101	LMT	O5B-C1B-O1B-C4'
19	h	103	LMT	O5B-C1B-O1B-C4'
14	A	818	CLA	CBA-CGA-O2A-C1
14	a	819	CLA	CBA-CGA-O2A-C1
14	1	817	CLA	CBA-CGA-O2A-C1
12	A	801	LHG	C24-C23-O8-C6
12	a	801	LHG	C24-C23-O8-C6
12	1	801	LHG	C24-C23-O8-C6
14	B	809	CLA	CBA-CGA-O2A-C1
14	b	809	CLA	CBA-CGA-O2A-C1
14	2	808	CLA	CBA-CGA-O2A-C1
14	A	814	CLA	O1A-CGA-O2A-C1
14	A	825	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	O1A-CGA-O2A-C1
14	B	808	CLA	O1A-CGA-O2A-C1
14	B	812	CLA	O1A-CGA-O2A-C1
14	B	816	CLA	O1A-CGA-O2A-C1
14	F	201	CLA	O1A-CGA-O2A-C1
14	a	815	CLA	O1A-CGA-O2A-C1
14	a	826	CLA	O1A-CGA-O2A-C1
14	a	837	CLA	O1A-CGA-O2A-C1
14	1	813	CLA	O1A-CGA-O2A-C1
14	1	824	CLA	O1A-CGA-O2A-C1
14	1	835	CLA	O1A-CGA-O2A-C1
14	1	841	CLA	O1A-CGA-O2A-C1
14	b	808	CLA	O1A-CGA-O2A-C1
14	b	812	CLA	O1A-CGA-O2A-C1
14	b	815	CLA	O1A-CGA-O2A-C1
14	2	807	CLA	O1A-CGA-O2A-C1
14	2	811	CLA	O1A-CGA-O2A-C1
14	2	815	CLA	O1A-CGA-O2A-C1
14	f	201	CLA	O1A-CGA-O2A-C1
14	B	817	CLA	O1A-CGA-O2A-C1
14	b	816	CLA	O1A-CGA-O2A-C1
14	2	816	CLA	O1A-CGA-O2A-C1
14	B	822	CLA	O1D-CGD-O2D-CED
14	K	4003	CLA	O1D-CGD-O2D-CED
14	b	821	CLA	O1D-CGD-O2D-CED
14	2	821	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	k	4003	CLA	O1D-CGD-O2D-CED
14	8	4003	CLA	O1D-CGD-O2D-CED
14	B	826	CLA	O1D-CGD-O2D-CED
14	B	844	CLA	O1D-CGD-O2D-CED
14	b	825	CLA	O1D-CGD-O2D-CED
14	b	843	CLA	O1D-CGD-O2D-CED
14	2	825	CLA	O1D-CGD-O2D-CED
14	2	843	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	832	CLA	CBD-CGD-O2D-CED
14	a	824	CLA	CBD-CGD-O2D-CED
14	a	833	CLA	CBD-CGD-O2D-CED
14	1	822	CLA	CBD-CGD-O2D-CED
14	1	831	CLA	CBD-CGD-O2D-CED
18	A	852	LMG	O9-C10-O7-C8
18	L	1506	LMG	O9-C10-O7-C8
18	a	852	LMG	O9-C10-O7-C8
18	l	4202	LMG	O9-C10-O7-C8
18	0	201	LMG	O9-C10-O7-C8
18	0	203	LMG	O9-C10-O7-C8
14	A	830	CLA	C3-C5-C6-C7
14	A	842	CLA	C3-C5-C6-C7
14	A	843	CLA	C3-C5-C6-C7
14	B	809	CLA	C3-C5-C6-C7
14	B	816	CLA	C3-C5-C6-C7
14	B	820	CLA	C3-C5-C6-C7
14	B	827	CLA	C3-C5-C6-C7
14	B	829	CLA	C3-C5-C6-C7
14	a	831	CLA	C3-C5-C6-C7
14	a	842	CLA	C3-C5-C6-C7
14	a	843	CLA	C3-C5-C6-C7
14	1	829	CLA	C3-C5-C6-C7
14	1	842	CLA	C3-C5-C6-C7
14	1	843	CLA	C3-C5-C6-C7
14	b	809	CLA	C3-C5-C6-C7
14	b	815	CLA	C3-C5-C6-C7
14	b	819	CLA	C3-C5-C6-C7
14	b	826	CLA	C3-C5-C6-C7
14	b	828	CLA	C3-C5-C6-C7
14	2	808	CLA	C3-C5-C6-C7
14	2	815	CLA	C3-C5-C6-C7
14	2	819	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	2	826	CLA	C3-C5-C6-C7
14	2	828	CLA	C3-C5-C6-C7
14	A	816	CLA	O1D-CGD-O2D-CED
14	a	817	CLA	O1D-CGD-O2D-CED
14	1	815	CLA	O1D-CGD-O2D-CED
14	A	814	CLA	CBA-CGA-O2A-C1
14	A	834	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	CBA-CGA-O2A-C1
14	B	808	CLA	CBA-CGA-O2A-C1
14	B	816	CLA	CBA-CGA-O2A-C1
14	B	829	CLA	CBA-CGA-O2A-C1
14	B	843	CLA	CBA-CGA-O2A-C1
14	a	815	CLA	CBA-CGA-O2A-C1
14	a	835	CLA	CBA-CGA-O2A-C1
14	a	837	CLA	CBA-CGA-O2A-C1
14	1	813	CLA	CBA-CGA-O2A-C1
14	1	833	CLA	CBA-CGA-O2A-C1
14	1	835	CLA	CBA-CGA-O2A-C1
14	b	808	CLA	CBA-CGA-O2A-C1
14	b	815	CLA	CBA-CGA-O2A-C1
14	b	828	CLA	CBA-CGA-O2A-C1
14	b	842	CLA	CBA-CGA-O2A-C1
14	2	807	CLA	CBA-CGA-O2A-C1
14	2	815	CLA	CBA-CGA-O2A-C1
14	2	828	CLA	CBA-CGA-O2A-C1
14	2	842	CLA	CBA-CGA-O2A-C1
14	A	804	CLA	CBD-CGD-O2D-CED
14	A	809	CLA	CBD-CGD-O2D-CED
14	A	812	CLA	CBD-CGD-O2D-CED
14	A	824	CLA	CBD-CGD-O2D-CED
14	A	837	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	A	844	CLA	CBD-CGD-O2D-CED
14	B	840	CLA	CBD-CGD-O2D-CED
14	a	805	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	CBD-CGD-O2D-CED
14	a	813	CLA	CBD-CGD-O2D-CED
14	a	825	CLA	CBD-CGD-O2D-CED
14	a	838	CLA	CBD-CGD-O2D-CED
14	a	844	CLA	CBD-CGD-O2D-CED
14	1	804	CLA	CBD-CGD-O2D-CED
14	1	808	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	1	811	CLA	CBD-CGD-O2D-CED
14	1	823	CLA	CBD-CGD-O2D-CED
14	1	836	CLA	CBD-CGD-O2D-CED
14	1	840	CLA	CBD-CGD-O2D-CED
14	1	844	CLA	CBD-CGD-O2D-CED
14	b	802	CLA	CBD-CGD-O2D-CED
14	b	839	CLA	CBD-CGD-O2D-CED
14	2	839	CLA	CBD-CGD-O2D-CED
14	A	813	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	O1D-CGD-O2D-CED
14	J	101	CLA	O1D-CGD-O2D-CED
14	a	814	CLA	O1D-CGD-O2D-CED
14	a	818	CLA	O1D-CGD-O2D-CED
14	1	812	CLA	O1D-CGD-O2D-CED
14	1	816	CLA	O1D-CGD-O2D-CED
14	j	101	CLA	O1D-CGD-O2D-CED
14	7	1102	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	O1A-CGA-O2A-C1
14	a	819	CLA	O1A-CGA-O2A-C1
14	1	817	CLA	O1A-CGA-O2A-C1
14	A	813	CLA	C4-C3-C5-C6
14	A	819	CLA	C4-C3-C5-C6
14	A	826	CLA	C4-C3-C5-C6
14	B	821	CLA	C4-C3-C5-C6
14	B	844	CLA	C4-C3-C5-C6
14	a	814	CLA	C4-C3-C5-C6
14	a	820	CLA	C4-C3-C5-C6
14	a	827	CLA	C4-C3-C5-C6
14	1	812	CLA	C4-C3-C5-C6
14	1	818	CLA	C4-C3-C5-C6
14	1	825	CLA	C4-C3-C5-C6
14	b	820	CLA	C4-C3-C5-C6
14	b	843	CLA	C4-C3-C5-C6
14	2	820	CLA	C4-C3-C5-C6
14	2	843	CLA	C4-C3-C5-C6
14	A	813	CLA	C2-C3-C5-C6
14	A	826	CLA	C2-C3-C5-C6
14	B	821	CLA	C2-C3-C5-C6
14	a	814	CLA	C2-C3-C5-C6
14	a	827	CLA	C2-C3-C5-C6
14	1	812	CLA	C2-C3-C5-C6
14	1	825	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	b	820	CLA	C2-C3-C5-C6
14	2	820	CLA	C2-C3-C5-C6
14	A	825	CLA	O1D-CGD-O2D-CED
14	a	826	CLA	O1D-CGD-O2D-CED
14	1	824	CLA	O1D-CGD-O2D-CED
14	B	815	CLA	C2A-CAA-CBA-CGA
14	b	814	CLA	C2A-CAA-CBA-CGA
14	2	814	CLA	C2A-CAA-CBA-CGA
14	B	801	CLA	C3-C5-C6-C7
14	B	812	CLA	C3-C5-C6-C7
14	a	804	CLA	C3-C5-C6-C7
14	b	812	CLA	C3-C5-C6-C7
14	2	801	CLA	C3-C5-C6-C7
14	2	811	CLA	C3-C5-C6-C7
14	A	825	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	CBA-CGA-O2A-C1
14	B	802	CLA	CBA-CGA-O2A-C1
14	B	806	CLA	CBA-CGA-O2A-C1
14	B	812	CLA	CBA-CGA-O2A-C1
14	B	840	CLA	CBA-CGA-O2A-C1
14	F	201	CLA	CBA-CGA-O2A-C1
14	a	826	CLA	CBA-CGA-O2A-C1
14	a	827	CLA	CBA-CGA-O2A-C1
14	1	824	CLA	CBA-CGA-O2A-C1
14	1	825	CLA	CBA-CGA-O2A-C1
14	1	841	CLA	CBA-CGA-O2A-C1
14	b	801	CLA	CBA-CGA-O2A-C1
14	b	806	CLA	CBA-CGA-O2A-C1
14	b	812	CLA	CBA-CGA-O2A-C1
14	b	839	CLA	CBA-CGA-O2A-C1
14	2	805	CLA	CBA-CGA-O2A-C1
14	2	811	CLA	CBA-CGA-O2A-C1
14	2	839	CLA	CBA-CGA-O2A-C1
14	f	201	CLA	CBA-CGA-O2A-C1
14	0	202	CLA	CBA-CGA-O2A-C1
17	A	850	BCR	C15-C16-C17-C18
17	B	850	BCR	C9-C10-C11-C12
17	B	851	BCR	C19-C20-C21-C22
17	a	850	BCR	C15-C16-C17-C18
17	1	850	BCR	C15-C16-C17-C18
17	b	849	BCR	C9-C10-C11-C12
17	b	850	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
17	2	849	BCR	C9-C10-C11-C12
17	2	850	BCR	C19-C20-C21-C22
14	A	815	CLA	O1A-CGA-O2A-C1
14	A	823	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	O1A-CGA-O2A-C1
14	B	801	CLA	O1A-CGA-O2A-C1
14	B	840	CLA	O1A-CGA-O2A-C1
14	a	804	CLA	O1A-CGA-O2A-C1
14	a	816	CLA	O1A-CGA-O2A-C1
14	a	824	CLA	O1A-CGA-O2A-C1
14	a	827	CLA	O1A-CGA-O2A-C1
14	1	814	CLA	O1A-CGA-O2A-C1
14	1	822	CLA	O1A-CGA-O2A-C1
14	1	825	CLA	O1A-CGA-O2A-C1
14	b	839	CLA	O1A-CGA-O2A-C1
14	2	801	CLA	O1A-CGA-O2A-C1
14	2	839	CLA	O1A-CGA-O2A-C1
14	A	834	CLA	O1D-CGD-O2D-CED
14	B	805	CLA	O1D-CGD-O2D-CED
14	a	835	CLA	O1D-CGD-O2D-CED
14	1	833	CLA	O1D-CGD-O2D-CED
14	b	805	CLA	O1D-CGD-O2D-CED
14	2	804	CLA	O1D-CGD-O2D-CED
14	A	814	CLA	C3-C5-C6-C7
14	a	815	CLA	C3-C5-C6-C7
14	1	813	CLA	C3-C5-C6-C7
14	A	821	CLA	CBD-CGD-O2D-CED
14	A	835	CLA	CBD-CGD-O2D-CED
14	B	814	CLA	CBD-CGD-O2D-CED
14	a	822	CLA	CBD-CGD-O2D-CED
14	a	836	CLA	CBD-CGD-O2D-CED
14	1	820	CLA	CBD-CGD-O2D-CED
14	1	834	CLA	CBD-CGD-O2D-CED
14	b	813	CLA	CBD-CGD-O2D-CED
14	2	813	CLA	CBD-CGD-O2D-CED
12	A	802	LHG	O2-C2-C3-O3
12	a	802	LHG	O2-C2-C3-O3
12	1	802	LHG	O2-C2-C3-O3
12	m	101	LHG	O2-C2-C3-O3
12	9	101	LHG	O2-C2-C3-O3
14	A	811	CLA	CBA-CGA-O2A-C1
14	A	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	839	CLA	CBA-CGA-O2A-C1
14	B	801	CLA	CBA-CGA-O2A-C1
14	B	821	CLA	CBA-CGA-O2A-C1
14	a	804	CLA	CBA-CGA-O2A-C1
14	a	812	CLA	CBA-CGA-O2A-C1
14	a	824	CLA	CBA-CGA-O2A-C1
14	a	840	CLA	CBA-CGA-O2A-C1
14	1	810	CLA	CBA-CGA-O2A-C1
14	1	822	CLA	CBA-CGA-O2A-C1
14	1	838	CLA	CBA-CGA-O2A-C1
14	b	820	CLA	CBA-CGA-O2A-C1
14	2	801	CLA	CBA-CGA-O2A-C1
14	2	820	CLA	CBA-CGA-O2A-C1
14	B	802	CLA	O1A-CGA-O2A-C1
14	B	806	CLA	O1A-CGA-O2A-C1
14	b	801	CLA	O1A-CGA-O2A-C1
14	b	806	CLA	O1A-CGA-O2A-C1
14	2	805	CLA	O1A-CGA-O2A-C1
14	0	202	CLA	O1A-CGA-O2A-C1
14	B	817	CLA	O1D-CGD-O2D-CED
14	b	816	CLA	O1D-CGD-O2D-CED
14	2	816	CLA	O1D-CGD-O2D-CED
14	F	205	CLA	CBD-CGD-O2D-CED
14	f	205	CLA	CBD-CGD-O2D-CED
14	6	4404	CLA	CBD-CGD-O2D-CED
17	J	104	BCR	C14-C15-C16-C17
17	j	104	BCR	C14-C15-C16-C17
17	7	1105	BCR	C14-C15-C16-C17
14	B	818	CLA	CBD-CGD-O2D-CED
14	2	817	CLA	CBD-CGD-O2D-CED
14	A	815	CLA	CBA-CGA-O2A-C1
14	a	816	CLA	CBA-CGA-O2A-C1
14	1	814	CLA	CBA-CGA-O2A-C1
14	B	801	CLA	C4-C3-C5-C6
14	a	804	CLA	C4-C3-C5-C6
14	2	801	CLA	C4-C3-C5-C6
14	A	819	CLA	C2-C3-C5-C6
14	B	801	CLA	C2-C3-C5-C6
14	a	804	CLA	C2-C3-C5-C6
14	a	820	CLA	C2-C3-C5-C6
14	1	818	CLA	C2-C3-C5-C6
14	2	801	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	839	CLA	O1A-CGA-O2A-C1
14	a	840	CLA	O1A-CGA-O2A-C1
14	1	838	CLA	O1A-CGA-O2A-C1
14	b	817	CLA	CBD-CGD-O2D-CED
18	L	1506	LMG	O6-C5-C6-O5
18	l	4202	LMG	O6-C5-C6-O5
18	0	201	LMG	O6-C5-C6-O5
14	B	812	CLA	C2A-CAA-CBA-CGA
14	b	812	CLA	C2A-CAA-CBA-CGA
14	2	811	CLA	C2A-CAA-CBA-CGA
14	B	815	CLA	O1D-CGD-O2D-CED
14	2	814	CLA	O1D-CGD-O2D-CED
14	A	811	CLA	O1A-CGA-O2A-C1
14	B	821	CLA	O1A-CGA-O2A-C1
14	a	812	CLA	O1A-CGA-O2A-C1
14	1	810	CLA	O1A-CGA-O2A-C1
14	b	820	CLA	O1A-CGA-O2A-C1
14	2	820	CLA	O1A-CGA-O2A-C1
18	L	1506	LMG	O6-C1-O1-C7
18	l	4202	LMG	O6-C1-O1-C7
18	0	201	LMG	O6-C1-O1-C7
19	F	202	LMT	O5'-C5'-C6'-O6'
19	f	202	LMT	O5'-C5'-C6'-O6'
19	6	4401	LMT	O5'-C5'-C6'-O6'
14	b	814	CLA	O1D-CGD-O2D-CED
14	A	821	CLA	CBA-CGA-O2A-C1
14	B	844	CLA	CBA-CGA-O2A-C1
14	a	822	CLA	CBA-CGA-O2A-C1
14	1	820	CLA	CBA-CGA-O2A-C1
14	b	843	CLA	CBA-CGA-O2A-C1
14	2	843	CLA	CBA-CGA-O2A-C1
14	A	810	CLA	CBD-CGD-O2D-CED
14	A	838	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	CBD-CGD-O2D-CED
14	B	809	CLA	CBD-CGD-O2D-CED
14	B	831	CLA	CBD-CGD-O2D-CED
14	a	811	CLA	CBD-CGD-O2D-CED
14	a	839	CLA	CBD-CGD-O2D-CED
14	a	843	CLA	CBD-CGD-O2D-CED
14	1	809	CLA	CBD-CGD-O2D-CED
14	1	837	CLA	CBD-CGD-O2D-CED
14	1	843	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	b	809	CLA	CBD-CGD-O2D-CED
14	b	830	CLA	CBD-CGD-O2D-CED
14	2	808	CLA	CBD-CGD-O2D-CED
14	2	830	CLA	CBD-CGD-O2D-CED
14	B	835	CLA	C2C-C3C-CAC-CBC
14	b	834	CLA	C2C-C3C-CAC-CBC
14	2	834	CLA	C2C-C3C-CAC-CBC
14	A	821	CLA	O1A-CGA-O2A-C1
14	a	822	CLA	O1A-CGA-O2A-C1
14	1	820	CLA	O1A-CGA-O2A-C1
14	A	812	CLA	O1D-CGD-O2D-CED
14	a	813	CLA	O1D-CGD-O2D-CED
14	a	833	CLA	O1D-CGD-O2D-CED
14	1	811	CLA	O1D-CGD-O2D-CED
14	1	831	CLA	O1D-CGD-O2D-CED
14	B	834	CLA	CBD-CGD-O2D-CED
14	b	833	CLA	CBD-CGD-O2D-CED
14	2	833	CLA	CBD-CGD-O2D-CED
14	B	819	CLA	C3-C5-C6-C7
14	b	818	CLA	C3-C5-C6-C7
14	2	818	CLA	C3-C5-C6-C7
14	A	832	CLA	O1D-CGD-O2D-CED
17	L	1504	BCR	C13-C14-C15-C16
17	l	4207	BCR	C13-C14-C15-C16
17	0	209	BCR	C13-C14-C15-C16
14	b	843	CLA	O1A-CGA-O2A-C1
18	B	803	LMG	O9-C10-O7-C8
18	b	803	LMG	O9-C10-O7-C8
18	2	802	LMG	O9-C10-O7-C8
12	A	802	LHG	C1-C2-C3-O3
12	a	802	LHG	C1-C2-C3-O3
12	1	802	LHG	C1-C2-C3-O3
14	A	807	CLA	CBA-CGA-O2A-C1
14	A	808	CLA	CBA-CGA-O2A-C1
14	A	810	CLA	CBA-CGA-O2A-C1
14	A	819	CLA	CBA-CGA-O2A-C1
14	B	820	CLA	CBA-CGA-O2A-C1
14	B	834	CLA	CBA-CGA-O2A-C1
14	L	1501	CLA	CBA-CGA-O2A-C1
14	L	1503	CLA	CBA-CGA-O2A-C1
14	a	808	CLA	CBA-CGA-O2A-C1
14	a	809	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	811	CLA	CBA-CGA-O2A-C1
14	a	820	CLA	CBA-CGA-O2A-C1
14	1	806	CLA	CBA-CGA-O2A-C1
14	1	807	CLA	CBA-CGA-O2A-C1
14	1	809	CLA	CBA-CGA-O2A-C1
14	1	818	CLA	CBA-CGA-O2A-C1
14	b	819	CLA	CBA-CGA-O2A-C1
14	b	833	CLA	CBA-CGA-O2A-C1
14	2	819	CLA	CBA-CGA-O2A-C1
14	2	833	CLA	CBA-CGA-O2A-C1
14	l	4204	CLA	CBA-CGA-O2A-C1
14	l	4206	CLA	CBA-CGA-O2A-C1
14	0	206	CLA	CBA-CGA-O2A-C1
14	0	208	CLA	CBA-CGA-O2A-C1
19	I	103	LMT	C4'-C5'-C6'-O6'
19	i	4101	LMT	C4'-C5'-C6'-O6'
19	h	103	LMT	C4'-C5'-C6'-O6'
14	A	823	CLA	O1D-CGD-O2D-CED
14	a	824	CLA	O1D-CGD-O2D-CED
14	1	822	CLA	O1D-CGD-O2D-CED
14	B	844	CLA	O1A-CGA-O2A-C1
14	2	843	CLA	O1A-CGA-O2A-C1
14	L	1503	CLA	C4-C3-C5-C6
14	l	4206	CLA	C4-C3-C5-C6
14	0	208	CLA	C4-C3-C5-C6
14	B	844	CLA	C2-C3-C5-C6
14	L	1503	CLA	C2-C3-C5-C6
14	b	843	CLA	C2-C3-C5-C6
14	2	843	CLA	C2-C3-C5-C6
14	l	4206	CLA	C2-C3-C5-C6
14	0	208	CLA	C2-C3-C5-C6
14	A	808	CLA	C3-C5-C6-C7
14	a	809	CLA	C3-C5-C6-C7
14	1	807	CLA	C3-C5-C6-C7
14	a	840	CLA	CBD-CGD-O2D-CED
14	1	838	CLA	CBD-CGD-O2D-CED
14	A	810	CLA	C6-C7-C8-C9
14	A	829	CLA	C6-C7-C8-C9
14	B	802	CLA	C6-C7-C8-C9
14	a	811	CLA	C6-C7-C8-C9
14	a	830	CLA	C6-C7-C8-C9
14	1	809	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	1	828	CLA	C6-C7-C8-C9
14	b	801	CLA	C6-C7-C8-C9
14	0	202	CLA	C6-C7-C8-C9
18	A	853	LMG	C2-C1-O1-C7
18	a	853	LMG	C2-C1-O1-C7
18	1	852	LMG	C2-C1-O1-C7
12	M	101	LHG	O2-C2-C3-O3
14	A	810	CLA	O1A-CGA-O2A-C1
14	a	811	CLA	O1A-CGA-O2A-C1
14	1	809	CLA	O1A-CGA-O2A-C1
14	A	839	CLA	CBD-CGD-O2D-CED
14	A	804	CLA	O1D-CGD-O2D-CED
14	a	805	CLA	O1D-CGD-O2D-CED
14	1	804	CLA	O1D-CGD-O2D-CED
17	A	847	BCR	C37-C22-C23-C24
17	A	848	BCR	C7-C8-C9-C34
17	A	848	BCR	C11-C12-C13-C35
17	A	849	BCR	C7-C8-C9-C34
17	A	851	BCR	C36-C18-C19-C20
17	B	847	BCR	C37-C22-C23-C24
17	B	849	BCR	C37-C22-C23-C24
17	B	850	BCR	C11-C12-C13-C35
17	B	851	BCR	C7-C8-C9-C34
17	B	851	BCR	C11-C12-C13-C35
17	F	203	BCR	C7-C8-C9-C34
17	J	103	BCR	C36-C18-C19-C20
17	J	103	BCR	C37-C22-C23-C24
17	L	1504	BCR	C7-C8-C9-C34
17	L	1505	BCR	C7-C8-C9-C34
17	M	102	BCR	C37-C22-C23-C24
17	K	4001	BCR	C37-C22-C23-C24
17	a	847	BCR	C37-C22-C23-C24
17	a	848	BCR	C7-C8-C9-C34
17	a	848	BCR	C11-C12-C13-C35
17	a	849	BCR	C7-C8-C9-C34
17	a	851	BCR	C36-C18-C19-C20
17	1	847	BCR	C37-C22-C23-C24
17	1	848	BCR	C7-C8-C9-C34
17	1	848	BCR	C11-C12-C13-C35
17	1	849	BCR	C7-C8-C9-C34
17	1	851	BCR	C36-C18-C19-C20
17	b	846	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	b	848	BCR	C37-C22-C23-C24
17	b	849	BCR	C11-C12-C13-C35
17	b	850	BCR	C7-C8-C9-C34
17	b	850	BCR	C11-C12-C13-C35
17	b	854	BCR	C37-C22-C23-C24
17	2	846	BCR	C37-C22-C23-C24
17	2	848	BCR	C37-C22-C23-C24
17	2	849	BCR	C11-C12-C13-C35
17	2	850	BCR	C7-C8-C9-C34
17	2	850	BCR	C11-C12-C13-C35
17	f	203	BCR	C7-C8-C9-C34
17	6	4402	BCR	C7-C8-C9-C34
17	j	103	BCR	C36-C18-C19-C20
17	j	103	BCR	C37-C22-C23-C24
17	7	1104	BCR	C36-C18-C19-C20
17	7	1104	BCR	C37-C22-C23-C24
17	k	4001	BCR	C37-C22-C23-C24
17	8	4001	BCR	C37-C22-C23-C24
17	l	4207	BCR	C7-C8-C9-C34
17	0	204	BCR	C7-C8-C9-C34
17	0	209	BCR	C7-C8-C9-C34
17	0	210	BCR	C7-C8-C9-C34
17	9	102	BCR	C37-C22-C23-C24
17	A	847	BCR	C21-C22-C23-C24
17	A	848	BCR	C7-C8-C9-C10
17	A	851	BCR	C21-C22-C23-C24
17	B	847	BCR	C7-C8-C9-C10
17	B	847	BCR	C21-C22-C23-C24
17	B	851	BCR	C7-C8-C9-C10
17	B	851	BCR	C21-C22-C23-C24
17	J	103	BCR	C21-C22-C23-C24
17	L	1504	BCR	C7-C8-C9-C10
17	L	1504	BCR	C21-C22-C23-C24
17	L	1505	BCR	C7-C8-C9-C10
17	K	4005	BCR	C21-C22-C23-C24
17	a	847	BCR	C21-C22-C23-C24
17	a	848	BCR	C7-C8-C9-C10
17	a	851	BCR	C21-C22-C23-C24
17	1	847	BCR	C21-C22-C23-C24
17	1	848	BCR	C7-C8-C9-C10
17	1	851	BCR	C21-C22-C23-C24
17	b	846	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
17	b	846	BCR	C21-C22-C23-C24
17	b	850	BCR	C7-C8-C9-C10
17	b	850	BCR	C21-C22-C23-C24
17	2	846	BCR	C7-C8-C9-C10
17	2	846	BCR	C21-C22-C23-C24
17	2	850	BCR	C7-C8-C9-C10
17	2	850	BCR	C21-C22-C23-C24
17	j	103	BCR	C21-C22-C23-C24
17	7	1104	BCR	C21-C22-C23-C24
17	k	4004	BCR	C21-C22-C23-C24
17	8	4005	BCR	C21-C22-C23-C24
17	l	4207	BCR	C7-C8-C9-C10
17	l	4207	BCR	C21-C22-C23-C24
17	0	204	BCR	C7-C8-C9-C10
17	0	209	BCR	C7-C8-C9-C10
17	0	209	BCR	C21-C22-C23-C24
17	0	210	BCR	C7-C8-C9-C10
14	B	820	CLA	C2A-CAA-CBA-CGA
14	b	819	CLA	C2A-CAA-CBA-CGA
14	2	819	CLA	C2A-CAA-CBA-CGA
12	B	853	LHG	C23-C24-C25-C26
12	b	852	LHG	C23-C24-C25-C26
12	2	852	LHG	C23-C24-C25-C26
14	A	808	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	O1A-CGA-O2A-C1
14	a	809	CLA	O1A-CGA-O2A-C1
14	a	820	CLA	O1A-CGA-O2A-C1
14	1	807	CLA	O1A-CGA-O2A-C1
14	1	818	CLA	O1A-CGA-O2A-C1
14	b	819	CLA	O1A-CGA-O2A-C1
14	2	819	CLA	O1A-CGA-O2A-C1
19	I	103	LMT	O5'-C5'-C6'-O6'
19	i	4101	LMT	O5'-C5'-C6'-O6'
19	h	103	LMT	O5'-C5'-C6'-O6'
12	M	101	LHG	C24-C23-O8-C6
12	m	101	LHG	C24-C23-O8-C6
12	9	101	LHG	C24-C23-O8-C6
14	B	832	CLA	CBA-CGA-O2A-C1
14	b	831	CLA	CBA-CGA-O2A-C1
14	2	831	CLA	CBA-CGA-O2A-C1
14	B	834	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	b	833	CLA	C2-C1-O2A-CGA
14	2	833	CLA	C2-C1-O2A-CGA
14	A	824	CLA	O1D-CGD-O2D-CED
14	A	841	CLA	O1D-CGD-O2D-CED
14	a	825	CLA	O1D-CGD-O2D-CED
14	1	823	CLA	O1D-CGD-O2D-CED
14	1	840	CLA	O1D-CGD-O2D-CED
14	b	802	CLA	O1D-CGD-O2D-CED
14	B	842	CLA	CBD-CGD-O2D-CED
14	2	841	CLA	CBD-CGD-O2D-CED
14	A	813	CLA	C8-C10-C11-C12
14	B	832	CLA	C5-C6-C7-C8
14	a	814	CLA	C8-C10-C11-C12
14	1	812	CLA	C8-C10-C11-C12
14	b	831	CLA	C5-C6-C7-C8
14	2	831	CLA	C5-C6-C7-C8
14	A	837	CLA	O1D-CGD-O2D-CED
14	a	838	CLA	O1D-CGD-O2D-CED
14	1	836	CLA	O1D-CGD-O2D-CED
14	b	841	CLA	CBD-CGD-O2D-CED
14	B	809	CLA	C11-C10-C8-C7
14	B	811	CLA	C11-C10-C8-C7
14	B	816	CLA	C12-C13-C15-C16
14	b	809	CLA	C11-C10-C8-C7
14	b	811	CLA	C11-C10-C8-C7
14	b	815	CLA	C12-C13-C15-C16
14	2	808	CLA	C11-C10-C8-C7
14	2	810	CLA	C11-C10-C8-C7
14	2	815	CLA	C12-C13-C15-C16
14	A	805	CLA	CBA-CGA-O2A-C1
14	a	806	CLA	CBA-CGA-O2A-C1
14	7	1101	CLA	CBA-CGA-O2A-C1
18	A	852	LMG	C10-C11-C12-C13
18	a	852	LMG	C10-C11-C12-C13
18	0	203	LMG	C10-C11-C12-C13
17	I	101	BCR	C9-C10-C11-C12
17	I	102	BCR	C9-C10-C11-C12
17	I	102	BCR	C13-C14-C15-C16
17	i	4102	BCR	C9-C10-C11-C12
17	i	4103	BCR	C9-C10-C11-C12
17	i	4103	BCR	C13-C14-C15-C16
17	h	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
17	h	102	BCR	C9-C10-C11-C12
17	h	102	BCR	C13-C14-C15-C16
18	A	853	LMG	O9-C10-O7-C8
18	a	853	LMG	O9-C10-O7-C8
18	1	852	LMG	O9-C10-O7-C8
14	A	844	CLA	O1D-CGD-O2D-CED
14	a	844	CLA	O1D-CGD-O2D-CED
14	1	844	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	C8-C10-C11-C12
14	B	806	CLA	C10-C11-C12-C13
14	a	806	CLA	C8-C10-C11-C12
14	b	806	CLA	C10-C11-C12-C13
14	2	805	CLA	C10-C11-C12-C13
14	7	1101	CLA	C8-C10-C11-C12
14	A	807	CLA	C15-C16-C17-C18
14	A	813	CLA	C15-C16-C17-C18
14	B	801	CLA	C5-C6-C7-C8
14	B	809	CLA	C13-C15-C16-C17
14	B	813	CLA	C8-C10-C11-C12
14	B	820	CLA	C5-C6-C7-C8
14	B	821	CLA	C8-C10-C11-C12
14	B	844	CLA	C13-C15-C16-C17
14	a	804	CLA	C5-C6-C7-C8
14	a	806	CLA	C5-C6-C7-C8
14	a	808	CLA	C15-C16-C17-C18
14	a	814	CLA	C15-C16-C17-C18
14	1	806	CLA	C15-C16-C17-C18
14	1	812	CLA	C15-C16-C17-C18
14	b	809	CLA	C13-C15-C16-C17
14	b	819	CLA	C5-C6-C7-C8
14	b	820	CLA	C8-C10-C11-C12
14	b	843	CLA	C13-C15-C16-C17
14	2	801	CLA	C5-C6-C7-C8
14	2	808	CLA	C13-C15-C16-C17
14	2	812	CLA	C8-C10-C11-C12
14	2	819	CLA	C5-C6-C7-C8
14	2	820	CLA	C8-C10-C11-C12
14	2	843	CLA	C13-C15-C16-C17
14	7	1101	CLA	C5-C6-C7-C8
14	l	4203	CLA	C8-C10-C11-C12
14	A	811	CLA	C2A-CAA-CBA-CGA
14	A	831	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	A	835	CLA	C2A-CAA-CBA-CGA
14	A	843	CLA	C2A-CAA-CBA-CGA
14	B	804	CLA	C2A-CAA-CBA-CGA
14	B	830	CLA	C2A-CAA-CBA-CGA
14	B	839	CLA	C2A-CAA-CBA-CGA
14	a	812	CLA	C2A-CAA-CBA-CGA
14	a	832	CLA	C2A-CAA-CBA-CGA
14	a	836	CLA	C2A-CAA-CBA-CGA
14	a	843	CLA	C2A-CAA-CBA-CGA
14	1	810	CLA	C2A-CAA-CBA-CGA
14	1	830	CLA	C2A-CAA-CBA-CGA
14	1	834	CLA	C2A-CAA-CBA-CGA
14	1	843	CLA	C2A-CAA-CBA-CGA
14	b	804	CLA	C2A-CAA-CBA-CGA
14	b	829	CLA	C2A-CAA-CBA-CGA
14	b	838	CLA	C2A-CAA-CBA-CGA
14	2	803	CLA	C2A-CAA-CBA-CGA
14	2	829	CLA	C2A-CAA-CBA-CGA
14	2	838	CLA	C2A-CAA-CBA-CGA
17	I	101	BCR	C10-C11-C12-C13
17	L	1504	BCR	C10-C11-C12-C13
17	i	4102	BCR	C10-C11-C12-C13
17	h	101	BCR	C10-C11-C12-C13
17	l	4207	BCR	C10-C11-C12-C13
17	0	209	BCR	C10-C11-C12-C13
14	A	805	CLA	C5-C6-C7-C8
14	A	805	CLA	C10-C11-C12-C13
14	A	807	CLA	C10-C11-C12-C13
14	A	829	CLA	C10-C11-C12-C13
14	A	830	CLA	C10-C11-C12-C13
14	A	832	CLA	C15-C16-C17-C18
14	A	843	CLA	C13-C15-C16-C17
14	B	831	CLA	C13-C15-C16-C17
14	a	806	CLA	C10-C11-C12-C13
14	a	808	CLA	C10-C11-C12-C13
14	a	830	CLA	C10-C11-C12-C13
14	a	831	CLA	C10-C11-C12-C13
14	a	832	CLA	C8-C10-C11-C12
14	a	833	CLA	C15-C16-C17-C18
14	a	843	CLA	C13-C15-C16-C17
14	1	806	CLA	C10-C11-C12-C13
14	1	828	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	1	829	CLA	C10-C11-C12-C13
14	1	830	CLA	C8-C10-C11-C12
14	1	831	CLA	C15-C16-C17-C18
14	1	843	CLA	C13-C15-C16-C17
14	b	830	CLA	C13-C15-C16-C17
14	2	830	CLA	C13-C15-C16-C17
14	7	1101	CLA	C10-C11-C12-C13
12	B	853	LHG	C7-C8-C9-C10
12	b	852	LHG	C7-C8-C9-C10
12	2	852	LHG	C7-C8-C9-C10
18	L	1506	LMG	C10-C11-C12-C13
18	l	4202	LMG	C10-C11-C12-C13
18	0	201	LMG	C10-C11-C12-C13
14	A	807	CLA	O1A-CGA-O2A-C1
14	B	834	CLA	O1A-CGA-O2A-C1
14	L	1501	CLA	O1A-CGA-O2A-C1
14	a	808	CLA	O1A-CGA-O2A-C1
14	1	806	CLA	O1A-CGA-O2A-C1
14	b	833	CLA	O1A-CGA-O2A-C1
14	2	833	CLA	O1A-CGA-O2A-C1
14	l	4204	CLA	O1A-CGA-O2A-C1
14	0	206	CLA	O1A-CGA-O2A-C1
14	B	833	CLA	CBD-CGD-O2D-CED
14	b	832	CLA	CBD-CGD-O2D-CED
14	2	832	CLA	CBD-CGD-O2D-CED
14	A	809	CLA	O1D-CGD-O2D-CED
14	a	810	CLA	O1D-CGD-O2D-CED
14	1	808	CLA	O1D-CGD-O2D-CED
14	b	839	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	C13-C15-C16-C17
14	A	831	CLA	C8-C10-C11-C12
14	A	839	CLA	C8-C10-C11-C12
14	A	839	CLA	C13-C15-C16-C17
14	A	842	CLA	C8-C10-C11-C12
14	B	809	CLA	C10-C11-C12-C13
14	B	816	CLA	C8-C10-C11-C12
14	B	830	CLA	C8-C10-C11-C12
14	L	1503	CLA	C13-C15-C16-C17
14	a	805	CLA	C13-C15-C16-C17
14	a	840	CLA	C8-C10-C11-C12
14	a	840	CLA	C13-C15-C16-C17
14	a	842	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	1	804	CLA	C13-C15-C16-C17
14	1	838	CLA	C8-C10-C11-C12
14	1	838	CLA	C13-C15-C16-C17
14	1	842	CLA	C8-C10-C11-C12
14	b	809	CLA	C10-C11-C12-C13
14	b	815	CLA	C8-C10-C11-C12
14	b	829	CLA	C8-C10-C11-C12
14	2	808	CLA	C10-C11-C12-C13
14	2	815	CLA	C8-C10-C11-C12
14	2	829	CLA	C8-C10-C11-C12
14	l	4206	CLA	C13-C15-C16-C17
14	0	208	CLA	C13-C15-C16-C17
14	A	823	CLA	C15-C16-C17-C18
14	B	811	CLA	C13-C15-C16-C17
14	a	824	CLA	C15-C16-C17-C18
14	1	822	CLA	C15-C16-C17-C18
14	b	811	CLA	C13-C15-C16-C17
14	2	810	CLA	C13-C15-C16-C17
14	A	808	CLA	C15-C16-C17-C18
14	A	832	CLA	C5-C6-C7-C8
14	A	834	CLA	C8-C10-C11-C12
14	A	839	CLA	C15-C16-C17-C18
14	a	809	CLA	C15-C16-C17-C18
14	a	833	CLA	C5-C6-C7-C8
14	a	835	CLA	C8-C10-C11-C12
14	a	840	CLA	C15-C16-C17-C18
14	1	831	CLA	C5-C6-C7-C8
14	1	833	CLA	C8-C10-C11-C12
14	1	838	CLA	C15-C16-C17-C18
14	B	832	CLA	O1A-CGA-O2A-C1
14	L	1503	CLA	O1A-CGA-O2A-C1
14	b	831	CLA	O1A-CGA-O2A-C1
14	2	831	CLA	O1A-CGA-O2A-C1
14	l	4206	CLA	O1A-CGA-O2A-C1
14	0	208	CLA	O1A-CGA-O2A-C1
14	A	835	CLA	O1D-CGD-O2D-CED
14	B	840	CLA	O1D-CGD-O2D-CED
14	a	836	CLA	O1D-CGD-O2D-CED
14	1	834	CLA	O1D-CGD-O2D-CED
14	2	839	CLA	O1D-CGD-O2D-CED
14	1	807	CLA	C15-C16-C17-C18
15	B	846	PQN	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
15	b	845	PQN	C20-C21-C22-C23
15	2	845	PQN	C20-C21-C22-C23
14	L	1502	CLA	CBA-CGA-O2A-C1
14	l	4205	CLA	CBA-CGA-O2A-C1
14	0	207	CLA	CBA-CGA-O2A-C1
14	B	814	CLA	O1D-CGD-O2D-CED
14	b	813	CLA	O1D-CGD-O2D-CED
14	2	813	CLA	O1D-CGD-O2D-CED
17	L	1505	BCR	C9-C10-C11-C12
17	0	204	BCR	C9-C10-C11-C12
17	0	210	BCR	C9-C10-C11-C12
14	B	801	CLA	C10-C11-C12-C13
14	a	804	CLA	C10-C11-C12-C13
14	2	801	CLA	C10-C11-C12-C13
14	A	810	CLA	C2A-CAA-CBA-CGA
14	A	819	CLA	C2A-CAA-CBA-CGA
14	B	823	CLA	C2A-CAA-CBA-CGA
14	B	829	CLA	C2A-CAA-CBA-CGA
14	a	811	CLA	C2A-CAA-CBA-CGA
14	a	820	CLA	C2A-CAA-CBA-CGA
14	1	809	CLA	C2A-CAA-CBA-CGA
14	1	818	CLA	C2A-CAA-CBA-CGA
14	b	822	CLA	C2A-CAA-CBA-CGA
14	b	828	CLA	C2A-CAA-CBA-CGA
14	2	822	CLA	C2A-CAA-CBA-CGA
14	2	828	CLA	C2A-CAA-CBA-CGA
17	i	4102	BCR	C14-C15-C16-C17
14	A	827	CLA	C13-C15-C16-C17
14	L	1503	CLA	C10-C11-C12-C13
14	a	828	CLA	C13-C15-C16-C17
14	1	826	CLA	C13-C15-C16-C17
14	l	4206	CLA	C10-C11-C12-C13
14	0	208	CLA	C10-C11-C12-C13
14	2	840	CLA	CBD-CGD-O2D-CED
14	A	805	CLA	O1A-CGA-O2A-C1
14	a	806	CLA	O1A-CGA-O2A-C1
14	7	1101	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	C13-C15-C16-C17
14	A	821	CLA	C13-C15-C16-C17
14	A	830	CLA	C13-C15-C16-C17
14	A	834	CLA	C5-C6-C7-C8
14	B	808	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	B	809	CLA	C5-C6-C7-C8
14	B	829	CLA	C5-C6-C7-C8
14	a	806	CLA	C13-C15-C16-C17
14	a	822	CLA	C13-C15-C16-C17
14	a	831	CLA	C13-C15-C16-C17
14	a	835	CLA	C5-C6-C7-C8
14	1	820	CLA	C13-C15-C16-C17
14	1	829	CLA	C13-C15-C16-C17
14	1	833	CLA	C5-C6-C7-C8
14	b	808	CLA	C10-C11-C12-C13
14	b	809	CLA	C5-C6-C7-C8
14	b	828	CLA	C5-C6-C7-C8
14	2	807	CLA	C10-C11-C12-C13
14	2	808	CLA	C5-C6-C7-C8
14	2	828	CLA	C5-C6-C7-C8
14	7	1101	CLA	C13-C15-C16-C17
14	B	841	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C5-C6-C7-C8
14	A	821	CLA	C10-C11-C12-C13
14	A	826	CLA	C5-C6-C7-C8
14	B	805	CLA	C8-C10-C11-C12
14	a	808	CLA	C5-C6-C7-C8
14	a	822	CLA	C10-C11-C12-C13
14	a	827	CLA	C5-C6-C7-C8
14	1	806	CLA	C5-C6-C7-C8
14	1	820	CLA	C10-C11-C12-C13
14	1	825	CLA	C5-C6-C7-C8
14	b	805	CLA	C8-C10-C11-C12
14	2	804	CLA	C8-C10-C11-C12
14	A	821	CLA	O1D-CGD-O2D-CED
14	a	822	CLA	O1D-CGD-O2D-CED
14	1	820	CLA	O1D-CGD-O2D-CED
14	f	205	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	C15-C16-C17-C18
14	B	835	CLA	C5-C6-C7-C8
14	a	811	CLA	C15-C16-C17-C18
14	1	809	CLA	C15-C16-C17-C18
14	b	834	CLA	C5-C6-C7-C8
14	2	834	CLA	C5-C6-C7-C8
14	B	832	CLA	C3-C5-C6-C7
14	b	831	CLA	C3-C5-C6-C7
14	2	831	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	b	840	CLA	CBD-CGD-O2D-CED
14	F	205	CLA	O1D-CGD-O2D-CED
14	6	4404	CLA	O1D-CGD-O2D-CED
14	2	812	CLA	C5-C6-C7-C8
12	A	801	LHG	O2-C2-C3-O3
12	a	801	LHG	O2-C2-C3-O3
12	1	801	LHG	O2-C2-C3-O3
14	A	821	CLA	C16-C17-C18-C19
14	a	822	CLA	C16-C17-C18-C19
14	1	820	CLA	C16-C17-C18-C19
14	B	813	CLA	C5-C6-C7-C8
14	l	4203	CLA	C5-C6-C7-C8
17	A	851	BCR	C11-C10-C9-C34
17	B	847	BCR	C16-C17-C18-C36
17	B	848	BCR	C11-C10-C9-C34
17	B	848	BCR	C20-C21-C22-C37
17	B	851	BCR	C20-C21-C22-C37
17	B	854	BCR	C11-C10-C9-C34
17	F	206	BCR	C35-C13-C14-C15
17	I	101	BCR	C16-C17-C18-C36
17	I	102	BCR	C11-C10-C9-C34
17	I	102	BCR	C35-C13-C14-C15
17	J	103	BCR	C16-C17-C18-C36
17	L	1505	BCR	C20-C21-C22-C37
17	K	4001	BCR	C11-C10-C9-C34
17	K	4001	BCR	C20-C21-C22-C37
17	a	851	BCR	C11-C10-C9-C34
17	1	851	BCR	C11-C10-C9-C34
17	b	846	BCR	C16-C17-C18-C36
17	b	847	BCR	C11-C10-C9-C34
17	b	847	BCR	C20-C21-C22-C37
17	b	850	BCR	C20-C21-C22-C37
17	b	853	BCR	C11-C10-C9-C34
17	2	846	BCR	C16-C17-C18-C36
17	2	847	BCR	C11-C10-C9-C34
17	2	847	BCR	C20-C21-C22-C37
17	2	850	BCR	C20-C21-C22-C37
17	f	206	BCR	C35-C13-C14-C15
17	6	4405	BCR	C35-C13-C14-C15
17	6	4406	BCR	C11-C10-C9-C34
17	i	4102	BCR	C16-C17-C18-C36
17	i	4103	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
17	i	4103	BCR	C35-C13-C14-C15
17	h	101	BCR	C16-C17-C18-C36
17	h	102	BCR	C11-C10-C9-C34
17	h	102	BCR	C35-C13-C14-C15
17	j	103	BCR	C35-C13-C14-C15
17	j	103	BCR	C16-C17-C18-C36
17	7	1104	BCR	C35-C13-C14-C15
17	7	1104	BCR	C16-C17-C18-C36
17	k	4001	BCR	C11-C10-C9-C34
17	k	4001	BCR	C20-C21-C22-C37
17	8	4001	BCR	C11-C10-C9-C34
17	8	4001	BCR	C20-C21-C22-C37
17	0	204	BCR	C20-C21-C22-C37
17	0	210	BCR	C20-C21-C22-C37
17	B	847	BCR	C7-C8-C9-C34
17	B	851	BCR	C36-C18-C19-C20
17	M	102	BCR	C11-C12-C13-C35
17	b	846	BCR	C7-C8-C9-C34
17	b	850	BCR	C36-C18-C19-C20
17	b	854	BCR	C11-C12-C13-C35
17	2	846	BCR	C7-C8-C9-C34
17	2	850	BCR	C36-C18-C19-C20
17	9	102	BCR	C11-C12-C13-C35
17	I	102	BCR	C7-C8-C9-C10
17	K	4001	BCR	C7-C8-C9-C10
17	i	4103	BCR	C7-C8-C9-C10
17	h	102	BCR	C7-C8-C9-C10
17	k	4001	BCR	C7-C8-C9-C10
17	8	4001	BCR	C7-C8-C9-C10
14	L	1502	CLA	O1A-CGA-O2A-C1
14	l	4205	CLA	O1A-CGA-O2A-C1
14	0	207	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	C2A-CAA-CBA-CGA
14	A	806	CLA	C2A-CAA-CBA-CGA
14	A	837	CLA	C2A-CAA-CBA-CGA
14	A	838	CLA	C2A-CAA-CBA-CGA
14	B	806	CLA	C2A-CAA-CBA-CGA
14	a	805	CLA	C2A-CAA-CBA-CGA
14	a	807	CLA	C2A-CAA-CBA-CGA
14	a	838	CLA	C2A-CAA-CBA-CGA
14	a	839	CLA	C2A-CAA-CBA-CGA
14	1	804	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	1	805	CLA	C2A-CAA-CBA-CGA
14	1	836	CLA	C2A-CAA-CBA-CGA
14	1	837	CLA	C2A-CAA-CBA-CGA
14	1	842	CLA	C2A-CAA-CBA-CGA
14	b	806	CLA	C2A-CAA-CBA-CGA
14	2	805	CLA	C2A-CAA-CBA-CGA
12	B	853	LHG	O1-C1-C2-C3
12	b	852	LHG	O1-C1-C2-C3
12	2	852	LHG	O1-C1-C2-C3
14	A	810	CLA	C16-C17-C18-C19
14	A	821	CLA	C16-C17-C18-C20
14	A	843	CLA	C16-C17-C18-C20
14	B	802	CLA	C16-C17-C18-C20
14	B	829	CLA	C16-C17-C18-C19
14	B	834	CLA	C6-C7-C8-C10
14	a	811	CLA	C16-C17-C18-C19
14	a	822	CLA	C16-C17-C18-C20
14	a	843	CLA	C16-C17-C18-C20
14	1	809	CLA	C16-C17-C18-C19
14	1	820	CLA	C16-C17-C18-C20
14	1	843	CLA	C16-C17-C18-C20
14	b	801	CLA	C16-C17-C18-C20
14	b	828	CLA	C16-C17-C18-C19
14	b	833	CLA	C6-C7-C8-C10
14	2	828	CLA	C16-C17-C18-C19
14	2	833	CLA	C6-C7-C8-C10
14	0	202	CLA	C16-C17-C18-C20
15	A	845	PQN	C26-C27-C28-C30
15	a	845	PQN	C26-C27-C28-C30
15	1	845	PQN	C26-C27-C28-C30
14	A	815	CLA	C3-C5-C6-C7
14	A	829	CLA	C3-C5-C6-C7
14	a	816	CLA	C3-C5-C6-C7
14	a	830	CLA	C3-C5-C6-C7
14	1	814	CLA	C3-C5-C6-C7
14	1	828	CLA	C3-C5-C6-C7
17	A	850	BCR	C12-C13-C14-C15
17	B	850	BCR	C11-C10-C9-C8
17	B	854	BCR	C20-C21-C22-C23
17	F	203	BCR	C11-C10-C9-C8
17	F	203	BCR	C12-C13-C14-C15
17	I	101	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	I	102	BCR	C16-C17-C18-C19
17	I	102	BCR	C20-C21-C22-C23
17	J	103	BCR	C12-C13-C14-C15
17	J	104	BCR	C20-C21-C22-C23
17	L	1505	BCR	C11-C10-C9-C8
17	M	102	BCR	C11-C10-C9-C8
17	M	102	BCR	C16-C17-C18-C19
17	M	102	BCR	C20-C21-C22-C23
17	a	850	BCR	C12-C13-C14-C15
17	1	850	BCR	C12-C13-C14-C15
17	b	849	BCR	C11-C10-C9-C8
17	b	853	BCR	C20-C21-C22-C23
17	b	854	BCR	C11-C10-C9-C8
17	b	854	BCR	C16-C17-C18-C19
17	b	854	BCR	C20-C21-C22-C23
17	2	849	BCR	C11-C10-C9-C8
17	f	203	BCR	C11-C10-C9-C8
17	f	203	BCR	C12-C13-C14-C15
17	6	4402	BCR	C11-C10-C9-C8
17	6	4402	BCR	C12-C13-C14-C15
17	6	4406	BCR	C20-C21-C22-C23
17	i	4102	BCR	C12-C13-C14-C15
17	i	4103	BCR	C16-C17-C18-C19
17	i	4103	BCR	C20-C21-C22-C23
17	h	101	BCR	C12-C13-C14-C15
17	h	102	BCR	C16-C17-C18-C19
17	h	102	BCR	C20-C21-C22-C23
17	j	103	BCR	C12-C13-C14-C15
17	j	104	BCR	C20-C21-C22-C23
17	7	1104	BCR	C12-C13-C14-C15
17	7	1105	BCR	C20-C21-C22-C23
17	0	204	BCR	C11-C10-C9-C8
17	0	210	BCR	C11-C10-C9-C8
17	9	102	BCR	C11-C10-C9-C8
17	9	102	BCR	C16-C17-C18-C19
17	9	102	BCR	C20-C21-C22-C23
18	l	4202	LMG	C4-C5-C6-O5
18	0	201	LMG	C4-C5-C6-O5
14	B	816	CLA	C15-C16-C17-C18
14	b	815	CLA	C15-C16-C17-C18
14	2	815	CLA	C15-C16-C17-C18
14	B	818	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	L	1506	LMG	C4-C5-C6-O5
14	a	811	CLA	O1D-CGD-O2D-CED
14	1	809	CLA	O1D-CGD-O2D-CED
14	b	817	CLA	O1D-CGD-O2D-CED
14	2	817	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	C10-C11-C12-C13
14	A	831	CLA	C15-C16-C17-C18
14	B	805	CLA	C13-C15-C16-C17
14	L	1502	CLA	C10-C11-C12-C13
14	a	811	CLA	C10-C11-C12-C13
14	a	832	CLA	C15-C16-C17-C18
14	1	809	CLA	C10-C11-C12-C13
14	1	830	CLA	C15-C16-C17-C18
14	2	804	CLA	C13-C15-C16-C17
14	l	4205	CLA	C10-C11-C12-C13
14	0	207	CLA	C10-C11-C12-C13
15	B	846	PQN	C15-C16-C17-C18
15	b	845	PQN	C15-C16-C17-C18
15	2	845	PQN	C15-C16-C17-C18
14	K	4004	CLA	C3-C5-C6-C7
14	a	854	CLA	C3-C5-C6-C7
14	8	4004	CLA	C3-C5-C6-C7
14	A	810	CLA	O1D-CGD-O2D-CED
14	A	814	CLA	C2-C1-O2A-CGA
14	a	815	CLA	C2-C1-O2A-CGA
14	1	813	CLA	C2-C1-O2A-CGA
14	A	810	CLA	C16-C17-C18-C20
14	B	802	CLA	C16-C17-C18-C19
14	a	811	CLA	C16-C17-C18-C20
14	1	809	CLA	C16-C17-C18-C20
14	b	801	CLA	C16-C17-C18-C19
14	0	202	CLA	C16-C17-C18-C19
15	A	845	PQN	C26-C27-C28-C29
15	a	845	PQN	C26-C27-C28-C29
15	1	845	PQN	C26-C27-C28-C29
14	A	810	CLA	C8-C10-C11-C12
14	a	811	CLA	C8-C10-C11-C12
14	1	809	CLA	C8-C10-C11-C12
14	b	805	CLA	C13-C15-C16-C17
12	9	101	LHG	C28-C29-C30-C31
14	B	842	CLA	CBA-CGA-O2A-C1
14	b	841	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	2	841	CLA	CBA-CGA-O2A-C1
17	B	854	BCR	C14-C15-C16-C17
17	I	101	BCR	C14-C15-C16-C17
17	b	853	BCR	C14-C15-C16-C17
17	6	4406	BCR	C14-C15-C16-C17
17	h	101	BCR	C14-C15-C16-C17
12	M	101	LHG	C28-C29-C30-C31
12	m	101	LHG	C28-C29-C30-C31
18	B	803	LMG	C14-C15-C16-C17
18	b	803	LMG	C14-C15-C16-C17
14	B	811	CLA	C5-C6-C7-C8
14	2	810	CLA	C5-C6-C7-C8
12	B	853	LHG	C30-C31-C32-C33
12	2	852	LHG	C30-C31-C32-C33
18	2	802	LMG	C14-C15-C16-C17
12	b	852	LHG	C30-C31-C32-C33
18	L	1506	LMG	C11-C12-C13-C14
18	l	4202	LMG	C11-C12-C13-C14
18	0	201	LMG	C11-C12-C13-C14
14	L	1503	CLA	C3-C5-C6-C7
14	B	809	CLA	O1D-CGD-O2D-CED
14	b	809	CLA	O1D-CGD-O2D-CED
14	2	808	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	C13-C15-C16-C17
14	a	808	CLA	C13-C15-C16-C17
14	1	806	CLA	C13-C15-C16-C17
14	A	814	CLA	C4B-C3B-CAB-CBB
14	A	820	CLA	C4B-C3B-CAB-CBB
14	A	835	CLA	C4B-C3B-CAB-CBB
14	A	837	CLA	C4B-C3B-CAB-CBB
14	A	840	CLA	C4B-C3B-CAB-CBB
14	A	841	CLA	C4B-C3B-CAB-CBB
14	A	844	CLA	C4B-C3B-CAB-CBB
14	B	804	CLA	C4B-C3B-CAB-CBB
14	B	810	CLA	C4B-C3B-CAB-CBB
14	B	813	CLA	C4B-C3B-CAB-CBB
14	B	820	CLA	C4B-C3B-CAB-CBB
14	B	829	CLA	C4B-C3B-CAB-CBB
14	B	834	CLA	C4B-C3B-CAB-CBB
14	B	841	CLA	C4B-C3B-CAB-CBB
14	a	815	CLA	C4B-C3B-CAB-CBB
14	a	821	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	a	836	CLA	C4B-C3B-CAB-CBB
14	a	838	CLA	C4B-C3B-CAB-CBB
14	a	841	CLA	C4B-C3B-CAB-CBB
14	a	844	CLA	C4B-C3B-CAB-CBB
14	1	813	CLA	C4B-C3B-CAB-CBB
14	1	819	CLA	C4B-C3B-CAB-CBB
14	1	834	CLA	C4B-C3B-CAB-CBB
14	1	836	CLA	C4B-C3B-CAB-CBB
14	1	839	CLA	C4B-C3B-CAB-CBB
14	1	840	CLA	C4B-C3B-CAB-CBB
14	1	844	CLA	C4B-C3B-CAB-CBB
14	b	802	CLA	C4B-C3B-CAB-CBB
14	b	804	CLA	C4B-C3B-CAB-CBB
14	b	810	CLA	C4B-C3B-CAB-CBB
14	b	819	CLA	C4B-C3B-CAB-CBB
14	b	828	CLA	C4B-C3B-CAB-CBB
14	b	833	CLA	C4B-C3B-CAB-CBB
14	b	840	CLA	C4B-C3B-CAB-CBB
14	2	803	CLA	C4B-C3B-CAB-CBB
14	2	809	CLA	C4B-C3B-CAB-CBB
14	2	812	CLA	C4B-C3B-CAB-CBB
14	2	819	CLA	C4B-C3B-CAB-CBB
14	2	828	CLA	C4B-C3B-CAB-CBB
14	2	833	CLA	C4B-C3B-CAB-CBB
14	2	840	CLA	C4B-C3B-CAB-CBB
14	l	4203	CLA	C4B-C3B-CAB-CBB
18	B	803	LMG	C28-C29-C30-C31
18	b	803	LMG	C28-C29-C30-C31
18	2	802	LMG	C28-C29-C30-C31
14	A	809	CLA	CBA-CGA-O2A-C1
14	a	810	CLA	CBA-CGA-O2A-C1
14	1	808	CLA	CBA-CGA-O2A-C1
14	A	843	CLA	C16-C17-C18-C19
14	B	829	CLA	C16-C17-C18-C20
14	B	834	CLA	C6-C7-C8-C9
14	L	1502	CLA	C16-C17-C18-C19
14	a	843	CLA	C16-C17-C18-C19
14	1	843	CLA	C16-C17-C18-C19
14	b	828	CLA	C16-C17-C18-C20
14	b	833	CLA	C6-C7-C8-C9
14	2	828	CLA	C16-C17-C18-C20
14	2	833	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	l	4205	CLA	C16-C17-C18-C19
14	0	207	CLA	C16-C17-C18-C19
14	A	838	CLA	O1D-CGD-O2D-CED
14	1	837	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	C2A-CAA-CBA-CGA
14	A	823	CLA	C2A-CAA-CBA-CGA
14	A	842	CLA	C2A-CAA-CBA-CGA
14	B	801	CLA	C2A-CAA-CBA-CGA
14	B	825	CLA	C2A-CAA-CBA-CGA
14	a	804	CLA	C2A-CAA-CBA-CGA
14	a	821	CLA	C2A-CAA-CBA-CGA
14	a	824	CLA	C2A-CAA-CBA-CGA
14	a	842	CLA	C2A-CAA-CBA-CGA
14	1	819	CLA	C2A-CAA-CBA-CGA
14	1	822	CLA	C2A-CAA-CBA-CGA
14	b	824	CLA	C2A-CAA-CBA-CGA
14	2	801	CLA	C2A-CAA-CBA-CGA
14	2	824	CLA	C2A-CAA-CBA-CGA
14	A	842	CLA	C10-C11-C12-C13
14	a	842	CLA	C10-C11-C12-C13
14	1	842	CLA	C10-C11-C12-C13
14	b	811	CLA	C5-C6-C7-C8
14	a	839	CLA	O1D-CGD-O2D-CED
14	A	831	CLA	C11-C12-C13-C15
14	a	832	CLA	C11-C12-C13-C15
14	1	830	CLA	C11-C12-C13-C15
14	L	1502	CLA	C2C-C3C-CAC-CBC
14	l	4205	CLA	C2C-C3C-CAC-CBC
14	0	207	CLA	C2C-C3C-CAC-CBC
14	B	808	CLA	C15-C16-C17-C18
14	b	808	CLA	C15-C16-C17-C18
14	2	807	CLA	C15-C16-C17-C18
18	A	852	LMG	C18-C19-C20-C21
18	0	203	LMG	C18-C19-C20-C21
14	l	4206	CLA	C3-C5-C6-C7
14	0	208	CLA	C3-C5-C6-C7
14	A	805	CLA	C3A-C2A-CAA-CBA
14	A	808	CLA	C3A-C2A-CAA-CBA
14	A	815	CLA	C3A-C2A-CAA-CBA
14	A	838	CLA	C3A-C2A-CAA-CBA
14	B	802	CLA	C3A-C2A-CAA-CBA
14	B	824	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	B	825	CLA	C3A-C2A-CAA-CBA
14	F	201	CLA	C3A-C2A-CAA-CBA
14	F	204	CLA	C3A-C2A-CAA-CBA
14	a	806	CLA	C3A-C2A-CAA-CBA
14	a	809	CLA	C3A-C2A-CAA-CBA
14	a	816	CLA	C3A-C2A-CAA-CBA
14	a	839	CLA	C3A-C2A-CAA-CBA
14	1	807	CLA	C3A-C2A-CAA-CBA
14	1	814	CLA	C3A-C2A-CAA-CBA
14	1	837	CLA	C3A-C2A-CAA-CBA
14	1	841	CLA	C3A-C2A-CAA-CBA
14	b	801	CLA	C3A-C2A-CAA-CBA
14	b	823	CLA	C3A-C2A-CAA-CBA
14	b	824	CLA	C3A-C2A-CAA-CBA
14	2	823	CLA	C3A-C2A-CAA-CBA
14	2	824	CLA	C3A-C2A-CAA-CBA
14	f	201	CLA	C3A-C2A-CAA-CBA
14	f	204	CLA	C3A-C2A-CAA-CBA
14	6	4403	CLA	C3A-C2A-CAA-CBA
14	7	1101	CLA	C3A-C2A-CAA-CBA
14	0	202	CLA	C3A-C2A-CAA-CBA
18	a	852	LMG	C18-C19-C20-C21
14	a	829	CLA	C5-C6-C7-C8
14	A	843	CLA	O1D-CGD-O2D-CED
14	a	843	CLA	O1D-CGD-O2D-CED
14	1	843	CLA	O1D-CGD-O2D-CED
17	B	848	BCR	C19-C20-C21-C22
17	b	847	BCR	C19-C20-C21-C22
17	2	847	BCR	C19-C20-C21-C22
14	A	807	CLA	C16-C17-C18-C19
14	B	805	CLA	C16-C17-C18-C19
14	L	1502	CLA	C16-C17-C18-C20
14	a	808	CLA	C16-C17-C18-C19
14	1	806	CLA	C16-C17-C18-C19
14	b	805	CLA	C16-C17-C18-C19
14	2	804	CLA	C16-C17-C18-C19
14	l	4205	CLA	C16-C17-C18-C20
14	0	207	CLA	C16-C17-C18-C20
12	b	852	LHG	C27-C28-C29-C30
12	B	853	LHG	C27-C28-C29-C30
12	2	852	LHG	C27-C28-C29-C30
14	A	829	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	830	CLA	CBA-CGA-O2A-C1
14	1	828	CLA	CBA-CGA-O2A-C1
12	B	853	LHG	C4-C5-C6-O8
12	b	852	LHG	C4-C5-C6-O8
12	2	852	LHG	C4-C5-C6-O8
18	L	1506	LMG	C7-C8-C9-O8
18	l	4202	LMG	C7-C8-C9-O8
18	0	201	LMG	C7-C8-C9-O8
14	A	828	CLA	C5-C6-C7-C8
14	1	827	CLA	C5-C6-C7-C8
18	A	852	LMG	C16-C17-C18-C19
18	a	852	LMG	C16-C17-C18-C19
18	0	203	LMG	C16-C17-C18-C19
14	B	843	CLA	C2C-C3C-CAC-CBC
14	b	842	CLA	C2C-C3C-CAC-CBC
14	B	831	CLA	O1D-CGD-O2D-CED
14	b	830	CLA	O1D-CGD-O2D-CED
14	2	830	CLA	O1D-CGD-O2D-CED
14	2	842	CLA	C2C-C3C-CAC-CBC
14	A	804	CLA	C2B-C3B-CAB-CBB
14	A	805	CLA	C2B-C3B-CAB-CBB
14	A	807	CLA	C2B-C3B-CAB-CBB
14	B	809	CLA	C2B-C3B-CAB-CBB
14	a	805	CLA	C2B-C3B-CAB-CBB
14	a	806	CLA	C2B-C3B-CAB-CBB
14	a	808	CLA	C2B-C3B-CAB-CBB
14	1	804	CLA	C2B-C3B-CAB-CBB
14	1	806	CLA	C2B-C3B-CAB-CBB
14	b	809	CLA	C2B-C3B-CAB-CBB
14	2	808	CLA	C2B-C3B-CAB-CBB
14	7	1101	CLA	C2B-C3B-CAB-CBB
17	A	851	BCR	C23-C24-C25-C26
17	A	851	BCR	C23-C24-C25-C30
17	B	854	BCR	C1-C6-C7-C8
17	B	854	BCR	C5-C6-C7-C8
17	I	101	BCR	C1-C6-C7-C8
17	I	102	BCR	C1-C6-C7-C8
17	M	102	BCR	C1-C6-C7-C8
17	M	102	BCR	C5-C6-C7-C8
17	a	851	BCR	C23-C24-C25-C26
17	a	851	BCR	C23-C24-C25-C30
17	1	851	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
17	1	851	BCR	C23-C24-C25-C30
17	b	853	BCR	C1-C6-C7-C8
17	b	853	BCR	C5-C6-C7-C8
17	b	854	BCR	C1-C6-C7-C8
17	b	854	BCR	C5-C6-C7-C8
17	6	4406	BCR	C1-C6-C7-C8
17	6	4406	BCR	C5-C6-C7-C8
17	i	4102	BCR	C1-C6-C7-C8
17	i	4103	BCR	C1-C6-C7-C8
17	h	101	BCR	C1-C6-C7-C8
17	h	102	BCR	C1-C6-C7-C8
17	0	204	BCR	C1-C6-C7-C8
17	9	102	BCR	C1-C6-C7-C8
17	9	102	BCR	C5-C6-C7-C8
18	B	803	LMG	C11-C10-O7-C8
18	b	803	LMG	C11-C10-O7-C8
18	2	802	LMG	C11-C10-O7-C8
14	A	823	CLA	C3-C5-C6-C7
14	B	804	CLA	C3-C5-C6-C7
14	a	824	CLA	C3-C5-C6-C7
14	1	822	CLA	C3-C5-C6-C7
14	b	804	CLA	C3-C5-C6-C7
14	2	803	CLA	C3-C5-C6-C7
18	A	852	LMG	C31-C32-C33-C34
18	a	852	LMG	C31-C32-C33-C34
18	0	203	LMG	C31-C32-C33-C34
12	A	801	LHG	C12-C13-C14-C15
12	a	801	LHG	C12-C13-C14-C15
12	1	801	LHG	C12-C13-C14-C15
14	A	839	CLA	C2A-CAA-CBA-CGA
14	B	831	CLA	C2A-CAA-CBA-CGA
14	a	840	CLA	C2A-CAA-CBA-CGA
14	1	838	CLA	C2A-CAA-CBA-CGA
14	b	830	CLA	C2A-CAA-CBA-CGA
14	2	830	CLA	C2A-CAA-CBA-CGA
14	B	829	CLA	C15-C16-C17-C18
14	b	828	CLA	C15-C16-C17-C18
14	2	828	CLA	C15-C16-C17-C18
14	B	806	CLA	C2C-C3C-CAC-CBC
14	b	806	CLA	C2C-C3C-CAC-CBC
14	2	805	CLA	C2C-C3C-CAC-CBC
17	A	847	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	B	852	BCR	C10-C11-C12-C13
17	F	206	BCR	C18-C19-C20-C21
17	K	4001	BCR	C10-C11-C12-C13
17	a	847	BCR	C10-C11-C12-C13
17	1	847	BCR	C10-C11-C12-C13
17	b	851	BCR	C10-C11-C12-C13
17	2	851	BCR	C10-C11-C12-C13
17	f	206	BCR	C18-C19-C20-C21
17	6	4405	BCR	C18-C19-C20-C21
17	k	4001	BCR	C10-C11-C12-C13
17	8	4001	BCR	C10-C11-C12-C13
18	A	852	LMG	C33-C34-C35-C36
18	a	852	LMG	C33-C34-C35-C36
18	0	203	LMG	C33-C34-C35-C36
14	A	843	CLA	CBA-CGA-O2A-C1
14	a	843	CLA	CBA-CGA-O2A-C1
14	1	843	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	C6-C7-C8-C9
14	A	843	CLA	C6-C7-C8-C9
14	a	806	CLA	C6-C7-C8-C9
14	a	843	CLA	C6-C7-C8-C9
14	1	843	CLA	C6-C7-C8-C9
14	7	1101	CLA	C6-C7-C8-C9
17	B	854	BCR	C6-C7-C8-C9
17	b	853	BCR	C6-C7-C8-C9
17	6	4406	BCR	C6-C7-C8-C9
12	9	101	LHG	C27-C28-C29-C30
12	M	101	LHG	C27-C28-C29-C30
12	m	101	LHG	C27-C28-C29-C30
12	B	853	LHG	C25-C26-C27-C28
12	b	852	LHG	C25-C26-C27-C28
18	B	803	LMG	C15-C16-C17-C18
18	b	803	LMG	C15-C16-C17-C18
18	2	802	LMG	C15-C16-C17-C18
17	K	4005	BCR	C15-C16-C17-C18
17	k	4004	BCR	C15-C16-C17-C18
17	8	4005	BCR	C15-C16-C17-C18
12	2	852	LHG	C25-C26-C27-C28
14	B	805	CLA	C5-C6-C7-C8
14	b	805	CLA	C5-C6-C7-C8
14	2	804	CLA	C5-C6-C7-C8
14	K	4003	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	8	4003	CLA	C4C-C3C-CAC-CBC
14	A	813	CLA	C3-C5-C6-C7
14	a	814	CLA	C3-C5-C6-C7
14	1	812	CLA	C3-C5-C6-C7
14	k	4003	CLA	C4C-C3C-CAC-CBC
17	M	102	BCR	C7-C8-C9-C10
17	b	854	BCR	C7-C8-C9-C10
17	9	102	BCR	C7-C8-C9-C10
14	B	809	CLA	C2A-CAA-CBA-CGA
14	B	834	CLA	C2A-CAA-CBA-CGA
14	b	809	CLA	C2A-CAA-CBA-CGA
14	b	833	CLA	C2A-CAA-CBA-CGA
14	2	833	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C16-C17-C18-C20
14	A	829	CLA	C16-C17-C18-C19
14	A	832	CLA	C16-C17-C18-C20
14	a	808	CLA	C16-C17-C18-C20
14	a	830	CLA	C16-C17-C18-C19
14	a	833	CLA	C16-C17-C18-C20
14	1	806	CLA	C16-C17-C18-C20
14	1	828	CLA	C16-C17-C18-C19
14	1	831	CLA	C16-C17-C18-C20
14	A	827	CLA	C4-C3-C5-C6
14	a	828	CLA	C4-C3-C5-C6
14	1	826	CLA	C4-C3-C5-C6
14	A	827	CLA	C2-C3-C5-C6
14	a	828	CLA	C2-C3-C5-C6
14	1	826	CLA	C2-C3-C5-C6
18	B	803	LMG	C12-C13-C14-C15
18	b	803	LMG	C12-C13-C14-C15
14	b	815	CLA	C5-C6-C7-C8
18	2	802	LMG	C12-C13-C14-C15
12	a	801	LHG	C24-C25-C26-C27
14	A	829	CLA	O1A-CGA-O2A-C1
14	a	830	CLA	O1A-CGA-O2A-C1
14	1	828	CLA	O1A-CGA-O2A-C1
14	A	808	CLA	C5-C6-C7-C8
14	A	841	CLA	C13-C15-C16-C17
14	B	805	CLA	C10-C11-C12-C13
14	B	816	CLA	C5-C6-C7-C8
14	1	807	CLA	C5-C6-C7-C8
14	1	840	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	b	802	CLA	C13-C15-C16-C17
14	2	804	CLA	C10-C11-C12-C13
14	2	815	CLA	C5-C6-C7-C8
12	A	801	LHG	C24-C25-C26-C27
12	1	801	LHG	C24-C25-C26-C27
14	B	834	CLA	O1D-CGD-O2D-CED
14	b	833	CLA	O1D-CGD-O2D-CED
14	2	833	CLA	O1D-CGD-O2D-CED
12	M	101	LHG	C23-C24-C25-C26
12	m	101	LHG	C23-C24-C25-C26
12	9	101	LHG	C23-C24-C25-C26
18	A	853	LMG	C11-C10-O7-C8
18	a	853	LMG	C11-C10-O7-C8
18	1	852	LMG	C11-C10-O7-C8
14	A	830	CLA	C15-C16-C17-C18
14	B	804	CLA	C5-C6-C7-C8
14	B	843	CLA	C10-C11-C12-C13
14	a	809	CLA	C5-C6-C7-C8
14	a	831	CLA	C15-C16-C17-C18
14	b	804	CLA	C5-C6-C7-C8
14	b	805	CLA	C10-C11-C12-C13
14	b	842	CLA	C10-C11-C12-C13
14	2	803	CLA	C5-C6-C7-C8
14	2	842	CLA	C10-C11-C12-C13
14	A	829	CLA	C16-C17-C18-C20
14	a	830	CLA	C16-C17-C18-C20
14	1	828	CLA	C16-C17-C18-C20
12	A	801	LHG	C14-C15-C16-C17
12	a	801	LHG	C14-C15-C16-C17
12	1	801	LHG	C14-C15-C16-C17
19	I	103	LMT	C5'-C4'-O1B-C1B
19	i	4101	LMT	C5'-C4'-O1B-C1B
19	h	103	LMT	C5'-C4'-O1B-C1B
12	M	101	LHG	C25-C26-C27-C28
12	m	101	LHG	C25-C26-C27-C28
12	9	101	LHG	C25-C26-C27-C28
14	f	201	CLA	C2C-C3C-CAC-CBC
14	a	843	CLA	C5-C6-C7-C8
14	1	829	CLA	C15-C16-C17-C18
14	1	843	CLA	C5-C6-C7-C8
14	B	808	CLA	C3-C5-C6-C7
14	b	808	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	2	807	CLA	C3-C5-C6-C7
18	B	803	LMG	O7-C8-C9-O8
18	b	803	LMG	O7-C8-C9-O8
18	2	802	LMG	O7-C8-C9-O8
12	A	801	LHG	C29-C30-C31-C32
12	A	801	LHG	C11-C12-C13-C14
12	a	801	LHG	C11-C12-C13-C14
12	a	801	LHG	C29-C30-C31-C32
12	1	801	LHG	C11-C12-C13-C14
12	1	801	LHG	C29-C30-C31-C32
18	A	852	LMG	C19-C20-C21-C22
18	a	852	LMG	C19-C20-C21-C22
14	A	843	CLA	C5-C6-C7-C8
18	b	803	LMG	O6-C5-C6-O5
18	2	802	LMG	O6-C5-C6-O5
18	0	203	LMG	C19-C20-C21-C22
14	F	201	CLA	C2C-C3C-CAC-CBC
14	1	841	CLA	C2C-C3C-CAC-CBC
12	B	853	LHG	C24-C25-C26-C27
12	M	101	LHG	C11-C10-C9-C8
12	b	852	LHG	C24-C25-C26-C27
12	2	852	LHG	C24-C25-C26-C27
12	m	101	LHG	C11-C10-C9-C8
12	9	101	LHG	C11-C10-C9-C8
14	B	835	CLA	C2-C1-O2A-CGA
14	b	834	CLA	C2-C1-O2A-CGA
14	2	834	CLA	C2-C1-O2A-CGA
18	B	803	LMG	O6-C5-C6-O5
18	0	201	LMG	C34-C35-C36-C37
14	b	815	CLA	C4-C3-C5-C6
14	2	815	CLA	C4-C3-C5-C6
12	M	101	LHG	C1-C2-C3-O3
12	m	101	LHG	C1-C2-C3-O3
12	9	101	LHG	C1-C2-C3-O3
12	A	801	LHG	C34-C35-C36-C37
12	a	801	LHG	C34-C35-C36-C37
12	1	801	LHG	C34-C35-C36-C37
18	L	1506	LMG	C34-C35-C36-C37
18	l	4202	LMG	C34-C35-C36-C37
14	2	808	CLA	C2A-CAA-CBA-CGA
14	b	809	CLA	C15-C16-C17-C18
14	2	808	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	B	809	CLA	C15-C16-C17-C18
12	A	802	LHG	O1-C1-C2-O2
12	a	802	LHG	O1-C1-C2-O2
12	1	802	LHG	O1-C1-C2-O2
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	C1A-C2A-CAA-CBA
14	A	821	CLA	C1A-C2A-CAA-CBA
14	A	823	CLA	C1A-C2A-CAA-CBA
14	A	832	CLA	C1A-C2A-CAA-CBA
14	A	833	CLA	C1A-C2A-CAA-CBA
14	A	838	CLA	C1A-C2A-CAA-CBA
14	A	842	CLA	C1A-C2A-CAA-CBA
14	B	807	CLA	C1A-C2A-CAA-CBA
14	B	812	CLA	C1A-C2A-CAA-CBA
14	B	814	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	C1A-C2A-CAA-CBA
14	B	821	CLA	C1A-C2A-CAA-CBA
14	B	826	CLA	C1A-C2A-CAA-CBA
14	B	833	CLA	C1A-C2A-CAA-CBA
14	B	834	CLA	C1A-C2A-CAA-CBA
14	B	837	CLA	C1A-C2A-CAA-CBA
14	B	839	CLA	C1A-C2A-CAA-CBA
14	F	204	CLA	C1A-C2A-CAA-CBA
14	a	810	CLA	C1A-C2A-CAA-CBA
14	a	812	CLA	C1A-C2A-CAA-CBA
14	a	822	CLA	C1A-C2A-CAA-CBA
14	a	824	CLA	C1A-C2A-CAA-CBA
14	a	833	CLA	C1A-C2A-CAA-CBA
14	a	834	CLA	C1A-C2A-CAA-CBA
14	a	839	CLA	C1A-C2A-CAA-CBA
14	a	842	CLA	C1A-C2A-CAA-CBA
14	1	808	CLA	C1A-C2A-CAA-CBA
14	1	810	CLA	C1A-C2A-CAA-CBA
14	1	820	CLA	C1A-C2A-CAA-CBA
14	1	822	CLA	C1A-C2A-CAA-CBA
14	1	831	CLA	C1A-C2A-CAA-CBA
14	1	832	CLA	C1A-C2A-CAA-CBA
14	1	837	CLA	C1A-C2A-CAA-CBA
14	1	842	CLA	C1A-C2A-CAA-CBA
14	b	807	CLA	C1A-C2A-CAA-CBA
14	b	812	CLA	C1A-C2A-CAA-CBA
14	b	813	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	815	CLA	C1A-C2A-CAA-CBA
14	b	820	CLA	C1A-C2A-CAA-CBA
14	b	825	CLA	C1A-C2A-CAA-CBA
14	b	832	CLA	C1A-C2A-CAA-CBA
14	b	833	CLA	C1A-C2A-CAA-CBA
14	b	836	CLA	C1A-C2A-CAA-CBA
14	b	838	CLA	C1A-C2A-CAA-CBA
14	2	806	CLA	C1A-C2A-CAA-CBA
14	2	811	CLA	C1A-C2A-CAA-CBA
14	2	813	CLA	C1A-C2A-CAA-CBA
14	2	815	CLA	C1A-C2A-CAA-CBA
14	2	820	CLA	C1A-C2A-CAA-CBA
14	2	825	CLA	C1A-C2A-CAA-CBA
14	2	832	CLA	C1A-C2A-CAA-CBA
14	2	833	CLA	C1A-C2A-CAA-CBA
14	2	836	CLA	C1A-C2A-CAA-CBA
14	2	838	CLA	C1A-C2A-CAA-CBA
14	f	204	CLA	C1A-C2A-CAA-CBA
14	6	4403	CLA	C1A-C2A-CAA-CBA
12	M	101	LHG	C24-C25-C26-C27
12	m	101	LHG	C24-C25-C26-C27
12	9	101	LHG	C24-C25-C26-C27
14	A	843	CLA	O1A-CGA-O2A-C1
18	B	803	LMG	C34-C35-C36-C37
18	b	803	LMG	C34-C35-C36-C37
18	2	802	LMG	C34-C35-C36-C37
12	A	802	LHG	O6-C4-C5-C6
12	a	802	LHG	O6-C4-C5-C6
12	1	802	LHG	O6-C4-C5-C6
14	B	821	CLA	C3-C5-C6-C7
14	b	820	CLA	C3-C5-C6-C7
14	2	820	CLA	C3-C5-C6-C7
13	A	803	CL0	C11-C10-C8-C7
13	a	803	CL0	C11-C10-C8-C7
13	1	803	CL0	C11-C10-C8-C7
14	A	821	CLA	C6-C7-C8-C10
14	A	842	CLA	C6-C7-C8-C10
14	B	802	CLA	C6-C7-C8-C10
14	B	804	CLA	C11-C10-C8-C7
14	B	806	CLA	C6-C7-C8-C10
14	B	806	CLA	C11-C10-C8-C7
14	B	809	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	B	810	CLA	C6-C7-C8-C10
14	B	821	CLA	C11-C10-C8-C7
14	B	830	CLA	C6-C7-C8-C10
14	B	832	CLA	C11-C10-C8-C7
14	B	844	CLA	C11-C10-C8-C7
14	L	1501	CLA	C6-C7-C8-C10
14	a	822	CLA	C6-C7-C8-C10
14	a	842	CLA	C6-C7-C8-C10
14	1	820	CLA	C6-C7-C8-C10
14	1	842	CLA	C6-C7-C8-C10
14	b	801	CLA	C6-C7-C8-C10
14	b	804	CLA	C11-C10-C8-C7
14	b	806	CLA	C6-C7-C8-C10
14	b	806	CLA	C11-C10-C8-C7
14	b	809	CLA	C6-C7-C8-C10
14	b	810	CLA	C6-C7-C8-C10
14	b	820	CLA	C11-C10-C8-C7
14	b	829	CLA	C6-C7-C8-C10
14	b	831	CLA	C11-C10-C8-C7
14	b	843	CLA	C11-C10-C8-C7
14	2	803	CLA	C11-C10-C8-C7
14	2	805	CLA	C6-C7-C8-C10
14	2	805	CLA	C11-C10-C8-C7
14	2	808	CLA	C6-C7-C8-C10
14	2	809	CLA	C6-C7-C8-C10
14	2	820	CLA	C11-C10-C8-C7
14	2	829	CLA	C6-C7-C8-C10
14	2	831	CLA	C11-C10-C8-C7
14	2	843	CLA	C11-C10-C8-C7
14	l	4204	CLA	C6-C7-C8-C10
14	0	202	CLA	C6-C7-C8-C10
14	0	206	CLA	C6-C7-C8-C10
15	B	846	PQN	C16-C17-C18-C20
15	b	845	PQN	C16-C17-C18-C20
15	2	845	PQN	C16-C17-C18-C20
14	a	843	CLA	O1A-CGA-O2A-C1
14	1	843	CLA	O1A-CGA-O2A-C1
14	B	816	CLA	C4-C3-C5-C6
14	A	814	CLA	C2-C3-C5-C6
14	B	816	CLA	C2-C3-C5-C6
14	a	815	CLA	C2-C3-C5-C6
14	1	813	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	b	815	CLA	C2-C3-C5-C6
14	2	815	CLA	C2-C3-C5-C6
12	A	801	LHG	C16-C17-C18-C19
12	1	801	LHG	C16-C17-C18-C19
14	A	821	CLA	C2A-CAA-CBA-CGA
14	A	824	CLA	C2A-CAA-CBA-CGA
14	B	832	CLA	C2A-CAA-CBA-CGA
14	a	822	CLA	C2A-CAA-CBA-CGA
14	a	825	CLA	C2A-CAA-CBA-CGA
14	1	820	CLA	C2A-CAA-CBA-CGA
14	1	823	CLA	C2A-CAA-CBA-CGA
14	b	831	CLA	C2A-CAA-CBA-CGA
14	2	831	CLA	C2A-CAA-CBA-CGA
13	A	803	CL0	C11-C10-C8-C9
13	a	803	CL0	C11-C10-C8-C9
13	1	803	CL0	C11-C10-C8-C9
14	A	821	CLA	C6-C7-C8-C9
14	A	830	CLA	C6-C7-C8-C9
14	A	831	CLA	C11-C12-C13-C14
14	A	843	CLA	C11-C10-C8-C9
14	B	806	CLA	C11-C10-C8-C9
14	B	812	CLA	C11-C12-C13-C14
14	B	832	CLA	C11-C10-C8-C9
14	a	822	CLA	C6-C7-C8-C9
14	a	831	CLA	C6-C7-C8-C9
14	a	832	CLA	C11-C12-C13-C14
14	a	843	CLA	C11-C10-C8-C9
14	1	820	CLA	C6-C7-C8-C9
14	1	829	CLA	C6-C7-C8-C9
14	1	830	CLA	C11-C12-C13-C14
14	1	843	CLA	C11-C10-C8-C9
14	b	806	CLA	C11-C10-C8-C9
14	b	812	CLA	C11-C12-C13-C14
14	b	831	CLA	C11-C10-C8-C9
14	2	805	CLA	C11-C10-C8-C9
14	2	811	CLA	C11-C12-C13-C14
14	2	831	CLA	C11-C10-C8-C9
15	B	846	PQN	C16-C17-C18-C19
15	b	845	PQN	C16-C17-C18-C19
15	2	845	PQN	C16-C17-C18-C19
12	B	853	LHG	C32-C33-C34-C35
12	a	801	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	2	852	LHG	C32-C33-C34-C35
14	A	826	CLA	C10-C11-C12-C13
14	a	827	CLA	C10-C11-C12-C13
14	1	825	CLA	C10-C11-C12-C13
14	A	822	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	B	835	CLA	CBA-CGA-O2A-C1
14	a	823	CLA	CBA-CGA-O2A-C1
14	a	833	CLA	CBA-CGA-O2A-C1
14	1	821	CLA	CBA-CGA-O2A-C1
14	1	831	CLA	CBA-CGA-O2A-C1
14	b	834	CLA	CBA-CGA-O2A-C1
14	2	834	CLA	CBA-CGA-O2A-C1
12	b	852	LHG	C32-C33-C34-C35
14	L	1503	CLA	C8-C10-C11-C12
14	l	4206	CLA	C8-C10-C11-C12
14	0	208	CLA	C8-C10-C11-C12
15	A	845	PQN	C25-C26-C27-C28
15	a	845	PQN	C25-C26-C27-C28
14	A	839	CLA	O1D-CGD-O2D-CED
14	a	840	CLA	O1D-CGD-O2D-CED
14	1	838	CLA	O1D-CGD-O2D-CED
15	1	845	PQN	C25-C26-C27-C28
14	B	810	CLA	CBA-CGA-O2A-C1
14	b	810	CLA	CBA-CGA-O2A-C1
14	2	809	CLA	CBA-CGA-O2A-C1
14	B	819	CLA	C6-C7-C8-C9
14	b	818	CLA	C6-C7-C8-C9
14	2	818	CLA	C6-C7-C8-C9
18	A	852	LMG	C17-C18-C19-C20
18	a	852	LMG	C17-C18-C19-C20
18	0	203	LMG	C17-C18-C19-C20
14	B	811	CLA	C8-C10-C11-C12
14	b	811	CLA	C8-C10-C11-C12
14	2	810	CLA	C8-C10-C11-C12
17	J	103	BCR	C35-C13-C14-C15
17	M	102	BCR	C16-C17-C18-C36
17	b	854	BCR	C16-C17-C18-C36
17	9	102	BCR	C16-C17-C18-C36
14	B	806	CLA	C13-C15-C16-C17
14	b	806	CLA	C13-C15-C16-C17
14	2	805	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	a	815	CLA	C4-C3-C5-C6
13	A	803	CL0	C2-C3-C5-C6
13	a	803	CL0	C2-C3-C5-C6
13	1	803	CL0	C2-C3-C5-C6
12	M	101	LHG	C30-C31-C32-C33
12	m	101	LHG	C30-C31-C32-C33
12	9	101	LHG	C30-C31-C32-C33
17	A	850	BCR	C7-C8-C9-C10
17	F	206	BCR	C11-C12-C13-C14
17	a	850	BCR	C7-C8-C9-C10
17	1	850	BCR	C7-C8-C9-C10
17	f	206	BCR	C11-C12-C13-C14
17	6	4405	BCR	C11-C12-C13-C14
15	A	845	PQN	C20-C21-C22-C23
14	A	833	CLA	C2A-CAA-CBA-CGA
14	B	807	CLA	C2A-CAA-CBA-CGA
14	a	834	CLA	C2A-CAA-CBA-CGA
14	1	832	CLA	C2A-CAA-CBA-CGA
14	b	807	CLA	C2A-CAA-CBA-CGA
14	2	806	CLA	C2A-CAA-CBA-CGA
14	B	806	CLA	C8-C10-C11-C12
14	b	806	CLA	C8-C10-C11-C12
14	2	805	CLA	C8-C10-C11-C12
15	a	845	PQN	C20-C21-C22-C23
17	I	101	BCR	C18-C19-C20-C21
17	J	103	BCR	C10-C11-C12-C13
17	i	4102	BCR	C18-C19-C20-C21
17	h	101	BCR	C18-C19-C20-C21
17	j	103	BCR	C10-C11-C12-C13
19	I	103	LMT	C4-C5-C6-C7
19	i	4101	LMT	C4-C5-C6-C7
19	h	103	LMT	C4-C5-C6-C7
15	1	845	PQN	C20-C21-C22-C23
14	b	841	CLA	O1D-CGD-O2D-CED
17	A	848	BCR	C20-C21-C22-C23
17	B	854	BCR	C11-C10-C9-C8
17	a	848	BCR	C20-C21-C22-C23
17	1	848	BCR	C20-C21-C22-C23
17	b	853	BCR	C11-C10-C9-C8
17	6	4406	BCR	C11-C10-C9-C8
12	A	802	LHG	O6-C4-C5-O7
12	a	802	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
12	1	802	LHG	O6-C4-C5-O7
14	L	1501	CLA	C5-C6-C7-C8
14	l	4204	CLA	C5-C6-C7-C8
14	0	206	CLA	C5-C6-C7-C8
14	B	842	CLA	O1D-CGD-O2D-CED
14	2	841	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	CBA-CGA-O2A-C1
14	B	807	CLA	CBA-CGA-O2A-C1
14	B	830	CLA	CBA-CGA-O2A-C1
14	a	829	CLA	CBA-CGA-O2A-C1
14	1	827	CLA	CBA-CGA-O2A-C1
14	b	807	CLA	CBA-CGA-O2A-C1
14	b	829	CLA	CBA-CGA-O2A-C1
14	2	806	CLA	CBA-CGA-O2A-C1
14	2	829	CLA	CBA-CGA-O2A-C1
14	2	830	CLA	CBA-CGA-O2A-C1
14	A	814	CLA	C4-C3-C5-C6
14	B	813	CLA	C4-C3-C5-C6
14	1	813	CLA	C4-C3-C5-C6
14	2	812	CLA	C4-C3-C5-C6
14	l	4203	CLA	C4-C3-C5-C6
14	A	823	CLA	C2-C3-C5-C6
14	a	824	CLA	C2-C3-C5-C6
14	1	822	CLA	C2-C3-C5-C6
14	A	819	CLA	C6-C7-C8-C9
14	a	820	CLA	C6-C7-C8-C9
14	1	818	CLA	C6-C7-C8-C9
14	B	835	CLA	C10-C11-C12-C13
14	2	834	CLA	C10-C11-C12-C13
14	B	831	CLA	CBA-CGA-O2A-C1
14	b	830	CLA	CBA-CGA-O2A-C1
14	b	834	CLA	C10-C11-C12-C13
14	A	826	CLA	C11-C12-C13-C14
14	a	827	CLA	C11-C12-C13-C14
14	1	825	CLA	C11-C12-C13-C14
14	A	815	CLA	C2A-CAA-CBA-CGA
14	a	816	CLA	C2A-CAA-CBA-CGA
14	1	814	CLA	C2A-CAA-CBA-CGA
14	A	822	CLA	O1A-CGA-O2A-C1
14	B	835	CLA	O1A-CGA-O2A-C1
14	a	823	CLA	O1A-CGA-O2A-C1
14	1	821	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	810	CLA	O1A-CGA-O2A-C1
14	b	834	CLA	O1A-CGA-O2A-C1
14	2	834	CLA	O1A-CGA-O2A-C1
12	A	801	LHG	C23-C24-C25-C26
12	a	801	LHG	C23-C24-C25-C26
12	1	801	LHG	C23-C24-C25-C26
13	A	803	CL0	CBA-CGA-O2A-C1
13	a	803	CL0	CBA-CGA-O2A-C1
13	1	803	CL0	CBA-CGA-O2A-C1
14	1	814	CLA	C2C-C3C-CAC-CBC
14	A	815	CLA	C2C-C3C-CAC-CBC
14	a	816	CLA	C2C-C3C-CAC-CBC
14	A	832	CLA	O1A-CGA-O2A-C1
14	B	810	CLA	O1A-CGA-O2A-C1
14	a	833	CLA	O1A-CGA-O2A-C1
14	1	831	CLA	O1A-CGA-O2A-C1
14	2	809	CLA	O1A-CGA-O2A-C1
18	B	803	LMG	C38-C39-C40-C41
18	b	803	LMG	C38-C39-C40-C41
14	B	833	CLA	O1D-CGD-O2D-CED
14	b	832	CLA	O1D-CGD-O2D-CED
14	2	832	CLA	O1D-CGD-O2D-CED
18	2	802	LMG	C38-C39-C40-C41
14	B	843	CLA	C8-C10-C11-C12
14	b	842	CLA	C8-C10-C11-C12
14	2	842	CLA	C8-C10-C11-C12
19	f	202	LMT	C4B-C5B-C6B-O6B
13	A	803	CL0	C4-C3-C5-C6
13	a	803	CL0	C4-C3-C5-C6
13	1	803	CL0	C4-C3-C5-C6
15	B	846	PQN	C14-C13-C15-C16
15	b	845	PQN	C14-C13-C15-C16
15	2	845	PQN	C14-C13-C15-C16
14	B	819	CLA	CBA-CGA-O2A-C1
14	b	818	CLA	CBA-CGA-O2A-C1
14	2	818	CLA	CBA-CGA-O2A-C1
14	B	816	CLA	C10-C11-C12-C13
14	b	815	CLA	C10-C11-C12-C13
14	2	815	CLA	C10-C11-C12-C13
19	F	202	LMT	C4B-C5B-C6B-O6B
19	6	4401	LMT	C4B-C5B-C6B-O6B
12	B	853	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
12	b	852	LHG	O1-C1-C2-O2
12	2	852	LHG	O1-C1-C2-O2
14	B	804	CLA	C11-C10-C8-C9
14	B	805	CLA	C11-C12-C13-C14
14	B	809	CLA	C6-C7-C8-C9
14	B	810	CLA	C6-C7-C8-C9
14	B	844	CLA	C11-C10-C8-C9
14	b	804	CLA	C11-C10-C8-C9
14	b	805	CLA	C11-C12-C13-C14
14	b	809	CLA	C6-C7-C8-C9
14	b	810	CLA	C6-C7-C8-C9
14	b	843	CLA	C11-C10-C8-C9
14	2	803	CLA	C11-C10-C8-C9
14	2	804	CLA	C11-C12-C13-C14
14	2	808	CLA	C6-C7-C8-C9
14	2	809	CLA	C6-C7-C8-C9
14	2	843	CLA	C11-C10-C8-C9
19	I	103	LMT	C3'-C4'-O1B-C1B
19	i	4101	LMT	C3'-C4'-O1B-C1B
14	A	805	CLA	C4B-C3B-CAB-CBB
14	A	808	CLA	C4B-C3B-CAB-CBB
14	A	813	CLA	C4B-C3B-CAB-CBB
14	A	815	CLA	C4B-C3B-CAB-CBB
14	A	825	CLA	C4B-C3B-CAB-CBB
14	A	833	CLA	C4B-C3B-CAB-CBB
14	B	822	CLA	C4B-C3B-CAB-CBB
14	B	826	CLA	C4B-C3B-CAB-CBB
14	B	833	CLA	C4B-C3B-CAB-CBB
14	a	806	CLA	C4B-C3B-CAB-CBB
14	a	809	CLA	C4B-C3B-CAB-CBB
14	a	814	CLA	C4B-C3B-CAB-CBB
14	a	816	CLA	C4B-C3B-CAB-CBB
14	a	826	CLA	C4B-C3B-CAB-CBB
14	a	834	CLA	C4B-C3B-CAB-CBB
14	1	807	CLA	C4B-C3B-CAB-CBB
14	1	812	CLA	C4B-C3B-CAB-CBB
14	1	814	CLA	C4B-C3B-CAB-CBB
14	1	824	CLA	C4B-C3B-CAB-CBB
14	1	832	CLA	C4B-C3B-CAB-CBB
14	b	821	CLA	C4B-C3B-CAB-CBB
14	b	825	CLA	C4B-C3B-CAB-CBB
14	b	832	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	2	821	CLA	C4B-C3B-CAB-CBB
14	2	825	CLA	C4B-C3B-CAB-CBB
14	2	832	CLA	C4B-C3B-CAB-CBB
14	7	1101	CLA	C4B-C3B-CAB-CBB
19	h	103	LMT	C3'-C4'-O1B-C1B
14	B	805	CLA	C16-C17-C18-C20
14	B	811	CLA	C16-C17-C18-C20
14	b	805	CLA	C16-C17-C18-C20
14	b	811	CLA	C16-C17-C18-C20
14	2	804	CLA	C16-C17-C18-C20
14	2	810	CLA	C16-C17-C18-C20
18	L	1506	LMG	C31-C32-C33-C34
18	0	201	LMG	C31-C32-C33-C34
14	A	825	CLA	C2A-CAA-CBA-CGA
14	B	810	CLA	C2A-CAA-CBA-CGA
14	a	826	CLA	C2A-CAA-CBA-CGA
14	1	824	CLA	C2A-CAA-CBA-CGA
14	b	810	CLA	C2A-CAA-CBA-CGA
14	2	809	CLA	C2A-CAA-CBA-CGA
18	l	4202	LMG	C31-C32-C33-C34
18	A	852	LMG	C2-C1-O1-C7
18	a	852	LMG	C2-C1-O1-C7
18	0	203	LMG	C2-C1-O1-C7
14	B	821	CLA	C5-C6-C7-C8
14	b	820	CLA	C5-C6-C7-C8
14	2	820	CLA	C5-C6-C7-C8
13	A	803	CL0	CAA-CBA-CGA-O2A
13	a	803	CL0	CAA-CBA-CGA-O2A
13	1	803	CL0	CAA-CBA-CGA-O2A
13	A	803	CL0	C6-C7-C8-C10
13	A	803	CL0	C11-C12-C13-C15
13	a	803	CL0	C6-C7-C8-C10
13	a	803	CL0	C11-C12-C13-C15
13	1	803	CL0	C6-C7-C8-C10
13	1	803	CL0	C11-C12-C13-C15
14	A	827	CLA	C6-C7-C8-C10
14	A	827	CLA	C12-C13-C15-C16
14	A	830	CLA	C6-C7-C8-C10
14	A	843	CLA	C11-C10-C8-C7
14	B	805	CLA	C11-C12-C13-C15
14	B	812	CLA	C11-C12-C13-C15
14	B	835	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	a	828	CLA	C6-C7-C8-C10
14	a	828	CLA	C12-C13-C15-C16
14	a	831	CLA	C6-C7-C8-C10
14	a	843	CLA	C11-C10-C8-C7
14	1	826	CLA	C6-C7-C8-C10
14	1	826	CLA	C12-C13-C15-C16
14	1	829	CLA	C6-C7-C8-C10
14	1	843	CLA	C11-C10-C8-C7
14	b	805	CLA	C11-C12-C13-C15
14	b	809	CLA	C12-C13-C15-C16
14	b	812	CLA	C11-C12-C13-C15
14	b	834	CLA	C11-C10-C8-C7
14	2	804	CLA	C11-C12-C13-C15
14	2	808	CLA	C12-C13-C15-C16
14	2	811	CLA	C11-C12-C13-C15
14	2	834	CLA	C11-C10-C8-C7
14	A	810	CLA	C13-C15-C16-C17
14	A	822	CLA	C8-C10-C11-C12
14	A	827	CLA	C10-C11-C12-C13
14	a	811	CLA	C13-C15-C16-C17
14	a	823	CLA	C8-C10-C11-C12
14	a	828	CLA	C10-C11-C12-C13
14	1	809	CLA	C13-C15-C16-C17
14	1	821	CLA	C8-C10-C11-C12
14	1	826	CLA	C10-C11-C12-C13
14	b	810	CLA	C10-C11-C12-C13
14	A	804	CLA	C4-C3-C5-C6
14	A	826	CLA	C3A-C2A-CAA-CBA
14	A	842	CLA	C3A-C2A-CAA-CBA
14	A	843	CLA	C3A-C2A-CAA-CBA
14	B	816	CLA	C3A-C2A-CAA-CBA
14	B	836	CLA	C3A-C2A-CAA-CBA
14	B	837	CLA	C3A-C2A-CAA-CBA
14	B	843	CLA	C3A-C2A-CAA-CBA
14	a	805	CLA	C4-C3-C5-C6
14	a	827	CLA	C3A-C2A-CAA-CBA
14	a	842	CLA	C3A-C2A-CAA-CBA
14	a	843	CLA	C3A-C2A-CAA-CBA
14	1	804	CLA	C4-C3-C5-C6
14	1	822	CLA	C4-C3-C5-C6
14	1	825	CLA	C3A-C2A-CAA-CBA
14	1	842	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	1	843	CLA	C3A-C2A-CAA-CBA
14	b	815	CLA	C3A-C2A-CAA-CBA
14	b	835	CLA	C3A-C2A-CAA-CBA
14	b	836	CLA	C3A-C2A-CAA-CBA
14	b	842	CLA	C3A-C2A-CAA-CBA
14	2	815	CLA	C3A-C2A-CAA-CBA
14	2	835	CLA	C3A-C2A-CAA-CBA
14	2	836	CLA	C3A-C2A-CAA-CBA
14	2	842	CLA	C3A-C2A-CAA-CBA
14	B	810	CLA	C10-C11-C12-C13
14	2	809	CLA	C10-C11-C12-C13
17	B	854	BCR	C9-C10-C11-C12
17	b	853	BCR	C9-C10-C11-C12
17	6	4406	BCR	C9-C10-C11-C12
14	J	102	CLA	C4C-C3C-CAC-CBC
14	j	102	CLA	C4C-C3C-CAC-CBC
14	7	1103	CLA	C4C-C3C-CAC-CBC
14	A	814	CLA	C6-C7-C8-C9
14	a	815	CLA	C6-C7-C8-C9
14	1	813	CLA	C6-C7-C8-C9
14	B	830	CLA	O1A-CGA-O2A-C1
14	b	829	CLA	O1A-CGA-O2A-C1
14	2	829	CLA	O1A-CGA-O2A-C1
14	A	834	CLA	C15-C16-C17-C18
14	B	843	CLA	C15-C16-C17-C18
14	a	835	CLA	C15-C16-C17-C18
14	1	833	CLA	C15-C16-C17-C18
14	b	842	CLA	C15-C16-C17-C18
14	2	842	CLA	C15-C16-C17-C18
17	J	103	BCR	C11-C12-C13-C14
17	j	103	BCR	C11-C12-C13-C14
12	M	101	LHG	C4-C5-C6-O8
12	m	101	LHG	C4-C5-C6-O8
12	9	101	LHG	C4-C5-C6-O8
14	A	823	CLA	C4-C3-C5-C6
14	a	824	CLA	C4-C3-C5-C6
14	A	809	CLA	O1A-CGA-O2A-C1
14	a	810	CLA	O1A-CGA-O2A-C1
14	1	808	CLA	O1A-CGA-O2A-C1
14	A	842	CLA	C2B-C3B-CAB-CBB
14	a	842	CLA	C2B-C3B-CAB-CBB
14	1	842	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	A	847	BCR	C1-C6-C7-C8
17	A	848	BCR	C1-C6-C7-C8
17	A	849	BCR	C1-C6-C7-C8
17	A	850	BCR	C1-C6-C7-C8
17	B	847	BCR	C1-C6-C7-C8
17	B	847	BCR	C23-C24-C25-C30
17	B	848	BCR	C1-C6-C7-C8
17	B	850	BCR	C1-C6-C7-C8
17	B	851	BCR	C23-C24-C25-C30
17	B	852	BCR	C23-C24-C25-C30
17	F	203	BCR	C1-C6-C7-C8
17	F	206	BCR	C1-C6-C7-C8
17	I	101	BCR	C5-C6-C7-C8
17	I	102	BCR	C23-C24-C25-C30
17	J	104	BCR	C23-C24-C25-C30
17	L	1504	BCR	C1-C6-C7-C8
17	L	1505	BCR	C1-C6-C7-C8
17	K	4001	BCR	C1-C6-C7-C8
17	a	847	BCR	C1-C6-C7-C8
17	a	848	BCR	C1-C6-C7-C8
17	a	849	BCR	C1-C6-C7-C8
17	a	850	BCR	C1-C6-C7-C8
17	1	847	BCR	C1-C6-C7-C8
17	1	848	BCR	C1-C6-C7-C8
17	1	849	BCR	C1-C6-C7-C8
17	1	850	BCR	C1-C6-C7-C8
17	b	846	BCR	C1-C6-C7-C8
17	b	846	BCR	C23-C24-C25-C30
17	b	847	BCR	C1-C6-C7-C8
17	b	849	BCR	C1-C6-C7-C8
17	b	850	BCR	C23-C24-C25-C30
17	b	851	BCR	C23-C24-C25-C30
17	2	846	BCR	C1-C6-C7-C8
17	2	846	BCR	C23-C24-C25-C30
17	2	847	BCR	C1-C6-C7-C8
17	2	849	BCR	C1-C6-C7-C8
17	2	850	BCR	C23-C24-C25-C30
17	2	851	BCR	C23-C24-C25-C30
17	f	203	BCR	C1-C6-C7-C8
17	f	206	BCR	C1-C6-C7-C8
17	6	4402	BCR	C1-C6-C7-C8
17	6	4405	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	i	4102	BCR	C5-C6-C7-C8
17	i	4103	BCR	C23-C24-C25-C30
17	h	101	BCR	C5-C6-C7-C8
17	h	102	BCR	C23-C24-C25-C30
17	j	104	BCR	C23-C24-C25-C30
17	7	1105	BCR	C23-C24-C25-C30
17	k	4001	BCR	C1-C6-C7-C8
17	8	4001	BCR	C1-C6-C7-C8
17	l	4207	BCR	C1-C6-C7-C8
17	0	209	BCR	C1-C6-C7-C8
17	0	210	BCR	C1-C6-C7-C8
14	a	822	CLA	C5-C6-C7-C8
14	b	831	CLA	C10-C11-C12-C13
14	2	831	CLA	C10-C11-C12-C13
18	l	4202	LMG	C32-C33-C34-C35
14	B	832	CLA	C10-C11-C12-C13
14	1	820	CLA	C5-C6-C7-C8
14	L	1501	CLA	CBD-CGD-O2D-CED
14	l	4204	CLA	CBD-CGD-O2D-CED
14	0	206	CLA	CBD-CGD-O2D-CED
18	L	1506	LMG	C32-C33-C34-C35
18	0	201	LMG	C32-C33-C34-C35
14	A	821	CLA	C5-C6-C7-C8
18	A	853	LMG	O1-C7-C8-O7
18	a	853	LMG	O1-C7-C8-O7
18	1	852	LMG	O1-C7-C8-O7
18	b	803	LMG	C31-C32-C33-C34
18	2	802	LMG	C31-C32-C33-C34
14	B	841	CLA	O1D-CGD-O2D-CED
17	A	850	BCR	C10-C11-C12-C13
17	a	850	BCR	C10-C11-C12-C13
17	1	850	BCR	C10-C11-C12-C13
17	7	1104	BCR	C10-C11-C12-C13
12	A	802	LHG	C12-C13-C14-C15
12	a	802	LHG	C12-C13-C14-C15
12	1	802	LHG	C12-C13-C14-C15
18	B	803	LMG	C31-C32-C33-C34
14	b	840	CLA	O1D-CGD-O2D-CED
14	A	834	CLA	C6-C7-C8-C9
14	B	804	CLA	C11-C12-C13-C14
14	B	821	CLA	C11-C10-C8-C9
14	a	835	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	1	833	CLA	C6-C7-C8-C9
14	b	804	CLA	C11-C12-C13-C14
14	b	820	CLA	C11-C10-C8-C9
14	2	803	CLA	C11-C12-C13-C14
14	2	820	CLA	C11-C10-C8-C9
14	2	840	CLA	O1D-CGD-O2D-CED
17	A	848	BCR	C22-C23-C24-C25
17	I	102	BCR	C22-C23-C24-C25
17	K	4001	BCR	C22-C23-C24-C25
17	a	848	BCR	C22-C23-C24-C25
17	1	848	BCR	C22-C23-C24-C25
17	i	4103	BCR	C22-C23-C24-C25
17	h	102	BCR	C22-C23-C24-C25
17	k	4001	BCR	C22-C23-C24-C25
17	8	4001	BCR	C22-C23-C24-C25
14	A	813	CLA	C13-C15-C16-C17
14	1	812	CLA	C13-C15-C16-C17
17	J	103	BCR	C9-C10-C11-C12
17	j	103	BCR	C9-C10-C11-C12
12	A	801	LHG	C35-C36-C37-C38
12	a	801	LHG	C35-C36-C37-C38
12	1	801	LHG	C35-C36-C37-C38
15	B	846	PQN	C12-C13-C15-C16
15	b	845	PQN	C12-C13-C15-C16
15	2	845	PQN	C12-C13-C15-C16
14	B	809	CLA	C16-C17-C18-C19
14	b	809	CLA	C16-C17-C18-C19
14	2	808	CLA	C16-C17-C18-C19
14	a	814	CLA	C13-C15-C16-C17
14	b	841	CLA	O1A-CGA-O2A-C1
14	2	841	CLA	O1A-CGA-O2A-C1
17	B	850	BCR	C11-C10-C9-C34
17	B	852	BCR	C20-C21-C22-C37
17	F	203	BCR	C16-C17-C18-C36
17	L	1504	BCR	C20-C21-C22-C37
17	b	849	BCR	C11-C10-C9-C34
17	b	851	BCR	C20-C21-C22-C37
17	2	849	BCR	C11-C10-C9-C34
17	2	851	BCR	C20-C21-C22-C37
17	f	203	BCR	C16-C17-C18-C36
17	6	4402	BCR	C16-C17-C18-C36
17	l	4207	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
17	0	209	BCR	C20-C21-C22-C37
12	M	101	LHG	O10-C23-O8-C6
12	m	101	LHG	O10-C23-O8-C6
12	9	101	LHG	O10-C23-O8-C6
12	b	852	LHG	C24-C23-O8-C6
19	f	202	LMT	C4'-C5'-C6'-O6'
14	A	829	CLA	C6-C7-C8-C10
14	A	834	CLA	C6-C7-C8-C10
14	A	841	CLA	C11-C10-C8-C7
14	B	809	CLA	C12-C13-C15-C16
14	B	811	CLA	C11-C12-C13-C15
14	L	1503	CLA	C11-C10-C8-C7
14	a	830	CLA	C6-C7-C8-C10
14	a	835	CLA	C6-C7-C8-C10
14	1	828	CLA	C6-C7-C8-C10
14	1	833	CLA	C6-C7-C8-C10
14	1	840	CLA	C11-C10-C8-C7
14	b	802	CLA	C11-C10-C8-C7
14	b	811	CLA	C11-C12-C13-C15
14	2	810	CLA	C11-C12-C13-C15
14	l	4206	CLA	C11-C10-C8-C7
14	0	208	CLA	C11-C10-C8-C7
17	7	1104	BCR	C11-C12-C13-C14
12	B	853	LHG	C24-C23-O8-C6
12	2	852	LHG	C24-C23-O8-C6
14	B	807	CLA	O1A-CGA-O2A-C1
14	B	831	CLA	O1A-CGA-O2A-C1
14	1	827	CLA	O1A-CGA-O2A-C1
14	b	807	CLA	O1A-CGA-O2A-C1
14	b	830	CLA	O1A-CGA-O2A-C1
14	2	806	CLA	O1A-CGA-O2A-C1
14	2	830	CLA	O1A-CGA-O2A-C1
19	F	202	LMT	C4'-C5'-C6'-O6'
19	6	4401	LMT	C4'-C5'-C6'-O6'
12	A	801	LHG	C7-C8-C9-C10
12	1	801	LHG	C7-C8-C9-C10
14	A	813	CLA	C10-C11-C12-C13
14	A	843	CLA	C15-C16-C17-C18
14	a	814	CLA	C10-C11-C12-C13
14	a	843	CLA	C15-C16-C17-C18
14	1	812	CLA	C10-C11-C12-C13
14	1	843	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	A	822	CLA	C2A-CAA-CBA-CGA
14	a	823	CLA	C2A-CAA-CBA-CGA
14	1	821	CLA	C2A-CAA-CBA-CGA
13	A	803	CL0	O1A-CGA-O2A-C1
13	a	803	CL0	O1A-CGA-O2A-C1
13	1	803	CL0	O1A-CGA-O2A-C1
14	A	828	CLA	O1A-CGA-O2A-C1
14	a	829	CLA	O1A-CGA-O2A-C1
18	A	852	LMG	O10-C28-O8-C9
18	a	852	LMG	O10-C28-O8-C9
18	0	203	LMG	O10-C28-O8-C9
14	B	842	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	C2-C3-C5-C6
14	a	805	CLA	C2-C3-C5-C6
14	1	804	CLA	C2-C3-C5-C6
12	a	801	LHG	C7-C8-C9-C10
12	A	801	LHG	C28-C29-C30-C31
12	a	801	LHG	C28-C29-C30-C31
12	1	801	LHG	C28-C29-C30-C31
14	B	819	CLA	O1A-CGA-O2A-C1
14	b	818	CLA	O1A-CGA-O2A-C1
14	2	818	CLA	O1A-CGA-O2A-C1
17	7	1104	BCR	C9-C10-C11-C12
14	B	819	CLA	C6-C7-C8-C10
14	a	833	CLA	C16-C17-C18-C19
14	b	818	CLA	C6-C7-C8-C10
14	2	818	CLA	C6-C7-C8-C10
18	A	852	LMG	C30-C31-C32-C33
18	a	852	LMG	C30-C31-C32-C33
18	0	203	LMG	C30-C31-C32-C33
14	B	844	CLA	C15-C16-C17-C18
14	b	843	CLA	C15-C16-C17-C18
14	2	843	CLA	C15-C16-C17-C18
14	A	824	CLA	O2A-C1-C2-C3
14	a	825	CLA	O2A-C1-C2-C3
14	1	823	CLA	O2A-C1-C2-C3
15	B	846	PQN	C25-C26-C27-C28
15	2	845	PQN	C25-C26-C27-C28
14	A	832	CLA	C16-C17-C18-C19
14	1	831	CLA	C16-C17-C18-C19
15	B	846	PQN	C26-C27-C28-C30
15	b	845	PQN	C26-C27-C28-C30

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Mol	Chain	Res	Type	Atoms
15	2	845	PQN	C26-C27-C28-C30
18	A	852	LMG	C11-C12-C13-C14
14	a	824	CLA	C5-C6-C7-C8
14	1	822	CLA	C5-C6-C7-C8
15	b	845	PQN	C25-C26-C27-C28
18	a	852	LMG	C11-C12-C13-C14
18	0	203	LMG	C11-C12-C13-C14
14	1	828	CLA	C4-C3-C5-C6
14	A	823	CLA	C5-C6-C7-C8
14	A	832	CLA	C13-C15-C16-C17
14	a	833	CLA	C13-C15-C16-C17
14	1	831	CLA	C13-C15-C16-C17
12	M	101	LHG	O7-C5-C6-O8
12	m	101	LHG	O7-C5-C6-O8
12	9	101	LHG	O7-C5-C6-O8
14	A	821	CLA	C11-C12-C13-C14
14	L	1503	CLA	C11-C10-C8-C9
14	a	822	CLA	C11-C12-C13-C14
14	1	820	CLA	C11-C12-C13-C14
14	l	4206	CLA	C11-C10-C8-C9
14	0	208	CLA	C11-C10-C8-C9
14	b	811	CLA	C16-C17-C18-C19
18	B	803	LMG	C16-C17-C18-C19
18	b	803	LMG	C16-C17-C18-C19
18	2	802	LMG	C16-C17-C18-C19
14	A	804	CLA	C15-C16-C17-C18
14	a	805	CLA	C15-C16-C17-C18
14	1	804	CLA	C15-C16-C17-C18
12	B	853	LHG	C26-C27-C28-C29
12	b	852	LHG	C26-C27-C28-C29
12	2	852	LHG	C26-C27-C28-C29
14	A	836	CLA	C2-C1-O2A-CGA
14	a	837	CLA	C2-C1-O2A-CGA
14	1	835	CLA	C2-C1-O2A-CGA
17	A	848	BCR	C19-C20-C21-C22
17	B	847	BCR	C19-C20-C21-C22
17	a	848	BCR	C19-C20-C21-C22
17	1	848	BCR	C19-C20-C21-C22
17	b	846	BCR	C19-C20-C21-C22
17	2	846	BCR	C19-C20-C21-C22
14	B	811	CLA	C16-C17-C18-C19
14	2	810	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	A	834	CLA	C13-C15-C16-C17
14	L	1501	CLA	C13-C15-C16-C17
14	a	835	CLA	C13-C15-C16-C17
14	1	833	CLA	C13-C15-C16-C17
14	l	4204	CLA	C13-C15-C16-C17
14	0	206	CLA	C13-C15-C16-C17
14	A	829	CLA	C4-C3-C5-C6
14	a	830	CLA	C4-C3-C5-C6
14	B	816	CLA	C13-C15-C16-C17
14	b	815	CLA	C13-C15-C16-C17
14	2	815	CLA	C13-C15-C16-C17
14	F	204	CLA	C2A-CAA-CBA-CGA
14	f	204	CLA	C2A-CAA-CBA-CGA
14	6	4403	CLA	C2A-CAA-CBA-CGA
14	B	809	CLA	C16-C17-C18-C20
14	B	844	CLA	C16-C17-C18-C20
14	b	809	CLA	C16-C17-C18-C20
14	b	843	CLA	C16-C17-C18-C20
14	2	808	CLA	C16-C17-C18-C20
14	2	843	CLA	C16-C17-C18-C20
14	2	842	CLA	C5-C6-C7-C8
17	A	851	BCR	C14-C15-C16-C17
14	B	810	CLA	C2C-C3C-CAC-CBC
14	B	843	CLA	C5-C6-C7-C8
14	A	834	CLA	C3-C5-C6-C7
14	B	813	CLA	C3-C5-C6-C7
14	a	835	CLA	C3-C5-C6-C7
14	1	833	CLA	C3-C5-C6-C7
14	2	812	CLA	C3-C5-C6-C7
14	l	4203	CLA	C3-C5-C6-C7
14	b	810	CLA	C2C-C3C-CAC-CBC
14	2	809	CLA	C2C-C3C-CAC-CBC
14	B	812	CLA	C14-C13-C15-C16
14	b	812	CLA	C14-C13-C15-C16
14	2	811	CLA	C14-C13-C15-C16
17	A	847	BCR	C18-C19-C20-C21
17	a	847	BCR	C18-C19-C20-C21
14	b	833	CLA	C5-C6-C7-C8
14	B	834	CLA	C5-C6-C7-C8
14	2	833	CLA	C5-C6-C7-C8
17	J	104	BCR	C11-C12-C13-C35
17	j	104	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
17	7	1105	BCR	C11-C12-C13-C35
14	F	201	CLA	C1A-C2A-CAA-CBA
14	K	4003	CLA	C1A-C2A-CAA-CBA
14	K	4003	CLA	C4B-C3B-CAB-CBB
14	1	841	CLA	C1A-C2A-CAA-CBA
14	f	201	CLA	C1A-C2A-CAA-CBA
14	k	4003	CLA	C1A-C2A-CAA-CBA
14	k	4003	CLA	C4B-C3B-CAB-CBB
14	8	4003	CLA	C1A-C2A-CAA-CBA
14	8	4003	CLA	C4B-C3B-CAB-CBB
14	0	202	CLA	C4-C3-C5-C6
14	b	842	CLA	C5-C6-C7-C8
17	A	850	BCR	C6-C7-C8-C9
17	a	850	BCR	C6-C7-C8-C9
17	1	850	BCR	C6-C7-C8-C9
17	I	101	BCR	C21-C22-C23-C24
17	i	4102	BCR	C21-C22-C23-C24
17	h	101	BCR	C21-C22-C23-C24
13	1	803	CL0	C3-C5-C6-C7
14	A	836	CLA	C2A-CAA-CBA-CGA
14	a	837	CLA	C2A-CAA-CBA-CGA
14	1	835	CLA	C2A-CAA-CBA-CGA
14	A	834	CLA	C10-C11-C12-C13
14	F	201	CLA	C2-C3-C5-C6
14	1	841	CLA	C2-C3-C5-C6
14	f	201	CLA	C2-C3-C5-C6
14	a	835	CLA	C10-C11-C12-C13
14	1	833	CLA	C10-C11-C12-C13
13	A	803	CL0	C3-C5-C6-C7
13	a	803	CL0	C3-C5-C6-C7
14	A	810	CLA	C11-C12-C13-C15
14	A	826	CLA	C11-C10-C8-C7
14	A	830	CLA	C12-C13-C15-C16
14	A	832	CLA	C12-C13-C15-C16
14	A	835	CLA	C12-C13-C15-C16
14	B	841	CLA	C11-C12-C13-C15
14	a	811	CLA	C11-C12-C13-C15
14	a	827	CLA	C11-C10-C8-C7
14	a	831	CLA	C12-C13-C15-C16
14	a	833	CLA	C12-C13-C15-C16
14	a	836	CLA	C12-C13-C15-C16
14	1	809	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	1	825	CLA	C11-C10-C8-C7
14	1	829	CLA	C12-C13-C15-C16
14	1	831	CLA	C12-C13-C15-C16
14	1	834	CLA	C12-C13-C15-C16
14	b	840	CLA	C11-C12-C13-C15
14	2	840	CLA	C11-C12-C13-C15
18	l	4202	LMG	C29-C30-C31-C32
14	B	820	CLA	C6-C7-C8-C9
14	b	819	CLA	C6-C7-C8-C9
14	2	819	CLA	C6-C7-C8-C9
18	L	1506	LMG	C29-C30-C31-C32
18	0	201	LMG	C29-C30-C31-C32
14	A	827	CLA	CBA-CGA-O2A-C1
14	a	828	CLA	CBA-CGA-O2A-C1
14	1	826	CLA	CBA-CGA-O2A-C1
14	A	815	CLA	CBD-CGD-O2D-CED
14	a	816	CLA	CBD-CGD-O2D-CED
14	1	814	CLA	CBD-CGD-O2D-CED
14	b	801	CLA	C4-C3-C5-C6
14	B	821	CLA	C11-C12-C13-C15
14	b	820	CLA	C11-C12-C13-C15
14	2	820	CLA	C11-C12-C13-C15
18	2	802	LMG	C13-C14-C15-C16
18	B	803	LMG	C13-C14-C15-C16
14	A	820	CLA	C3-C5-C6-C7
14	a	821	CLA	C3-C5-C6-C7
14	1	819	CLA	C3-C5-C6-C7
14	B	840	CLA	C2C-C3C-CAC-CBC
13	A	803	CL0	C6-C7-C8-C9
13	a	803	CL0	C6-C7-C8-C9
13	1	803	CL0	C6-C7-C8-C9
14	A	841	CLA	C11-C10-C8-C9
14	B	811	CLA	C11-C10-C8-C9
14	B	811	CLA	C11-C12-C13-C14
14	B	835	CLA	C11-C10-C8-C9
14	B	844	CLA	C6-C7-C8-C9
14	1	840	CLA	C11-C10-C8-C9
14	b	802	CLA	C11-C10-C8-C9
14	b	811	CLA	C11-C10-C8-C9
14	b	811	CLA	C11-C12-C13-C14
14	b	834	CLA	C11-C10-C8-C9
14	b	843	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	2	810	CLA	C11-C10-C8-C9
14	2	810	CLA	C11-C12-C13-C14
14	2	834	CLA	C11-C10-C8-C9
18	b	803	LMG	C13-C14-C15-C16
18	B	803	LMG	C32-C33-C34-C35
18	b	803	LMG	C32-C33-C34-C35
18	2	802	LMG	C32-C33-C34-C35
17	I	102	BCR	C15-C16-C17-C18
17	i	4103	BCR	C15-C16-C17-C18
17	h	102	BCR	C15-C16-C17-C18
14	b	839	CLA	C2C-C3C-CAC-CBC
18	2	802	LMG	C17-C18-C19-C20
14	A	824	CLA	C1-C2-C3-C4
14	a	825	CLA	C1-C2-C3-C4
14	1	823	CLA	C1-C2-C3-C4
18	B	803	LMG	C17-C18-C19-C20
18	b	803	LMG	C17-C18-C19-C20
14	A	836	CLA	C3-C5-C6-C7
14	a	837	CLA	C3-C5-C6-C7
14	1	835	CLA	C3-C5-C6-C7
14	2	839	CLA	C2C-C3C-CAC-CBC
12	B	853	LHG	O7-C5-C6-O8
12	b	852	LHG	O7-C5-C6-O8
12	2	852	LHG	O7-C5-C6-O8
18	L	1506	LMG	O7-C8-C9-O8
18	l	4202	LMG	O7-C8-C9-O8
18	0	201	LMG	O7-C8-C9-O8
14	A	828	CLA	C6-C7-C8-C9
14	a	829	CLA	C6-C7-C8-C9
14	1	827	CLA	C6-C7-C8-C9
14	A	832	CLA	CAD-CBD-CGD-O2D
14	B	816	CLA	CAD-CBD-CGD-O2D
14	B	840	CLA	CAD-CBD-CGD-O2D
14	B	844	CLA	CAD-CBD-CGD-O2D
14	L	1501	CLA	CAD-CBD-CGD-O2D
14	K	4002	CLA	CAD-CBD-CGD-O2D
14	a	833	CLA	CAD-CBD-CGD-O2D
14	1	831	CLA	CAD-CBD-CGD-O2D
14	b	815	CLA	CAD-CBD-CGD-O2D
14	b	839	CLA	CAD-CBD-CGD-O2D
14	b	843	CLA	CAD-CBD-CGD-O2D
14	2	815	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	2	839	CLA	CAD-CBD-CGD-O2D
14	2	843	CLA	CAD-CBD-CGD-O2D
14	k	4002	CLA	CAD-CBD-CGD-O2D
14	8	4002	CLA	CAD-CBD-CGD-O2D
14	l	4204	CLA	CAD-CBD-CGD-O2D
14	0	206	CLA	CAD-CBD-CGD-O2D
18	A	852	LMG	C15-C16-C17-C18
14	A	830	CLA	C2A-CAA-CBA-CGA
14	a	831	CLA	C2A-CAA-CBA-CGA
14	1	829	CLA	C2A-CAA-CBA-CGA
18	a	852	LMG	C15-C16-C17-C18
18	0	203	LMG	C15-C16-C17-C18
12	A	801	LHG	C3-O3-P-O6
12	M	101	LHG	C3-O3-P-O5
12	M	101	LHG	C4-O6-P-O3
12	a	801	LHG	C3-O3-P-O6
12	1	801	LHG	C3-O3-P-O6
12	m	101	LHG	C3-O3-P-O5
12	m	101	LHG	C4-O6-P-O3
12	9	101	LHG	C3-O3-P-O5
12	9	101	LHG	C4-O6-P-O3
14	A	821	CLA	CHA-CBD-CGD-O1D
14	A	821	CLA	CHA-CBD-CGD-O2D
14	A	832	CLA	CAD-CBD-CGD-O1D
14	A	834	CLA	CAD-CBD-CGD-O1D
14	B	816	CLA	CAD-CBD-CGD-O1D
14	B	835	CLA	CAD-CBD-CGD-O1D
14	B	840	CLA	CAD-CBD-CGD-O1D
14	B	844	CLA	CAD-CBD-CGD-O1D
14	L	1501	CLA	CAD-CBD-CGD-O1D
14	K	4002	CLA	CAD-CBD-CGD-O1D
14	K	4003	CLA	CAD-CBD-CGD-O1D
14	a	822	CLA	CHA-CBD-CGD-O1D
14	a	822	CLA	CHA-CBD-CGD-O2D
14	a	833	CLA	CAD-CBD-CGD-O1D
14	a	835	CLA	CAD-CBD-CGD-O1D
14	1	820	CLA	CHA-CBD-CGD-O1D
14	1	820	CLA	CHA-CBD-CGD-O2D
14	1	831	CLA	CAD-CBD-CGD-O1D
14	1	833	CLA	CAD-CBD-CGD-O1D
14	b	815	CLA	CAD-CBD-CGD-O1D
14	b	834	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	b	839	CLA	CAD-CBD-CGD-O1D
14	b	843	CLA	CAD-CBD-CGD-O1D
14	2	815	CLA	CAD-CBD-CGD-O1D
14	2	834	CLA	CAD-CBD-CGD-O1D
14	2	839	CLA	CAD-CBD-CGD-O1D
14	2	843	CLA	CAD-CBD-CGD-O1D
14	k	4002	CLA	CAD-CBD-CGD-O1D
14	k	4003	CLA	CAD-CBD-CGD-O1D
14	8	4002	CLA	CAD-CBD-CGD-O1D
14	8	4003	CLA	CAD-CBD-CGD-O1D
14	l	4204	CLA	CAD-CBD-CGD-O1D
14	0	206	CLA	CAD-CBD-CGD-O1D
17	J	104	BCR	C19-C20-C21-C22
17	j	104	BCR	C19-C20-C21-C22
17	7	1105	BCR	C19-C20-C21-C22
14	A	807	CLA	C3-C5-C6-C7
14	A	810	CLA	C3-C5-C6-C7
14	a	808	CLA	C3-C5-C6-C7
14	a	811	CLA	C3-C5-C6-C7
14	1	806	CLA	C3-C5-C6-C7
14	1	809	CLA	C3-C5-C6-C7
17	a	851	BCR	C14-C15-C16-C17
17	1	851	BCR	C14-C15-C16-C17
14	B	802	CLA	C4-C3-C5-C6
14	A	832	CLA	C2B-C3B-CAB-CBB
14	B	834	CLA	C2B-C3B-CAB-CBB
14	B	836	CLA	C2B-C3B-CAB-CBB
14	B	841	CLA	C2B-C3B-CAB-CBB
14	B	844	CLA	C2B-C3B-CAB-CBB
14	J	102	CLA	C2B-C3B-CAB-CBB
14	L	1502	CLA	C2B-C3B-CAB-CBB
14	K	4003	CLA	C2B-C3B-CAB-CBB
14	a	833	CLA	C2B-C3B-CAB-CBB
14	1	831	CLA	C2B-C3B-CAB-CBB
14	b	833	CLA	C2B-C3B-CAB-CBB
14	b	835	CLA	C2B-C3B-CAB-CBB
14	b	840	CLA	C2B-C3B-CAB-CBB
14	b	843	CLA	C2B-C3B-CAB-CBB
14	2	833	CLA	C2B-C3B-CAB-CBB
14	2	835	CLA	C2B-C3B-CAB-CBB
14	2	840	CLA	C2B-C3B-CAB-CBB
14	2	843	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	j	102	CLA	C2B-C3B-CAB-CBB
14	7	1103	CLA	C2B-C3B-CAB-CBB
14	k	4003	CLA	C2B-C3B-CAB-CBB
14	8	4003	CLA	C2B-C3B-CAB-CBB
14	l	4205	CLA	C2B-C3B-CAB-CBB
14	0	207	CLA	C2B-C3B-CAB-CBB
17	A	849	BCR	C23-C24-C25-C30
17	K	4001	BCR	C23-C24-C25-C30
17	a	849	BCR	C23-C24-C25-C30
17	1	849	BCR	C23-C24-C25-C30
17	k	4001	BCR	C23-C24-C25-C30
17	8	4001	BCR	C23-C24-C25-C30
12	A	802	LHG	C13-C14-C15-C16
12	a	802	LHG	C13-C14-C15-C16
12	1	802	LHG	C13-C14-C15-C16
14	A	829	CLA	C2-C3-C5-C6
14	B	813	CLA	C2-C3-C5-C6
14	a	830	CLA	C2-C3-C5-C6
14	1	828	CLA	C2-C3-C5-C6
14	2	812	CLA	C2-C3-C5-C6
14	l	4203	CLA	C2-C3-C5-C6
14	B	806	CLA	C3-C5-C6-C7
14	b	806	CLA	C3-C5-C6-C7
14	2	805	CLA	C3-C5-C6-C7
18	A	852	LMG	C37-C38-C39-C40
18	0	203	LMG	C37-C38-C39-C40
14	A	827	CLA	O1A-CGA-O2A-C1
14	a	828	CLA	O1A-CGA-O2A-C1
14	1	826	CLA	O1A-CGA-O2A-C1
18	a	852	LMG	C37-C38-C39-C40
12	a	801	LHG	C18-C19-C20-C21
12	1	801	LHG	C18-C19-C20-C21
12	2	852	LHG	C11-C10-C9-C8
17	1	847	BCR	C18-C19-C20-C21
12	A	801	LHG	C18-C19-C20-C21
18	A	852	LMG	C34-C35-C36-C37
18	a	852	LMG	C34-C35-C36-C37
18	0	203	LMG	C34-C35-C36-C37
12	B	853	LHG	C11-C10-C9-C8
12	b	852	LHG	C11-C10-C9-C8
18	b	803	LMG	C18-C19-C20-C21
17	B	852	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
17	b	851	BCR	C19-C20-C21-C22
17	2	851	BCR	C19-C20-C21-C22
14	b	816	CLA	C4C-C3C-CAC-CBC
14	A	804	CLA	C16-C17-C18-C20
14	B	820	CLA	C6-C7-C8-C10
14	a	805	CLA	C16-C17-C18-C20
14	1	804	CLA	C16-C17-C18-C20
14	b	819	CLA	C6-C7-C8-C10
14	2	819	CLA	C6-C7-C8-C10
14	B	817	CLA	C4C-C3C-CAC-CBC
14	2	816	CLA	C4C-C3C-CAC-CBC
14	A	832	CLA	C6-C7-C8-C9
14	B	809	CLA	C11-C10-C8-C9
14	a	833	CLA	C6-C7-C8-C9
14	1	831	CLA	C6-C7-C8-C9
14	b	809	CLA	C11-C10-C8-C9
14	2	808	CLA	C11-C10-C8-C9
14	2	843	CLA	C6-C7-C8-C9
18	B	803	LMG	C18-C19-C20-C21
14	B	805	CLA	C6-C7-C8-C10
14	b	805	CLA	C6-C7-C8-C10
14	2	804	CLA	C6-C7-C8-C10
18	2	802	LMG	C18-C19-C20-C21
14	B	844	CLA	C16-C17-C18-C19
14	a	829	CLA	C6-C7-C8-C10
14	1	827	CLA	C6-C7-C8-C10
14	b	843	CLA	C16-C17-C18-C19
14	2	843	CLA	C16-C17-C18-C19
18	l	4202	LMG	C29-C28-O8-C9
18	0	201	LMG	C29-C28-O8-C9
14	B	805	CLA	CAA-CBA-CGA-O2A
14	b	805	CLA	CAA-CBA-CGA-O2A
14	2	804	CLA	CAA-CBA-CGA-O2A
17	F	206	BCR	C14-C15-C16-C17
17	f	206	BCR	C14-C15-C16-C17
17	6	4405	BCR	C14-C15-C16-C17
18	L	1506	LMG	C29-C28-O8-C9
14	A	841	CLA	C2C-C3C-CAC-CBC
14	1	840	CLA	C2C-C3C-CAC-CBC
14	b	802	CLA	C2C-C3C-CAC-CBC
14	A	828	CLA	C6-C7-C8-C10
14	A	812	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	A	841	CLA	C2A-CAA-CBA-CGA
14	a	813	CLA	C2A-CAA-CBA-CGA
14	1	811	CLA	C2A-CAA-CBA-CGA
14	1	840	CLA	C2A-CAA-CBA-CGA
14	b	802	CLA	C2A-CAA-CBA-CGA
14	B	835	CLA	C4-C3-C5-C6
14	b	834	CLA	C4-C3-C5-C6
14	2	834	CLA	C4-C3-C5-C6
18	B	803	LMG	C7-C8-C9-O8
18	b	803	LMG	C7-C8-C9-O8
18	2	802	LMG	C7-C8-C9-O8
14	A	822	CLA	C2C-C3C-CAC-CBC
14	1	821	CLA	C2C-C3C-CAC-CBC
14	b	818	CLA	C5-C6-C7-C8
14	2	818	CLA	C5-C6-C7-C8
14	a	823	CLA	C2C-C3C-CAC-CBC
17	K	4005	BCR	C13-C14-C15-C16
17	k	4004	BCR	C13-C14-C15-C16
17	8	4005	BCR	C13-C14-C15-C16
15	B	846	PQN	C26-C27-C28-C29
15	b	845	PQN	C26-C27-C28-C29
15	2	845	PQN	C26-C27-C28-C29
14	B	819	CLA	C5-C6-C7-C8
14	0	206	CLA	O1D-CGD-O2D-CED
14	l	4204	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	CAA-CBA-CGA-O2A
14	b	818	CLA	CAA-CBA-CGA-O2A
14	2	818	CLA	CAA-CBA-CGA-O2A
14	A	821	CLA	C14-C13-C15-C16
14	B	805	CLA	C6-C7-C8-C9
14	L	1502	CLA	C11-C12-C13-C14
14	a	822	CLA	C14-C13-C15-C16
14	b	805	CLA	C6-C7-C8-C9
14	2	804	CLA	C6-C7-C8-C9
14	l	4205	CLA	C11-C12-C13-C14
14	0	207	CLA	C11-C12-C13-C14
14	A	813	CLA	CBA-CGA-O2A-C1
14	a	814	CLA	CBA-CGA-O2A-C1
14	1	812	CLA	CBA-CGA-O2A-C1
14	B	814	CLA	C4B-C3B-CAB-CBB
14	B	839	CLA	C4B-C3B-CAB-CBB
14	b	813	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	838	CLA	C4B-C3B-CAB-CBB
14	2	813	CLA	C4B-C3B-CAB-CBB
14	2	838	CLA	C4B-C3B-CAB-CBB
18	L	1506	LMG	C33-C34-C35-C36
18	l	4202	LMG	C33-C34-C35-C36
18	0	201	LMG	C33-C34-C35-C36
14	L	1501	CLA	O1D-CGD-O2D-CED
14	A	831	CLA	C16-C17-C18-C20
14	a	832	CLA	C16-C17-C18-C20
14	1	830	CLA	C16-C17-C18-C20
14	A	842	CLA	CBA-CGA-O2A-C1
14	K	4004	CLA	CBA-CGA-O2A-C1
14	a	842	CLA	CBA-CGA-O2A-C1
14	a	854	CLA	CBA-CGA-O2A-C1
14	1	842	CLA	CBA-CGA-O2A-C1
14	8	4004	CLA	CBA-CGA-O2A-C1
14	K	4004	CLA	O1A-CGA-O2A-C1
14	a	814	CLA	O1A-CGA-O2A-C1
14	a	854	CLA	O1A-CGA-O2A-C1
14	8	4004	CLA	O1A-CGA-O2A-C1
14	B	812	CLA	C4-C3-C5-C6
14	L	1501	CLA	C4-C3-C5-C6
14	b	812	CLA	C4-C3-C5-C6
14	2	811	CLA	C4-C3-C5-C6
14	l	4204	CLA	C4-C3-C5-C6
14	0	206	CLA	C4-C3-C5-C6
14	L	1503	CLA	CAA-CBA-CGA-O2A
14	B	835	CLA	C2-C3-C5-C6
14	b	834	CLA	C2-C3-C5-C6
14	2	834	CLA	C2-C3-C5-C6
14	A	813	CLA	O1A-CGA-O2A-C1
14	1	812	CLA	O1A-CGA-O2A-C1
14	l	4206	CLA	CAA-CBA-CGA-O2A
14	0	208	CLA	CAA-CBA-CGA-O2A
14	A	808	CLA	C11-C12-C13-C15
14	A	826	CLA	C6-C7-C8-C10
14	B	801	CLA	C11-C10-C8-C7
14	a	804	CLA	C11-C10-C8-C7
14	a	809	CLA	C11-C12-C13-C15
14	a	827	CLA	C6-C7-C8-C10
14	1	807	CLA	C11-C12-C13-C15
14	1	825	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	2	801	CLA	C11-C10-C8-C7
14	A	804	CLA	C16-C17-C18-C19
14	B	821	CLA	C11-C12-C13-C14
14	a	805	CLA	C16-C17-C18-C19
14	1	804	CLA	C16-C17-C18-C19
14	b	820	CLA	C11-C12-C13-C14
14	2	820	CLA	C11-C12-C13-C14
12	B	853	LHG	C29-C30-C31-C32
12	b	852	LHG	C29-C30-C31-C32
12	2	852	LHG	C29-C30-C31-C32
12	a	801	LHG	C27-C28-C29-C30
12	1	801	LHG	C27-C28-C29-C30
12	A	801	LHG	C27-C28-C29-C30
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	832	CLA	C4-C3-C5-C6
14	B	815	CLA	C3A-C2A-CAA-CBA
14	a	807	CLA	C3A-C2A-CAA-CBA
14	a	833	CLA	C4-C3-C5-C6
14	1	805	CLA	C3A-C2A-CAA-CBA
14	1	831	CLA	C4-C3-C5-C6
14	b	814	CLA	C3A-C2A-CAA-CBA
14	2	814	CLA	C3A-C2A-CAA-CBA
14	2	829	CLA	C4C-C3C-CAC-CBC
17	A	851	BCR	C16-C17-C18-C36
17	B	849	BCR	C20-C21-C22-C37
17	B	850	BCR	C35-C13-C14-C15
17	B	851	BCR	C11-C10-C9-C34
17	L	1504	BCR	C16-C17-C18-C36
17	a	851	BCR	C16-C17-C18-C36
17	1	851	BCR	C16-C17-C18-C36
17	b	848	BCR	C20-C21-C22-C37
17	b	849	BCR	C35-C13-C14-C15
17	b	850	BCR	C11-C10-C9-C34
17	2	848	BCR	C20-C21-C22-C37
17	2	849	BCR	C35-C13-C14-C15
17	2	850	BCR	C11-C10-C9-C34
14	A	829	CLA	C5-C6-C7-C8
14	L	1502	CLA	C8-C10-C11-C12
14	a	830	CLA	C5-C6-C7-C8
14	1	828	CLA	C5-C6-C7-C8
14	l	4205	CLA	C8-C10-C11-C12
14	0	207	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	1	827	CLA	C2C-C3C-CAC-CBC
18	b	803	LMG	C11-C12-C13-C14
14	B	830	CLA	C4C-C3C-CAC-CBC
14	b	829	CLA	C4C-C3C-CAC-CBC
14	A	828	CLA	C2C-C3C-CAC-CBC
14	a	829	CLA	C2C-C3C-CAC-CBC
18	B	803	LMG	C11-C12-C13-C14
18	2	802	LMG	C11-C12-C13-C14
14	F	201	CLA	C2-C1-O2A-CGA
14	1	841	CLA	C2-C1-O2A-CGA
14	f	201	CLA	C2-C1-O2A-CGA
17	B	851	BCR	C15-C16-C17-C18
17	F	203	BCR	C13-C14-C15-C16
17	b	850	BCR	C15-C16-C17-C18
17	2	850	BCR	C15-C16-C17-C18
17	f	203	BCR	C13-C14-C15-C16
17	6	4402	BCR	C13-C14-C15-C16
17	A	851	BCR	C7-C8-C9-C34
17	a	851	BCR	C7-C8-C9-C34
14	F	201	CLA	C4-C3-C5-C6
14	1	841	CLA	C4-C3-C5-C6
14	f	201	CLA	C4-C3-C5-C6
17	A	851	BCR	C11-C12-C13-C14
17	B	849	BCR	C21-C22-C23-C24
17	a	851	BCR	C11-C12-C13-C14
17	b	848	BCR	C21-C22-C23-C24
17	2	848	BCR	C21-C22-C23-C24
14	B	825	CLA	CAA-CBA-CGA-O1A
14	b	824	CLA	CAA-CBA-CGA-O1A
14	2	824	CLA	CAA-CBA-CGA-O1A
14	A	810	CLA	C11-C12-C13-C14
14	A	832	CLA	C14-C13-C15-C16
14	B	813	CLA	C11-C10-C8-C9
14	B	816	CLA	C11-C12-C13-C14
14	a	811	CLA	C11-C12-C13-C14
14	a	833	CLA	C14-C13-C15-C16
14	1	809	CLA	C11-C12-C13-C14
14	1	820	CLA	C14-C13-C15-C16
14	1	831	CLA	C14-C13-C15-C16
14	b	815	CLA	C11-C12-C13-C14
14	2	812	CLA	C11-C10-C8-C9
14	2	815	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	l	4203	CLA	C11-C10-C8-C9
15	B	846	PQN	C24-C23-C25-C26
15	b	845	PQN	C24-C23-C25-C26
15	2	845	PQN	C24-C23-C25-C26
14	B	811	CLA	C4-C3-C5-C6
14	b	811	CLA	C4-C3-C5-C6
14	2	810	CLA	C4-C3-C5-C6
12	A	802	LHG	C7-C8-C9-C10
12	1	802	LHG	C7-C8-C9-C10
14	l	4204	CLA	C2-C3-C5-C6
14	0	206	CLA	C2-C3-C5-C6
14	1	842	CLA	O1A-CGA-O2A-C1
14	B	826	CLA	CAA-CBA-CGA-O2A
14	b	825	CLA	CAA-CBA-CGA-O2A
14	2	825	CLA	CAA-CBA-CGA-O2A
12	a	802	LHG	C7-C8-C9-C10
14	a	828	CLA	C8-C10-C11-C12
14	A	816	CLA	C1A-C2A-CAA-CBA
14	A	818	CLA	C1A-C2A-CAA-CBA
14	A	826	CLA	C1A-C2A-CAA-CBA
14	B	822	CLA	C1A-C2A-CAA-CBA
14	B	844	CLA	C1A-C2A-CAA-CBA
14	a	817	CLA	C1A-C2A-CAA-CBA
14	a	819	CLA	C1A-C2A-CAA-CBA
14	a	827	CLA	C1A-C2A-CAA-CBA
14	1	815	CLA	C1A-C2A-CAA-CBA
14	1	817	CLA	C1A-C2A-CAA-CBA
14	1	825	CLA	C1A-C2A-CAA-CBA
14	b	821	CLA	C1A-C2A-CAA-CBA
14	b	843	CLA	C1A-C2A-CAA-CBA
14	2	821	CLA	C1A-C2A-CAA-CBA
14	2	843	CLA	C1A-C2A-CAA-CBA
17	A	851	BCR	C11-C10-C9-C8
17	B	849	BCR	C20-C21-C22-C23
17	B	850	BCR	C16-C17-C18-C19
17	a	851	BCR	C11-C10-C9-C8
17	1	851	BCR	C11-C10-C9-C8
17	b	848	BCR	C20-C21-C22-C23
17	b	849	BCR	C16-C17-C18-C19
17	2	848	BCR	C20-C21-C22-C23
17	2	849	BCR	C16-C17-C18-C19
14	B	816	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	b	815	CLA	C4C-C3C-CAC-CBC
14	2	815	CLA	C4C-C3C-CAC-CBC
14	A	827	CLA	C8-C10-C11-C12
14	1	826	CLA	C8-C10-C11-C12
14	A	842	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	C2B-C3B-CAB-CBB
14	A	826	CLA	C2B-C3B-CAB-CBB
14	A	834	CLA	C2B-C3B-CAB-CBB
14	A	838	CLA	C2B-C3B-CAB-CBB
14	B	807	CLA	C2B-C3B-CAB-CBB
14	B	808	CLA	C2B-C3B-CAB-CBB
14	B	811	CLA	C2B-C3B-CAB-CBB
14	B	814	CLA	C2B-C3B-CAB-CBB
14	B	815	CLA	C2B-C3B-CAB-CBB
14	B	823	CLA	C2B-C3B-CAB-CBB
14	B	824	CLA	C2B-C3B-CAB-CBB
14	B	825	CLA	C2B-C3B-CAB-CBB
14	B	838	CLA	C2B-C3B-CAB-CBB
14	B	843	CLA	C2B-C3B-CAB-CBB
14	F	205	CLA	C2B-C3B-CAB-CBB
14	J	101	CLA	C2B-C3B-CAB-CBB
14	K	4002	CLA	C2B-C3B-CAB-CBB
14	a	819	CLA	C2B-C3B-CAB-CBB
14	a	827	CLA	C2B-C3B-CAB-CBB
14	a	828	CLA	C2B-C3B-CAB-CBB
14	a	835	CLA	C2B-C3B-CAB-CBB
14	a	839	CLA	C2B-C3B-CAB-CBB
14	1	817	CLA	C2B-C3B-CAB-CBB
14	1	825	CLA	C2B-C3B-CAB-CBB
14	1	826	CLA	C2B-C3B-CAB-CBB
14	1	833	CLA	C2B-C3B-CAB-CBB
14	1	837	CLA	C2B-C3B-CAB-CBB
14	b	807	CLA	C2B-C3B-CAB-CBB
14	b	808	CLA	C2B-C3B-CAB-CBB
14	b	811	CLA	C2B-C3B-CAB-CBB
14	b	813	CLA	C2B-C3B-CAB-CBB
14	b	814	CLA	C2B-C3B-CAB-CBB
14	b	822	CLA	C2B-C3B-CAB-CBB
14	b	823	CLA	C2B-C3B-CAB-CBB
14	b	824	CLA	C2B-C3B-CAB-CBB
14	b	837	CLA	C2B-C3B-CAB-CBB
14	b	842	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	2	806	CLA	C2B-C3B-CAB-CBB
14	2	807	CLA	C2B-C3B-CAB-CBB
14	2	810	CLA	C2B-C3B-CAB-CBB
14	2	813	CLA	C2B-C3B-CAB-CBB
14	2	814	CLA	C2B-C3B-CAB-CBB
14	2	822	CLA	C2B-C3B-CAB-CBB
14	2	823	CLA	C2B-C3B-CAB-CBB
14	2	824	CLA	C2B-C3B-CAB-CBB
14	2	837	CLA	C2B-C3B-CAB-CBB
14	2	842	CLA	C2B-C3B-CAB-CBB
14	f	205	CLA	C2B-C3B-CAB-CBB
14	6	4404	CLA	C2B-C3B-CAB-CBB
14	j	101	CLA	C2B-C3B-CAB-CBB
14	7	1102	CLA	C2B-C3B-CAB-CBB
14	k	4002	CLA	C2B-C3B-CAB-CBB
14	8	4002	CLA	C2B-C3B-CAB-CBB
17	A	847	BCR	C5-C6-C7-C8
17	A	847	BCR	C23-C24-C25-C30
17	A	848	BCR	C5-C6-C7-C8
17	A	849	BCR	C5-C6-C7-C8
17	A	849	BCR	C23-C24-C25-C26
17	A	850	BCR	C5-C6-C7-C8
17	A	850	BCR	C23-C24-C25-C30
17	B	847	BCR	C5-C6-C7-C8
17	B	847	BCR	C23-C24-C25-C26
17	B	848	BCR	C5-C6-C7-C8
17	B	850	BCR	C5-C6-C7-C8
17	B	851	BCR	C1-C6-C7-C8
17	B	851	BCR	C5-C6-C7-C8
17	B	851	BCR	C23-C24-C25-C26
17	B	852	BCR	C1-C6-C7-C8
17	B	852	BCR	C23-C24-C25-C26
17	B	854	BCR	C23-C24-C25-C30
17	F	203	BCR	C5-C6-C7-C8
17	F	206	BCR	C5-C6-C7-C8
17	I	102	BCR	C23-C24-C25-C26
17	J	104	BCR	C23-C24-C25-C26
17	L	1504	BCR	C5-C6-C7-C8
17	L	1505	BCR	C5-C6-C7-C8
17	L	1505	BCR	C23-C24-C25-C30
17	M	102	BCR	C23-C24-C25-C30
17	K	4001	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	K	4001	BCR	C23-C24-C25-C26
17	K	4005	BCR	C1-C6-C7-C8
17	a	847	BCR	C5-C6-C7-C8
17	a	847	BCR	C23-C24-C25-C30
17	a	848	BCR	C5-C6-C7-C8
17	a	849	BCR	C5-C6-C7-C8
17	a	849	BCR	C23-C24-C25-C26
17	a	850	BCR	C5-C6-C7-C8
17	a	850	BCR	C23-C24-C25-C30
17	1	847	BCR	C5-C6-C7-C8
17	1	847	BCR	C23-C24-C25-C30
17	1	848	BCR	C5-C6-C7-C8
17	1	849	BCR	C5-C6-C7-C8
17	1	849	BCR	C23-C24-C25-C26
17	1	850	BCR	C5-C6-C7-C8
17	1	850	BCR	C23-C24-C25-C30
17	b	846	BCR	C5-C6-C7-C8
17	b	846	BCR	C23-C24-C25-C26
17	b	847	BCR	C5-C6-C7-C8
17	b	849	BCR	C5-C6-C7-C8
17	b	850	BCR	C1-C6-C7-C8
17	b	850	BCR	C5-C6-C7-C8
17	b	850	BCR	C23-C24-C25-C26
17	b	851	BCR	C1-C6-C7-C8
17	b	851	BCR	C23-C24-C25-C26
17	b	853	BCR	C23-C24-C25-C30
17	b	854	BCR	C23-C24-C25-C30
17	2	846	BCR	C5-C6-C7-C8
17	2	846	BCR	C23-C24-C25-C26
17	2	847	BCR	C5-C6-C7-C8
17	2	849	BCR	C5-C6-C7-C8
17	2	850	BCR	C1-C6-C7-C8
17	2	850	BCR	C5-C6-C7-C8
17	2	850	BCR	C23-C24-C25-C26
17	2	851	BCR	C1-C6-C7-C8
17	2	851	BCR	C23-C24-C25-C26
17	f	203	BCR	C5-C6-C7-C8
17	f	206	BCR	C5-C6-C7-C8
17	6	4402	BCR	C5-C6-C7-C8
17	6	4405	BCR	C5-C6-C7-C8
17	6	4406	BCR	C23-C24-C25-C30
17	i	4103	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
17	h	102	BCR	C23-C24-C25-C26
17	j	104	BCR	C23-C24-C25-C26
17	7	1105	BCR	C23-C24-C25-C26
17	k	4001	BCR	C5-C6-C7-C8
17	k	4001	BCR	C23-C24-C25-C26
17	k	4004	BCR	C1-C6-C7-C8
17	8	4001	BCR	C5-C6-C7-C8
17	8	4001	BCR	C23-C24-C25-C26
17	8	4005	BCR	C1-C6-C7-C8
17	l	4207	BCR	C5-C6-C7-C8
17	0	204	BCR	C5-C6-C7-C8
17	0	204	BCR	C23-C24-C25-C30
17	0	209	BCR	C5-C6-C7-C8
17	0	210	BCR	C5-C6-C7-C8
17	0	210	BCR	C23-C24-C25-C30
17	9	102	BCR	C23-C24-C25-C30
18	A	852	LMG	C28-C29-C30-C31
18	0	203	LMG	C28-C29-C30-C31
14	B	826	CLA	CAA-CBA-CGA-O1A
14	K	4002	CLA	CAA-CBA-CGA-O2A
14	2	825	CLA	CAA-CBA-CGA-O1A
14	k	4002	CLA	CAA-CBA-CGA-O2A
14	8	4002	CLA	CAA-CBA-CGA-O2A
18	B	803	LMG	C29-C28-O8-C9
12	A	801	LHG	C2-C3-O3-P
12	a	801	LHG	C2-C3-O3-P
12	1	801	LHG	C2-C3-O3-P
14	b	825	CLA	CAA-CBA-CGA-O1A
14	A	810	CLA	C4-C3-C5-C6
14	a	811	CLA	C4-C3-C5-C6
14	1	809	CLA	C4-C3-C5-C6
14	L	1501	CLA	C2-C3-C5-C6
18	a	852	LMG	C28-C29-C30-C31
18	b	803	LMG	C29-C28-O8-C9
18	2	802	LMG	C29-C28-O8-C9
14	a	842	CLA	O1A-CGA-O2A-C1
14	A	808	CLA	C12-C13-C15-C16
14	A	813	CLA	C6-C7-C8-C10
14	A	813	CLA	C11-C10-C8-C7
14	A	821	CLA	C11-C12-C13-C15
14	A	839	CLA	C11-C12-C13-C15
14	B	816	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	B	821	CLA	C6-C7-C8-C10
14	B	844	CLA	C11-C12-C13-C15
14	L	1502	CLA	C11-C12-C13-C15
14	a	809	CLA	C12-C13-C15-C16
14	a	814	CLA	C6-C7-C8-C10
14	a	814	CLA	C11-C10-C8-C7
14	a	822	CLA	C11-C12-C13-C15
14	a	840	CLA	C11-C12-C13-C15
14	1	807	CLA	C12-C13-C15-C16
14	1	812	CLA	C6-C7-C8-C10
14	1	812	CLA	C11-C10-C8-C7
14	1	820	CLA	C11-C12-C13-C15
14	1	838	CLA	C11-C12-C13-C15
14	b	815	CLA	C6-C7-C8-C10
14	b	820	CLA	C6-C7-C8-C10
14	b	843	CLA	C11-C12-C13-C15
14	2	815	CLA	C6-C7-C8-C10
14	2	820	CLA	C6-C7-C8-C10
14	2	843	CLA	C11-C12-C13-C15
14	l	4205	CLA	C11-C12-C13-C15
14	0	207	CLA	C11-C12-C13-C15
14	B	821	CLA	C2A-CAA-CBA-CGA
14	b	820	CLA	C2A-CAA-CBA-CGA
14	2	820	CLA	C2A-CAA-CBA-CGA
18	L	1506	LMG	C35-C36-C37-C38
18	l	4202	LMG	C35-C36-C37-C38
18	0	201	LMG	C35-C36-C37-C38
17	1	851	BCR	C7-C8-C9-C34
14	B	808	CLA	C4-C3-C5-C6
14	B	834	CLA	C4-C3-C5-C6
14	b	808	CLA	C4-C3-C5-C6
14	b	833	CLA	C4-C3-C5-C6
14	2	807	CLA	C4-C3-C5-C6
14	2	833	CLA	C4-C3-C5-C6
14	B	806	CLA	C2-C3-C5-C6
14	B	812	CLA	C2-C3-C5-C6
14	b	806	CLA	C2-C3-C5-C6
14	b	812	CLA	C2-C3-C5-C6
14	2	805	CLA	C2-C3-C5-C6
14	2	811	CLA	C2-C3-C5-C6
14	F	205	CLA	CAA-CBA-CGA-O1A
14	f	205	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	6	4404	CLA	CAA-CBA-CGA-O1A
17	1	851	BCR	C11-C12-C13-C14
14	a	816	CLA	O1D-CGD-O2D-CED
14	1	814	CLA	O1D-CGD-O2D-CED
14	A	813	CLA	C5-C6-C7-C8
14	a	814	CLA	C5-C6-C7-C8
14	1	812	CLA	C5-C6-C7-C8
14	A	815	CLA	O1D-CGD-O2D-CED
14	F	205	CLA	CAA-CBA-CGA-O2A
14	K	4002	CLA	CAA-CBA-CGA-O1A
14	f	205	CLA	CAA-CBA-CGA-O2A
14	6	4404	CLA	CAA-CBA-CGA-O2A
14	k	4002	CLA	CAA-CBA-CGA-O1A
14	B	816	CLA	C14-C13-C15-C16
14	b	815	CLA	C14-C13-C15-C16
14	2	815	CLA	C14-C13-C15-C16
13	A	803	CL0	CAA-CBA-CGA-O1A
13	a	803	CL0	CAA-CBA-CGA-O1A
14	8	4002	CLA	CAA-CBA-CGA-O1A
13	1	803	CL0	CAA-CBA-CGA-O1A
17	L	1504	BCR	C22-C23-C24-C25
17	l	4207	BCR	C22-C23-C24-C25
17	0	209	BCR	C22-C23-C24-C25
14	A	805	CLA	C4-C3-C5-C6
14	A	830	CLA	C4-C3-C5-C6
14	B	806	CLA	C4-C3-C5-C6
14	a	806	CLA	C4-C3-C5-C6
14	a	831	CLA	C4-C3-C5-C6
14	1	829	CLA	C4-C3-C5-C6
14	b	806	CLA	C4-C3-C5-C6
14	2	805	CLA	C4-C3-C5-C6
14	7	1101	CLA	C4-C3-C5-C6
14	B	802	CLA	C2-C3-C5-C6
14	b	801	CLA	C2-C3-C5-C6
14	0	202	CLA	C2-C3-C5-C6
12	m	101	LHG	C32-C33-C34-C35
14	A	837	CLA	CAA-CBA-CGA-O2A
14	a	838	CLA	CAA-CBA-CGA-O2A
14	1	836	CLA	CAA-CBA-CGA-O2A
12	M	101	LHG	C32-C33-C34-C35
12	9	101	LHG	C32-C33-C34-C35
18	A	853	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	a	853	LMG	O1-C7-C8-C9
18	1	852	LMG	O1-C7-C8-C9
14	A	814	CLA	C2A-CAA-CBA-CGA
14	B	819	CLA	C2A-CAA-CBA-CGA
14	B	841	CLA	C2A-CAA-CBA-CGA
14	a	815	CLA	C2A-CAA-CBA-CGA
14	1	813	CLA	C2A-CAA-CBA-CGA
14	b	818	CLA	C2A-CAA-CBA-CGA
14	b	840	CLA	C2A-CAA-CBA-CGA
14	2	818	CLA	C2A-CAA-CBA-CGA
14	2	840	CLA	C2A-CAA-CBA-CGA
14	B	804	CLA	C4-C3-C5-C6
14	B	807	CLA	C4-C3-C5-C6
14	b	804	CLA	C4-C3-C5-C6
14	b	807	CLA	C4-C3-C5-C6
14	2	803	CLA	C4-C3-C5-C6
14	2	806	CLA	C4-C3-C5-C6
14	A	844	CLA	CAA-CBA-CGA-O2A
14	a	844	CLA	CAA-CBA-CGA-O2A
14	1	844	CLA	CAA-CBA-CGA-O2A
14	B	807	CLA	C2-C3-C5-C6
14	2	806	CLA	C2-C3-C5-C6
14	7	1101	CLA	C2-C3-C5-C6
14	6	4403	CLA	C4C-C3C-CAC-CBC
14	A	807	CLA	C4B-C3B-CAB-CBB
14	B	818	CLA	C4B-C3B-CAB-CBB
14	B	827	CLA	C4B-C3B-CAB-CBB
14	F	204	CLA	C4C-C3C-CAC-CBC
14	a	808	CLA	C4B-C3B-CAB-CBB
14	1	806	CLA	C4B-C3B-CAB-CBB
14	b	826	CLA	C4B-C3B-CAB-CBB
14	2	817	CLA	C4B-C3B-CAB-CBB
14	2	826	CLA	C4B-C3B-CAB-CBB
14	f	204	CLA	C4C-C3C-CAC-CBC
14	2	823	CLA	CAA-CBA-CGA-O2A
14	B	824	CLA	CAA-CBA-CGA-O2A
14	b	823	CLA	CAA-CBA-CGA-O2A
14	1	840	CLA	C16-C17-C18-C20
14	b	802	CLA	C16-C17-C18-C20
17	A	849	BCR	C16-C17-C18-C36
17	A	850	BCR	C16-C17-C18-C36
17	B	850	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
17	I	102	BCR	C20-C21-C22-C37
17	a	849	BCR	C16-C17-C18-C36
17	a	850	BCR	C16-C17-C18-C36
17	1	849	BCR	C16-C17-C18-C36
17	1	850	BCR	C16-C17-C18-C36
17	b	849	BCR	C16-C17-C18-C36
17	2	849	BCR	C16-C17-C18-C36
17	i	4103	BCR	C20-C21-C22-C37
17	h	102	BCR	C20-C21-C22-C37
17	l	4207	BCR	C16-C17-C18-C36
17	0	209	BCR	C16-C17-C18-C36
14	A	808	CLA	C10-C11-C12-C13
14	a	809	CLA	C10-C11-C12-C13
14	1	807	CLA	C10-C11-C12-C13
18	A	852	LMG	C14-C15-C16-C17
18	a	852	LMG	C14-C15-C16-C17
14	B	815	CLA	CAA-CBA-CGA-O2A
14	B	825	CLA	CAA-CBA-CGA-O2A
14	b	814	CLA	CAA-CBA-CGA-O2A
14	b	824	CLA	CAA-CBA-CGA-O2A
14	2	814	CLA	CAA-CBA-CGA-O2A
14	2	824	CLA	CAA-CBA-CGA-O2A
18	0	203	LMG	C14-C15-C16-C17
14	A	841	CLA	C16-C17-C18-C20
18	A	853	LMG	O7-C8-C9-O8
18	a	853	LMG	O7-C8-C9-O8
18	1	852	LMG	O7-C8-C9-O8
14	A	805	CLA	C2-C3-C5-C6
14	a	806	CLA	C2-C3-C5-C6
14	b	807	CLA	C2-C3-C5-C6
14	B	812	CLA	C11-C10-C8-C7
14	b	812	CLA	C11-C10-C8-C7
14	2	811	CLA	C11-C10-C8-C7
17	K	4005	BCR	C9-C10-C11-C12
17	k	4004	BCR	C9-C10-C11-C12
17	8	4005	BCR	C9-C10-C11-C12
14	A	832	CLA	C11-C10-C8-C9
14	a	833	CLA	C11-C10-C8-C9
14	1	831	CLA	C11-C10-C8-C9
14	K	4003	CLA	CAA-CBA-CGA-O2A
14	k	4003	CLA	CAA-CBA-CGA-O2A
14	8	4003	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	A	805	CLA	C2-C1-O2A-CGA
14	a	806	CLA	C2-C1-O2A-CGA
14	7	1101	CLA	C2-C1-O2A-CGA
14	A	811	CLA	C3A-C2A-CAA-CBA
14	A	816	CLA	C3A-C2A-CAA-CBA
14	B	808	CLA	C3A-C2A-CAA-CBA
14	K	4004	CLA	C3A-C2A-CAA-CBA
14	a	812	CLA	C3A-C2A-CAA-CBA
14	a	817	CLA	C3A-C2A-CAA-CBA
14	a	854	CLA	C3A-C2A-CAA-CBA
14	1	810	CLA	C3A-C2A-CAA-CBA
14	1	815	CLA	C3A-C2A-CAA-CBA
14	b	808	CLA	C3A-C2A-CAA-CBA
14	2	807	CLA	C3A-C2A-CAA-CBA
14	8	4004	CLA	C3A-C2A-CAA-CBA
14	a	844	CLA	CAA-CBA-CGA-O1A
14	1	844	CLA	CAA-CBA-CGA-O1A
14	A	844	CLA	CAA-CBA-CGA-O1A
14	B	824	CLA	CAA-CBA-CGA-O1A
14	b	823	CLA	CAA-CBA-CGA-O1A
14	2	823	CLA	CAA-CBA-CGA-O1A
14	a	804	CLA	C2C-C3C-CAC-CBC
14	2	801	CLA	C2C-C3C-CAC-CBC
14	A	837	CLA	CAA-CBA-CGA-O1A
14	a	838	CLA	CAA-CBA-CGA-O1A
14	1	836	CLA	CAA-CBA-CGA-O1A
14	2	822	CLA	CAA-CBA-CGA-O2A
14	B	823	CLA	CAA-CBA-CGA-O2A
14	b	822	CLA	CAA-CBA-CGA-O2A
17	A	851	BCR	C16-C17-C18-C19
17	B	850	BCR	C12-C13-C14-C15
17	F	206	BCR	C12-C13-C14-C15
17	I	101	BCR	C20-C21-C22-C23
17	a	851	BCR	C16-C17-C18-C19
17	1	851	BCR	C16-C17-C18-C19
17	b	849	BCR	C12-C13-C14-C15
17	2	849	BCR	C12-C13-C14-C15
17	f	206	BCR	C12-C13-C14-C15
17	6	4405	BCR	C12-C13-C14-C15
17	i	4102	BCR	C20-C21-C22-C23
17	h	101	BCR	C20-C21-C22-C23
12	B	853	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
12	b	852	LHG	O6-C4-C5-O7
12	2	852	LHG	O6-C4-C5-O7
14	a	828	CLA	C5-C6-C7-C8
14	2	801	CLA	C8-C10-C11-C12
14	k	4003	CLA	CAA-CBA-CGA-O1A
14	B	801	CLA	C2C-C3C-CAC-CBC
14	B	827	CLA	C4-C3-C5-C6
14	b	826	CLA	C4-C3-C5-C6
14	2	826	CLA	C4-C3-C5-C6
14	B	823	CLA	CAA-CBA-CGA-O1A
14	K	4003	CLA	CAA-CBA-CGA-O1A
14	b	822	CLA	CAA-CBA-CGA-O1A
14	2	822	CLA	CAA-CBA-CGA-O1A
14	8	4003	CLA	CAA-CBA-CGA-O1A
12	A	801	LHG	C10-C11-C12-C13
14	A	827	CLA	C5-C6-C7-C8
14	B	801	CLA	C8-C10-C11-C12
14	a	804	CLA	C8-C10-C11-C12
14	1	826	CLA	C5-C6-C7-C8
12	a	801	LHG	C10-C11-C12-C13
12	1	801	LHG	C10-C11-C12-C13
14	B	815	CLA	CAA-CBA-CGA-O1A
14	2	814	CLA	CAA-CBA-CGA-O1A
14	a	811	CLA	CAA-CBA-CGA-O2A
14	1	809	CLA	CAA-CBA-CGA-O2A
14	b	814	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	C11-C10-C8-C9
14	A	835	CLA	C14-C13-C15-C16
14	B	841	CLA	C11-C12-C13-C14
14	L	1503	CLA	C11-C12-C13-C14
14	L	1503	CLA	C14-C13-C15-C16
14	a	814	CLA	C11-C10-C8-C9
14	a	836	CLA	C14-C13-C15-C16
14	1	812	CLA	C11-C10-C8-C9
14	1	834	CLA	C14-C13-C15-C16
14	b	840	CLA	C11-C12-C13-C14
14	2	840	CLA	C11-C12-C13-C14
14	l	4206	CLA	C11-C12-C13-C14
14	l	4206	CLA	C14-C13-C15-C16
14	0	208	CLA	C11-C12-C13-C14
14	0	208	CLA	C14-C13-C15-C16
14	A	810	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	B	853	LHG	O6-C4-C5-C6
12	b	852	LHG	O6-C4-C5-C6
12	2	852	LHG	O6-C4-C5-C6
18	a	853	LMG	O7-C10-C11-C12
14	B	804	CLA	C6-C7-C8-C10
14	L	1501	CLA	C12-C13-C15-C16
14	b	804	CLA	C6-C7-C8-C10
14	2	803	CLA	C6-C7-C8-C10
14	l	4204	CLA	C12-C13-C15-C16
14	0	206	CLA	C12-C13-C15-C16
14	A	824	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	C2B-C3B-CAB-CBB
14	A	819	CLA	C2B-C3B-CAB-CBB
14	A	822	CLA	C2B-C3B-CAB-CBB
14	A	827	CLA	C2B-C3B-CAB-CBB
14	A	844	CLA	C2B-C3B-CAB-CBB
14	B	804	CLA	C2B-C3B-CAB-CBB
14	B	810	CLA	C2B-C3B-CAB-CBB
14	B	816	CLA	C2B-C3B-CAB-CBB
14	F	204	CLA	C2B-C3B-CAB-CBB
14	a	812	CLA	C2B-C3B-CAB-CBB
14	a	820	CLA	C2B-C3B-CAB-CBB
14	a	823	CLA	C2B-C3B-CAB-CBB
14	a	844	CLA	C2B-C3B-CAB-CBB
14	1	810	CLA	C2B-C3B-CAB-CBB
14	1	818	CLA	C2B-C3B-CAB-CBB
14	1	821	CLA	C2B-C3B-CAB-CBB
14	1	844	CLA	C2B-C3B-CAB-CBB
14	b	804	CLA	C2B-C3B-CAB-CBB
14	b	810	CLA	C2B-C3B-CAB-CBB
14	b	815	CLA	C2B-C3B-CAB-CBB
14	2	803	CLA	C2B-C3B-CAB-CBB
14	2	809	CLA	C2B-C3B-CAB-CBB
14	2	815	CLA	C2B-C3B-CAB-CBB
14	f	204	CLA	C2B-C3B-CAB-CBB
14	6	4403	CLA	C2B-C3B-CAB-CBB
17	A	850	BCR	C23-C24-C25-C26
17	B	852	BCR	C5-C6-C7-C8
17	B	854	BCR	C23-C24-C25-C26
17	F	203	BCR	C23-C24-C25-C26
17	F	203	BCR	C23-C24-C25-C30
17	F	206	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
17	F	206	BCR	C23-C24-C25-C30
17	J	103	BCR	C1-C6-C7-C8
17	J	103	BCR	C5-C6-C7-C8
17	J	104	BCR	C5-C6-C7-C8
17	L	1505	BCR	C23-C24-C25-C26
17	M	102	BCR	C23-C24-C25-C26
17	K	4005	BCR	C23-C24-C25-C26
17	K	4005	BCR	C23-C24-C25-C30
17	a	850	BCR	C23-C24-C25-C26
17	1	850	BCR	C23-C24-C25-C26
17	b	851	BCR	C5-C6-C7-C8
17	b	853	BCR	C23-C24-C25-C26
17	b	854	BCR	C23-C24-C25-C26
17	2	851	BCR	C5-C6-C7-C8
17	f	203	BCR	C23-C24-C25-C26
17	f	203	BCR	C23-C24-C25-C30
17	f	206	BCR	C23-C24-C25-C26
17	6	4402	BCR	C23-C24-C25-C26
17	6	4402	BCR	C23-C24-C25-C30
17	6	4405	BCR	C23-C24-C25-C26
17	6	4406	BCR	C23-C24-C25-C26
17	j	103	BCR	C1-C6-C7-C8
17	j	103	BCR	C5-C6-C7-C8
17	j	104	BCR	C5-C6-C7-C8
17	7	1104	BCR	C1-C6-C7-C8
17	7	1104	BCR	C5-C6-C7-C8
17	7	1105	BCR	C5-C6-C7-C8
17	k	4004	BCR	C23-C24-C25-C26
17	k	4004	BCR	C23-C24-C25-C30
17	8	4005	BCR	C23-C24-C25-C26
17	8	4005	BCR	C23-C24-C25-C30
17	0	204	BCR	C23-C24-C25-C26
17	0	210	BCR	C23-C24-C25-C26
17	9	102	BCR	C23-C24-C25-C26
18	A	853	LMG	O7-C10-C11-C12
18	1	852	LMG	O7-C10-C11-C12
14	A	822	CLA	C2-C1-O2A-CGA
14	B	809	CLA	C2-C1-O2A-CGA
14	a	823	CLA	C2-C1-O2A-CGA
14	1	821	CLA	C2-C1-O2A-CGA
14	b	809	CLA	C2-C1-O2A-CGA
14	2	808	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	a	825	CLA	O1A-CGA-O2A-C1
14	A	823	CLA	CAA-CBA-CGA-O2A
14	a	824	CLA	CAA-CBA-CGA-O2A
14	1	822	CLA	CAA-CBA-CGA-O2A
14	B	832	CLA	C4-C3-C5-C6
14	b	831	CLA	C4-C3-C5-C6
14	a	837	CLA	CAA-CBA-CGA-O2A
14	1	835	CLA	CAA-CBA-CGA-O2A
12	B	853	LHG	O2-C2-C3-O3
12	2	852	LHG	O2-C2-C3-O3
14	1	823	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	CAA-CBA-CGA-O2A
12	A	802	LHG	C11-C10-C9-C8
12	a	802	LHG	C11-C10-C9-C8
12	1	802	LHG	C11-C10-C9-C8
18	L	1506	LMG	C37-C38-C39-C40
18	0	201	LMG	C37-C38-C39-C40
14	B	812	CLA	C12-C13-C15-C16
14	b	812	CLA	C12-C13-C15-C16
14	2	811	CLA	C12-C13-C15-C16
18	l	4202	LMG	C37-C38-C39-C40
14	2	831	CLA	C4-C3-C5-C6
14	A	832	CLA	C2-C3-C5-C6
14	a	833	CLA	C2-C3-C5-C6
14	1	831	CLA	C2-C3-C5-C6
14	a	843	CLA	C2C-C3C-CAC-CBC
14	A	812	CLA	CAA-CBA-CGA-O2A
14	a	813	CLA	CAA-CBA-CGA-O2A
14	1	811	CLA	CAA-CBA-CGA-O2A
14	A	843	CLA	C2C-C3C-CAC-CBC
14	1	843	CLA	C2C-C3C-CAC-CBC
14	A	807	CLA	C11-C10-C8-C9
14	A	808	CLA	C14-C13-C15-C16
14	A	826	CLA	C11-C10-C8-C9
14	A	839	CLA	C11-C12-C13-C14
14	B	816	CLA	C6-C7-C8-C9
14	a	808	CLA	C11-C10-C8-C9
14	a	809	CLA	C14-C13-C15-C16
14	a	827	CLA	C11-C10-C8-C9
14	a	840	CLA	C11-C12-C13-C14
14	1	806	CLA	C11-C10-C8-C9
14	1	807	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	1	825	CLA	C11-C10-C8-C9
14	1	838	CLA	C11-C12-C13-C14
14	b	815	CLA	C6-C7-C8-C9
14	2	815	CLA	C6-C7-C8-C9
12	M	101	LHG	O8-C23-C24-C25
12	9	101	LHG	O8-C23-C24-C25
14	b	842	CLA	CAA-CBA-CGA-O2A
12	b	852	LHG	O2-C2-C3-O3
14	B	802	CLA	C4B-C3B-CAB-CBB
14	B	808	CLA	C1A-C2A-CAA-CBA
14	B	813	CLA	C1A-C2A-CAA-CBA
14	B	832	CLA	C4B-C3B-CAB-CBB
14	B	835	CLA	C4B-C3B-CAB-CBB
14	L	1503	CLA	C4B-C3B-CAB-CBB
14	K	4004	CLA	C4B-C3B-CAB-CBB
14	a	854	CLA	C4B-C3B-CAB-CBB
14	b	801	CLA	C4B-C3B-CAB-CBB
14	b	808	CLA	C1A-C2A-CAA-CBA
14	b	817	CLA	C4B-C3B-CAB-CBB
14	b	831	CLA	C4B-C3B-CAB-CBB
14	b	834	CLA	C4B-C3B-CAB-CBB
14	2	807	CLA	C1A-C2A-CAA-CBA
14	2	812	CLA	C1A-C2A-CAA-CBA
14	2	831	CLA	C4B-C3B-CAB-CBB
14	2	834	CLA	C4B-C3B-CAB-CBB
14	8	4004	CLA	C4B-C3B-CAB-CBB
14	l	4203	CLA	C1A-C2A-CAA-CBA
14	l	4206	CLA	C4B-C3B-CAB-CBB
14	0	202	CLA	C4B-C3B-CAB-CBB
14	0	208	CLA	C4B-C3B-CAB-CBB
14	B	811	CLA	CBA-CGA-O2A-C1
14	b	811	CLA	CBA-CGA-O2A-C1
14	2	810	CLA	CBA-CGA-O2A-C1
18	A	852	LMG	O6-C1-O1-C7
18	a	852	LMG	O6-C1-O1-C7
18	0	203	LMG	O6-C1-O1-C7
12	m	101	LHG	O8-C23-C24-C25
14	B	809	CLA	CAA-CBA-CGA-O2A
14	2	829	CLA	CAA-CBA-CGA-O2A
14	A	812	CLA	CAA-CBA-CGA-O1A
14	a	813	CLA	CAA-CBA-CGA-O1A
14	1	811	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	B	854	BCR	C21-C22-C23-C24
17	b	853	BCR	C21-C22-C23-C24
17	6	4406	BCR	C21-C22-C23-C24
17	a	851	BCR	C19-C20-C21-C22
17	1	851	BCR	C19-C20-C21-C22
14	B	843	CLA	CAA-CBA-CGA-O2A
14	1	823	CLA	CAA-CBA-CGA-O2A
14	b	809	CLA	CAA-CBA-CGA-O2A
14	2	808	CLA	CAA-CBA-CGA-O2A
14	2	842	CLA	CAA-CBA-CGA-O2A
14	B	827	CLA	C2A-CAA-CBA-CGA
14	b	826	CLA	C2A-CAA-CBA-CGA
14	2	826	CLA	C2A-CAA-CBA-CGA
14	B	811	CLA	C15-C16-C17-C18
14	b	811	CLA	C15-C16-C17-C18
14	A	824	CLA	CAA-CBA-CGA-O2A
14	B	830	CLA	CAA-CBA-CGA-O2A
14	a	825	CLA	CAA-CBA-CGA-O2A
14	b	829	CLA	CAA-CBA-CGA-O2A
14	2	810	CLA	C15-C16-C17-C18
14	A	813	CLA	C2-C1-O2A-CGA
14	B	816	CLA	C2-C1-O2A-CGA
14	a	814	CLA	C2-C1-O2A-CGA
14	1	812	CLA	C2-C1-O2A-CGA
14	b	815	CLA	C2-C1-O2A-CGA
14	2	815	CLA	C2-C1-O2A-CGA
14	1	810	CLA	CAA-CBA-CGA-O2A
14	A	822	CLA	C6-C7-C8-C10
14	A	832	CLA	C11-C10-C8-C7
14	A	842	CLA	C11-C10-C8-C7
14	a	823	CLA	C6-C7-C8-C10
14	a	833	CLA	C11-C10-C8-C7
14	a	842	CLA	C11-C10-C8-C7
14	1	821	CLA	C6-C7-C8-C10
14	1	831	CLA	C11-C10-C8-C7
14	1	842	CLA	C11-C10-C8-C7
14	A	824	CLA	CBA-CGA-O2A-C1
14	a	825	CLA	CBA-CGA-O2A-C1
14	1	823	CLA	CBA-CGA-O2A-C1
18	2	802	LMG	C35-C36-C37-C38
14	A	811	CLA	CAA-CBA-CGA-O2A
14	a	812	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	b	803	LMG	C35-C36-C37-C38
17	A	851	BCR	C19-C20-C21-C22
18	B	803	LMG	C35-C36-C37-C38
14	b	840	CLA	C5-C6-C7-C8
14	2	808	CLA	C8-C10-C11-C12
14	B	809	CLA	C8-C10-C11-C12
14	b	809	CLA	C8-C10-C11-C12
14	2	840	CLA	C5-C6-C7-C8
14	B	833	CLA	CAA-CBA-CGA-O2A
14	2	832	CLA	CAA-CBA-CGA-O2A
14	A	813	CLA	C3A-C2A-CAA-CBA
14	B	817	CLA	C3A-C2A-CAA-CBA
14	B	835	CLA	C3A-C2A-CAA-CBA
14	a	814	CLA	C3A-C2A-CAA-CBA
14	1	812	CLA	C3A-C2A-CAA-CBA
14	b	816	CLA	C3A-C2A-CAA-CBA
14	b	834	CLA	C3A-C2A-CAA-CBA
14	2	816	CLA	C3A-C2A-CAA-CBA
14	2	834	CLA	C3A-C2A-CAA-CBA
14	B	841	CLA	C5-C6-C7-C8
14	A	810	CLA	C2-C3-C5-C6
12	A	801	LHG	C11-C10-C9-C8
12	a	801	LHG	C11-C10-C9-C8
17	A	848	BCR	C12-C13-C14-C15
17	1	848	BCR	C12-C13-C14-C15
14	b	832	CLA	CAA-CBA-CGA-O2A
14	A	836	CLA	CAA-CBA-CGA-O1A
14	1	835	CLA	CAA-CBA-CGA-O1A
12	1	801	LHG	C11-C10-C9-C8
14	a	824	CLA	CAA-CBA-CGA-O1A
14	a	837	CLA	CAA-CBA-CGA-O1A
14	1	806	CLA	C2A-CAA-CBA-CGA
14	b	827	CLA	CBA-CGA-O2A-C1
14	A	830	CLA	C14-C13-C15-C16
14	A	842	CLA	C11-C10-C8-C9
14	B	804	CLA	C6-C7-C8-C9
14	B	844	CLA	C11-C12-C13-C14
14	a	831	CLA	C14-C13-C15-C16
14	a	842	CLA	C11-C10-C8-C9
14	1	829	CLA	C14-C13-C15-C16
14	1	842	CLA	C11-C10-C8-C9
14	b	804	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	b	843	CLA	C11-C12-C13-C14
14	2	803	CLA	C6-C7-C8-C9
14	2	843	CLA	C11-C12-C13-C14
14	A	823	CLA	CAA-CBA-CGA-O1A
14	1	822	CLA	CAA-CBA-CGA-O1A
14	A	826	CLA	C3-C5-C6-C7
14	a	827	CLA	C3-C5-C6-C7
14	1	825	CLA	C3-C5-C6-C7
18	a	852	LMG	O6-C5-C6-O5
14	B	828	CLA	CBA-CGA-O2A-C1
14	2	827	CLA	CBA-CGA-O2A-C1
14	a	811	CLA	C2-C3-C5-C6
14	1	809	CLA	C2-C3-C5-C6
14	A	838	CLA	C4-C3-C5-C6
14	a	839	CLA	C4-C3-C5-C6
14	1	837	CLA	C4-C3-C5-C6
14	B	828	CLA	O1A-CGA-O2A-C1
14	b	827	CLA	O1A-CGA-O2A-C1
14	2	806	CLA	C6-C7-C8-C9
14	B	807	CLA	C6-C7-C8-C9
14	b	807	CLA	C6-C7-C8-C9
14	A	810	CLA	CAA-CBA-CGA-O1A
14	a	811	CLA	CAA-CBA-CGA-O1A
14	1	809	CLA	CAA-CBA-CGA-O1A
14	2	842	CLA	CAA-CBA-CGA-O1A
18	L	1506	LMG	C8-C7-O1-C1
18	l	4202	LMG	C8-C7-O1-C1
18	0	201	LMG	C8-C7-O1-C1
14	2	827	CLA	O1A-CGA-O2A-C1
18	A	852	LMG	O7-C8-C9-O8
18	a	852	LMG	O7-C8-C9-O8
18	0	203	LMG	O7-C8-C9-O8
14	B	843	CLA	CAA-CBA-CGA-O1A
14	a	828	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	C2A-CAA-CBA-CGA
14	a	808	CLA	C2A-CAA-CBA-CGA
18	0	203	LMG	O6-C5-C6-O5
14	b	842	CLA	CAA-CBA-CGA-O1A
18	l	4202	LMG	O10-C28-C29-C30
18	A	852	LMG	O6-C5-C6-O5
14	A	827	CLA	CAA-CBA-CGA-O2A
14	1	826	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	B	834	CLA	C2-C3-C5-C6
14	b	833	CLA	C2-C3-C5-C6
14	2	833	CLA	C2-C3-C5-C6
12	A	801	LHG	C15-C16-C17-C18
12	a	801	LHG	C15-C16-C17-C18
12	1	801	LHG	C15-C16-C17-C18
14	A	834	CLA	CAD-CBD-CGD-O2D
14	B	822	CLA	CAD-CBD-CGD-O2D
14	B	835	CLA	CAD-CBD-CGD-O2D
14	a	835	CLA	CAD-CBD-CGD-O2D
14	1	833	CLA	CAD-CBD-CGD-O2D
14	b	821	CLA	CAD-CBD-CGD-O2D
14	b	834	CLA	CAD-CBD-CGD-O2D
14	2	821	CLA	CAD-CBD-CGD-O2D
14	2	834	CLA	CAD-CBD-CGD-O2D
14	f	204	CLA	CAA-CBA-CGA-O2A
14	6	4403	CLA	CAA-CBA-CGA-O2A
18	L	1506	LMG	O10-C28-C29-C30
14	F	204	CLA	CAA-CBA-CGA-O2A
14	A	824	CLA	CAA-CBA-CGA-O1A
14	1	810	CLA	CAA-CBA-CGA-O1A
18	0	201	LMG	O10-C28-C29-C30
14	a	832	CLA	CAA-CBA-CGA-O2A
14	B	833	CLA	CAA-CBA-CGA-O1A
14	b	832	CLA	CAA-CBA-CGA-O1A
14	2	832	CLA	CAA-CBA-CGA-O1A
14	a	812	CLA	CAA-CBA-CGA-O1A
14	a	825	CLA	CAA-CBA-CGA-O1A
14	1	823	CLA	CAA-CBA-CGA-O1A
14	2	810	CLA	O1A-CGA-O2A-C1
14	A	831	CLA	CAA-CBA-CGA-O2A
14	1	830	CLA	CAA-CBA-CGA-O2A
14	A	811	CLA	CAA-CBA-CGA-O1A
14	f	204	CLA	CAA-CBA-CGA-O1A
14	B	809	CLA	CAA-CBA-CGA-O1A
14	b	809	CLA	CAA-CBA-CGA-O1A
14	2	808	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

359 monomers are involved in 953 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	821	CLA	4	0
14	2	805	CLA	3	0
17	i	4103	BCR	3	0
14	b	843	CLA	5	0
14	A	832	CLA	7	0
17	1	850	BCR	6	0
17	b	846	BCR	2	0
14	1	829	CLA	11	0
14	1	826	CLA	8	0
14	2	819	CLA	3	0
14	A	820	CLA	4	0
14	A	828	CLA	4	0
14	b	816	CLA	1	0
14	b	833	CLA	1	0
14	a	829	CLA	3	0
17	J	104	BCR	2	0
14	B	822	CLA	2	0
14	B	830	CLA	2	0
14	A	810	CLA	7	0
19	I	103	LMT	1	0
14	B	804	CLA	7	0
17	B	848	BCR	2	0
14	B	817	CLA	1	0
14	B	835	CLA	1	0
14	a	843	CLA	5	0
14	a	842	CLA	7	0
14	1	823	CLA	1	0
14	a	813	CLA	2	0
14	l	4205	CLA	4	0
17	l	4207	BCR	1	0
17	I	102	BCR	4	0
19	h	103	LMT	1	0
17	6	4402	BCR	4	0
17	i	4102	BCR	2	0
17	9	102	BCR	4	0
14	A	804	CLA	5	0
14	a	814	CLA	4	0
14	b	835	CLA	3	0
14	A	837	CLA	1	0
14	2	825	CLA	5	0
14	A	817	CLA	1	0
14	2	831	CLA	8	0
14	7	1101	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	830	CLA	4	0
14	2	803	CLA	9	0
14	B	844	CLA	5	0
14	1	835	CLA	6	0
16	3	102	SF4	1	0
14	a	820	CLA	1	0
14	2	817	CLA	2	0
14	b	820	CLA	2	0
17	A	847	BCR	2	0
17	J	103	BCR	3	0
14	b	804	CLA	8	0
14	L	1502	CLA	2	0
14	J	101	CLA	1	0
17	2	851	BCR	5	0
14	B	825	CLA	1	0
14	A	821	CLA	3	0
17	M	102	BCR	5	0
14	8	4003	CLA	1	0
14	A	825	CLA	1	0
17	h	102	BCR	3	0
14	6	4403	CLA	3	0
14	a	840	CLA	5	0
14	2	827	CLA	1	0
12	b	852	LHG	2	0
14	2	821	CLA	2	0
15	a	845	PQN	1	0
14	B	805	CLA	2	0
14	A	836	CLA	6	0
14	1	822	CLA	4	0
14	k	4003	CLA	1	0
17	1	849	BCR	1	0
14	F	205	CLA	2	0
14	2	842	CLA	5	0
14	a	806	CLA	6	0
13	a	803	CL0	3	0
14	B	818	CLA	2	0
14	f	204	CLA	1	0
14	2	813	CLA	1	0
14	a	804	CLA	10	0
14	k	4002	CLA	2	0
14	B	836	CLA	2	0
14	A	808	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	834	CLA	1	0
14	a	837	CLA	6	0
14	J	102	CLA	1	0
14	B	808	CLA	4	0
17	7	1104	BCR	7	0
15	A	845	PQN	1	0
14	A	827	CLA	8	0
14	2	807	CLA	2	0
14	2	833	CLA	1	0
17	B	854	BCR	6	0
15	1	845	PQN	1	0
14	2	841	CLA	2	0
18	L	1506	LMG	1	0
18	a	852	LMG	1	0
14	A	842	CLA	9	0
17	a	847	BCR	4	0
17	b	847	BCR	2	0
14	2	811	CLA	6	0
14	7	1103	CLA	1	0
14	a	812	CLA	2	0
14	b	826	CLA	2	0
14	1	813	CLA	2	0
14	1	836	CLA	1	0
14	a	818	CLA	1	0
17	8	4005	BCR	3	0
12	m	101	LHG	1	0
14	a	839	CLA	2	0
14	b	822	CLA	2	0
14	b	802	CLA	5	0
14	b	828	CLA	1	0
14	B	843	CLA	6	0
14	A	841	CLA	4	0
14	b	806	CLA	4	0
14	A	834	CLA	3	0
14	f	205	CLA	2	0
14	b	834	CLA	2	0
14	A	805	CLA	7	0
14	1	843	CLA	6	0
14	1	842	CLA	8	0
14	A	813	CLA	4	0
14	a	808	CLA	5	0
14	B	813	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	806	CLA	5	0
14	b	808	CLA	4	0
14	2	809	CLA	4	0
14	B	828	CLA	1	0
14	B	841	CLA	3	0
14	a	827	CLA	2	0
15	b	845	PQN	8	0
14	A	833	CLA	1	0
14	1	837	CLA	2	0
18	l	4202	LMG	1	0
17	b	854	BCR	5	0
17	A	851	BCR	4	0
14	2	837	CLA	2	0
14	L	1503	CLA	8	0
14	B	833	CLA	3	0
17	1	848	BCR	4	0
14	b	841	CLA	2	0
14	b	842	CLA	5	0
14	0	202	CLA	2	0
14	1	808	CLA	1	0
14	B	811	CLA	5	0
17	B	852	BCR	7	0
14	l	4203	CLA	9	0
14	A	830	CLA	9	0
14	A	811	CLA	2	0
14	1	834	CLA	4	0
17	B	847	BCR	2	0
14	a	838	CLA	1	0
14	L	1501	CLA	6	0
14	2	810	CLA	3	0
14	j	102	CLA	1	0
14	a	841	CLA	2	0
14	2	812	CLA	8	0
14	1	841	CLA	4	0
17	a	848	BCR	3	0
14	1	804	CLA	6	0
14	A	829	CLA	5	0
14	B	809	CLA	10	0
17	b	849	BCR	4	0
14	A	838	CLA	2	0
14	b	813	CLA	1	0
14	A	822	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	820	CLA	3	0
14	a	816	CLA	5	0
14	B	812	CLA	4	0
14	a	833	CLA	7	0
14	1	811	CLA	2	0
17	k	4004	BCR	3	0
14	2	806	CLA	2	0
17	K	4005	BCR	4	0
14	1	825	CLA	2	0
14	a	825	CLA	1	0
14	a	830	CLA	5	0
14	a	811	CLA	7	0
14	1	831	CLA	5	0
14	b	824	CLA	1	0
14	A	835	CLA	4	0
14	a	810	CLA	1	0
18	A	852	LMG	1	0
14	l	4204	CLA	6	0
14	1	840	CLA	4	0
14	A	831	CLA	5	0
14	b	830	CLA	3	0
17	B	851	BCR	8	0
14	b	817	CLA	2	0
12	1	801	LHG	4	0
14	K	4003	CLA	1	0
14	b	805	CLA	3	0
14	1	812	CLA	3	0
14	a	854	CLA	2	0
17	A	848	BCR	4	0
14	2	834	CLA	2	0
14	1	824	CLA	1	0
14	B	819	CLA	2	0
14	a	832	CLA	5	0
17	b	851	BCR	5	0
17	2	846	BCR	3	0
17	I	101	BCR	2	0
14	1	818	CLA	1	0
14	A	823	CLA	5	0
14	a	822	CLA	3	0
17	2	848	BCR	1	0
17	F	203	BCR	3	0
17	6	4406	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	2	843	CLA	4	0
14	b	819	CLA	2	0
14	a	821	CLA	4	0
17	K	4001	BCR	2	0
14	b	839	CLA	3	0
17	j	103	BCR	4	0
14	K	4004	CLA	2	0
17	1	851	BCR	3	0
14	2	801	CLA	8	0
14	B	831	CLA	4	0
14	2	822	CLA	2	0
14	B	840	CLA	4	0
14	a	835	CLA	4	0
16	c	102	SF4	1	0
14	K	4002	CLA	2	0
17	0	209	BCR	2	0
12	1	802	LHG	1	0
14	1	819	CLA	4	0
12	a	802	LHG	1	0
14	b	831	CLA	5	0
17	6	4405	BCR	1	0
17	2	849	BCR	4	0
14	b	825	CLA	6	0
14	B	827	CLA	2	0
14	A	809	CLA	1	0
17	h	101	BCR	3	0
14	2	835	CLA	2	0
14	2	829	CLA	2	0
14	b	821	CLA	2	0
14	2	815	CLA	9	0
14	2	826	CLA	2	0
14	0	208	CLA	12	0
14	b	829	CLA	2	0
14	8	4004	CLA	1	0
14	0	206	CLA	6	0
14	0	207	CLA	3	0
14	a	831	CLA	12	0
14	A	843	CLA	7	0
14	A	839	CLA	6	0
14	2	832	CLA	3	0
17	A	849	BCR	1	0
14	F	201	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	849	BCR	1	0
14	B	842	CLA	3	0
14	B	810	CLA	5	0
14	1	809	CLA	8	0
17	2	850	BCR	7	0
14	1	816	CLA	1	0
14	a	809	CLA	5	0
14	2	816	CLA	1	0
14	1	838	CLA	5	0
14	b	810	CLA	7	0
14	8	4002	CLA	2	0
16	C	102	SF4	1	0
12	2	852	LHG	2	0
14	6	4404	CLA	2	0
14	b	827	CLA	1	0
14	B	832	CLA	7	0
14	B	807	CLA	2	0
14	b	809	CLA	8	0
17	8	4001	BCR	2	0
14	b	832	CLA	3	0
14	B	837	CLA	1	0
14	b	807	CLA	1	0
14	1	827	CLA	3	0
14	b	811	CLA	5	0
17	a	849	BCR	1	0
17	a	850	BCR	6	0
14	f	201	CLA	4	0
14	A	812	CLA	2	0
14	1	807	CLA	7	0
14	B	801	CLA	9	0
14	A	840	CLA	2	0
14	1	810	CLA	2	0
14	1	832	CLA	1	0
14	A	824	CLA	1	0
14	2	820	CLA	1	0
14	B	816	CLA	8	0
17	F	206	BCR	1	0
14	a	823	CLA	3	0
17	L	1504	BCR	1	0
14	b	837	CLA	3	0
14	A	807	CLA	6	0
14	B	820	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	814	CLA	5	0
14	2	840	CLA	3	0
15	2	845	PQN	6	0
17	L	1505	BCR	9	0
12	B	853	LHG	2	0
17	b	853	BCR	8	0
19	i	4101	LMT	1	0
14	A	814	CLA	2	0
14	B	806	CLA	4	0
14	B	814	CLA	1	0
14	B	821	CLA	2	0
14	l	4206	CLA	12	0
14	b	812	CLA	5	0
12	a	801	LHG	6	0
14	A	815	CLA	5	0
14	A	826	CLA	2	0
14	b	840	CLA	2	0
14	a	805	CLA	5	0
14	2	836	CLA	1	0
14	1	833	CLA	4	0
14	a	824	CLA	5	0
14	b	818	CLA	2	0
14	b	801	CLA	2	0
18	0	203	LMG	1	0
14	B	838	CLA	2	0
14	j	101	CLA	1	0
17	k	4001	BCR	2	0
18	0	201	LMG	2	0
17	2	847	BCR	3	0
17	f	206	BCR	1	0
14	B	802	CLA	3	0
17	1	847	BCR	2	0
17	a	851	BCR	2	0
17	0	204	BCR	8	0
14	1	828	CLA	5	0
14	B	834	CLA	1	0
14	b	815	CLA	9	0
14	2	818	CLA	1	0
14	2	828	CLA	1	0
14	2	839	CLA	3	0
17	A	850	BCR	6	0
14	2	830	CLA	4	0

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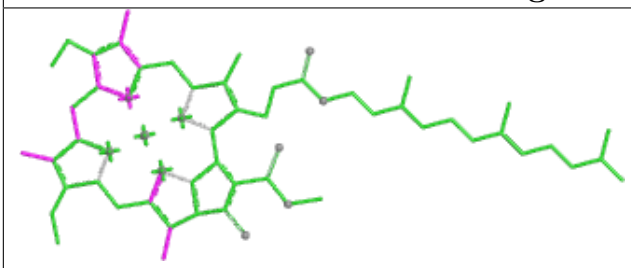
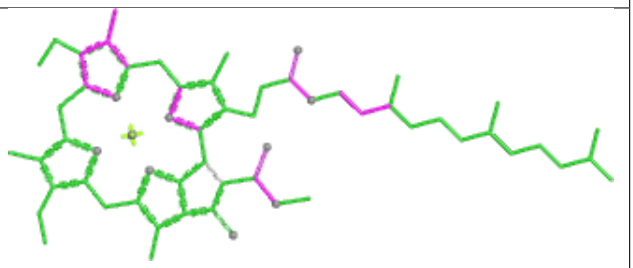
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	828	CLA	7	0
14	1	839	CLA	2	0
17	B	850	BCR	4	0
17	f	203	BCR	4	0
14	B	829	CLA	2	0
14	B	826	CLA	5	0
12	A	801	LHG	4	0
14	2	808	CLA	10	0
12	A	802	LHG	1	0
18	B	803	LMG	4	0
14	A	819	CLA	1	0
17	b	850	BCR	8	0
17	0	210	BCR	8	0
14	a	815	CLA	2	0
14	a	826	CLA	1	0
15	B	846	PQN	9	0
18	2	802	LMG	3	0
14	a	836	CLA	5	0
14	b	836	CLA	2	0
18	b	803	LMG	3	0
14	B	823	CLA	2	0
14	2	804	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.

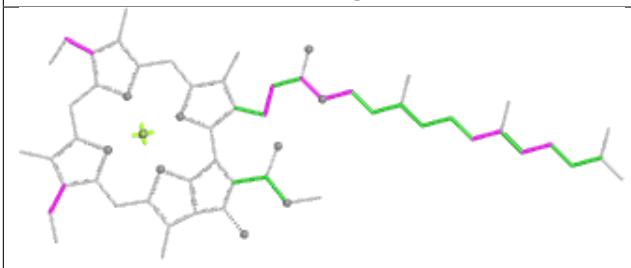
Ligand CLA 1 821



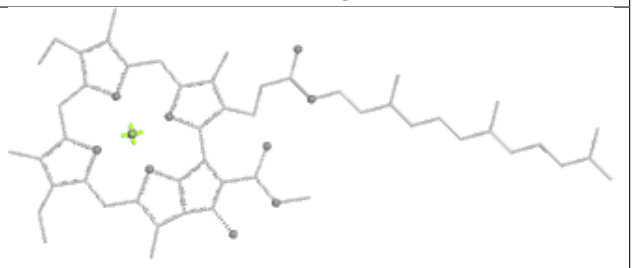
Bond lengths



Bond angles

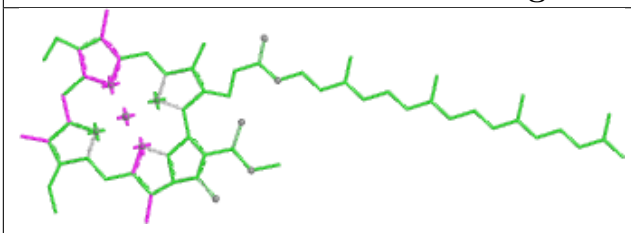


Torsions

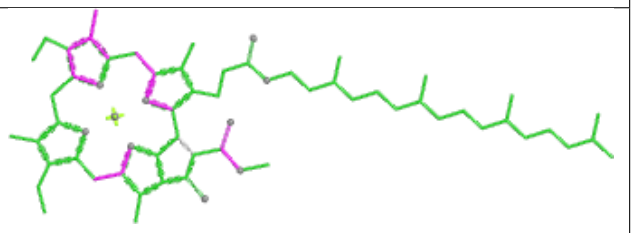


Rings

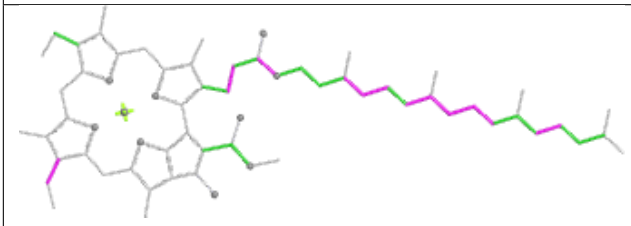
Ligand CLA 2 805



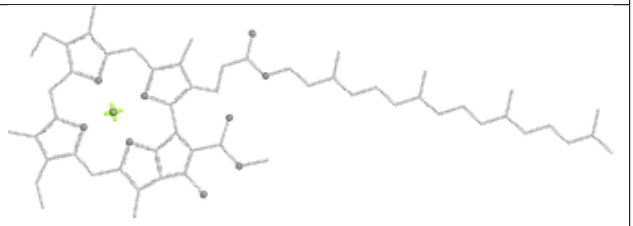
Bond lengths



Bond angles



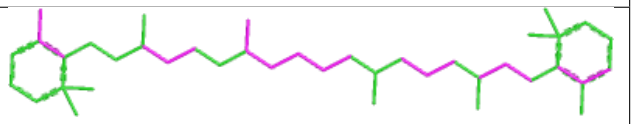
Torsions



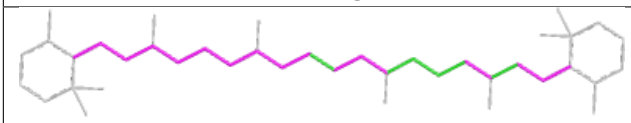
Rings

Ligand BCR i 4103

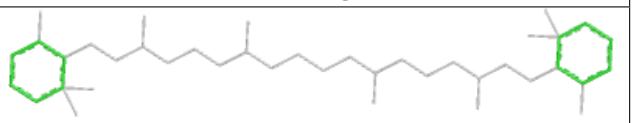
Bond lengths



Bond angles

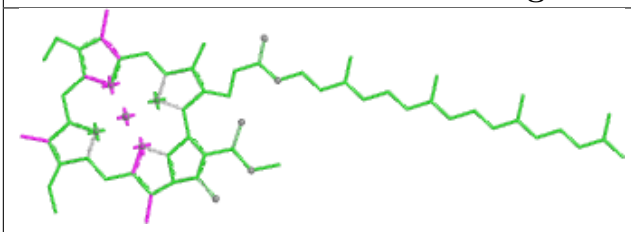


Torsions

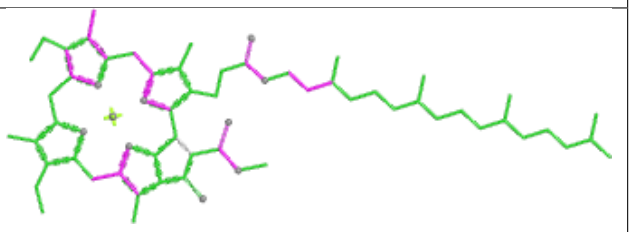


Rings

Ligand CLA b 843



Bond lengths



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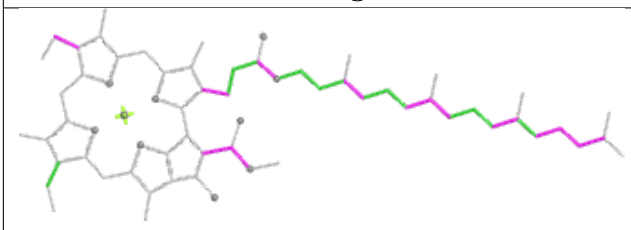
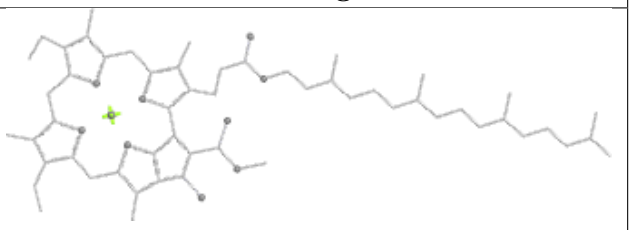
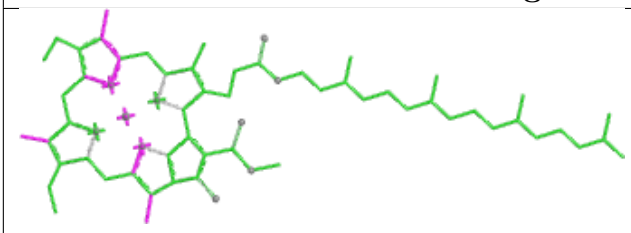


Torsions

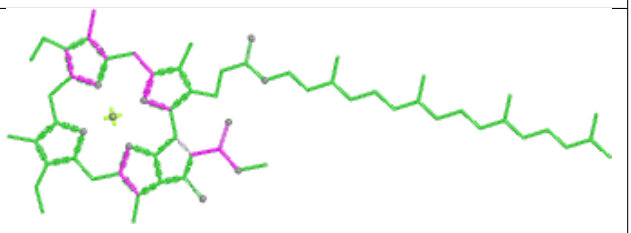


Rings

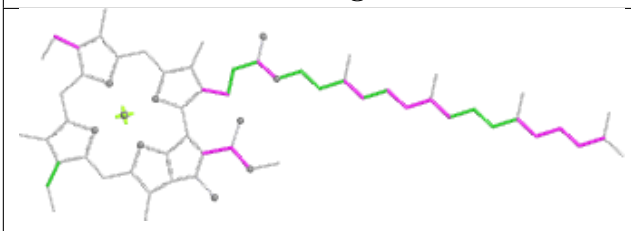
Ligand CLA A 832



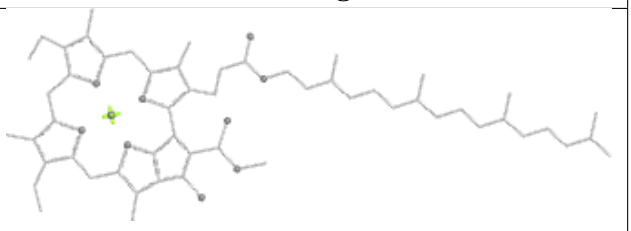
Bond lengths



Bond angles

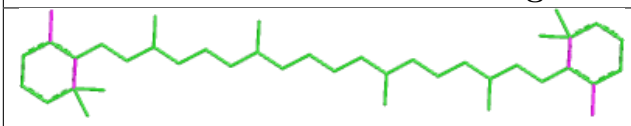


Torsions



Rings

Ligand BCR 1 850



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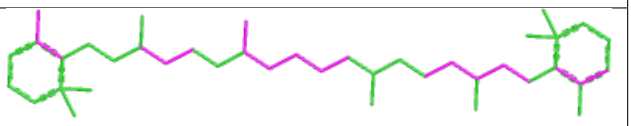
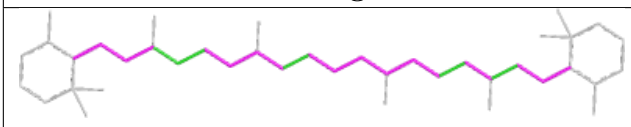
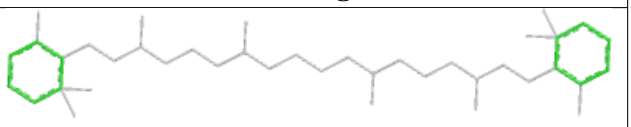


Bond angles

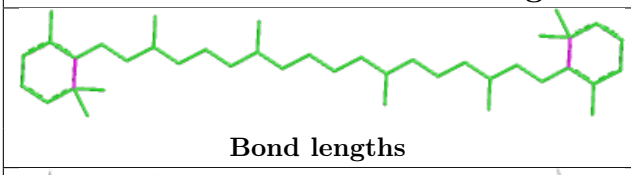


Torsions

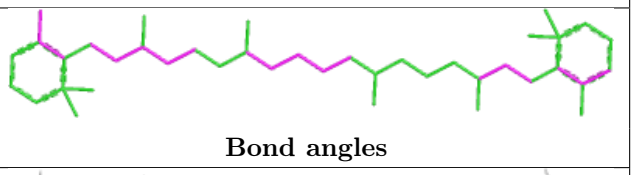


Rings

Ligand BCR b 846



Bond lengths



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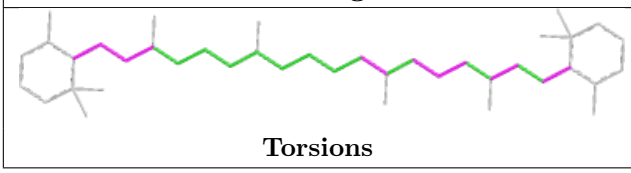

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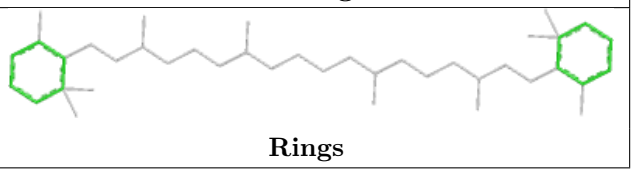
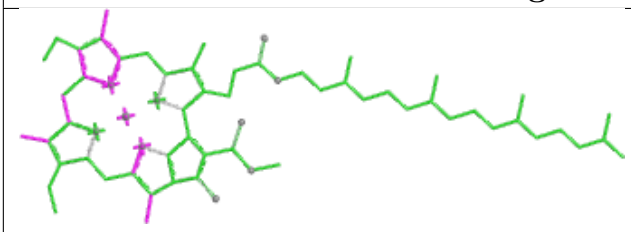


Rings

Ligand CLA 1 829



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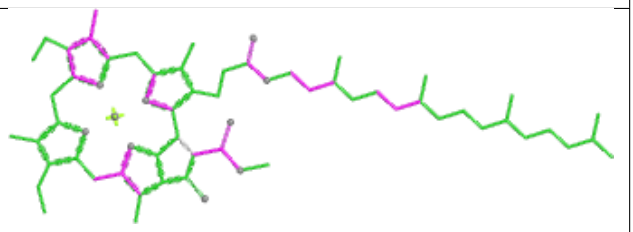
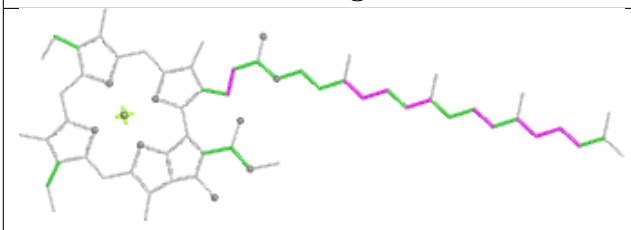
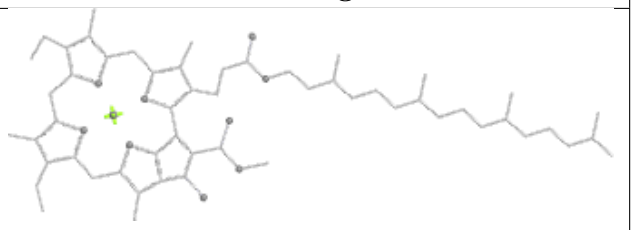


Bond angles

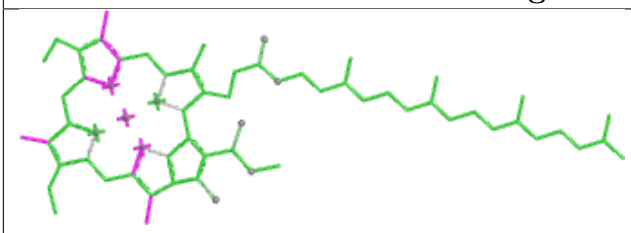


Torsions

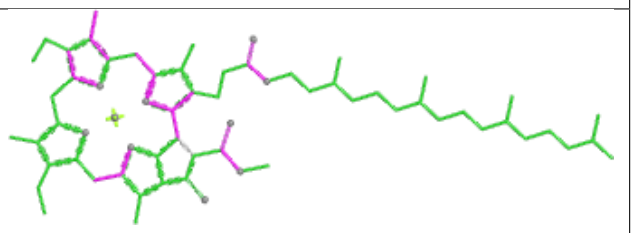


Rings

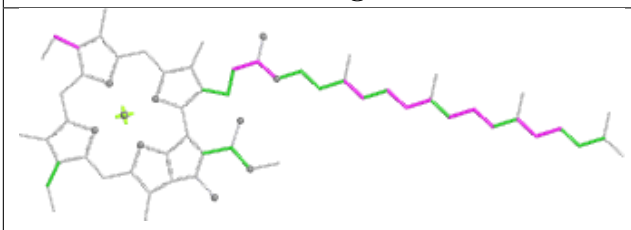
Ligand CLA 1 826



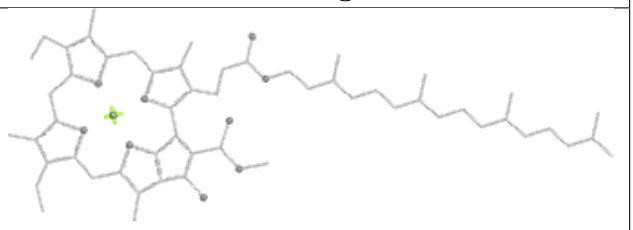
Bond lengths



Bond angles

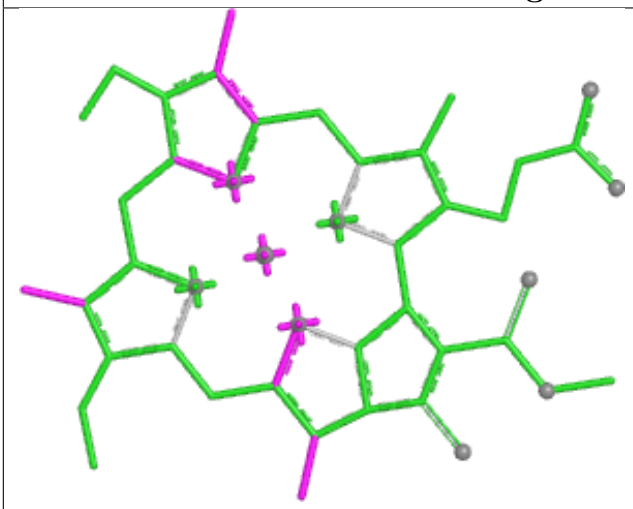


Torsions



Rings

Ligand CLA F 204



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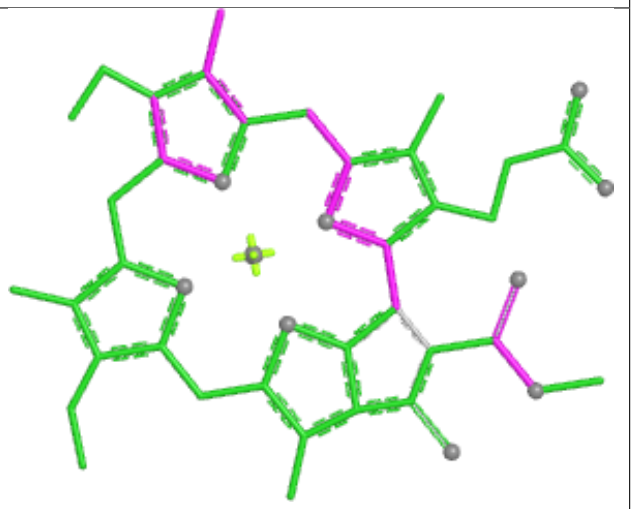
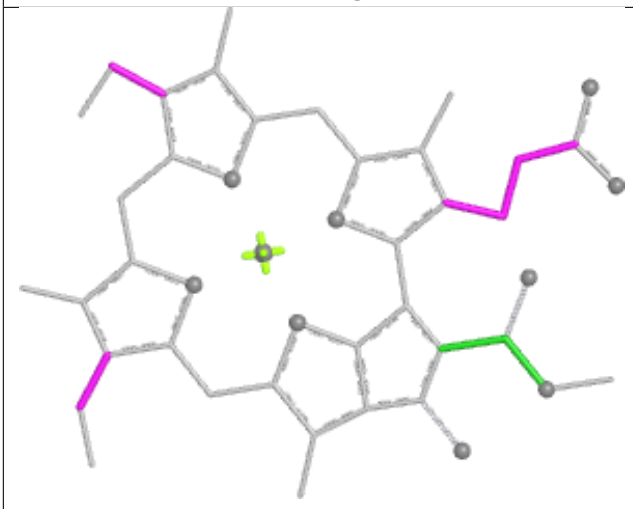


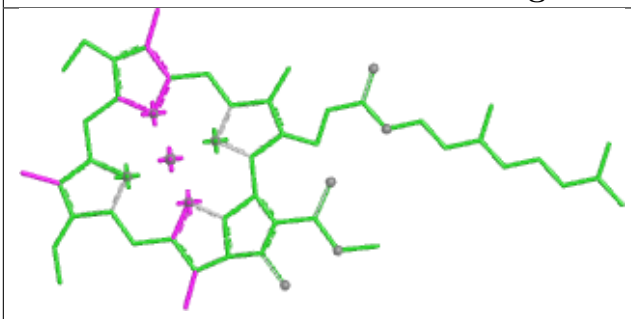
Bond angles



Torsions

Rings

Ligand CLA 2 819



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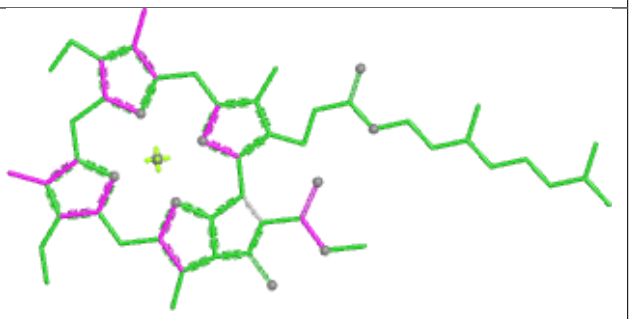
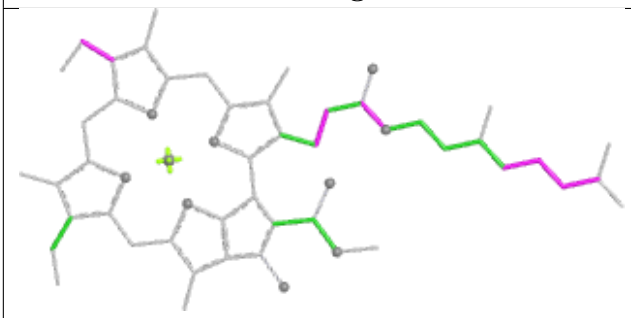


Bond angles



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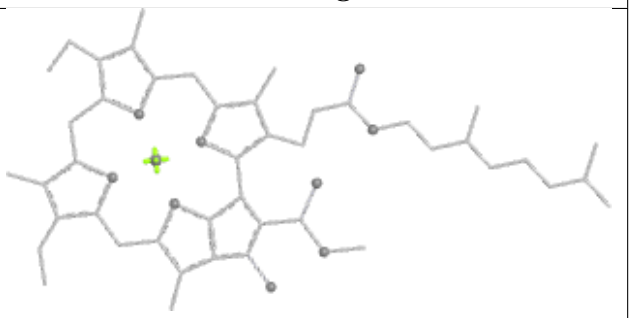
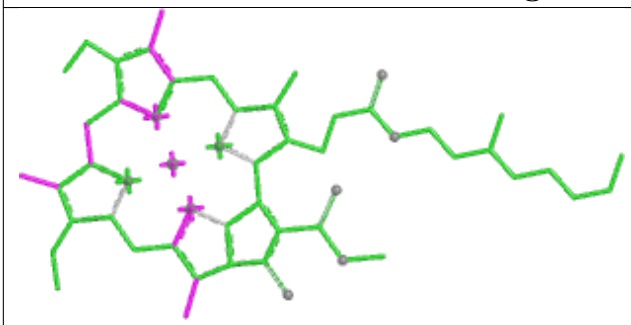


Rings

Ligand CLA A 820



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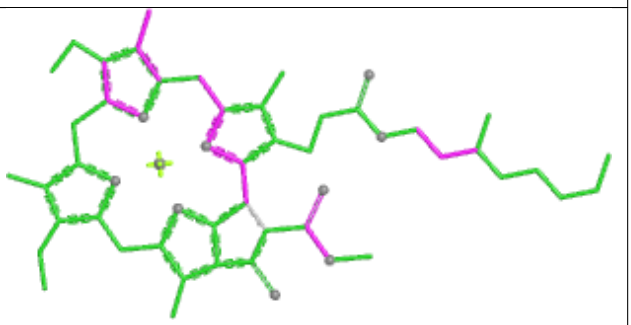
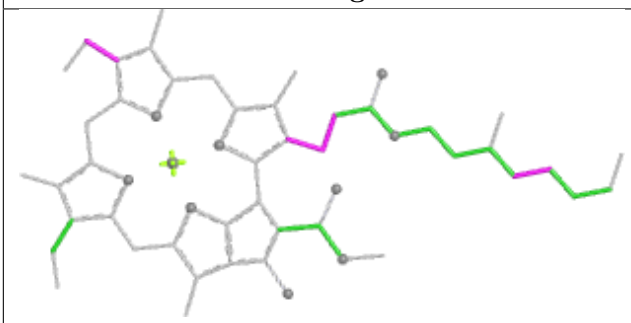
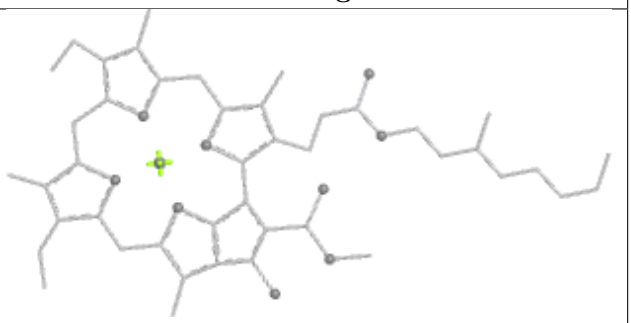


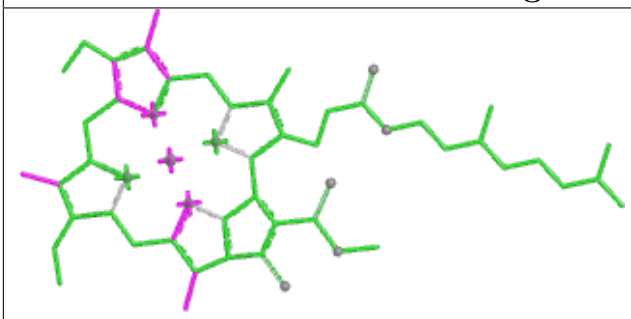
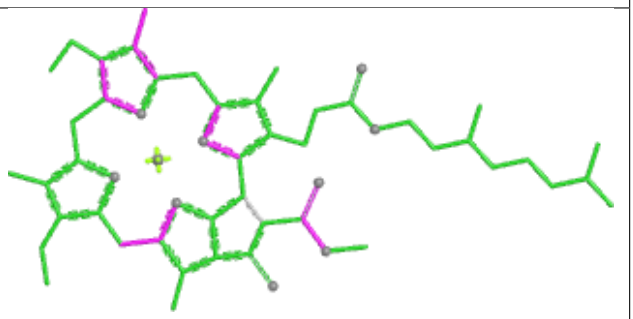
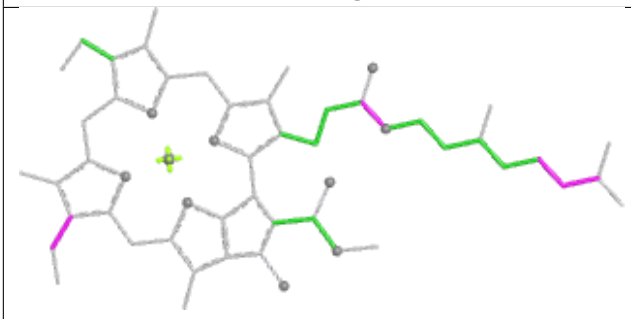
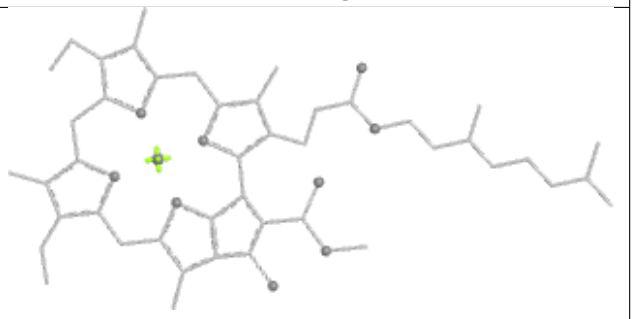
Bond angles



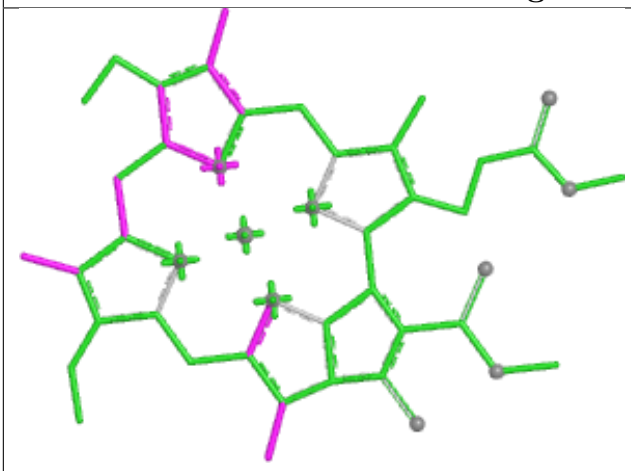
Torsions



Rings

Ligand CLA A 828	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b 816



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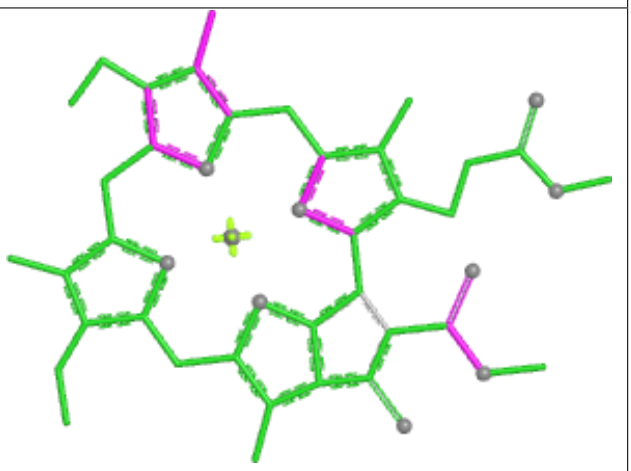
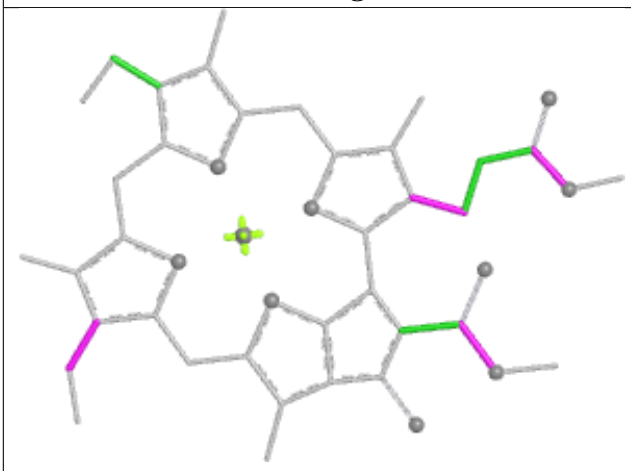
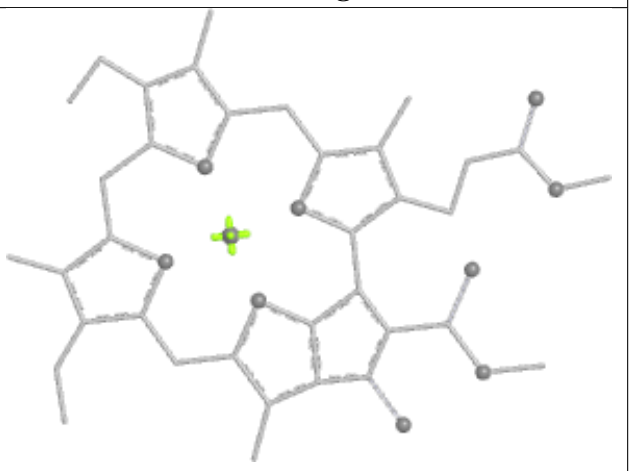


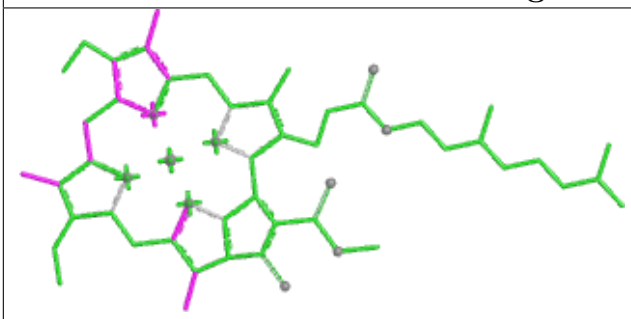
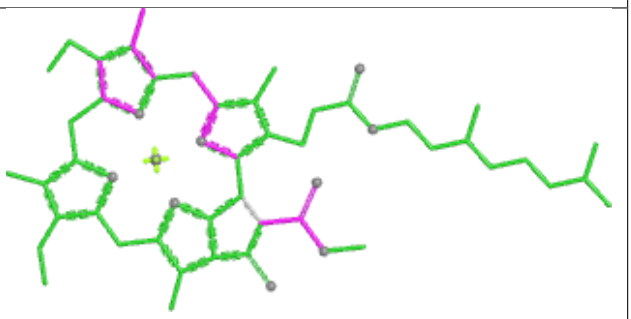
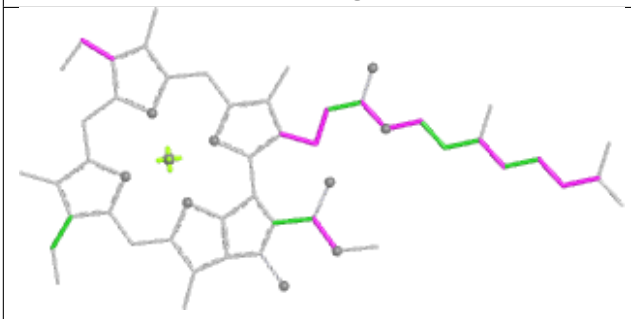
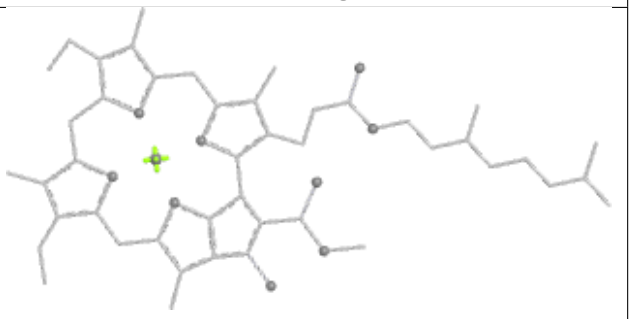
Bond angles



Torsions



Rings

Ligand CLA b 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

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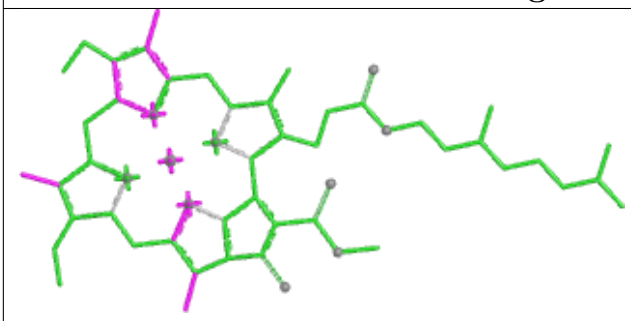
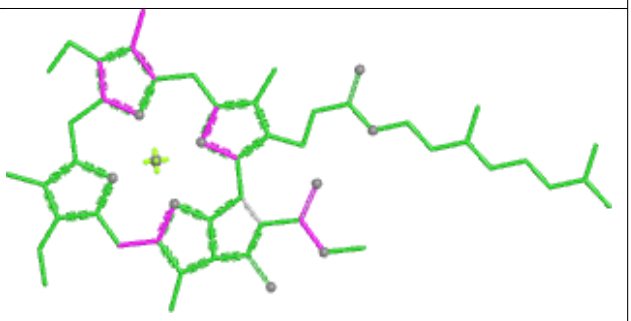
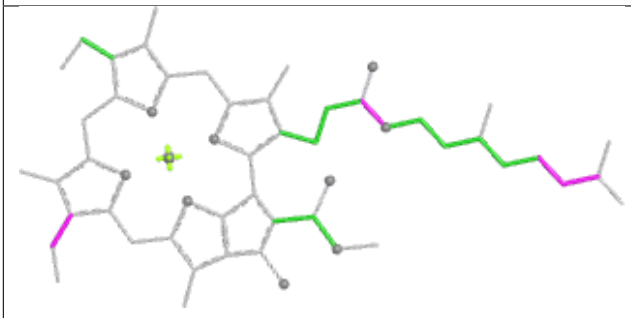
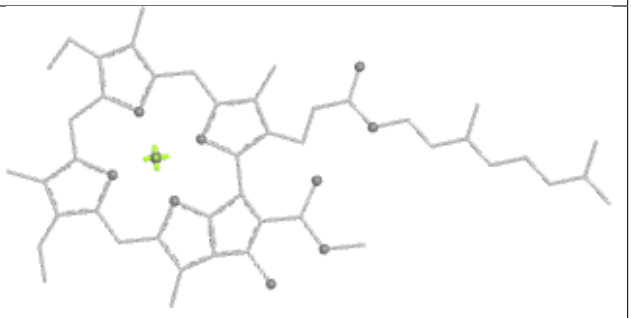
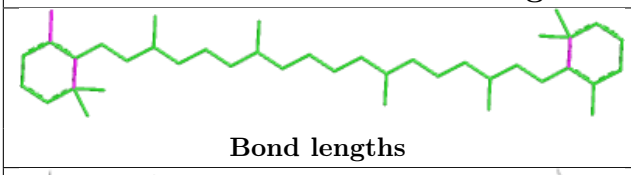
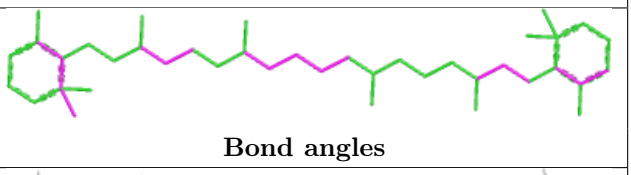
 Bond lengths	 Bond angles
 Torsions	 Rings

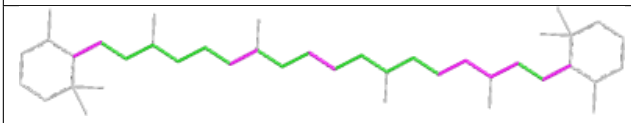
Ligand BCR J 104



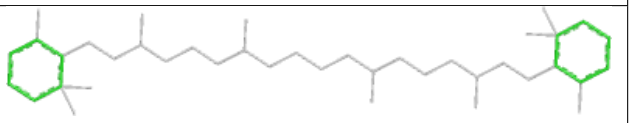
Bond lengths



Bond angles

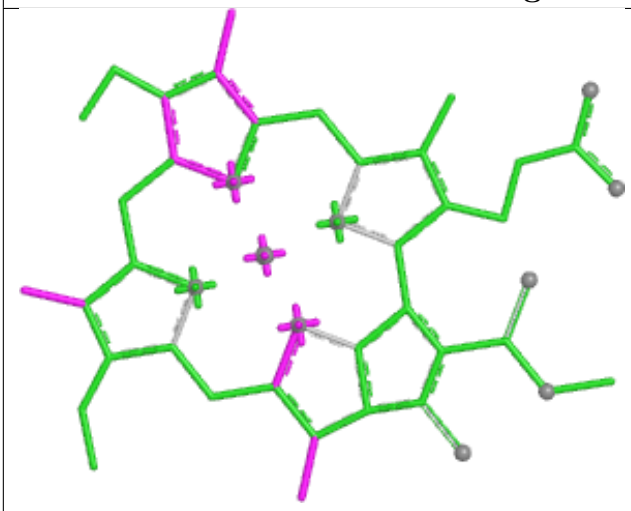


Torsions



Rings

Ligand CLA A 844



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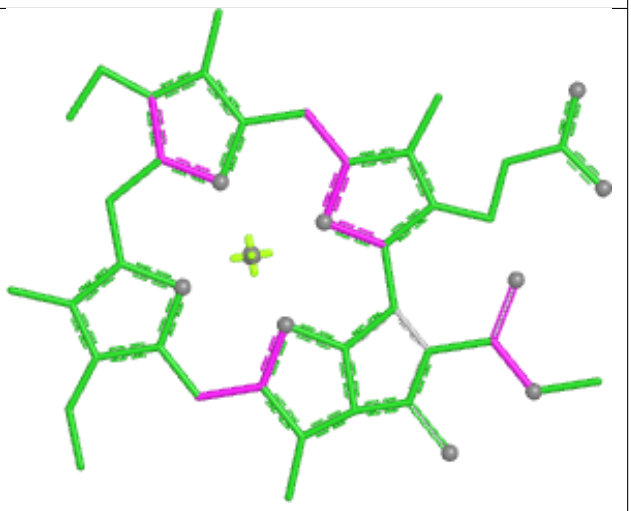
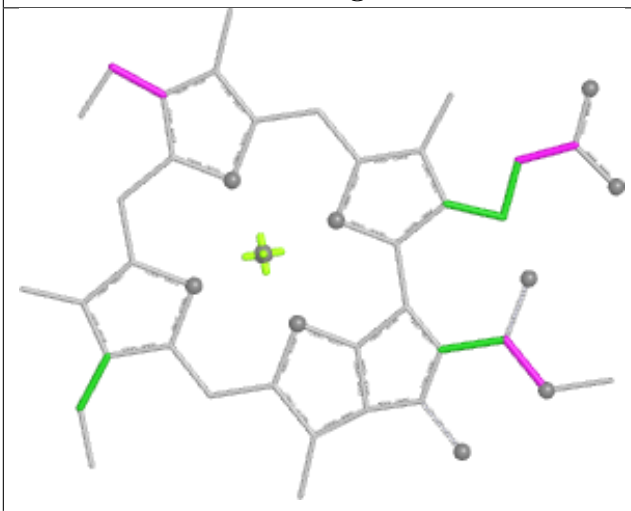


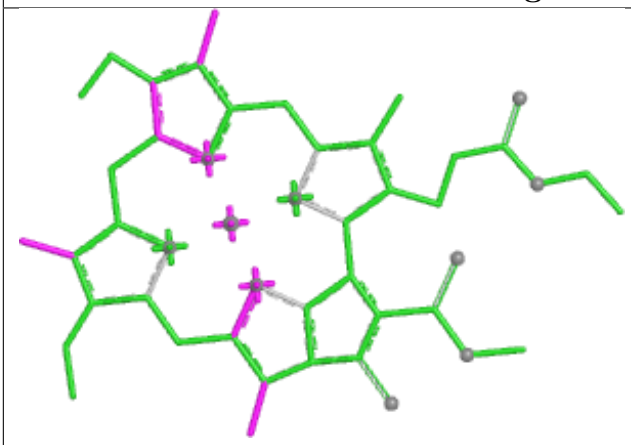
Bond angles



Torsions

Rings

Ligand CLA B 822



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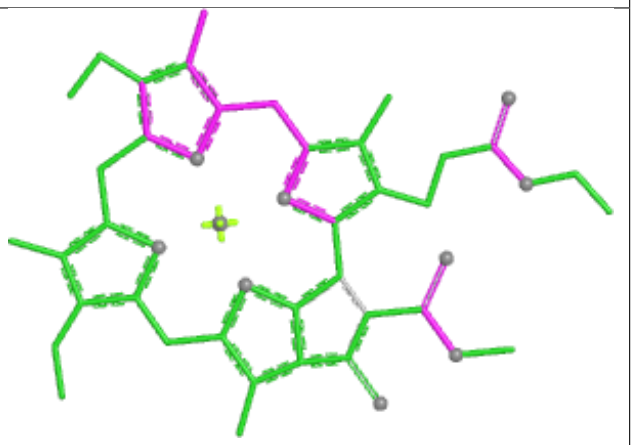
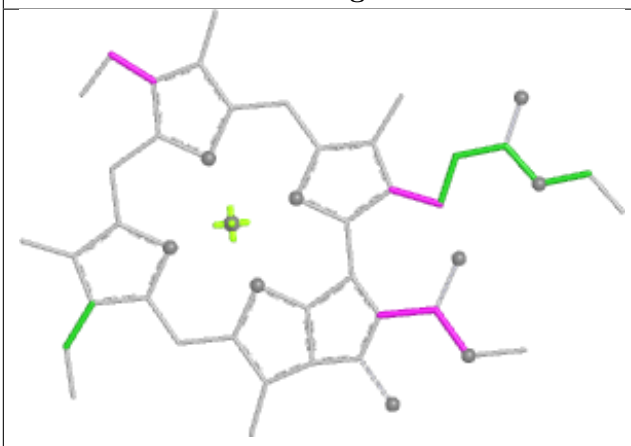


Bond angles



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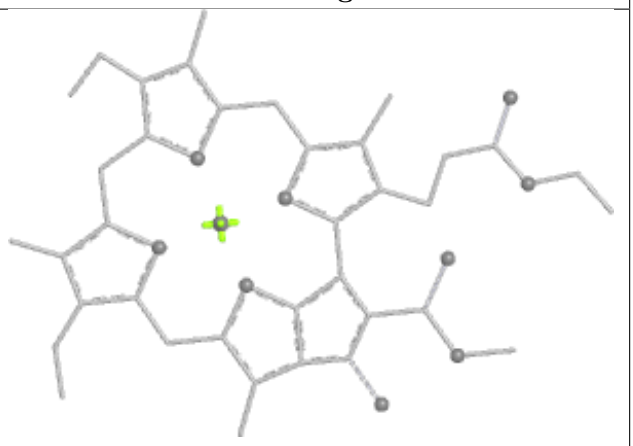
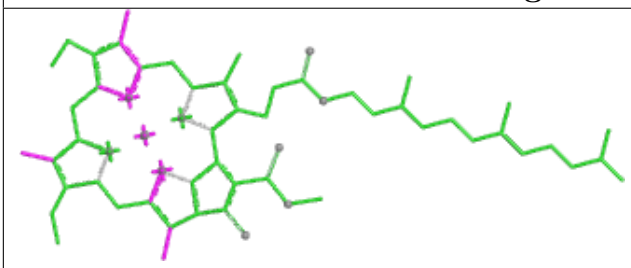


Rings

Ligand CLA B 830



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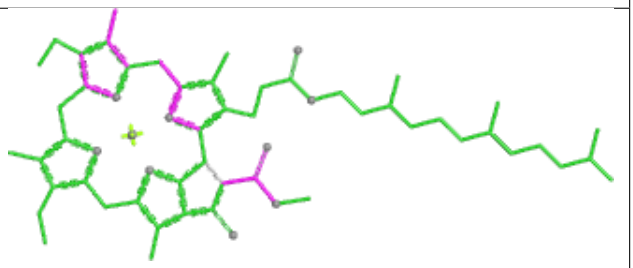
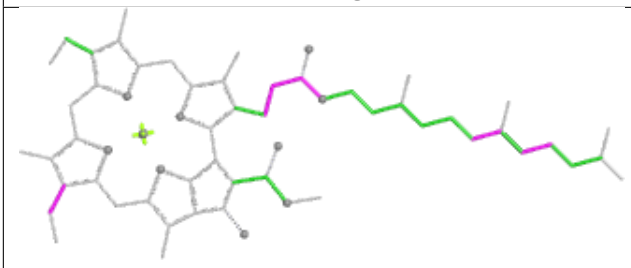
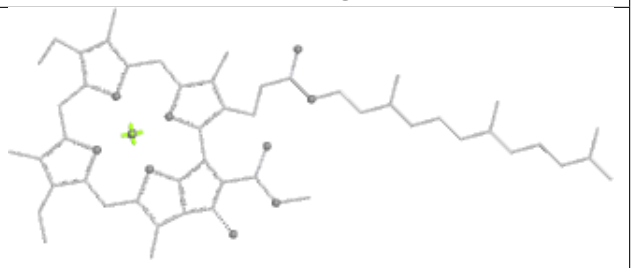


Bond angles

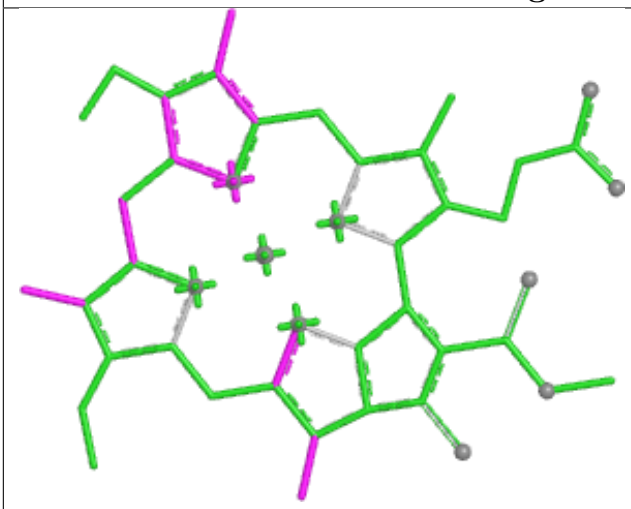


Torsions



Rings

Ligand CLA 2 823



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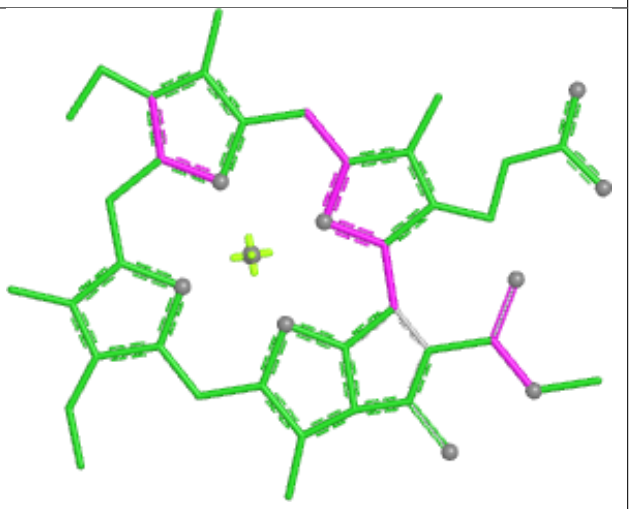
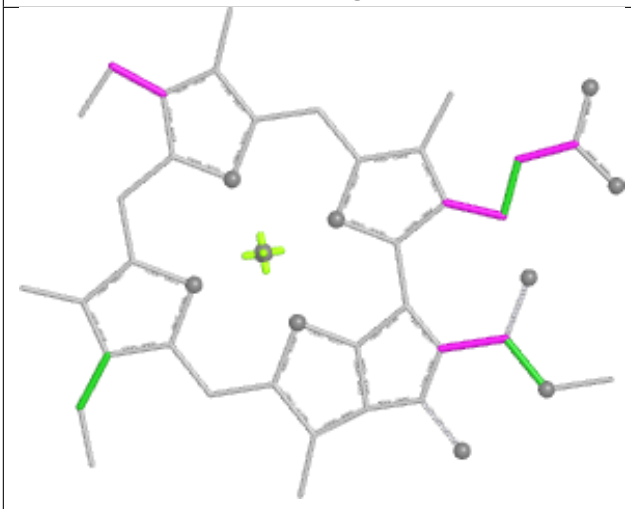


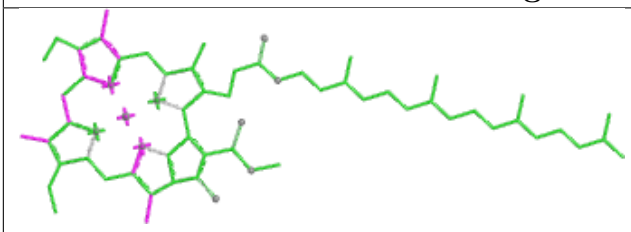
Bond angles



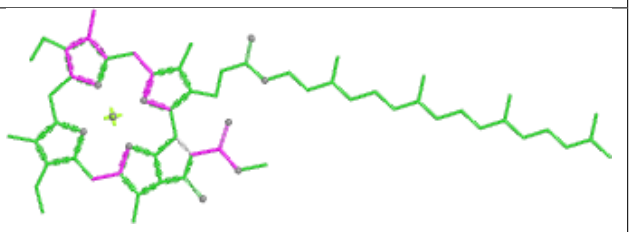
Torsions

Rings

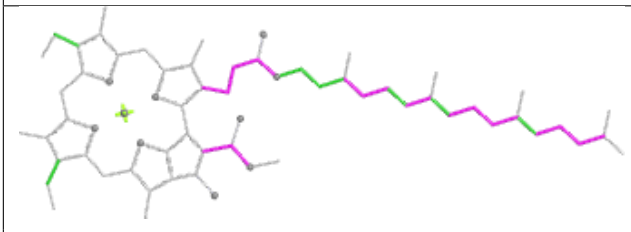
Ligand CLA A 810



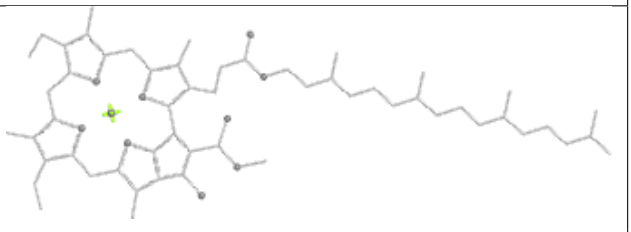
Bond lengths



Bond angles

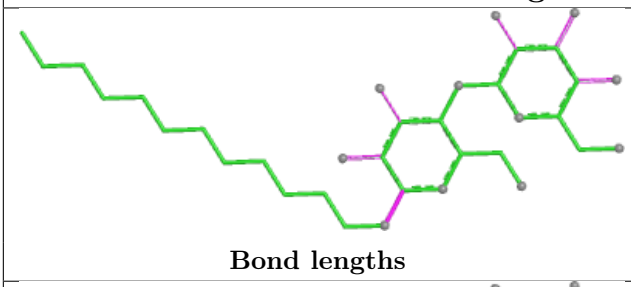


Torsions

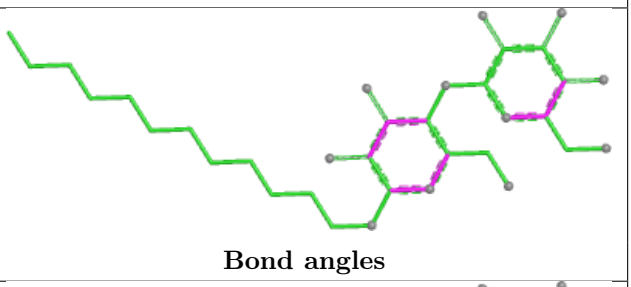


Rings

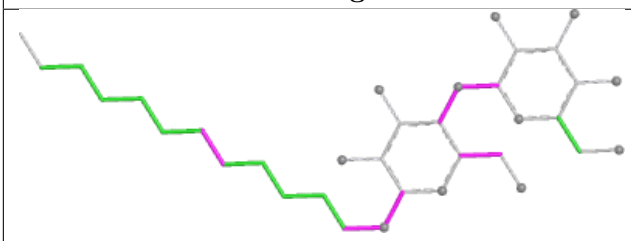
Ligand LMT I 103



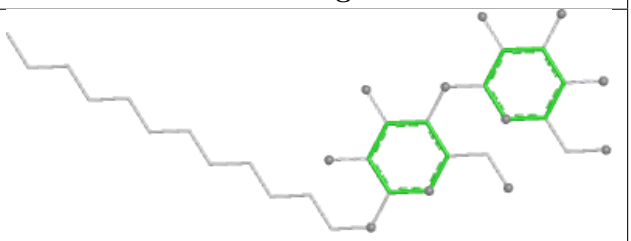
Bond lengths



Bond angles

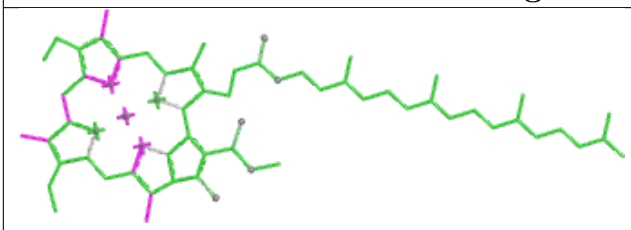


Torsions

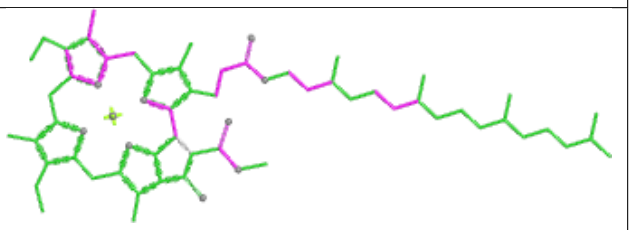


Rings

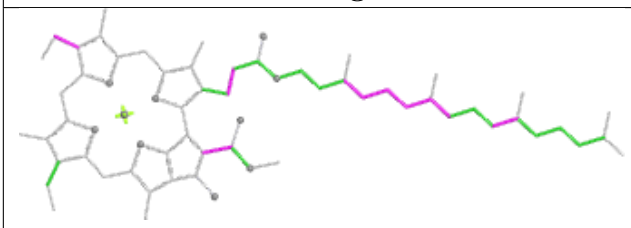
Ligand CLA B 804



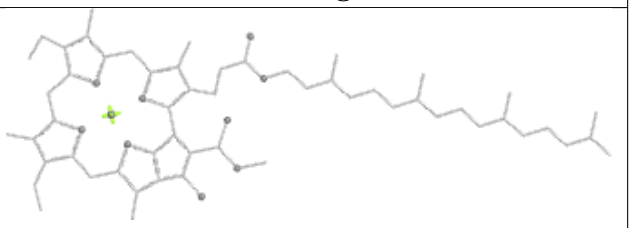
Bond lengths



Bond angles



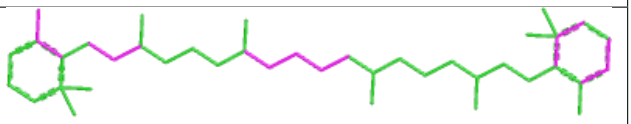
Torsions



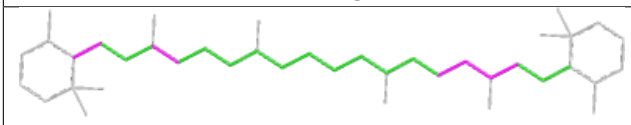
Rings

Ligand BCR B 848

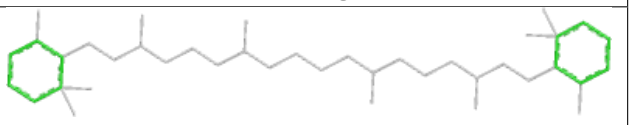
Bond lengths



Bond angles

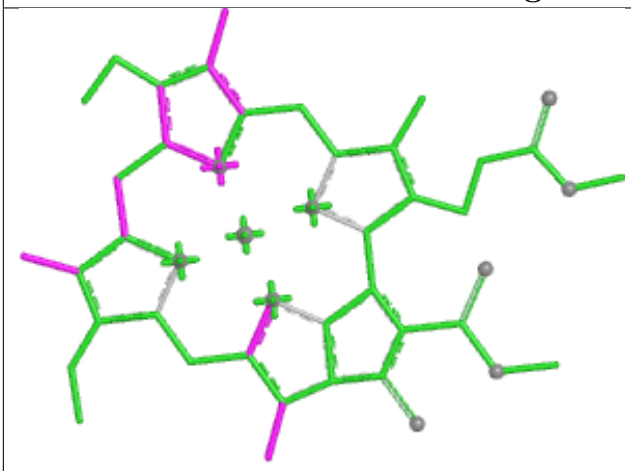


Torsions

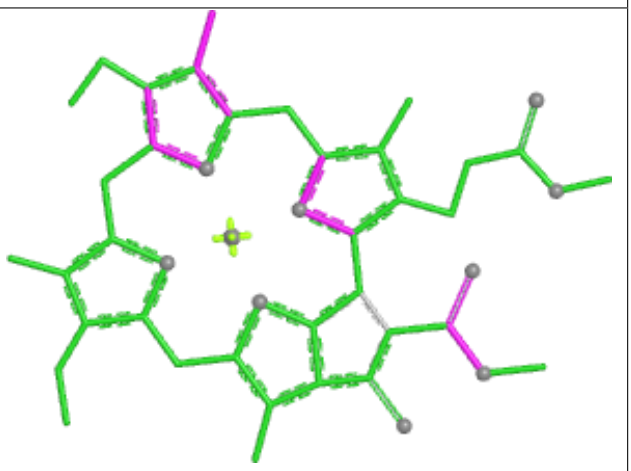


Rings

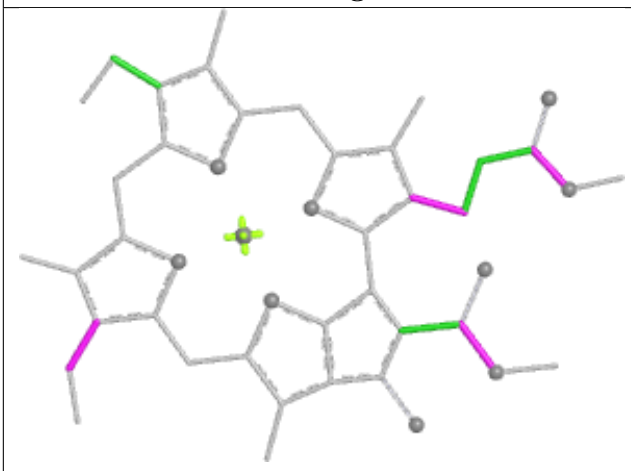
Ligand CLA B 817



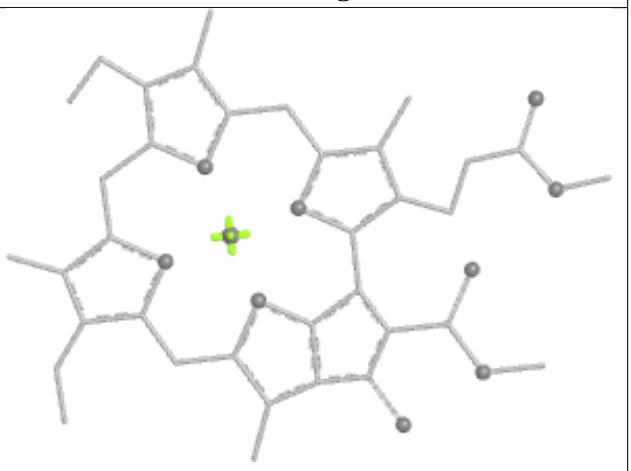
Bond lengths



Bond angles

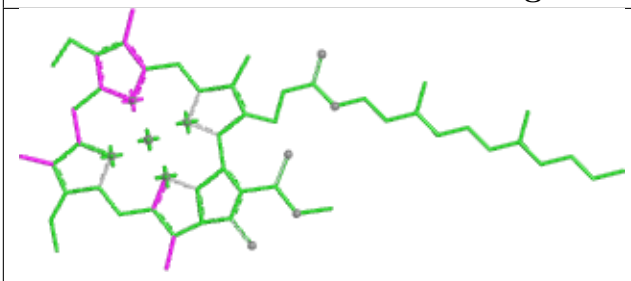


Torsions

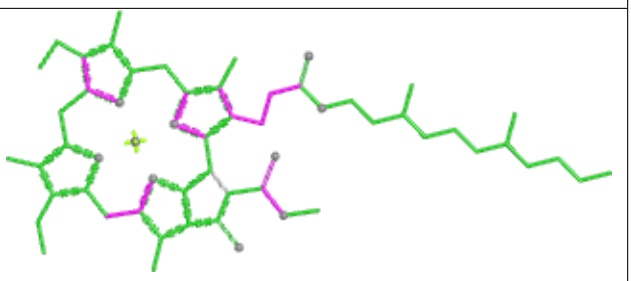


Rings

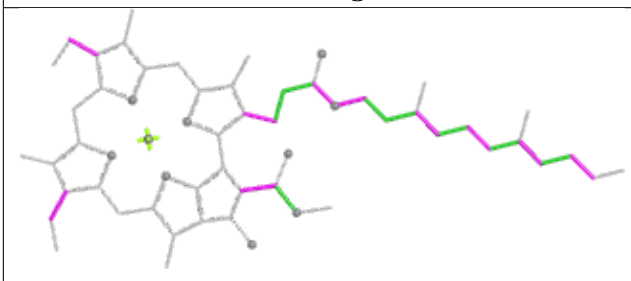
Ligand CLA B 835



Bond lengths



Bond angles



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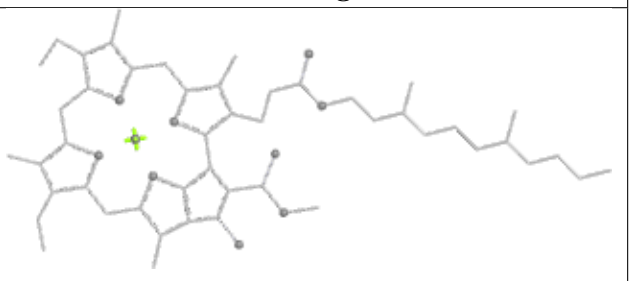
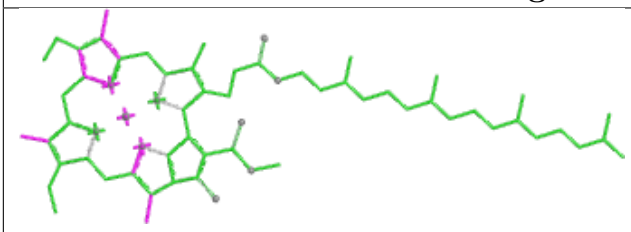


Rings

Ligand CLA a 843



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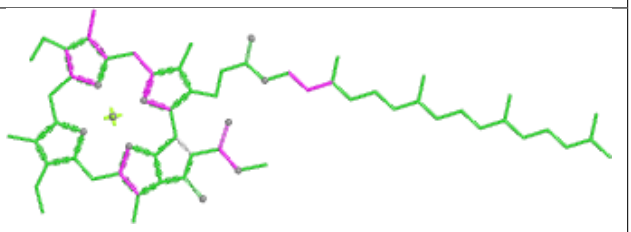
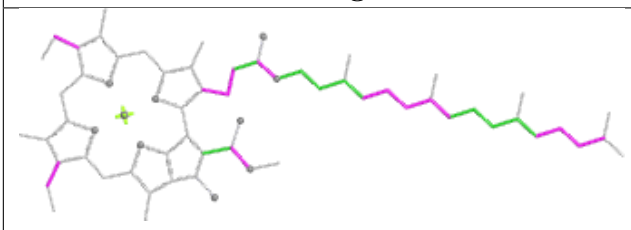


Bond angles



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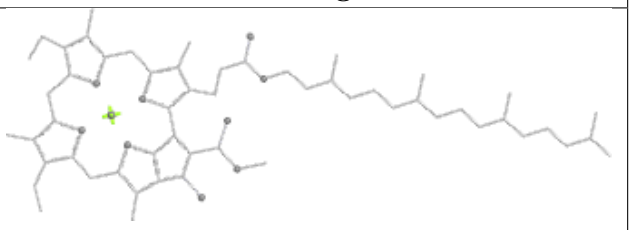
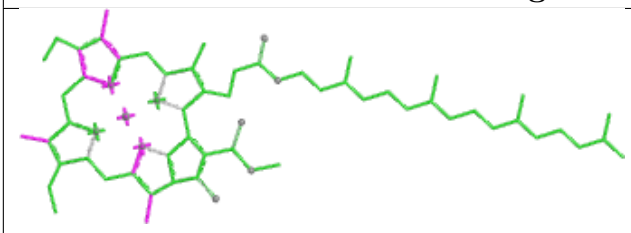
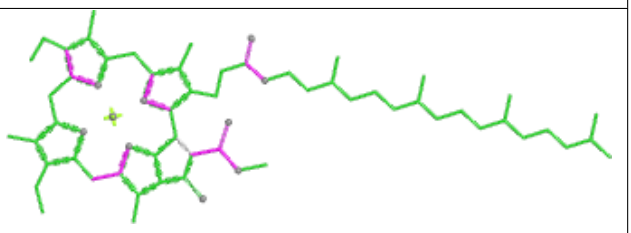


Rings

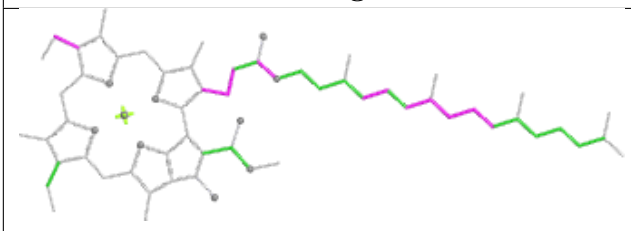
Ligand CLA a 842



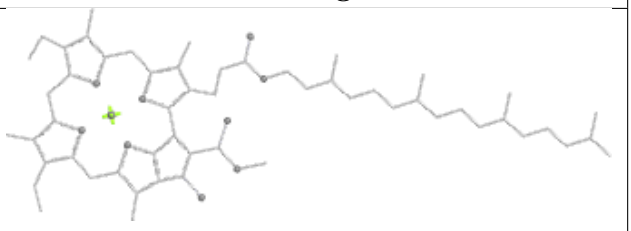
Bond lengths



Bond angles

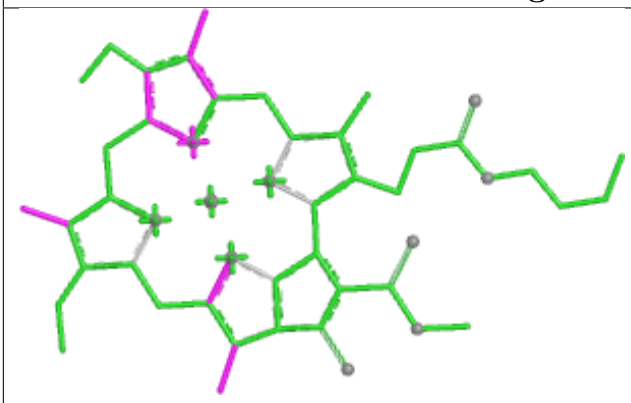


Torsions



Rings

Ligand CLA 1 823



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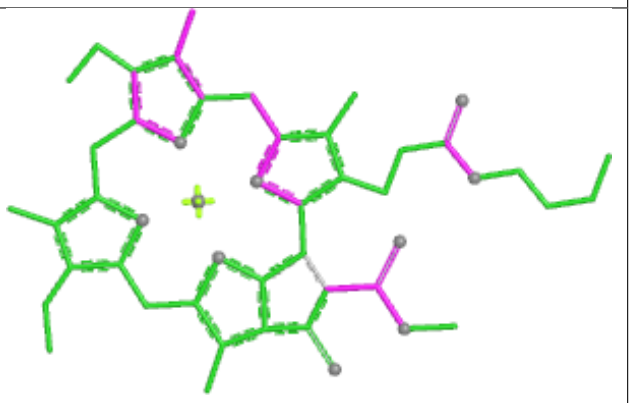
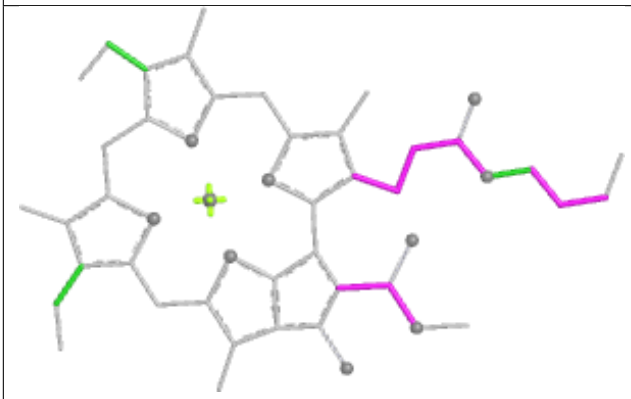
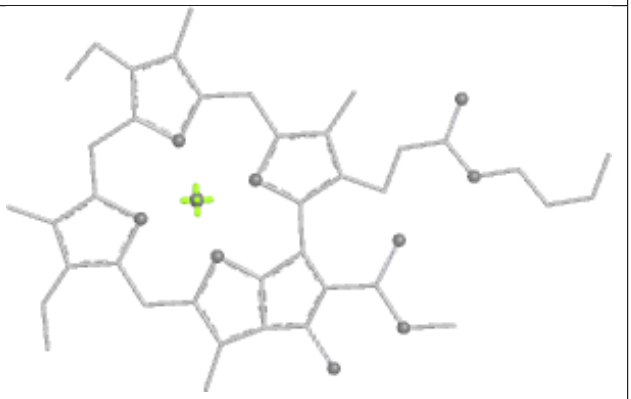


Bond angles

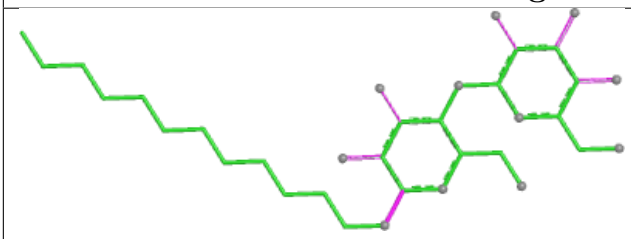


Torsions



Rings

Ligand LMT f 202



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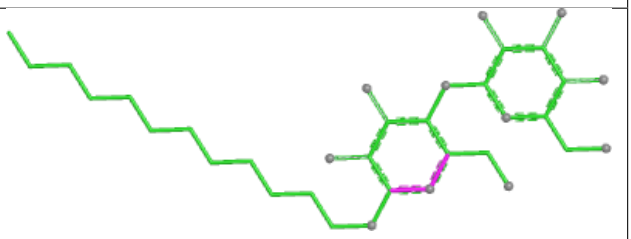
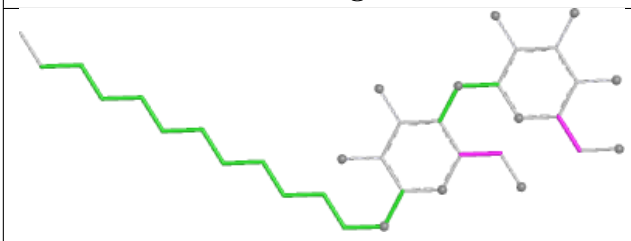


Bond angles



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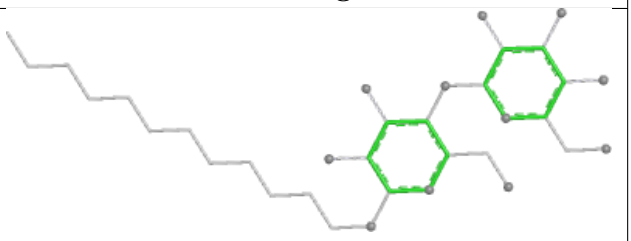
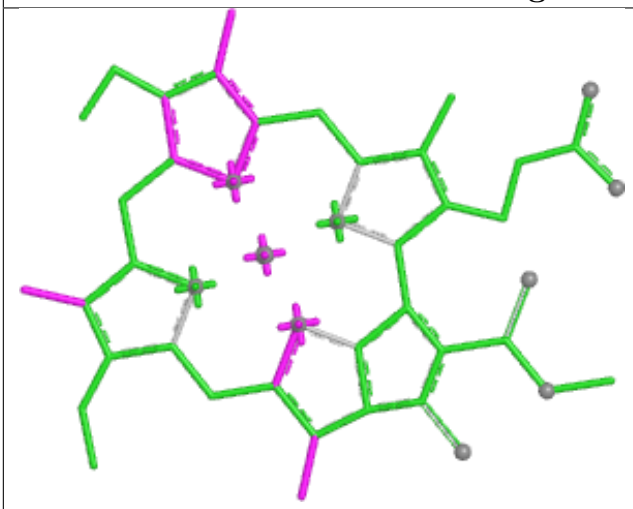


Rings

Ligand CLA a 813



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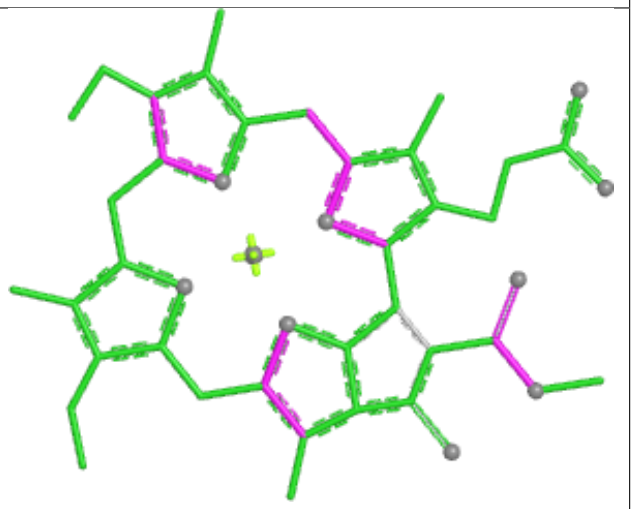
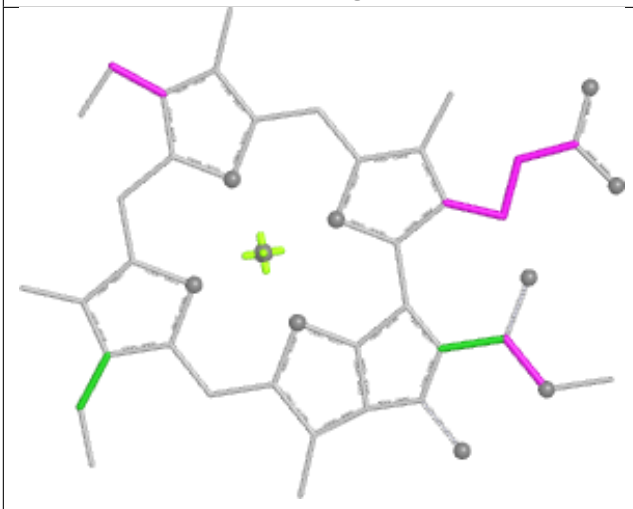


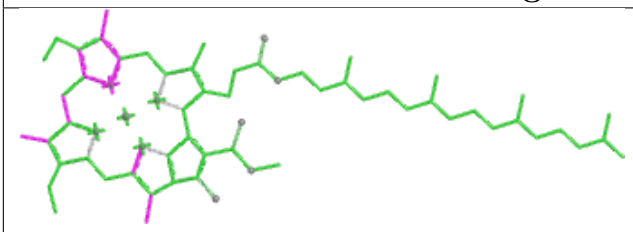
Bond angles



Torsions

Rings

Ligand CLA l 4205



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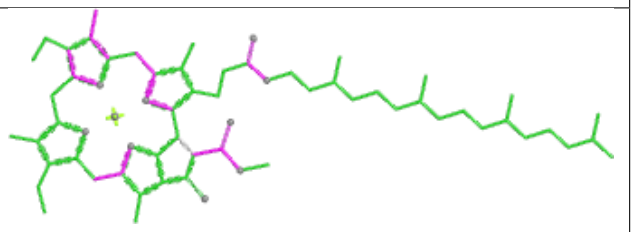
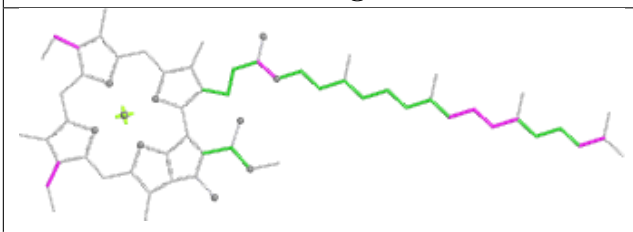


Bond angles



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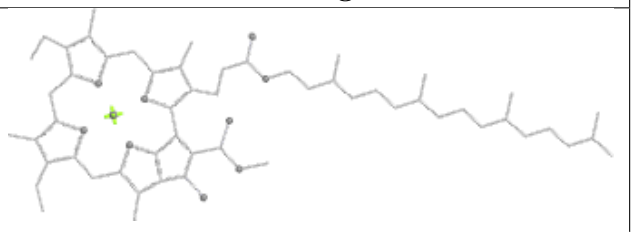
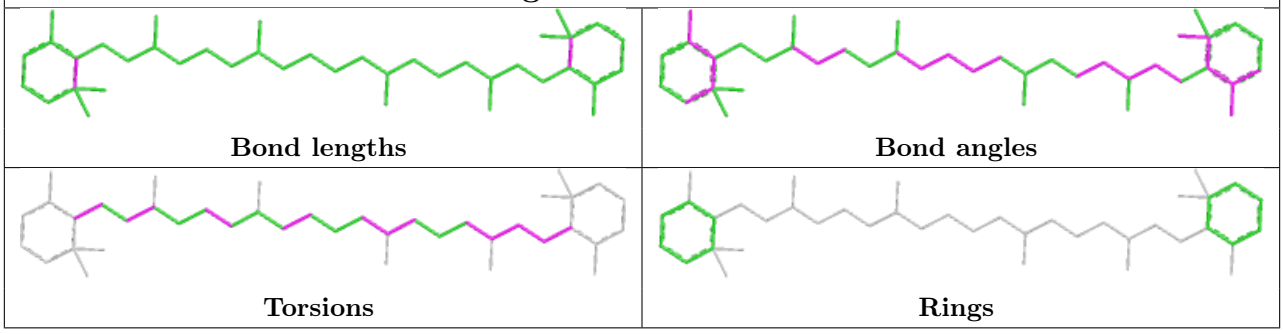
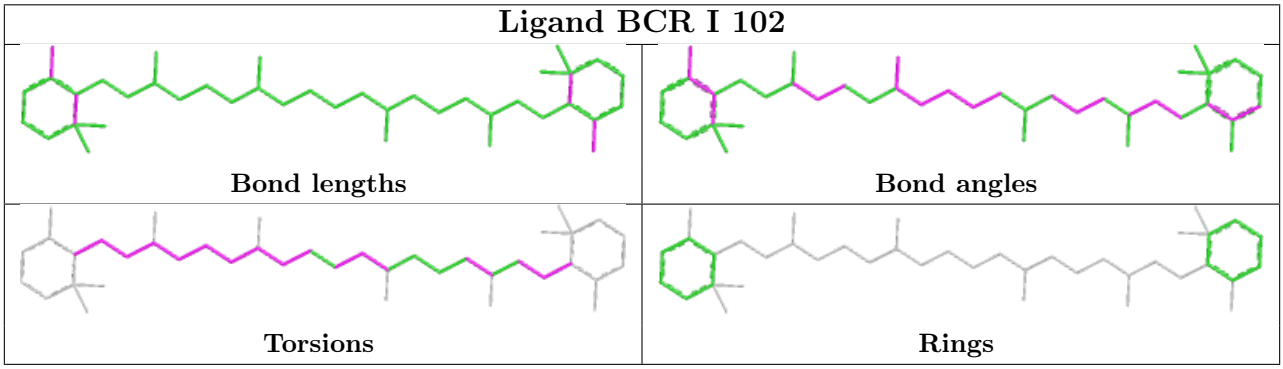


Rings

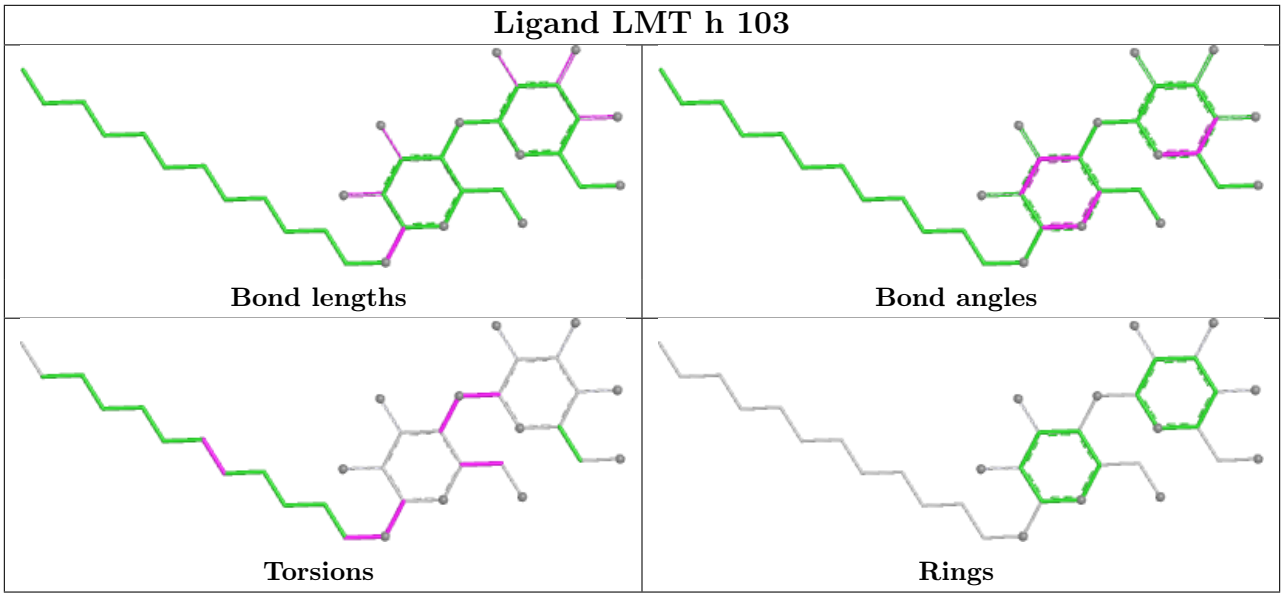
Ligand BCR l 4207



Ligand BCR I 102



Ligand LMT h 103



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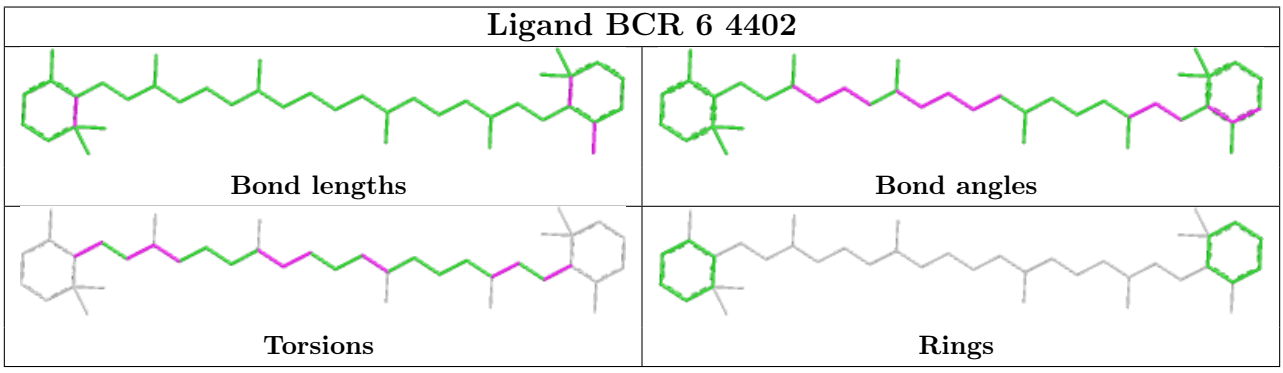
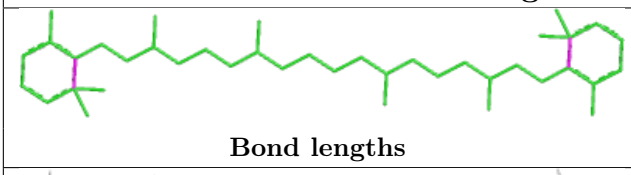
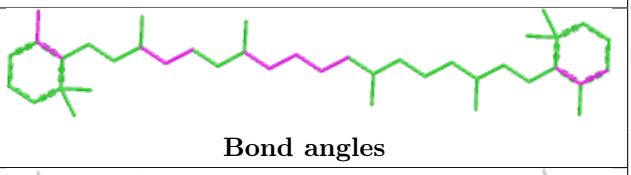


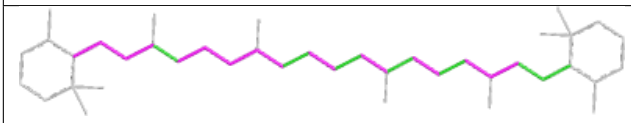
Ligand BCR i 4102



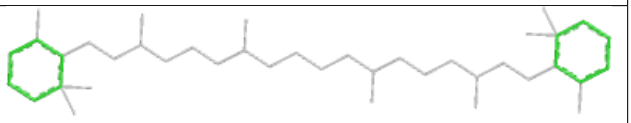
Bond lengths



Bond angles

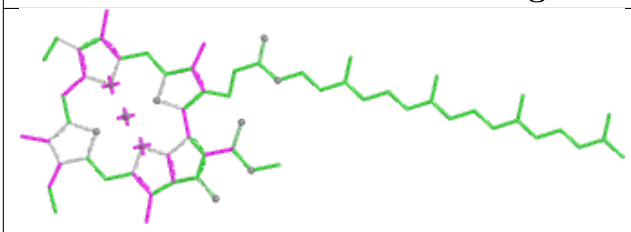


Torsions

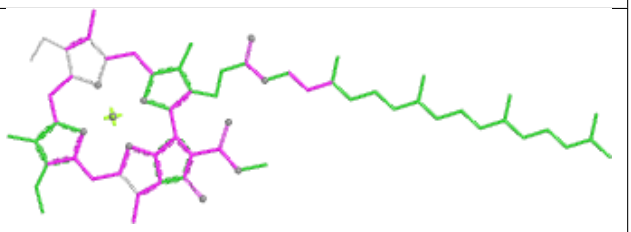


Rings

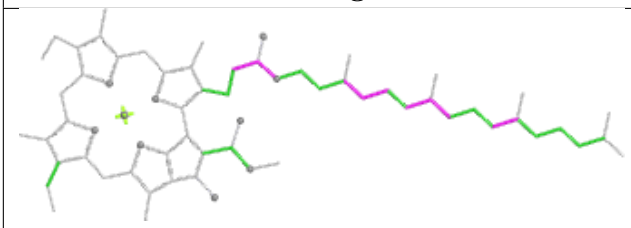
Ligand CL0 A 803



Bond lengths



Bond angles



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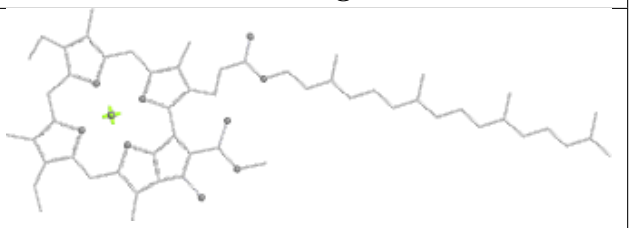
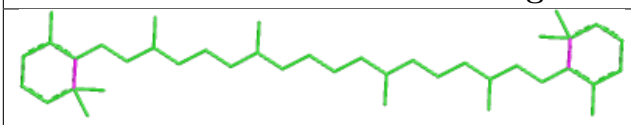
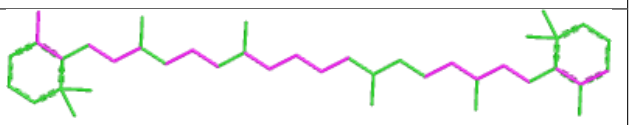


Rings

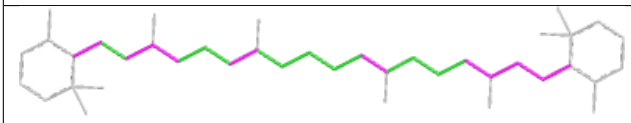
Ligand BCR 9 102



Bond lengths



Bond angles



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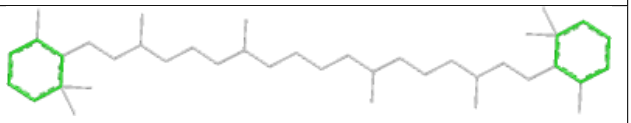
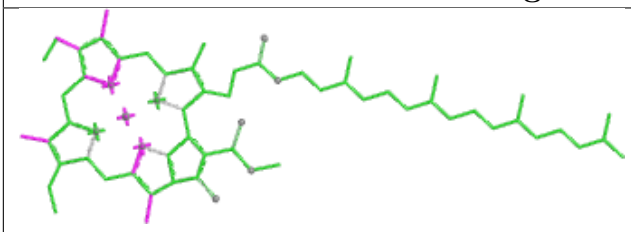
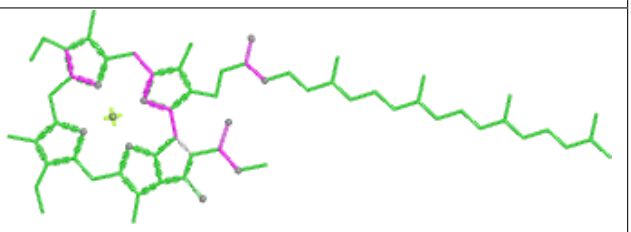


Rings

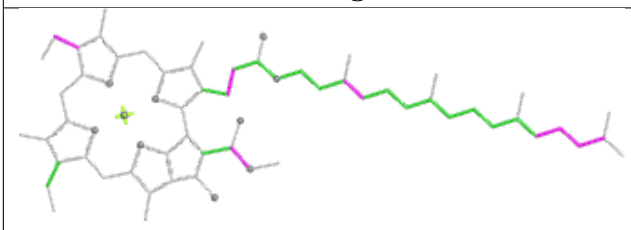
Ligand CLA A 804



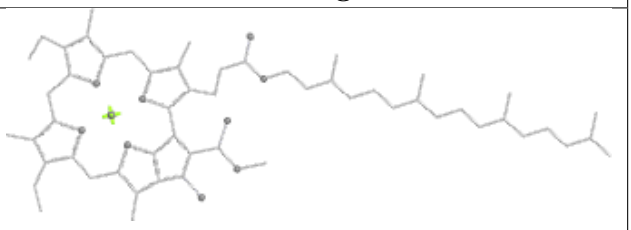
Bond lengths



Bond angles

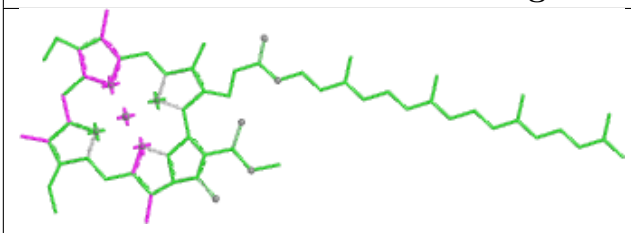


Torsions



Rings

Ligand CLA a 814



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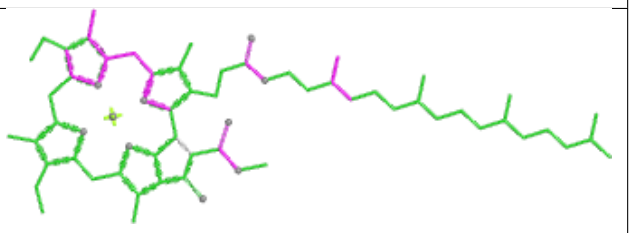

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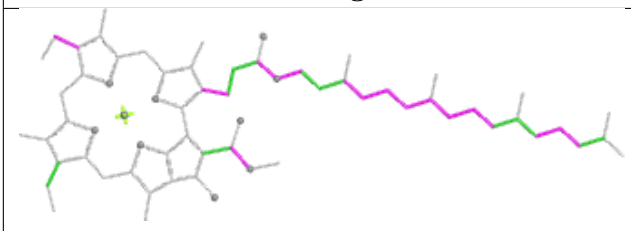
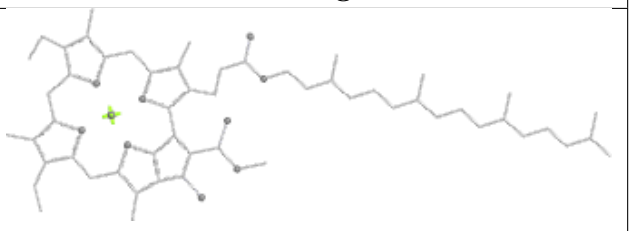
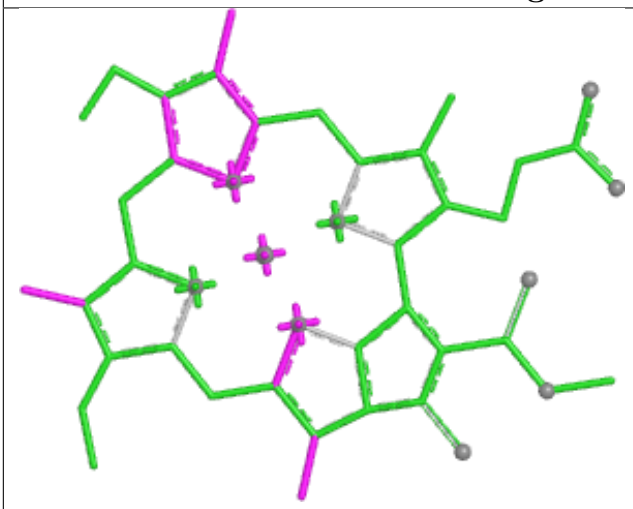


Torsions



Rings

Ligand CLA b 835



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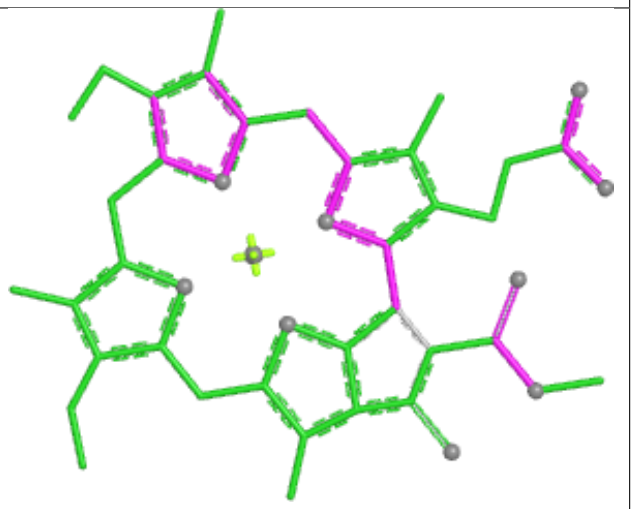

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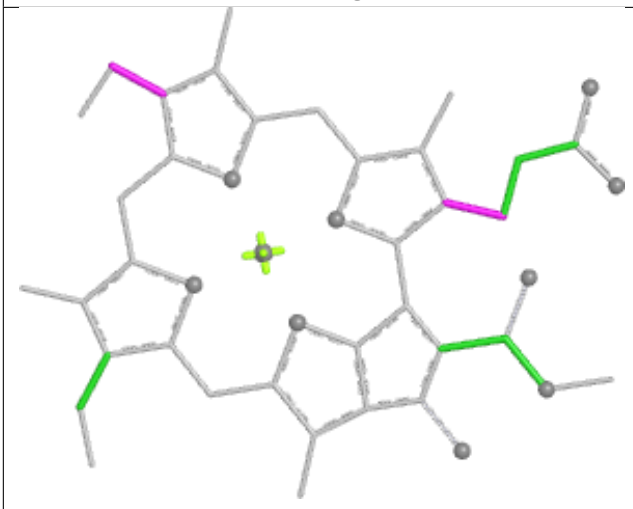
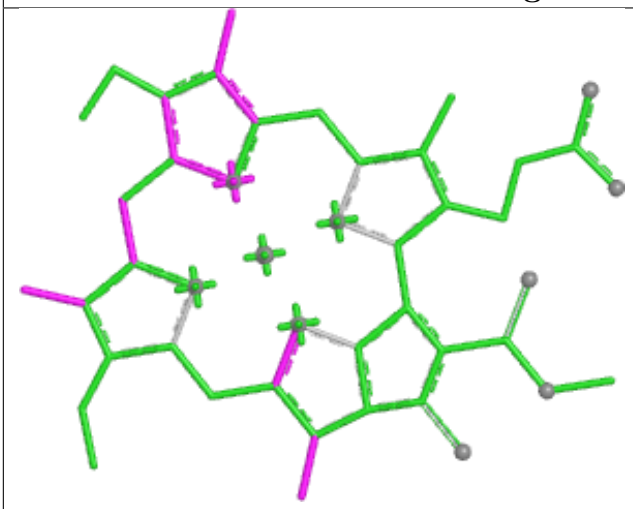


Torsions

Rings

Ligand CLA A 837



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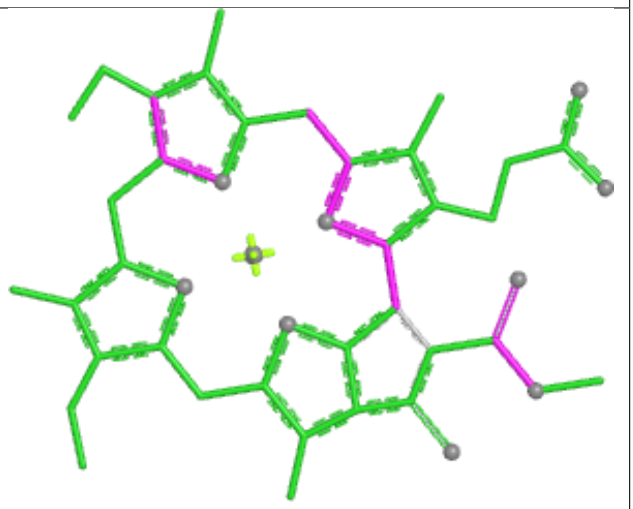

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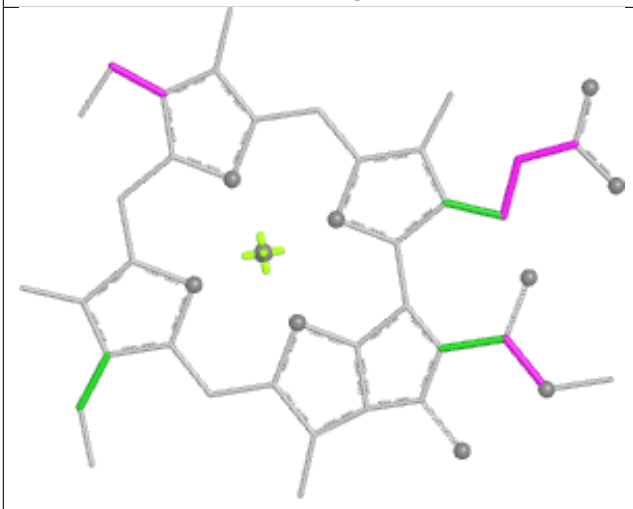
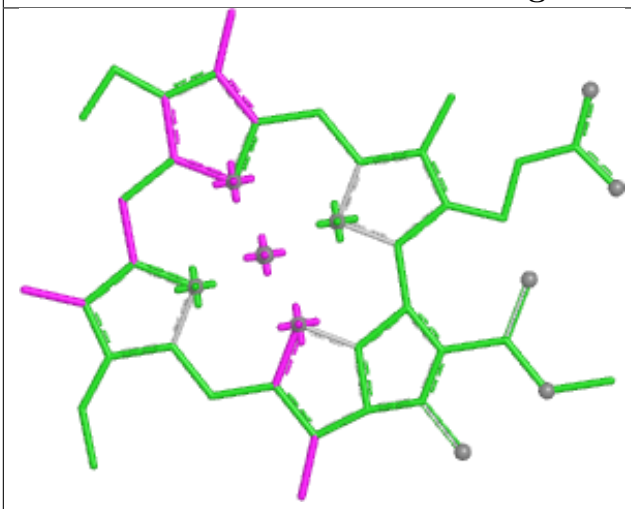


Torsions

Rings

Ligand CLA 2 825



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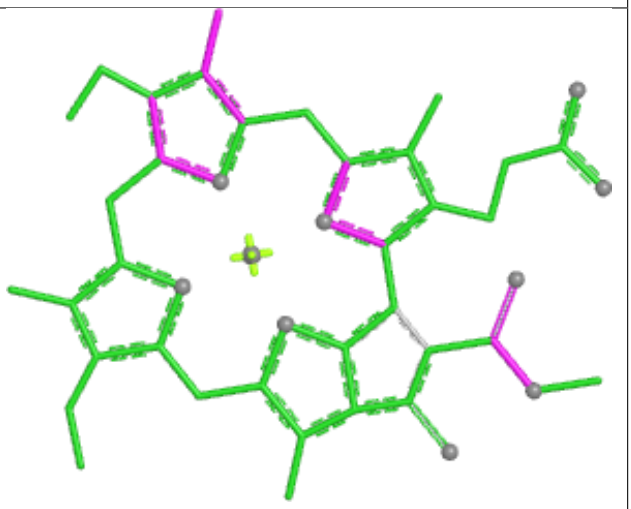
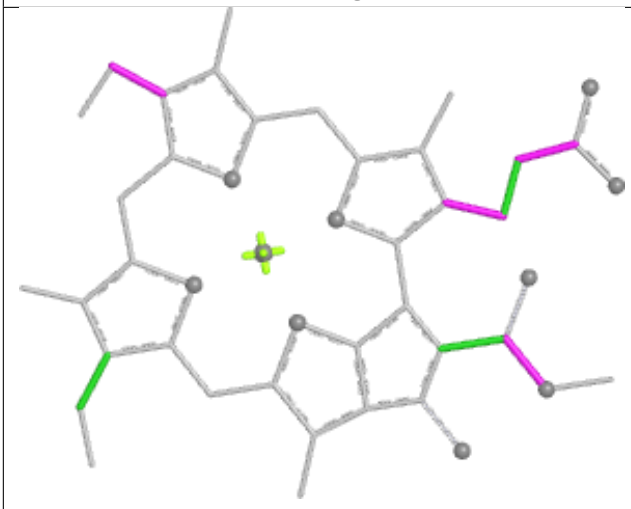


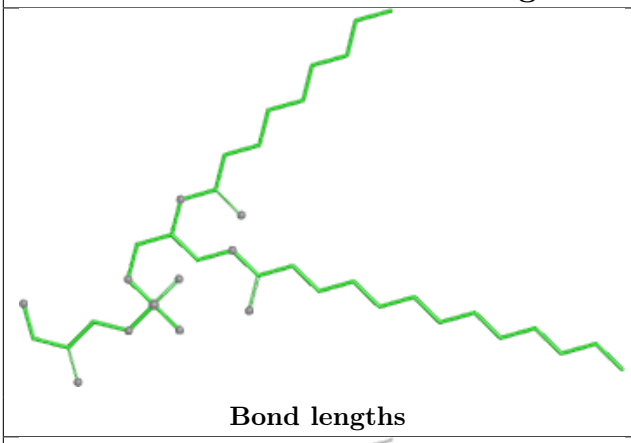
Bond angles



Torsions

Rings

Ligand LHG M 101



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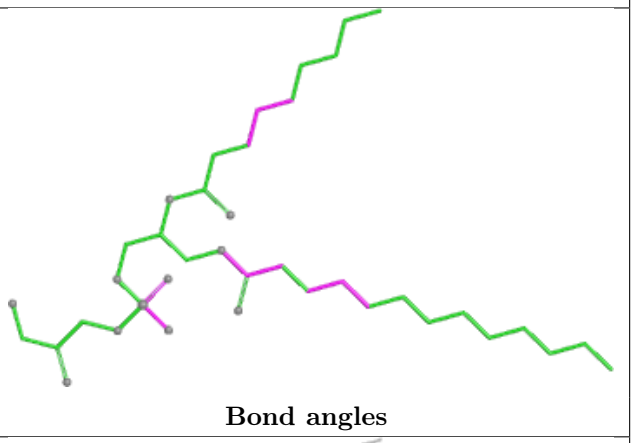
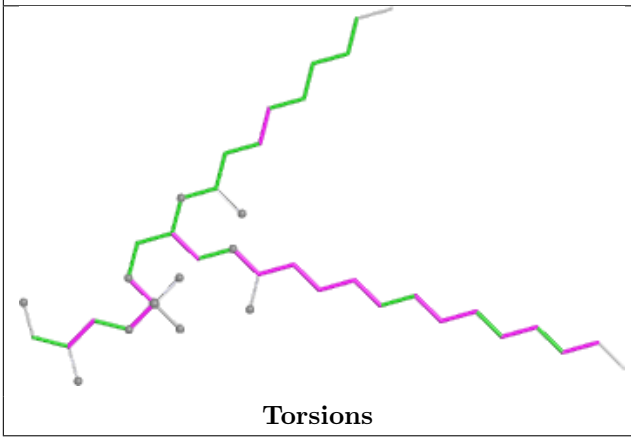


Bond angles



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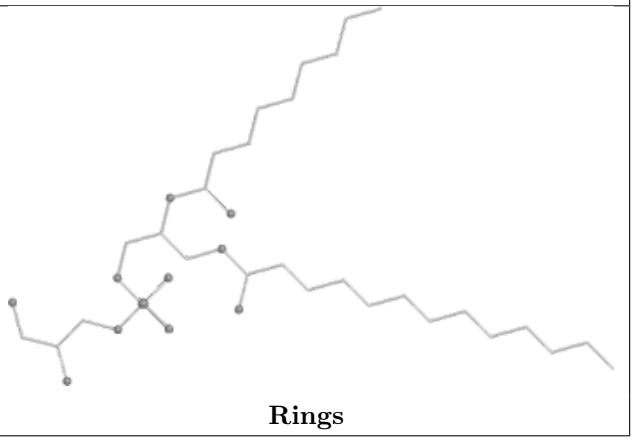
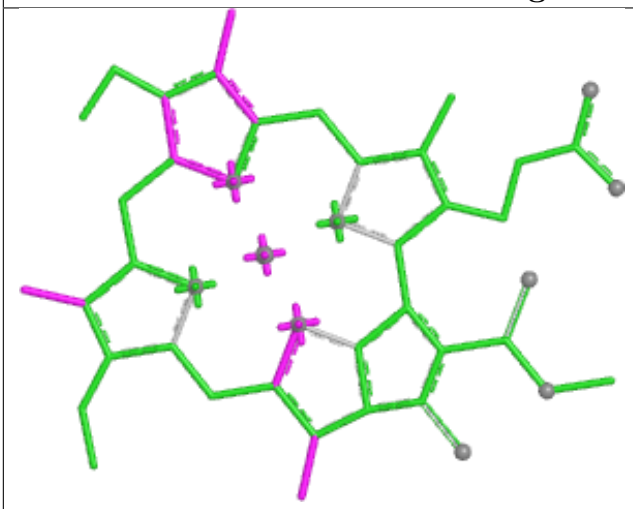


Rings

Ligand CLA 2 824



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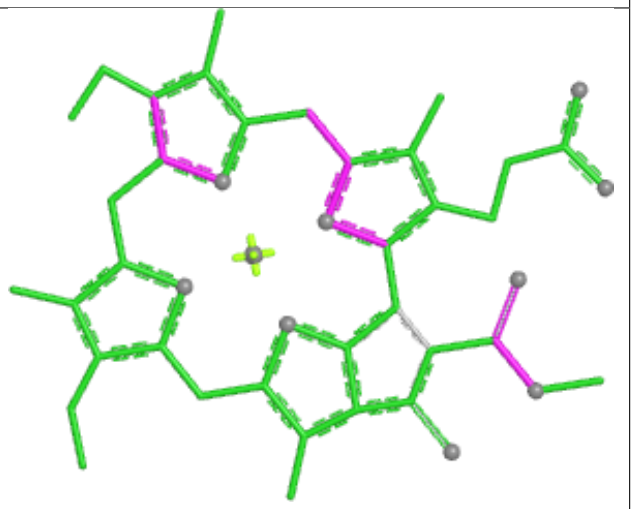
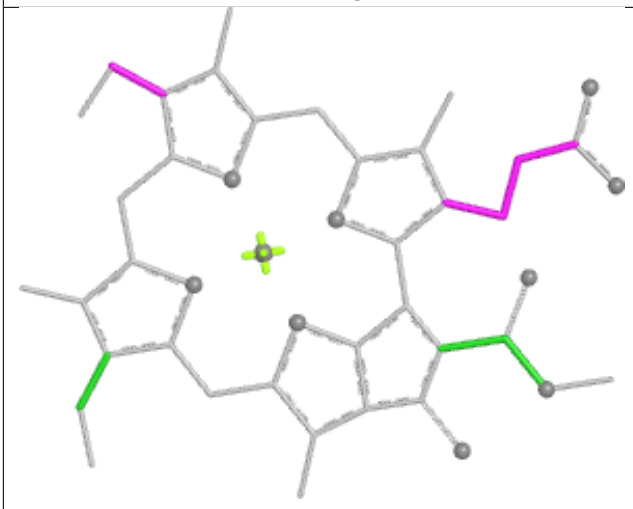


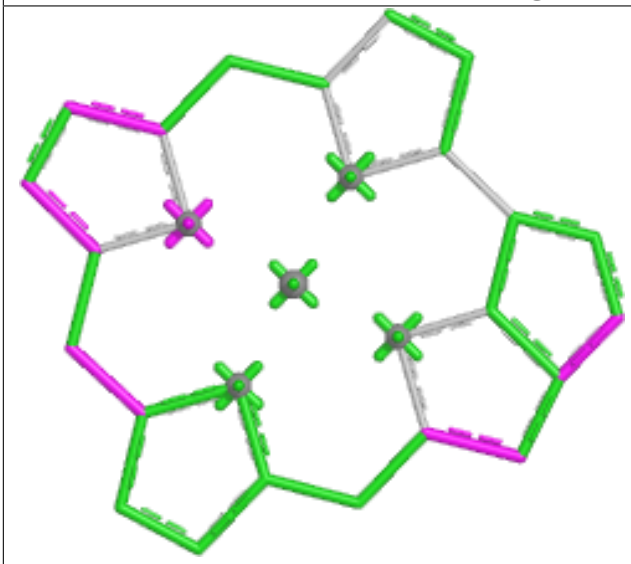
Bond angles



Torsions

Rings

Ligand CLA 2 844



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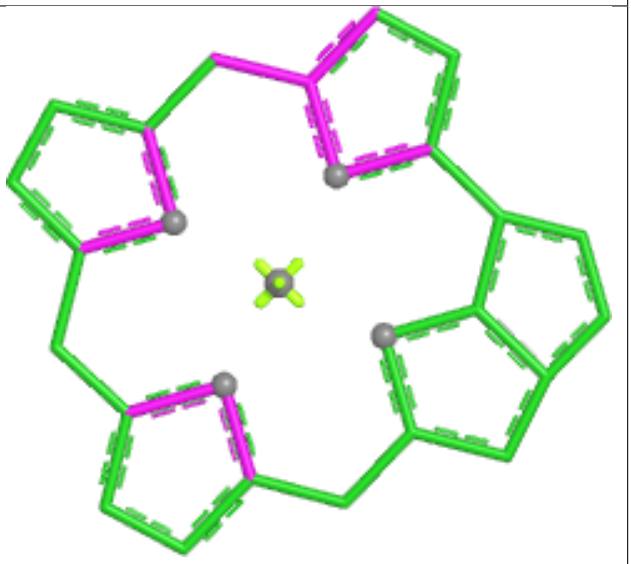
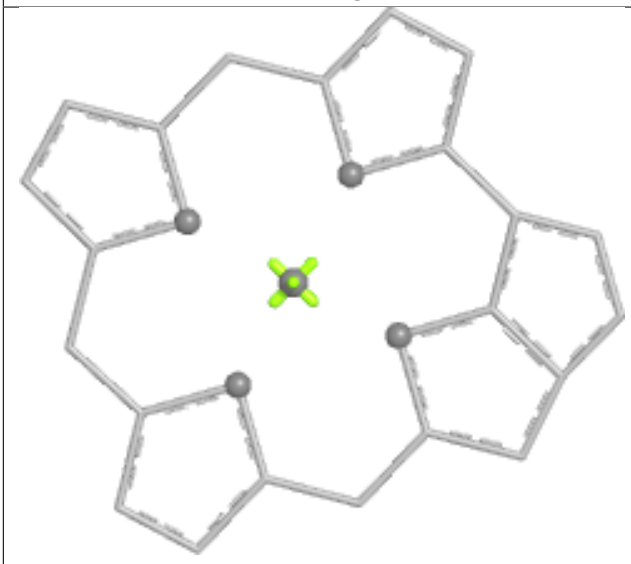
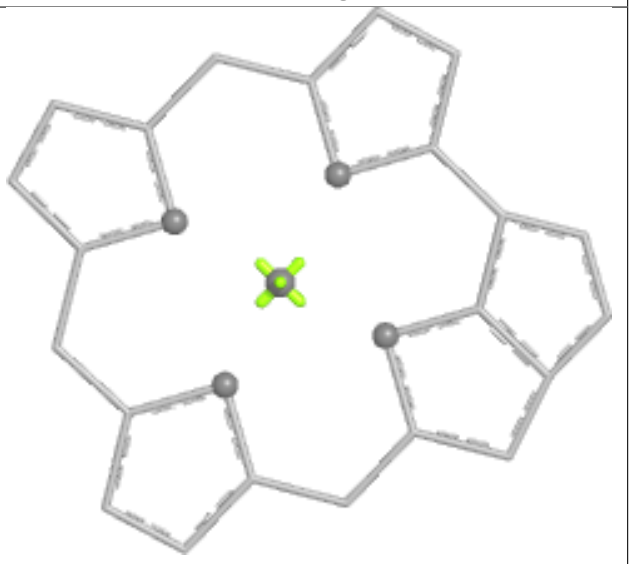


Bond angles

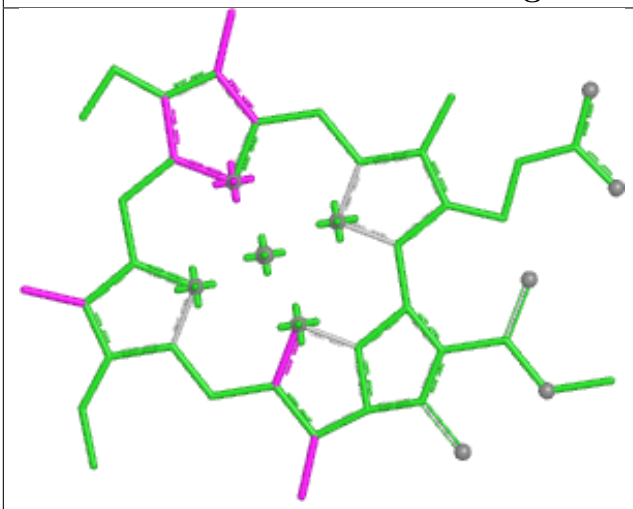


Torsions



Rings

Ligand CLA A 817



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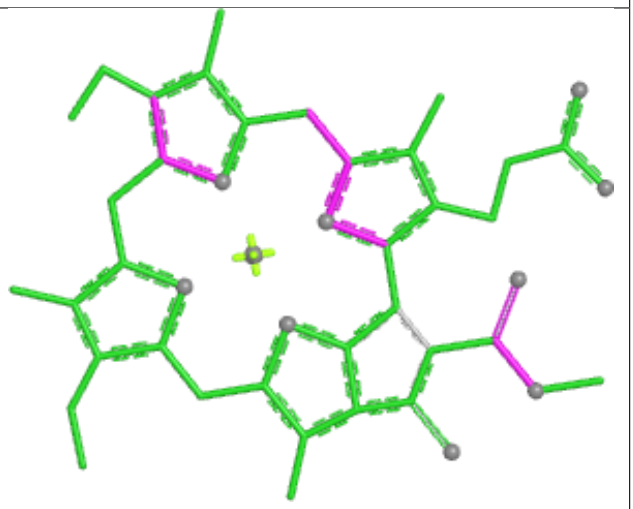

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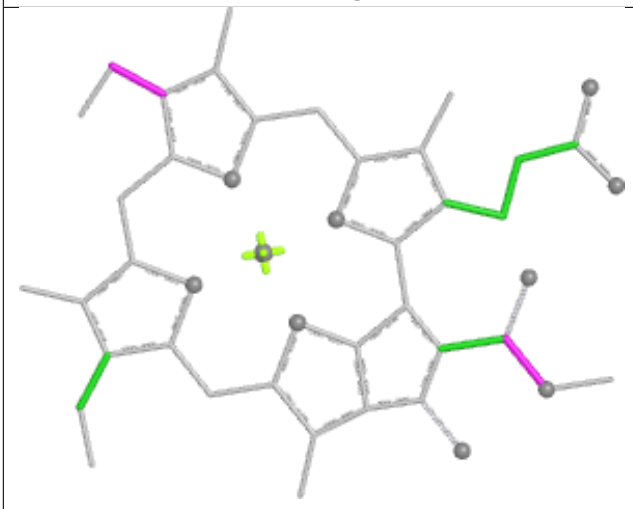
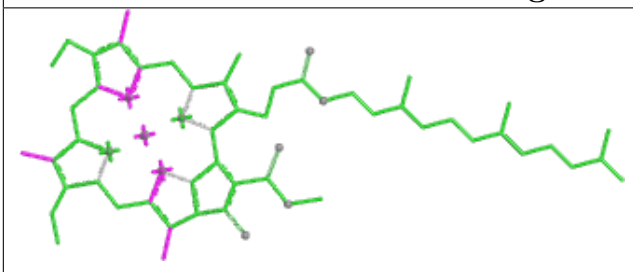


Torsions

Rings

Ligand CLA 2 831



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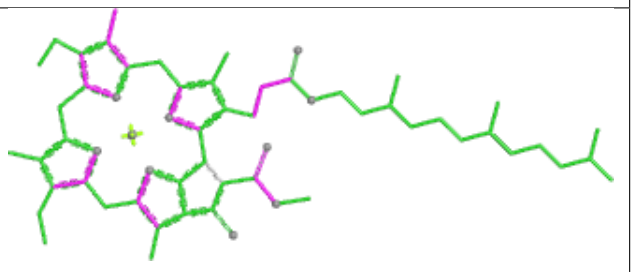
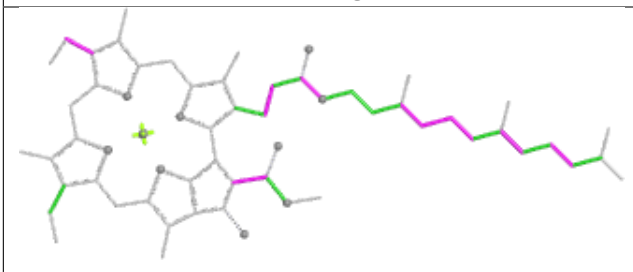
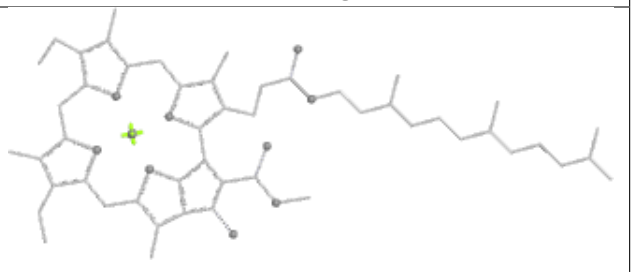


Bond angles

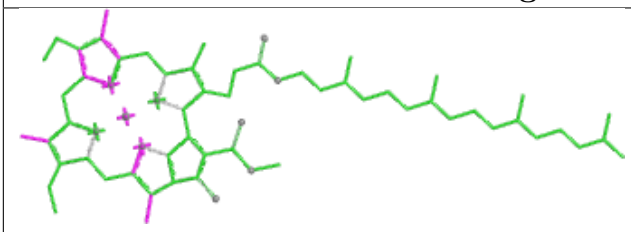


Torsions



Rings

Ligand CLA 7 1101



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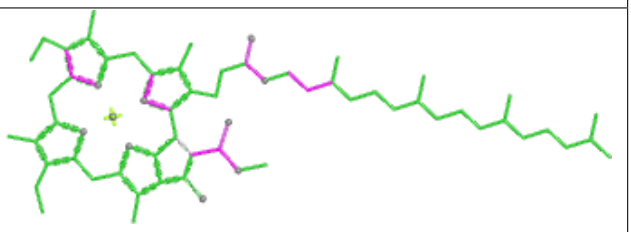

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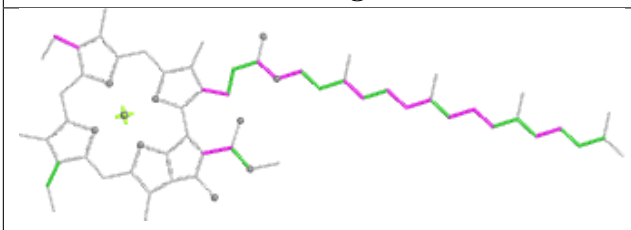

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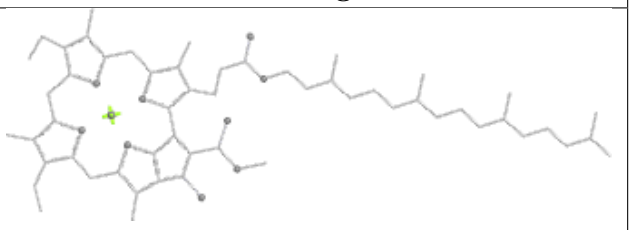
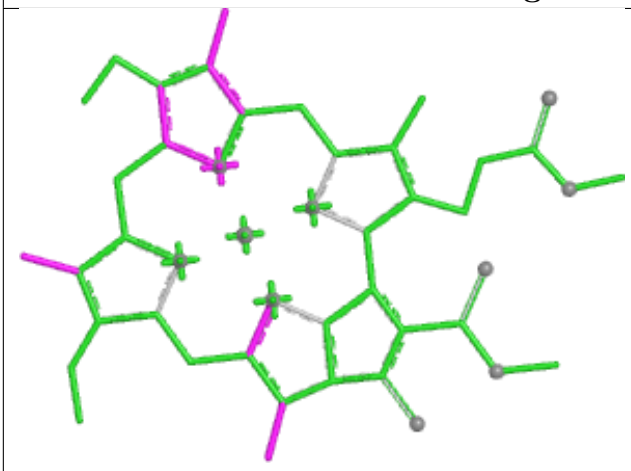


Rings

Ligand CLA A 818



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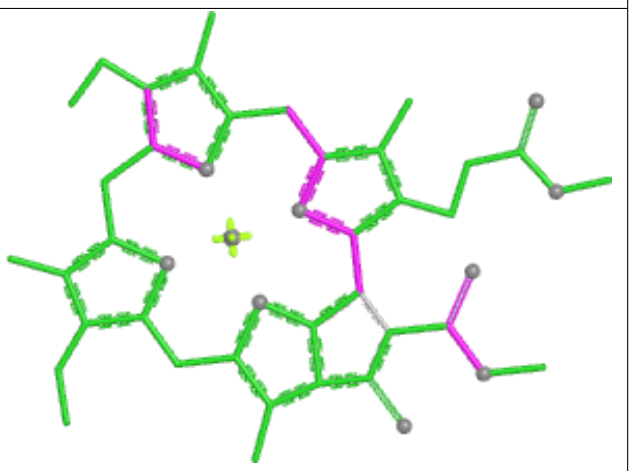
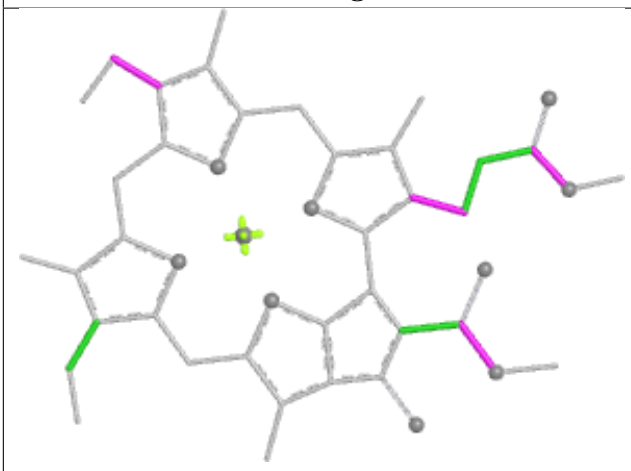


Bond angles



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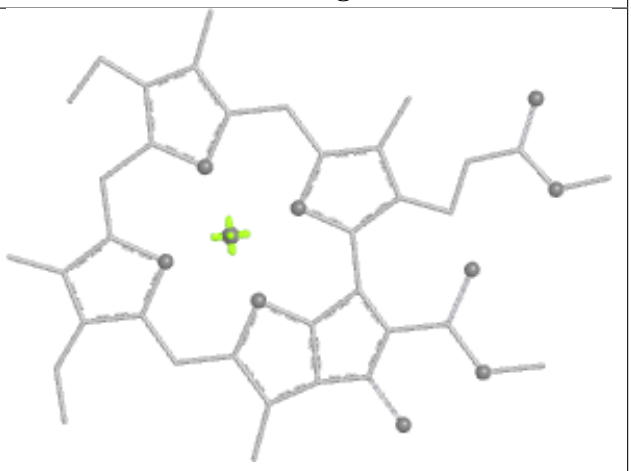
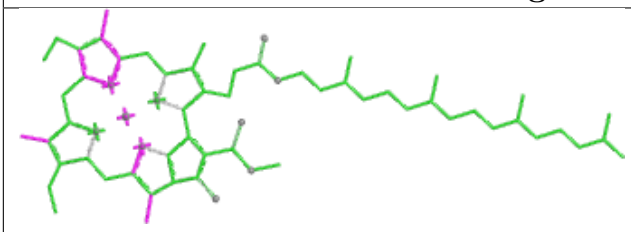


Rings

Ligand CLA 1 830



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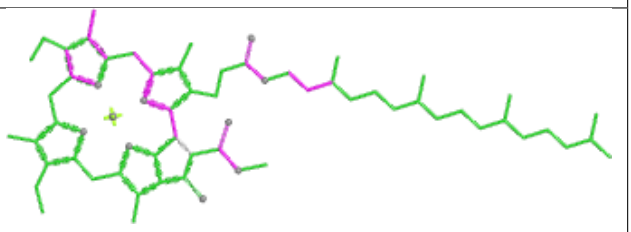
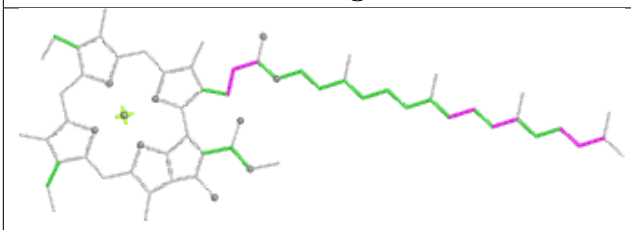
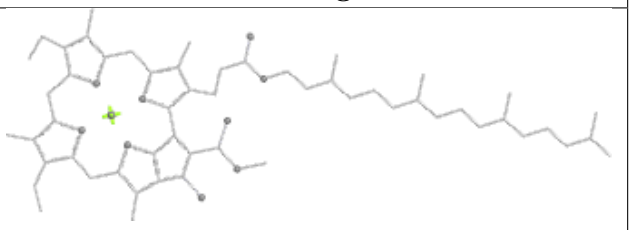


Bond angles

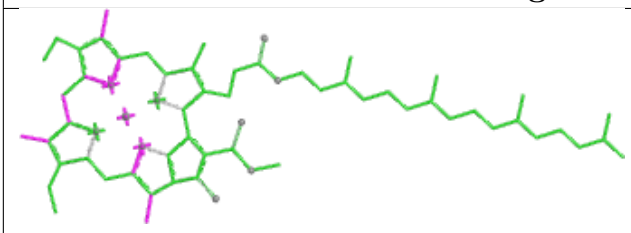


Torsions



Rings

Ligand CLA 2 803



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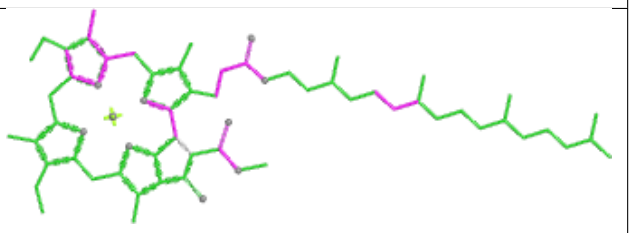
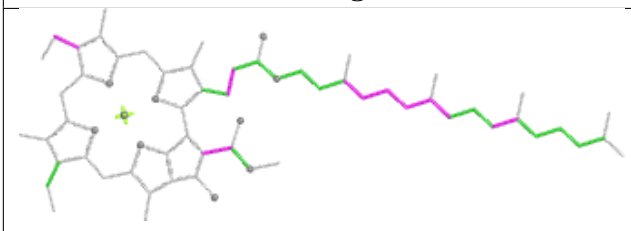


Bond angles



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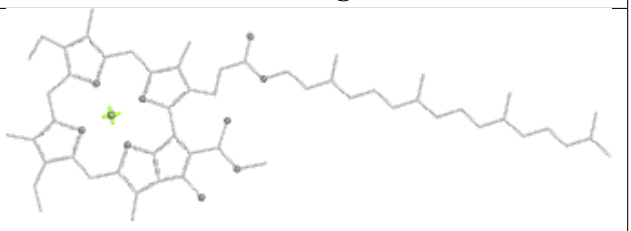
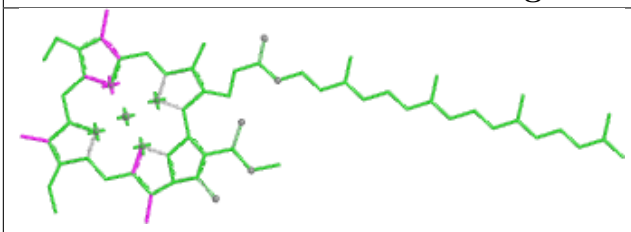
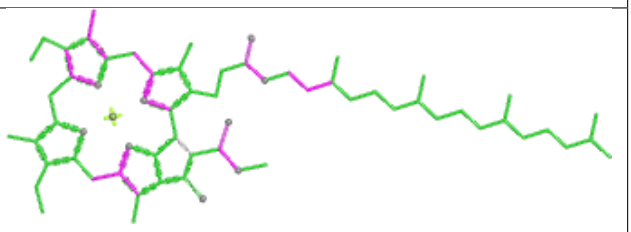


Rings

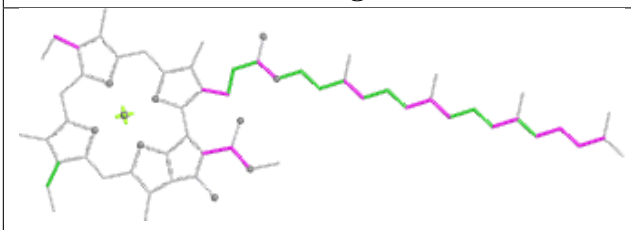
Ligand CLA B 844



Bond lengths



Bond angles



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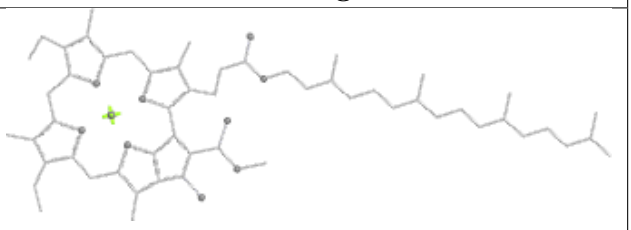
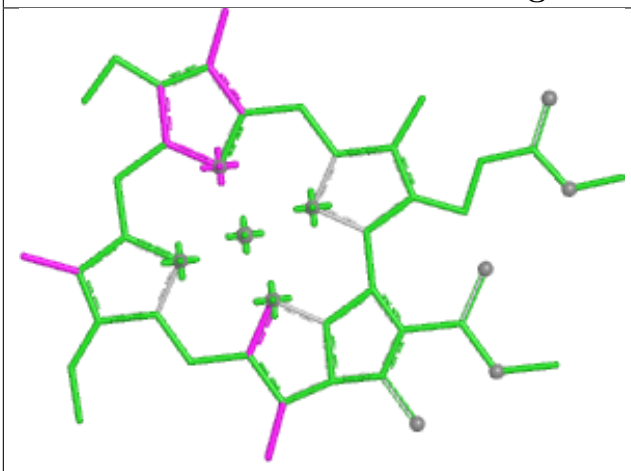
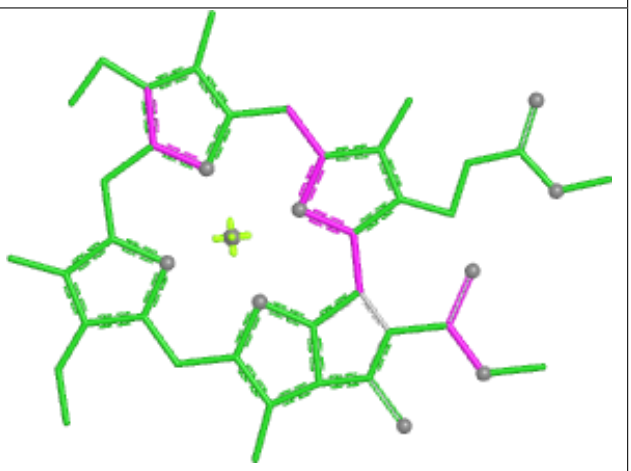


Rings

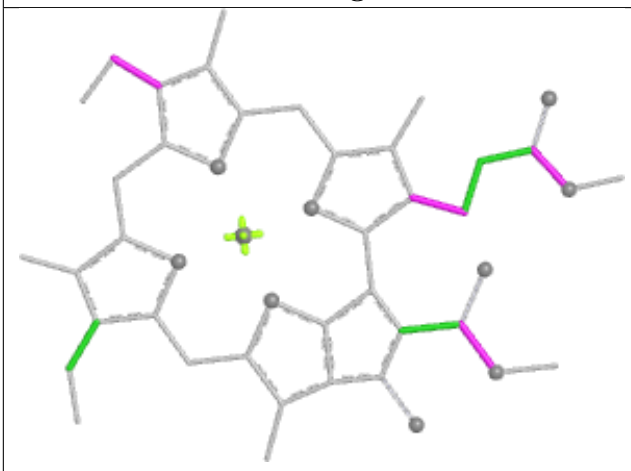
Ligand CLA 1 817



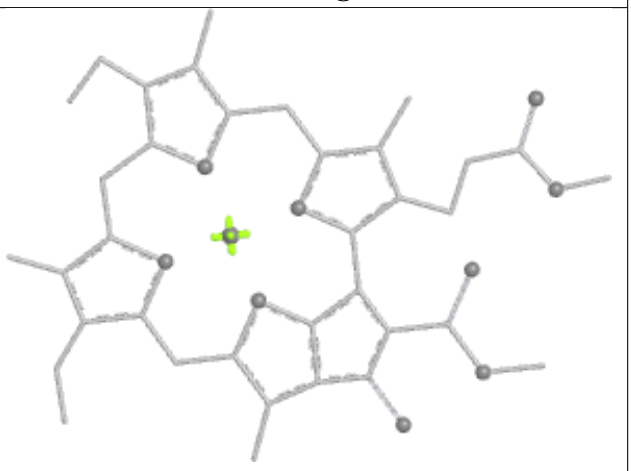
Bond lengths



Bond angles

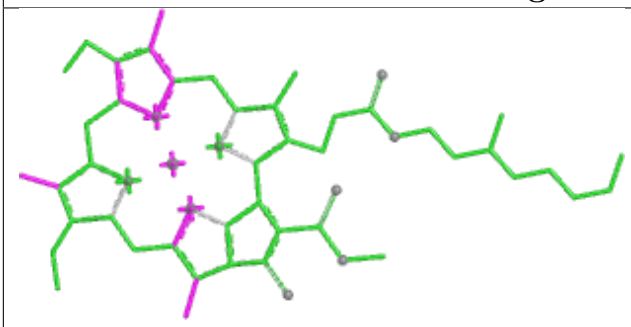


Torsions

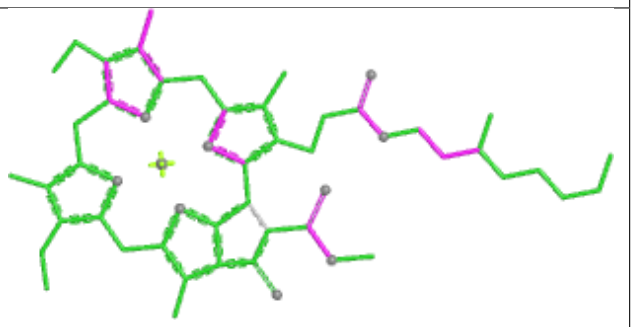


Rings

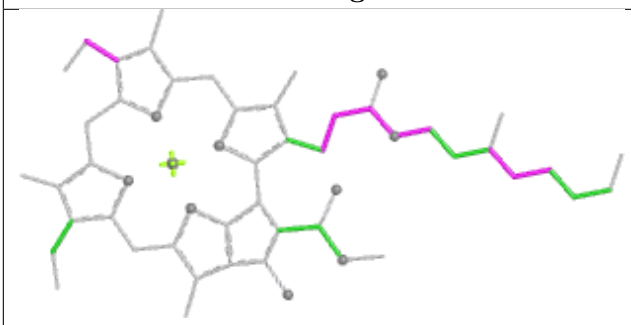
Ligand CLA 1 835



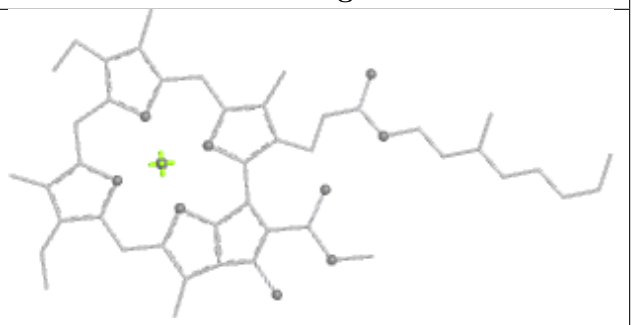
Bond lengths



Bond angles

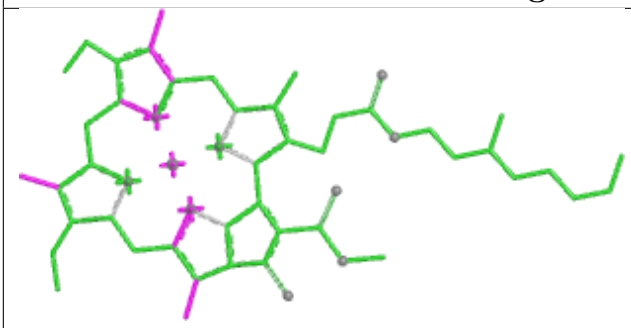


Torsions

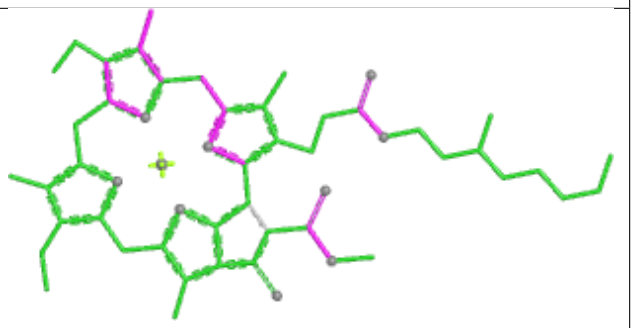


Rings

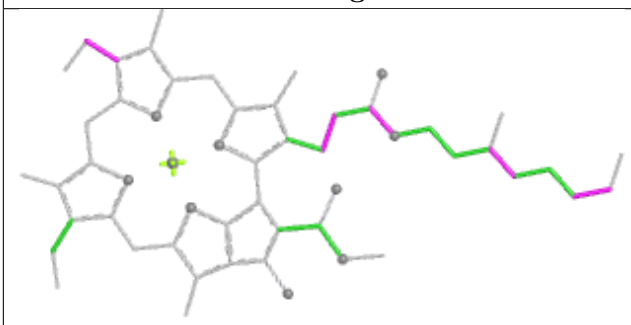
Ligand CLA a 820



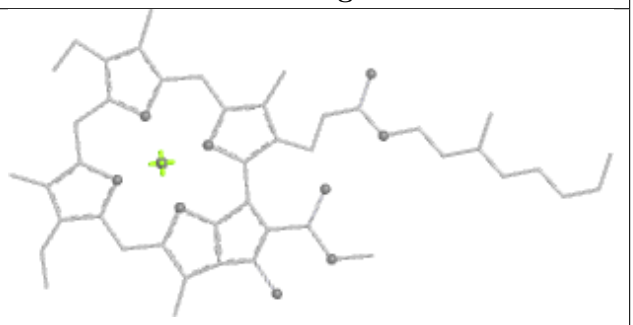
Bond lengths



Bond angles

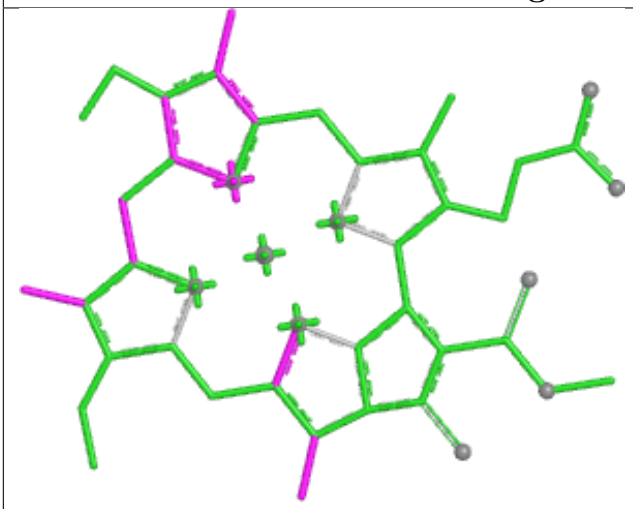


Torsions

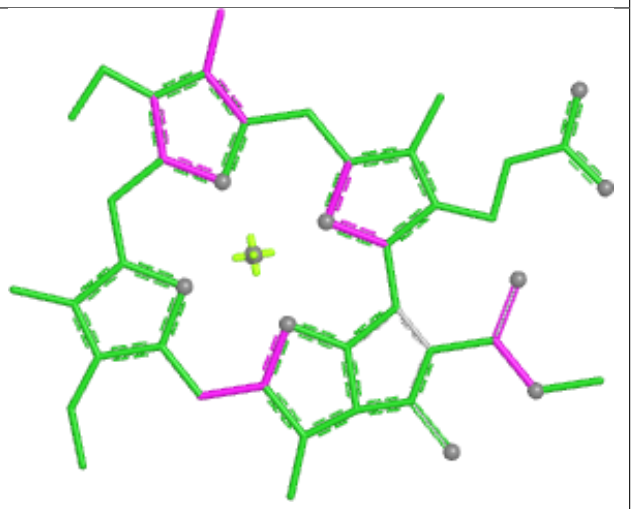


Rings

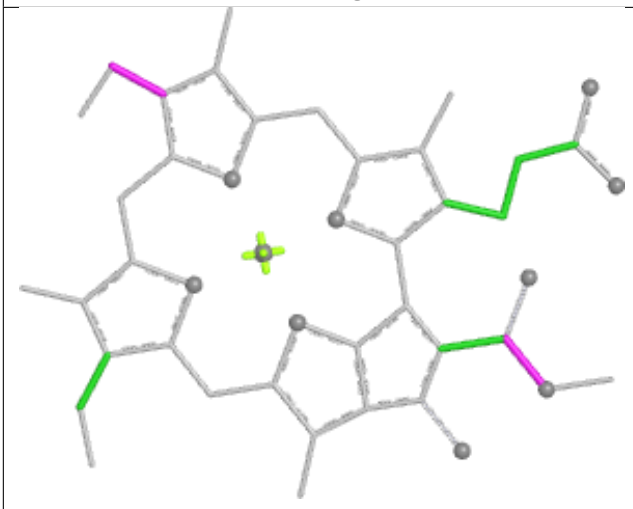
Ligand CLA 2 817



Bond lengths



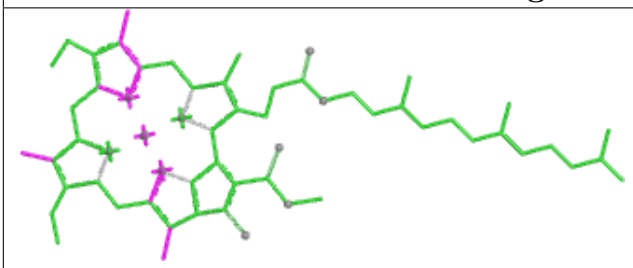
Bond angles



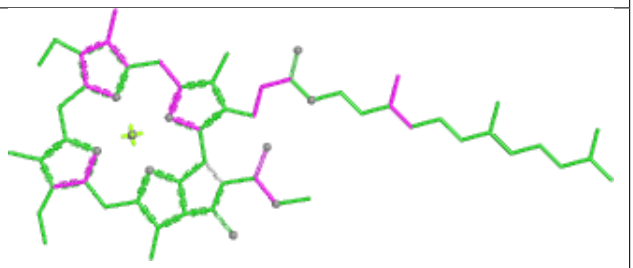
Torsions

Rings

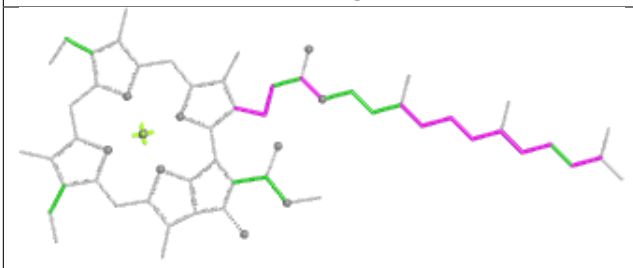
Ligand CLA b 820



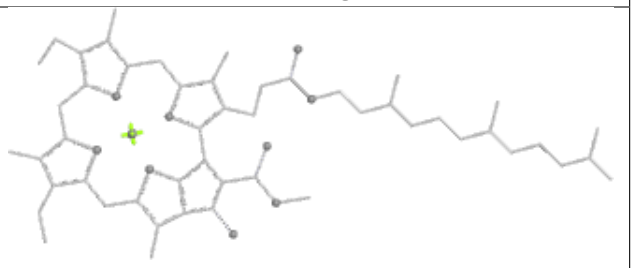
Bond lengths



Bond angles

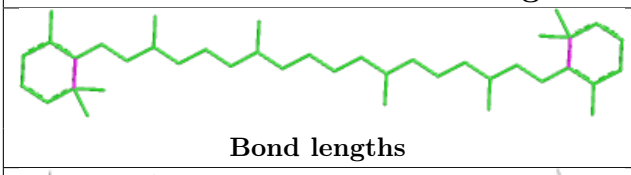


Torsions

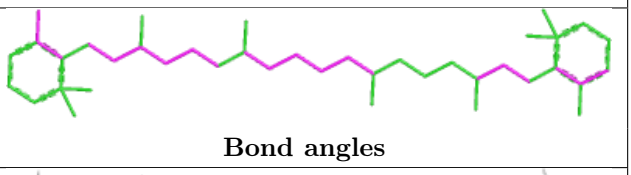


Rings

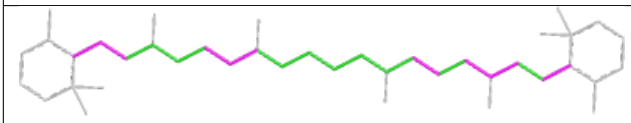
Ligand BCR A 847



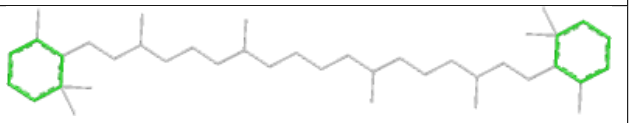
Bond lengths



Bond angles



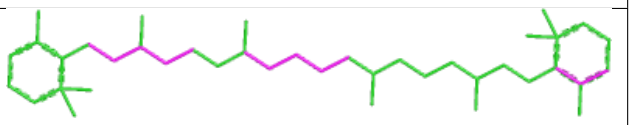
Torsions



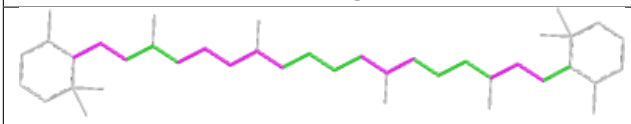
Rings

Ligand BCR J 103

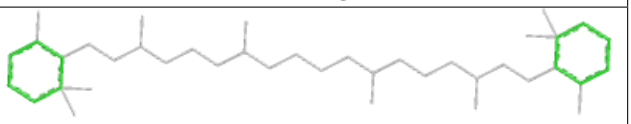
Bond lengths



Bond angles

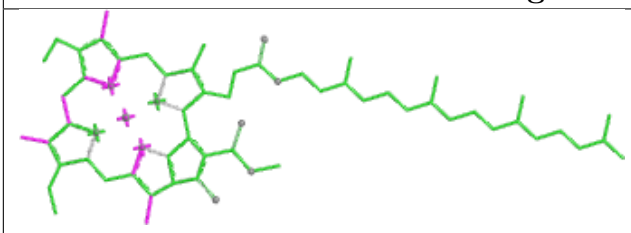


Torsions

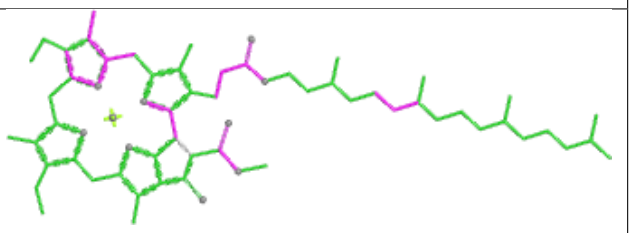


Rings

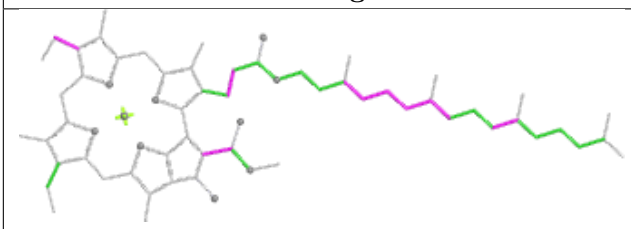
Ligand CLA b 804



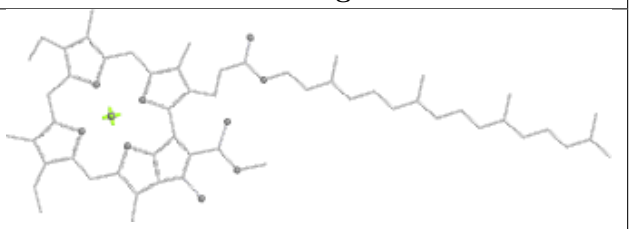
Bond lengths



Bond angles

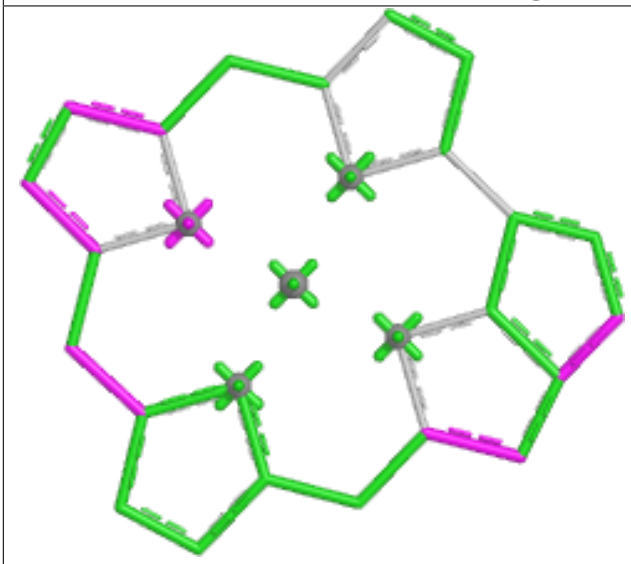


Torsions

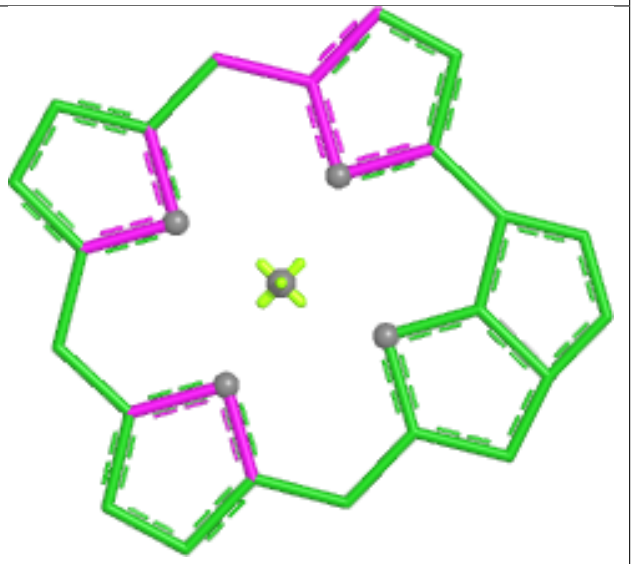


Rings

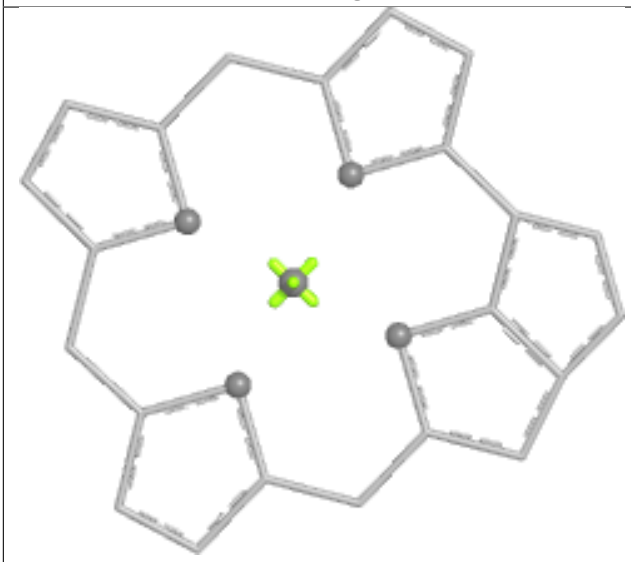
Ligand CLA b 844



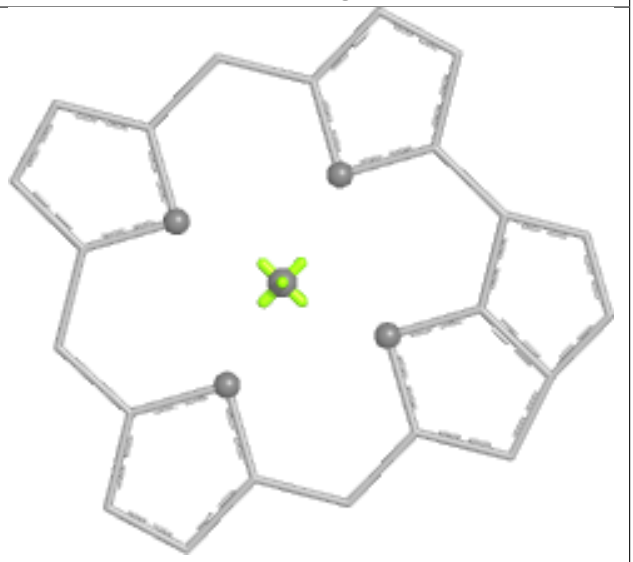
Bond lengths



Bond angles

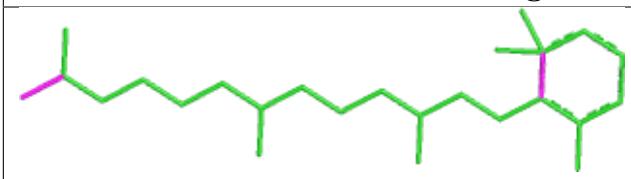


Torsions

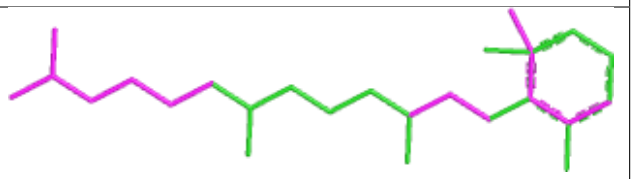


Rings

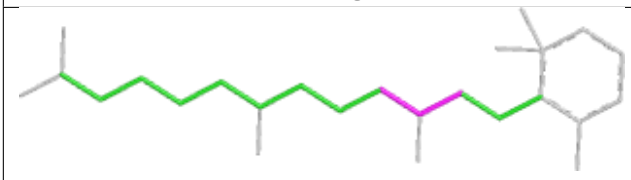
Ligand BCR b 848



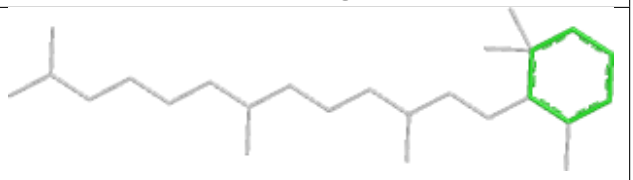
Bond lengths



Bond angles

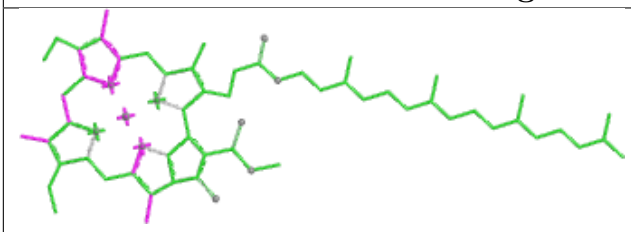


Torsions

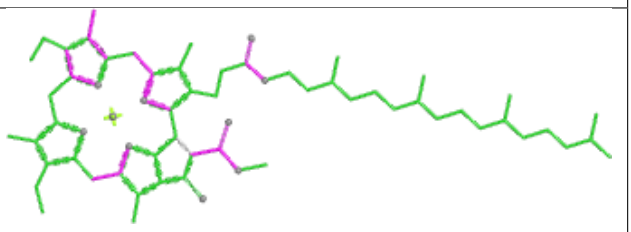


Rings

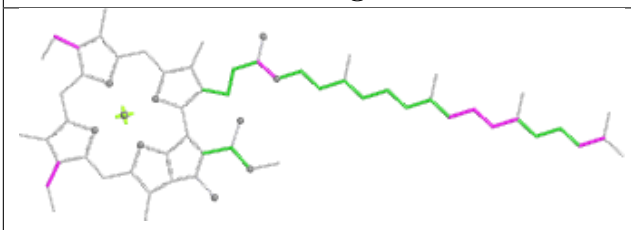
Ligand CLA L 1502



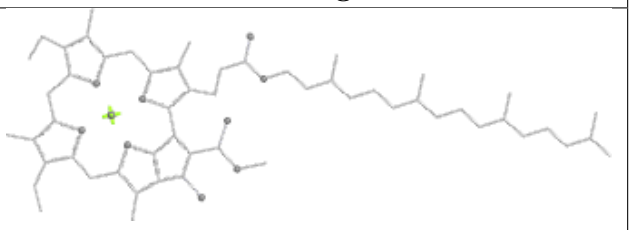
Bond lengths



Bond angles

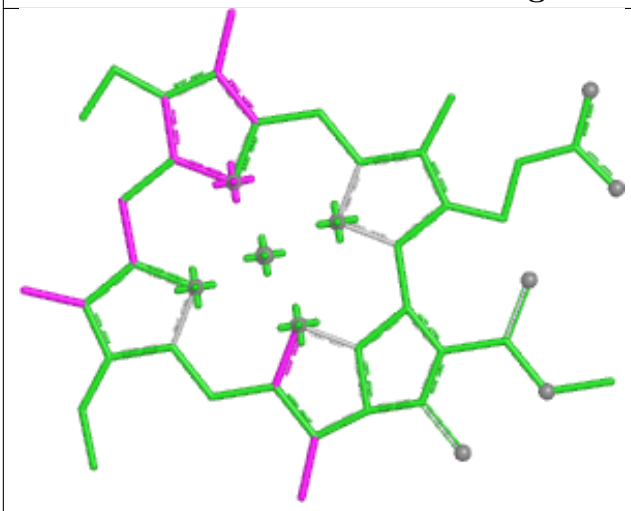


Torsions

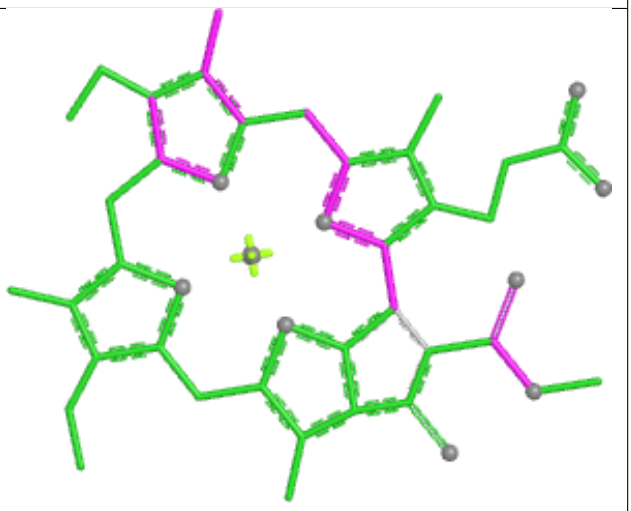


Rings

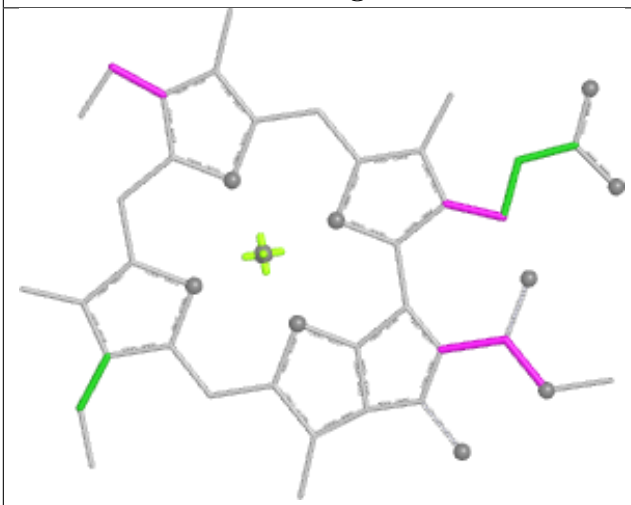
Ligand CLA J 101



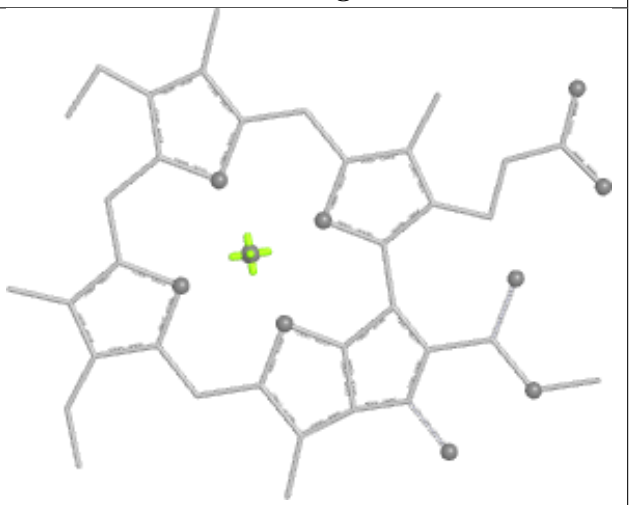
Bond lengths



Bond angles

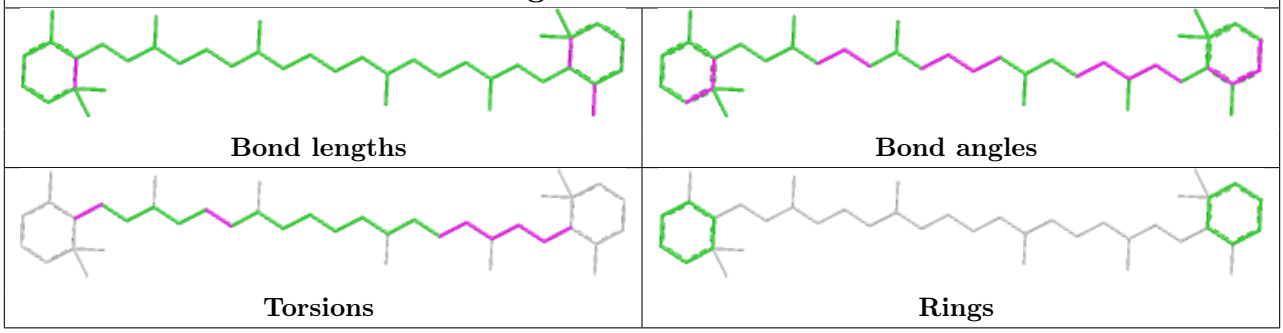


Torsions



Rings

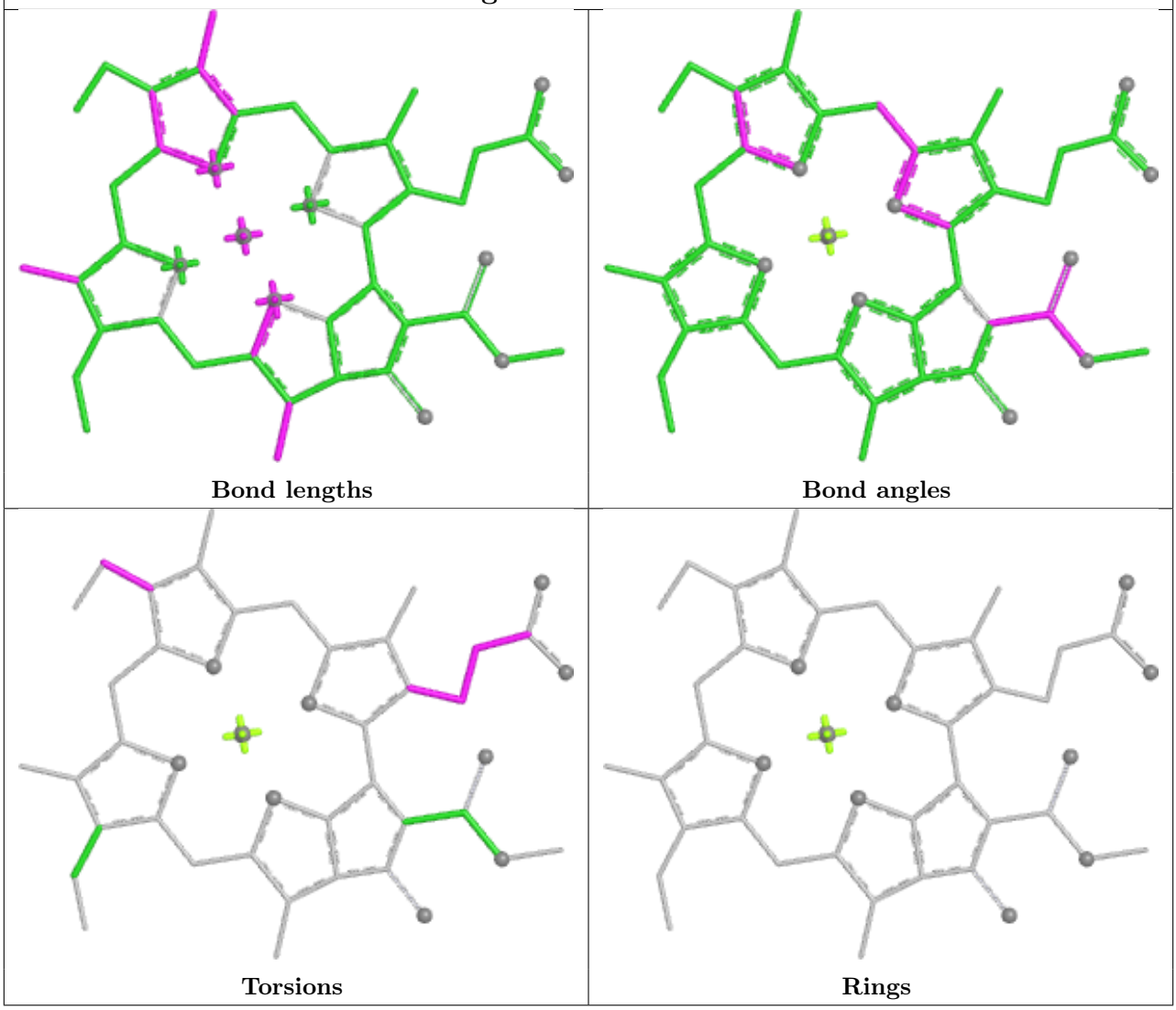
Ligand BCR 2 851



Bond lengths | Bond angles

Torsions | Rings

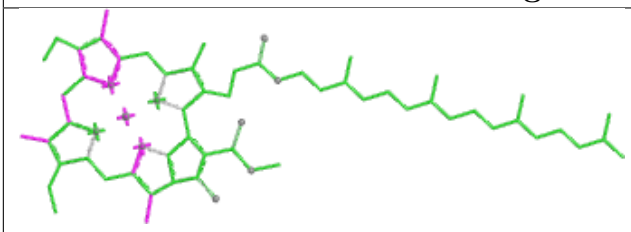
Ligand CLA B 825



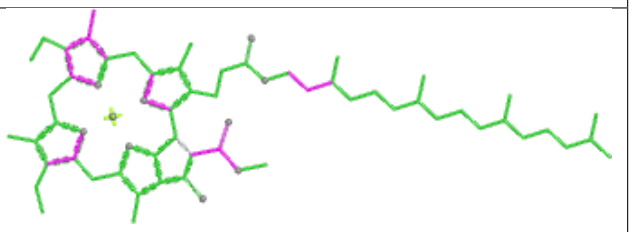
Bond lengths | Bond angles

Torsions | Rings

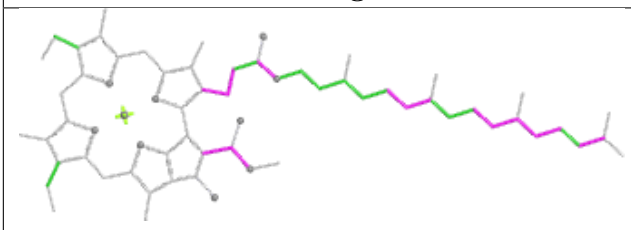
Ligand CLA A 821



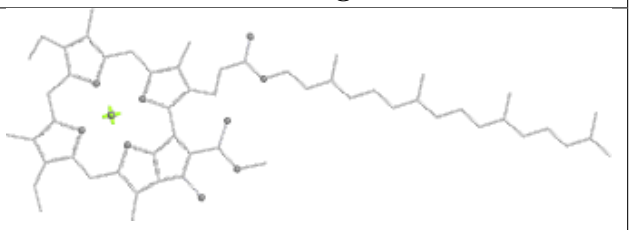
Bond lengths



Bond angles



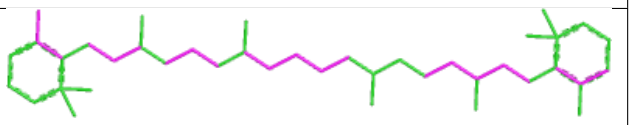
Torsions



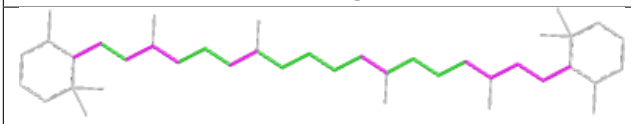
Rings

Ligand BCR M 102

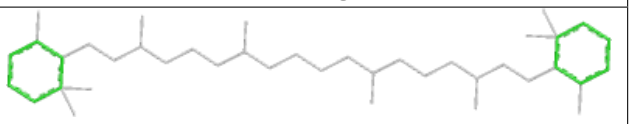
Bond lengths



Bond angles

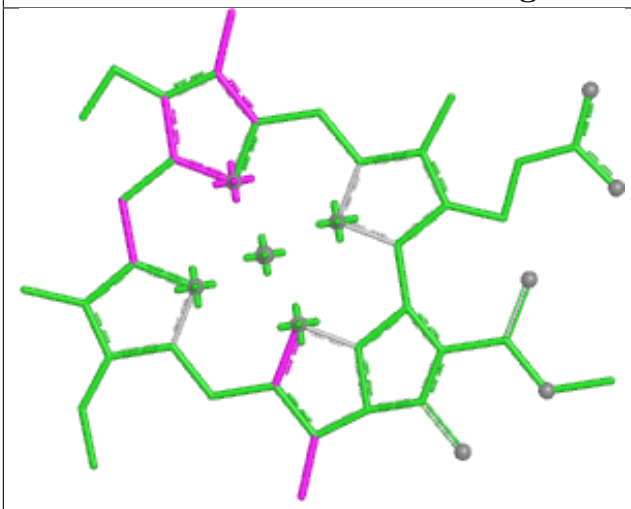


Torsions

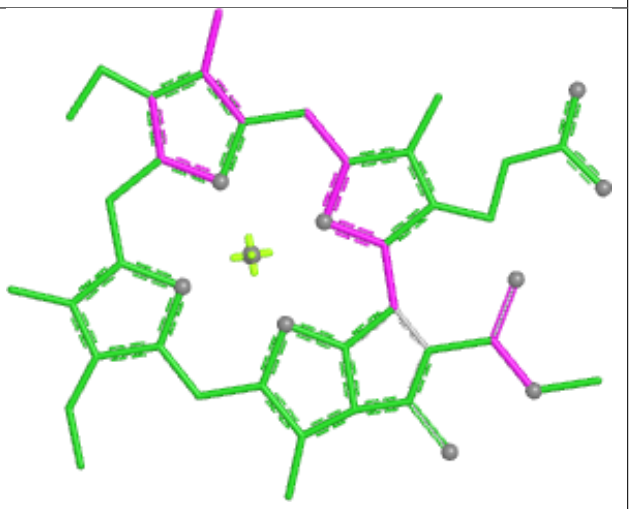


Rings

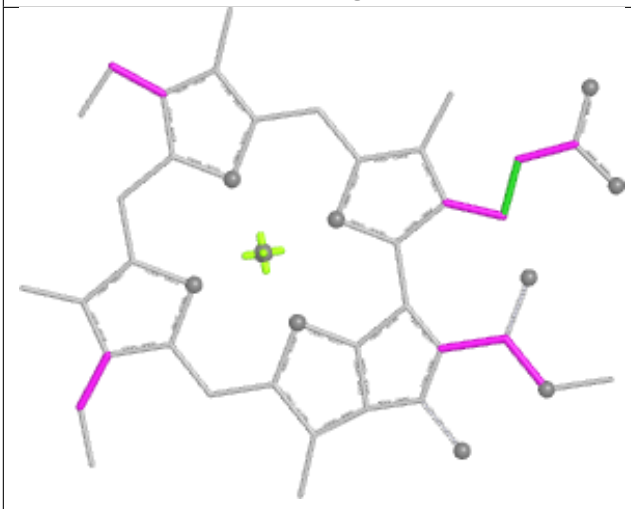
Ligand CLA 8 4003



Bond lengths



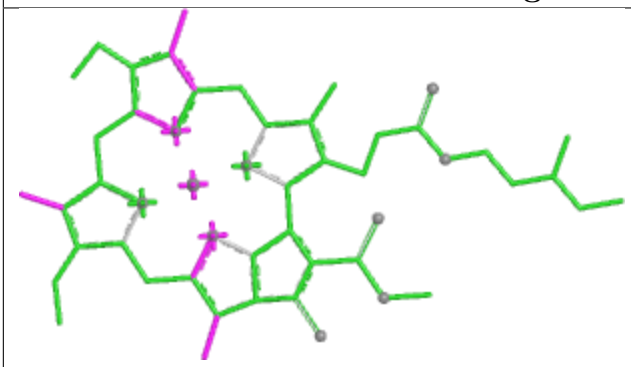
Bond angles



Torsions

Rings

Ligand CLA A 825



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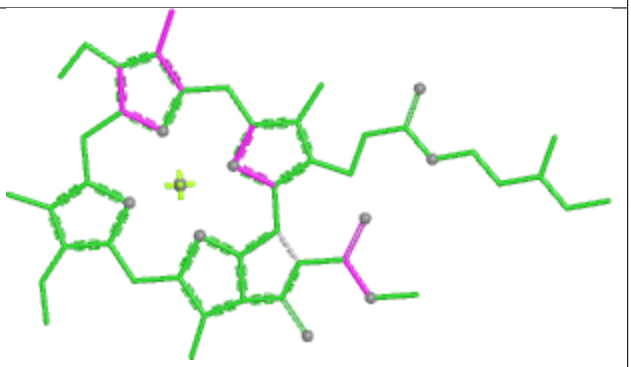
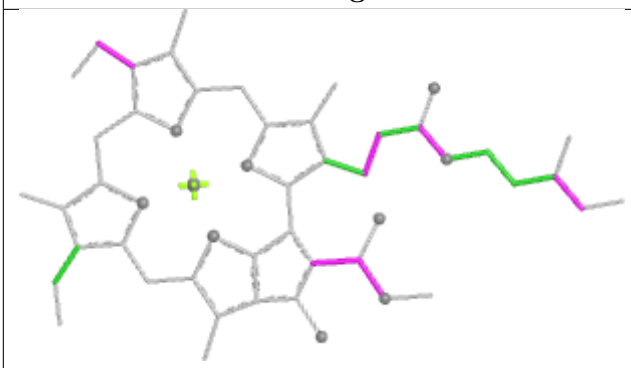
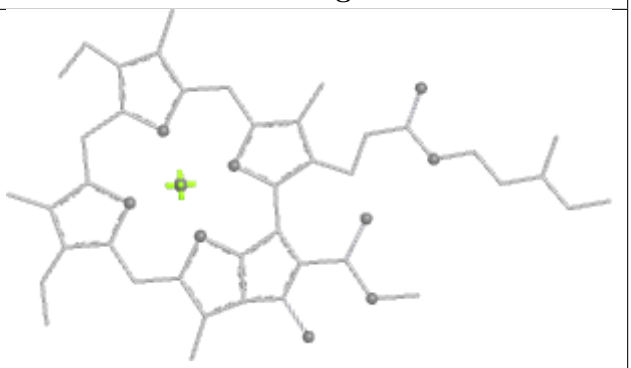


Bond angles

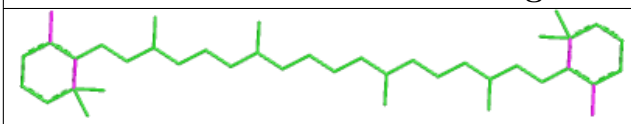


Torsions



Rings

Ligand BCR h 102



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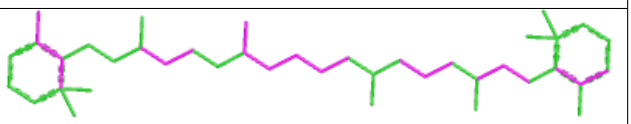
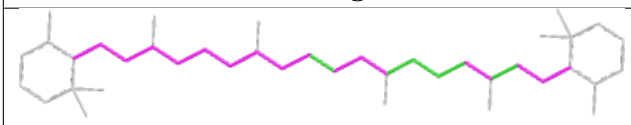
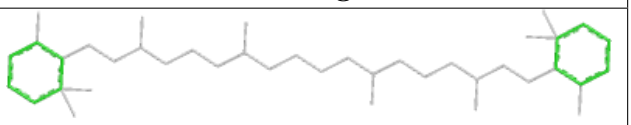


Bond angles

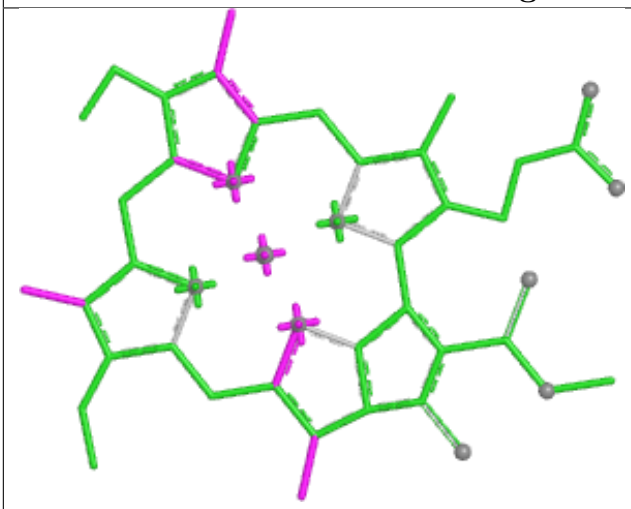


Torsions



Rings

Ligand CLA 6 4403



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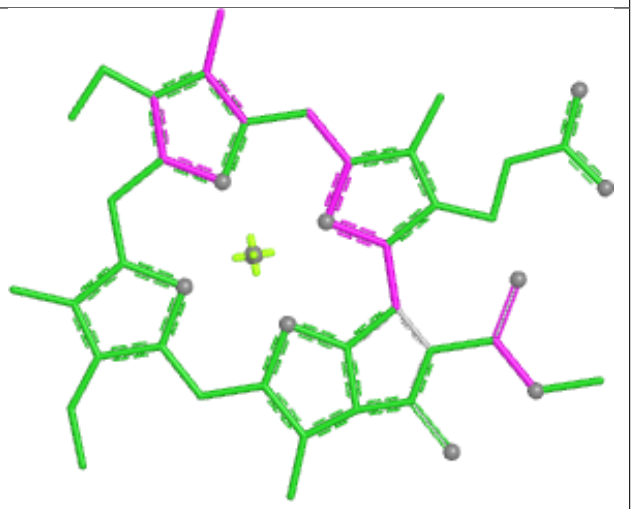
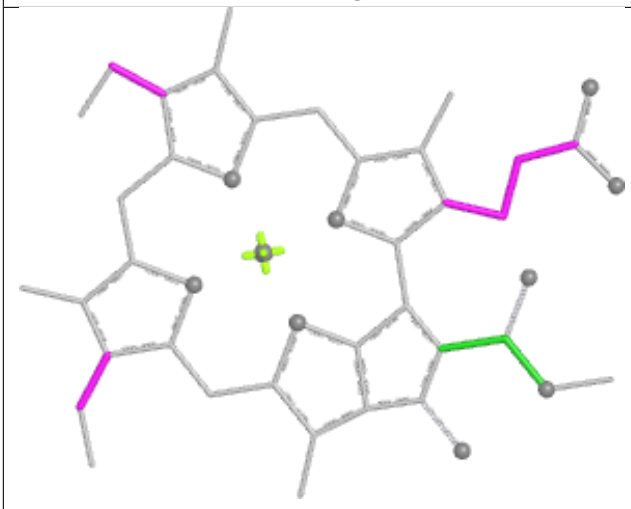


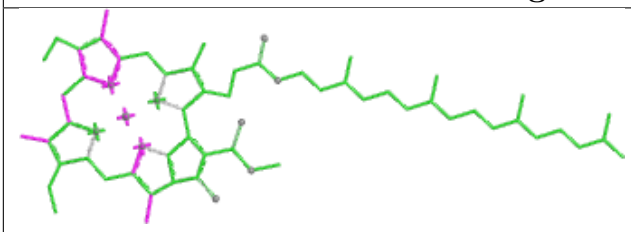
Bond angles



Torsions

Rings

Ligand CLA a 840



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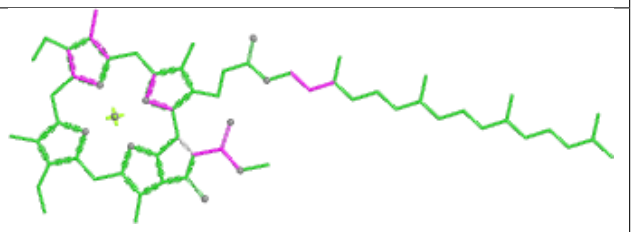
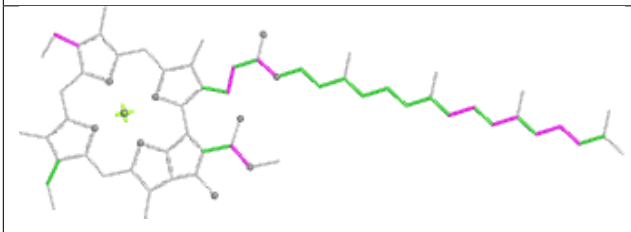
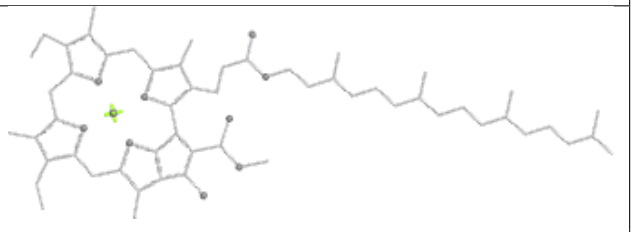


Bond angles

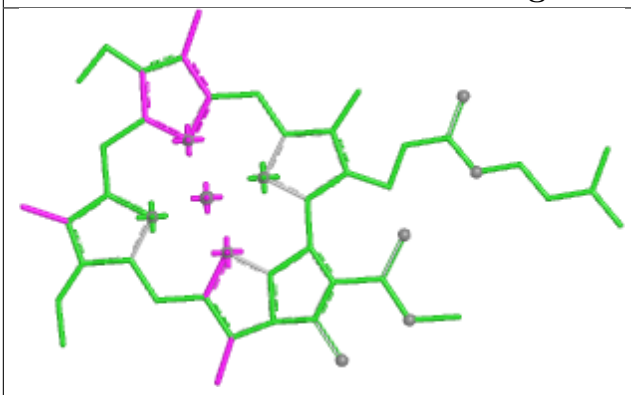


Torsions



Rings

Ligand CLA 2 827



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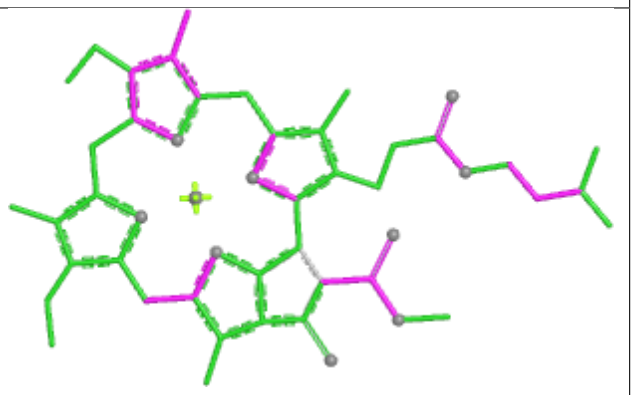
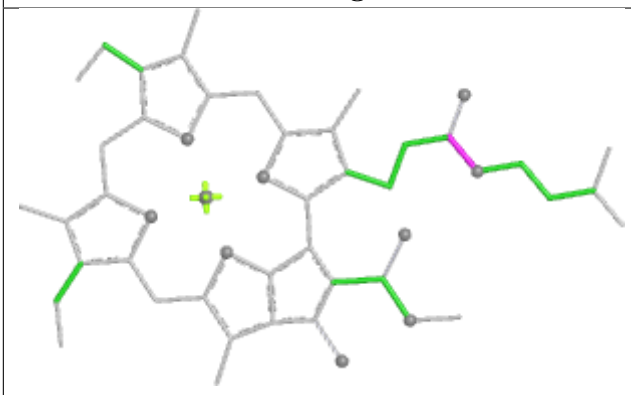
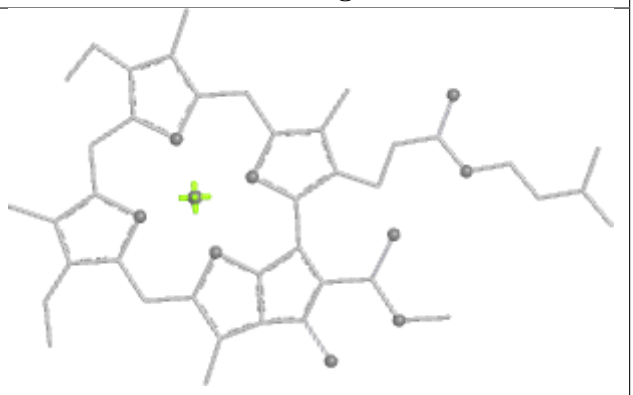


Bond angles

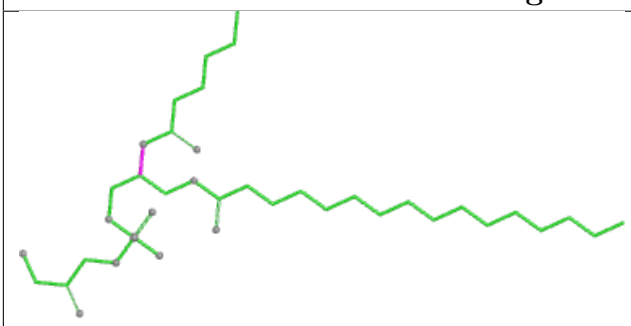


Torsions

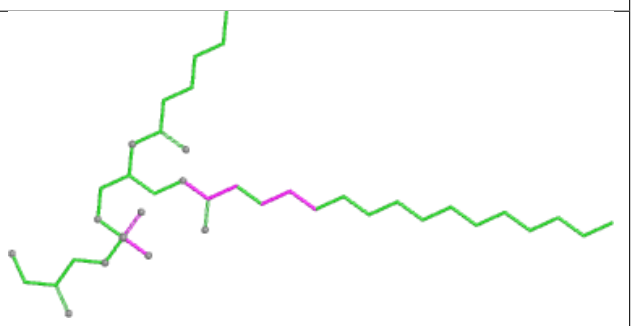


Rings

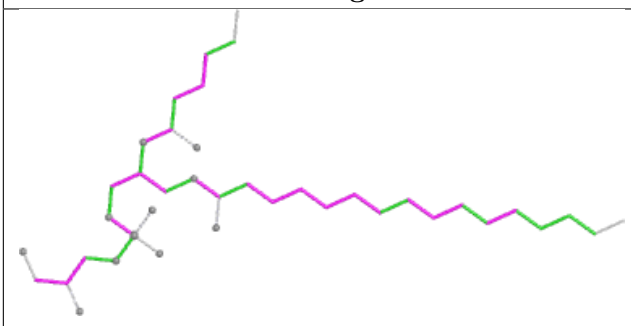
Ligand LHG b 852



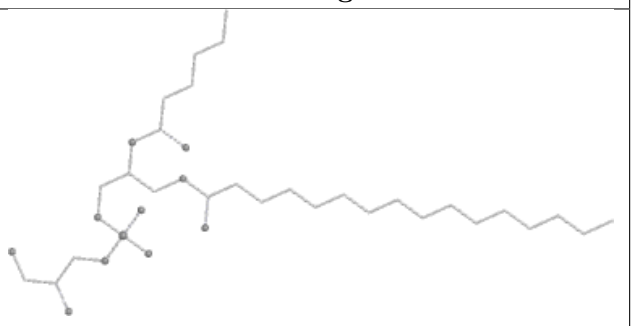
Bond lengths



Bond angles

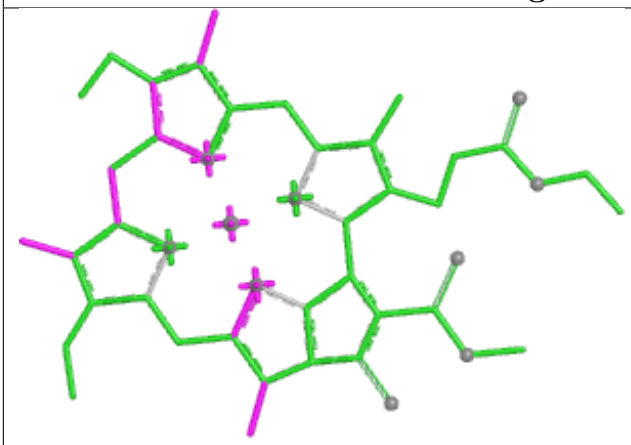


Torsions



Rings

Ligand CLA 2 821



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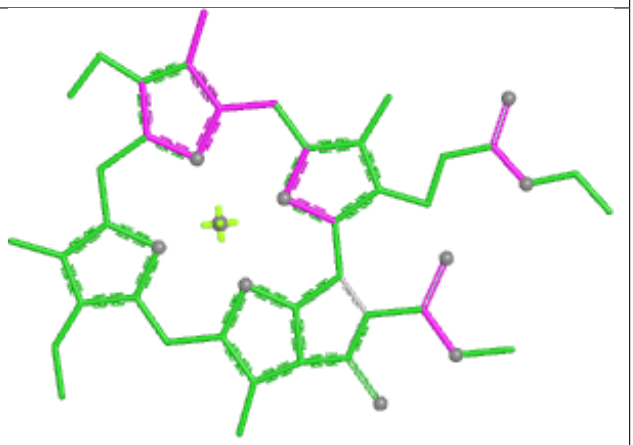
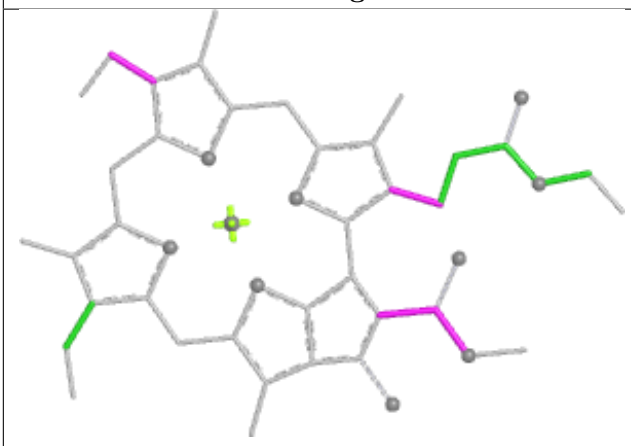
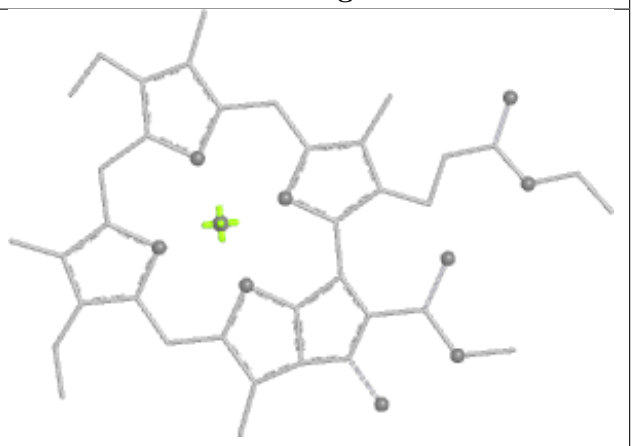


Bond angles

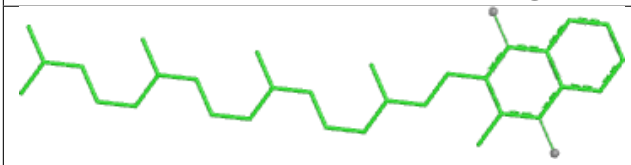


Torsions



Rings

Ligand PQN a 845



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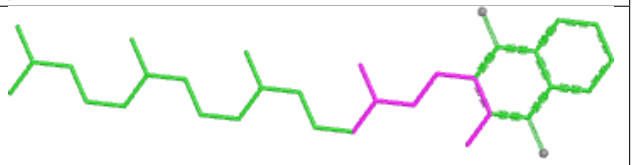
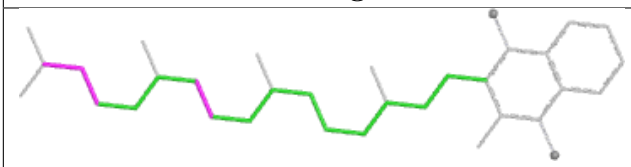
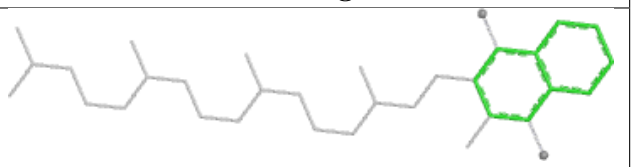


Bond angles

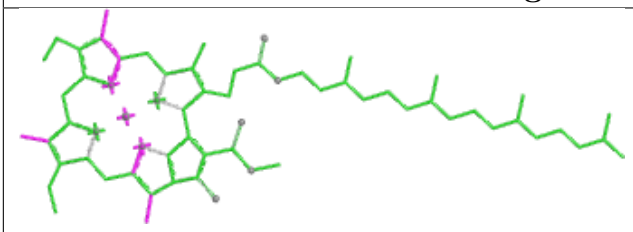


Torsions



Rings

Ligand CLA B 805



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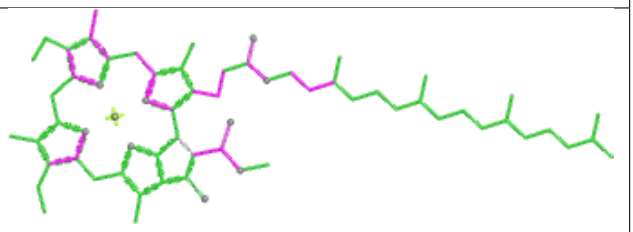
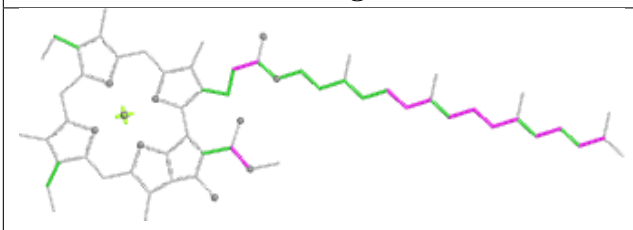
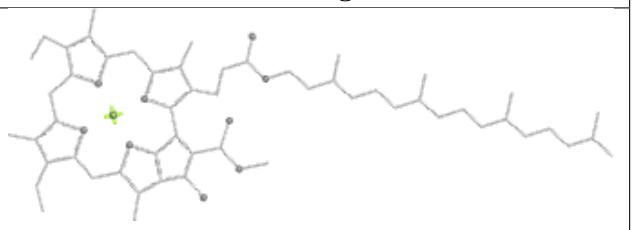


Bond angles

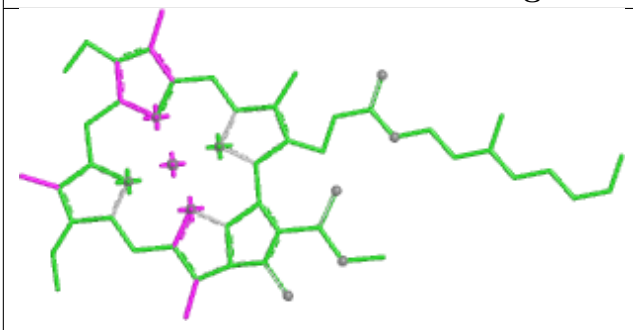


Torsions



Rings

Ligand CLA A 836



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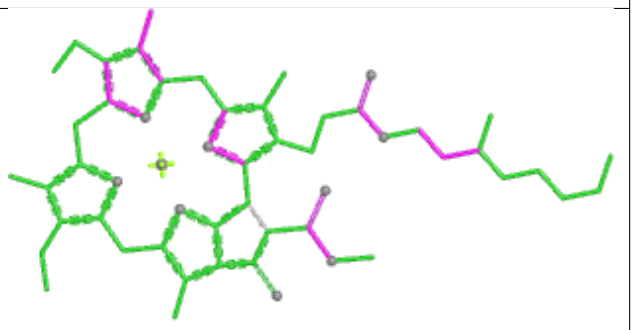
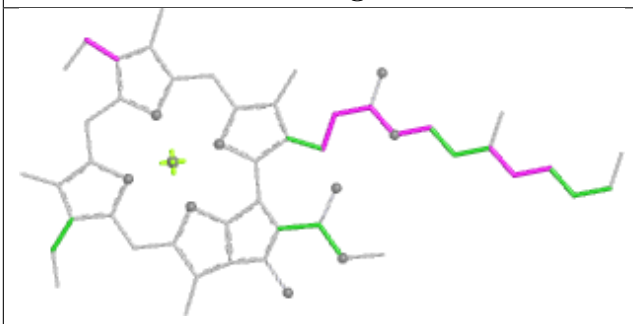
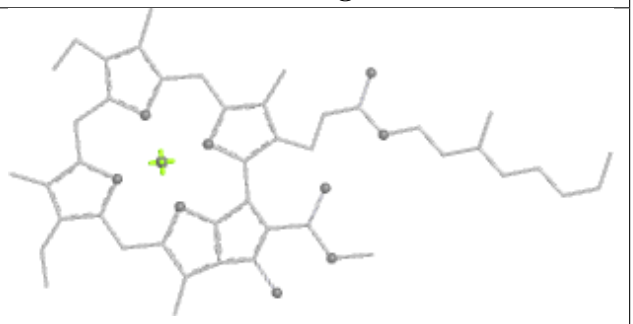


Bond angles

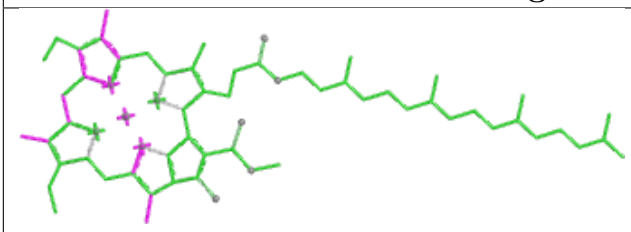


Torsions



Rings

Ligand CLA 1 822



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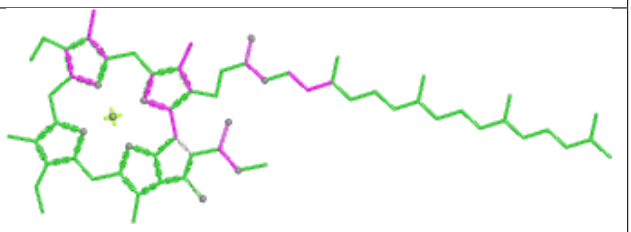
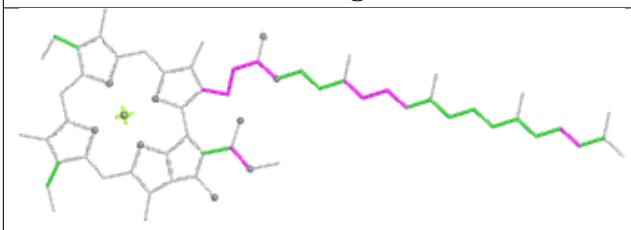
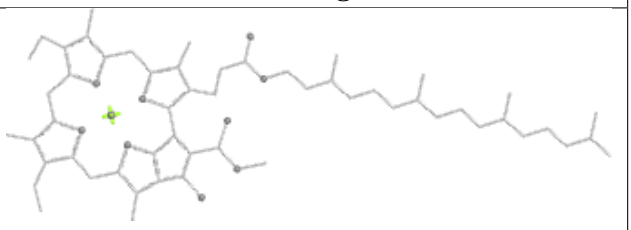


Bond angles

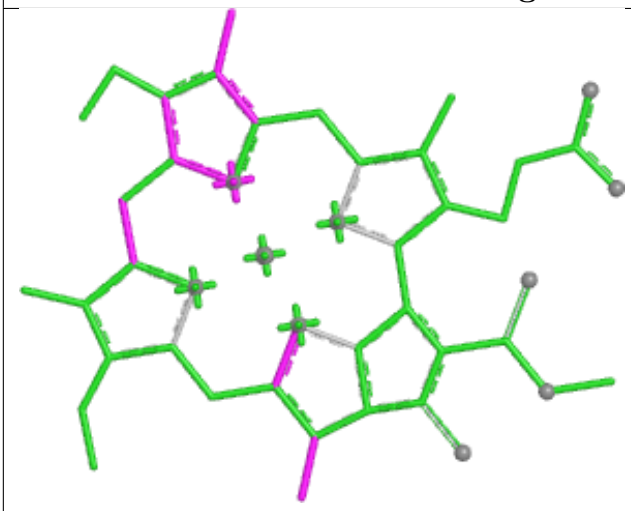


Torsions

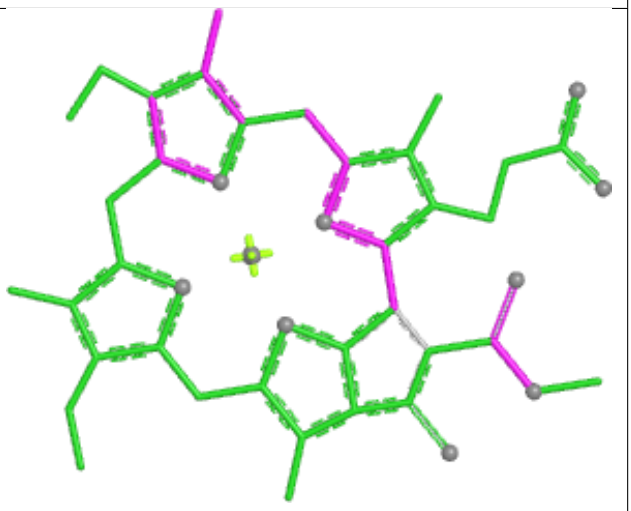


Rings

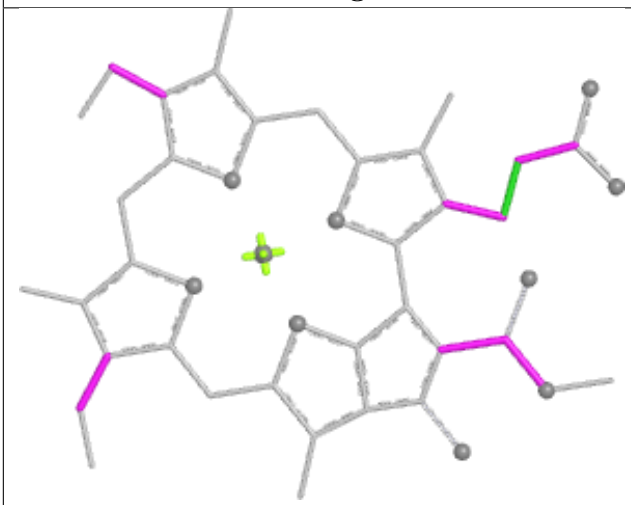
Ligand CLA k 4003



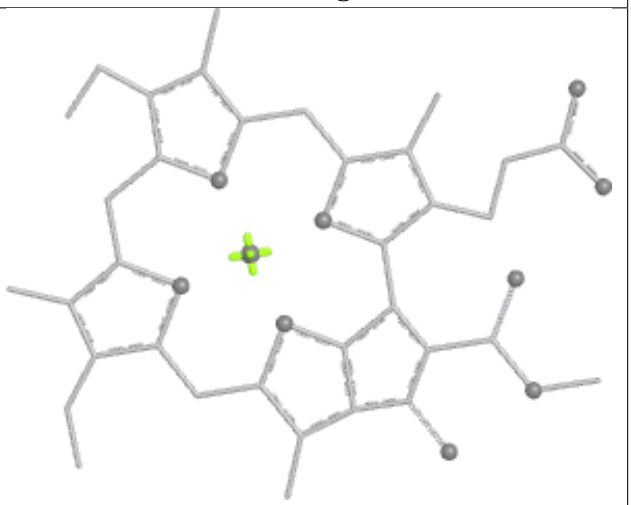
Bond lengths



Bond angles

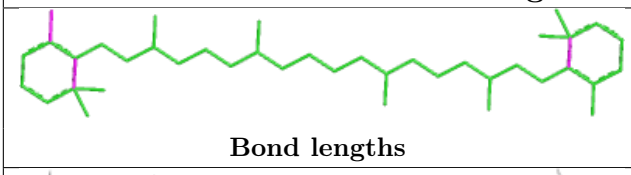


Torsions

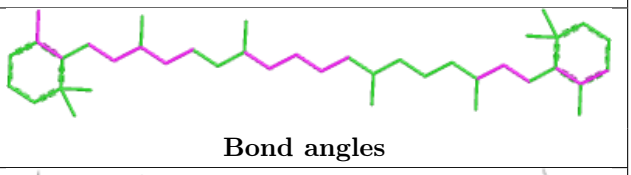


Rings

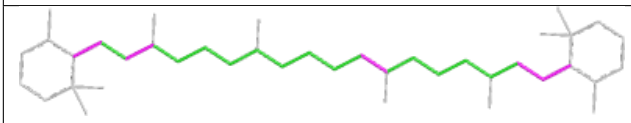
Ligand BCR 1 849



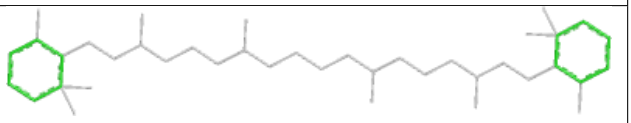
Bond lengths



Bond angles

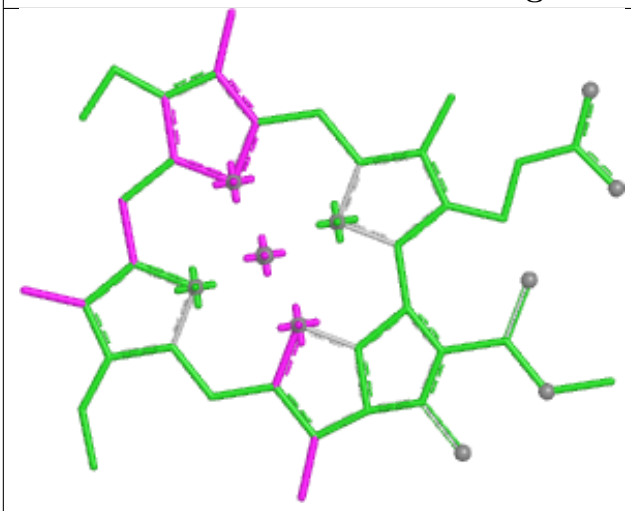


Torsions

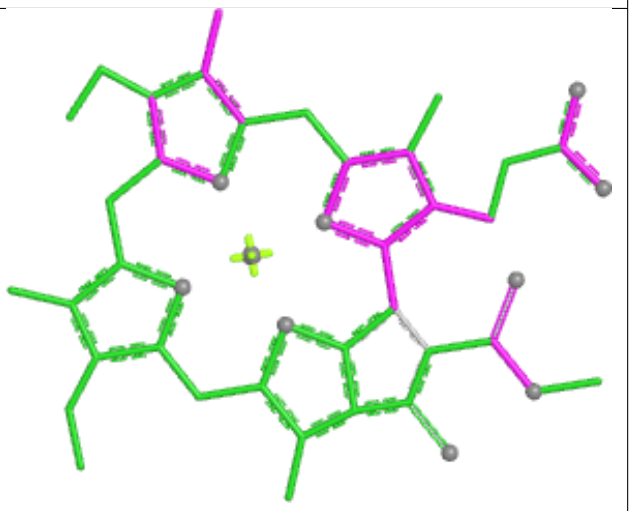


Rings

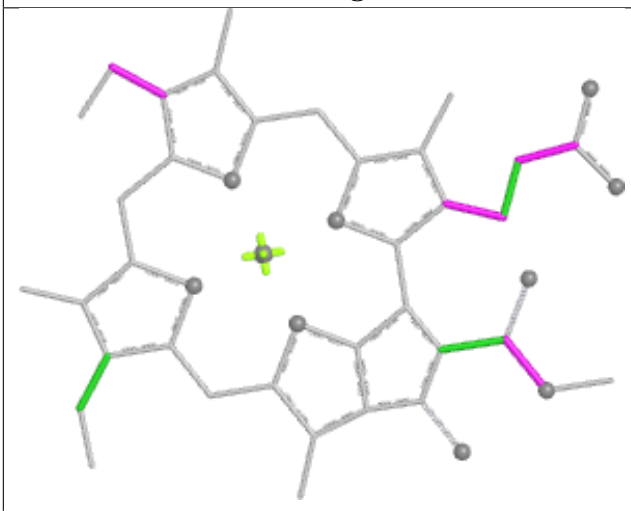
Ligand CLA F 205



Bond lengths



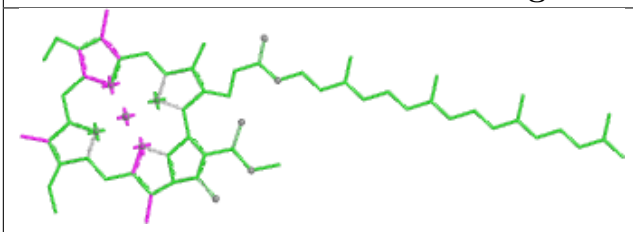
Bond angles



Torsions

Rings

Ligand CLA 2 842



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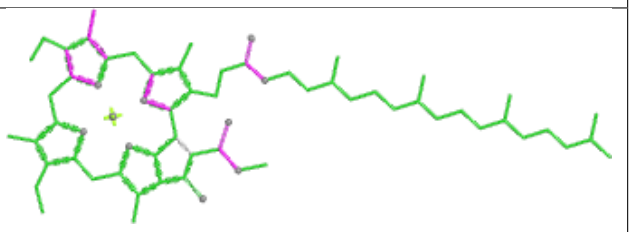
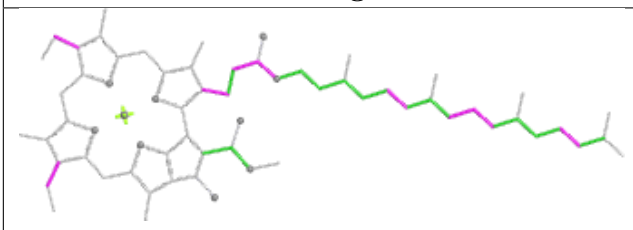
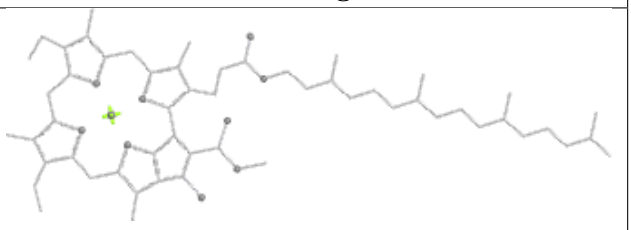


Bond angles

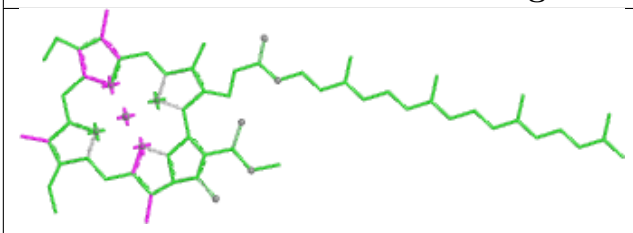


Torsions



Rings

Ligand CLA a 806



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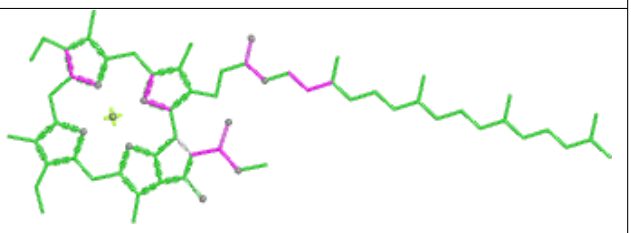
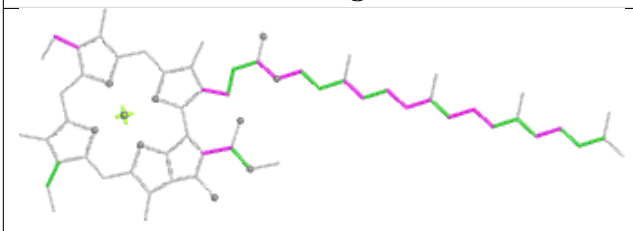
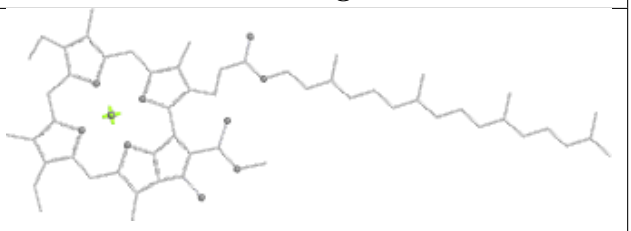


Bond angles

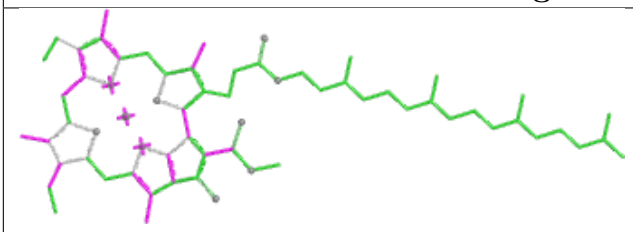


Torsions



Rings

Ligand CL0 a 803



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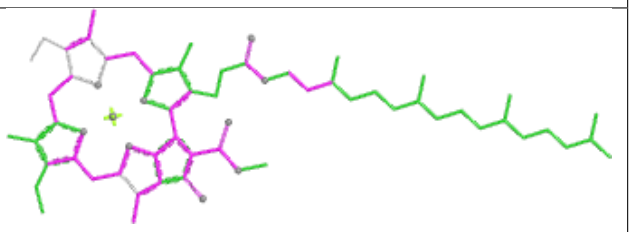

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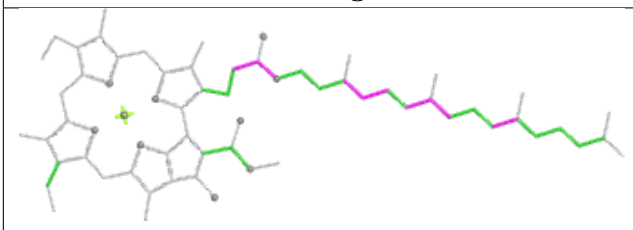
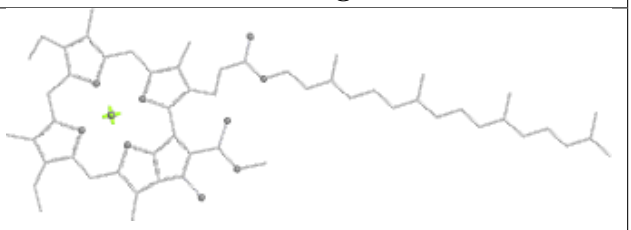
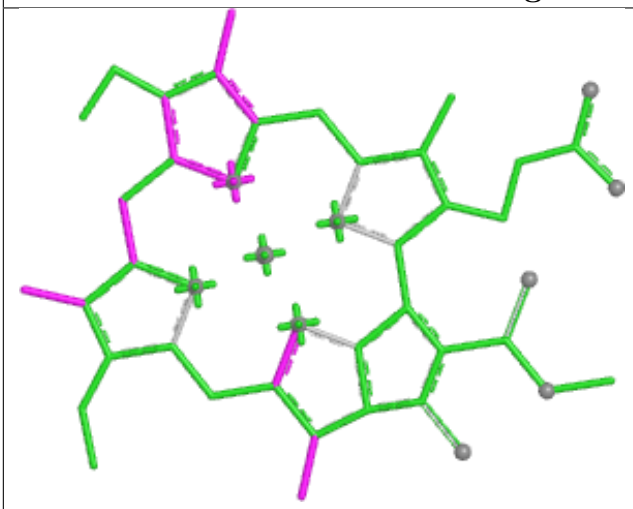


Torsions



Rings

Ligand CLA B 818



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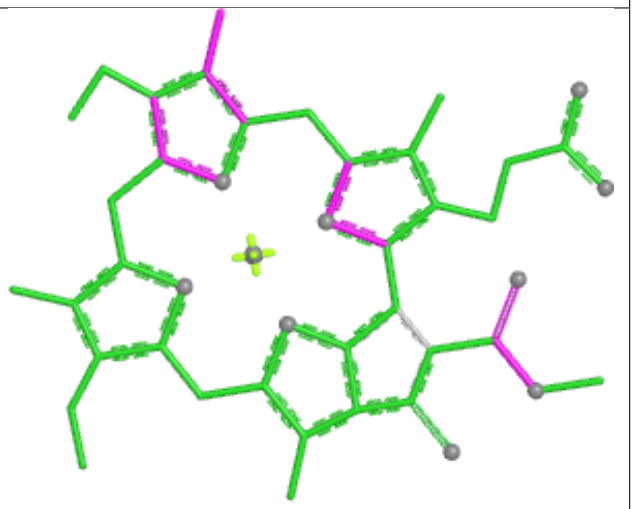
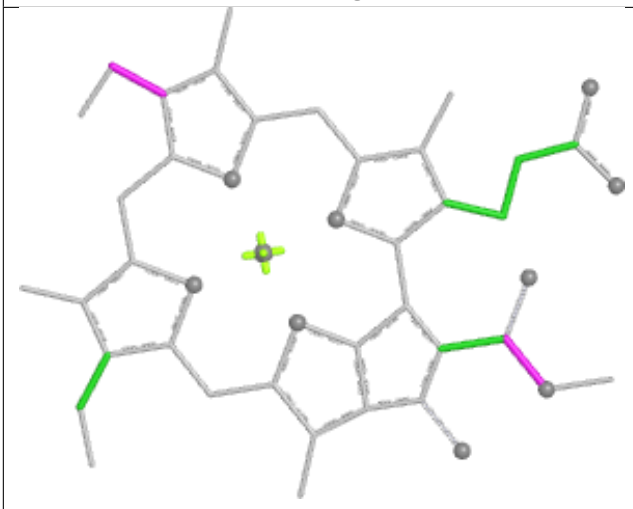


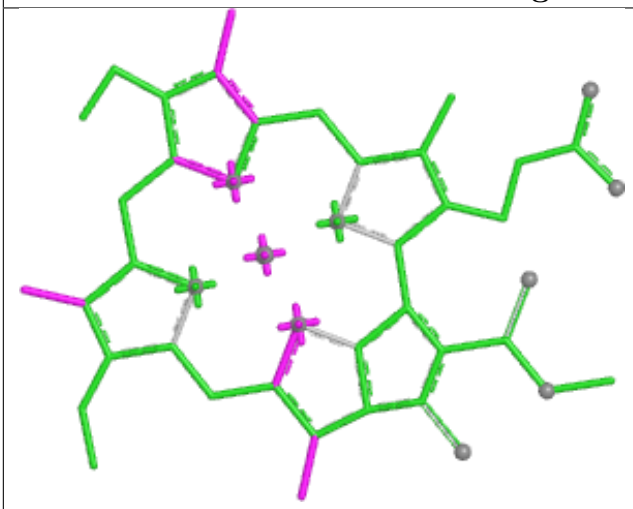
Bond angles



Torsions

Rings

Ligand CLA f 204



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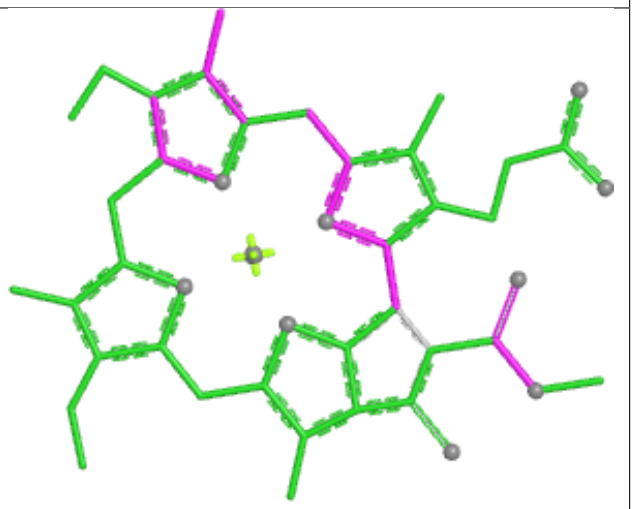

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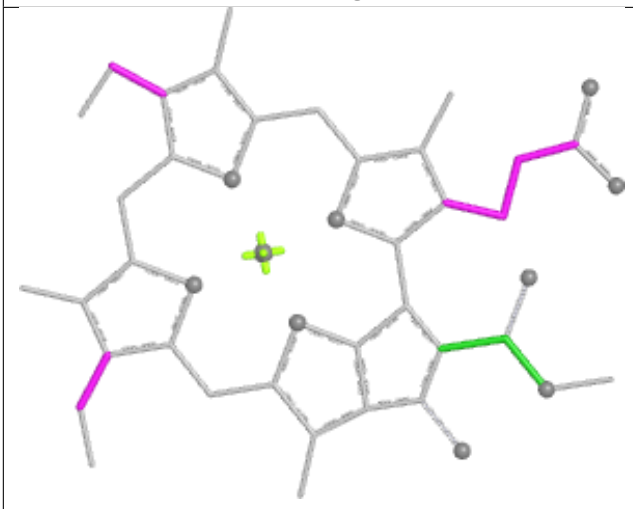
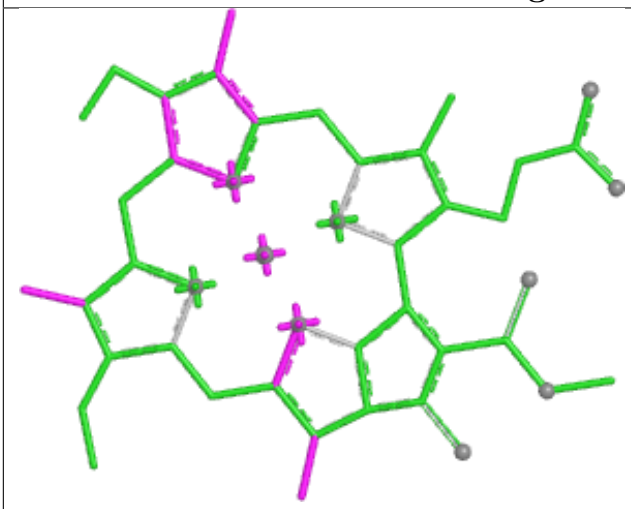


Torsions

Rings

Ligand CLA 2 813



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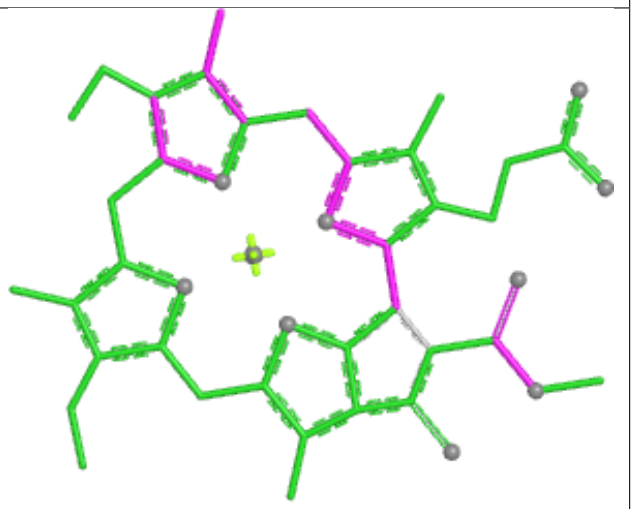

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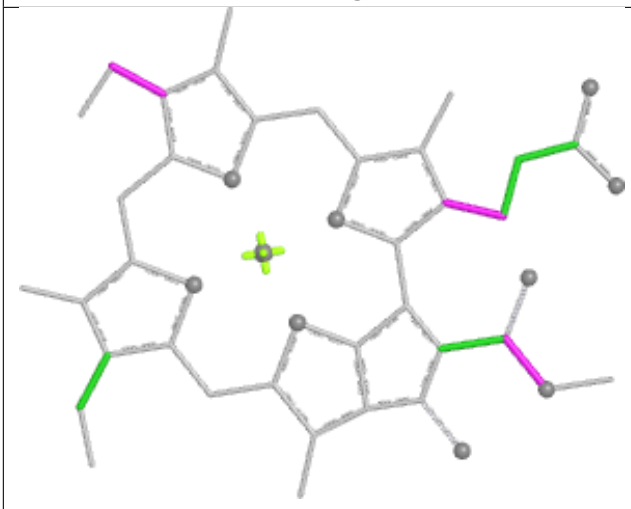
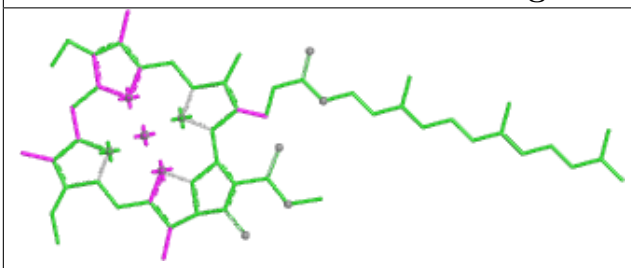


Torsions

Rings

Ligand CLA a 804



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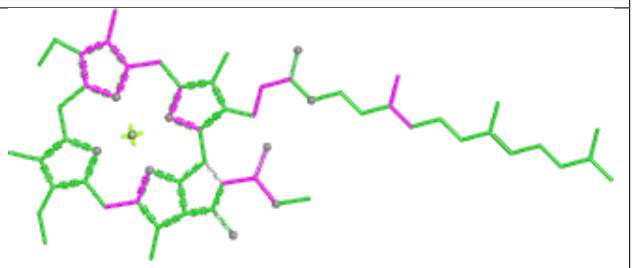
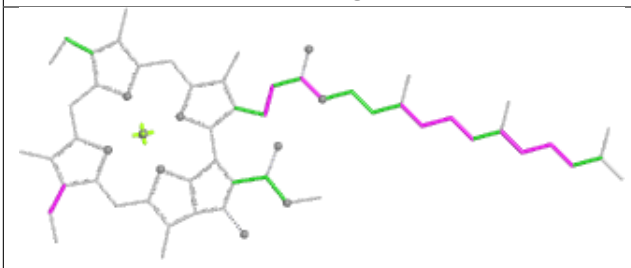
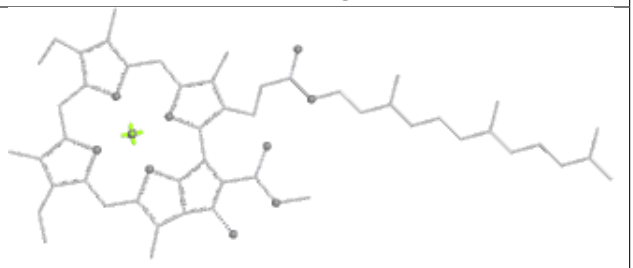


Bond angles

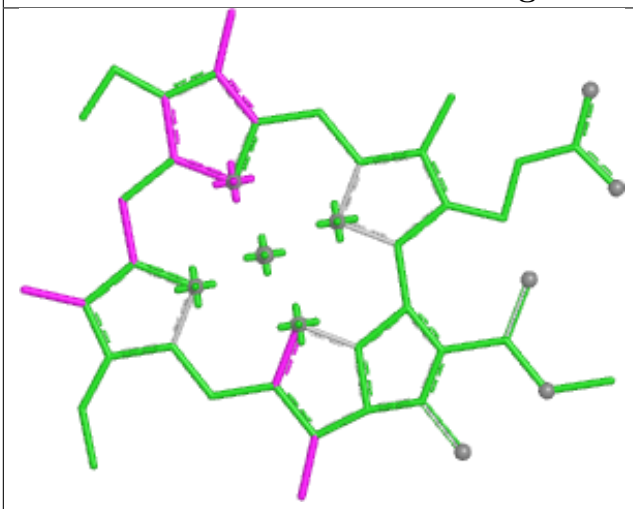


Torsions



Rings

Ligand CLA k 4002



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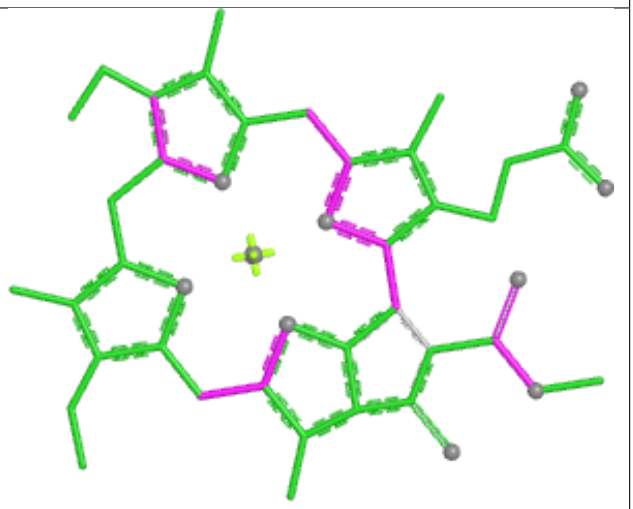
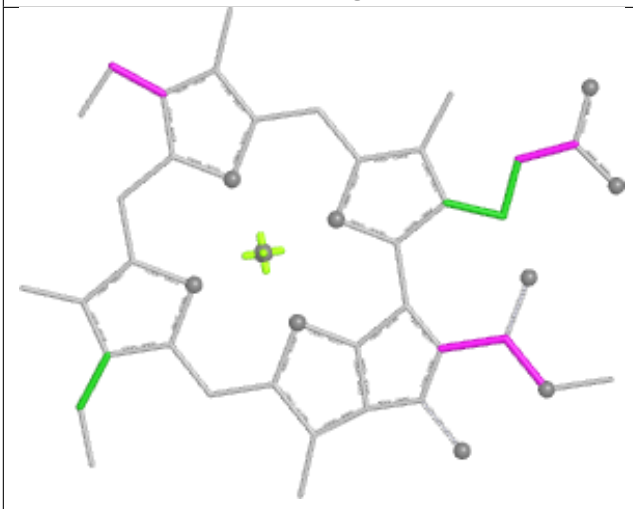


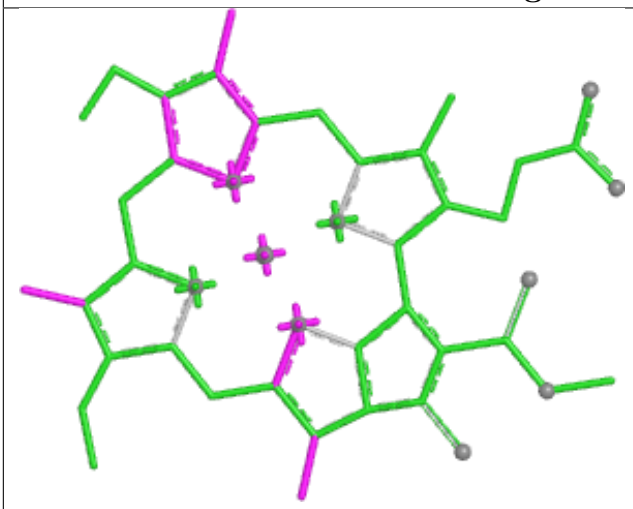
Bond angles



Torsions

Rings

Ligand CLA B 836



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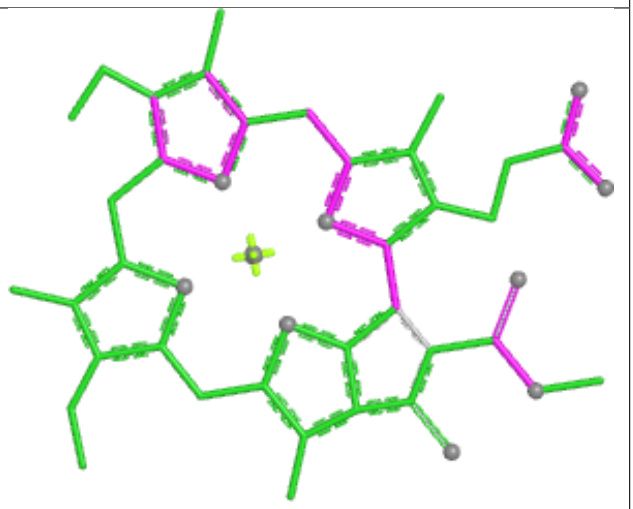
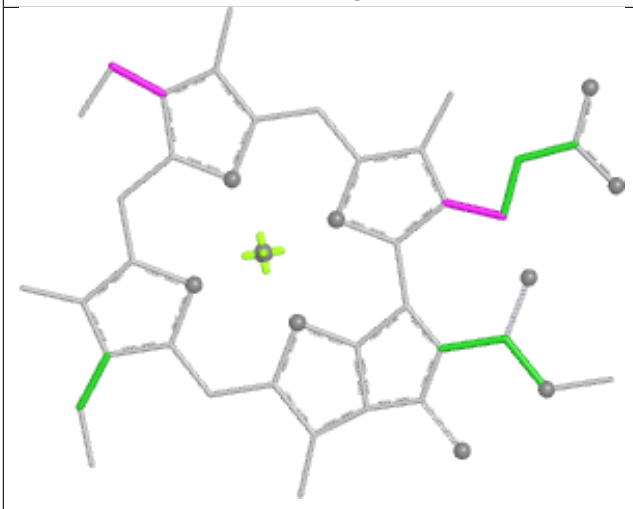


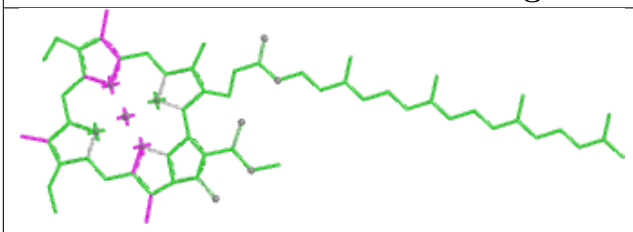
Bond angles



Torsions

Rings

Ligand CLA A 808



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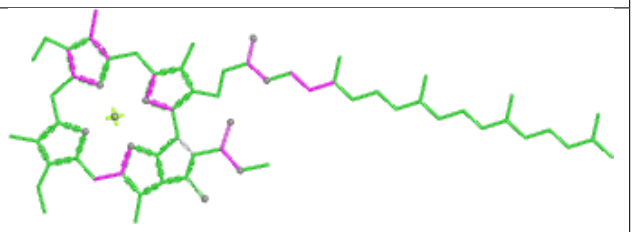
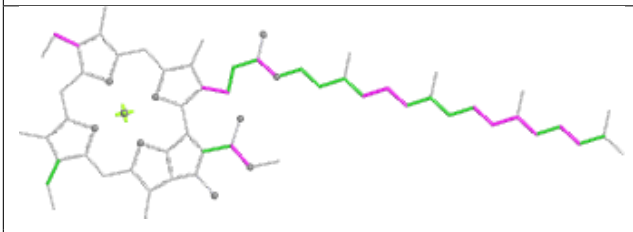


Bond angles



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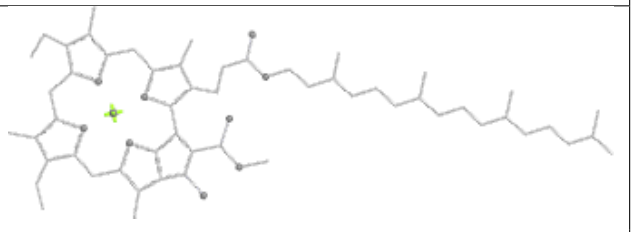
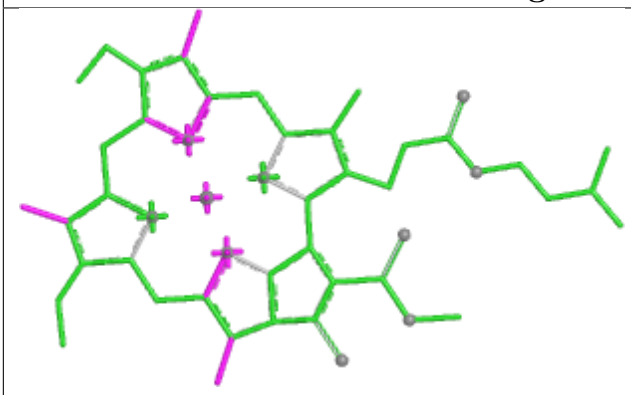


Rings

Ligand CLA a 834



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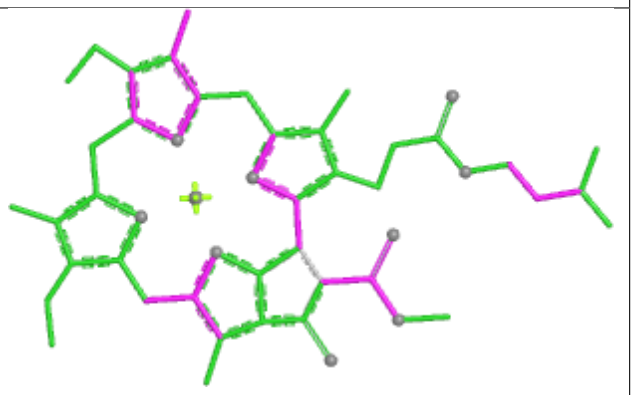
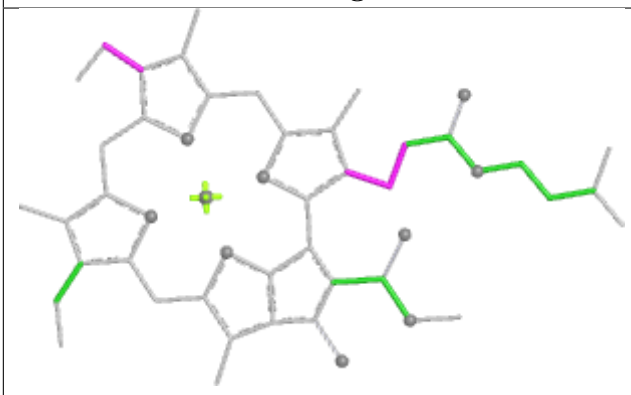
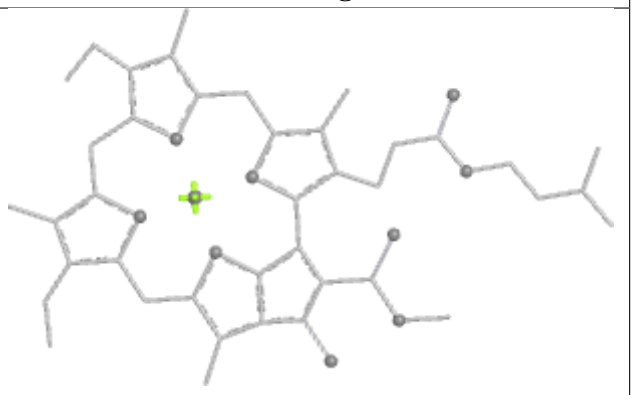


Bond angles

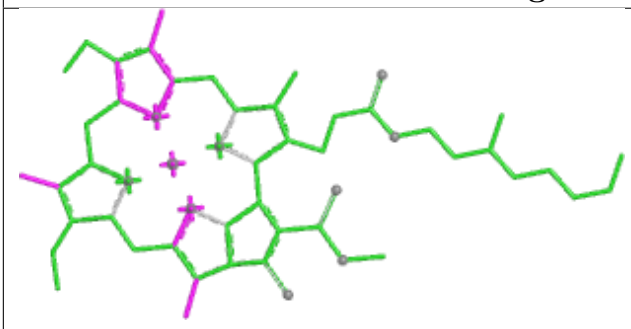


Torsions



Rings

Ligand CLA a 837



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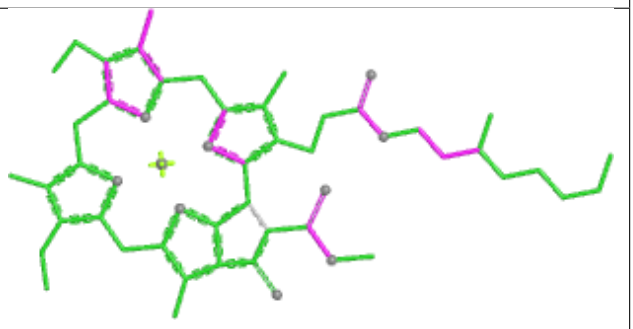
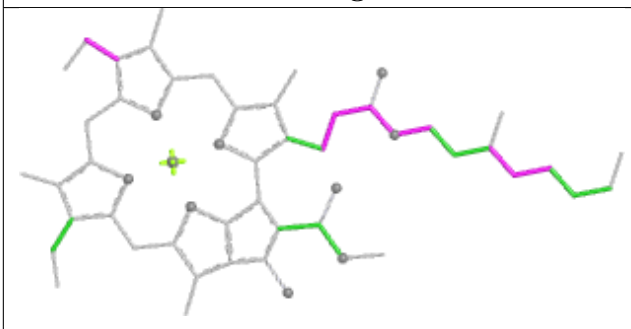
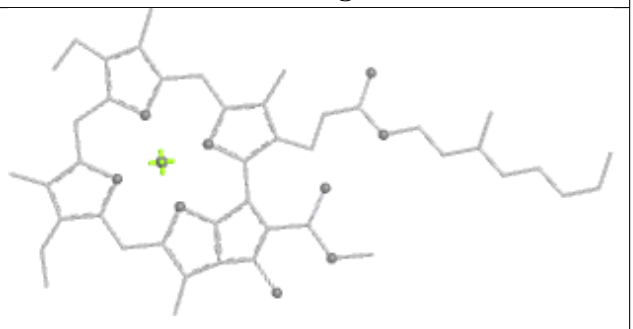


Bond angles

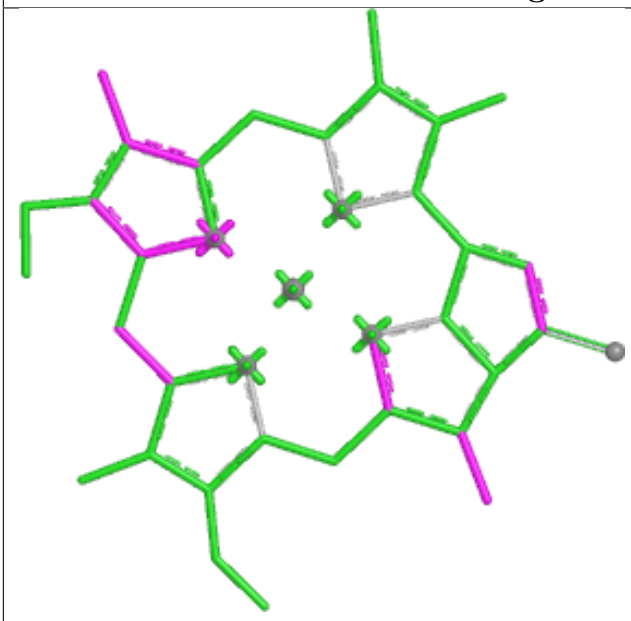


Torsions



Rings

Ligand CLA J 102



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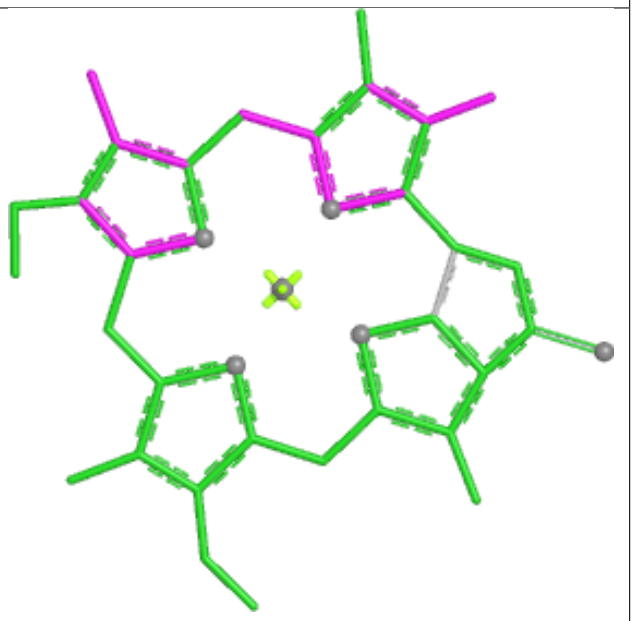
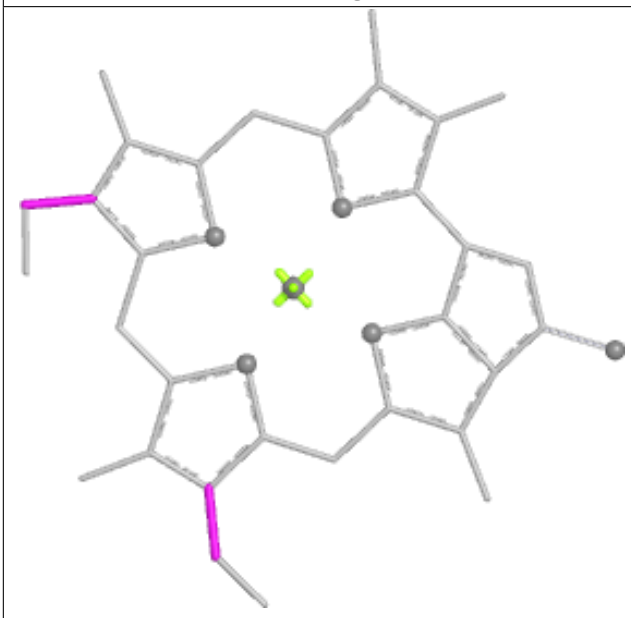
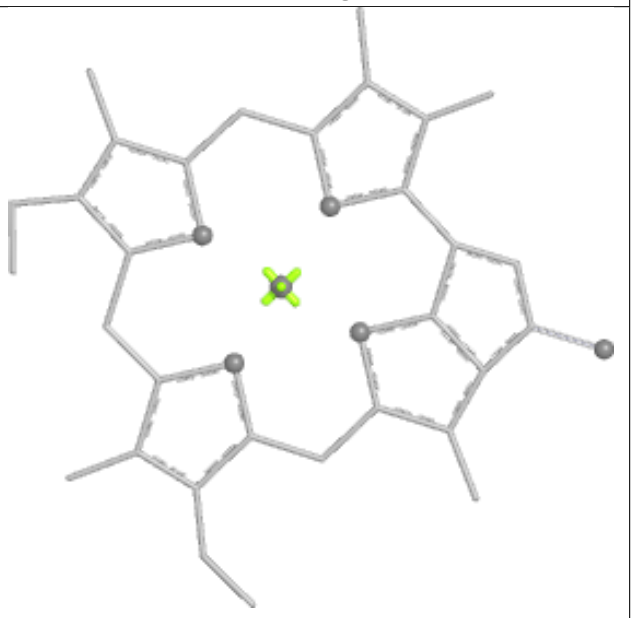


Bond angles

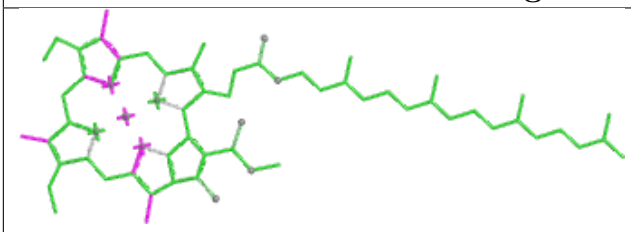


Torsions



Rings

Ligand CLA B 808



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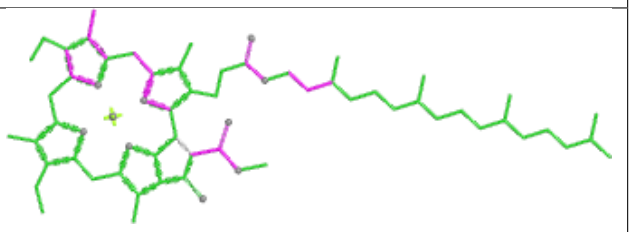
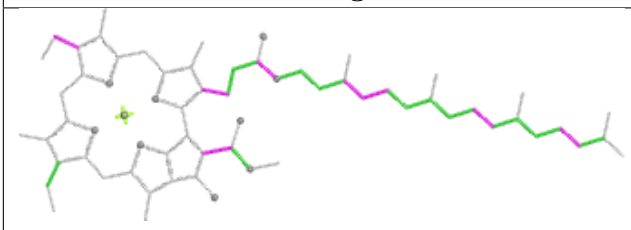
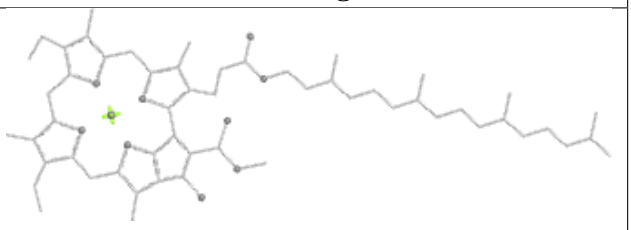


Bond angles



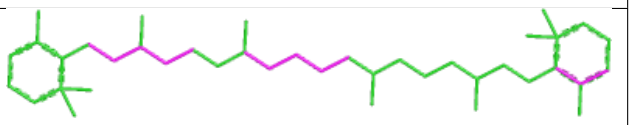
Torsions



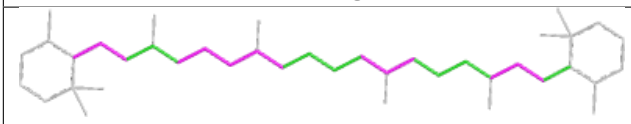
Rings

Ligand BCR 7 1104

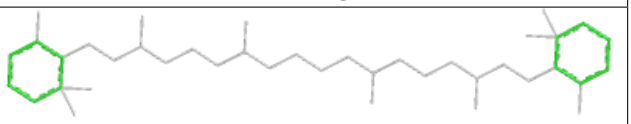
Bond lengths



Bond angles

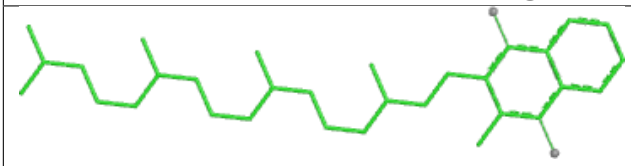


Torsions

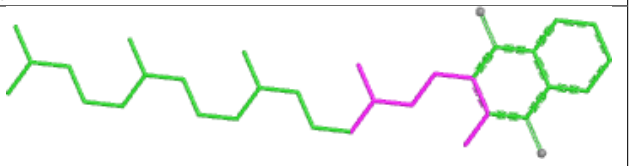


Rings

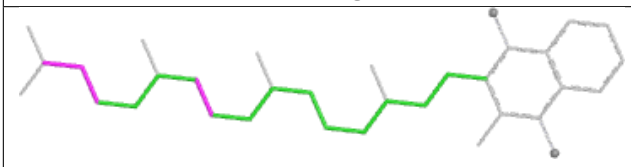
Ligand PQN A 845



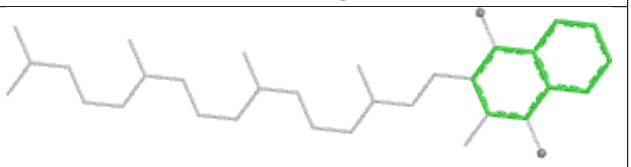
Bond lengths



Bond angles

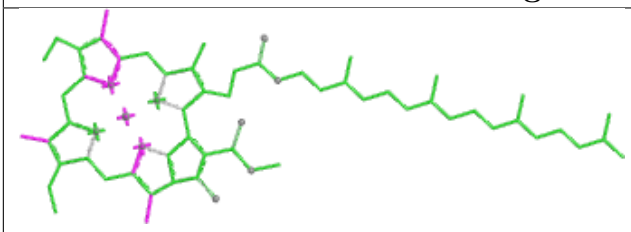


Torsions



Rings

Ligand CLA A 827



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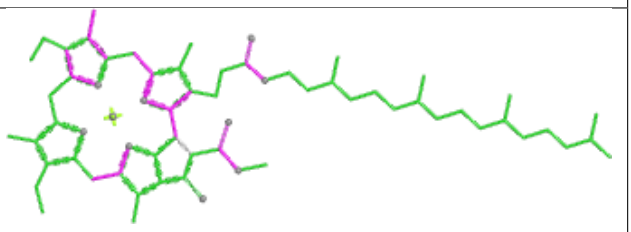
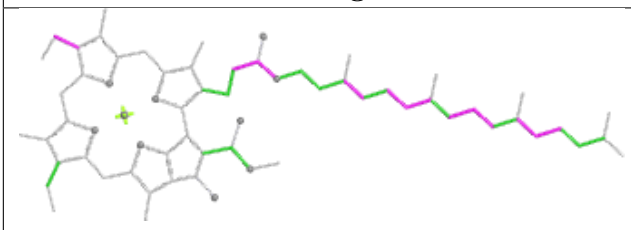


Bond angles



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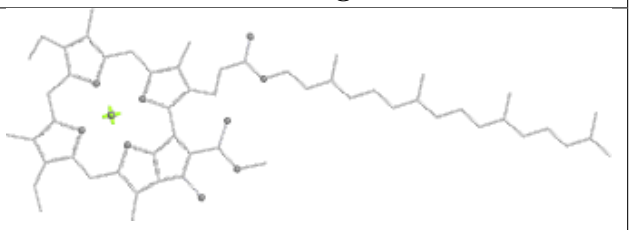
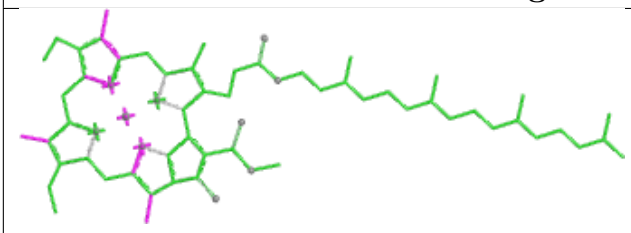


Rings

Ligand CLA 2 807



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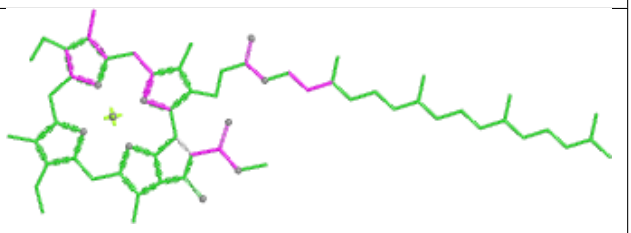
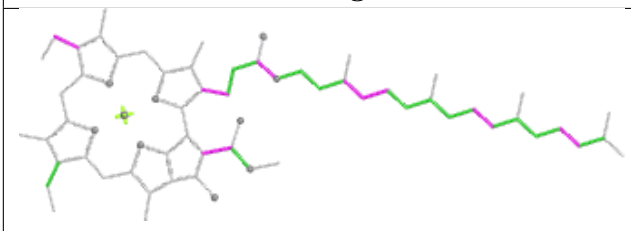


Bond angles



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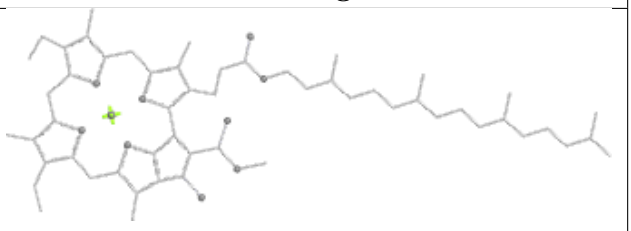
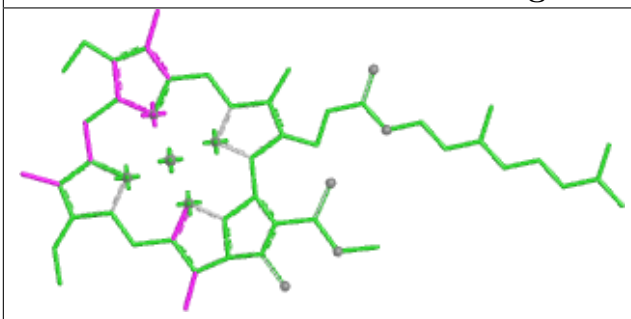


Rings

Ligand CLA 2 833



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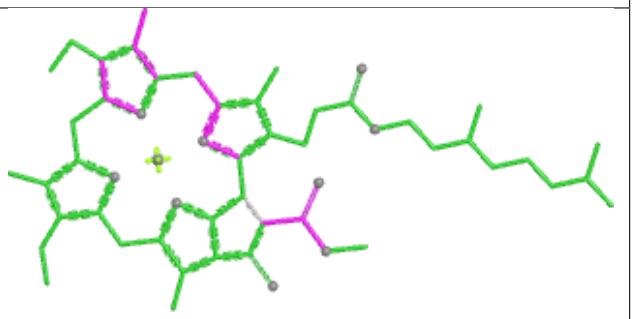
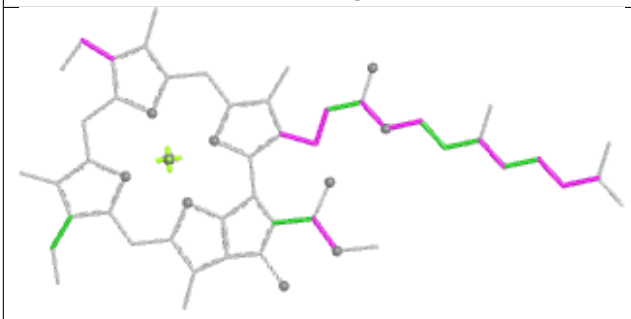
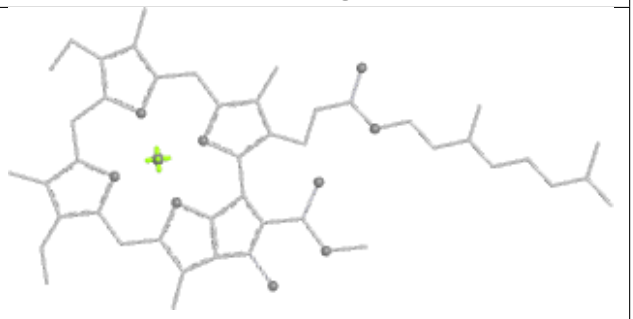


Bond angles

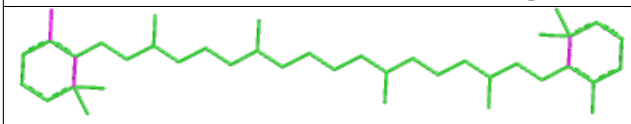


Torsions



Rings

Ligand BCR B 854



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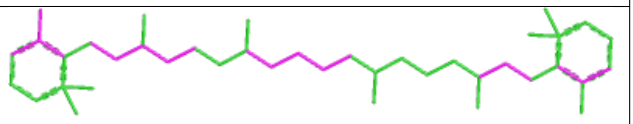
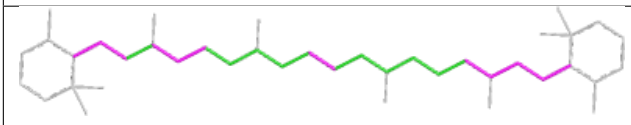


Bond angles



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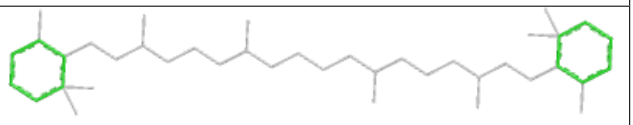
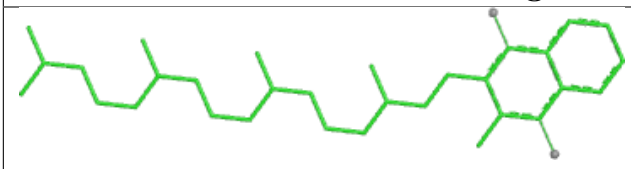


Rings

Ligand PQN 1 845



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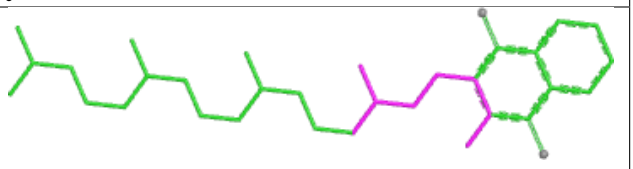
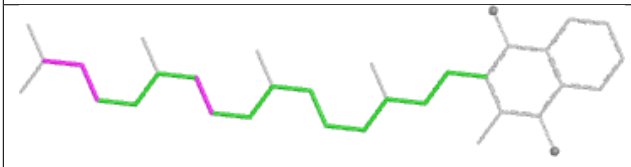


Bond angles



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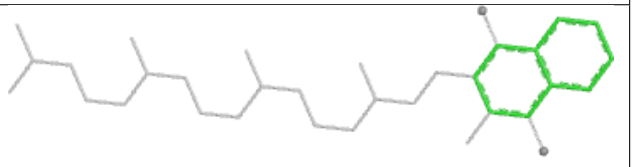
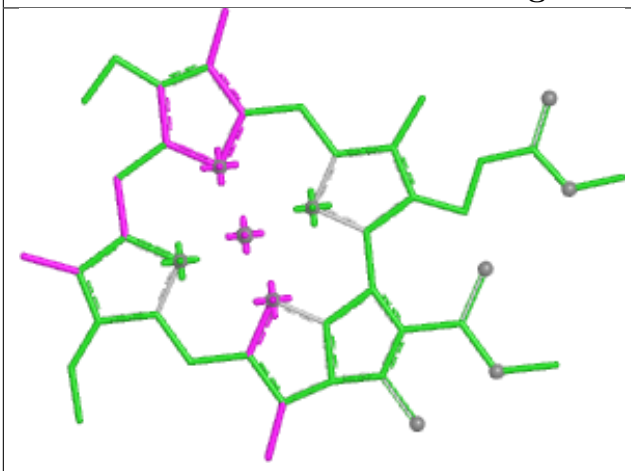


Rings

Ligand CLA 2 841



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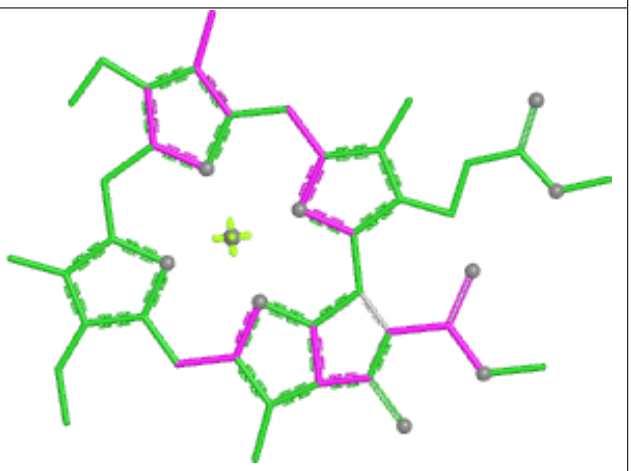

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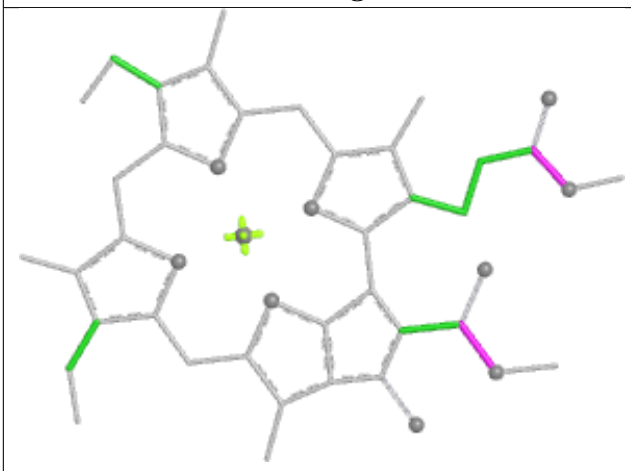

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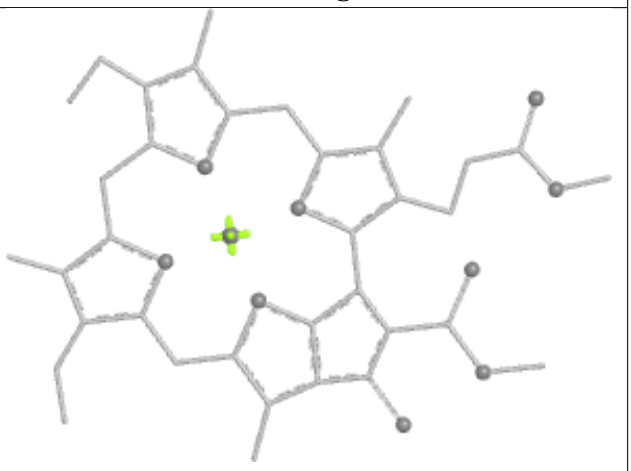
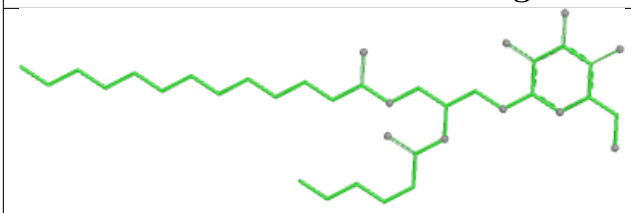


Rings

Ligand LMG L 1506



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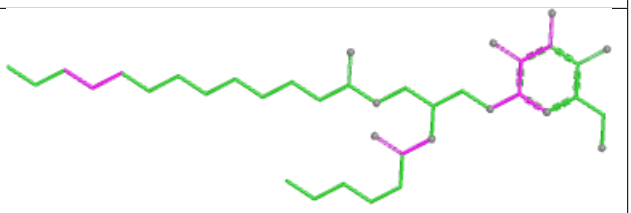

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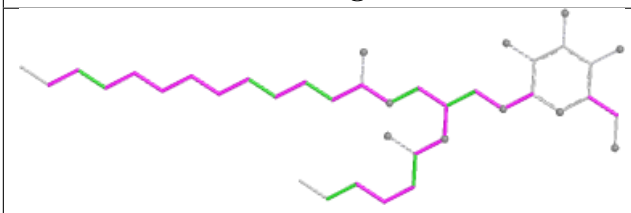

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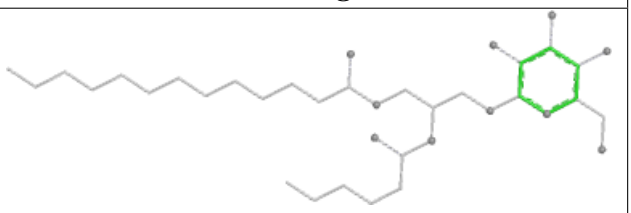
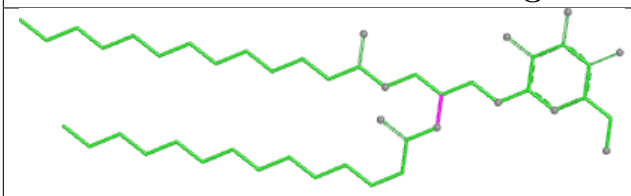


Rings

Ligand LMG a 852



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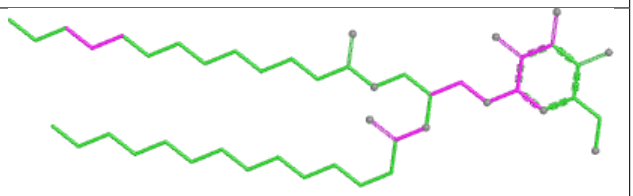
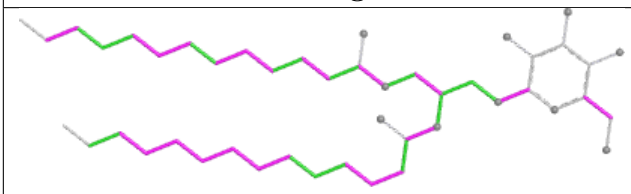


Bond angles



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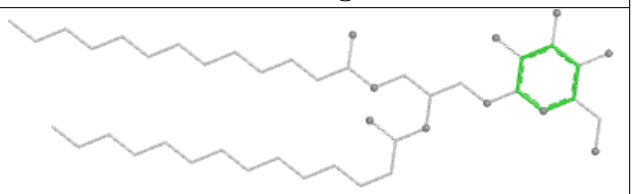
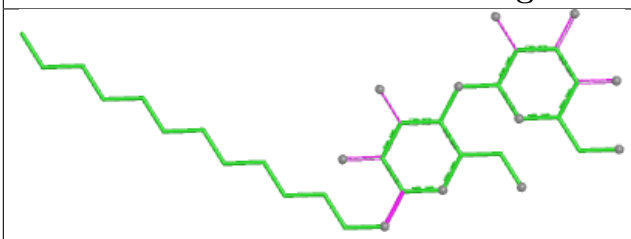


Rings

Ligand LMT 6 4401



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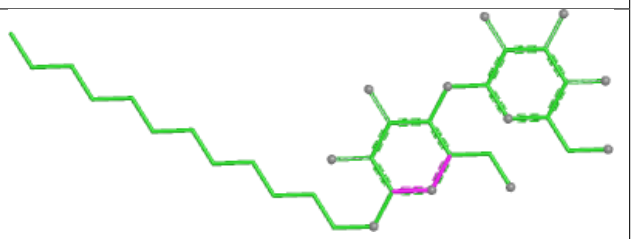

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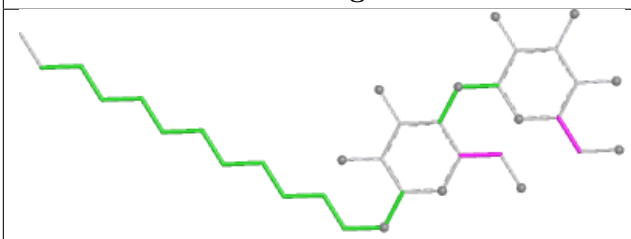

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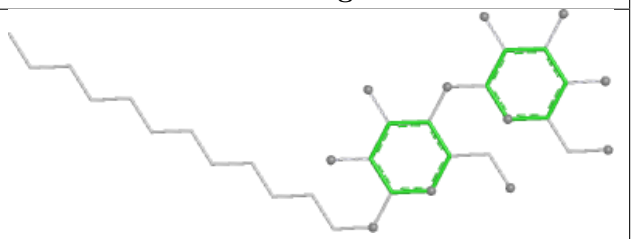
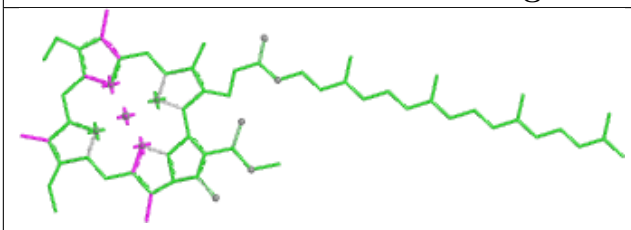


Rings

Ligand CLA A 842



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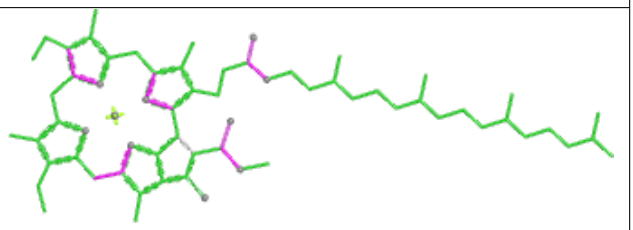
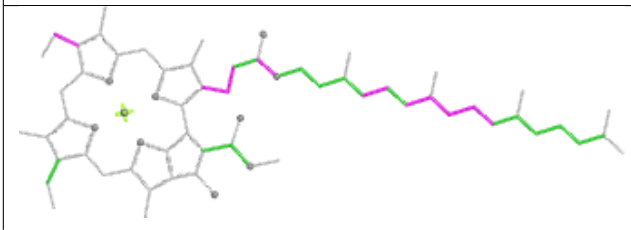


Bond angles



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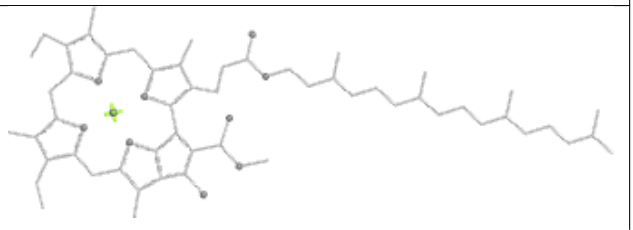
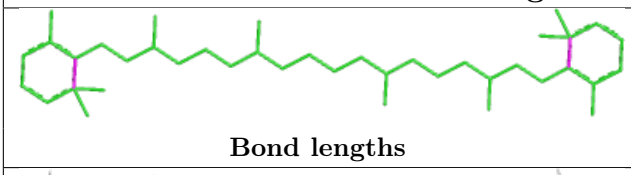


Rings

Ligand BCR a 847



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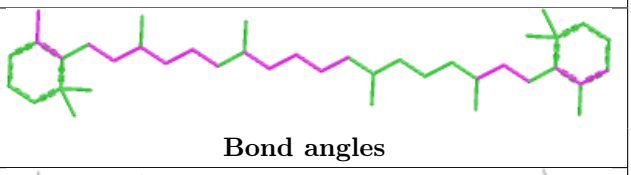
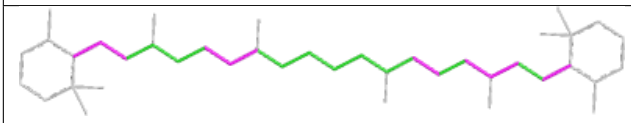
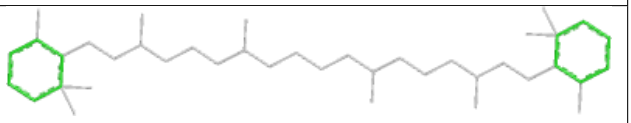


Bond angles



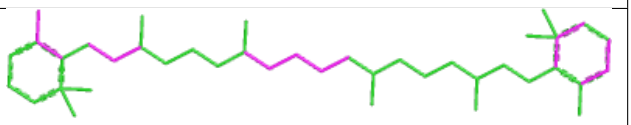
Torsions



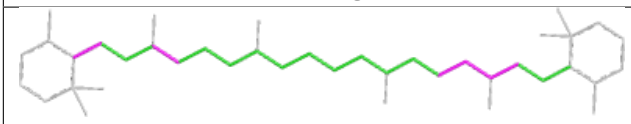
Rings

Ligand BCR b 847

Bond lengths



Bond angles



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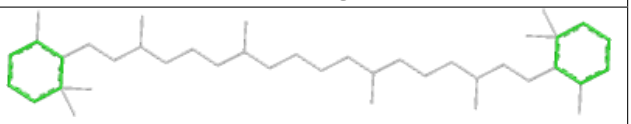
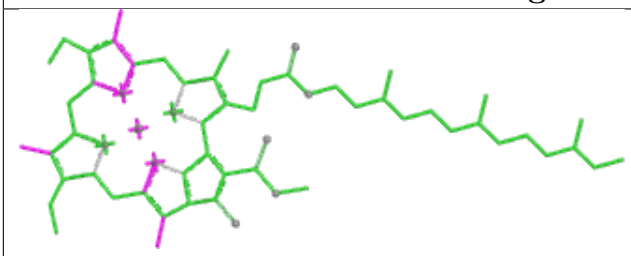


Rings

Ligand CLA 2 811



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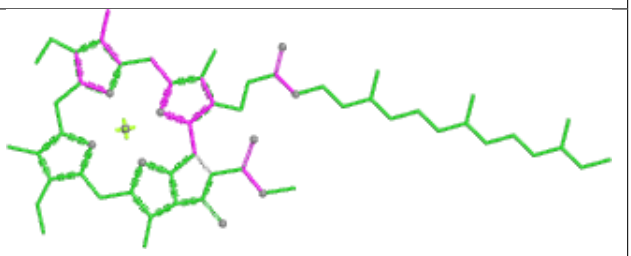
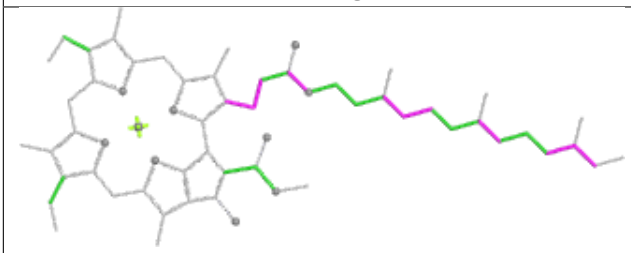


Bond angles



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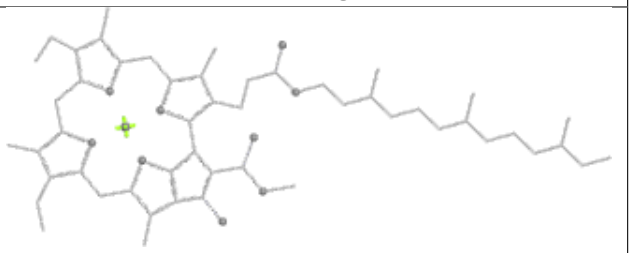
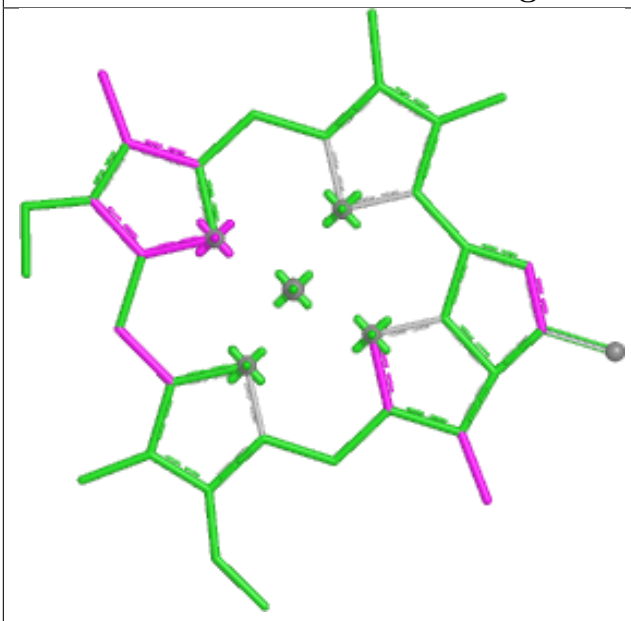
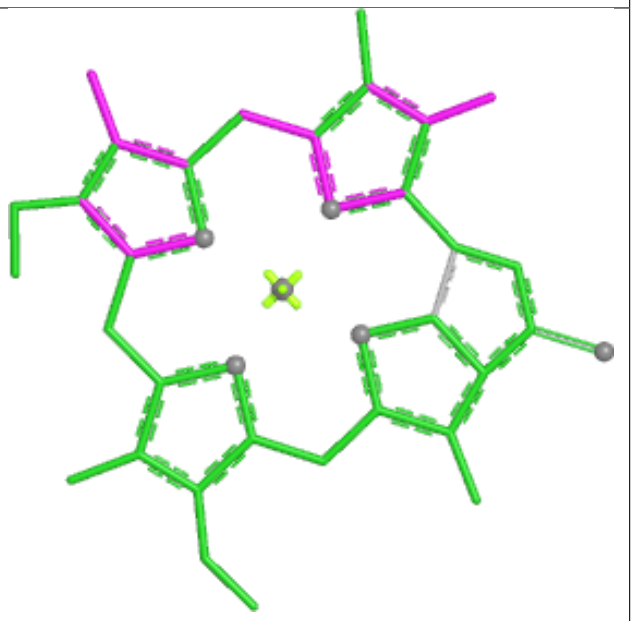


Rings

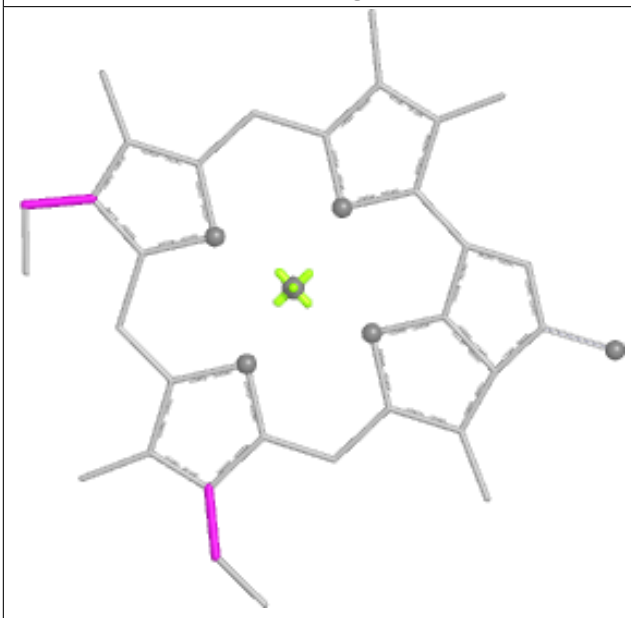
Ligand CLA 7 1103



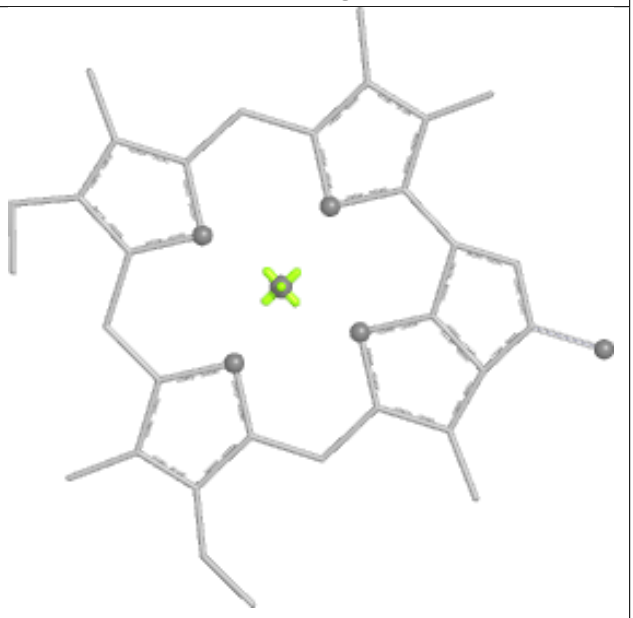
Bond lengths



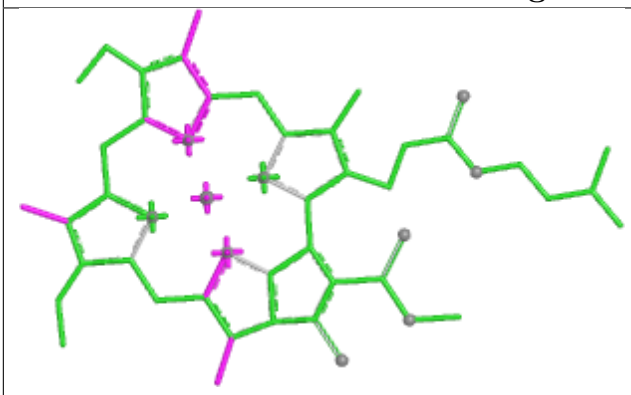
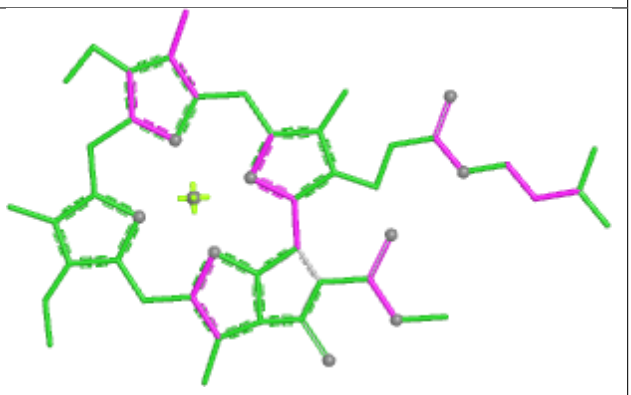
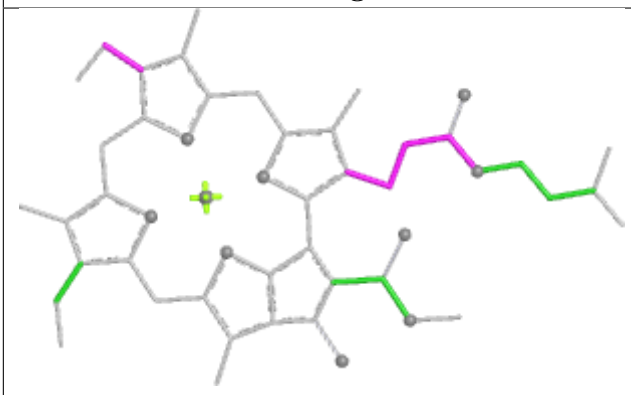
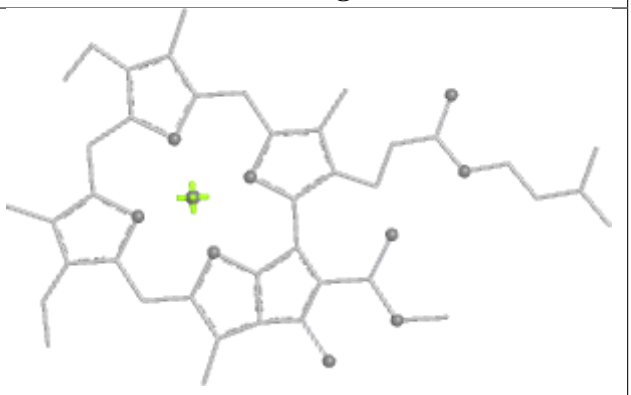
Bond angles

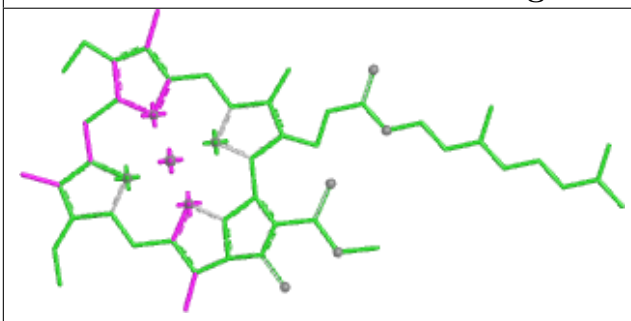
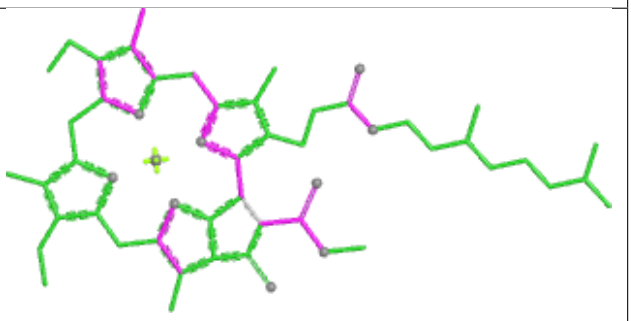
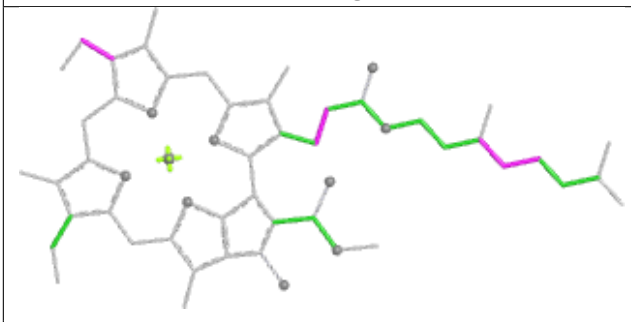
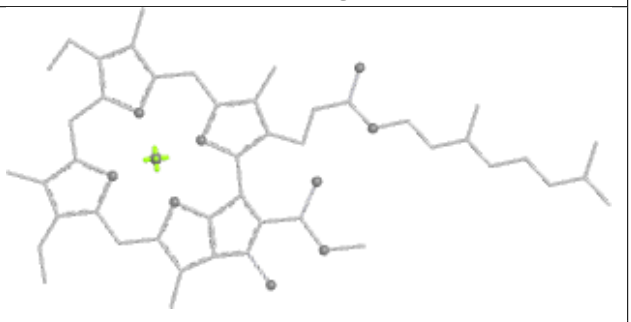


Torsions

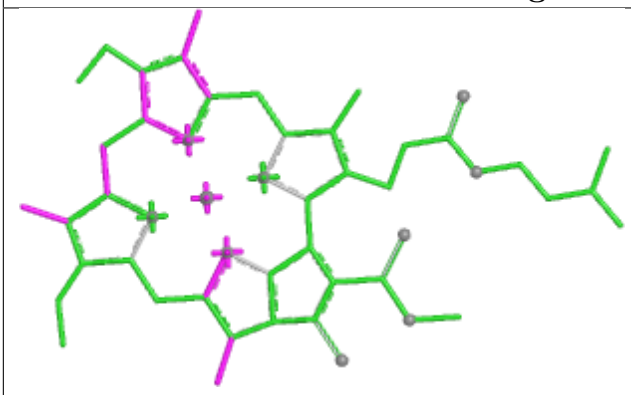


Rings

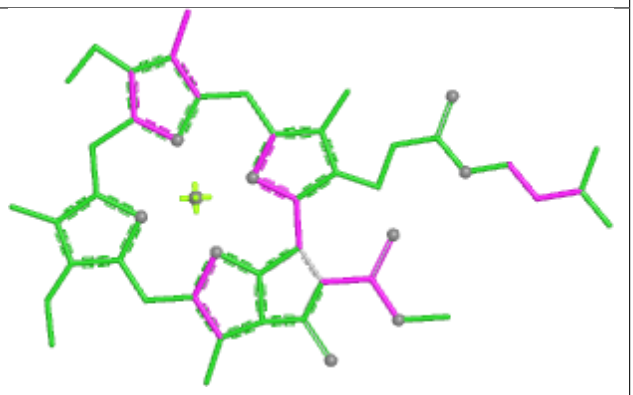
Ligand CLA a 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

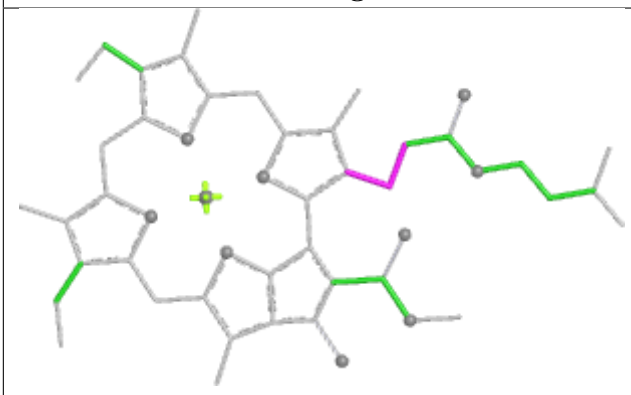
Ligand CLA 1 805



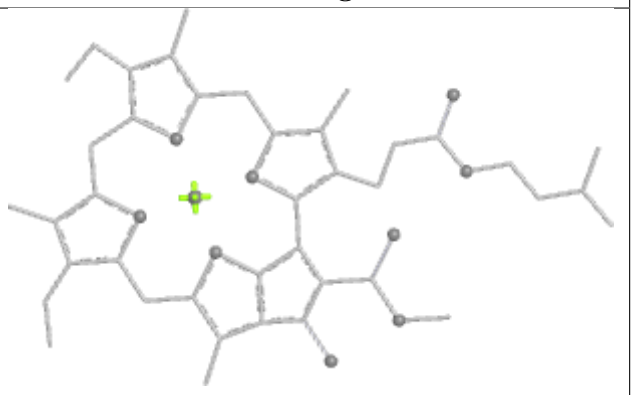
Bond lengths



Bond angles

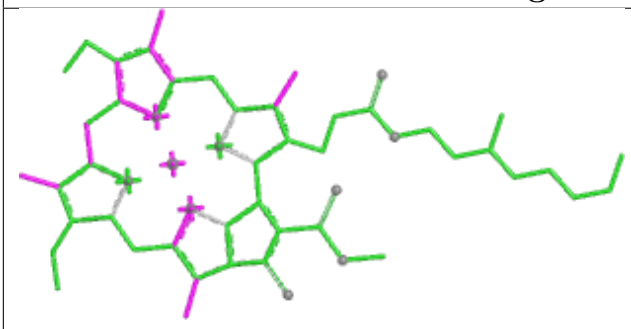


Torsions

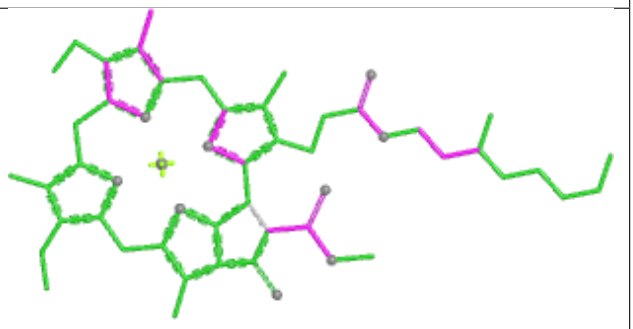


Rings

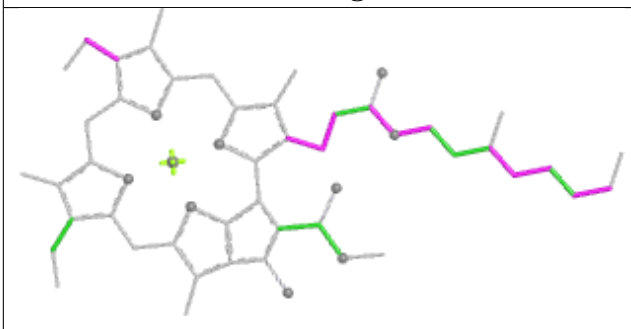
Ligand CLA 1 813



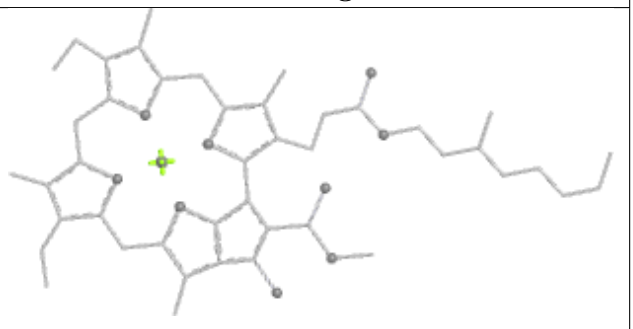
Bond lengths



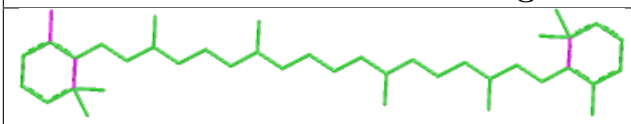
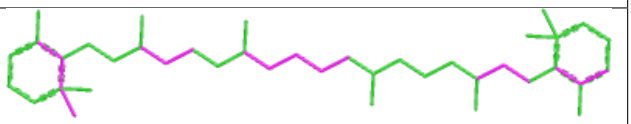
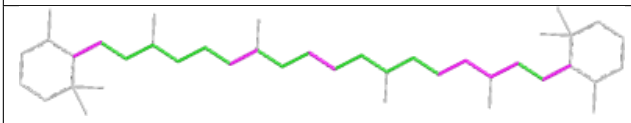
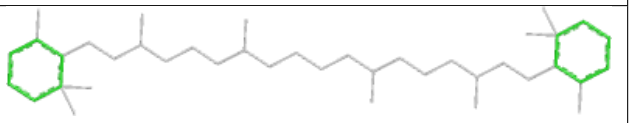
Bond angles

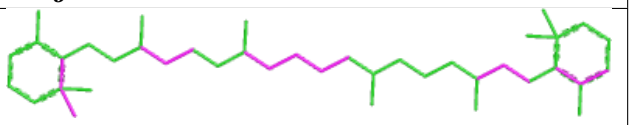
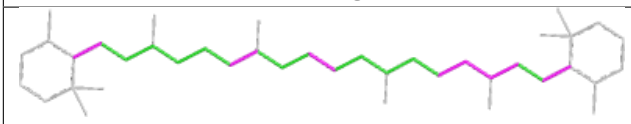
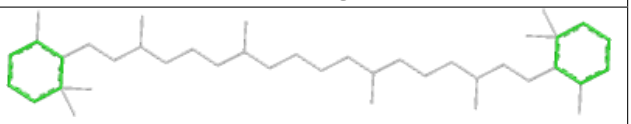


Torsions

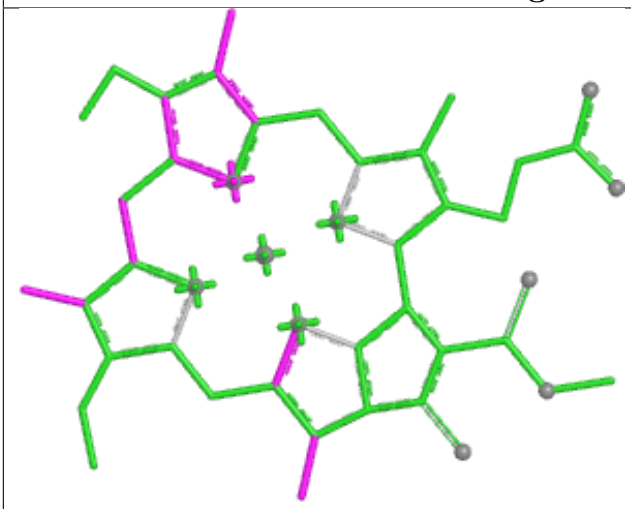


Rings

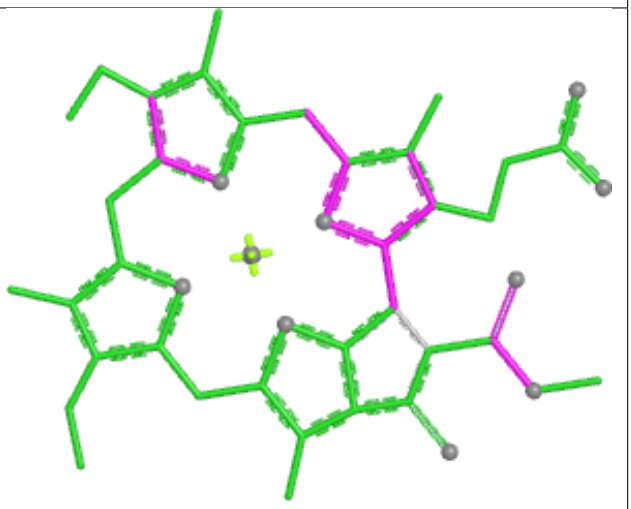
Ligand BCR 7 1105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR j 104	
Bond lengths	 Bond angles
 Torsions	 Rings

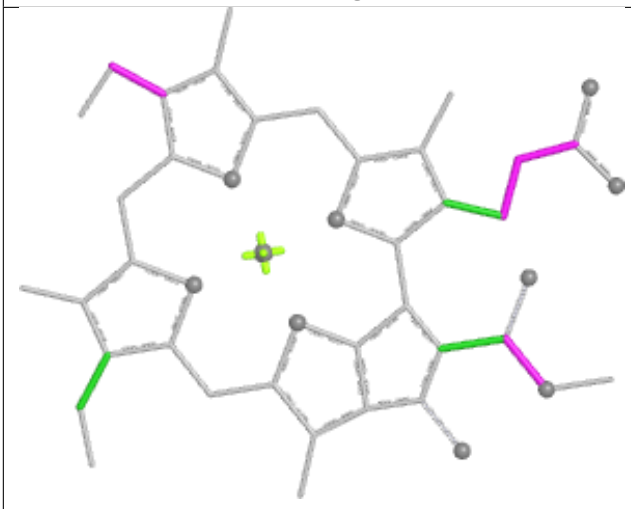
Ligand CLA 1 836



Bond lengths



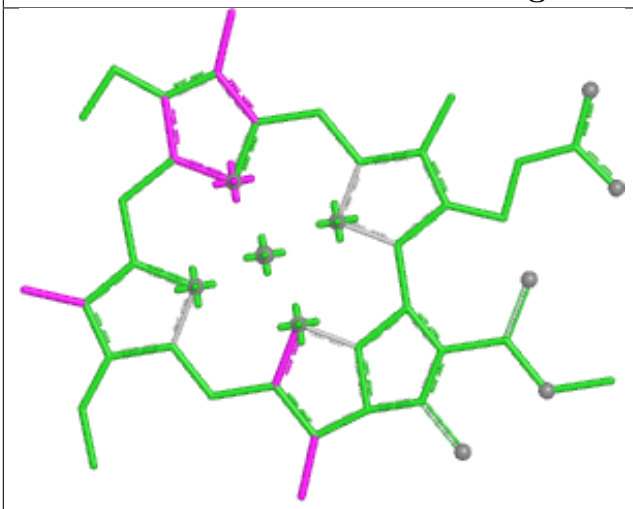
Bond angles



Torsions

Rings

Ligand CLA a 818



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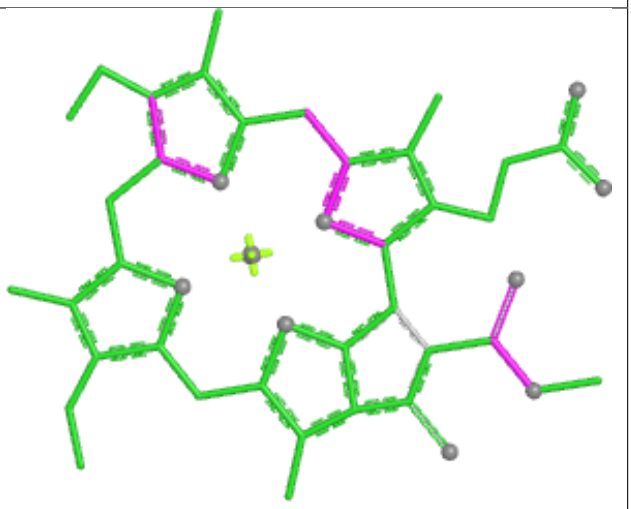
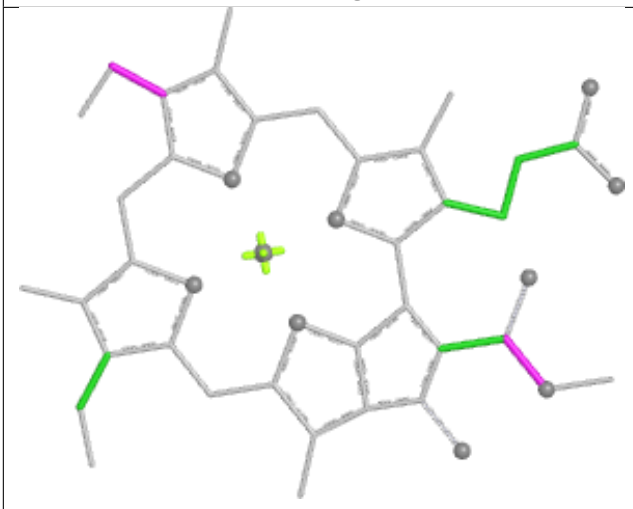


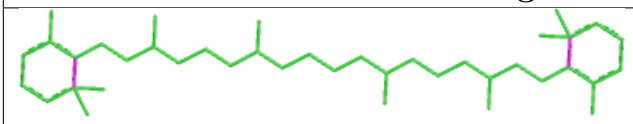
Bond angles



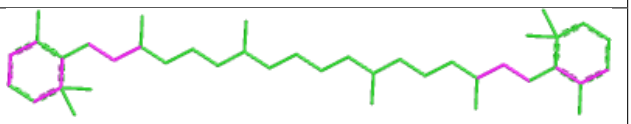
Torsions

Rings

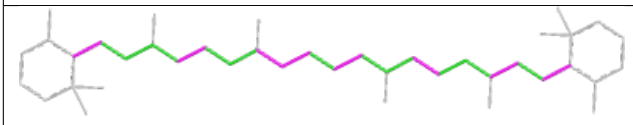
Ligand BCR 8 4005



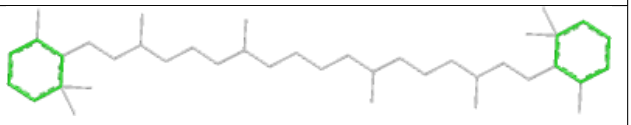
Bond lengths



Bond angles

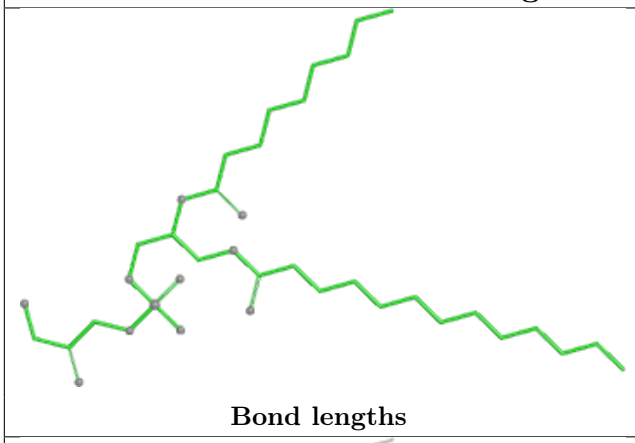


Torsions



Rings

Ligand LHG m 101



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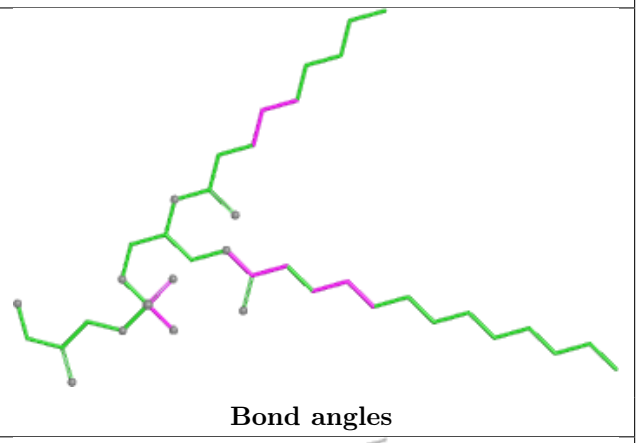
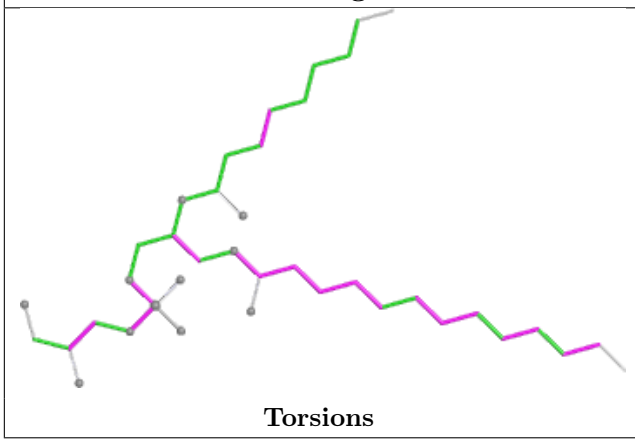
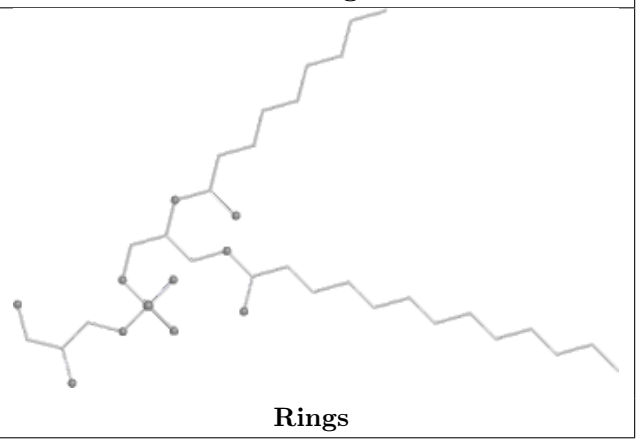


Bond angles

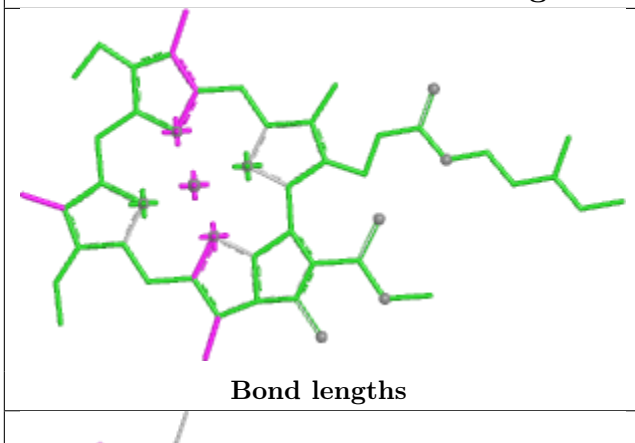


Torsions

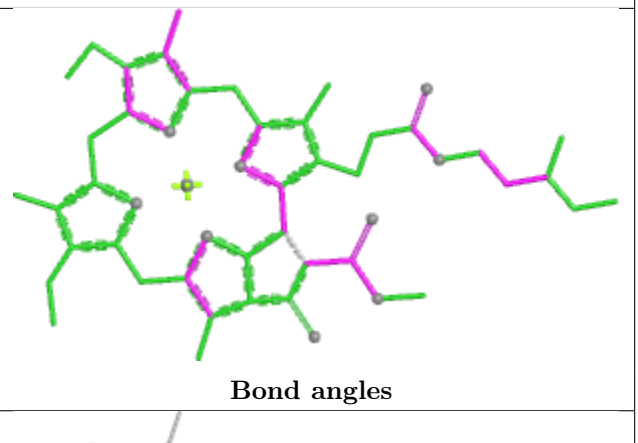


Rings

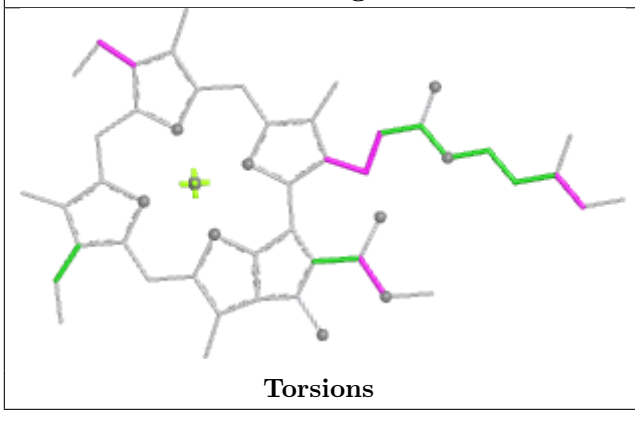
Ligand CLA a 839



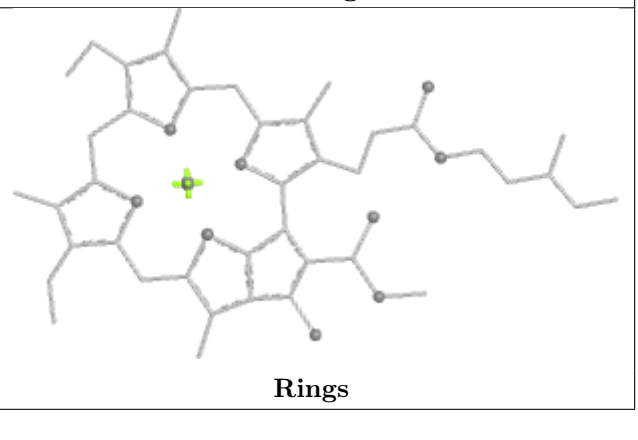
Bond lengths



Bond angles

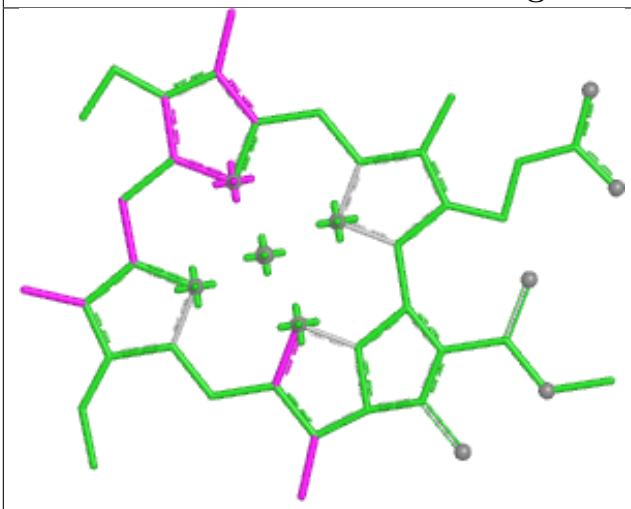


Torsions

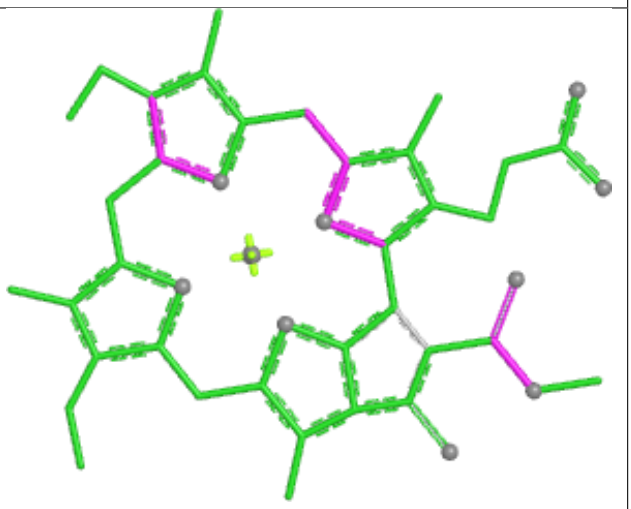


Rings

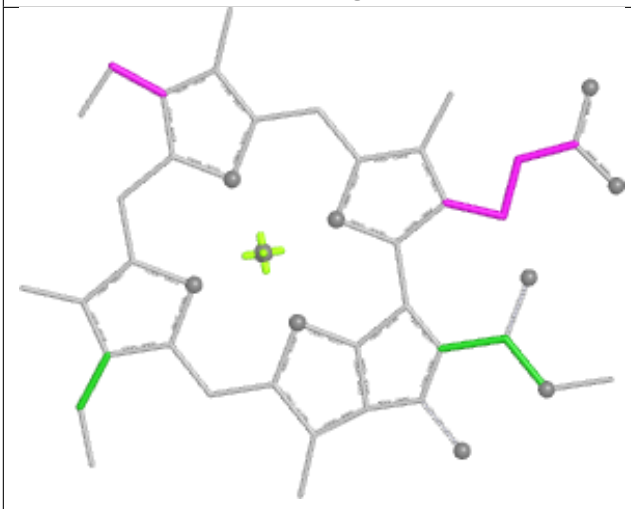
Ligand CLA b 822



Bond lengths



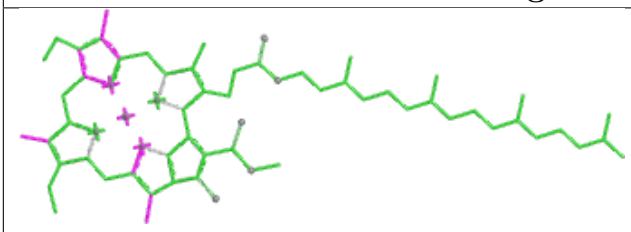
Bond angles



Torsions

Rings

Ligand CLA b 802



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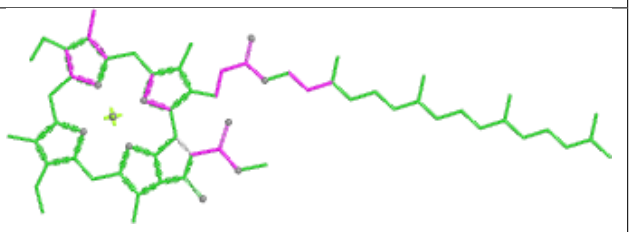
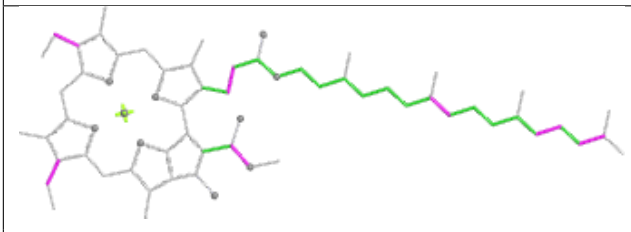
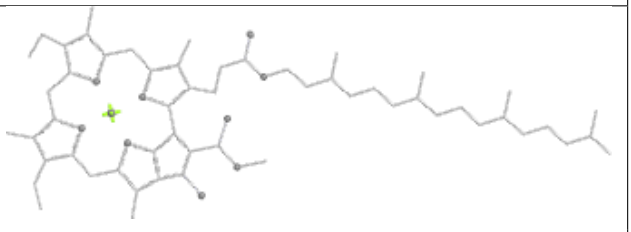


Bond angles

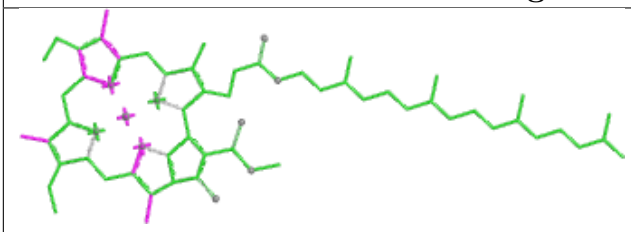


Torsions

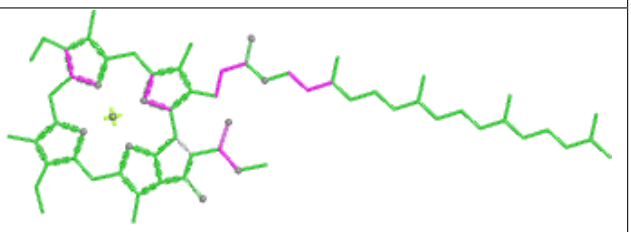


Rings

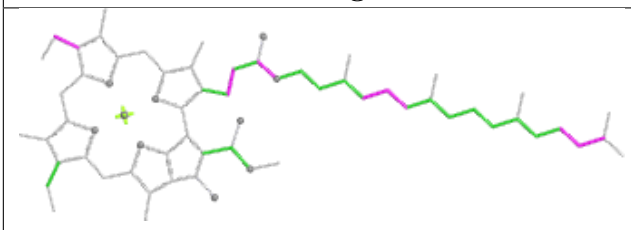
Ligand CLA b 828



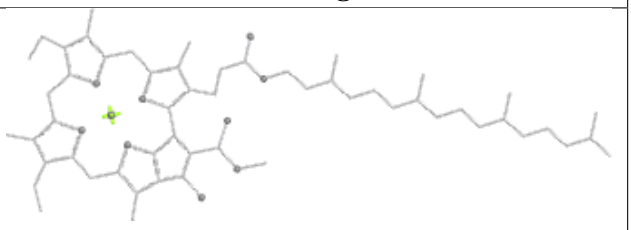
Bond lengths



Bond angles

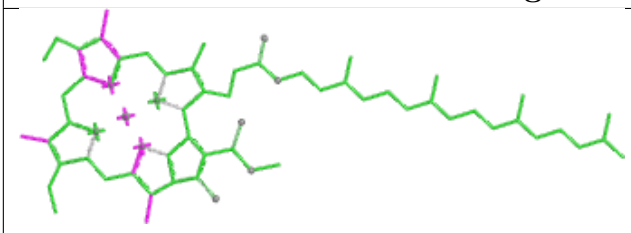


Torsions

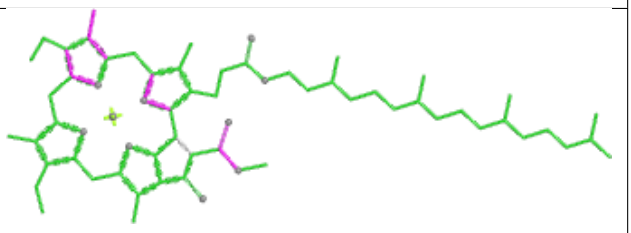


Rings

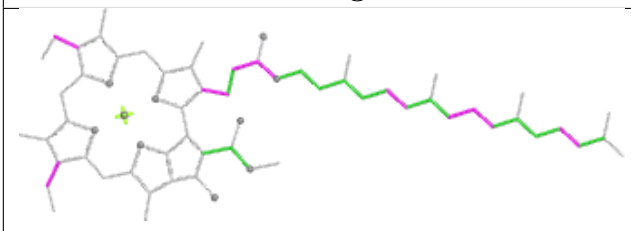
Ligand CLA B 843



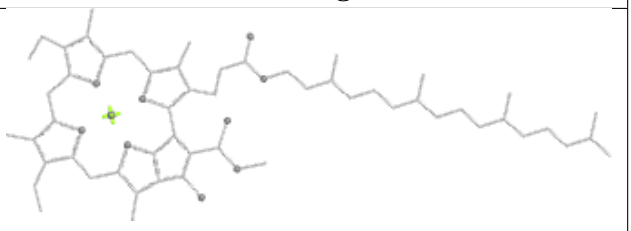
Bond lengths



Bond angles

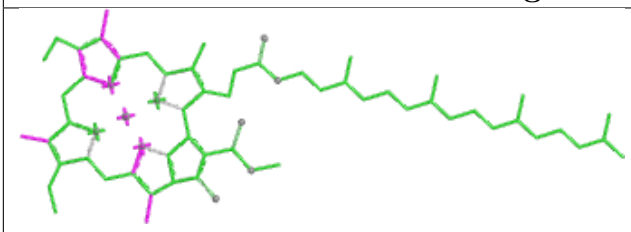


Torsions



Rings

Ligand CLA A 841



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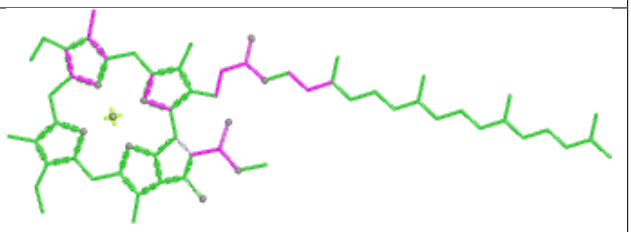

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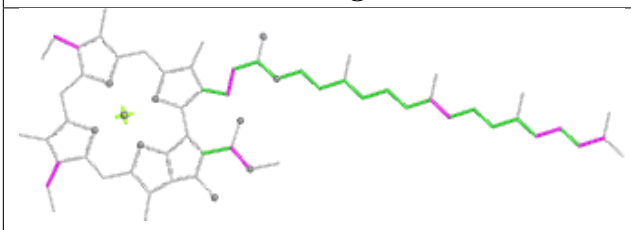

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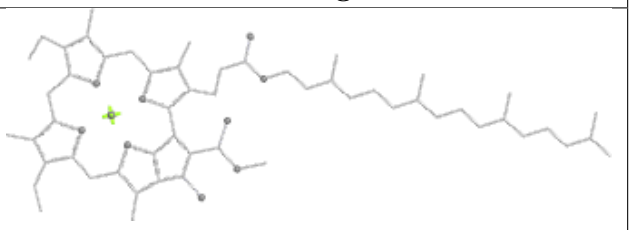
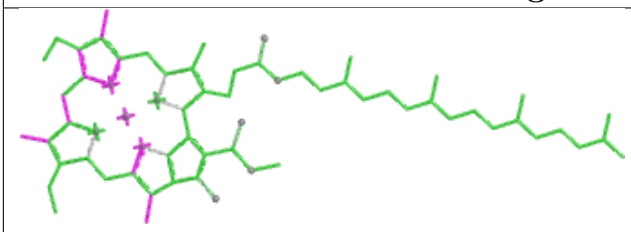


Rings

Ligand CLA b 806



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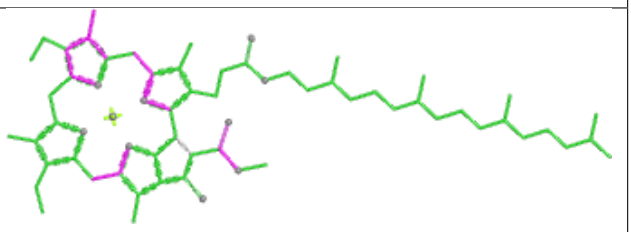
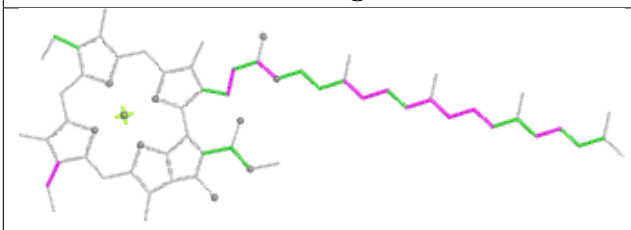


Bond angles



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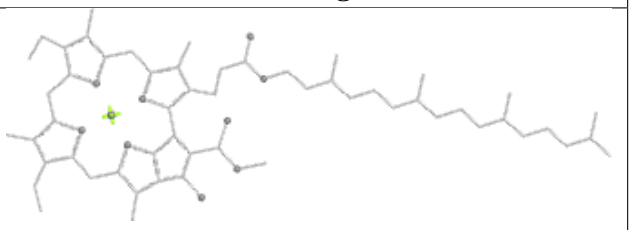
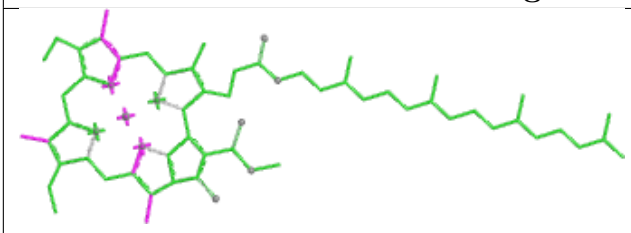


Rings

Ligand CLA A 834



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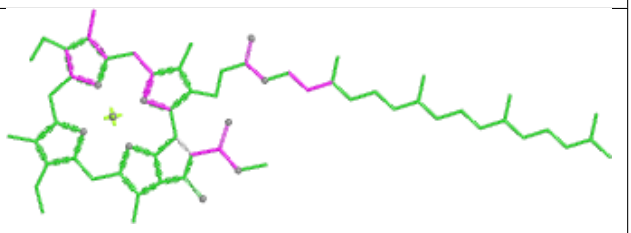
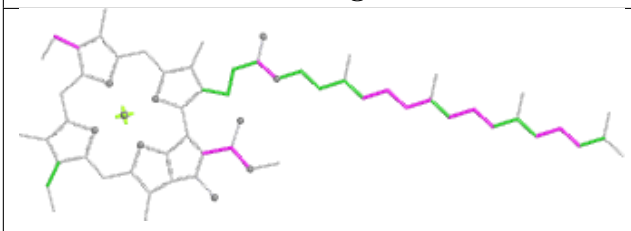
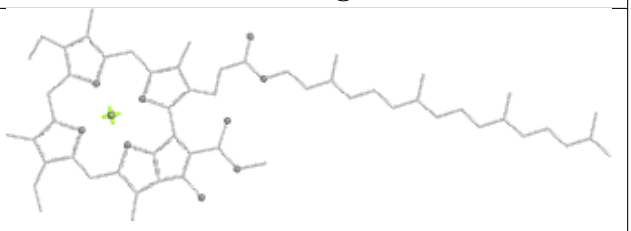


Bond angles

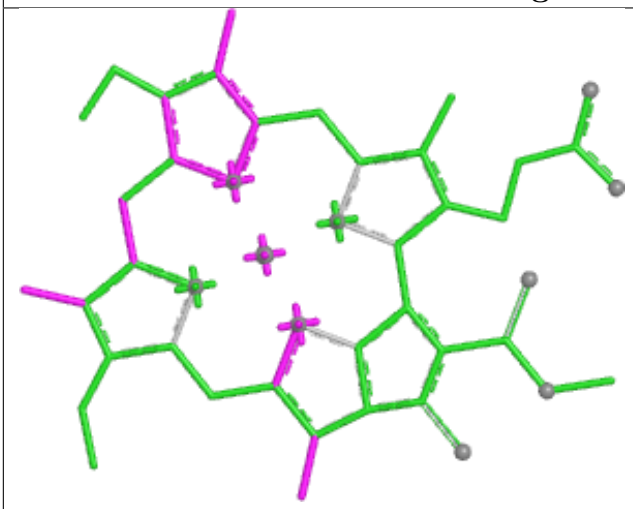


Torsions



Rings

Ligand CLA f 205



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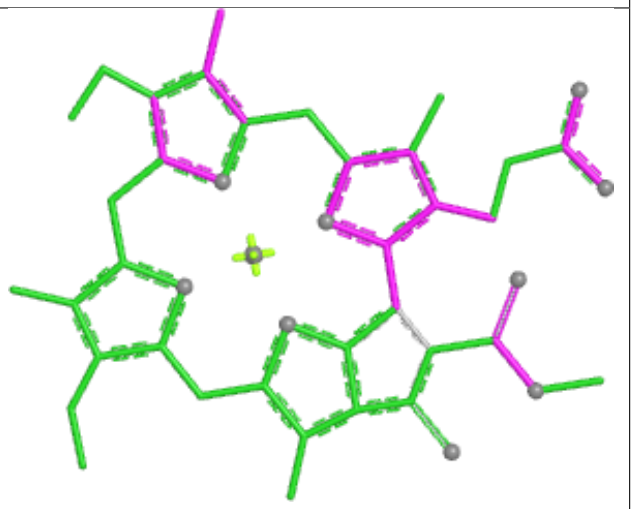
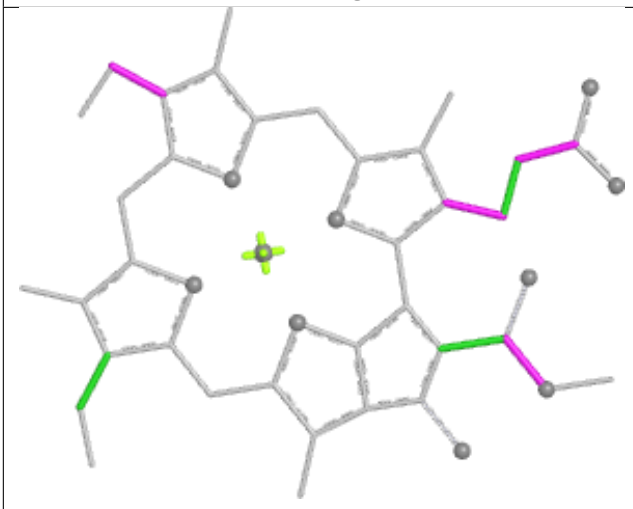


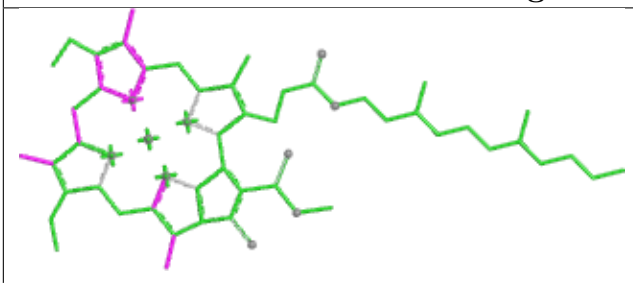
Bond angles



Torsions

Rings

Ligand CLA b 834



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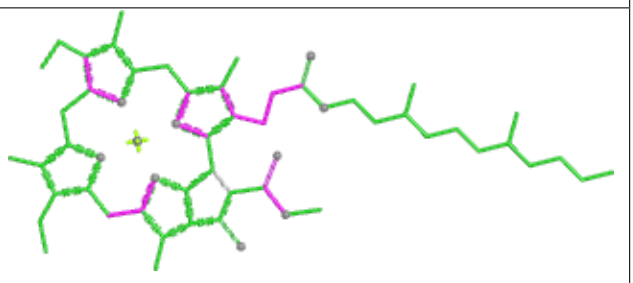
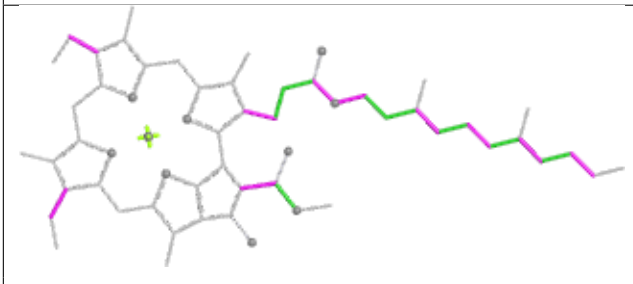


Bond angles



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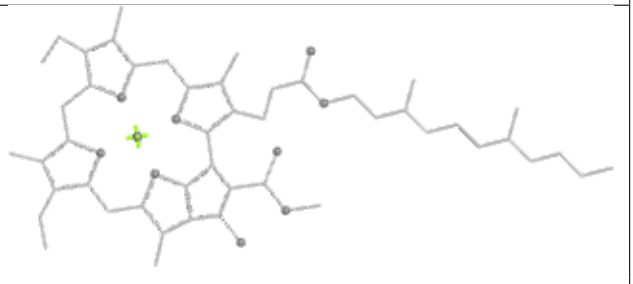
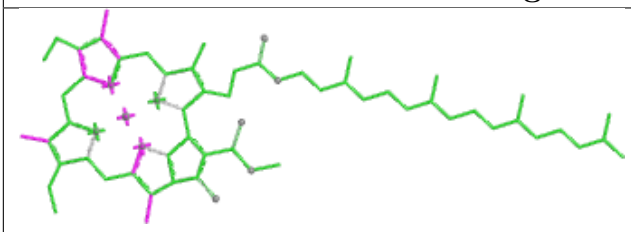


Rings

Ligand CLA A 805



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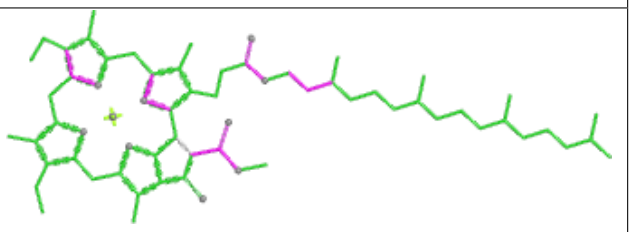
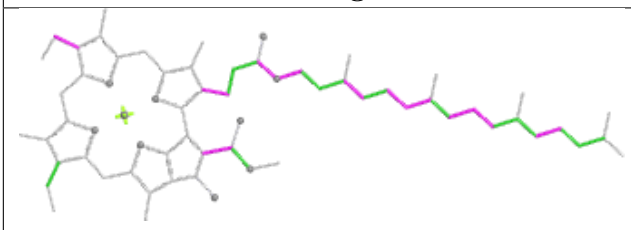


Bond angles



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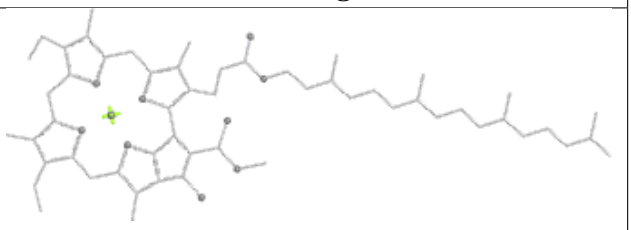
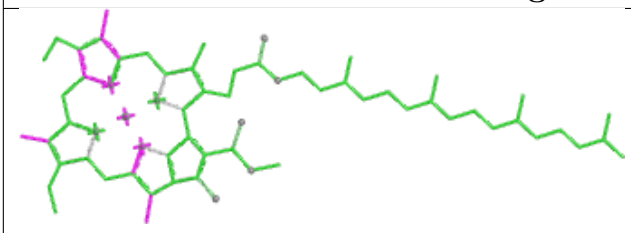


Rings

Ligand CLA 1 843



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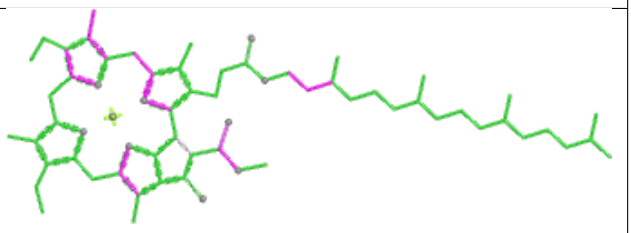
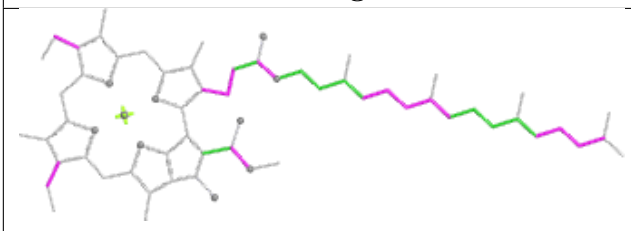
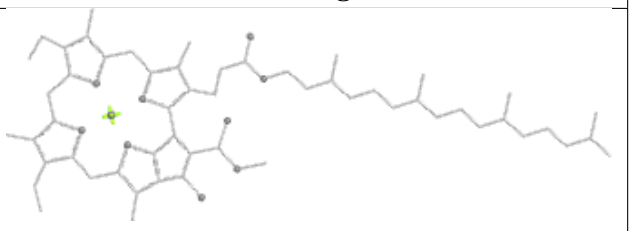


Bond angles

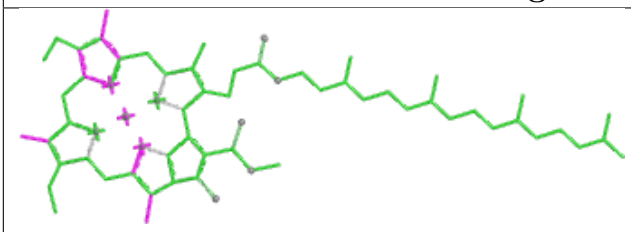


Torsions

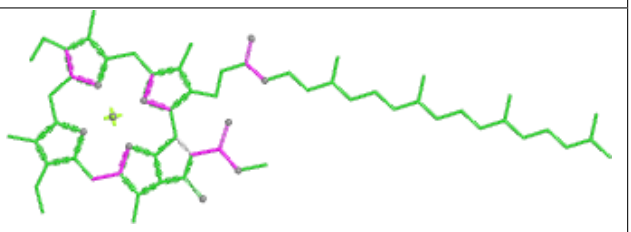


Rings

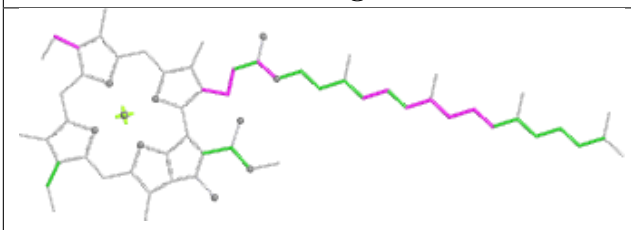
Ligand CLA 1 842



Bond lengths



Bond angles



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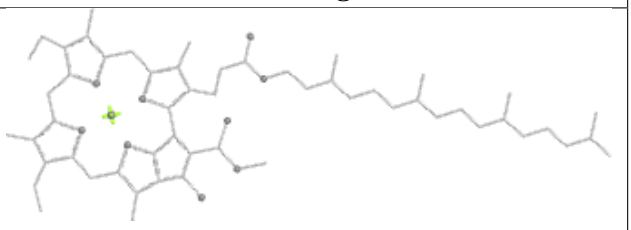
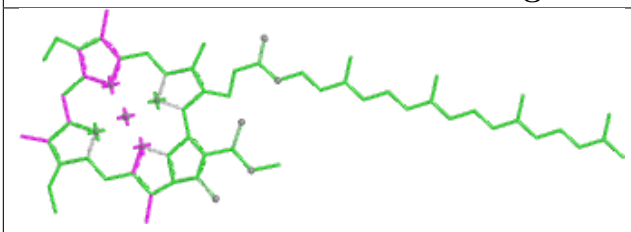


Rings

Ligand CLA A 813



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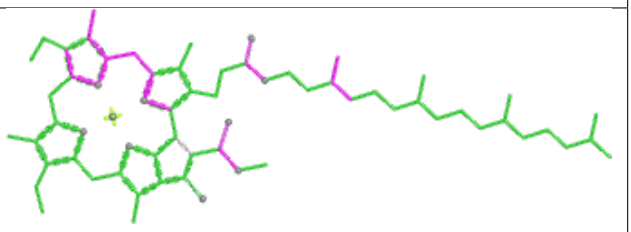
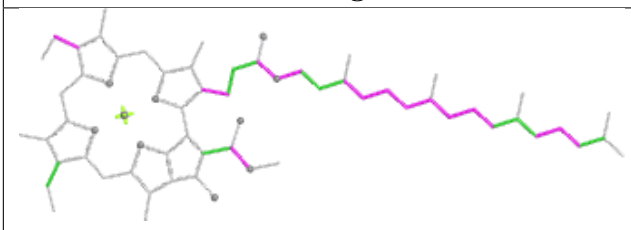


Bond angles



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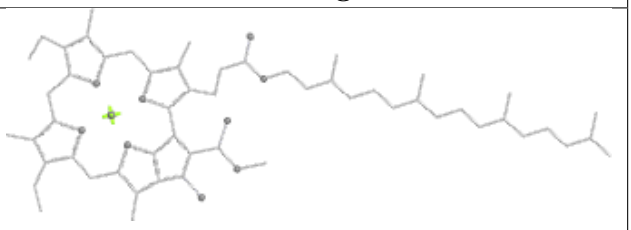
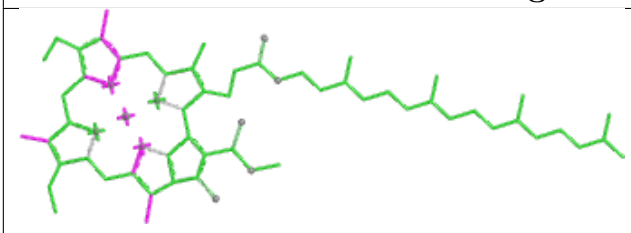


Rings

Ligand CLA a 808



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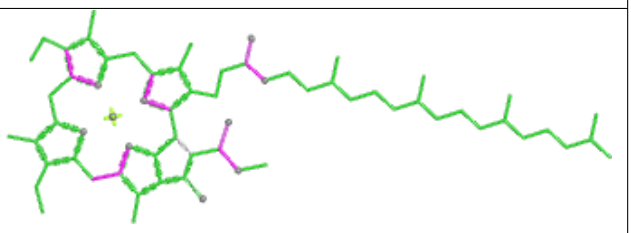
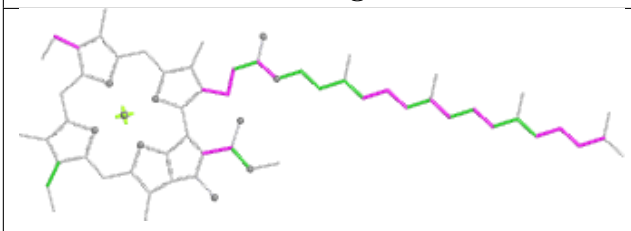
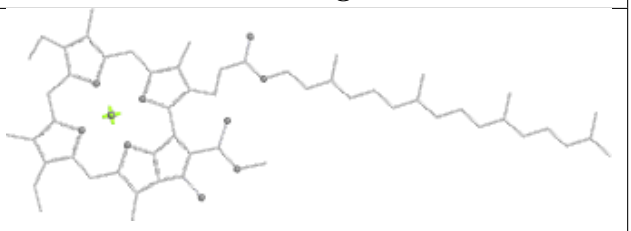


Bond angles

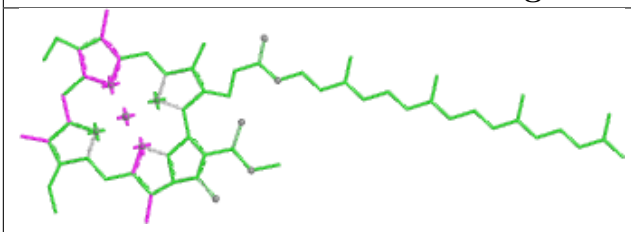


Torsions



Rings

Ligand CLA B 813



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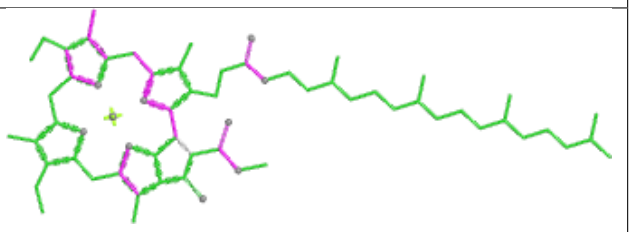
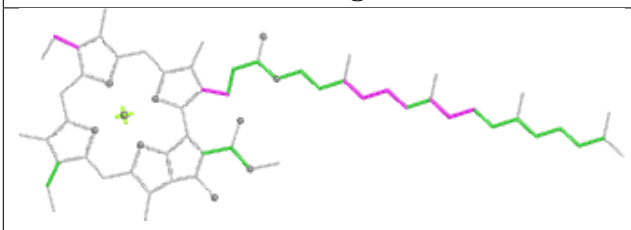
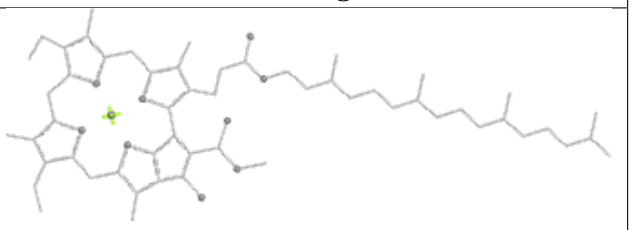


Bond angles

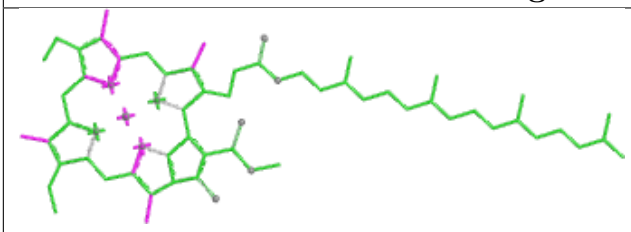


Torsions

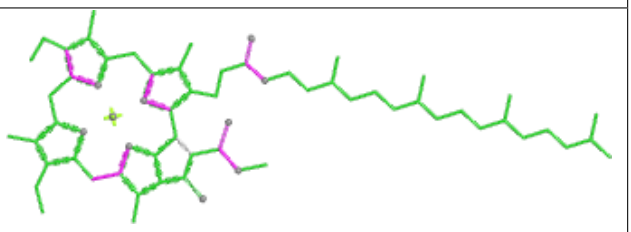


Rings

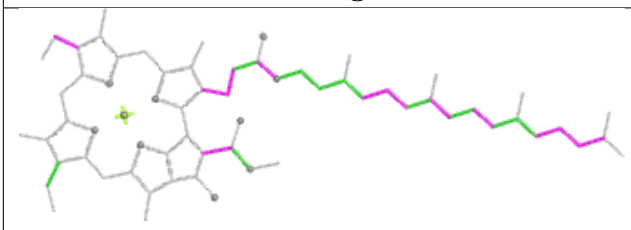
Ligand CLA 1 806



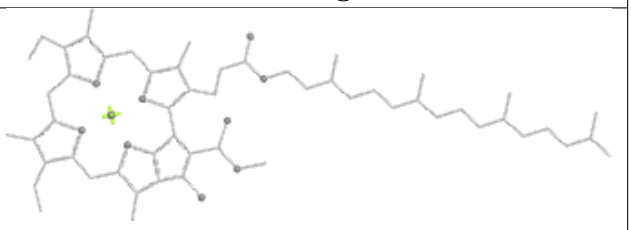
Bond lengths



Bond angles

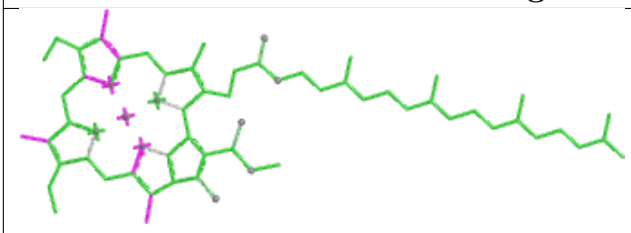


Torsions



Rings

Ligand CLA b 808



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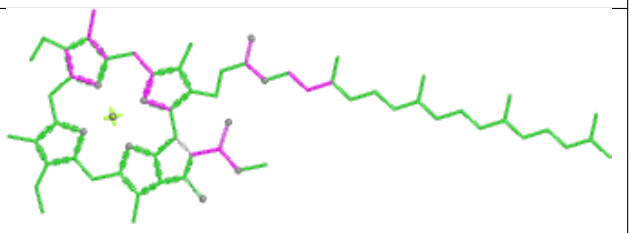
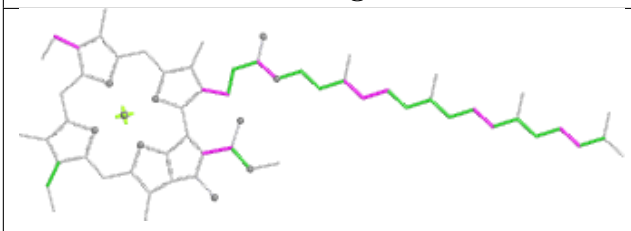
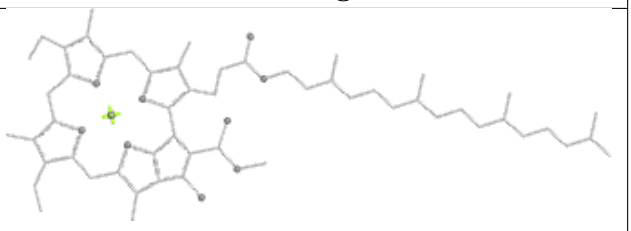


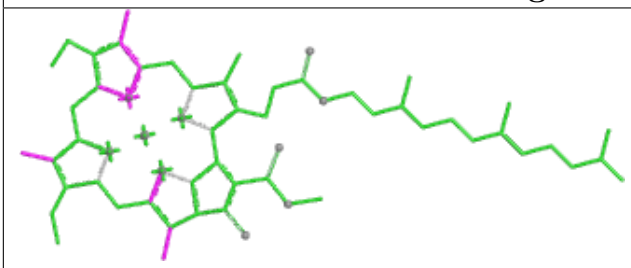
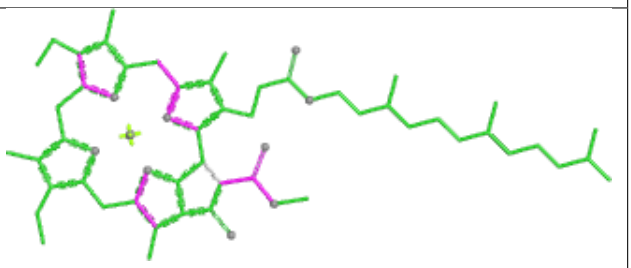
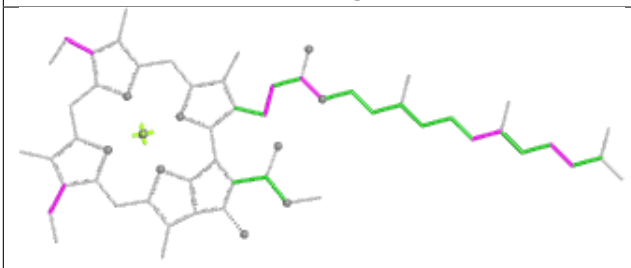
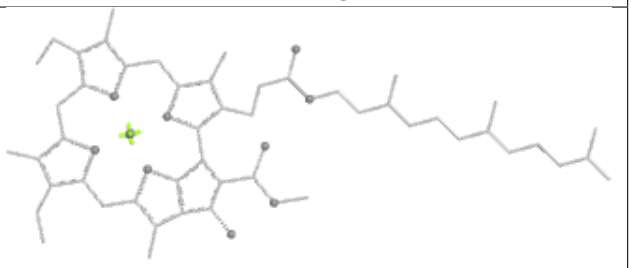
Bond angles

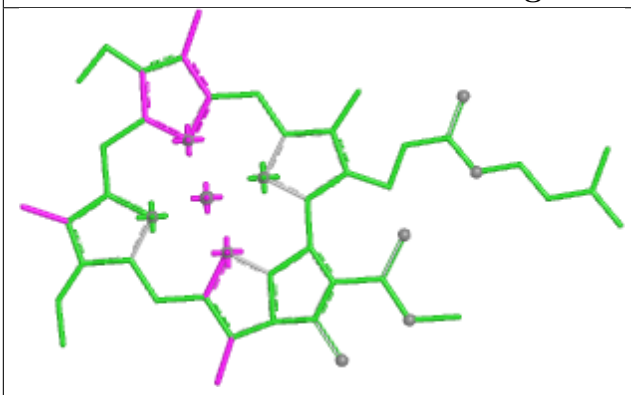
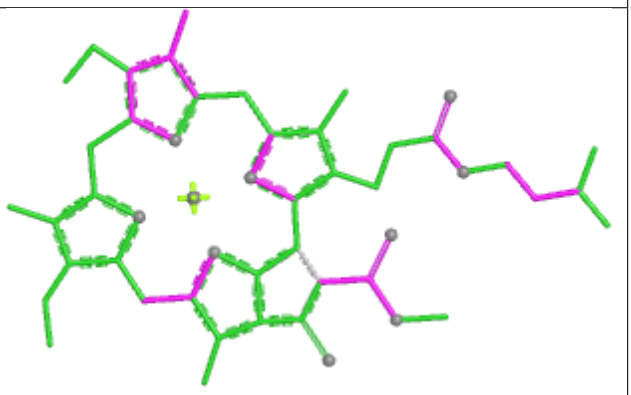
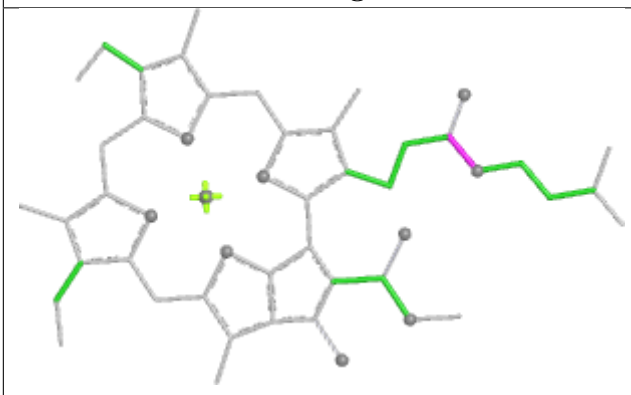
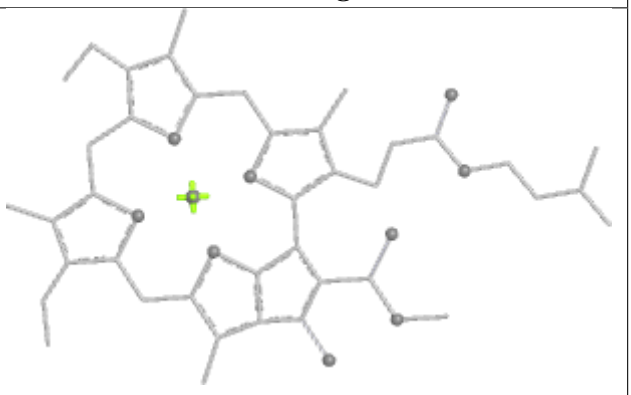


Torsions

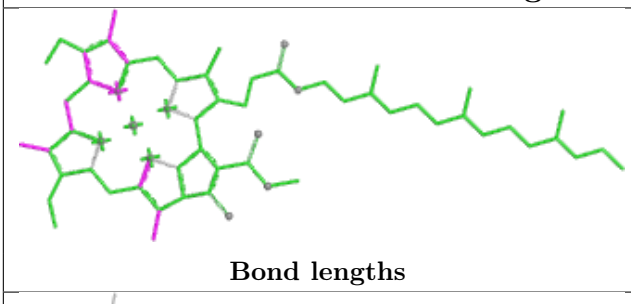


Rings

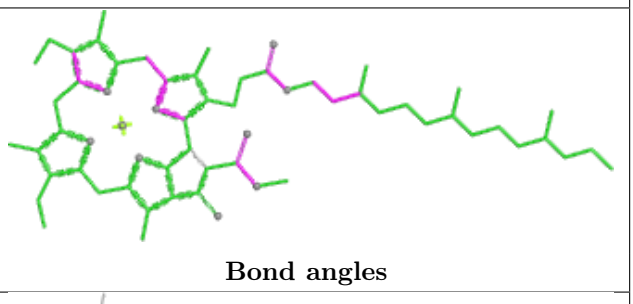
Ligand CLA 2 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

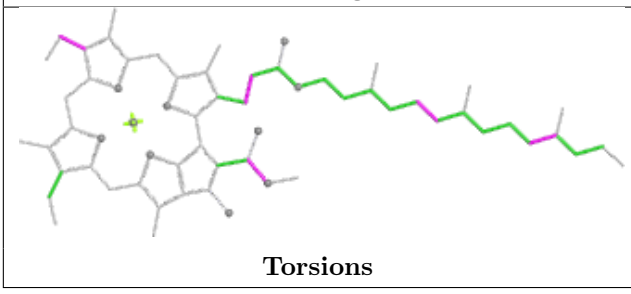
Ligand CLA B 841



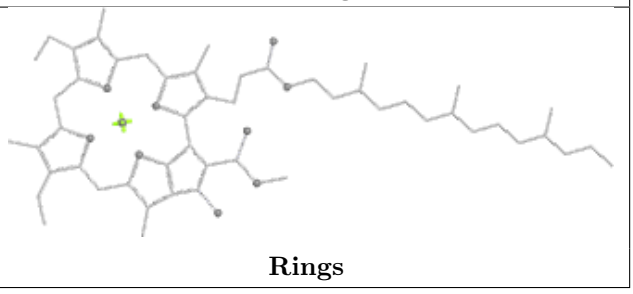
Bond lengths



Bond angles

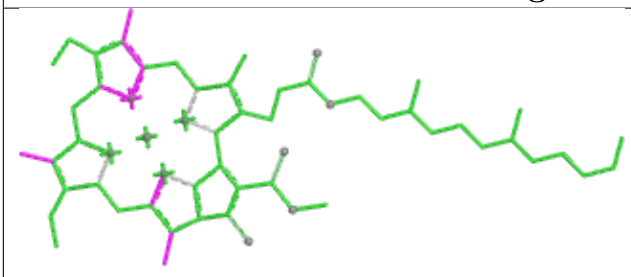


Torsions

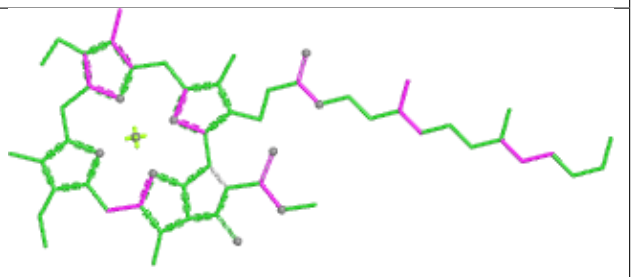


Rings

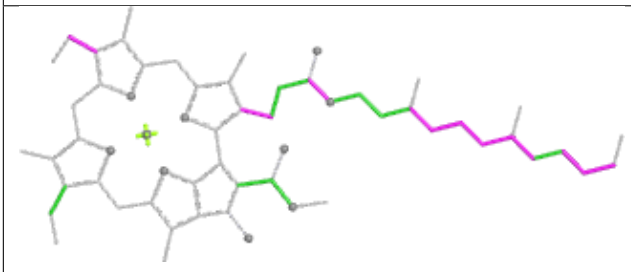
Ligand CLA a 827



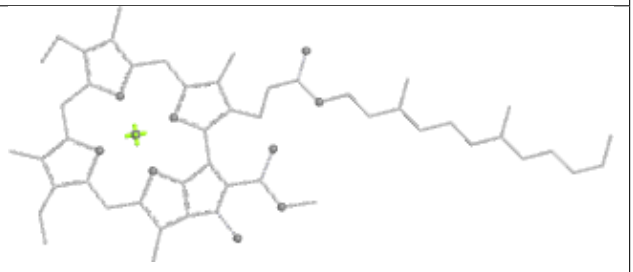
Bond lengths



Bond angles

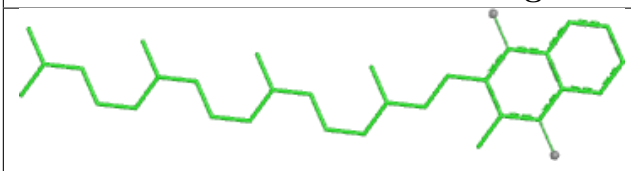


Torsions

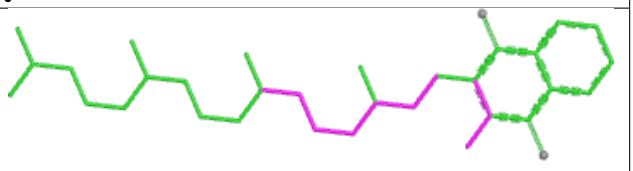


Rings

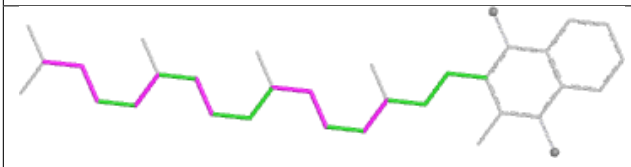
Ligand PQN b 845



Bond lengths



Bond angles



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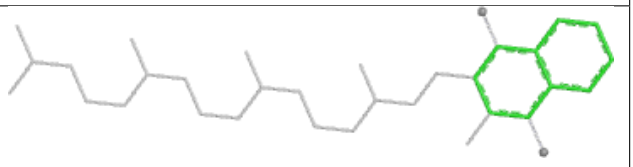
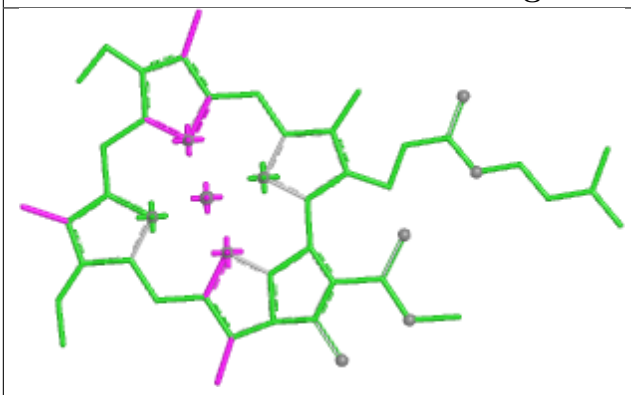


Rings

Ligand CLA A 833



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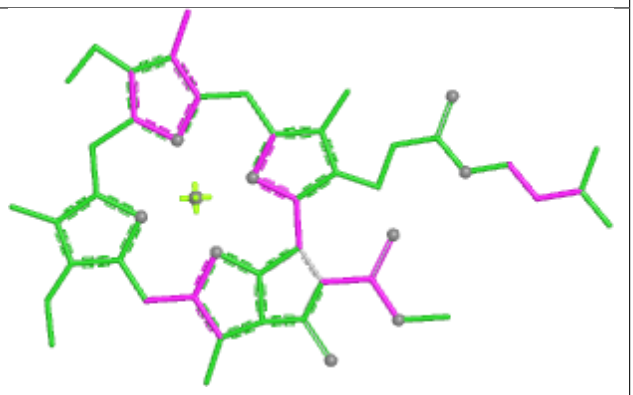
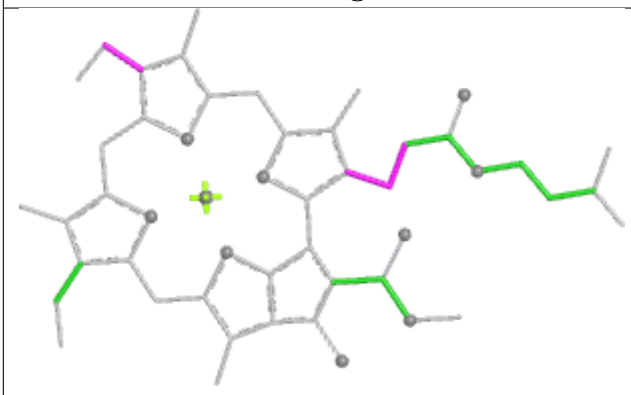


Bond angles



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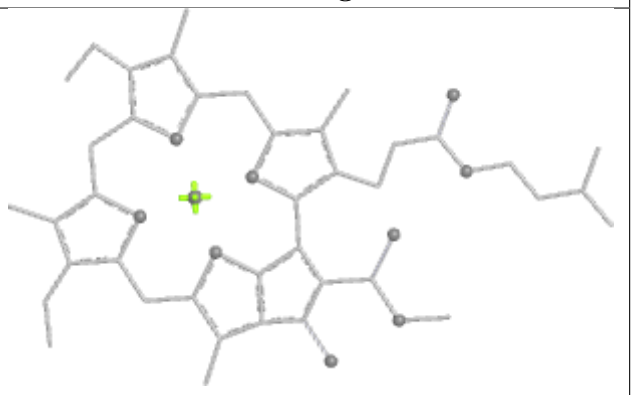
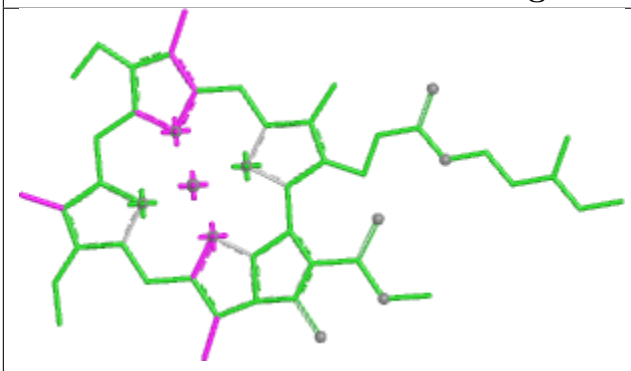
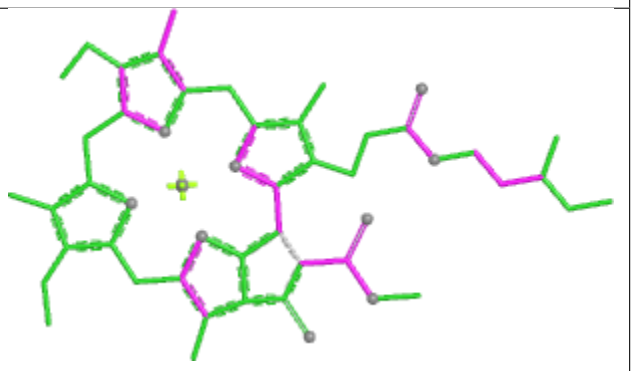


Rings

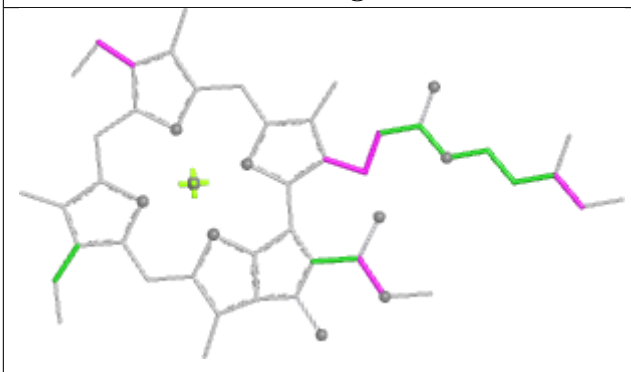
Ligand CLA 1 837



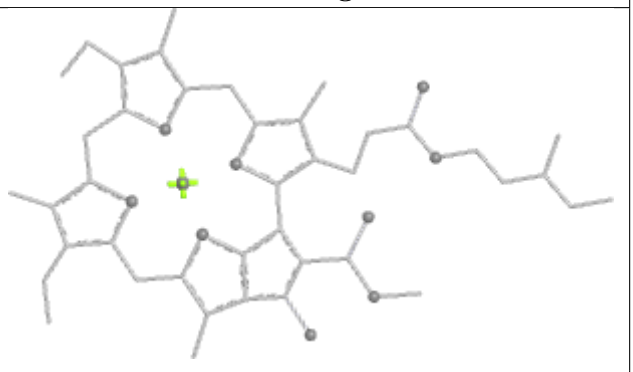
Bond lengths



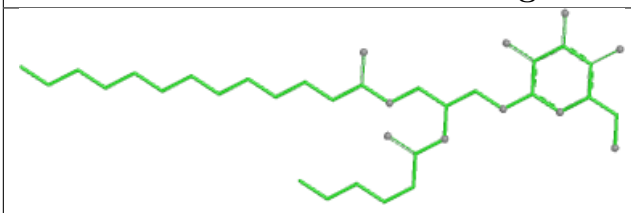
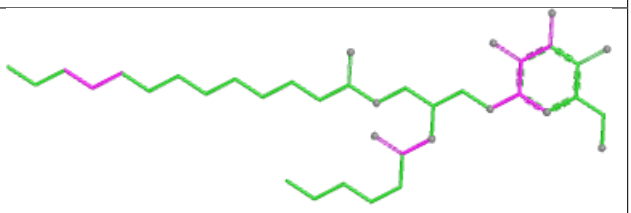
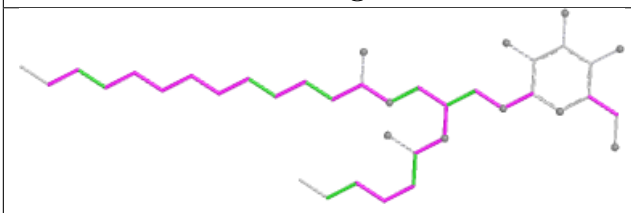
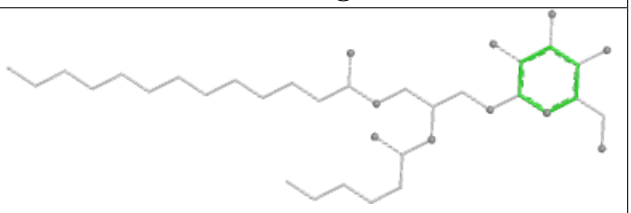
Bond angles

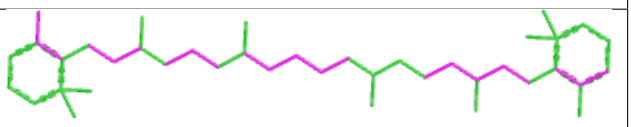
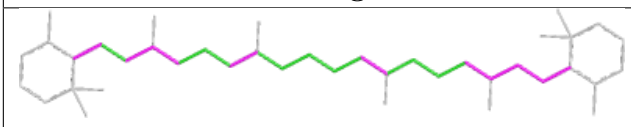
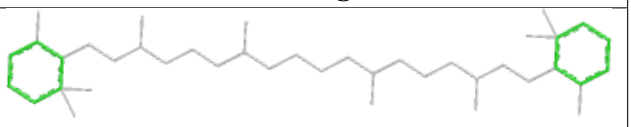


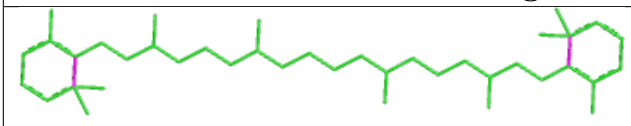
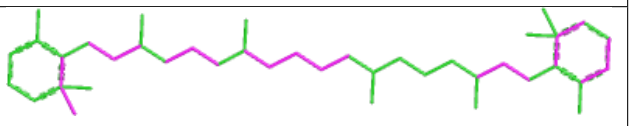
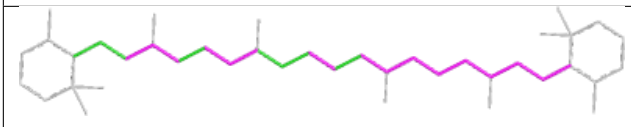
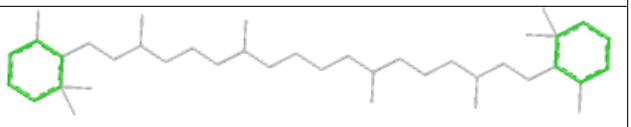
Torsions



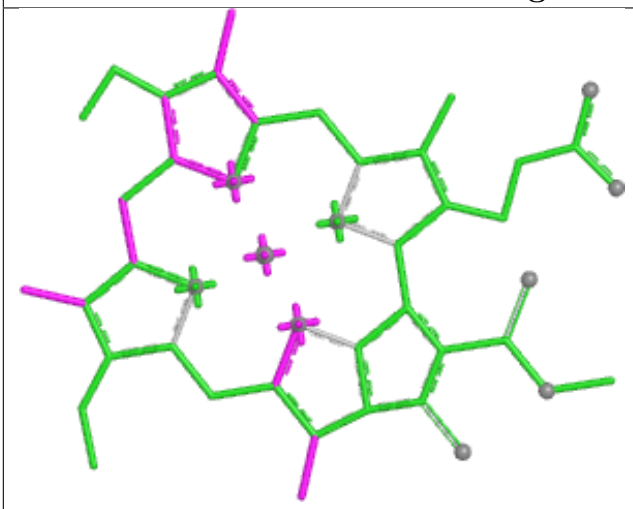
Rings

Ligand LMG l 4202	
 Bond lengths	 Bond angles
 Torsions	 Rings

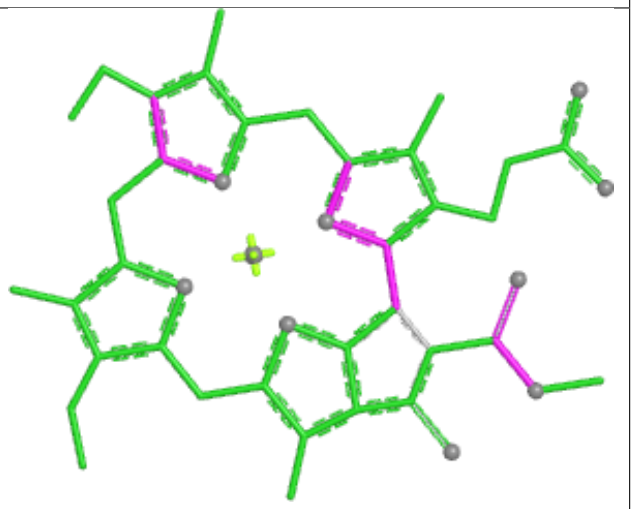
Ligand BCR b 854	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

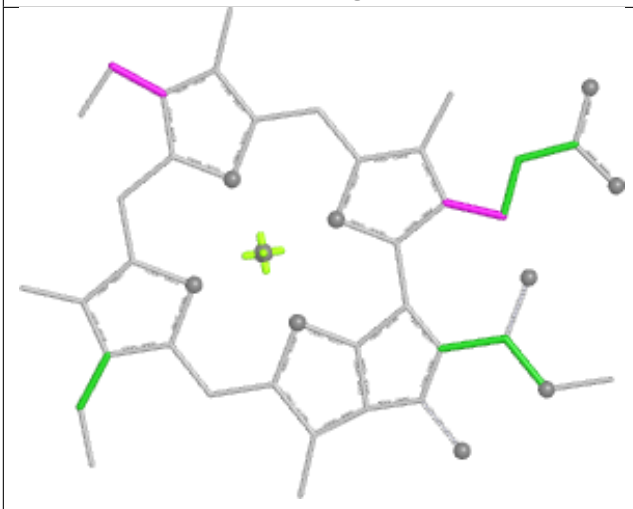
Ligand CLA 2 837



Bond lengths



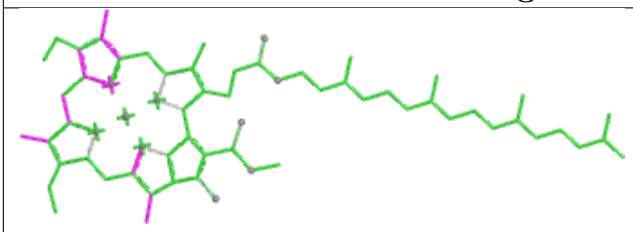
Bond angles



Torsions

Rings

Ligand CLA L 1503



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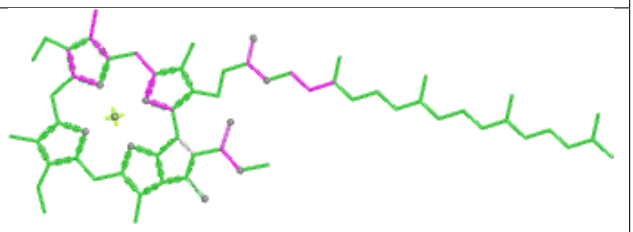
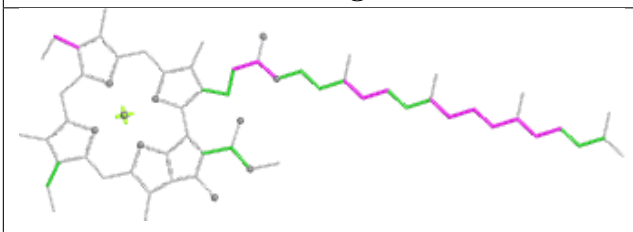
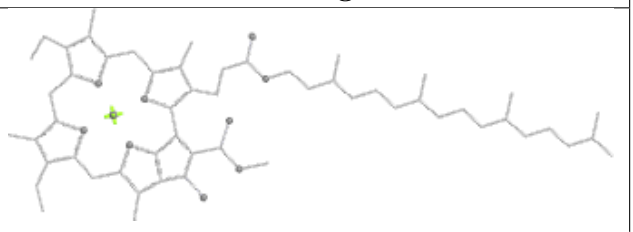


Bond angles

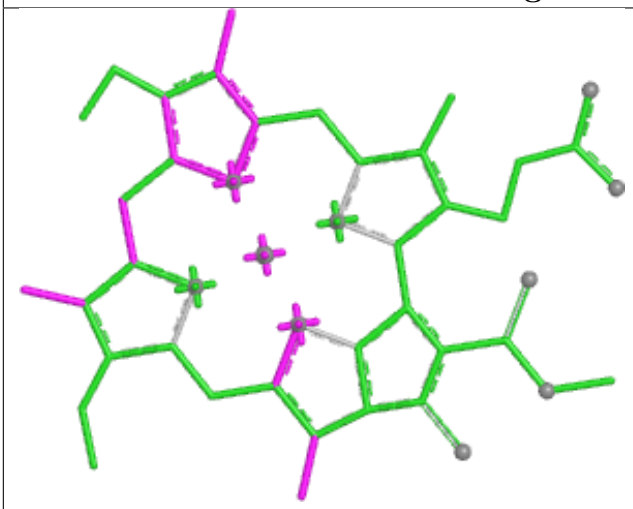


Torsions

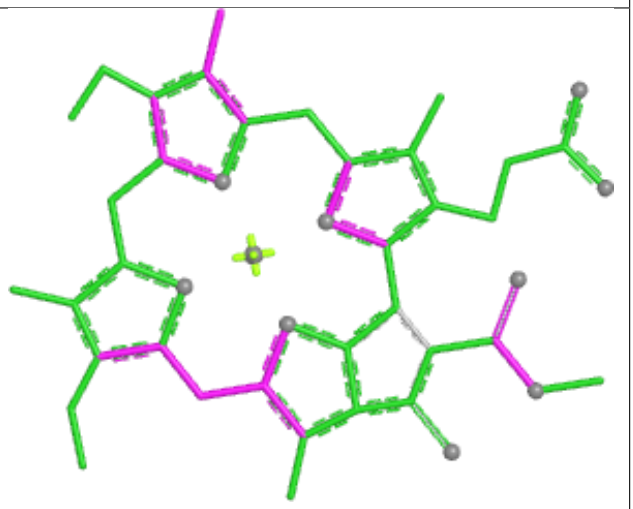


Rings

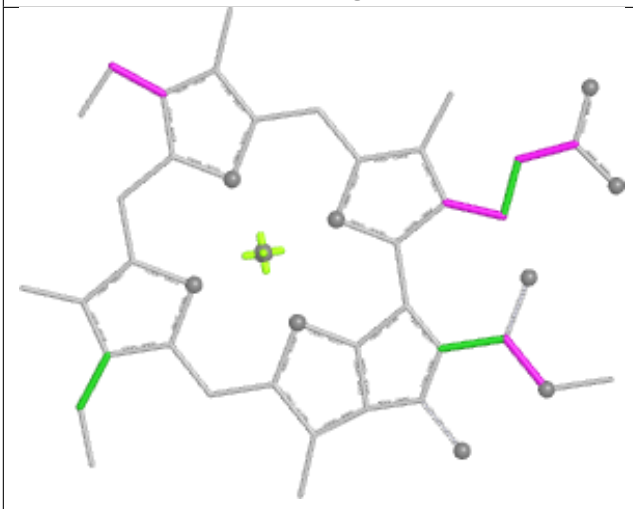
Ligand CLA B 833



Bond lengths



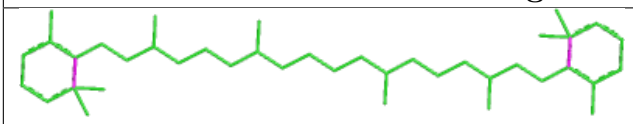
Bond angles



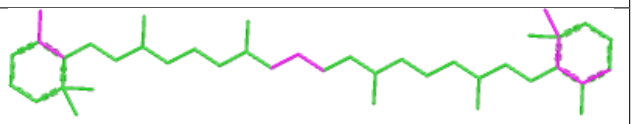
Torsions

Rings

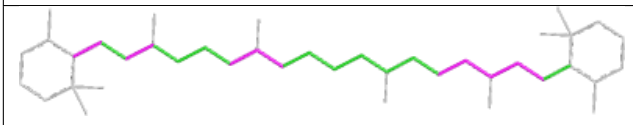
Ligand BCR 1 848



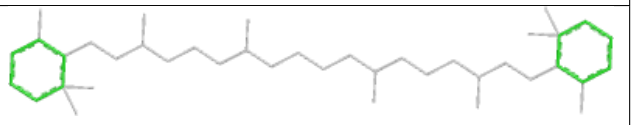
Bond lengths



Bond angles

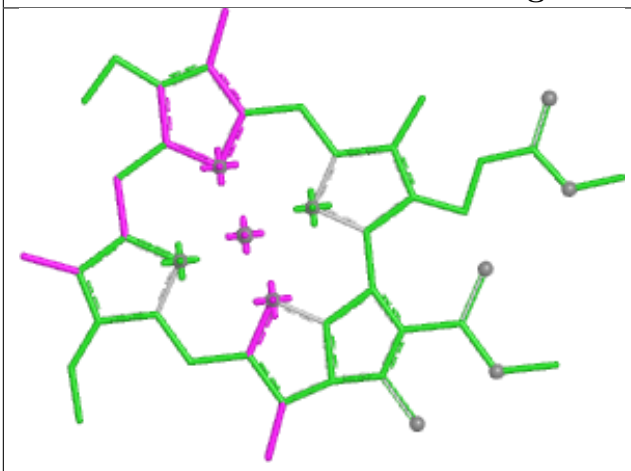


Torsions

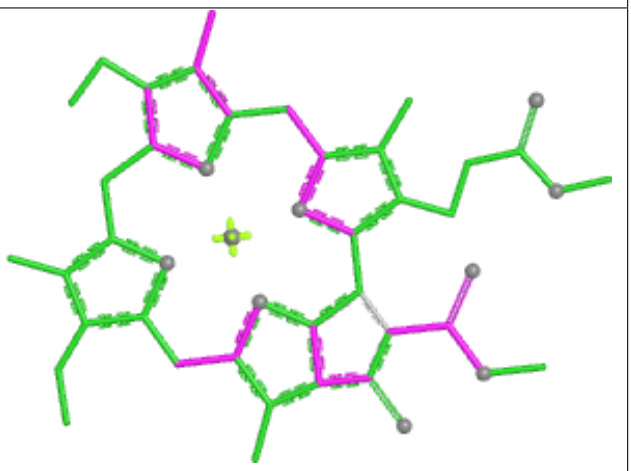


Rings

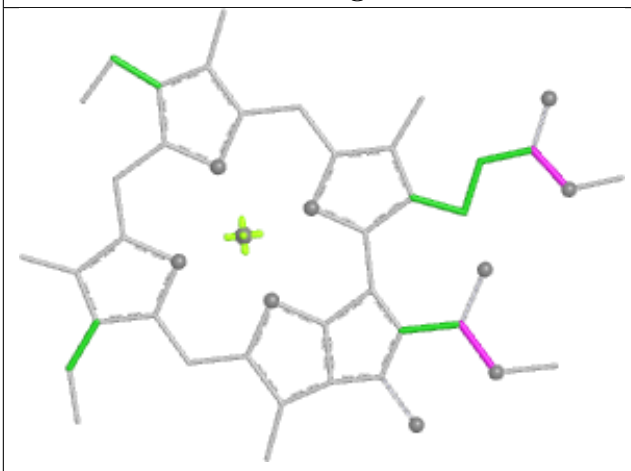
Ligand CLA b 841



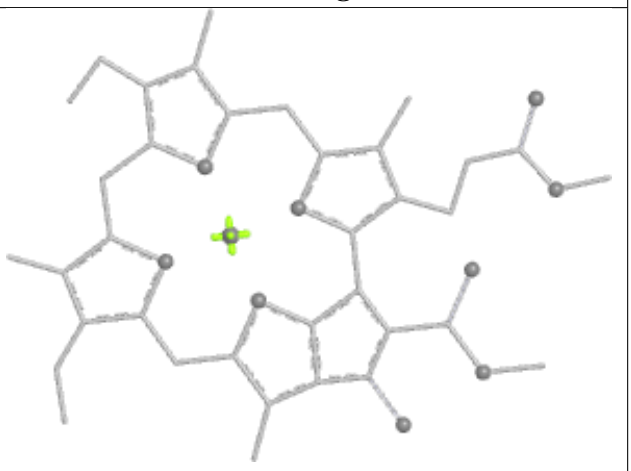
Bond lengths



Bond angles

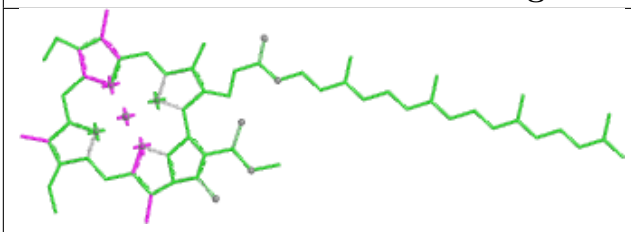


Torsions

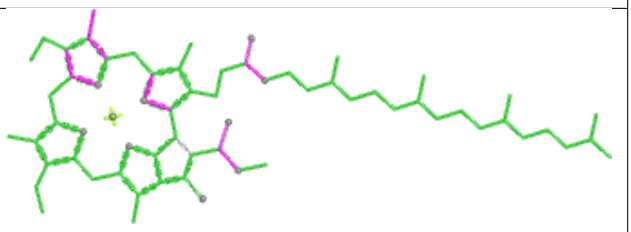


Rings

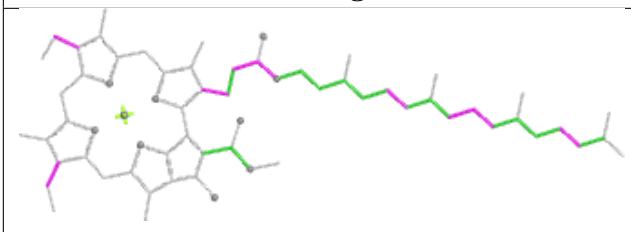
Ligand CLA b 842



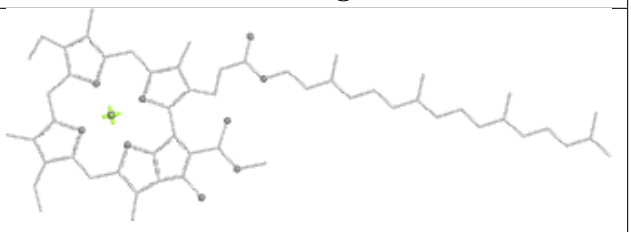
Bond lengths



Bond angles

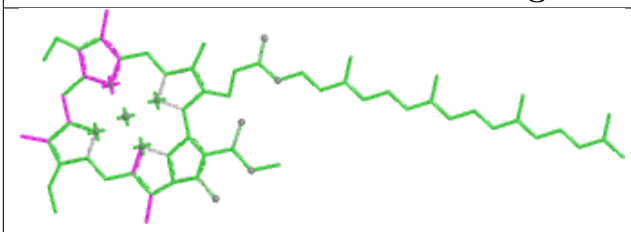


Torsions

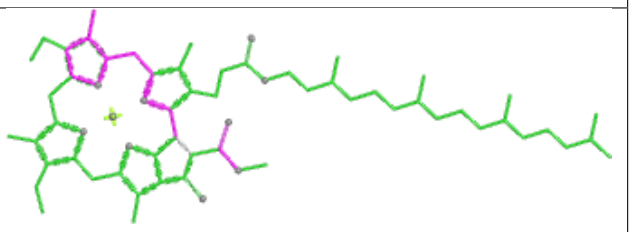


Rings

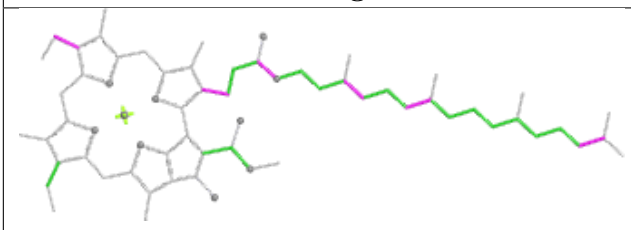
Ligand CLA 0 202



Bond lengths



Bond angles



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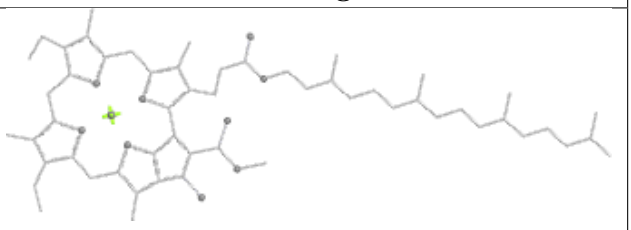
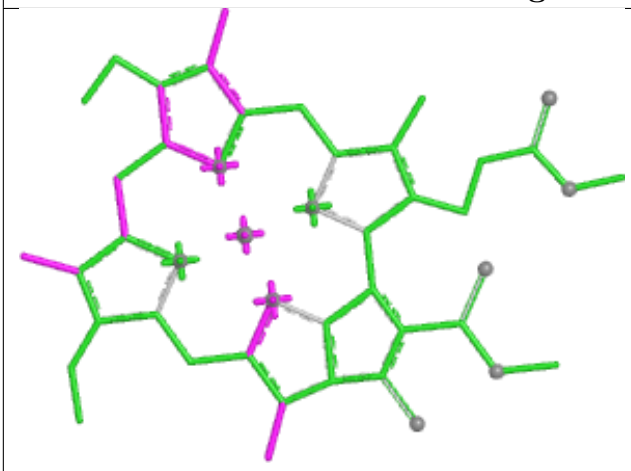
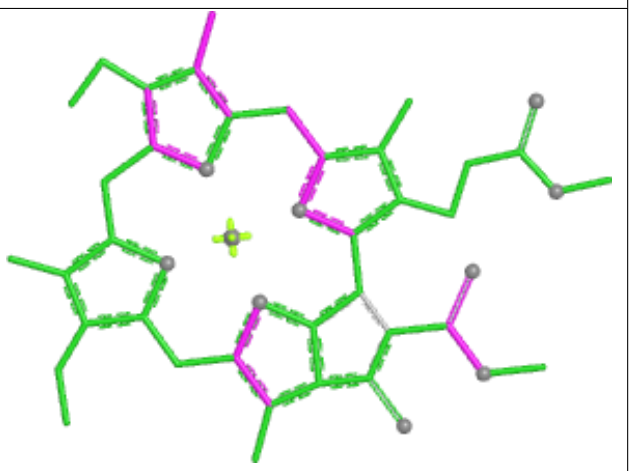


Rings

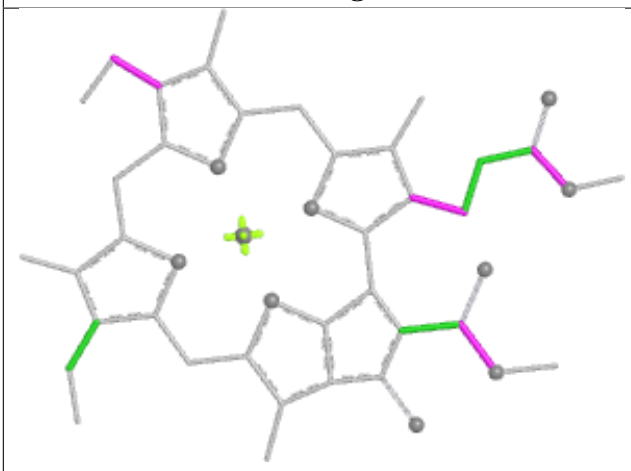
Ligand CLA 1 808



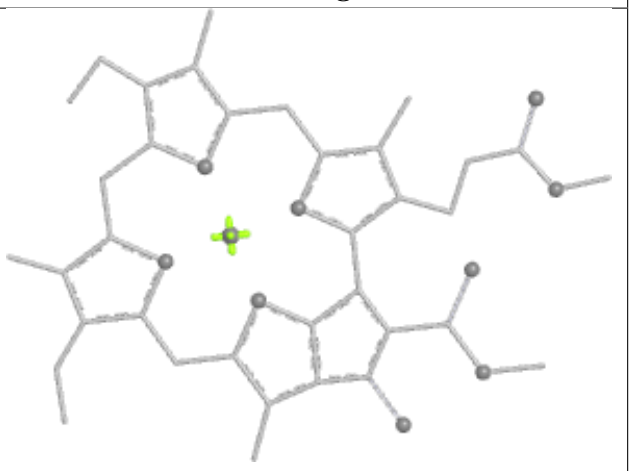
Bond lengths



Bond angles

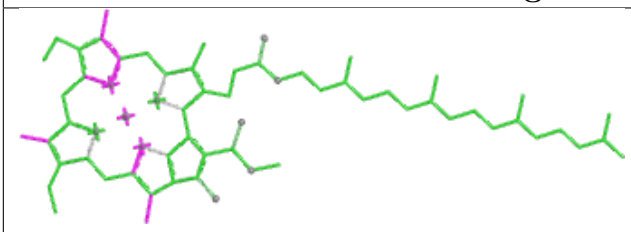


Torsions

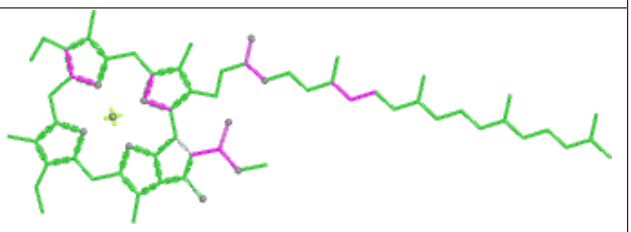


Rings

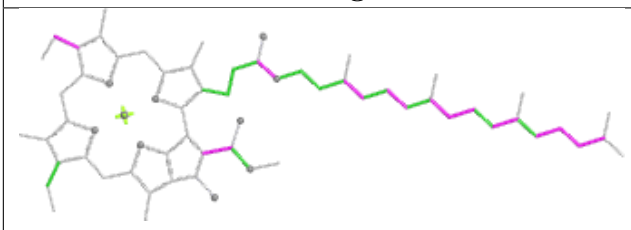
Ligand CLA B 811



Bond lengths



Bond angles



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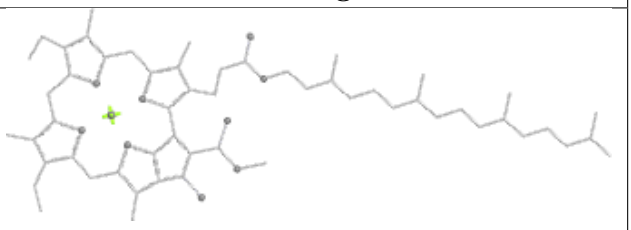
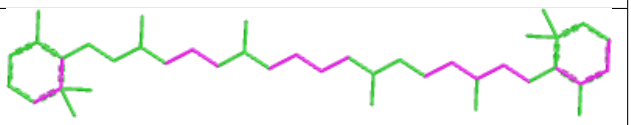


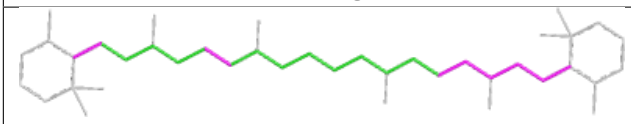
Rings

Ligand BCR B 852

Bond lengths



Bond angles



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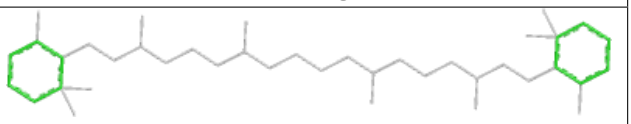
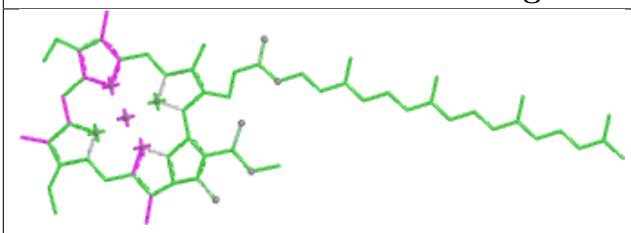
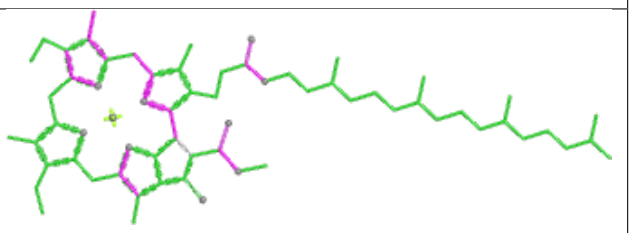


Rings

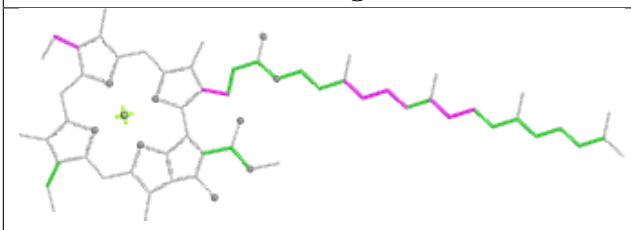
Ligand CLA l 4203



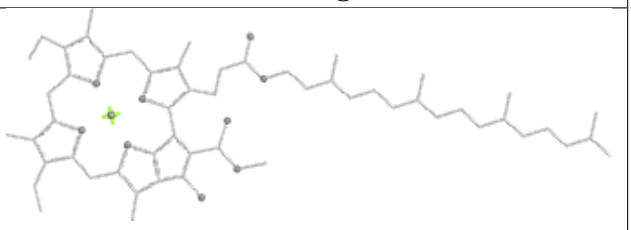
Bond lengths



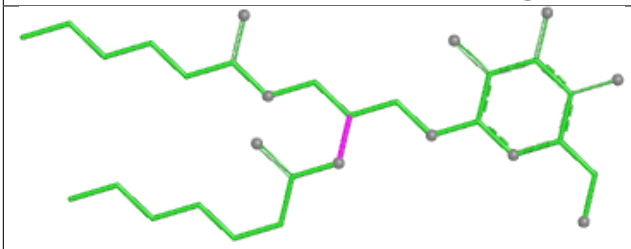
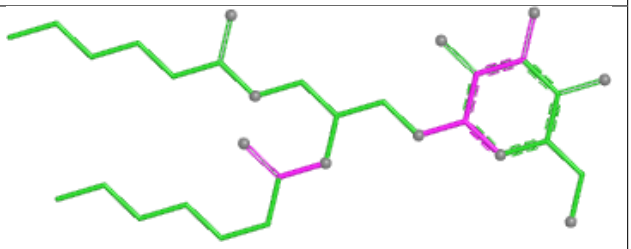
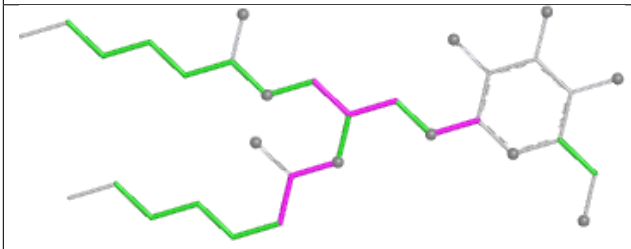
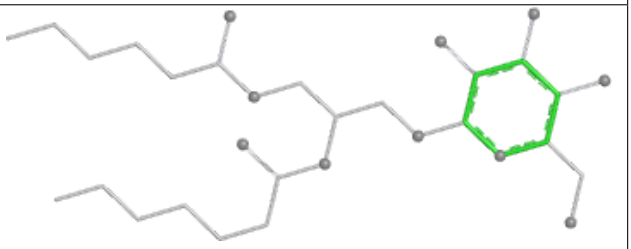
Bond angles

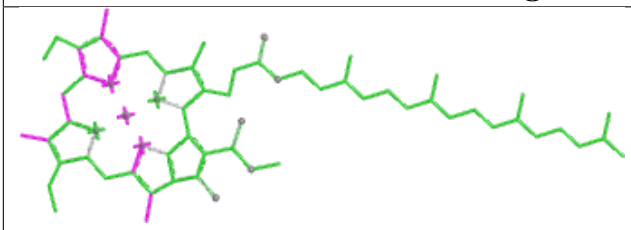
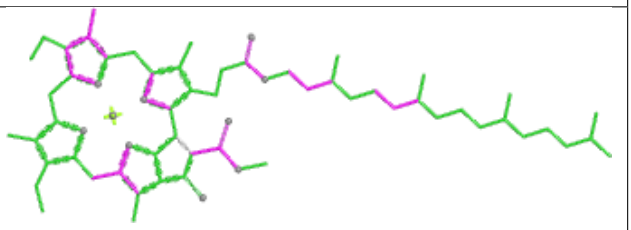
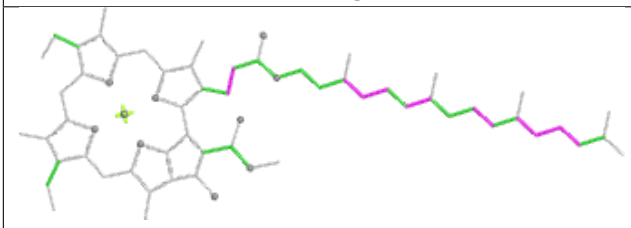
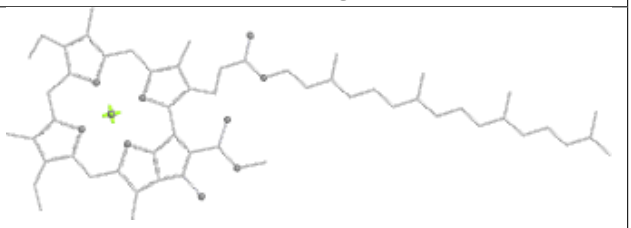


Torsions

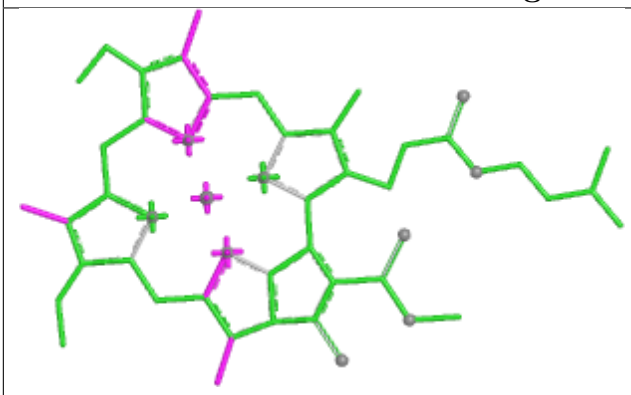


Rings

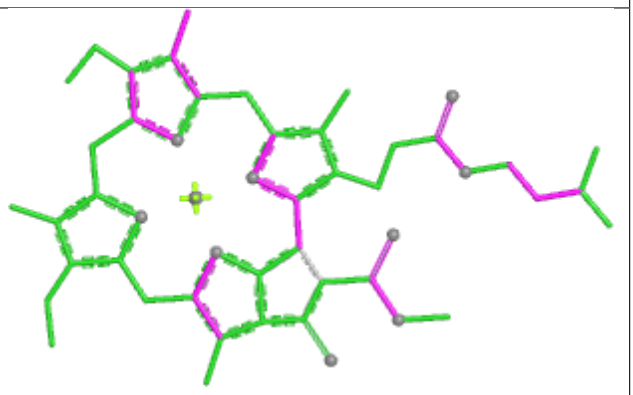
Ligand LMG A 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

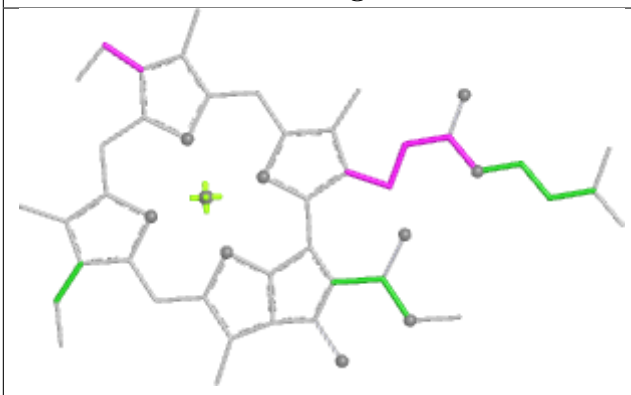
Ligand CLA A 811



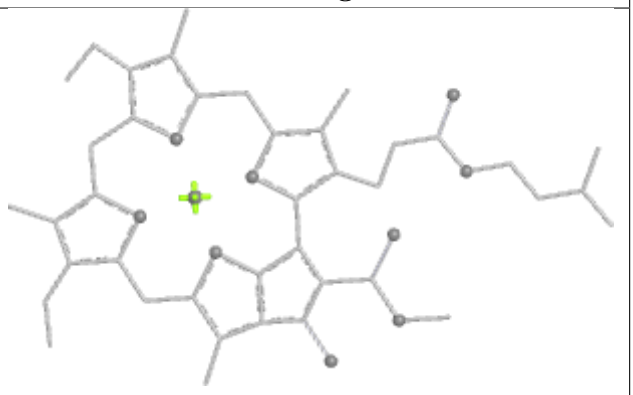
Bond lengths



Bond angles

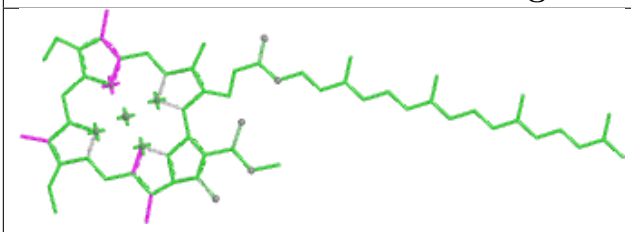


Torsions



Rings

Ligand CLA 1 834



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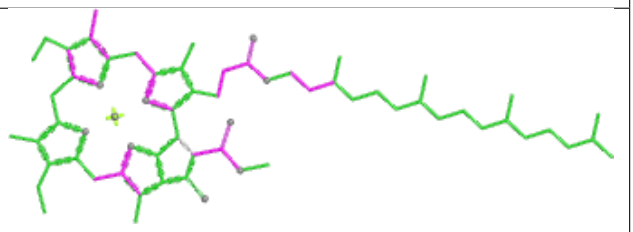
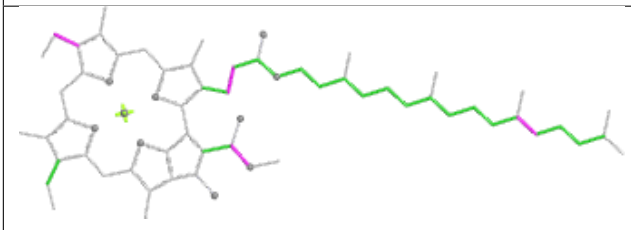
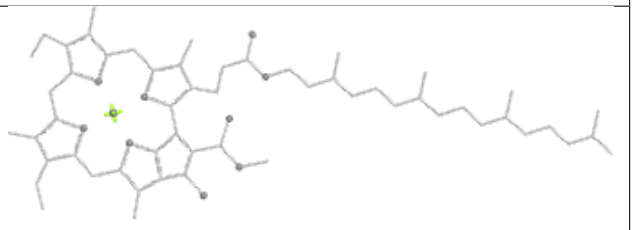


Bond angles

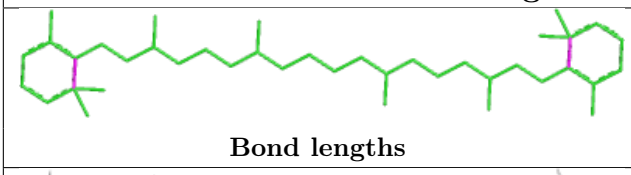


Torsions



Rings

Ligand BCR B 847



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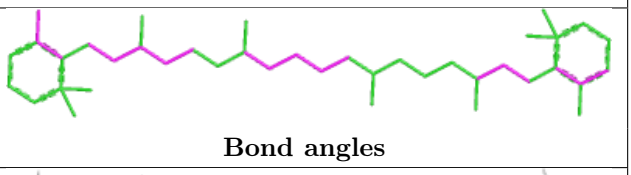
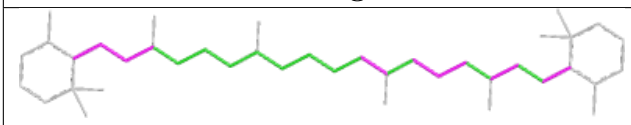
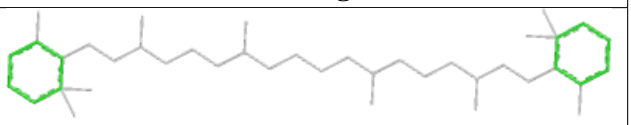


Bond angles

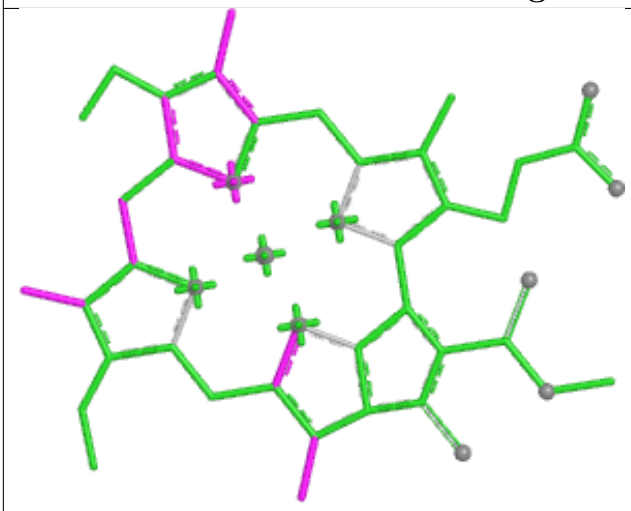


Torsions



Rings

Ligand CLA a 838



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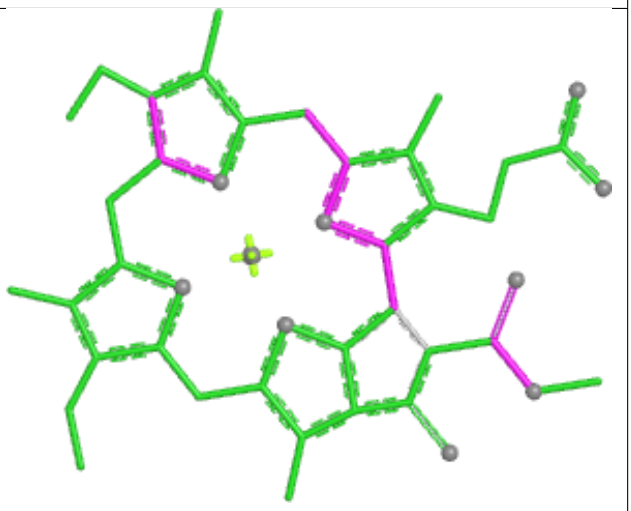
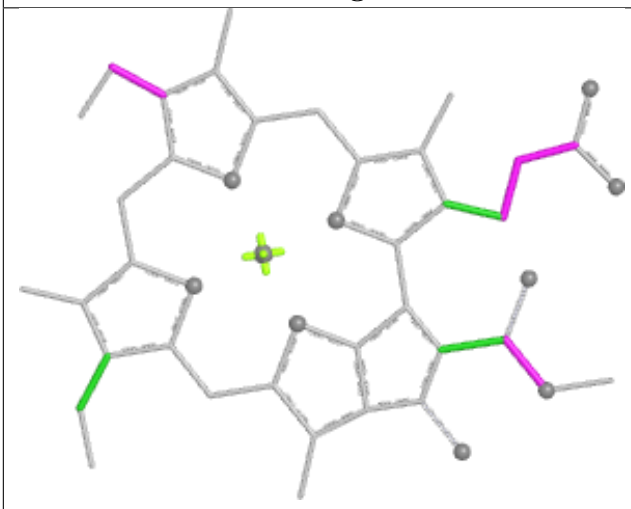


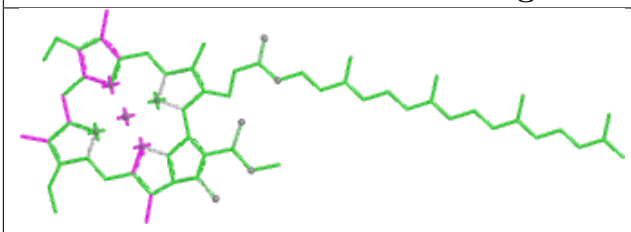
Bond angles



Torsions

Rings

Ligand CLA L 1501



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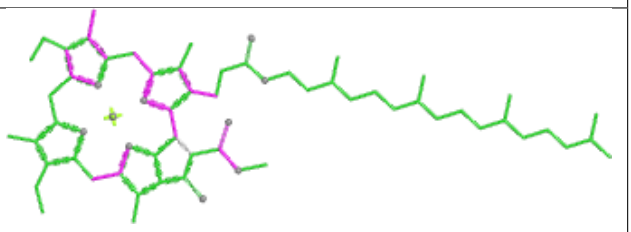
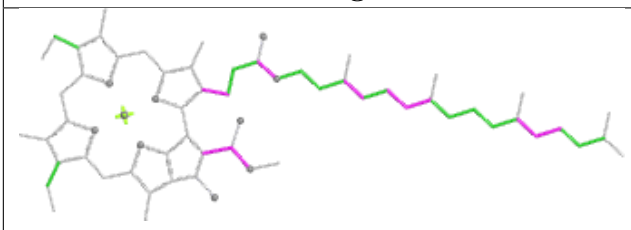
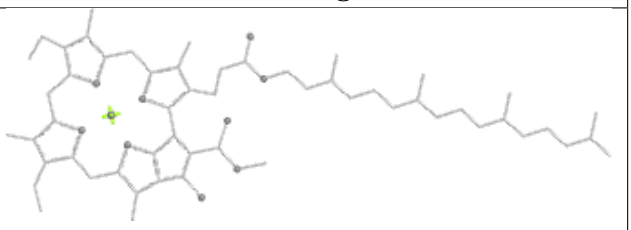


Bond angles

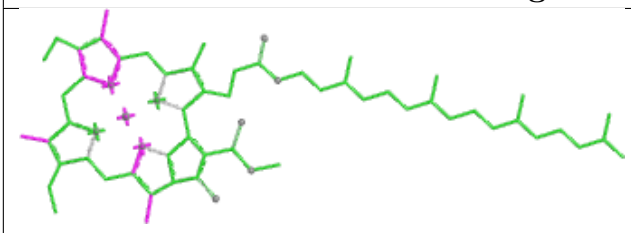


Torsions

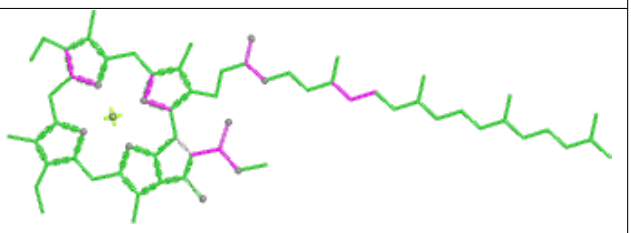


Rings

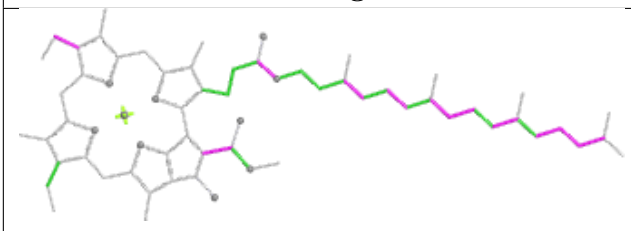
Ligand CLA 2 810



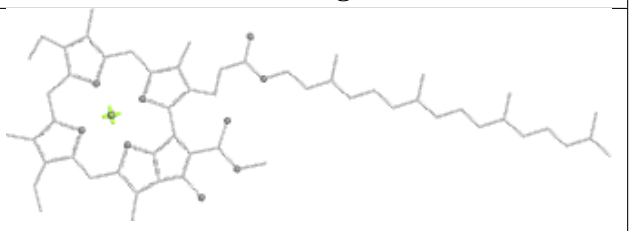
Bond lengths



Bond angles

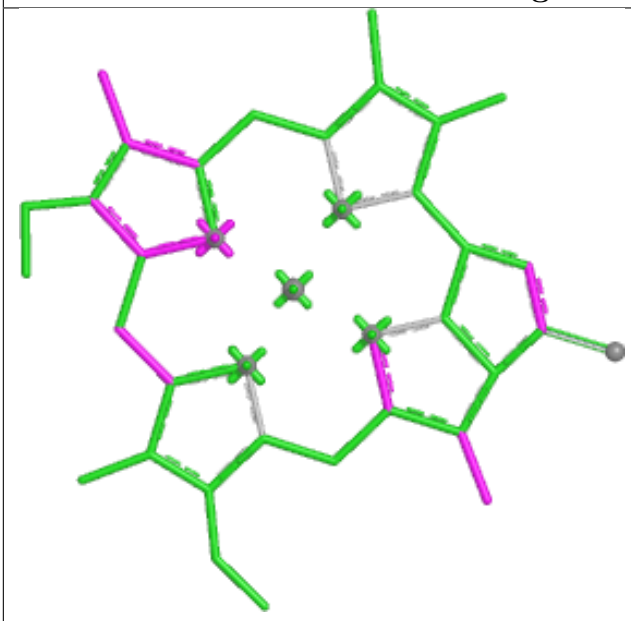


Torsions

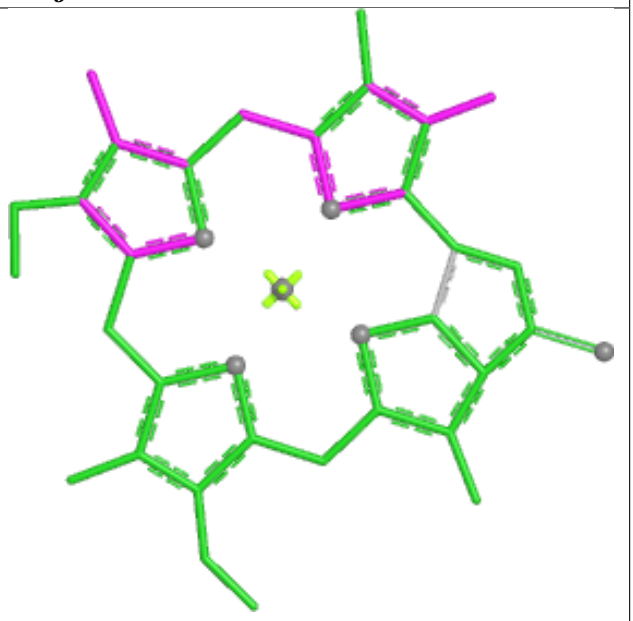


Rings

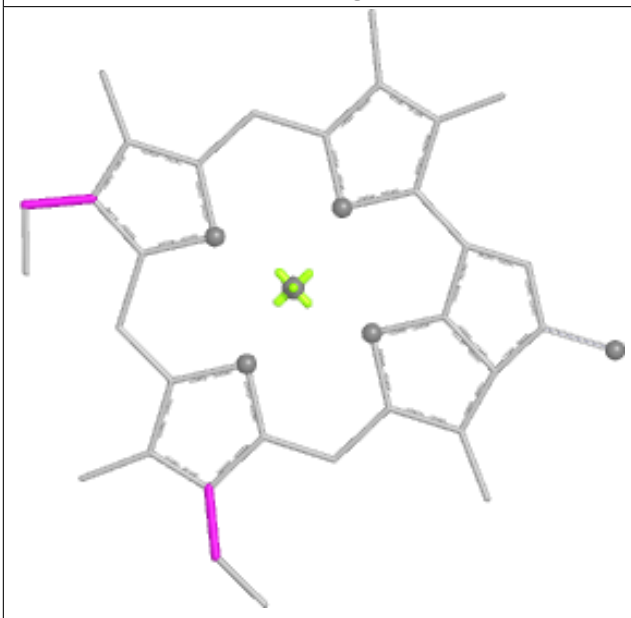
Ligand CLA j 102



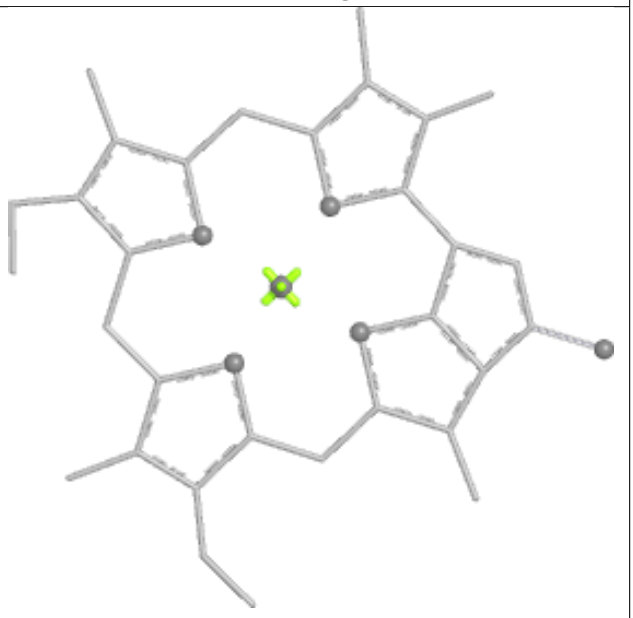
Bond lengths



Bond angles

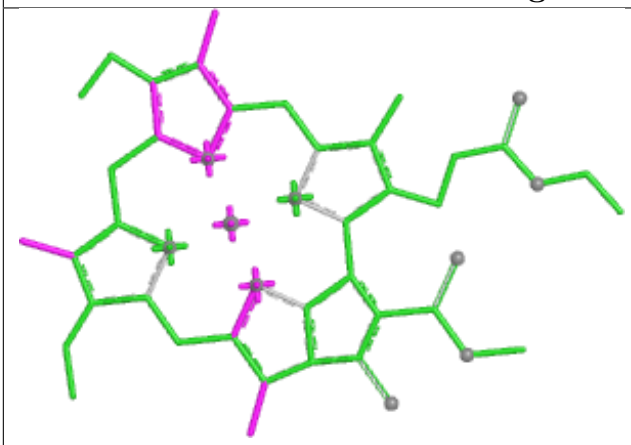


Torsions

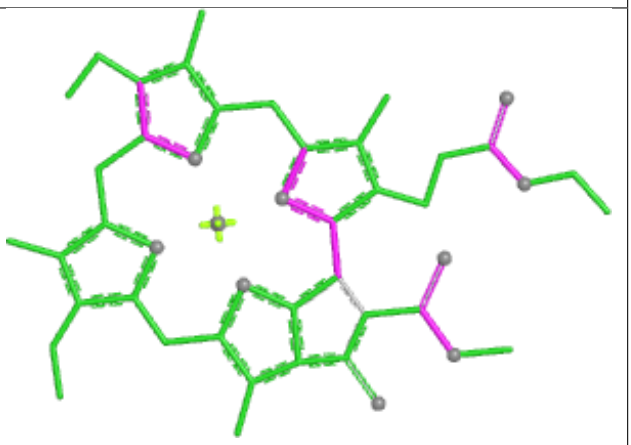


Rings

Ligand CLA a 841



Bond lengths



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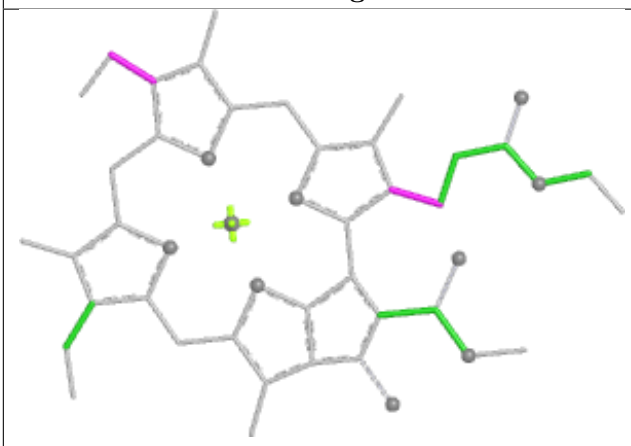
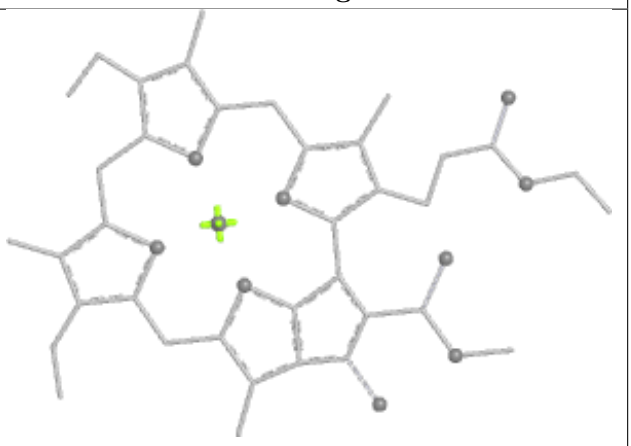
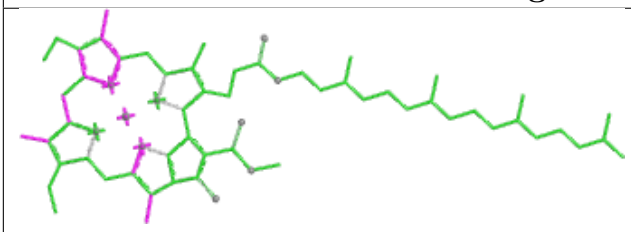


Torsions



Rings

Ligand CLA 2 812



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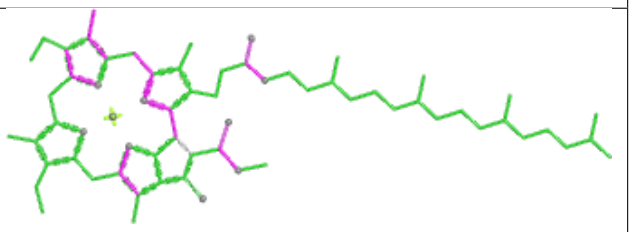

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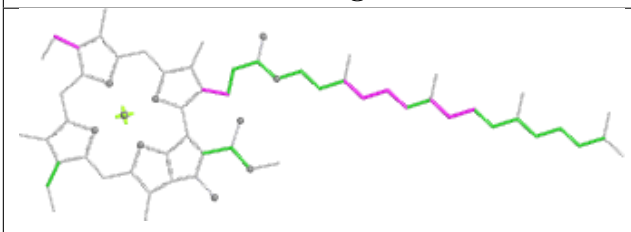
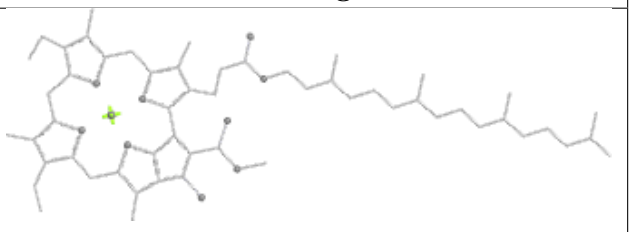
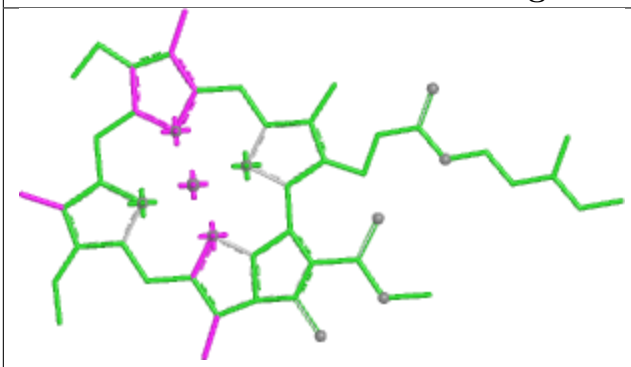


Torsions



Rings

Ligand CLA 1 841



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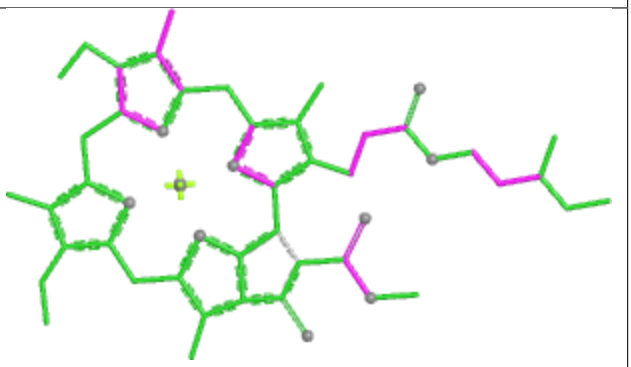
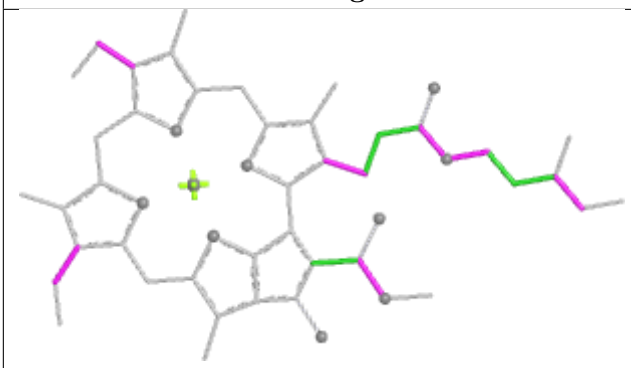


Bond angles



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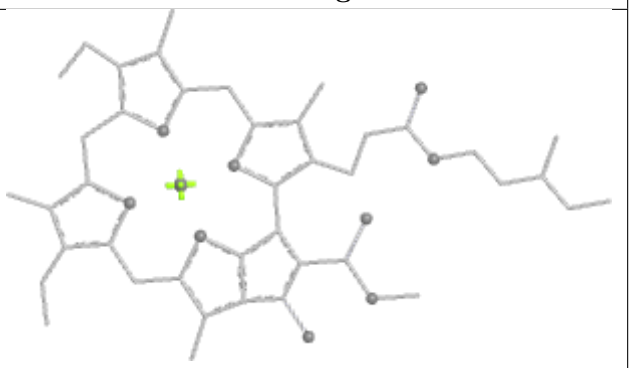
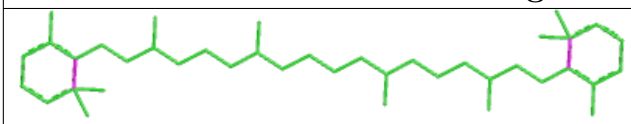


Rings

Ligand BCR a 848



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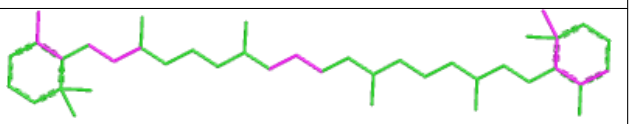
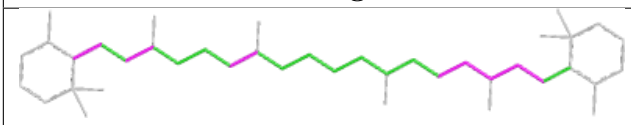


Bond angles



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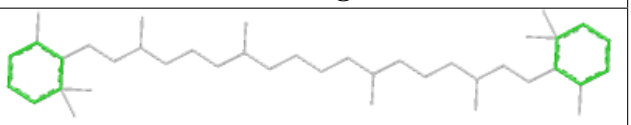
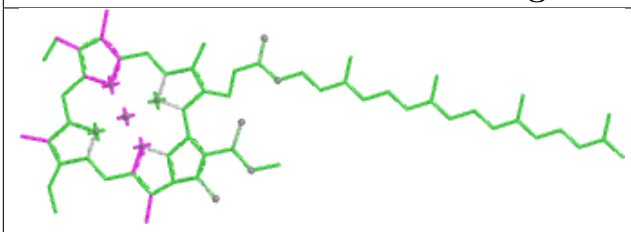


Rings

Ligand CLA 1 804



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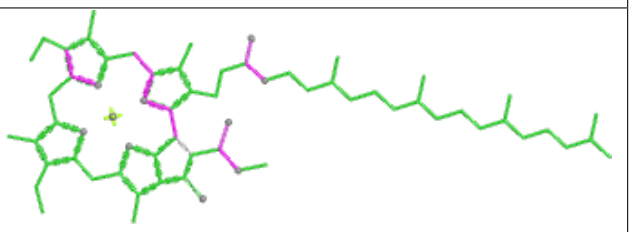
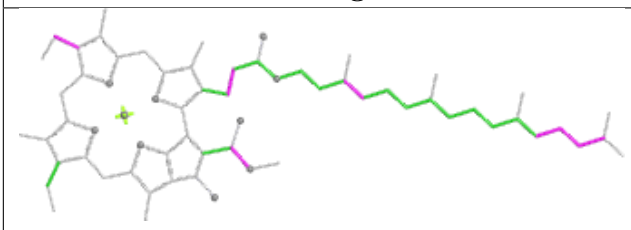


Bond angles



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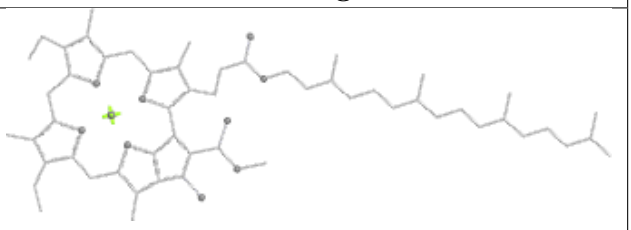
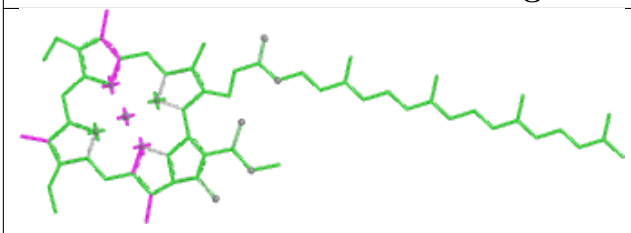


Rings

Ligand CLA A 829



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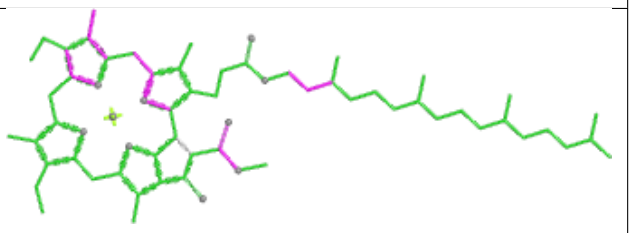
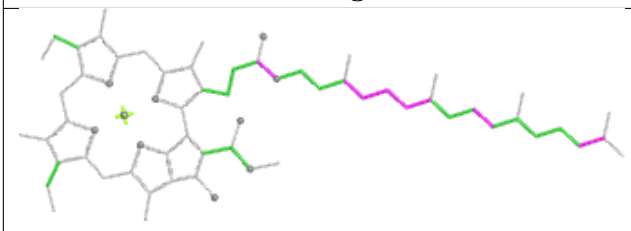


Bond angles



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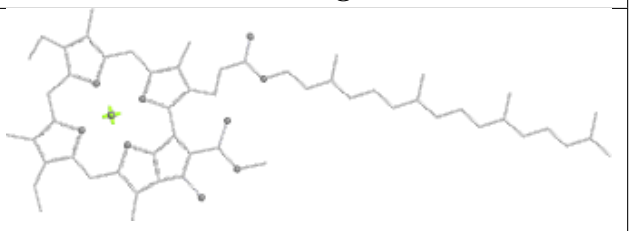
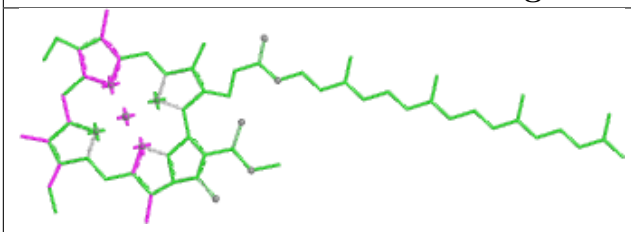


Rings

Ligand CLA B 809



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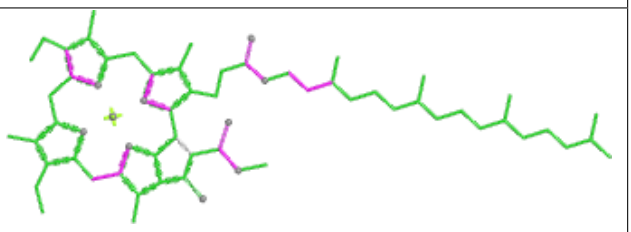

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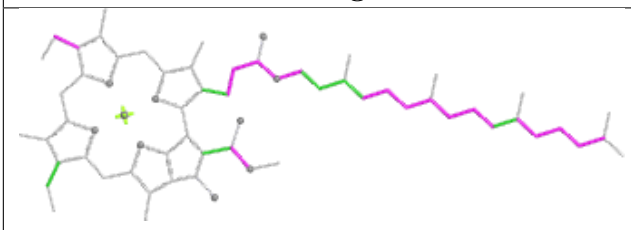

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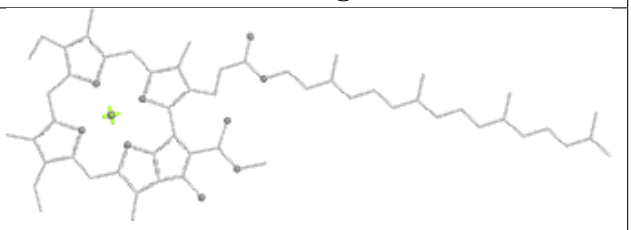
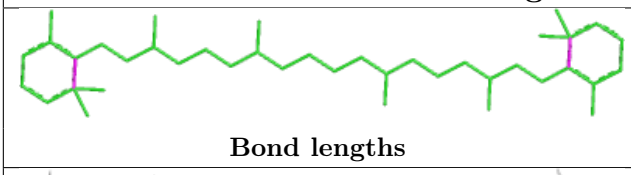


Rings

Ligand BCR b 849



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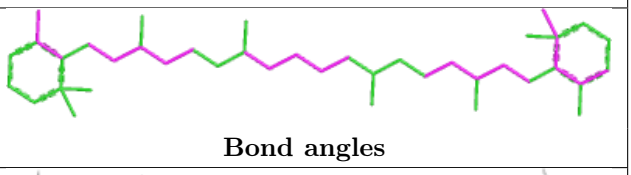

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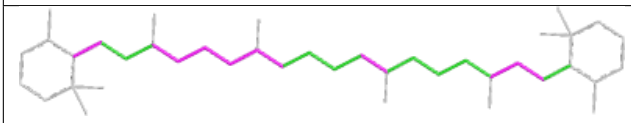

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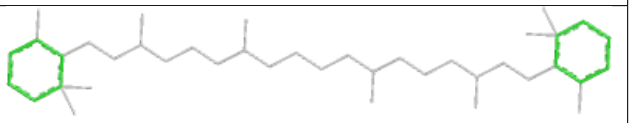
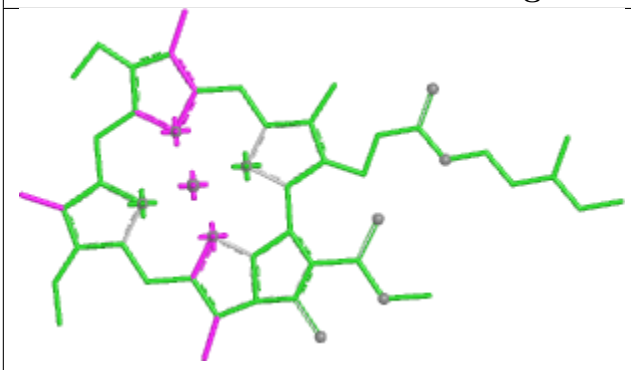


Rings

Ligand CLA A 838



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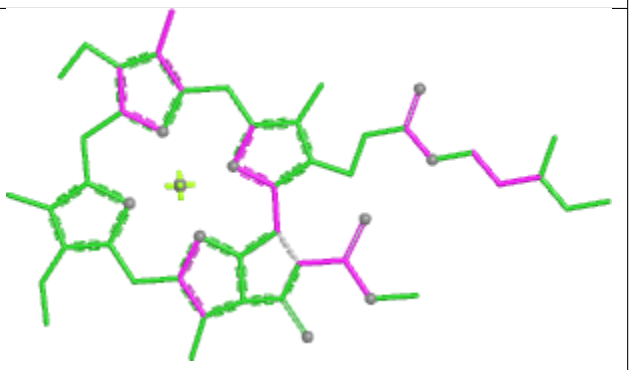
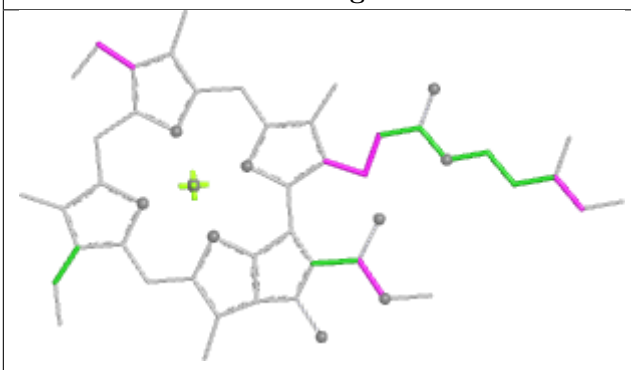


Bond angles



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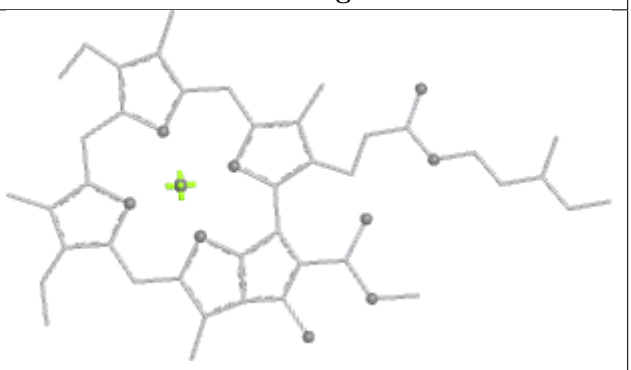
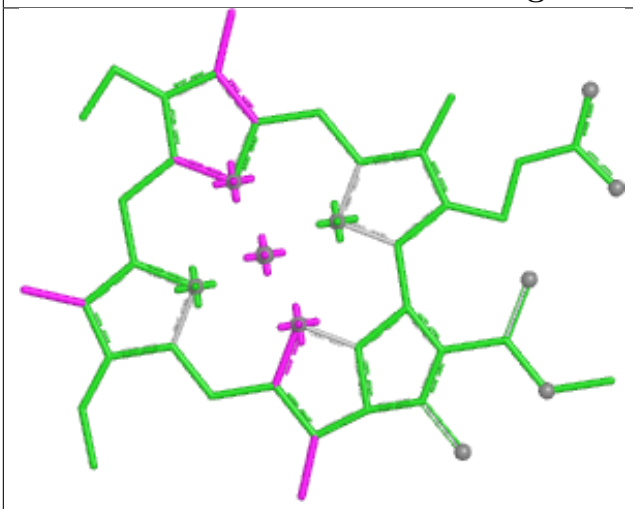


Rings

Ligand CLA b 813



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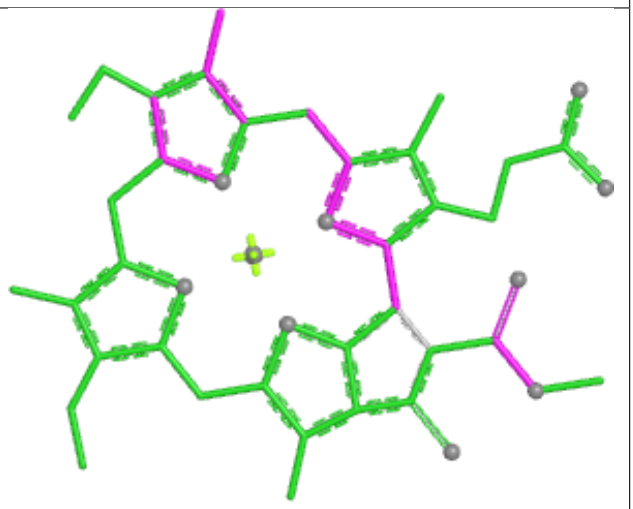
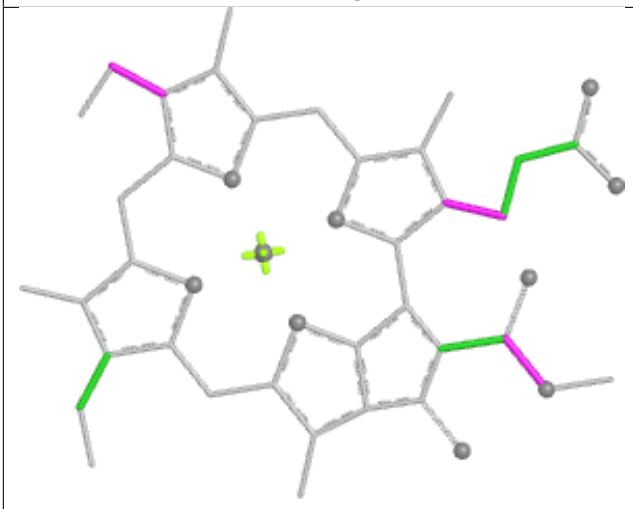


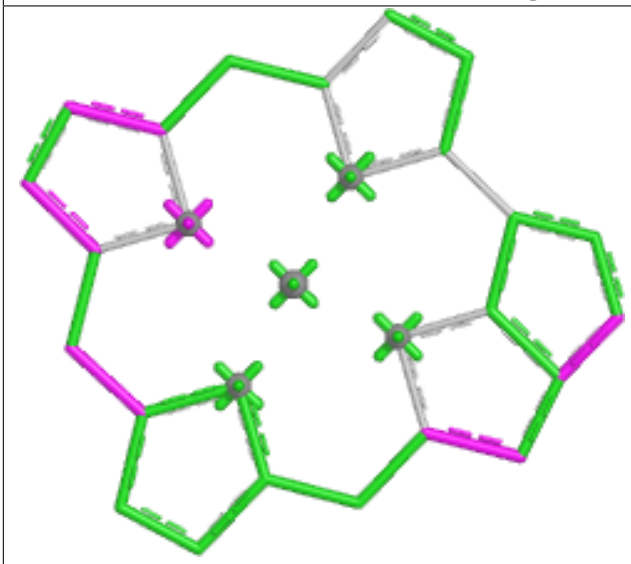
Bond angles



Torsions

Rings

Ligand CLA B 845



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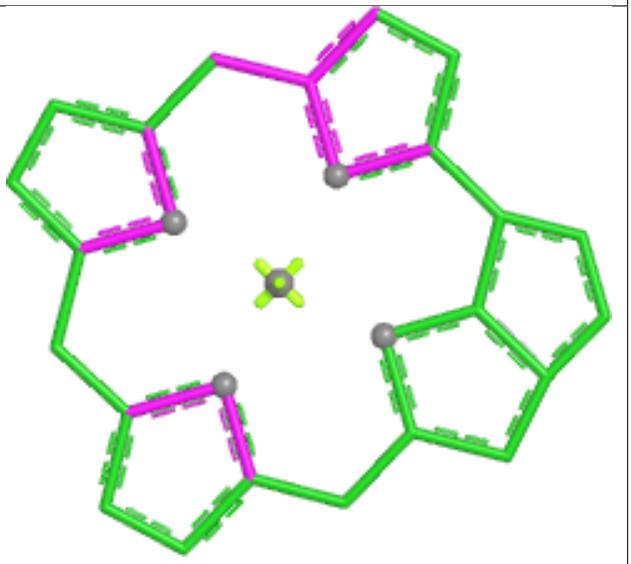
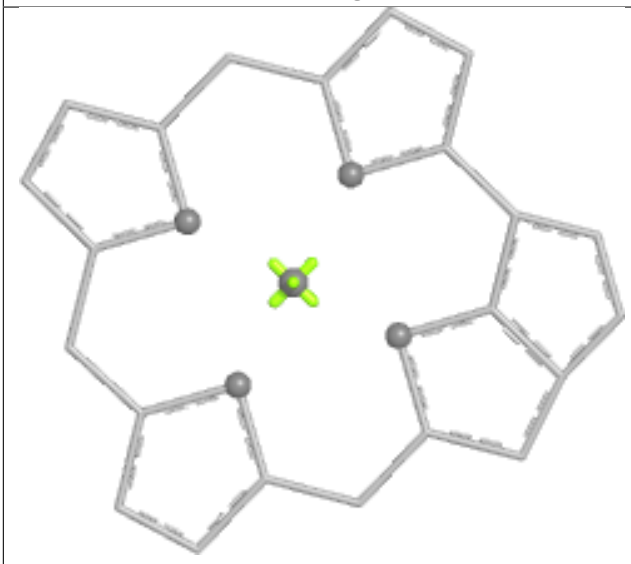
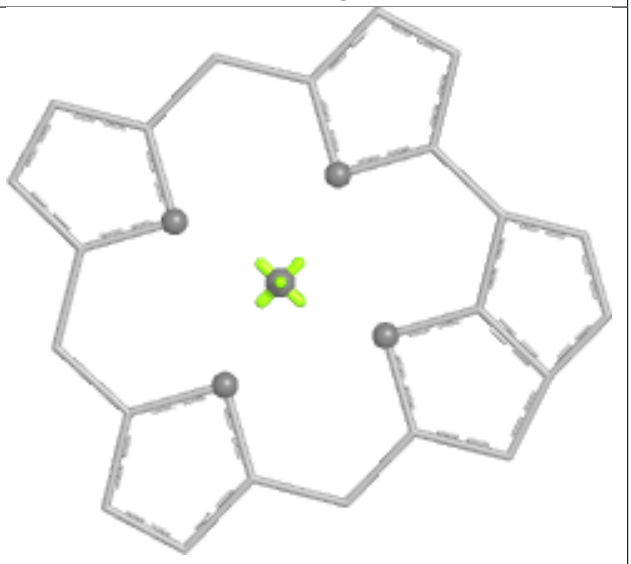


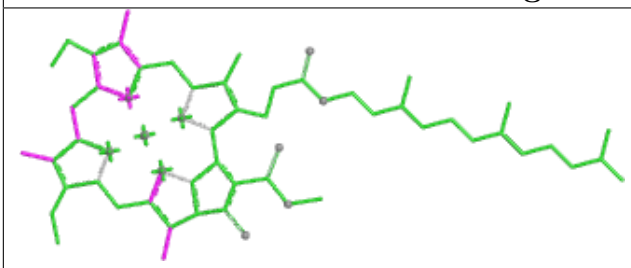
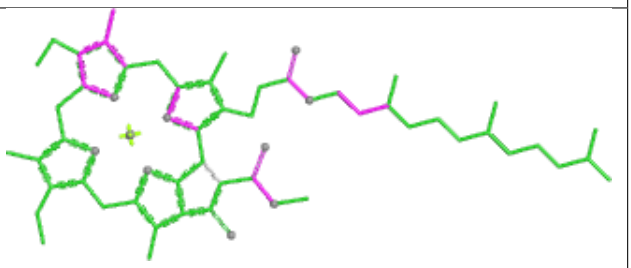
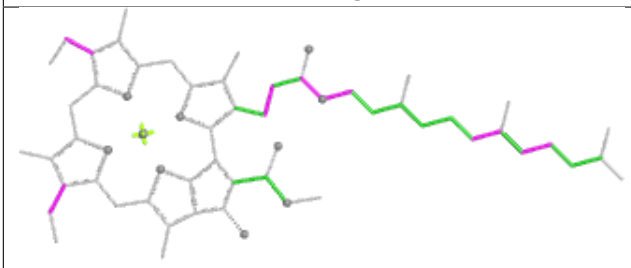
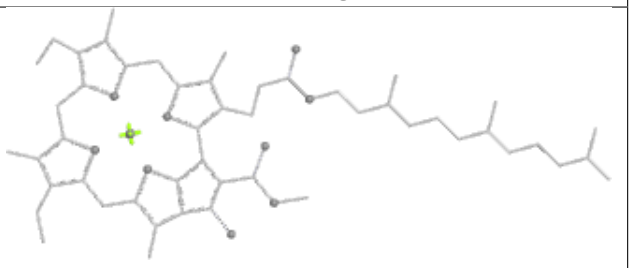
Bond angles

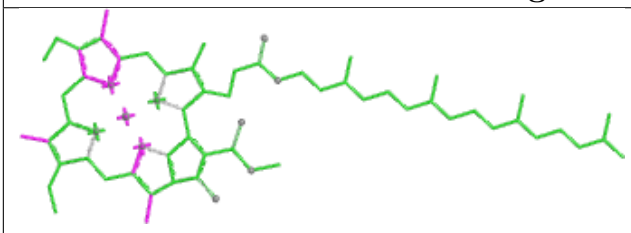
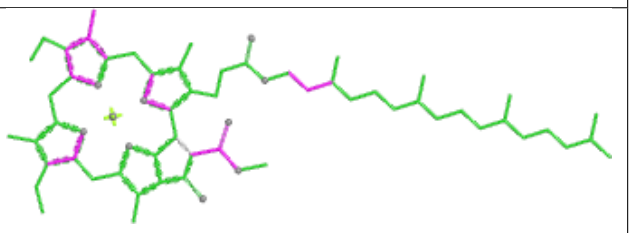
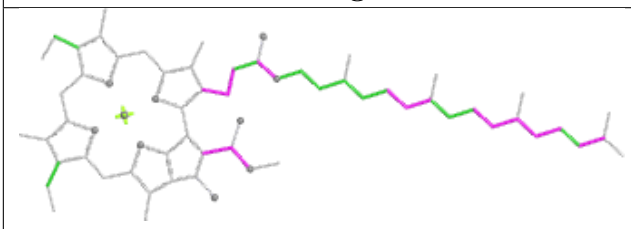
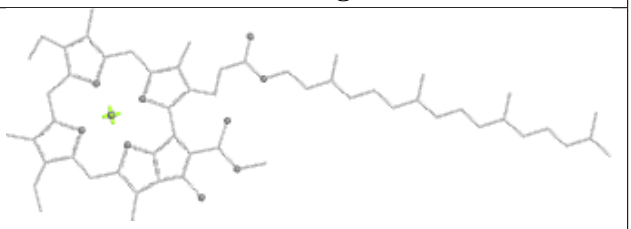


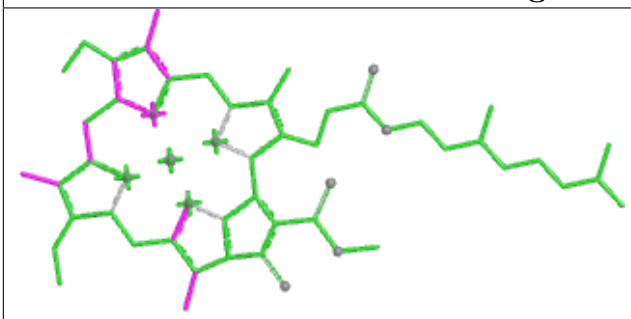
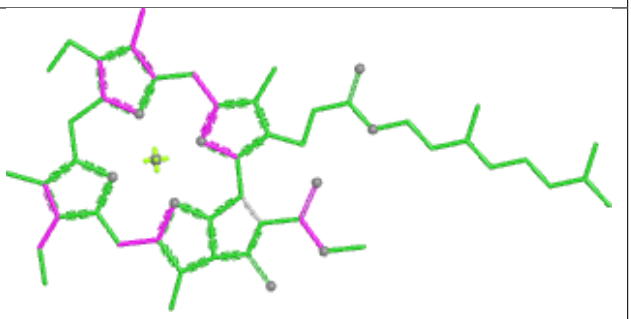
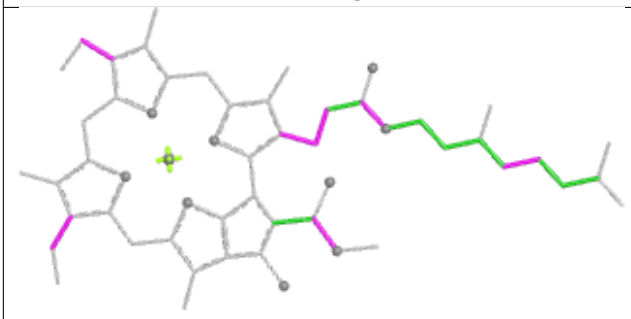
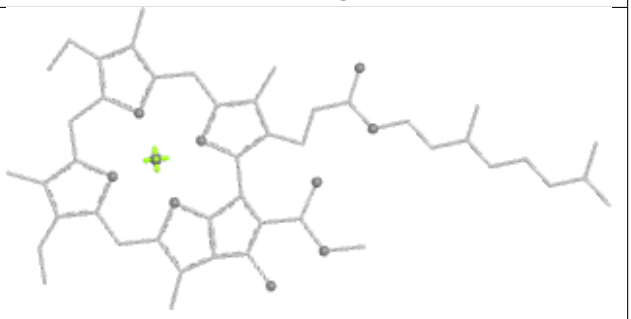
Torsions

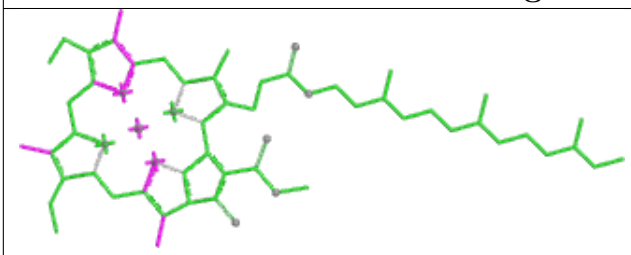
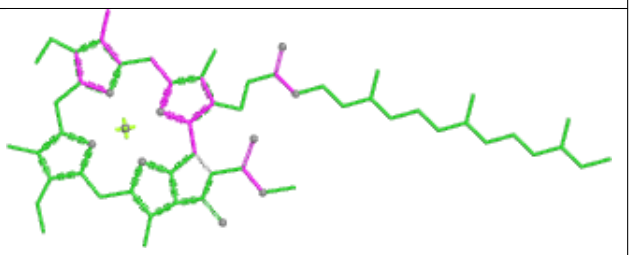
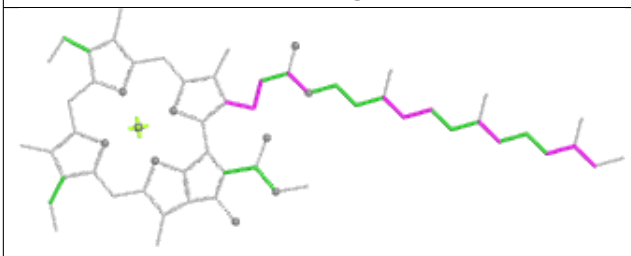
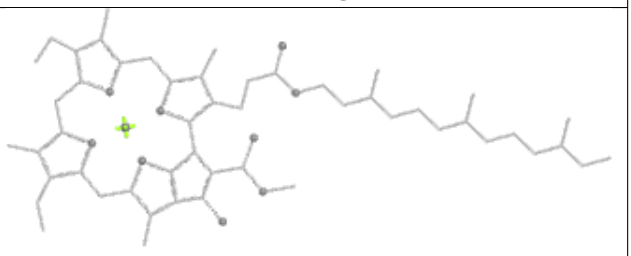


Rings

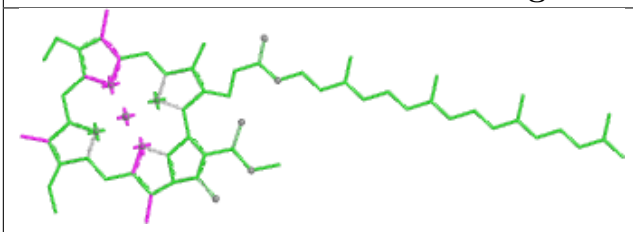
Ligand CLA A 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 833



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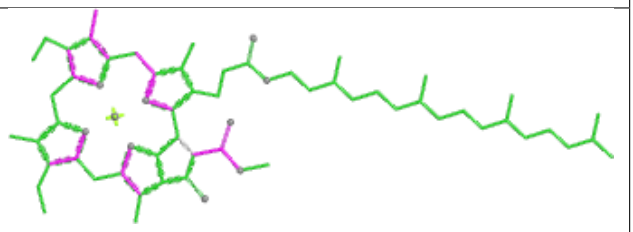
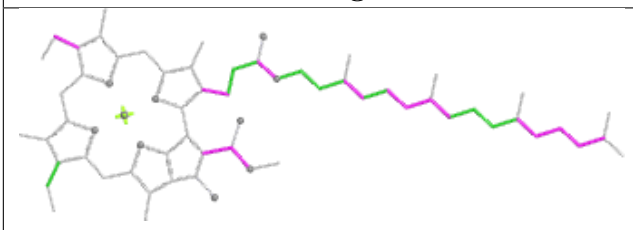
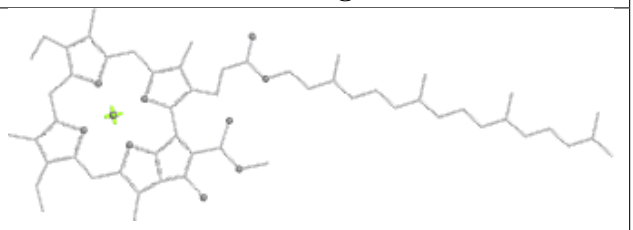


Bond angles

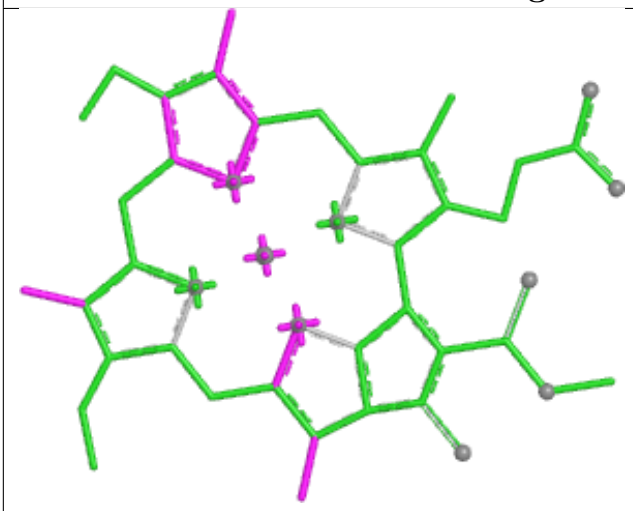


Torsions



Rings

Ligand CLA 1 811



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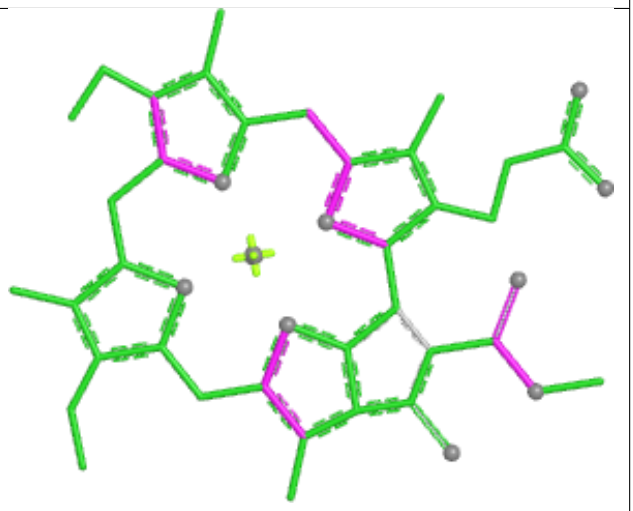

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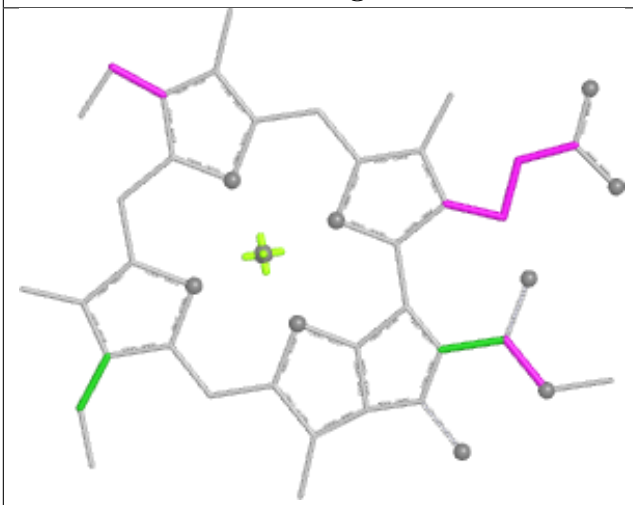
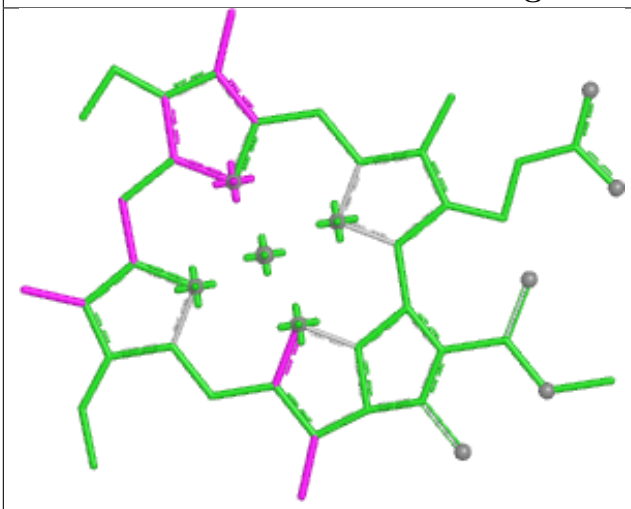


Torsions

Rings

Ligand CLA B 824



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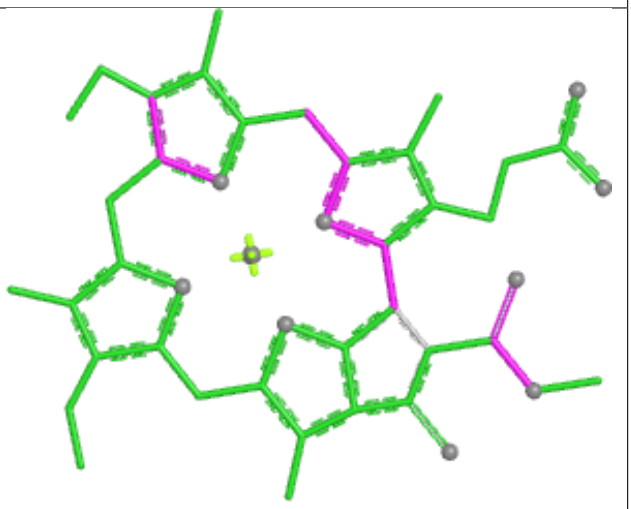
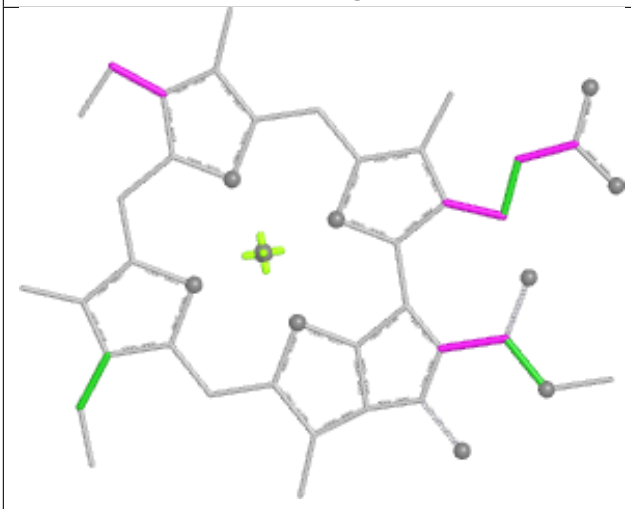


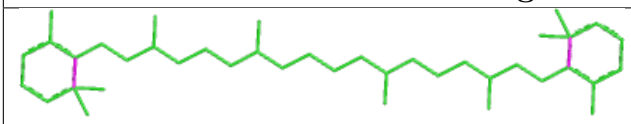
Bond angles



Torsions

Rings

Ligand BCR k 4004



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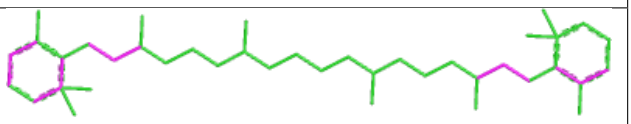

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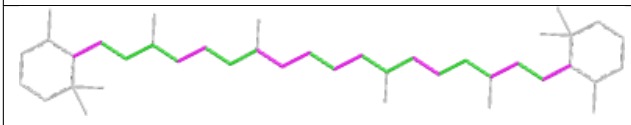

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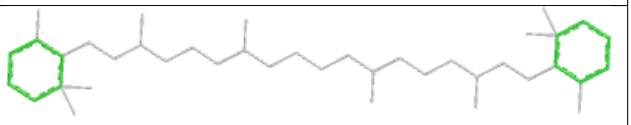
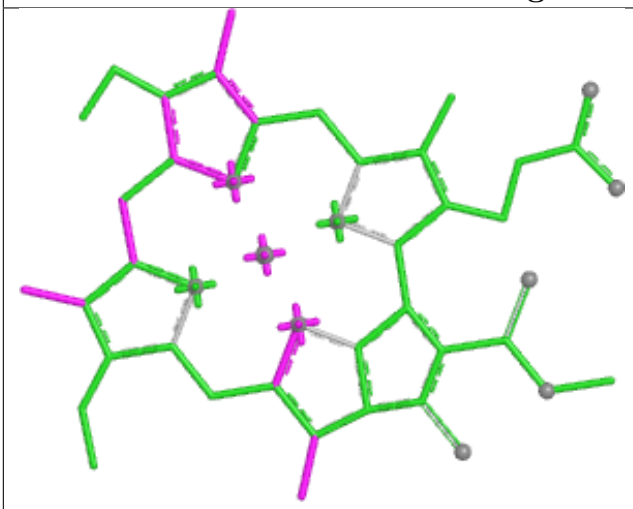


Rings

Ligand CLA b 814



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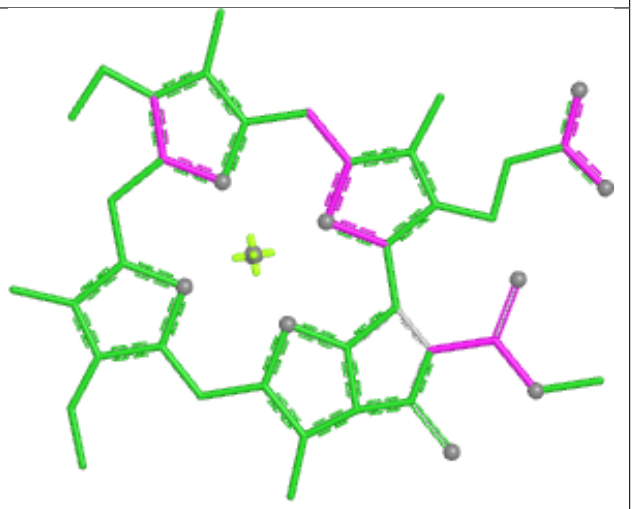

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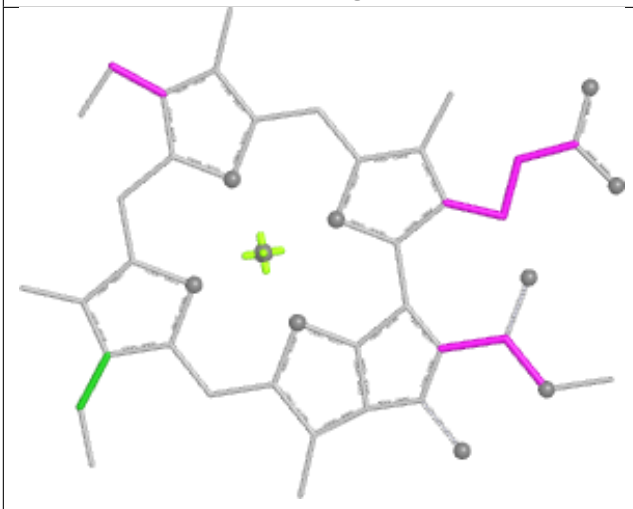
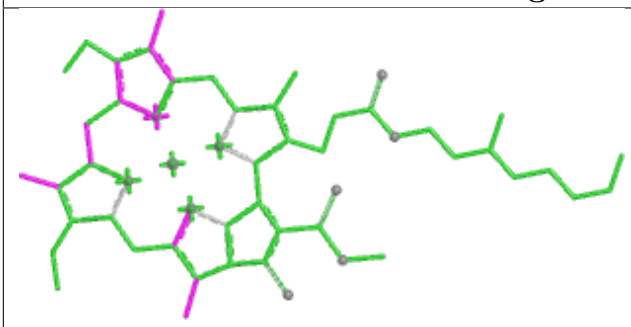


Torsions

Rings

Ligand CLA 2 806



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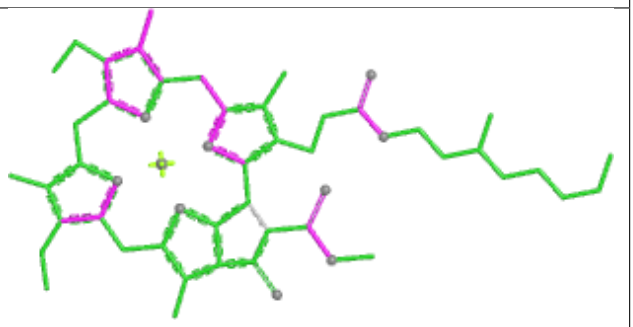

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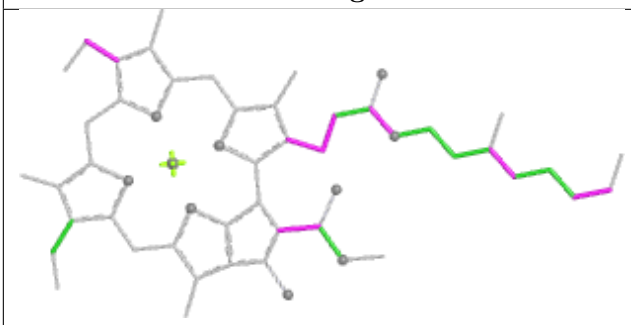

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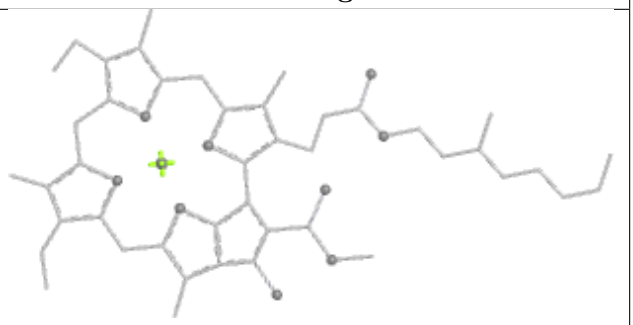
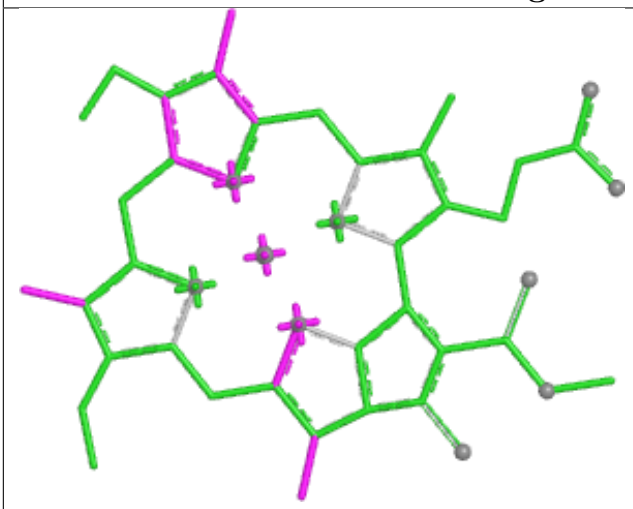


Rings

Ligand CLA 1 844



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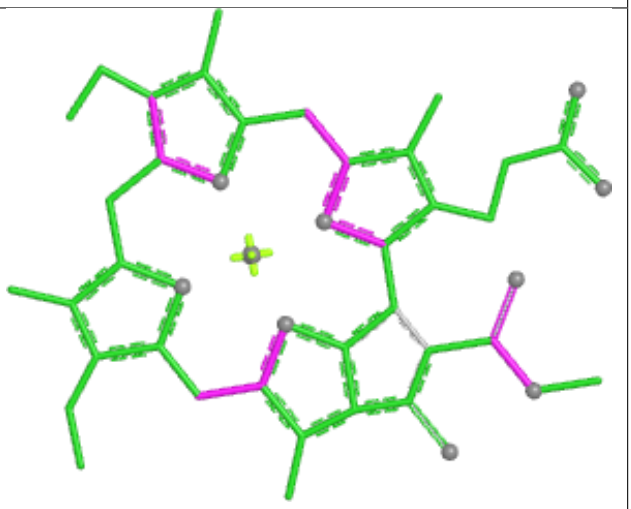
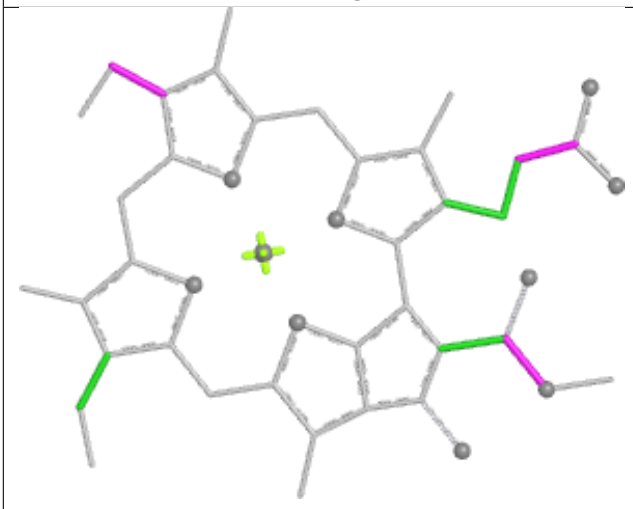


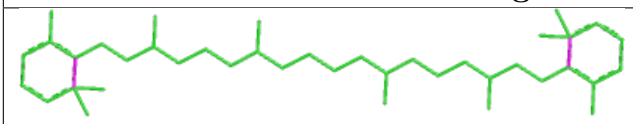
Bond angles



Torsions

Rings

Ligand BCR K 4005



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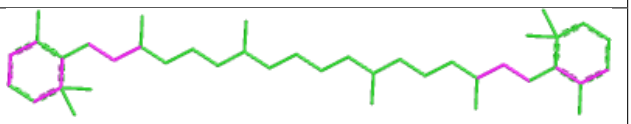

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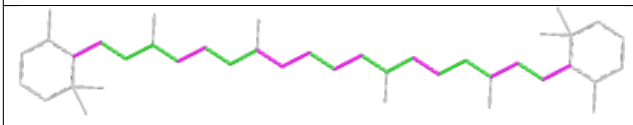
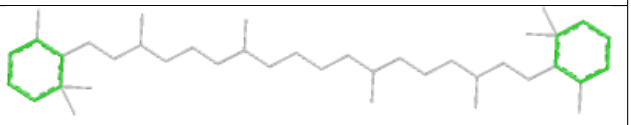
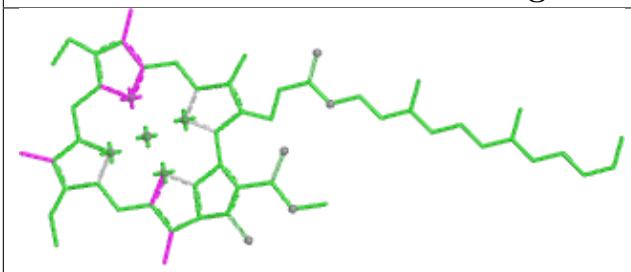
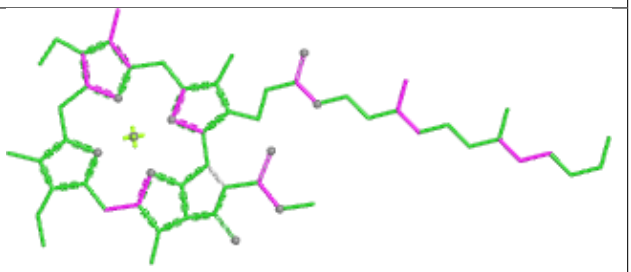
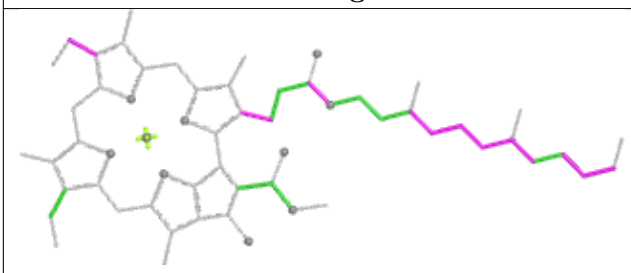
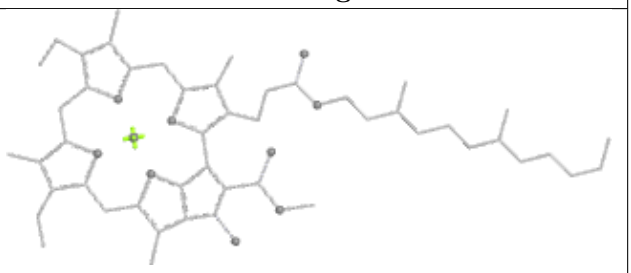
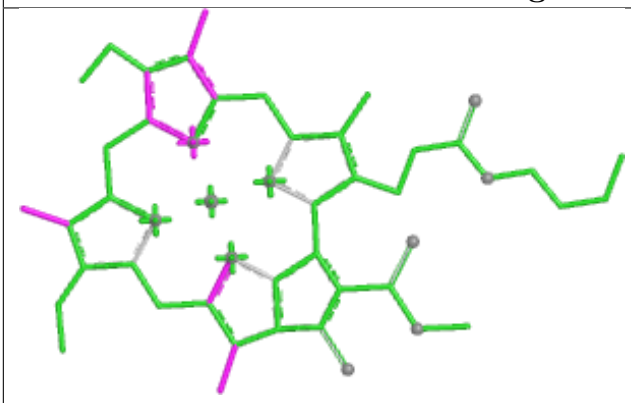
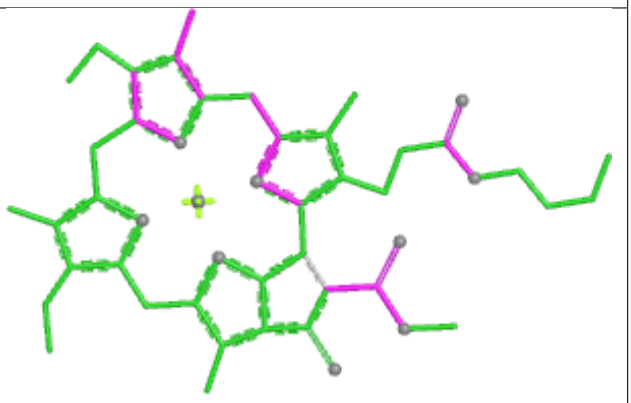
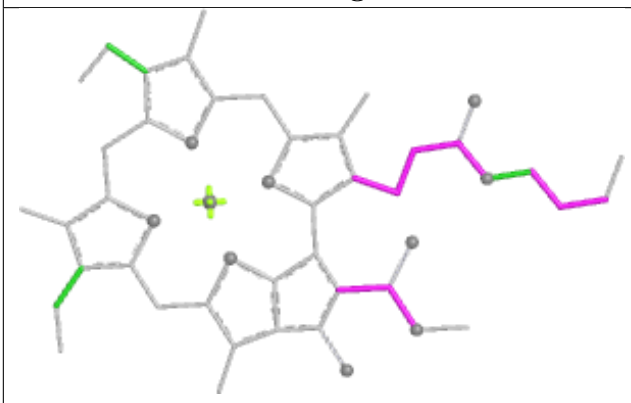
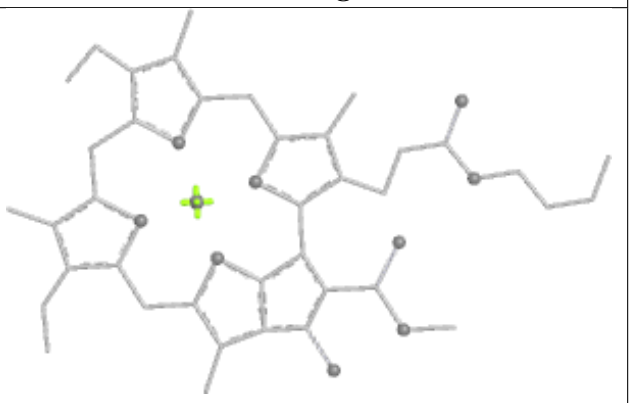


Torsions

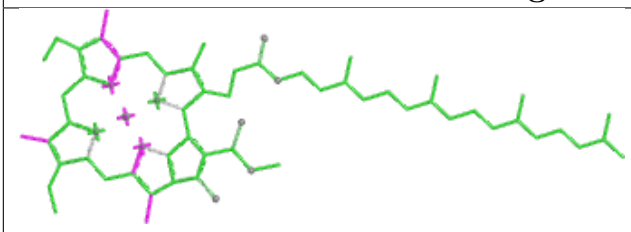


Rings

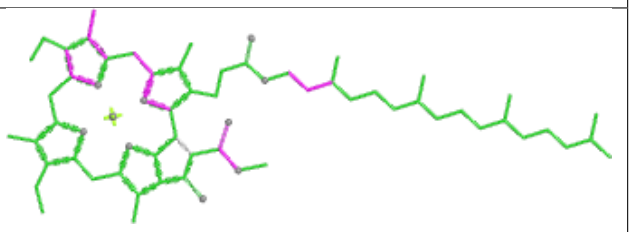
Ligand CLA 1 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

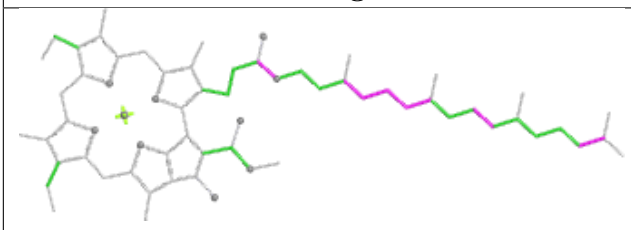
Ligand CLA a 830



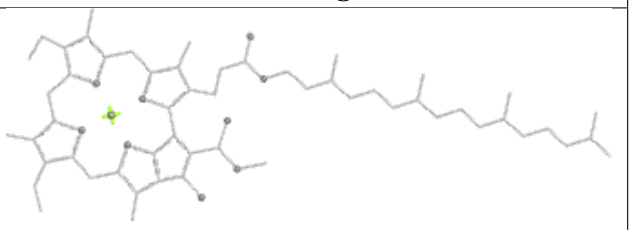
Bond lengths



Bond angles

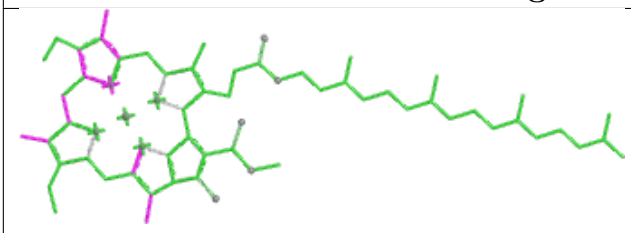


Torsions



Rings

Ligand CLA a 811



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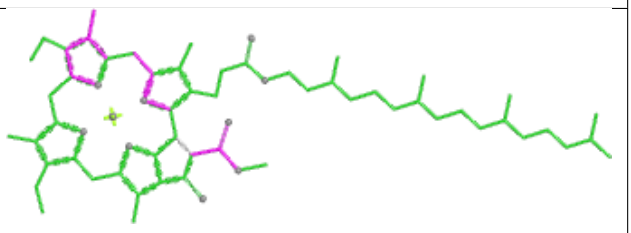
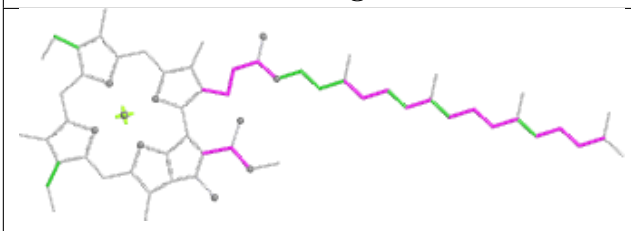


Bond angles



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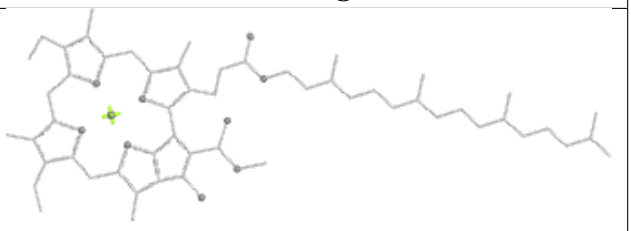
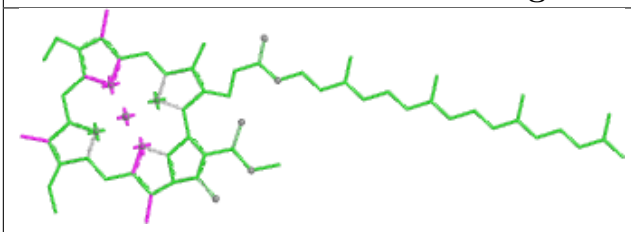
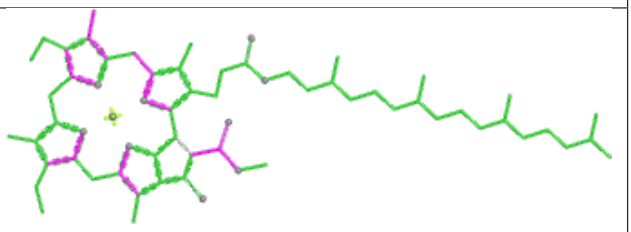


Rings

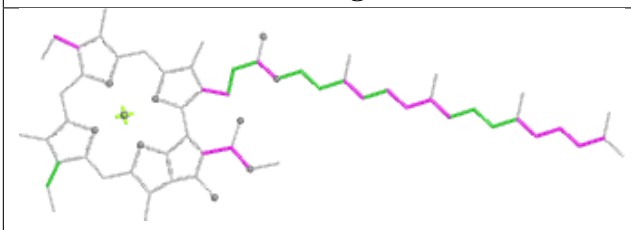
Ligand CLA 1 831



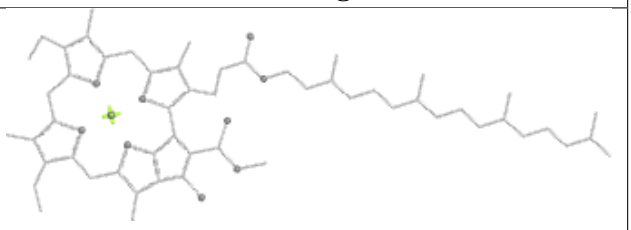
Bond lengths



Bond angles

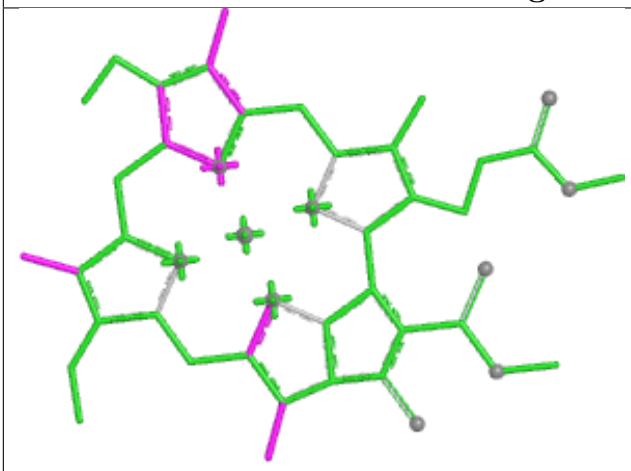


Torsions

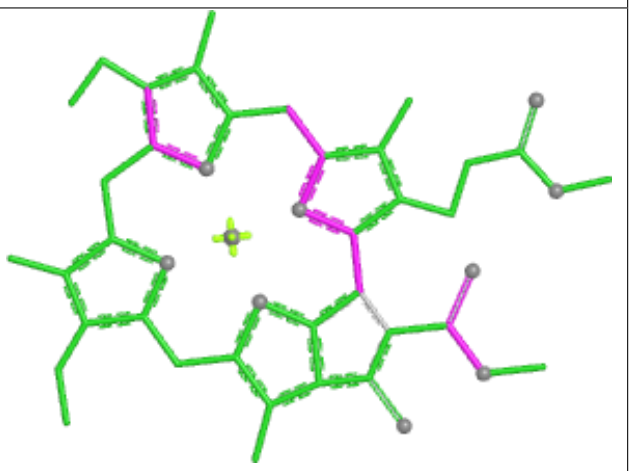


Rings

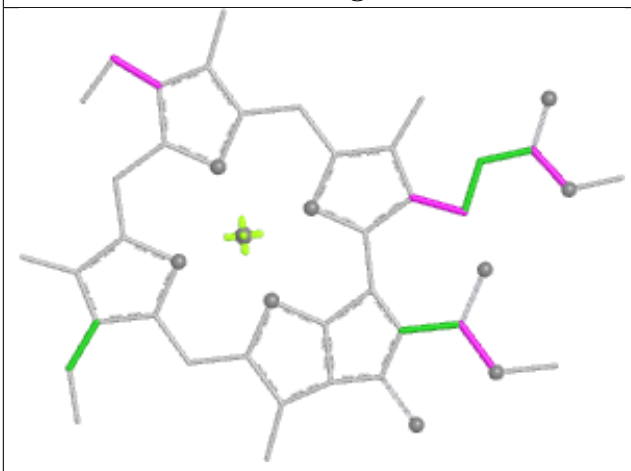
Ligand CLA a 819



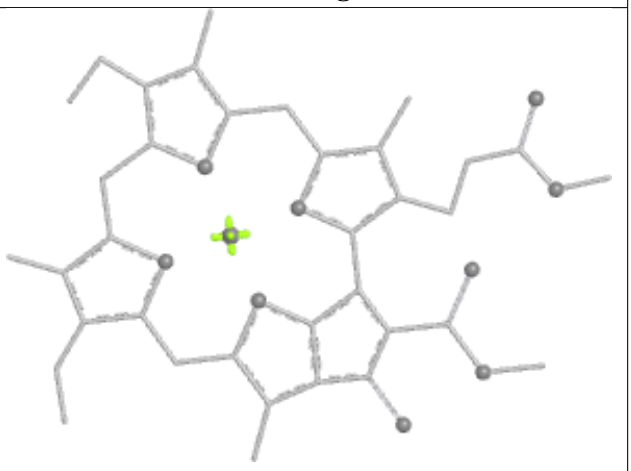
Bond lengths



Bond angles

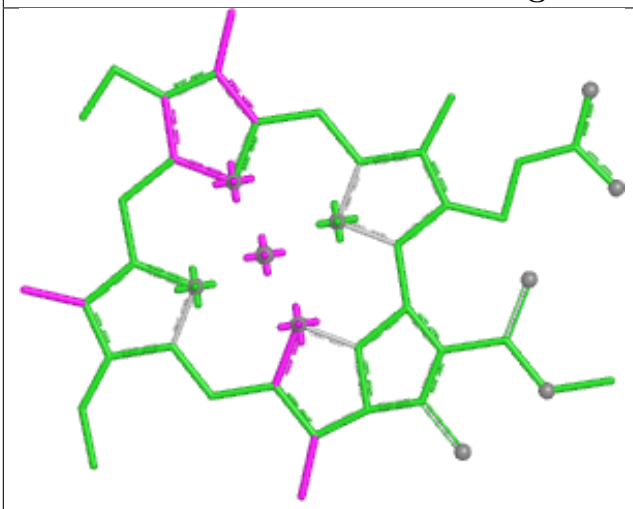


Torsions



Rings

Ligand CLA a 844



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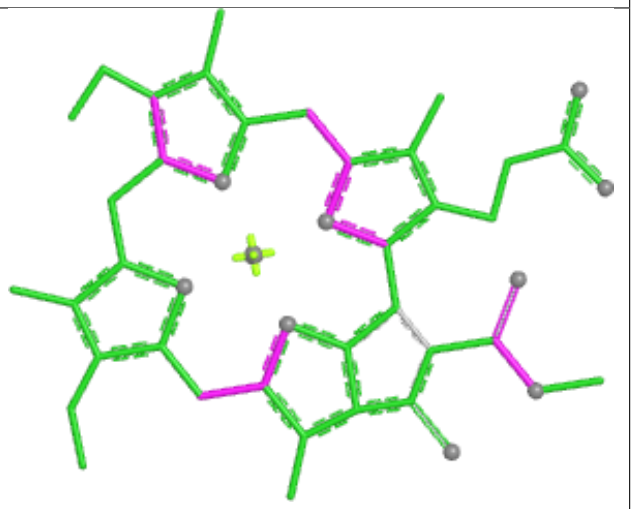
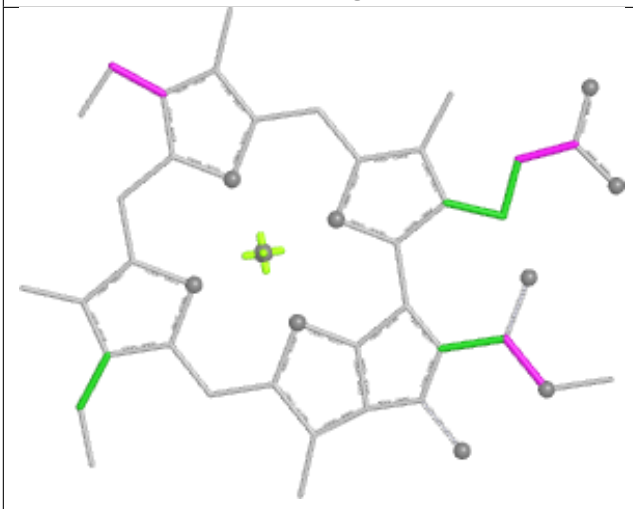


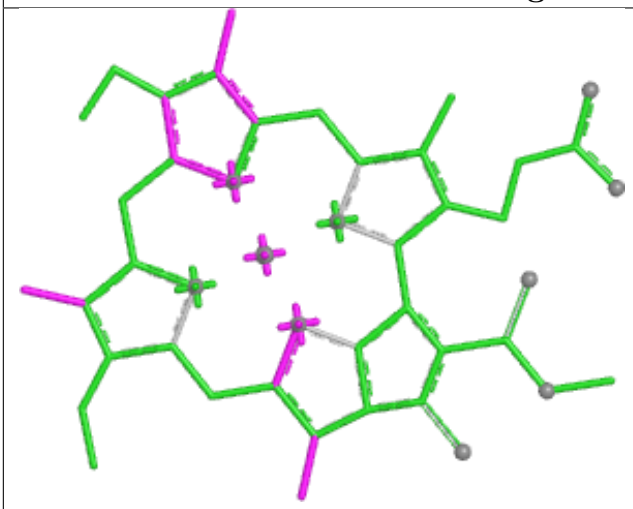
Bond angles



Torsions

Rings

Ligand CLA b 824



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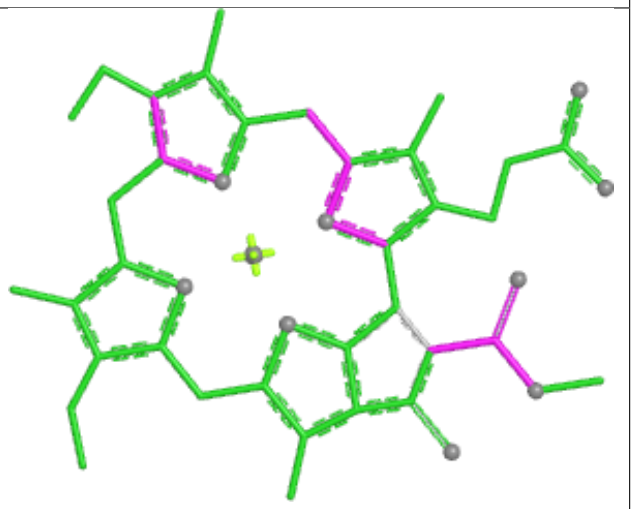
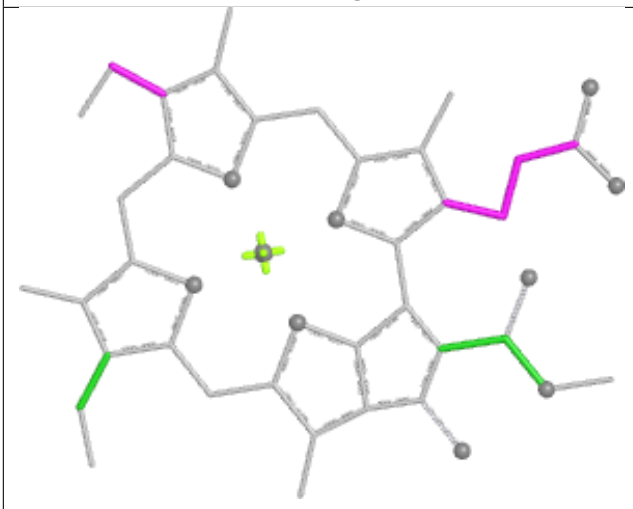


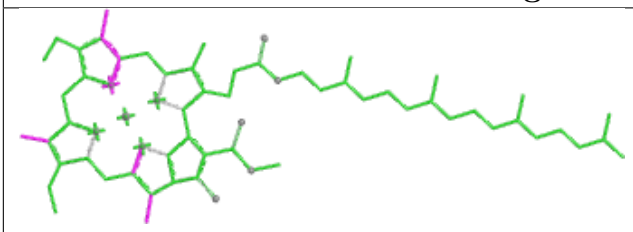
Bond angles



Torsions

Rings

Ligand CLA A 835



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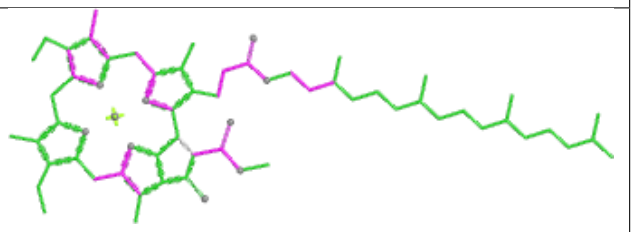
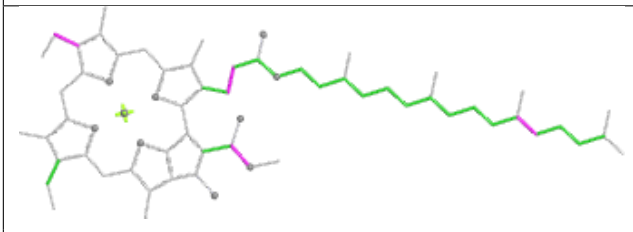
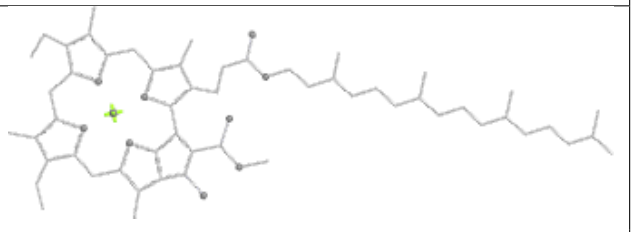


Bond angles

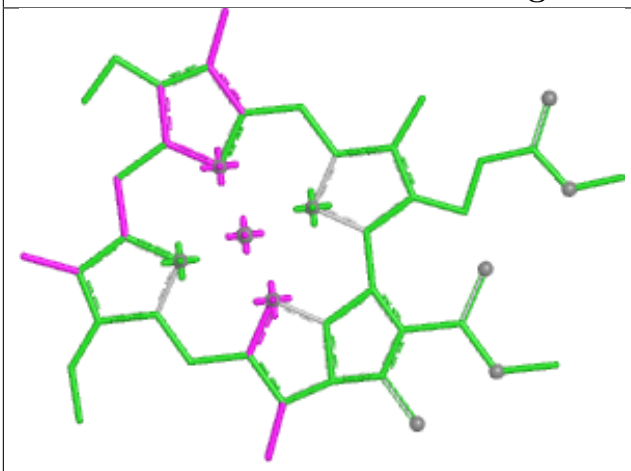


Torsions

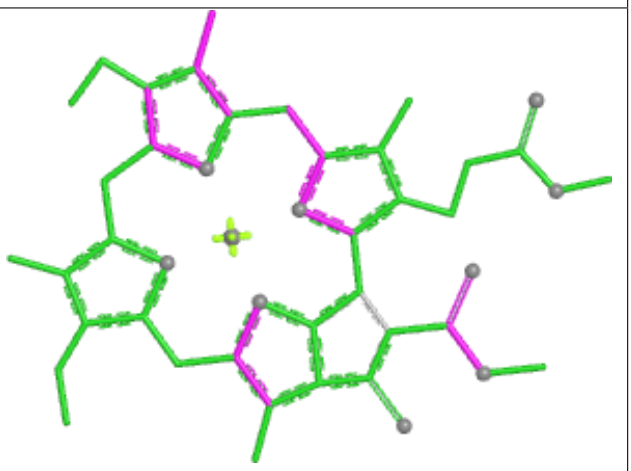


Rings

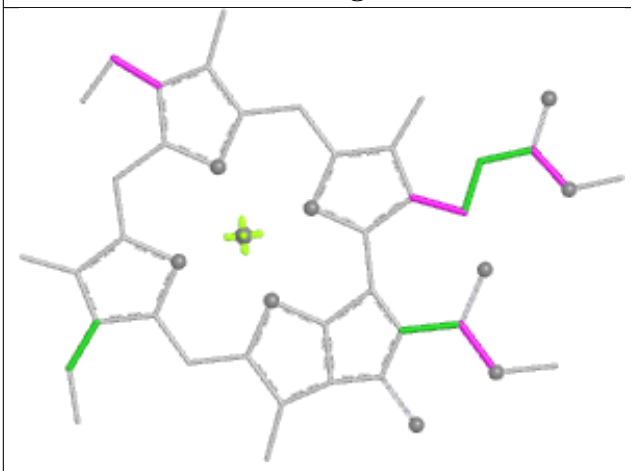
Ligand CLA a 810



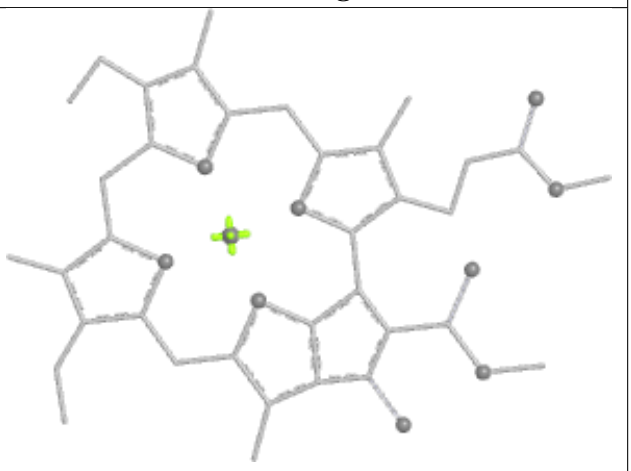
Bond lengths



Bond angles

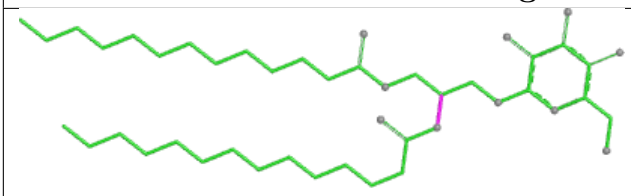


Torsions



Rings

Ligand LMG A 852



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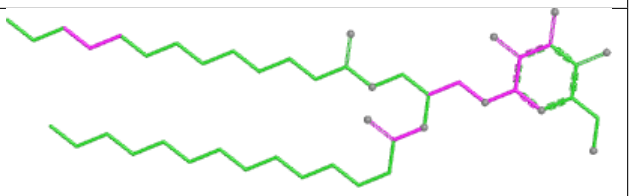
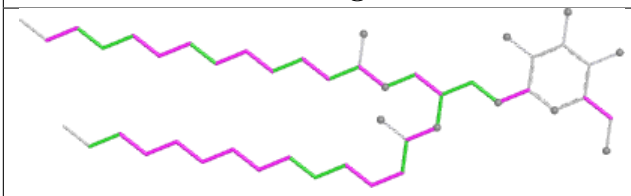


Bond angles



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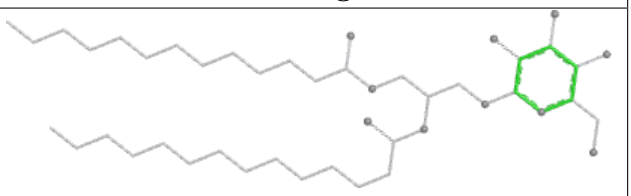
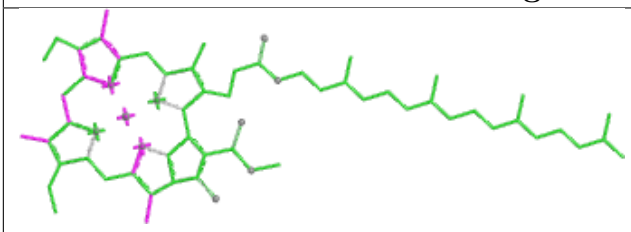


Rings

Ligand CLA l 4204



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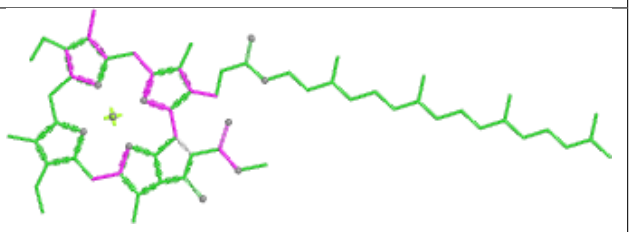
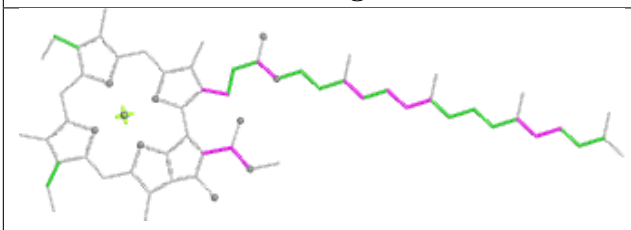


Bond angles



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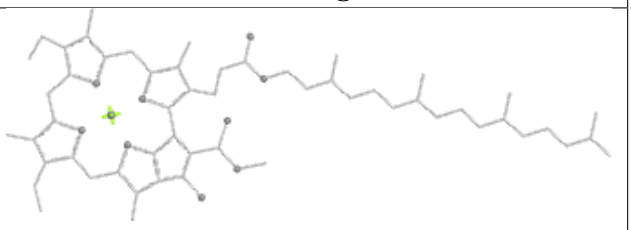
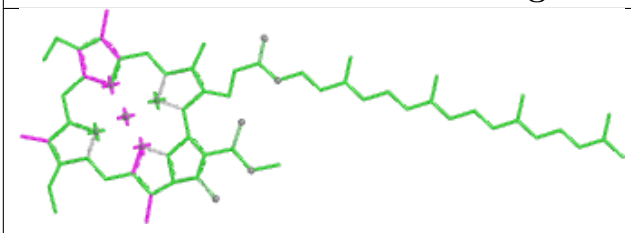
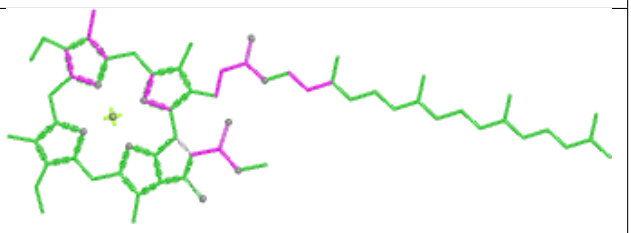


Rings

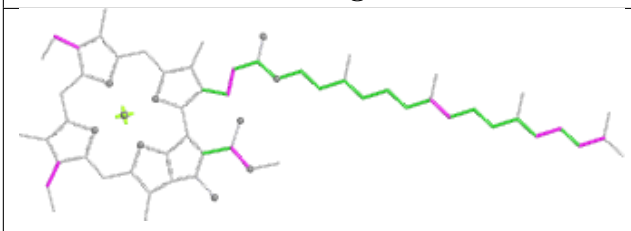
Ligand CLA 1 840



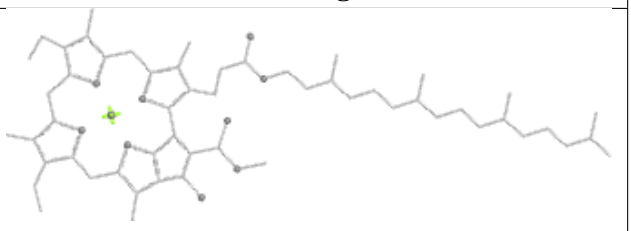
Bond lengths



Bond angles

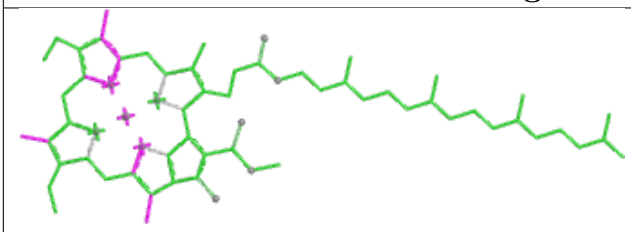


Torsions

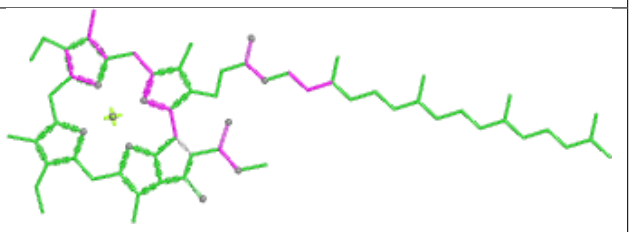


Rings

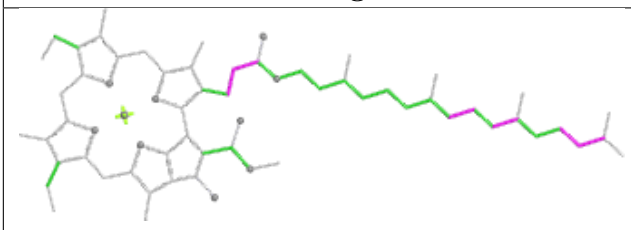
Ligand CLA A 831



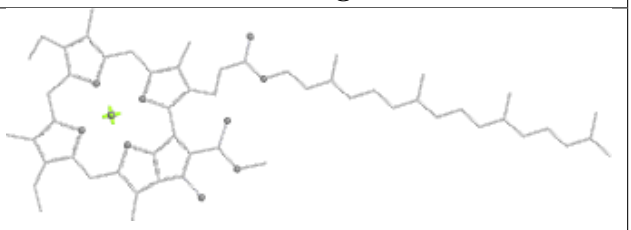
Bond lengths



Bond angles

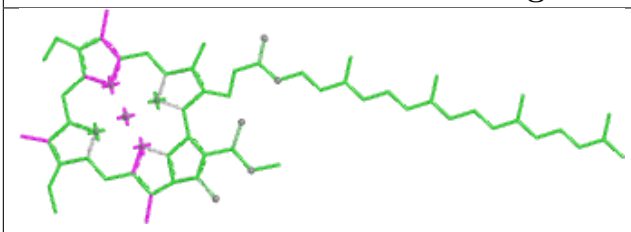


Torsions



Rings

Ligand CLA b 830



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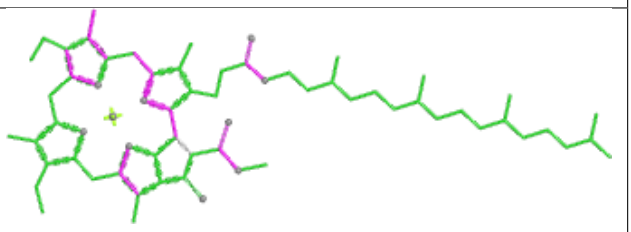

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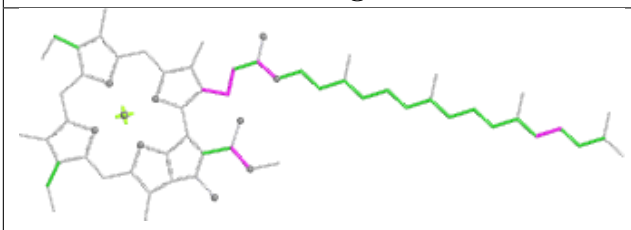
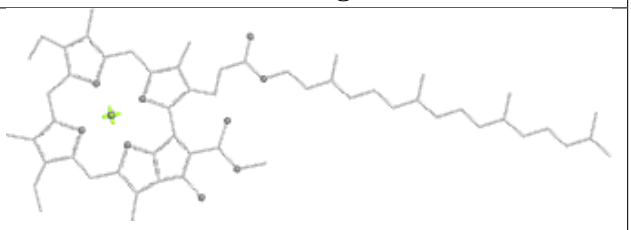


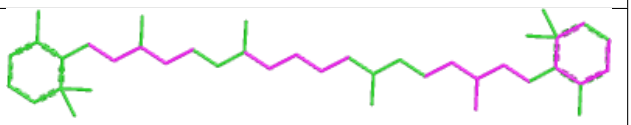
Torsions



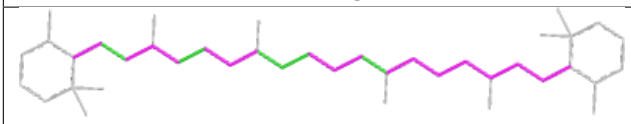
Rings

Ligand BCR B 851

Bond lengths



Bond angles



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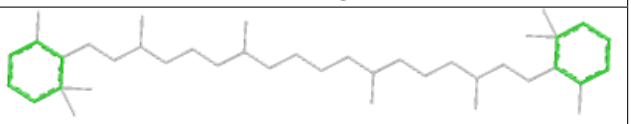
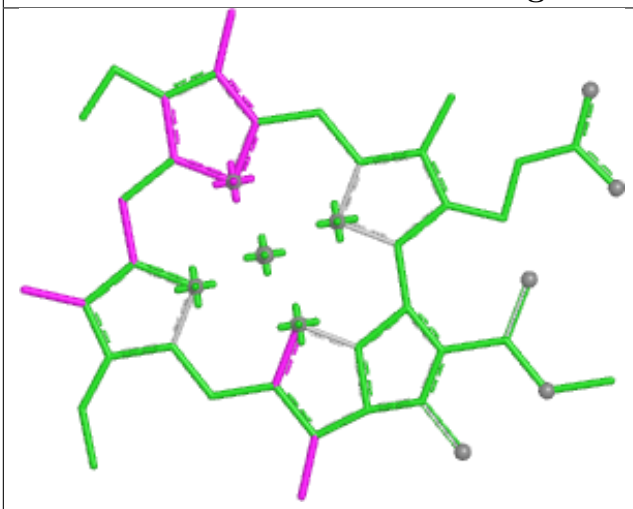


Rings

Ligand CLA b 817



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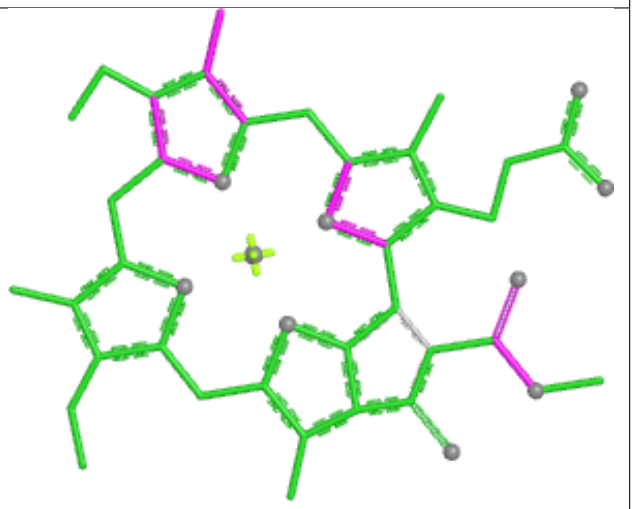
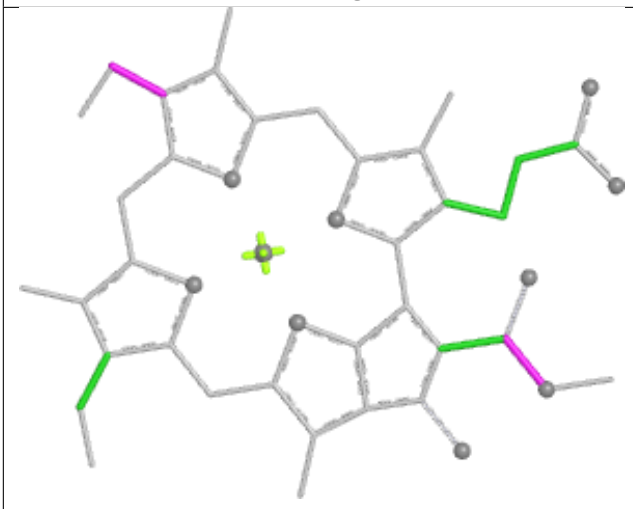


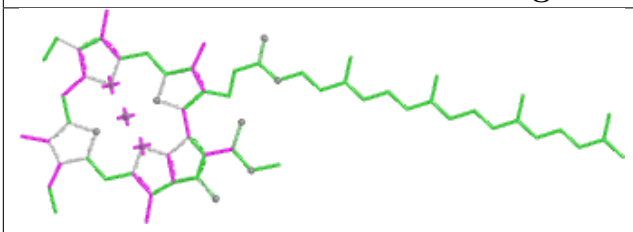
Bond angles



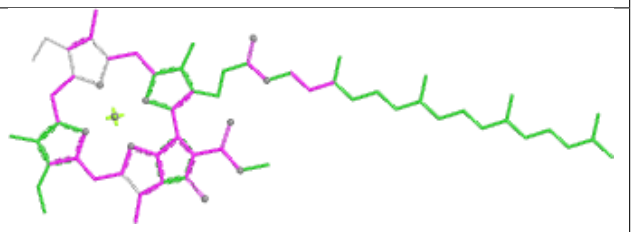
Torsions

Rings

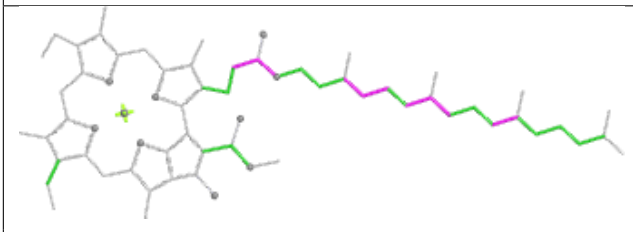
Ligand CL0 1 803



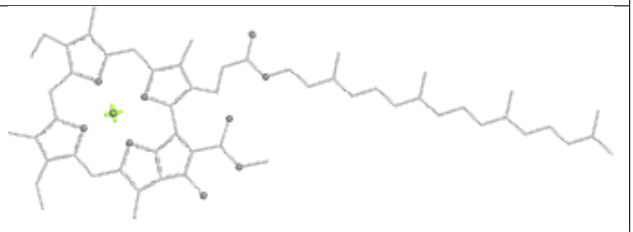
Bond lengths



Bond angles

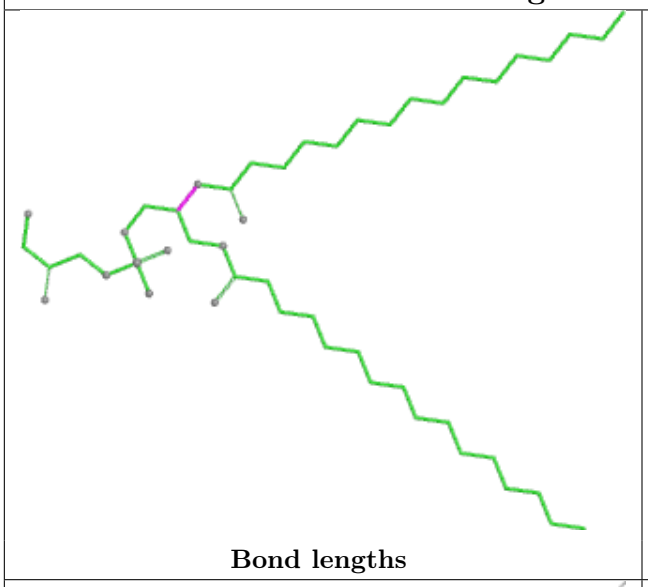


Torsions



Rings

Ligand LHG 1 801



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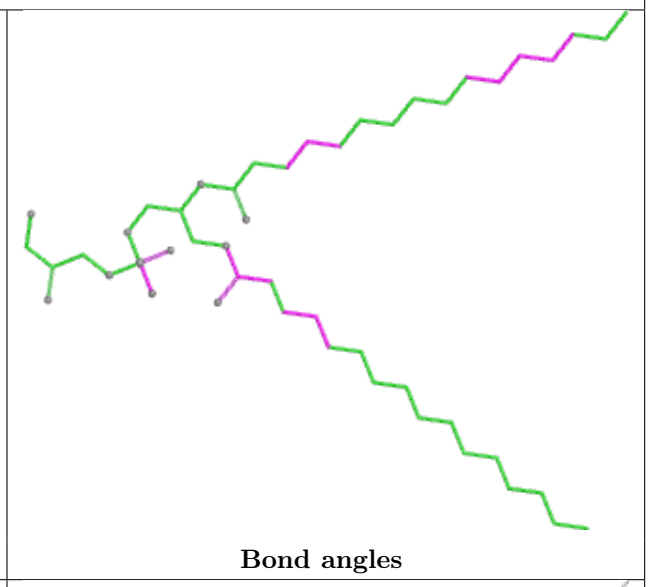
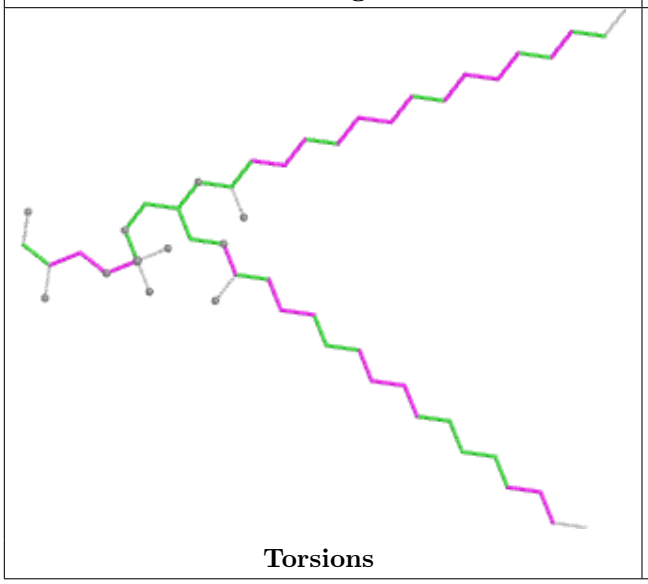
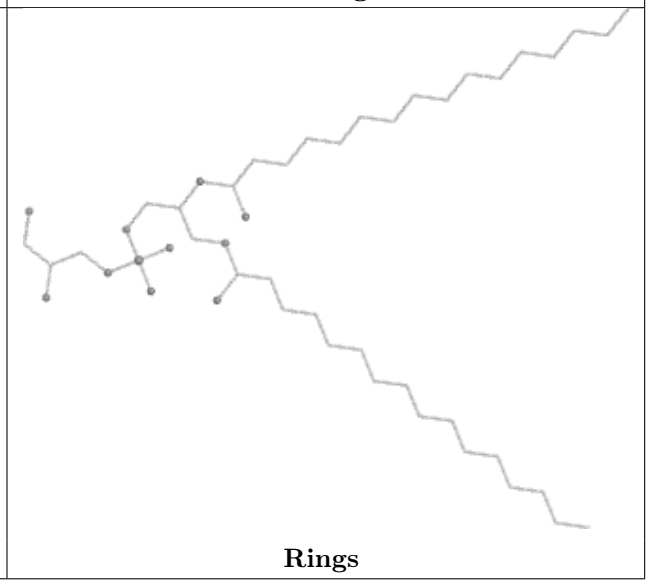


Bond angles

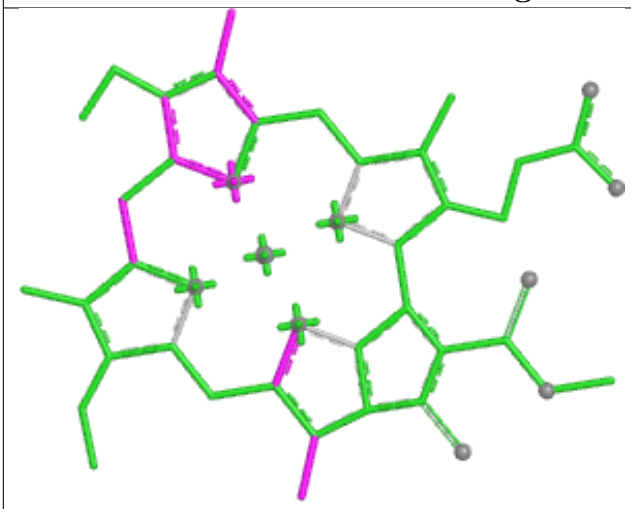


Torsions

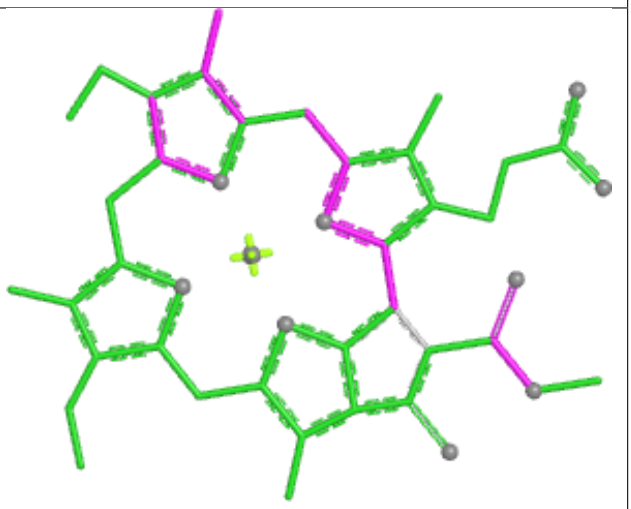


Rings

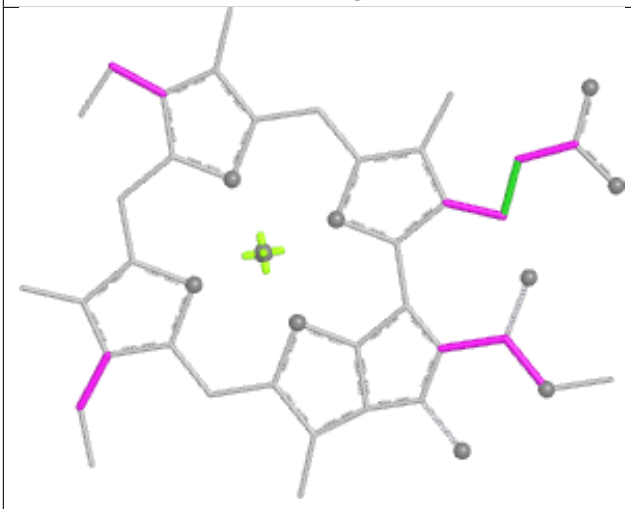
Ligand CLA K 4003



Bond lengths



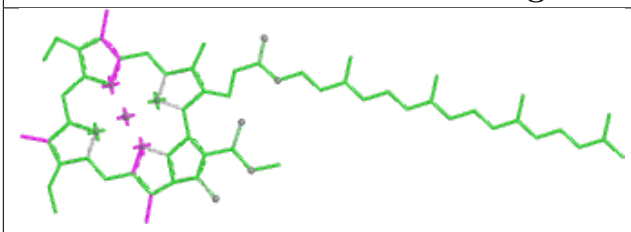
Bond angles



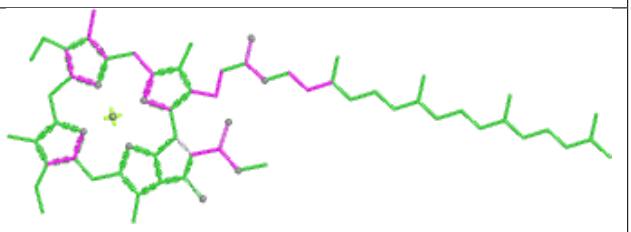
Torsions

Rings

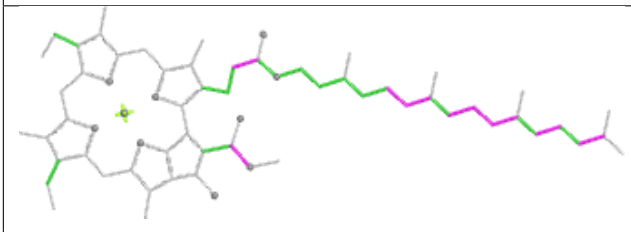
Ligand CLA b 805



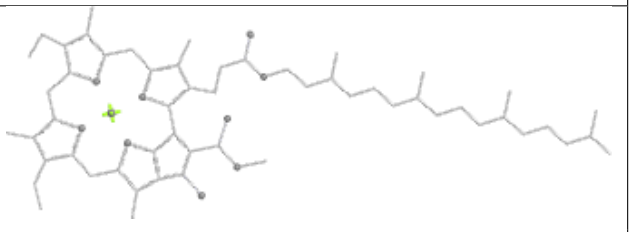
Bond lengths



Bond angles

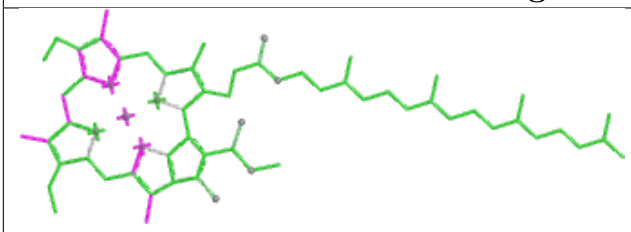


Torsions

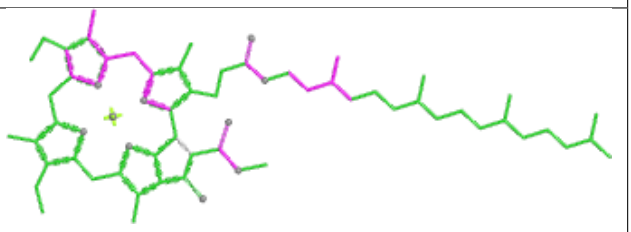


Rings

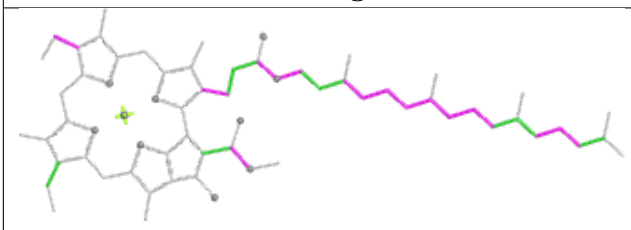
Ligand CLA 1 812



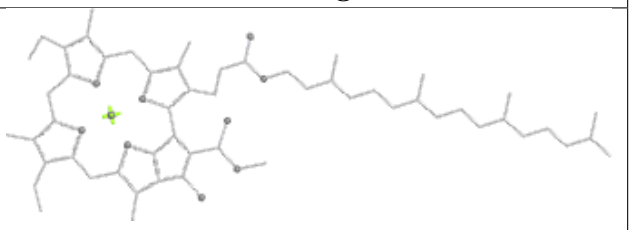
Bond lengths



Bond angles

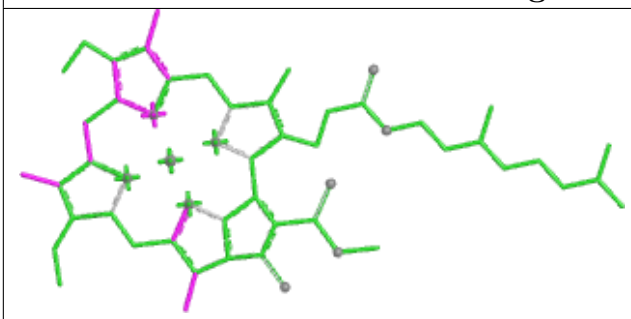


Torsions



Rings

Ligand CLA a 854



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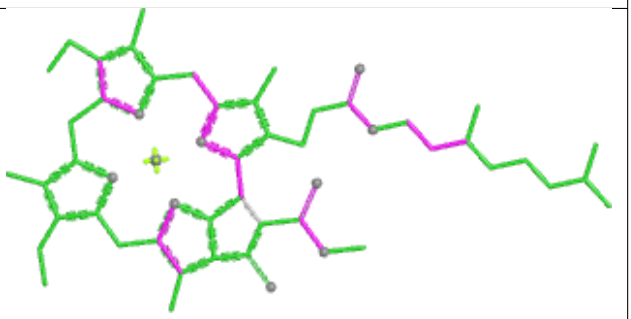
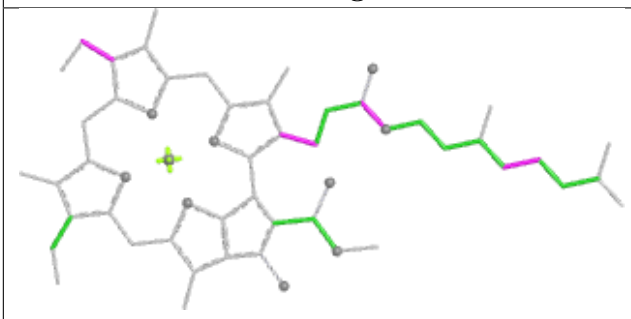
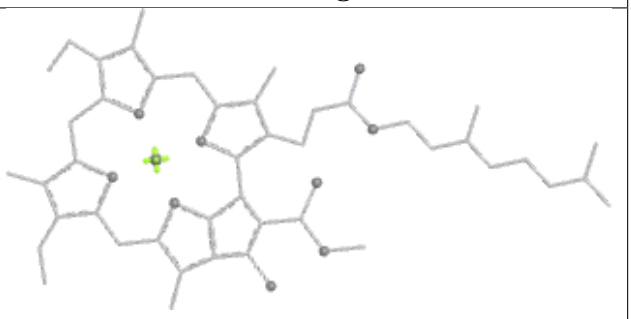


Bond angles

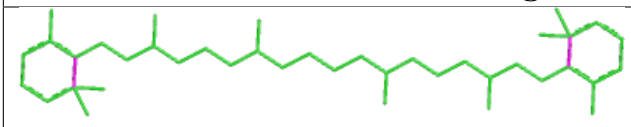


Torsions

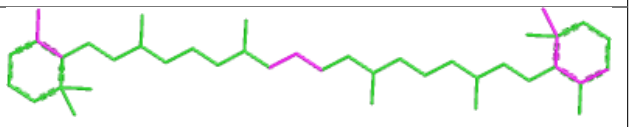


Rings

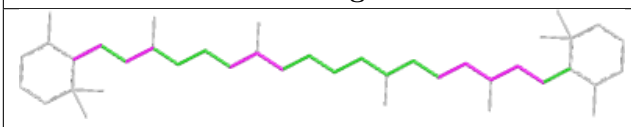
Ligand BCR A 848



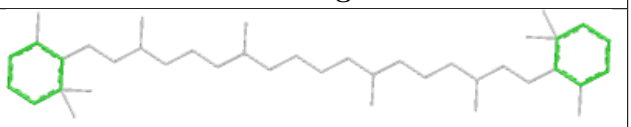
Bond lengths



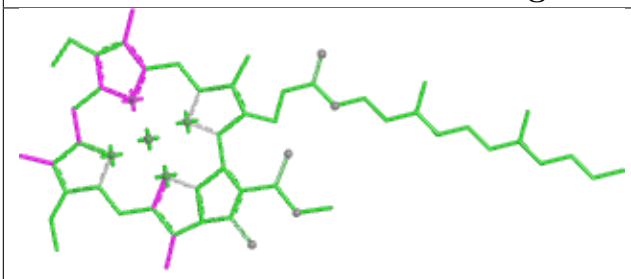
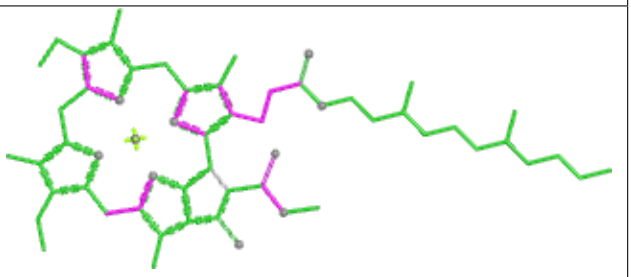
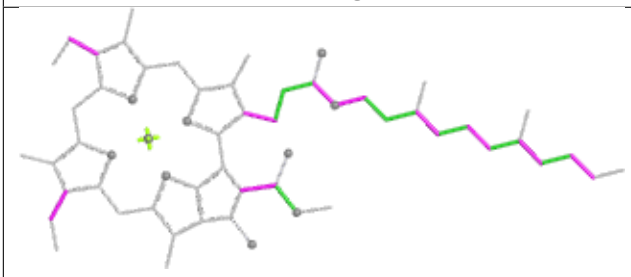
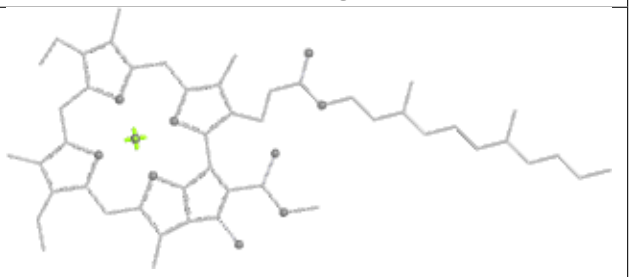
Bond angles

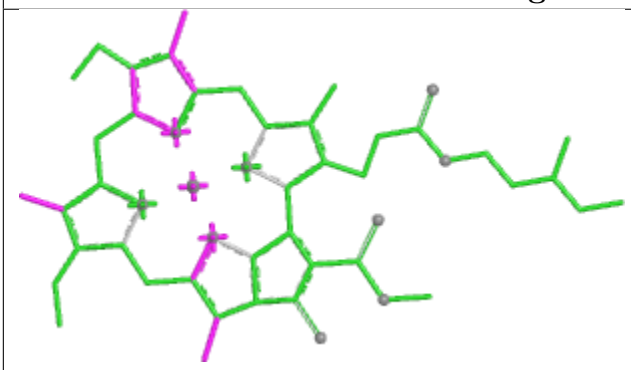
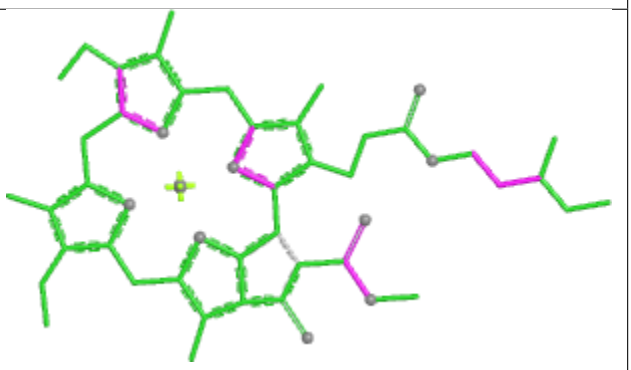
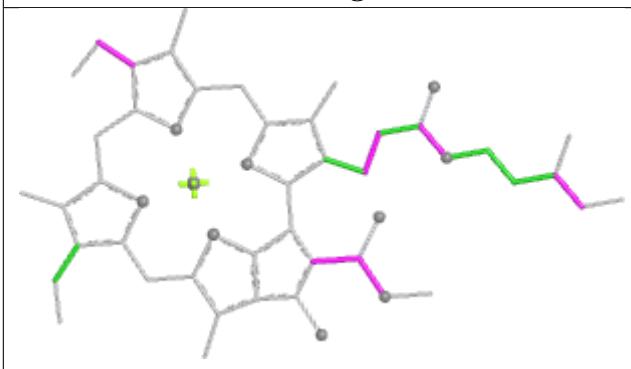
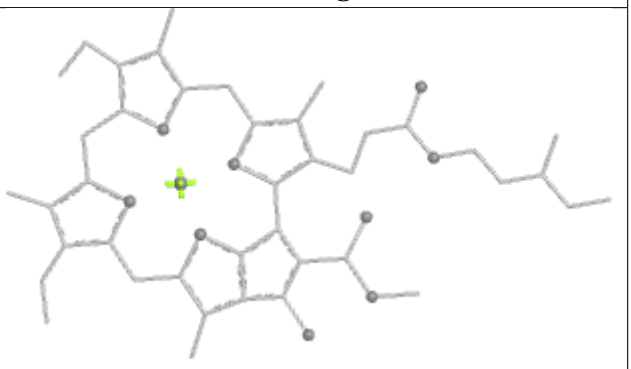


Torsions

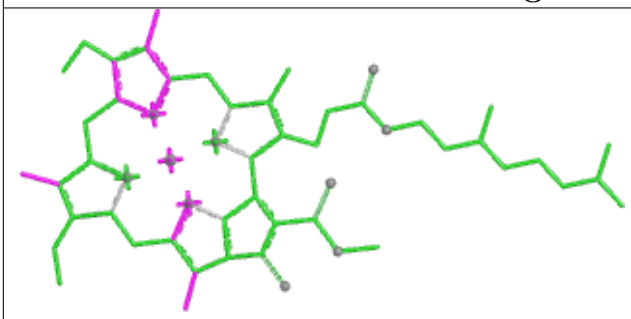


Rings

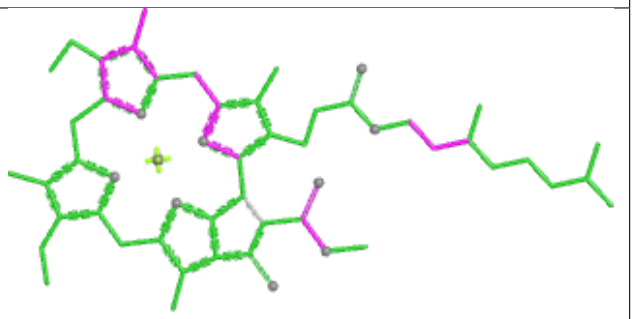
Ligand CLA 2 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

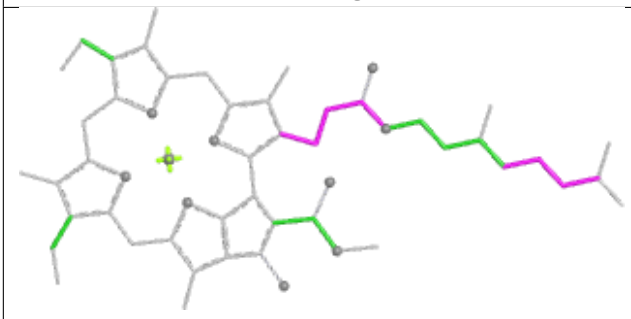
Ligand CLA B 819



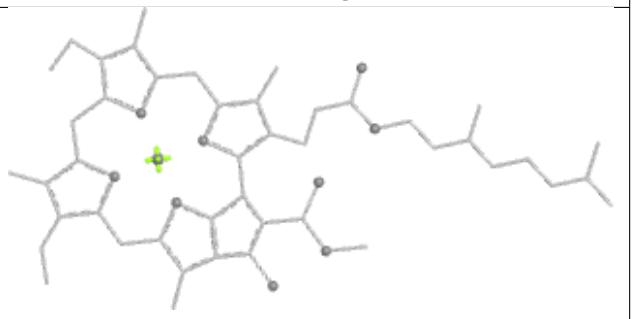
Bond lengths



Bond angles

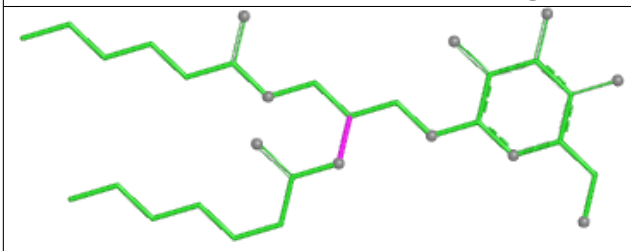


Torsions



Rings

Ligand LMG a 853



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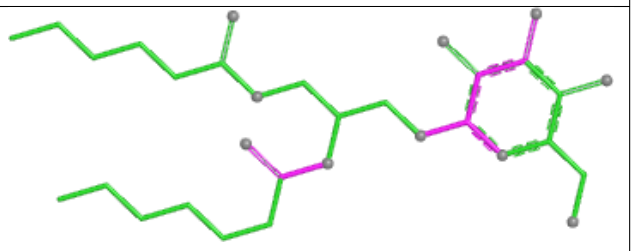
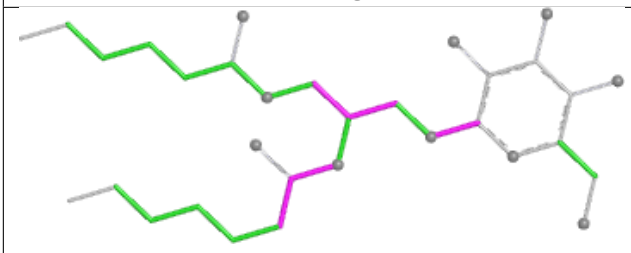
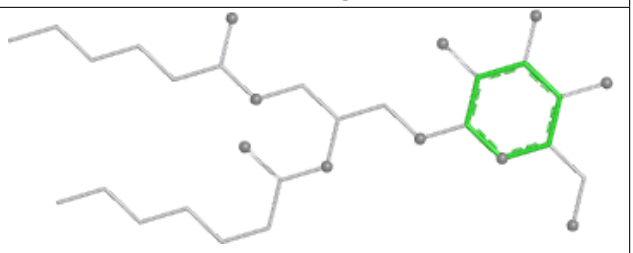


Bond angles

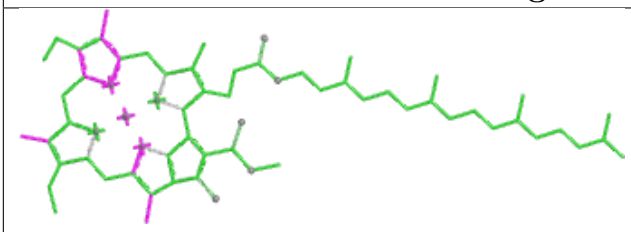


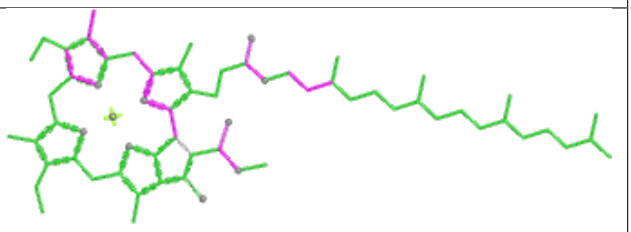
Torsions

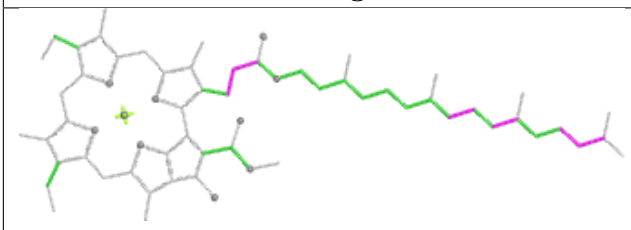


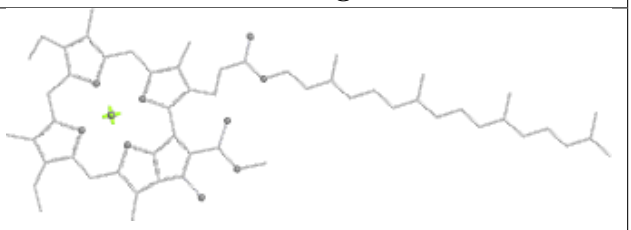
Rings

Ligand CLA a 832


Bond lengths

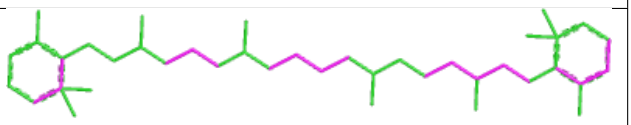

Bond angles

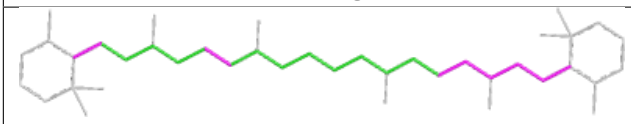

Torsions

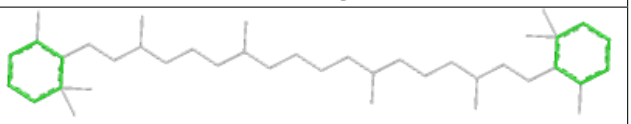

Rings

Ligand BCR b 851

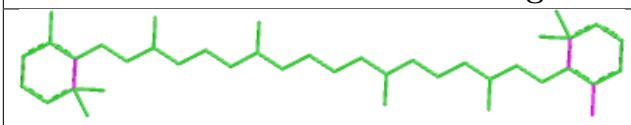
Bond lengths

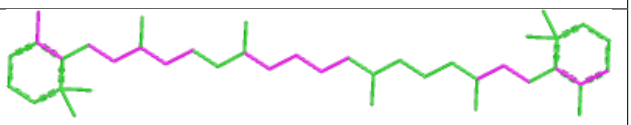

Bond angles

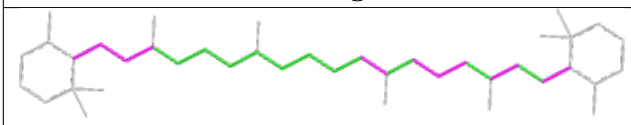

Torsions


Rings

Ligand BCR 2 846


Bond lengths


Bond angles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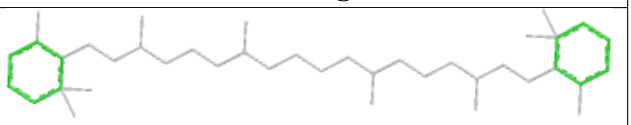
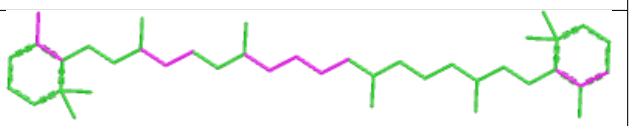
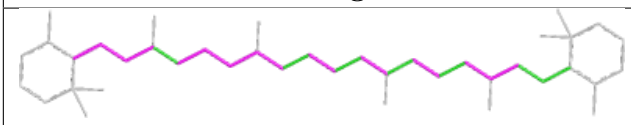

Rings

Ligand BCR I 101

Bond lengths


Bond angles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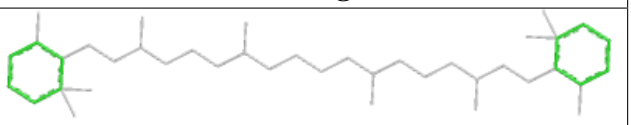
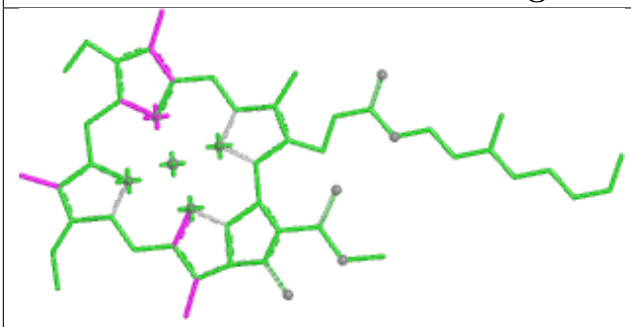
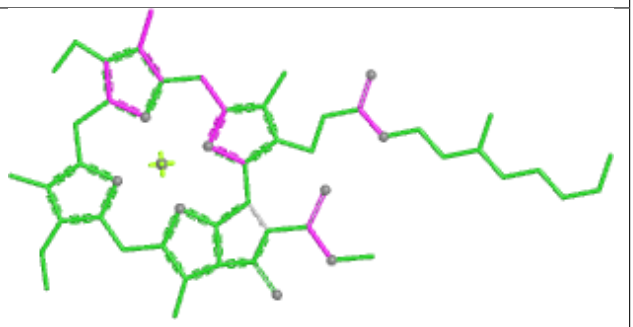

Rings

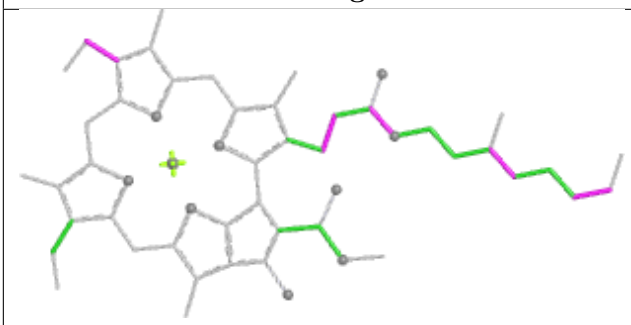
Ligand CLA 1 818



Bond lengths



Bond angles



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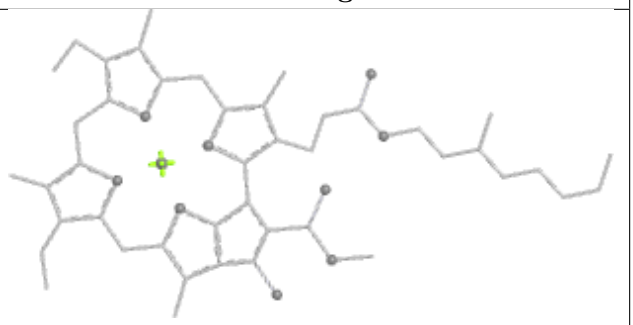
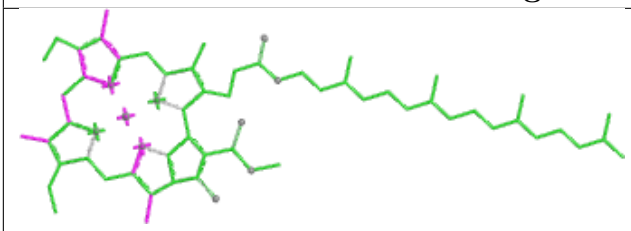
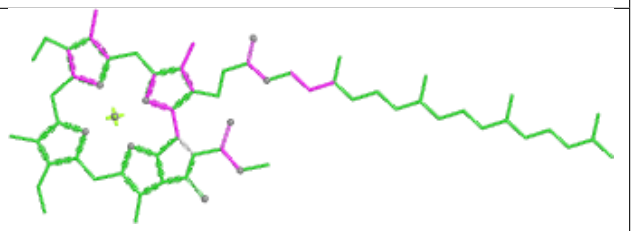


Rings

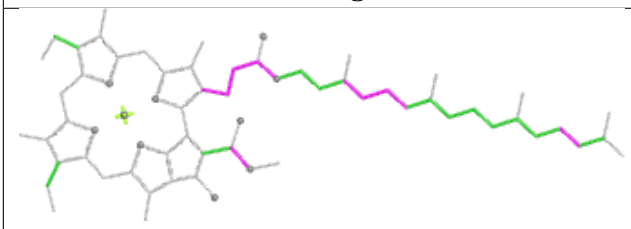
Ligand CLA A 823



Bond lengths



Bond angles



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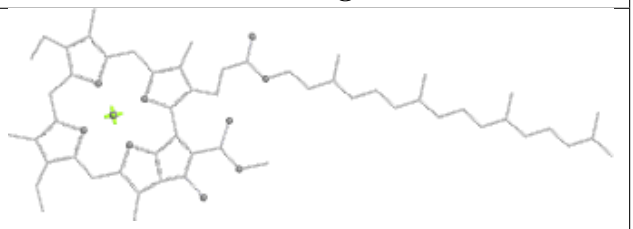
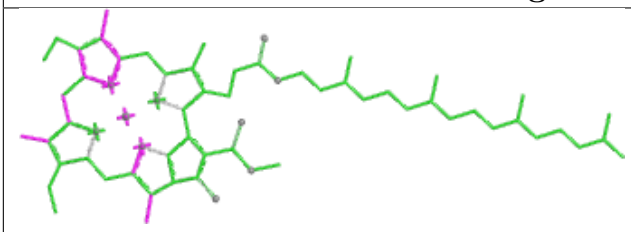
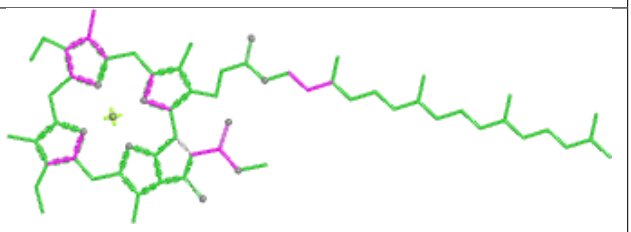


Rings

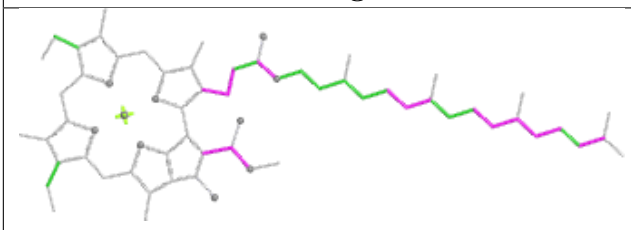
Ligand CLA a 822



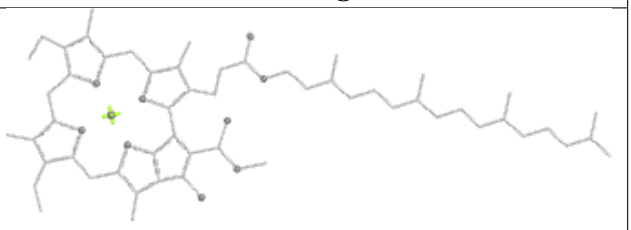
Bond lengths



Bond angles

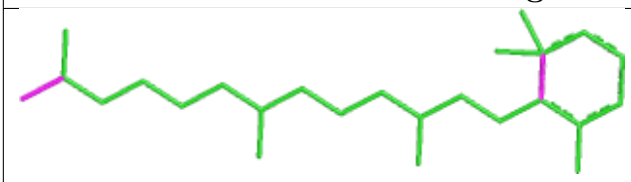


Torsions

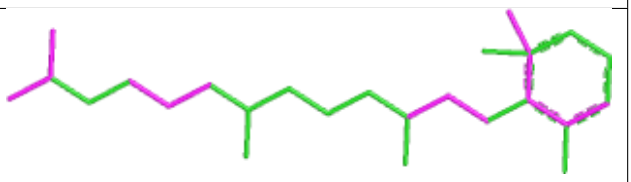


Rings

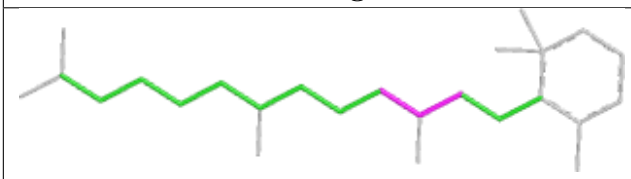
Ligand BCR 2 848



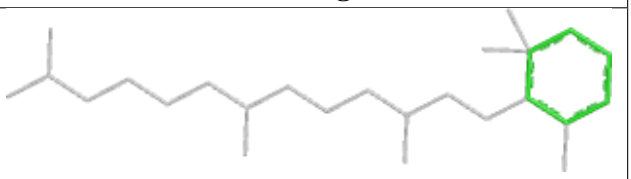
Bond lengths



Bond angles



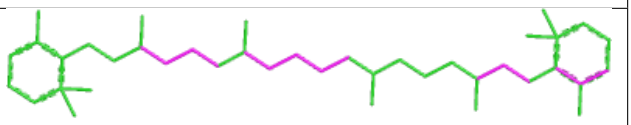
Torsions



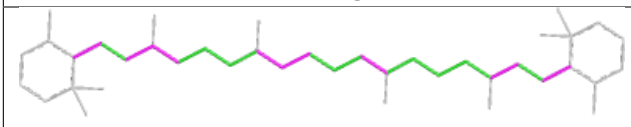
Rings

Ligand BCR F 203

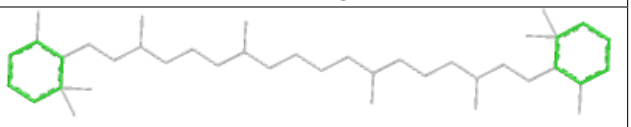
Bond lengths



Bond angles

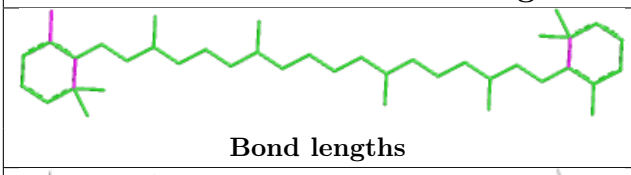


Torsions

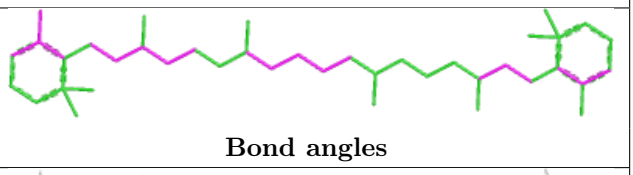


Rings

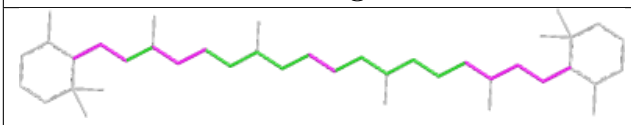
Ligand BCR 6 4406



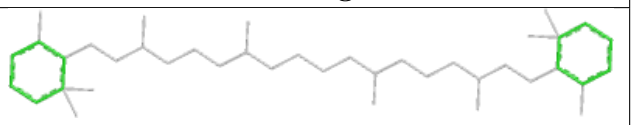
Bond lengths



Bond angles

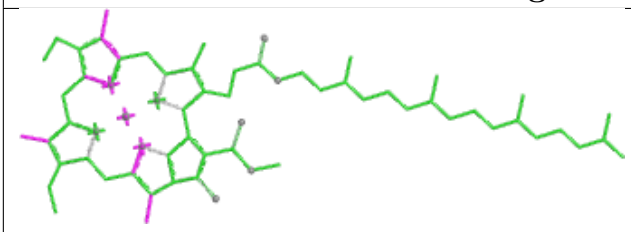


Torsions

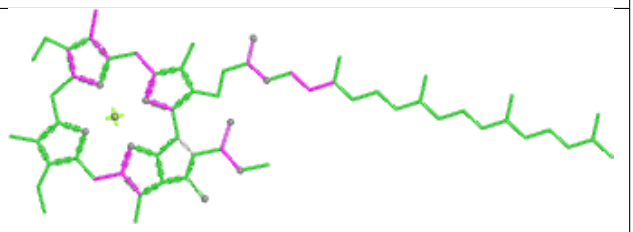


Rings

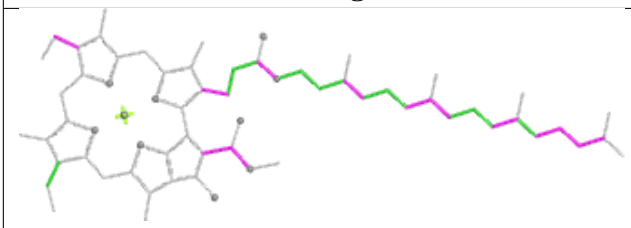
Ligand CLA 2 843



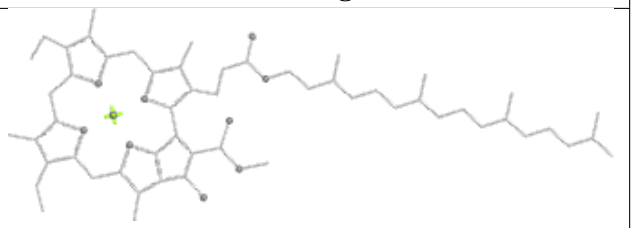
Bond lengths



Bond angles

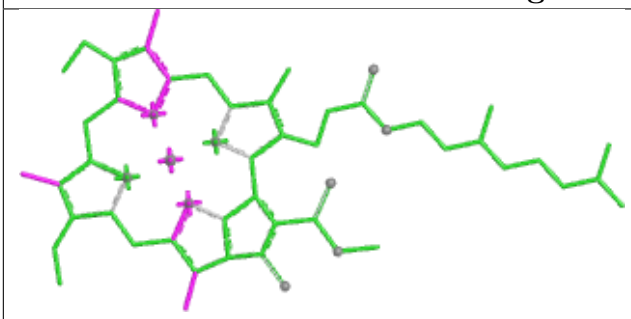


Torsions



Rings

Ligand CLA b 819



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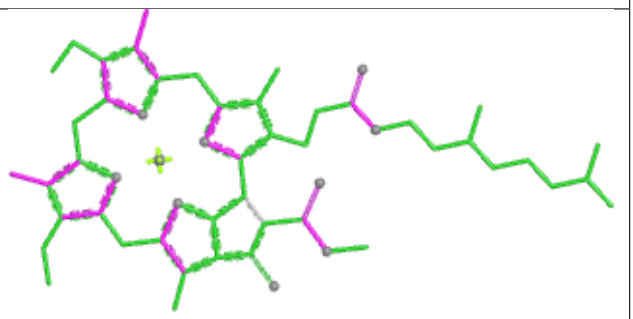
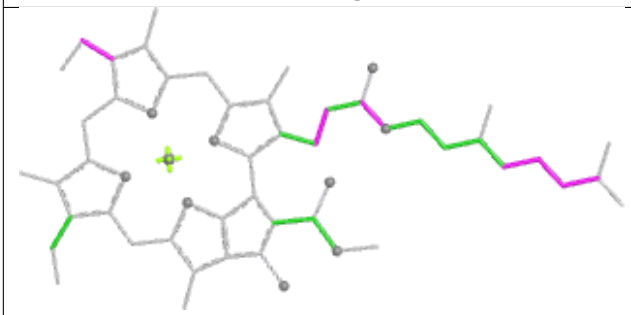


Bond angles



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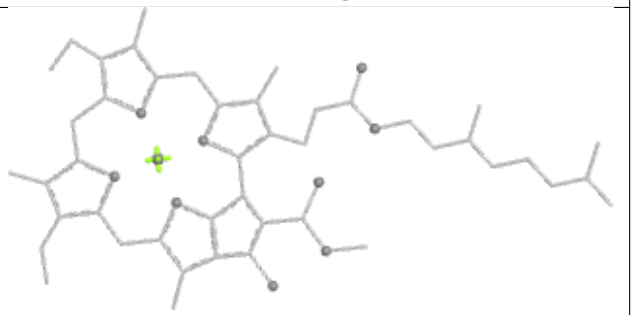
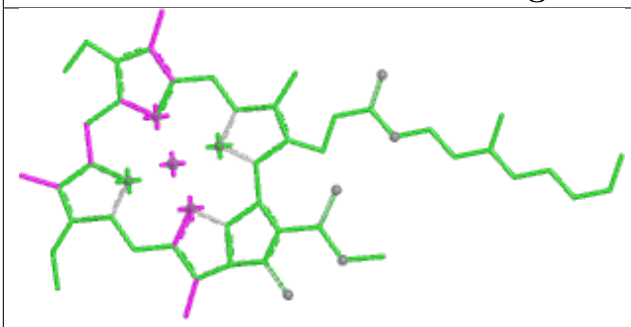


Rings

Ligand CLA a 821



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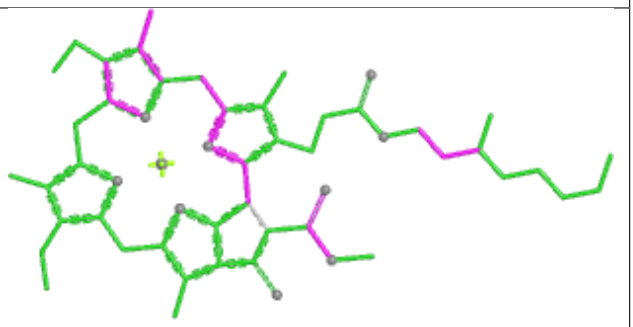
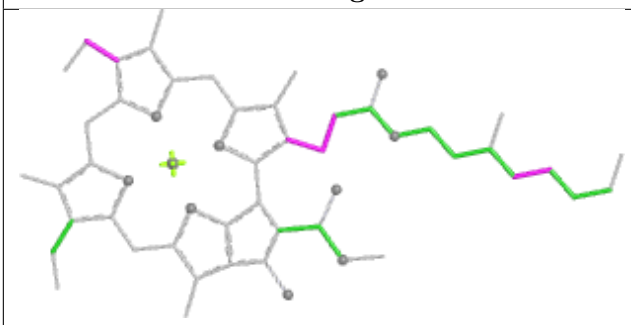


Bond angles



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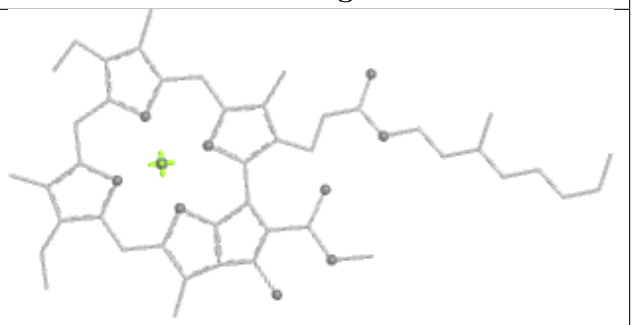
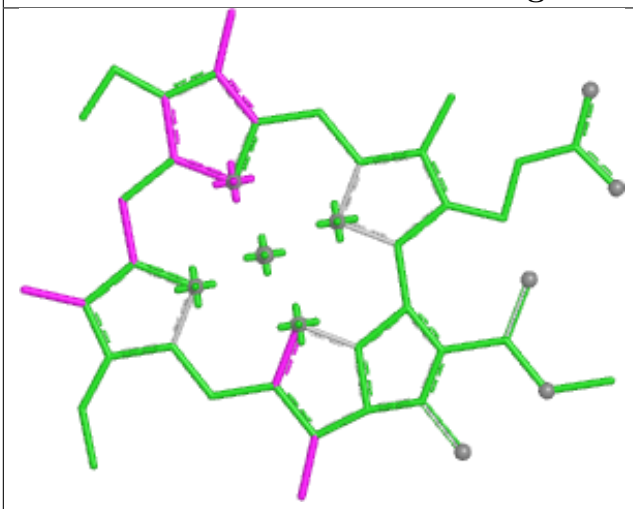


Rings

Ligand CLA b 823



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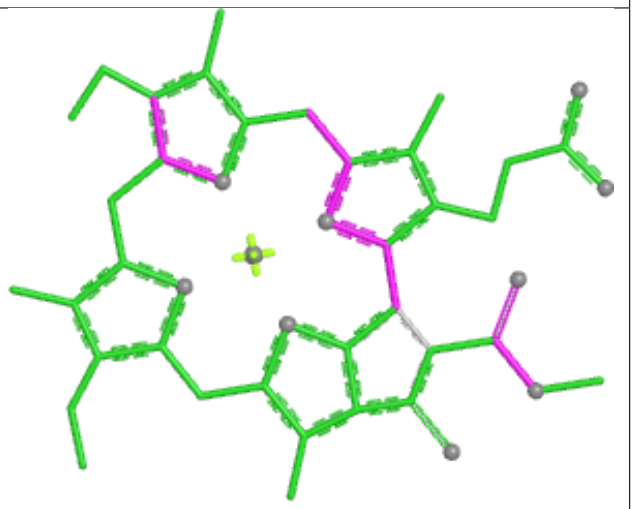
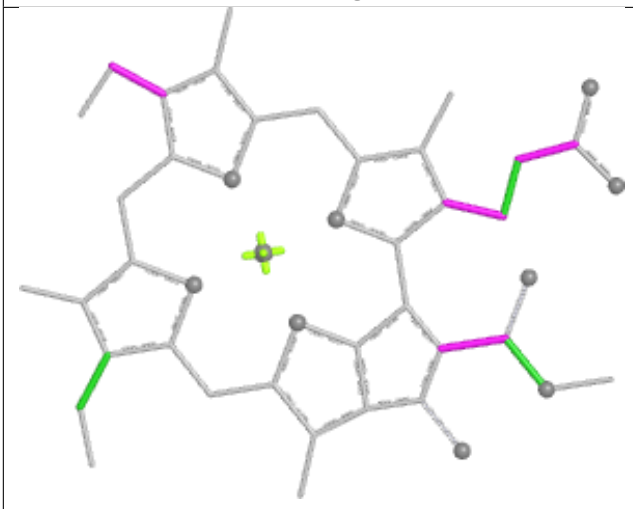


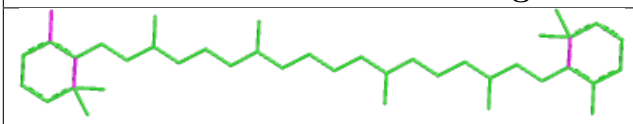
Bond angles



Torsions

Rings

Ligand BCR K 4001



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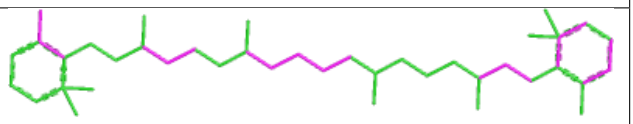
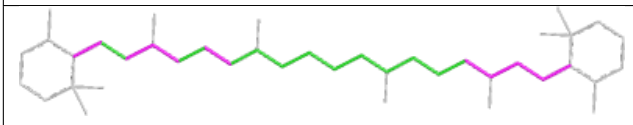
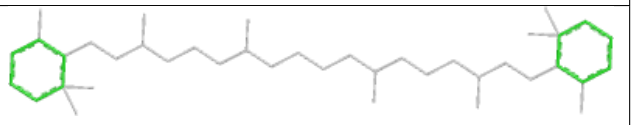


Bond angles

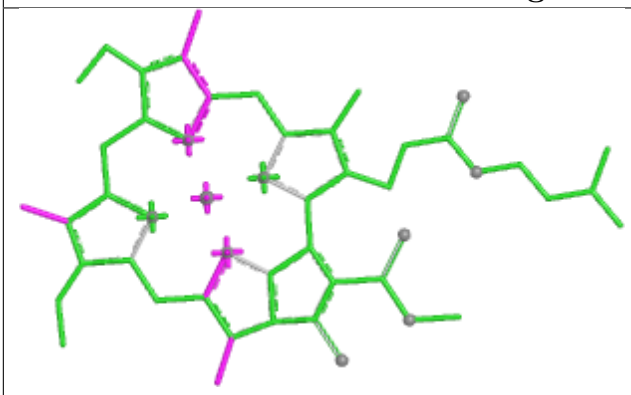


Torsions

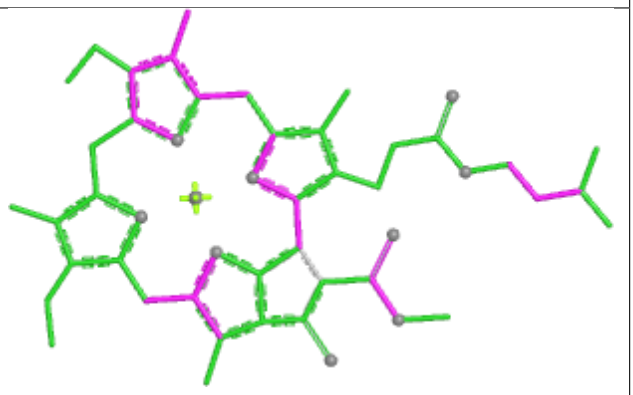


Rings

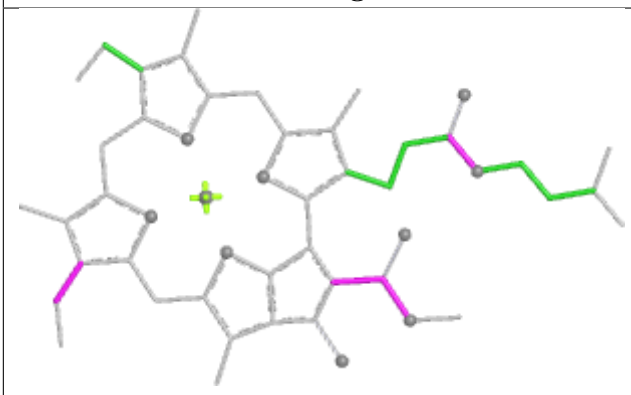
Ligand CLA b 839



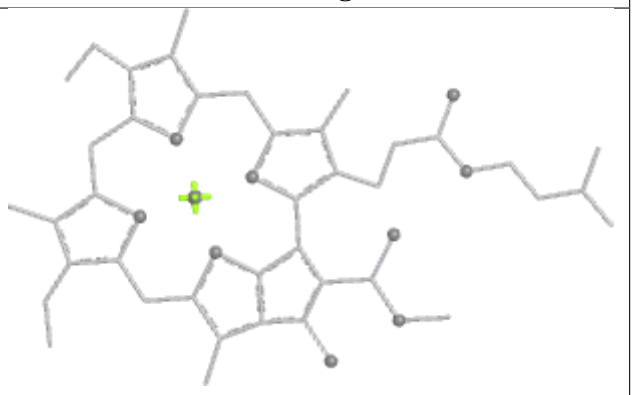
Bond lengths



Bond angles



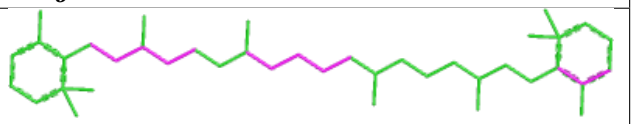
Torsions



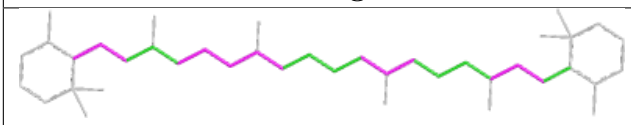
Rings

Ligand BCR j 103

Bond lengths



Bond angles



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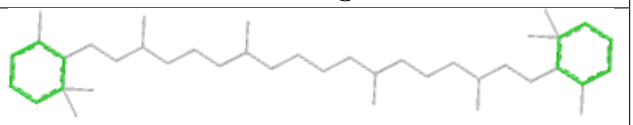
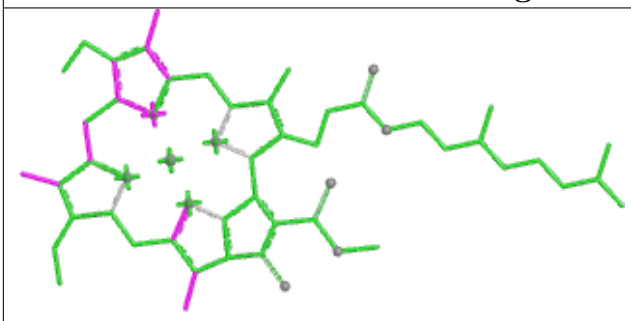


Rings

Ligand CLA K 4004



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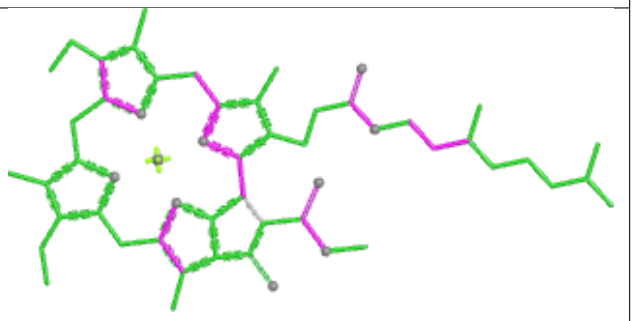
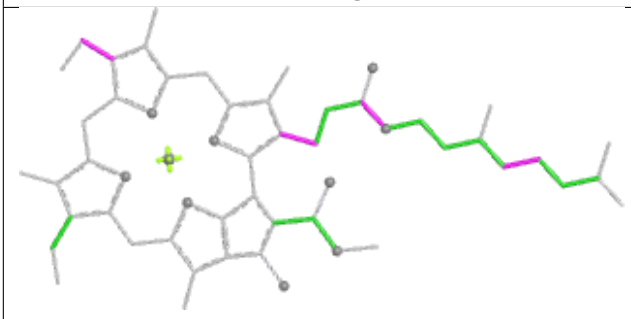


Bond angles



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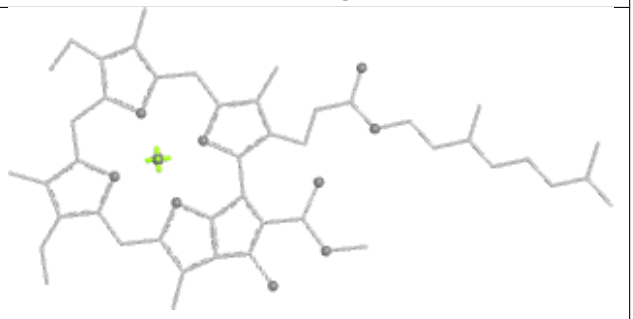
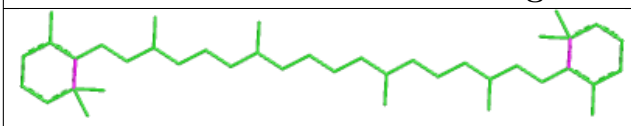


Rings

Ligand BCR 1 851



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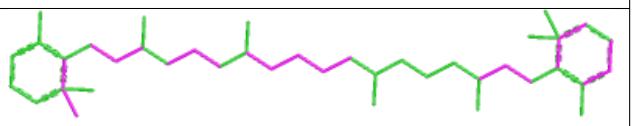
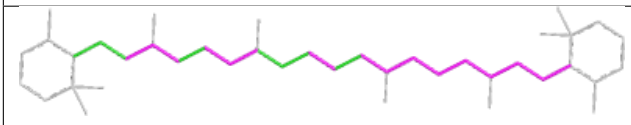
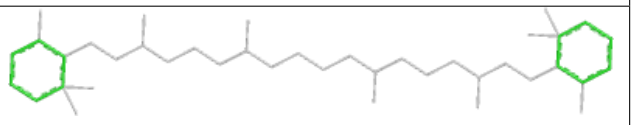


Bond angles

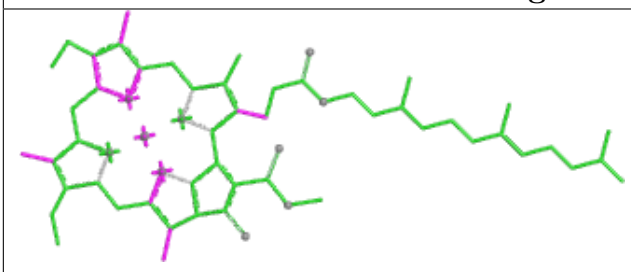


Torsions

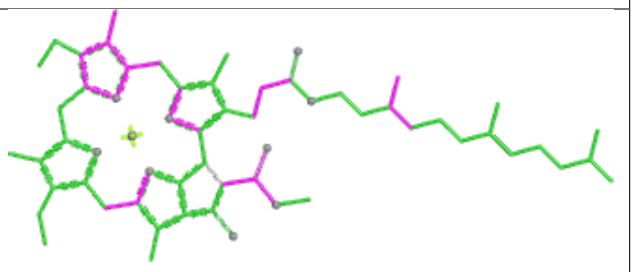


Rings

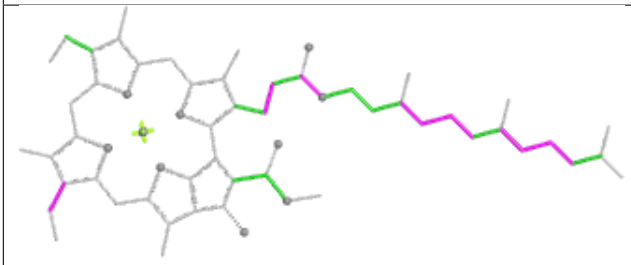
Ligand CLA 2 801



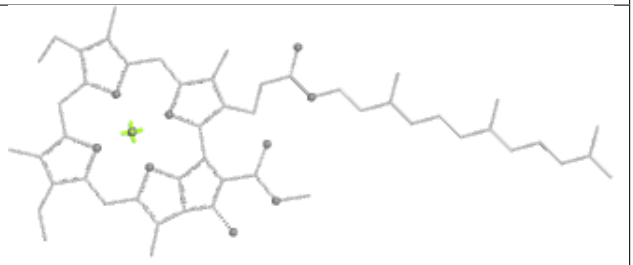
Bond lengths



Bond angles

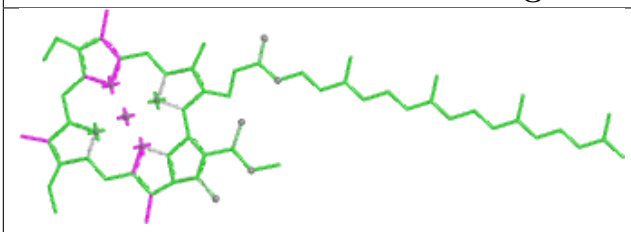


Torsions

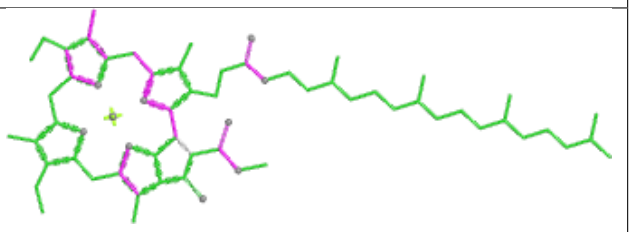


Rings

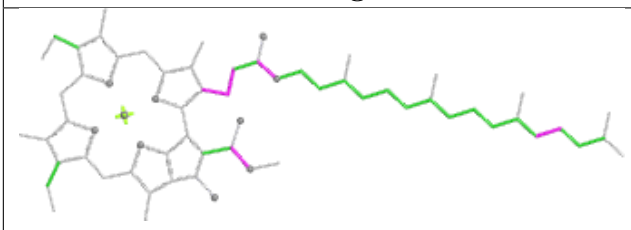
Ligand CLA B 831



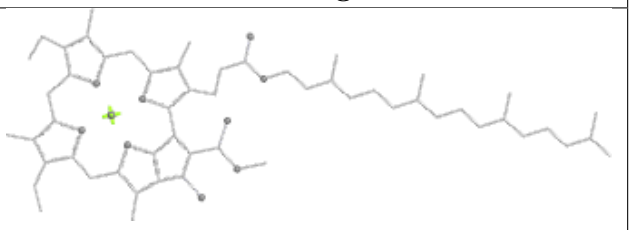
Bond lengths



Bond angles

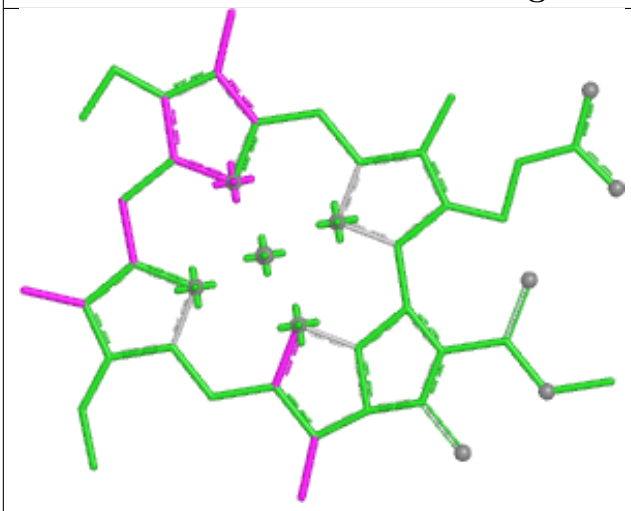


Torsions

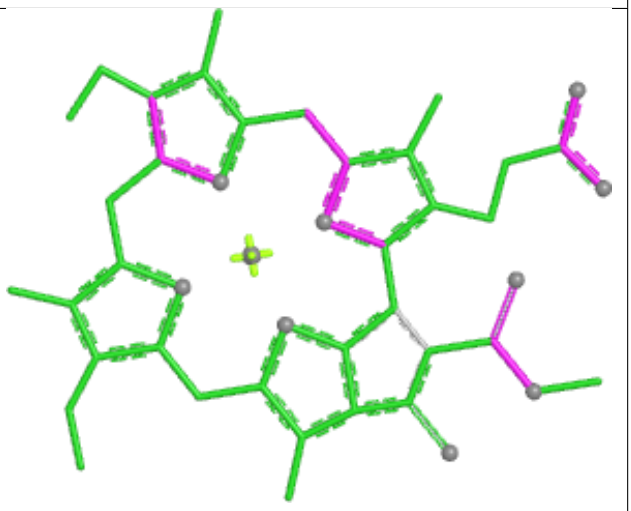


Rings

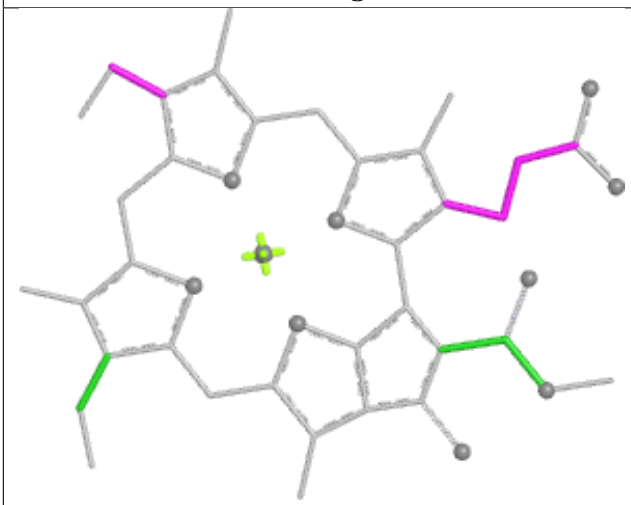
Ligand CLA 2 822



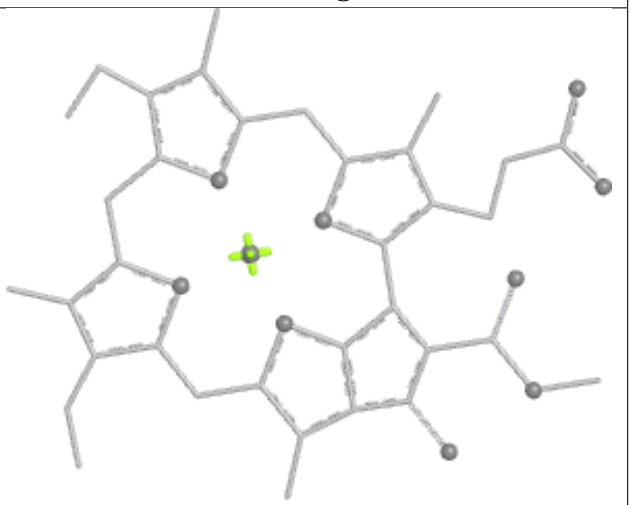
Bond lengths



Bond angles

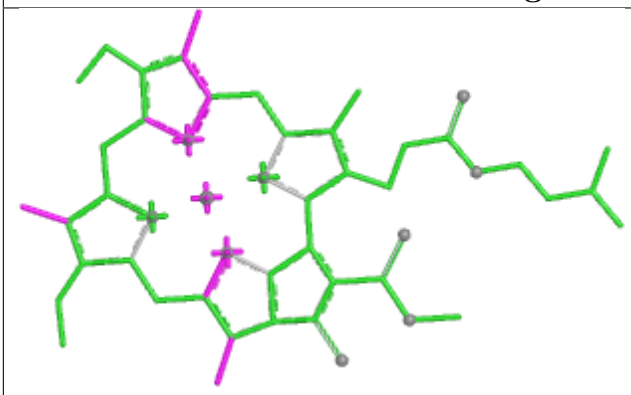


Torsions



Rings

Ligand CLA B 840



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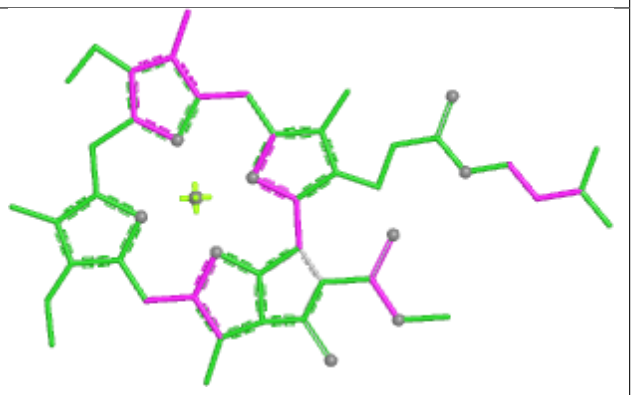
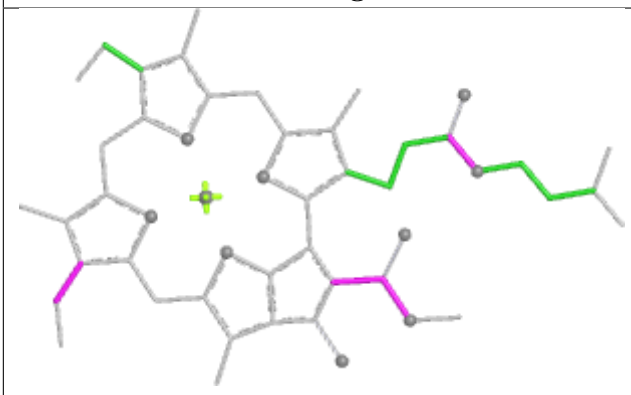


Bond angles



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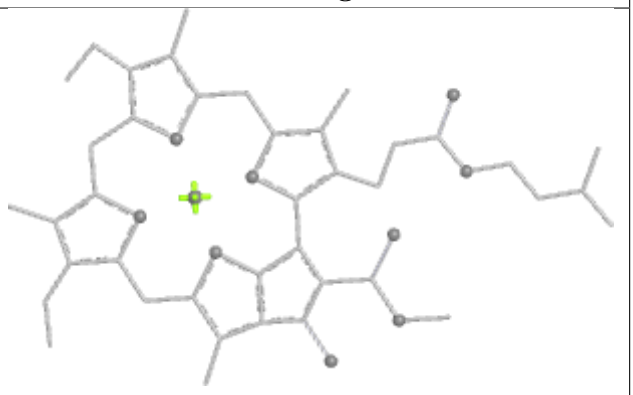
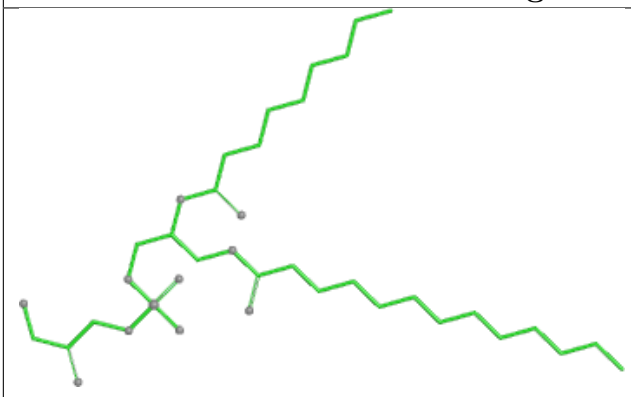


Rings

Ligand LHG 9 101



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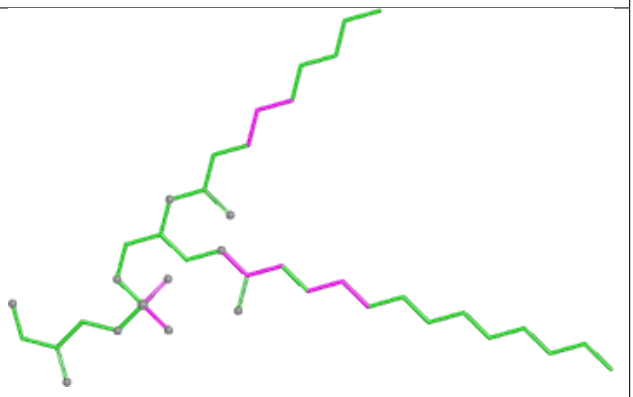
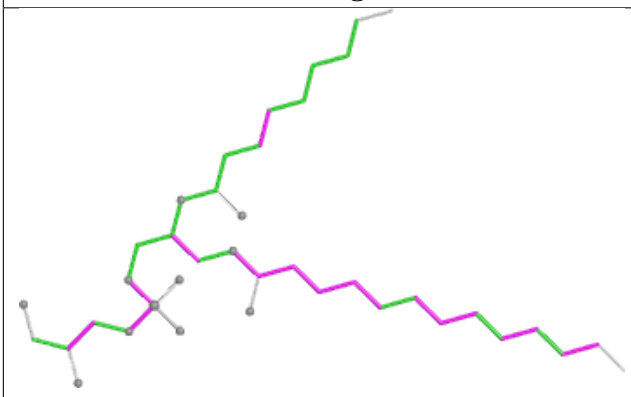
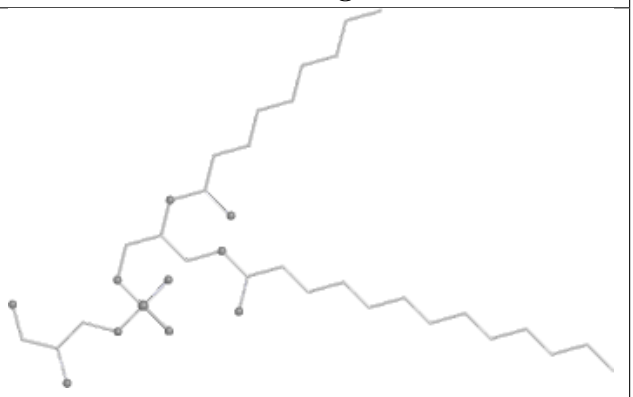


Bond angles

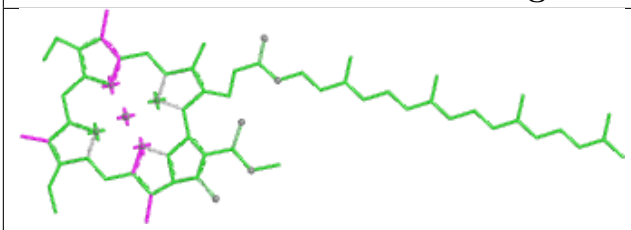


Torsions



Rings

Ligand CLA a 835



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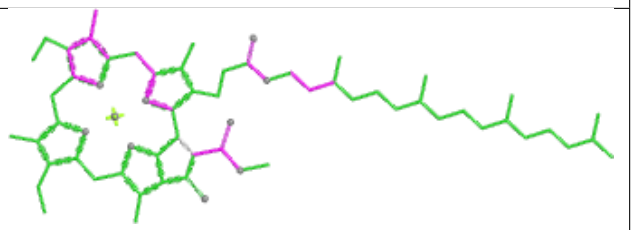
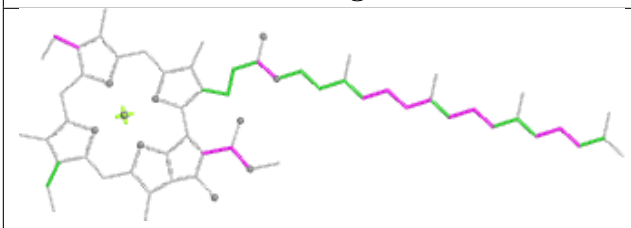


Bond angles



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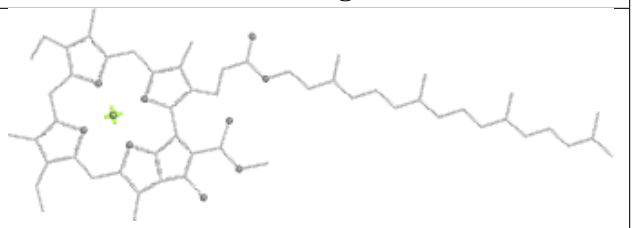
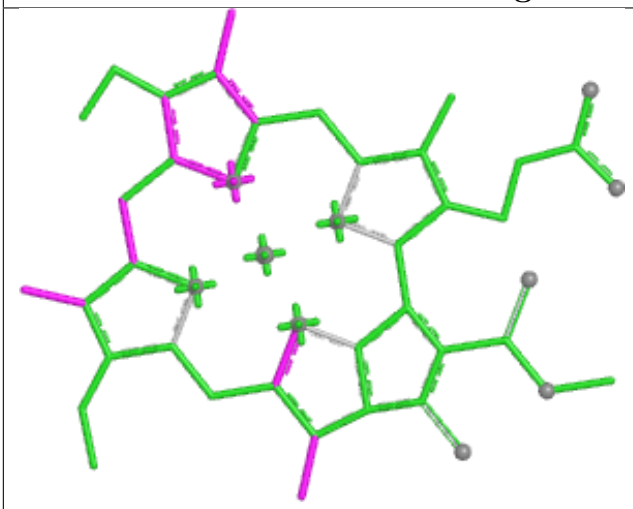


Rings

Ligand CLA K 4002



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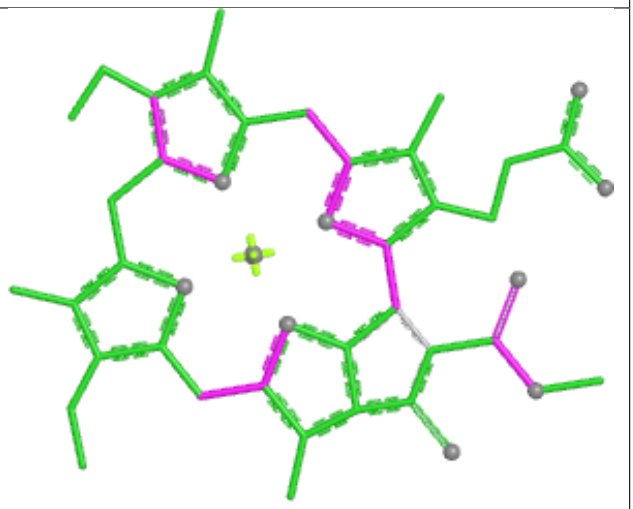
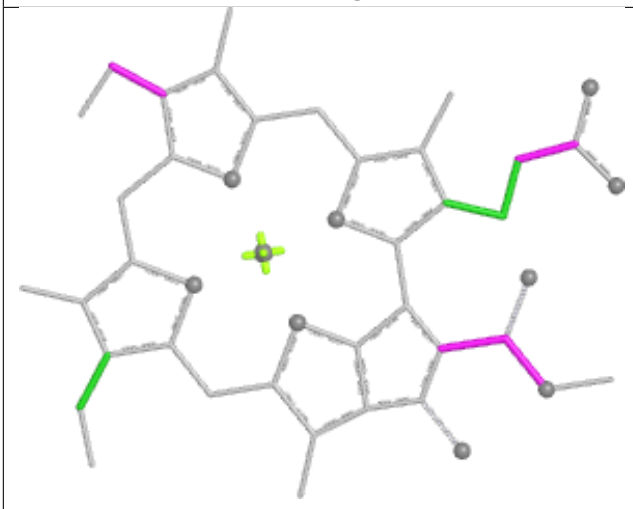


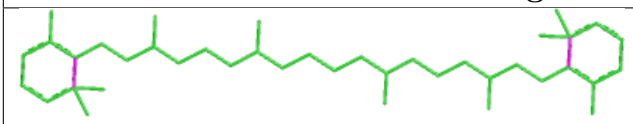
Bond angles



Torsions

Rings

Ligand BCR 0 209



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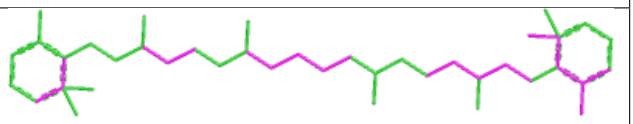

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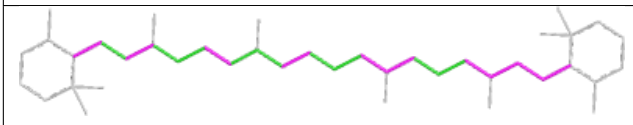

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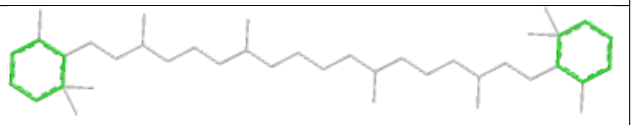
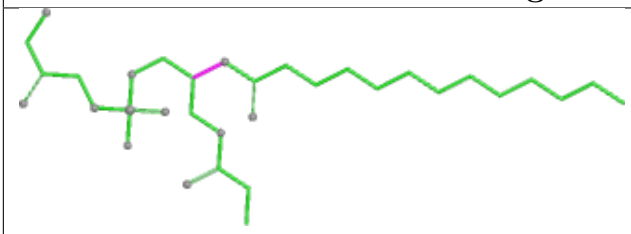


Rings

Ligand LHG 1 802



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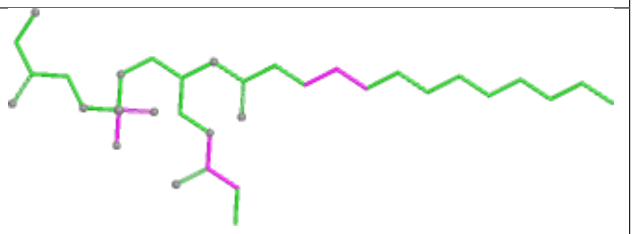
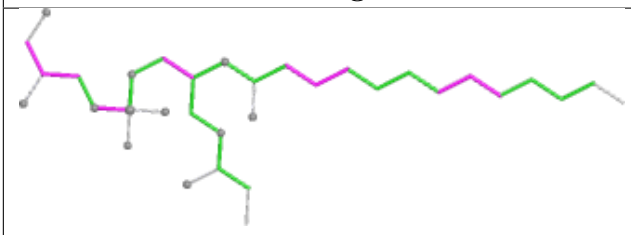


Bond angles



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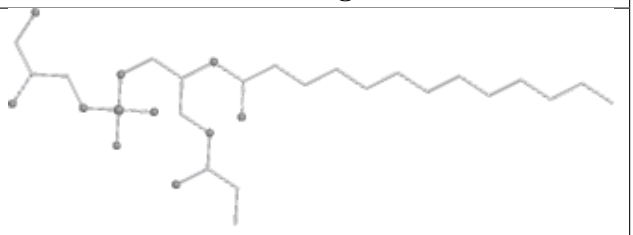
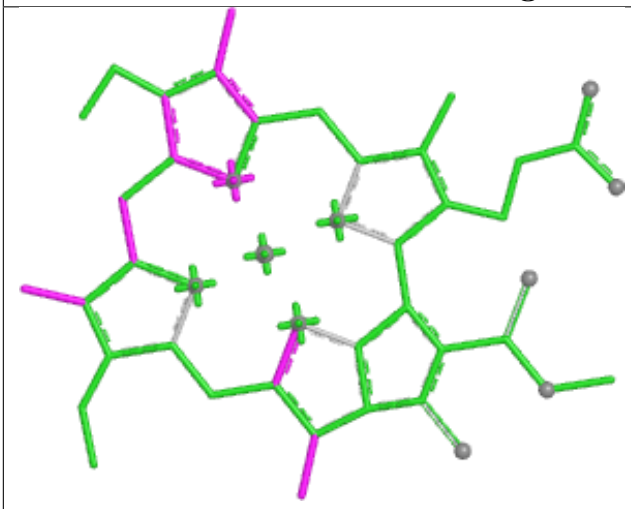


Rings

Ligand CLA 7 1102



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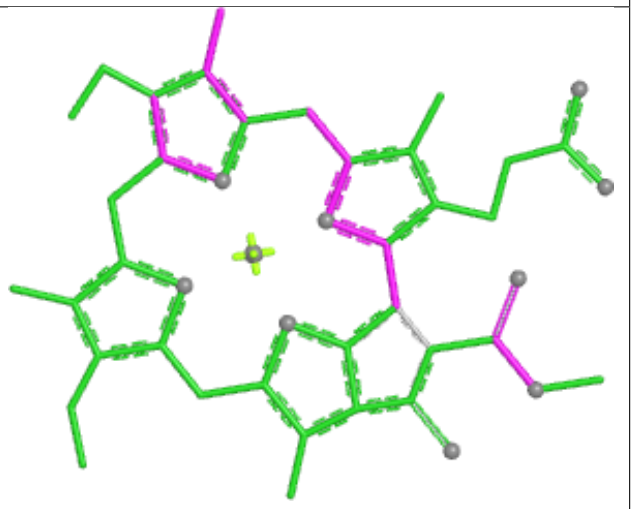

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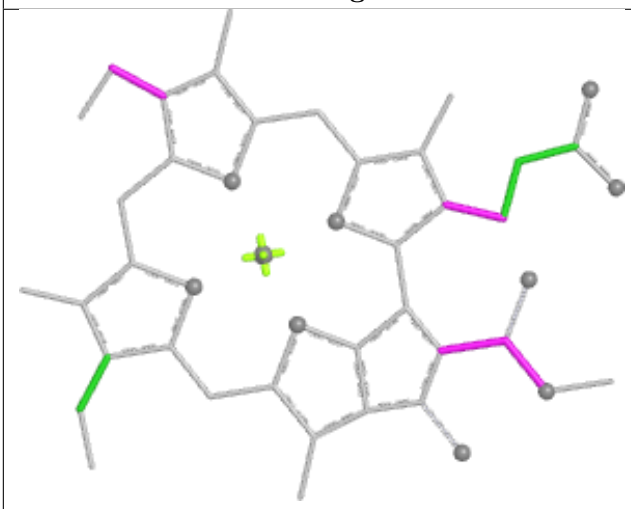
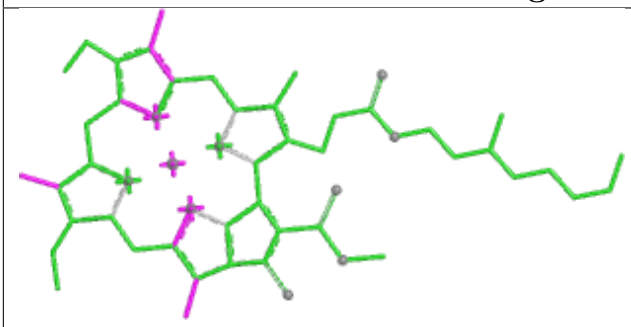


Torsions

Rings

Ligand CLA 1 819



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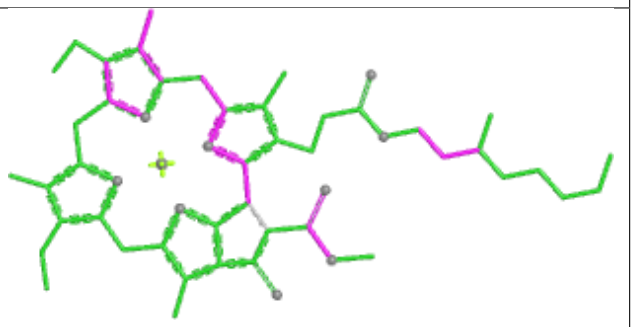
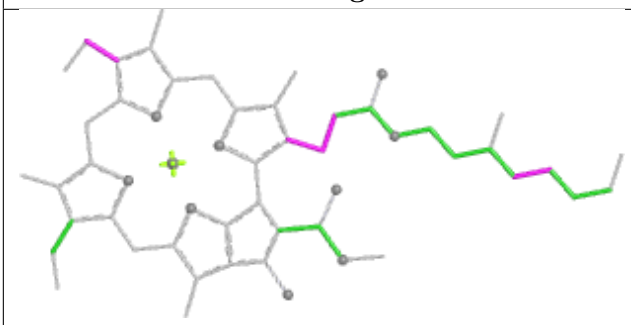
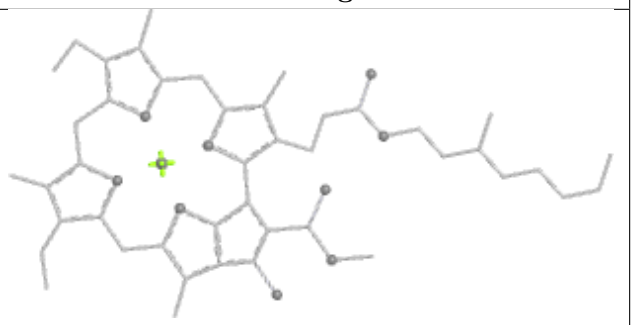


Bond angles

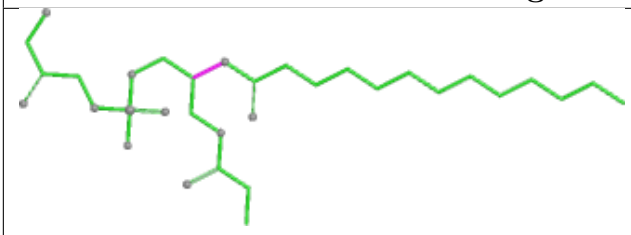


Torsions



Rings

Ligand LHG a 802



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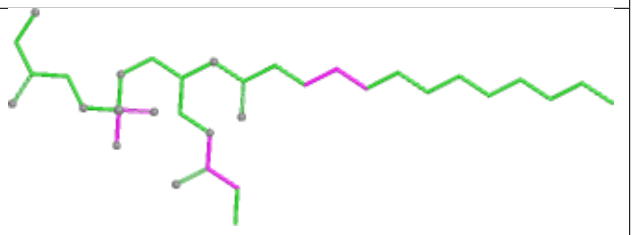
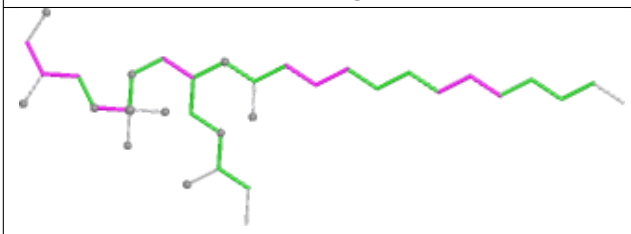


Bond angles



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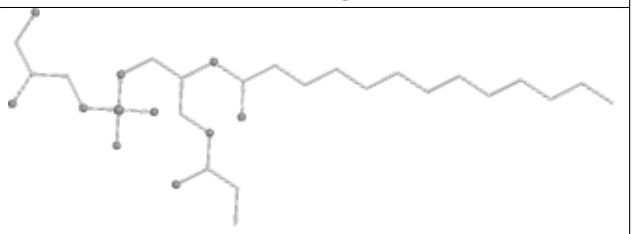
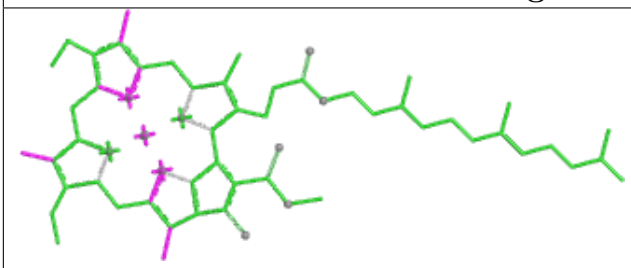


Rings

Ligand CLA b 831



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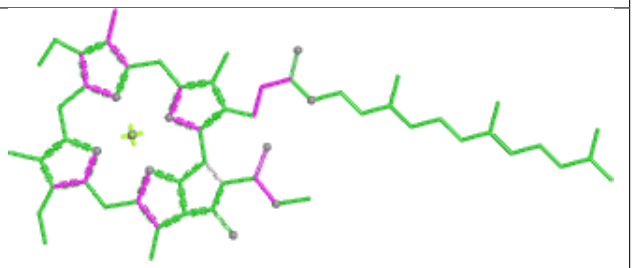
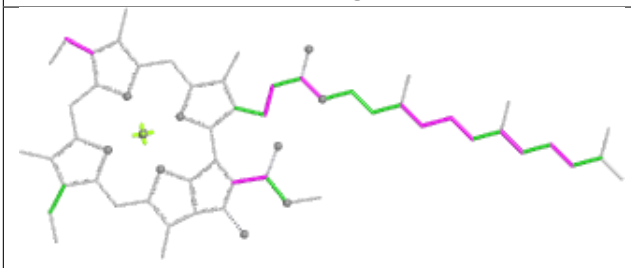


Bond angles



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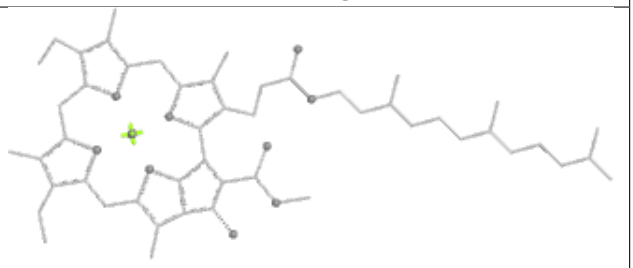
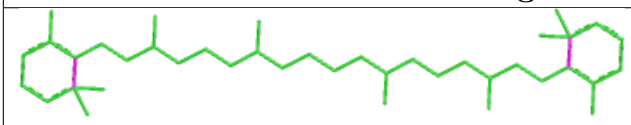


Rings

Ligand BCR 6 4405



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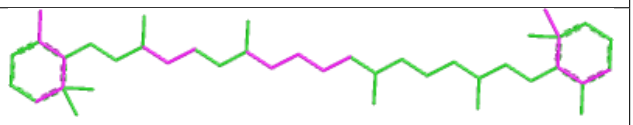
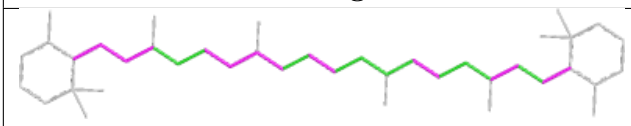


Bond angles



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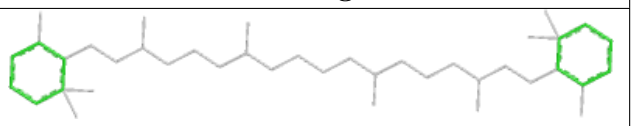
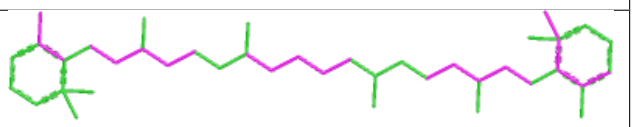


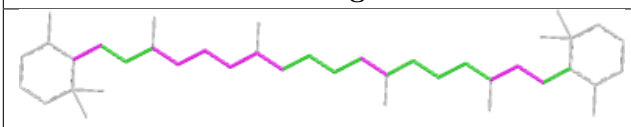
Rings

Ligand BCR 2 849

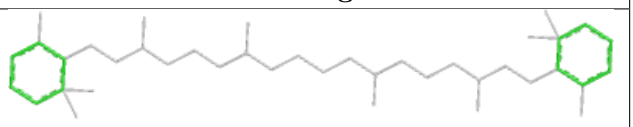
Bond lengths



Bond angles

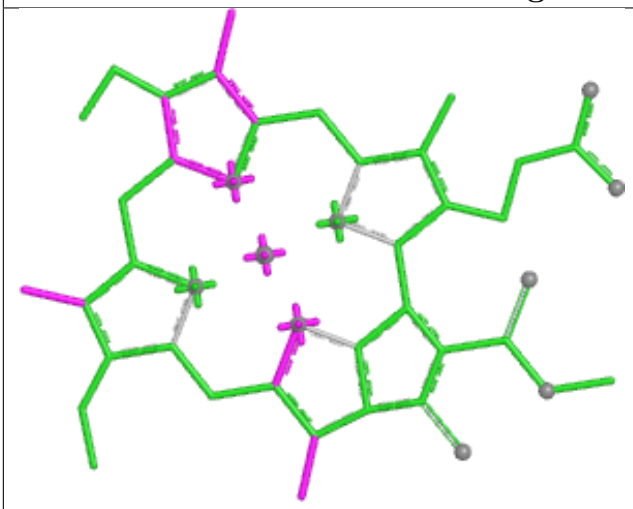


Torsions



Rings

Ligand CLA b 825



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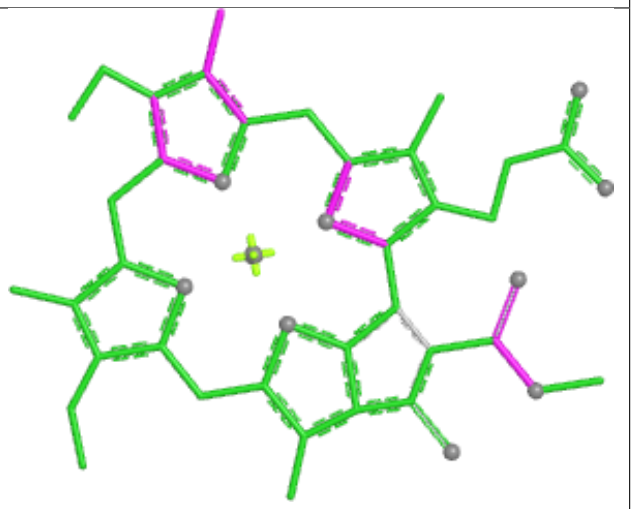
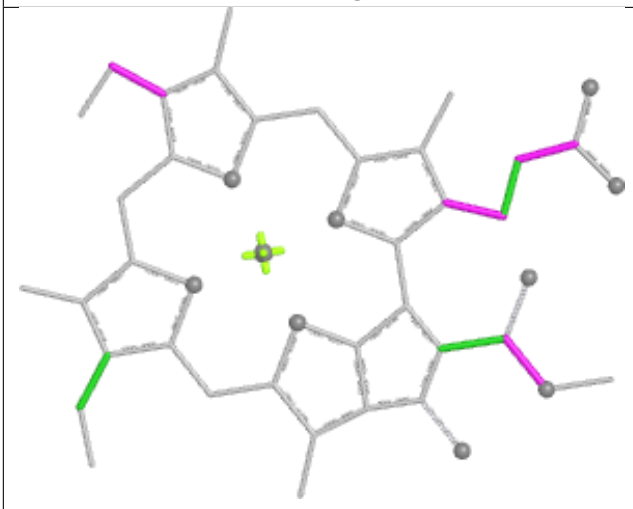


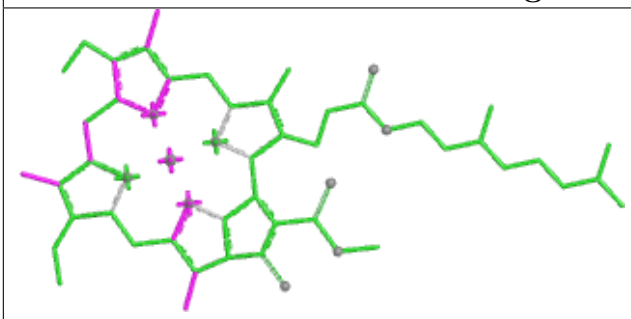
Bond angles



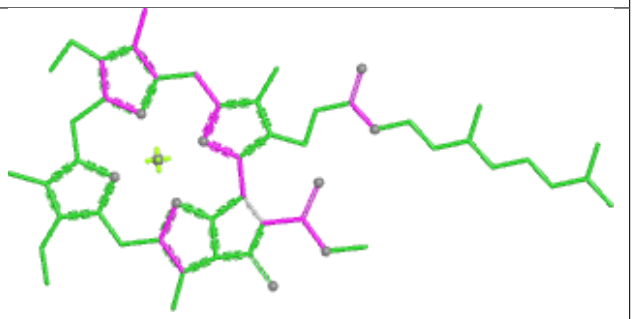
Torsions

Rings

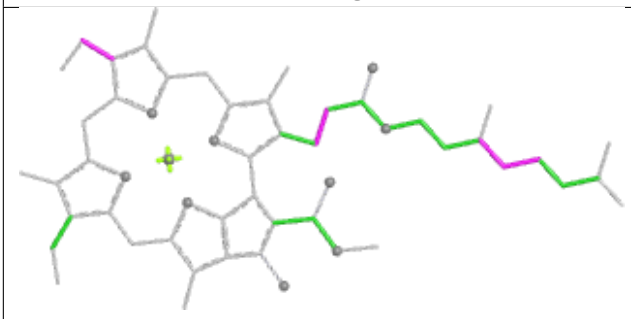
Ligand CLA B 827



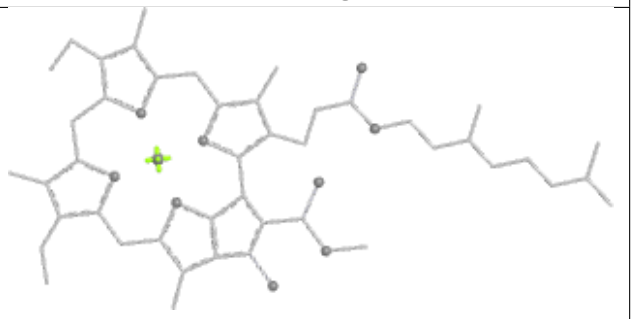
Bond lengths



Bond angles

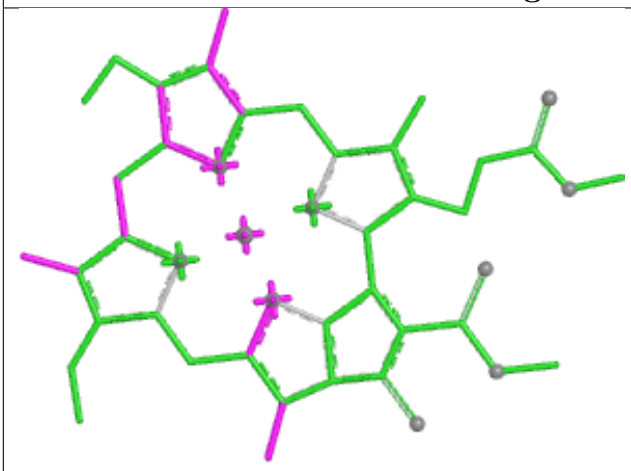


Torsions

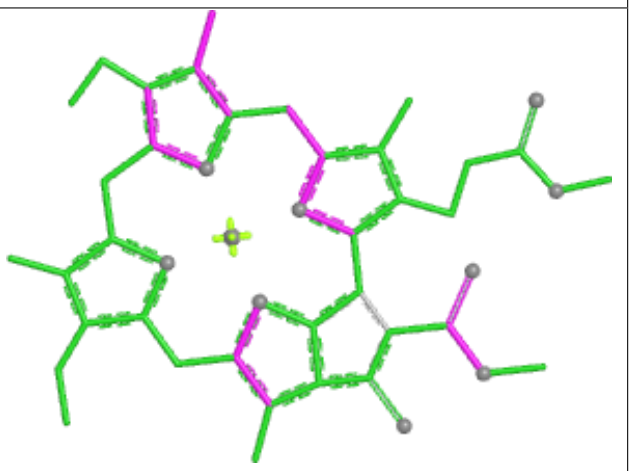


Rings

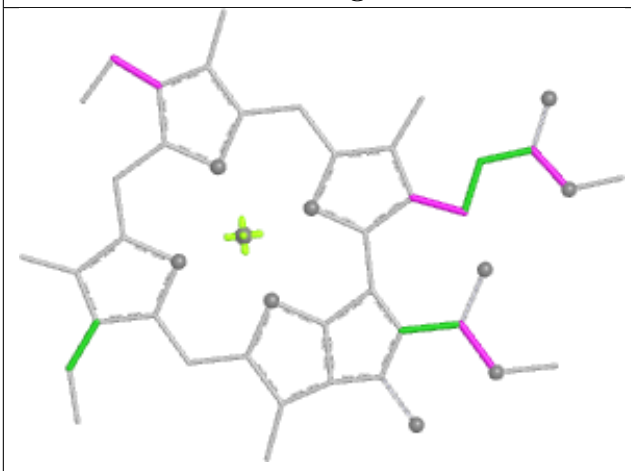
Ligand CLA A 809



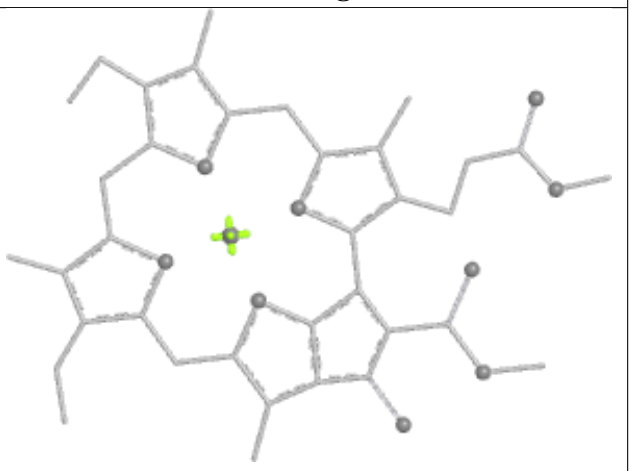
Bond lengths



Bond angles



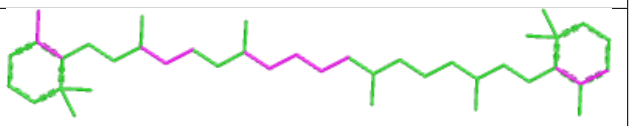
Torsions



Rings

Ligand BCR h 101

Bond lengths



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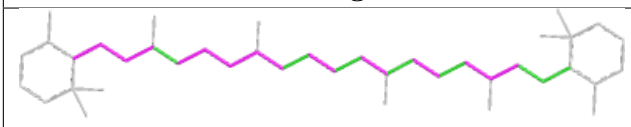
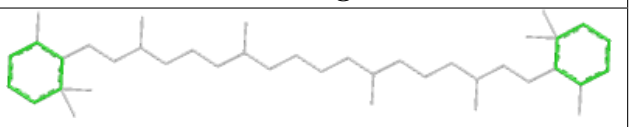
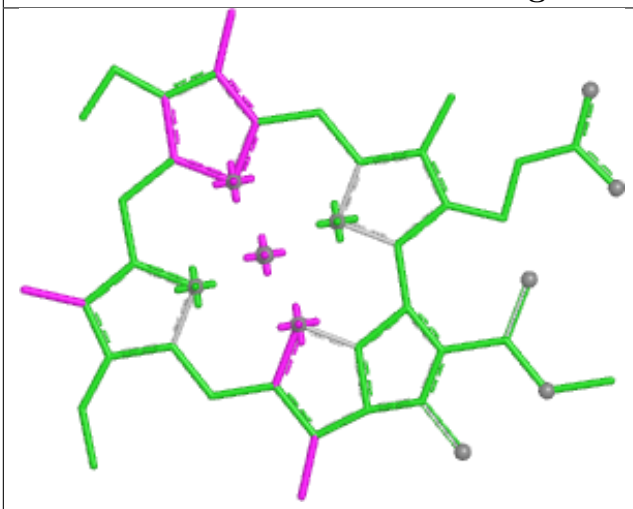


Torsions



Rings

Ligand CLA 2 835



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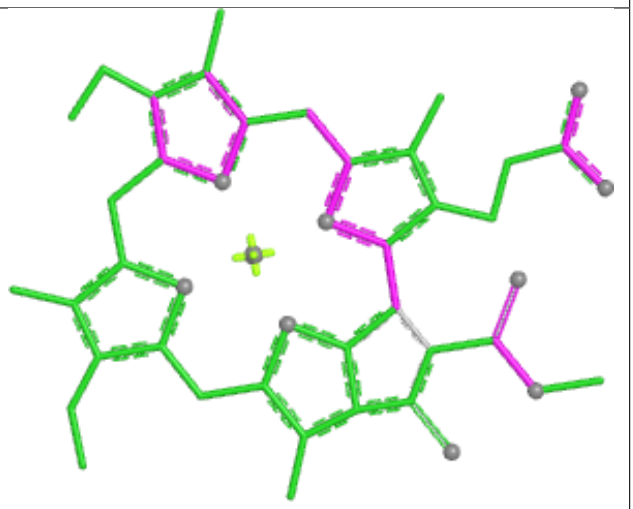
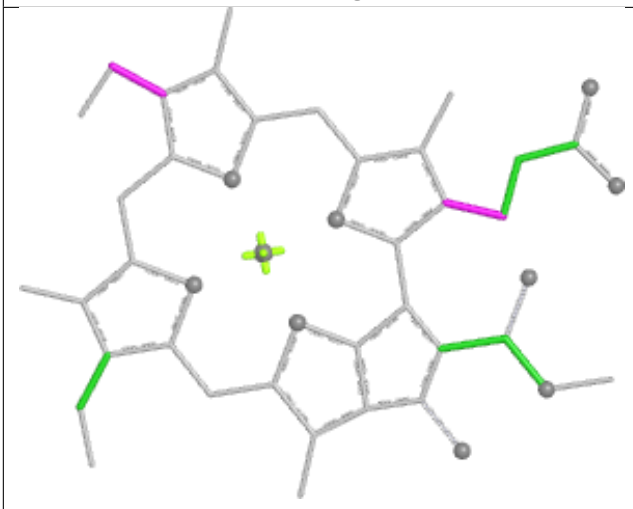


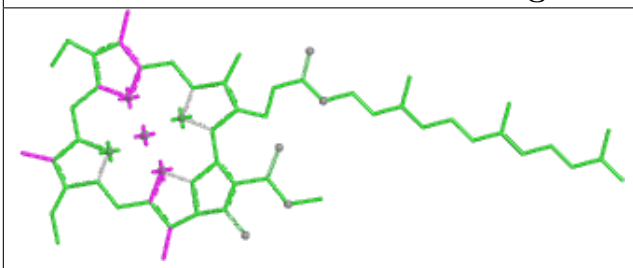
Bond angles



Torsions

Rings

Ligand CLA 2 829



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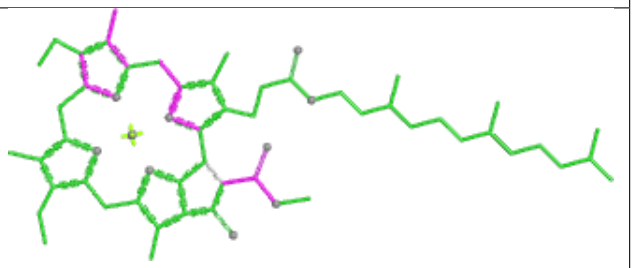

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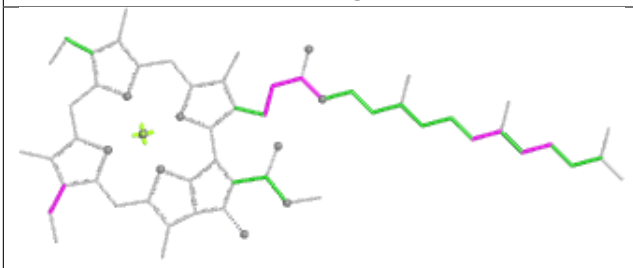
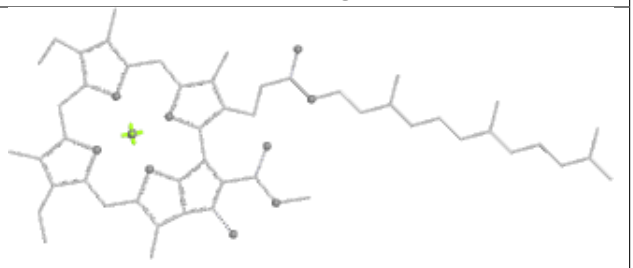
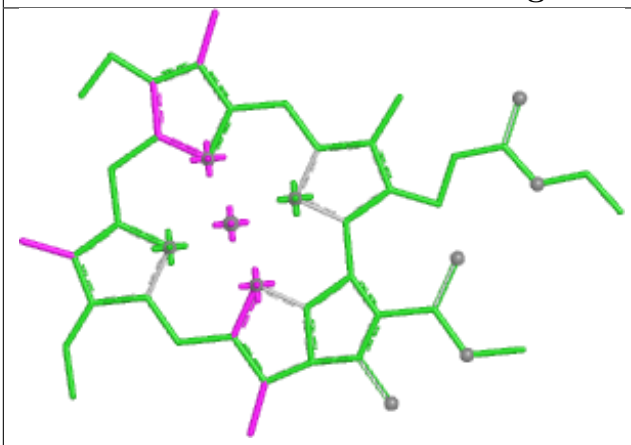


Torsions



Rings

Ligand CLA b 821



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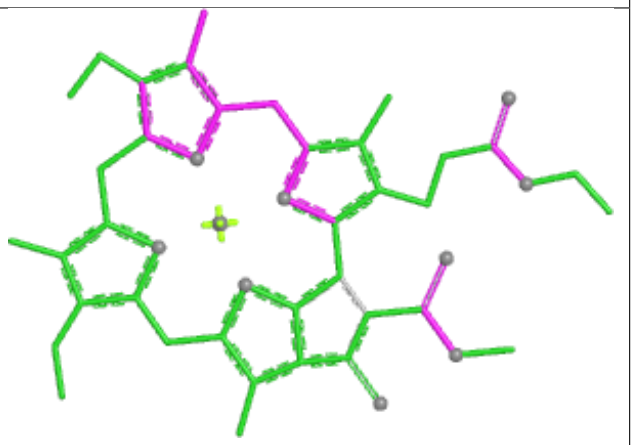
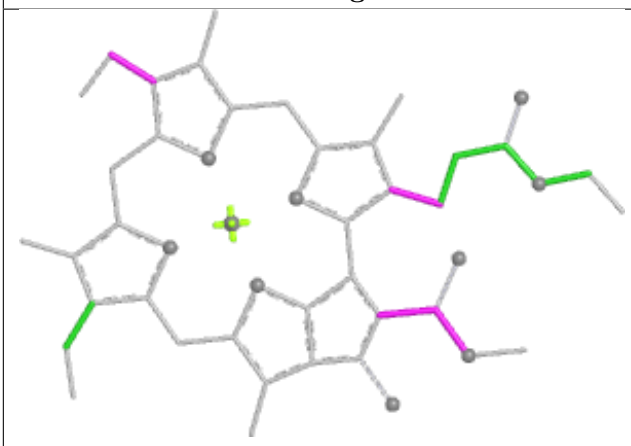


Bond angles



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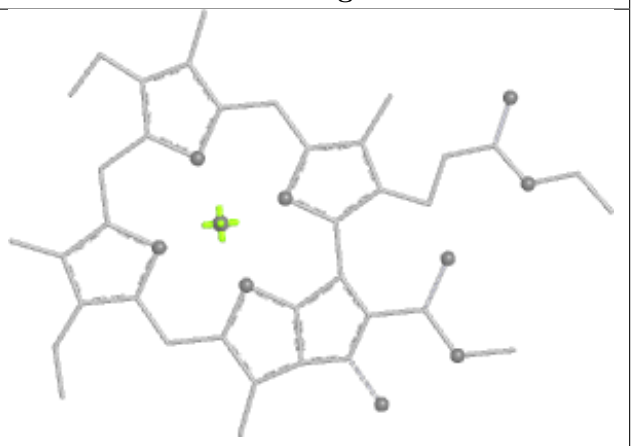
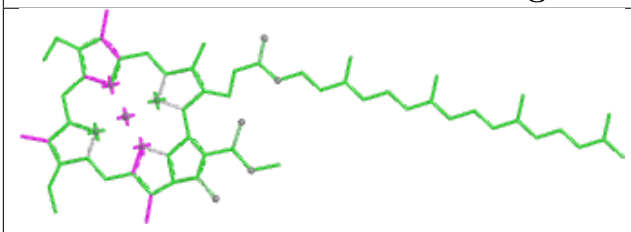


Rings

Ligand CLA 2 815



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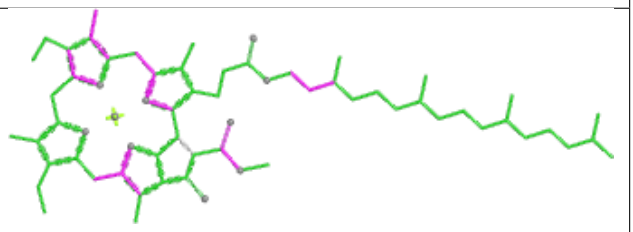

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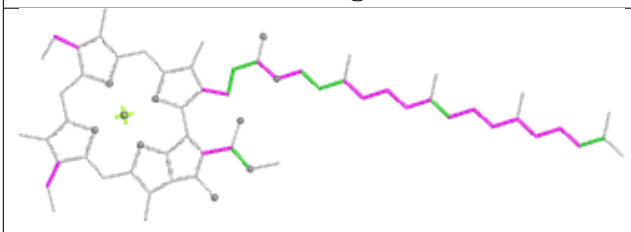

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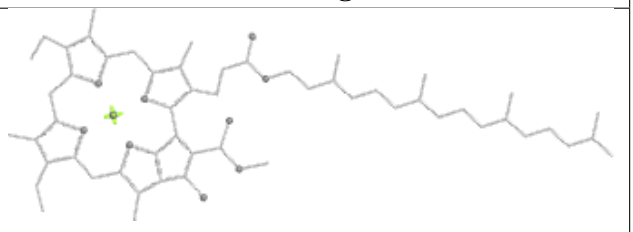
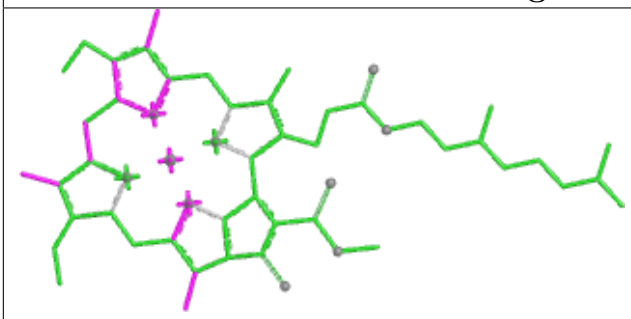


Rings

Ligand CLA 2 826



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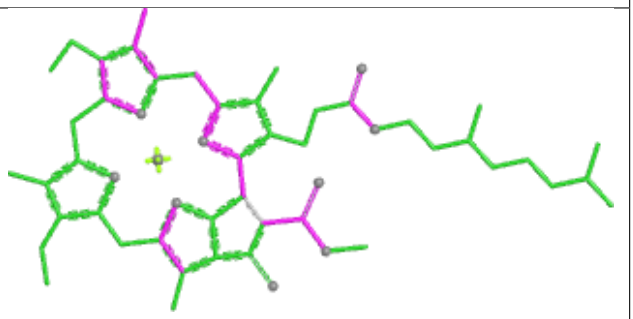
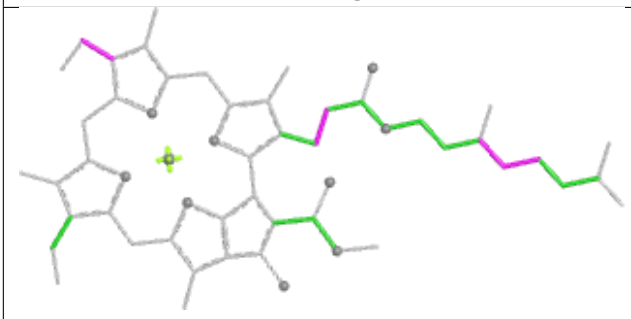


Bond angles



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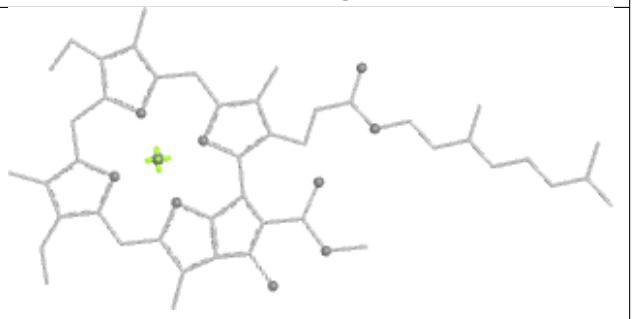
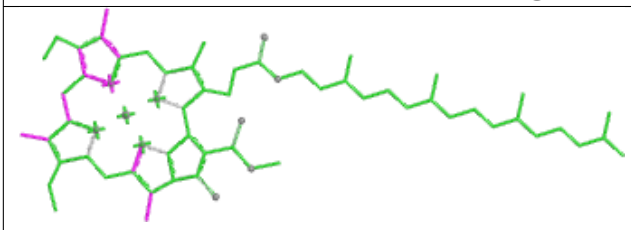


Rings

Ligand CLA 0 208



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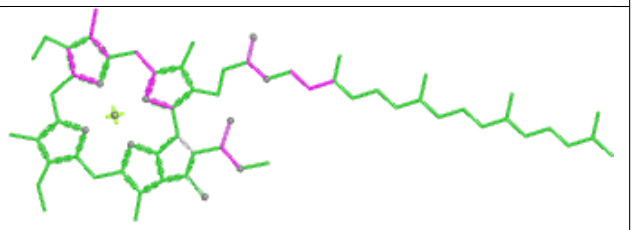

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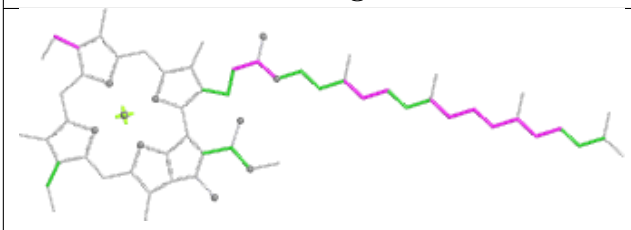

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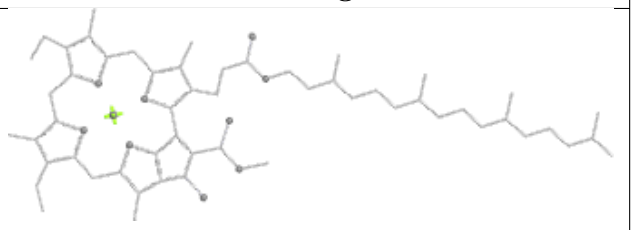
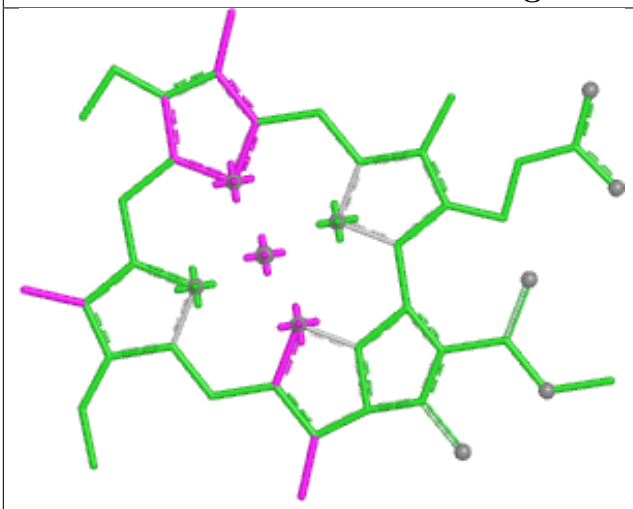


Rings

Ligand CLA A 816



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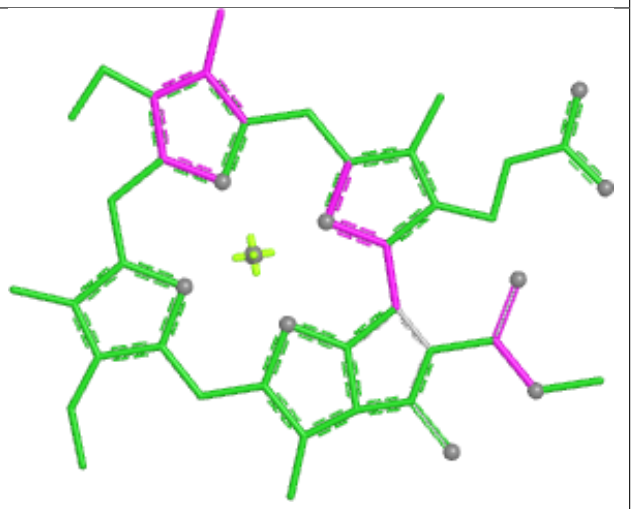
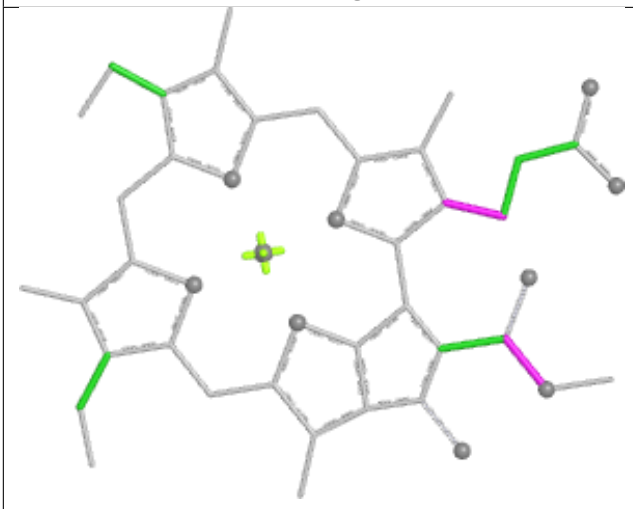


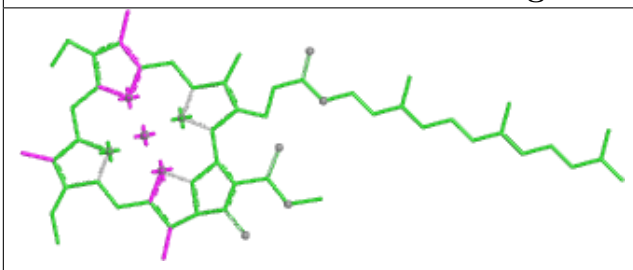
Bond angles



Torsions

Rings

Ligand CLA b 829



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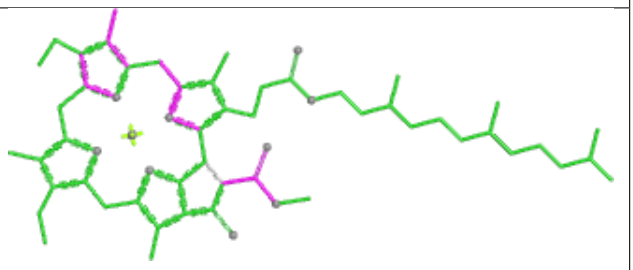

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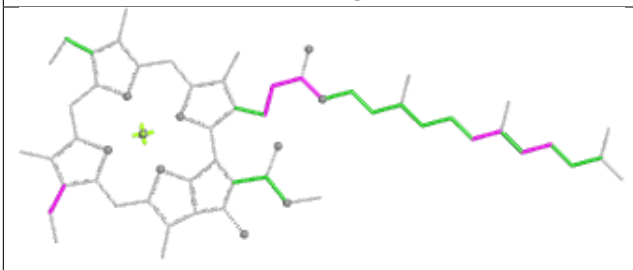
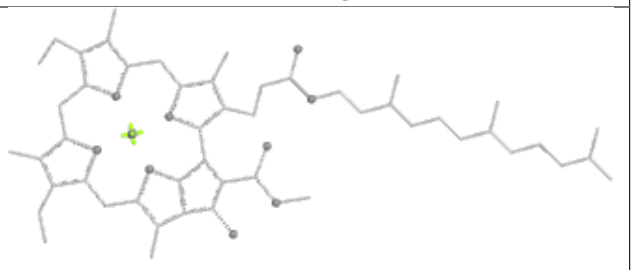
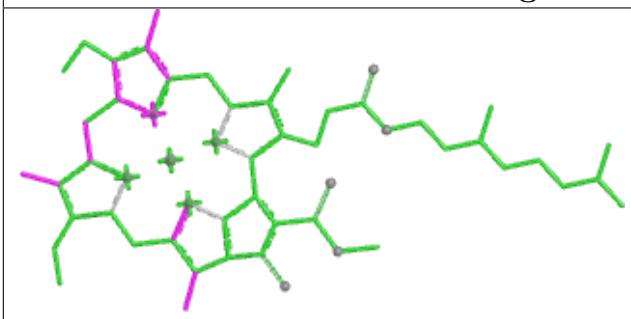
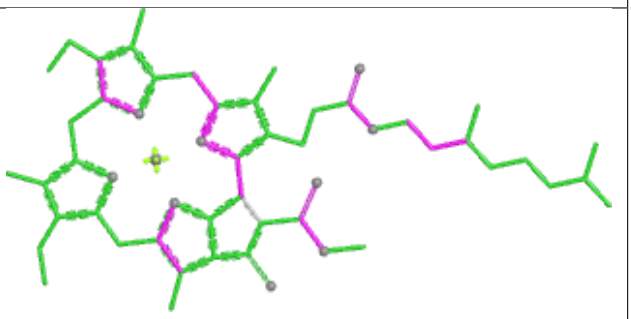
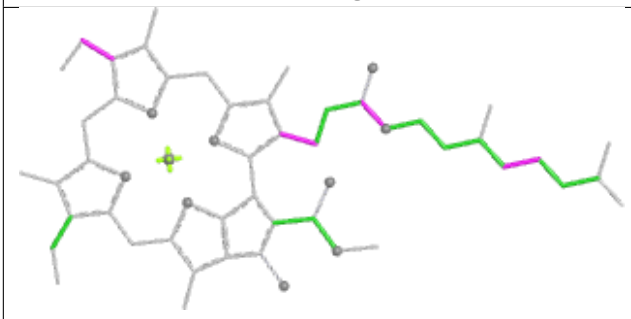
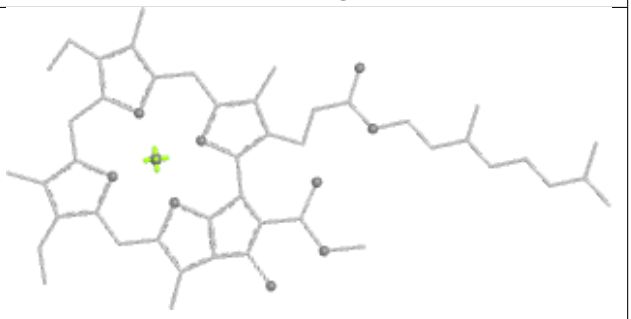
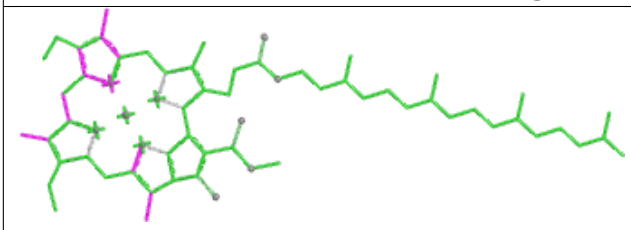
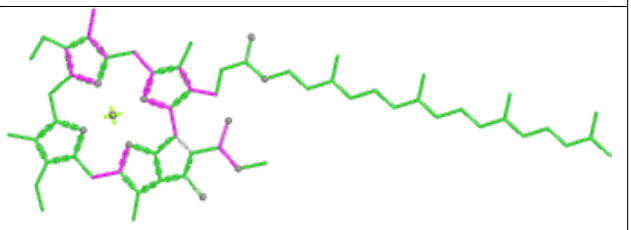
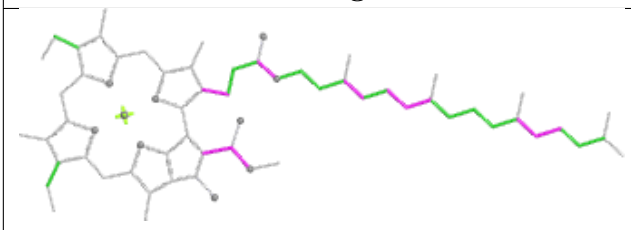
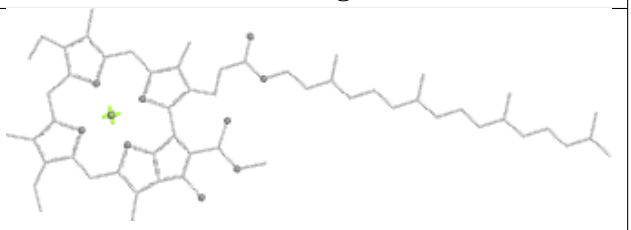


Torsions

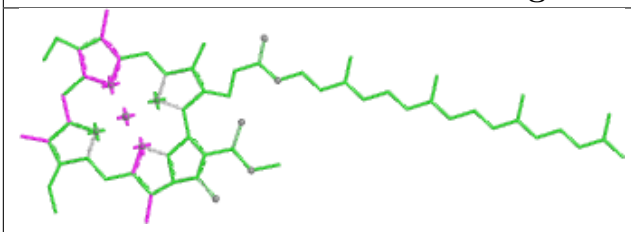


Rings

Ligand CLA 8 4004	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 0 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 0 207



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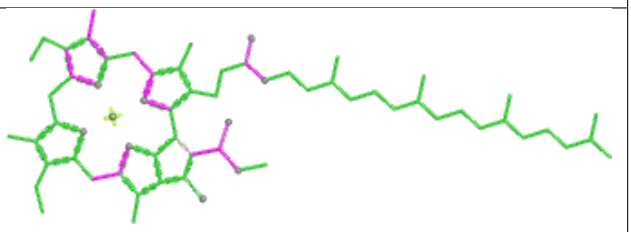
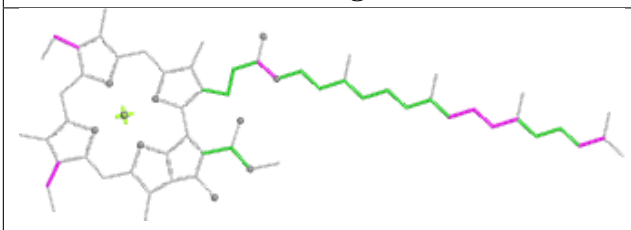
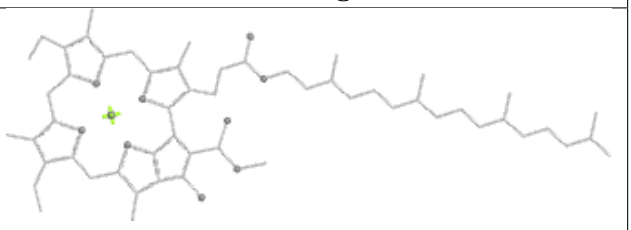


Bond angles

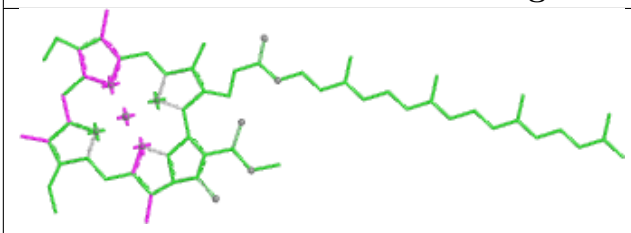


Torsions

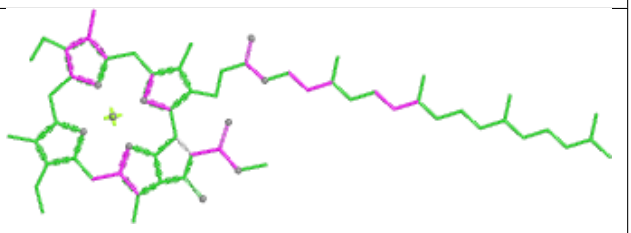


Rings

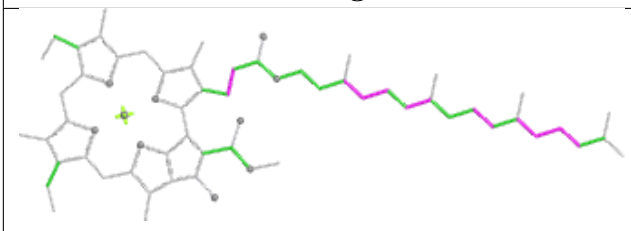
Ligand CLA a 831



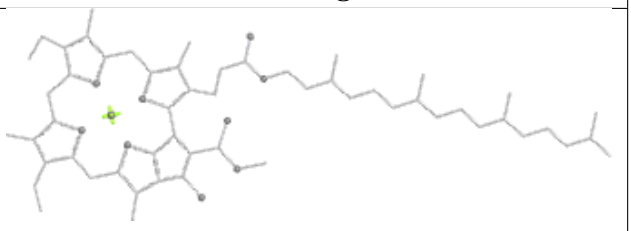
Bond lengths



Bond angles

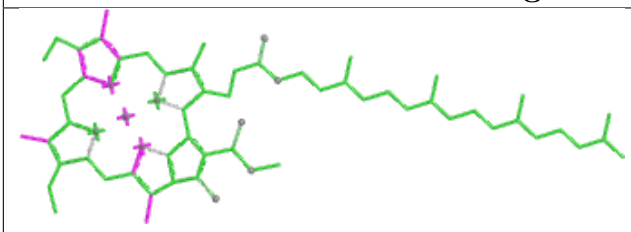


Torsions



Rings

Ligand CLA A 843



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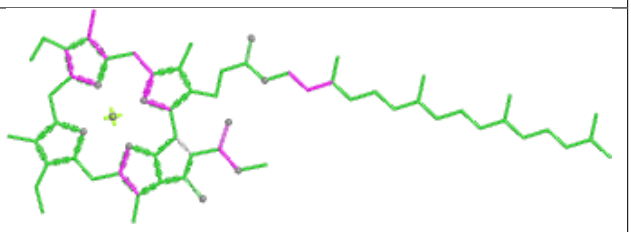
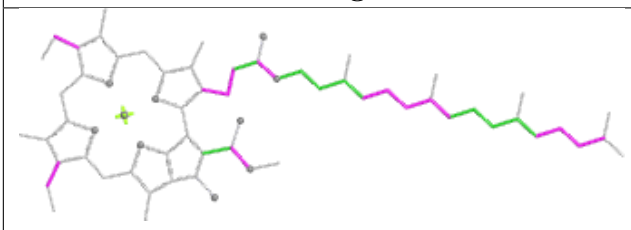
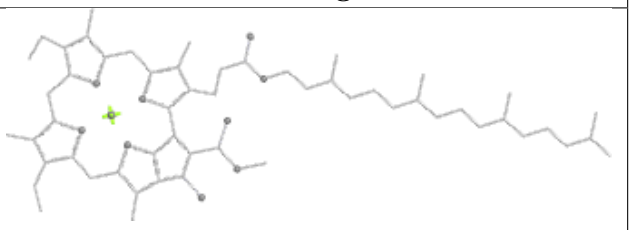


Bond angles

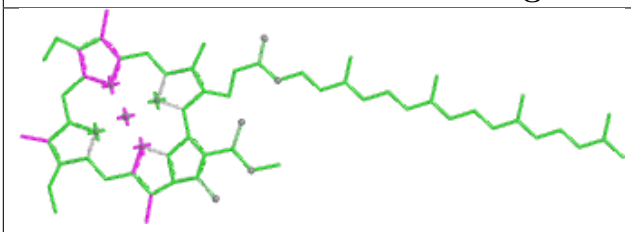


Torsions

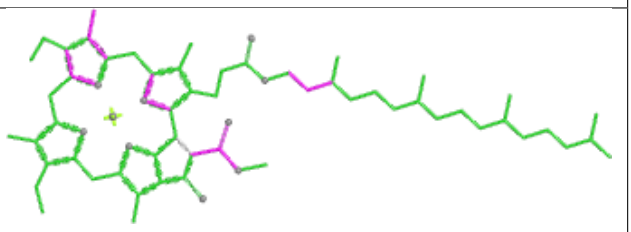


Rings

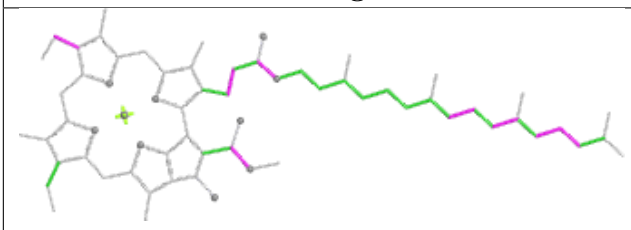
Ligand CLA A 839



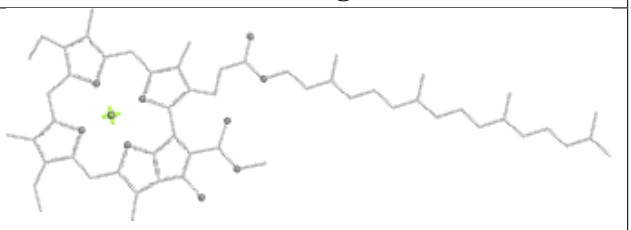
Bond lengths



Bond angles

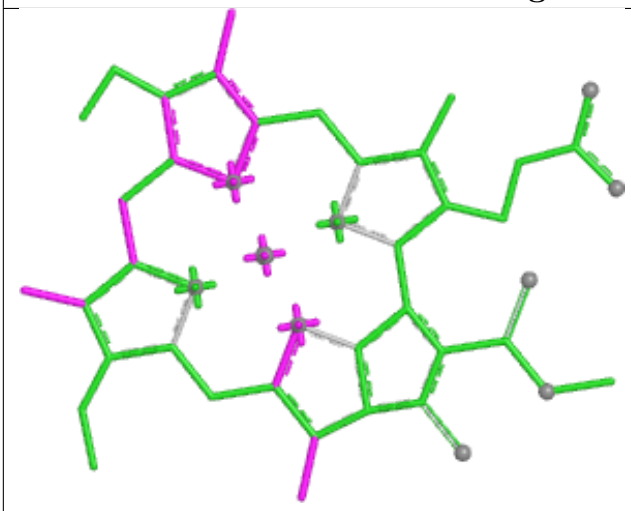


Torsions



Rings

Ligand CLA 2 832



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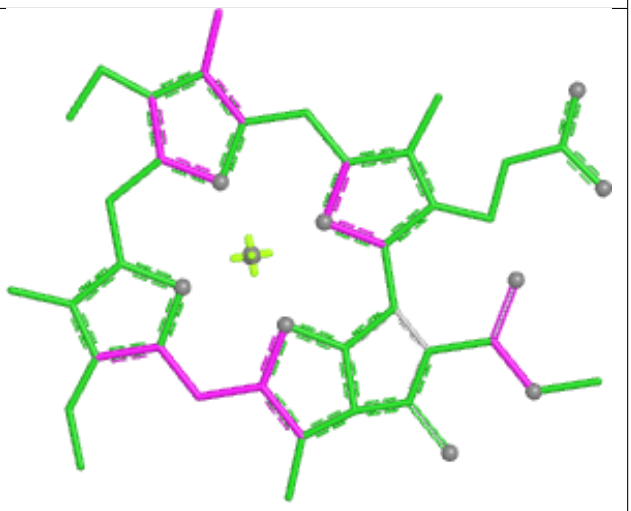
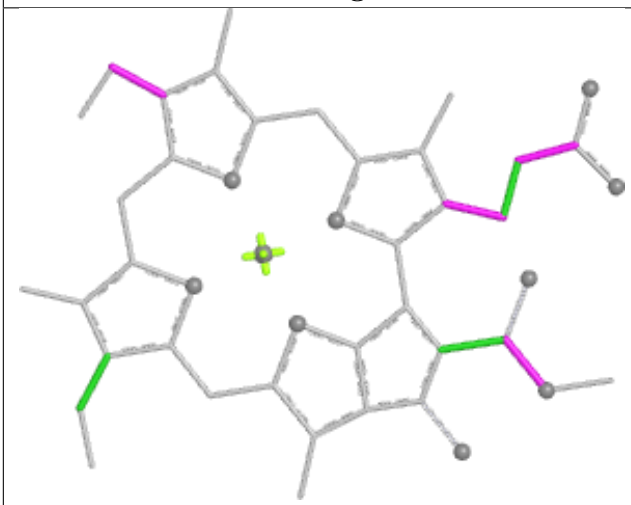
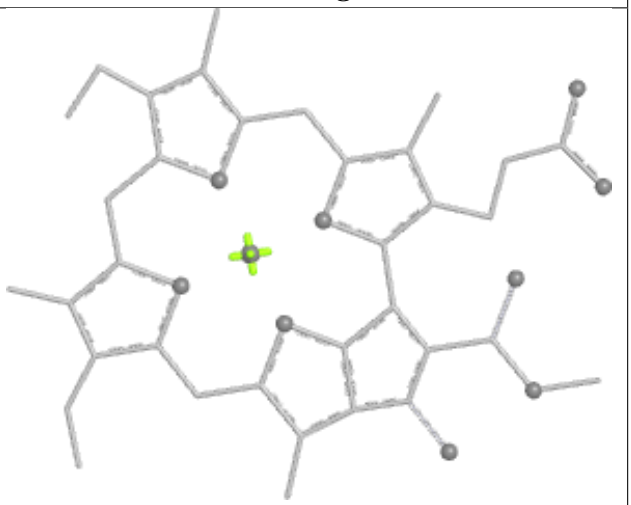


Bond angles

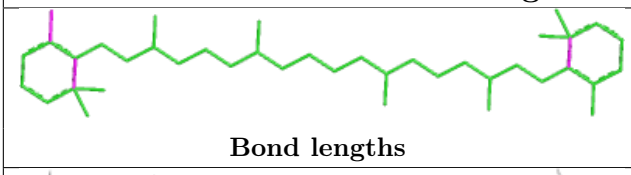


Torsions



Rings

Ligand BCR A 849



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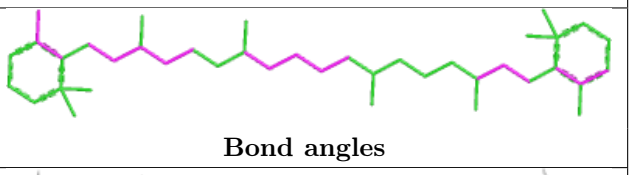
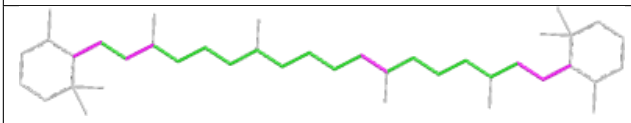
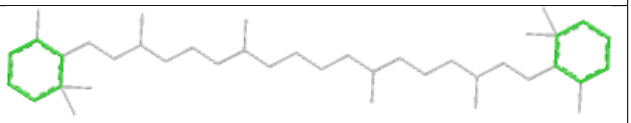


Bond angles

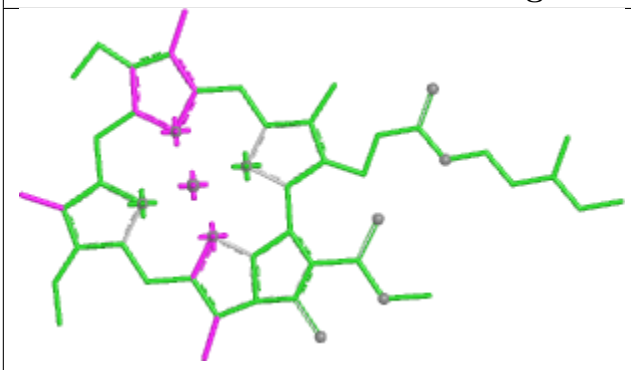


Torsions

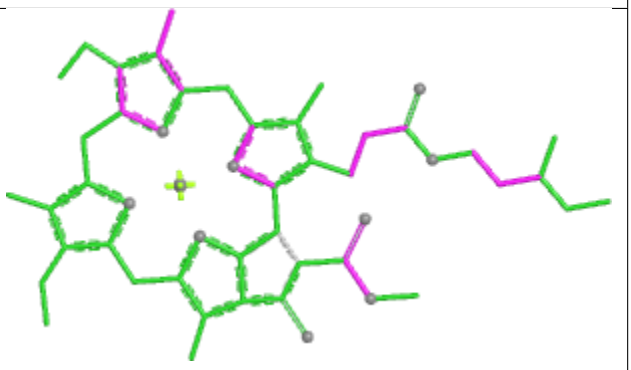


Rings

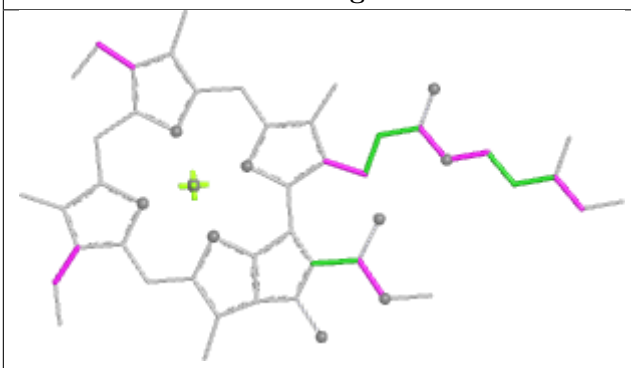
Ligand CLA F 201



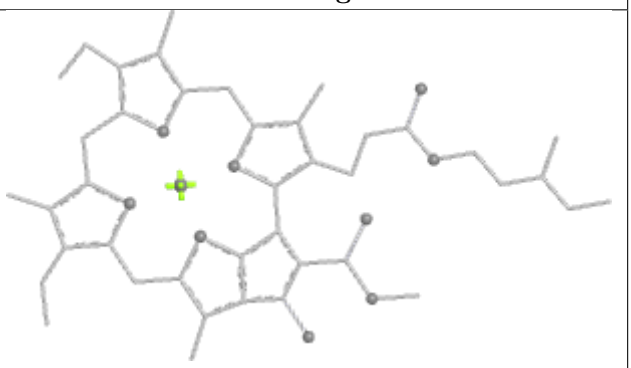
Bond lengths



Bond angles

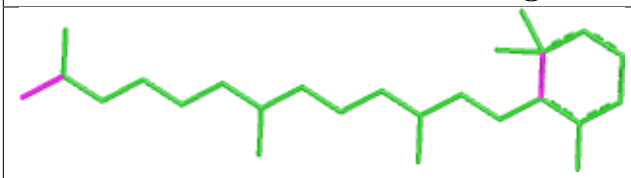


Torsions



Rings

Ligand BCR B 849



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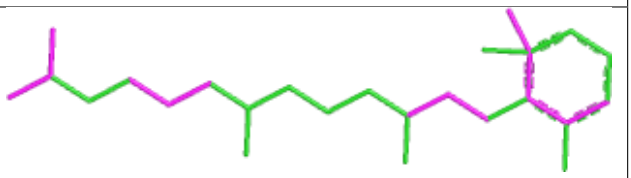
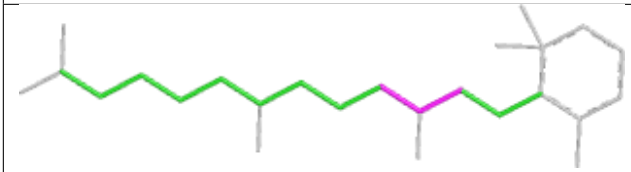


Bond angles



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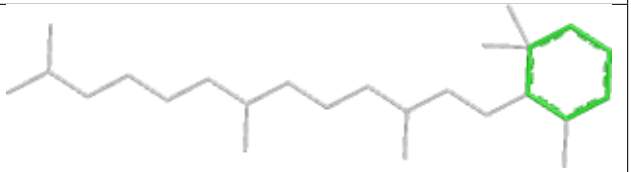
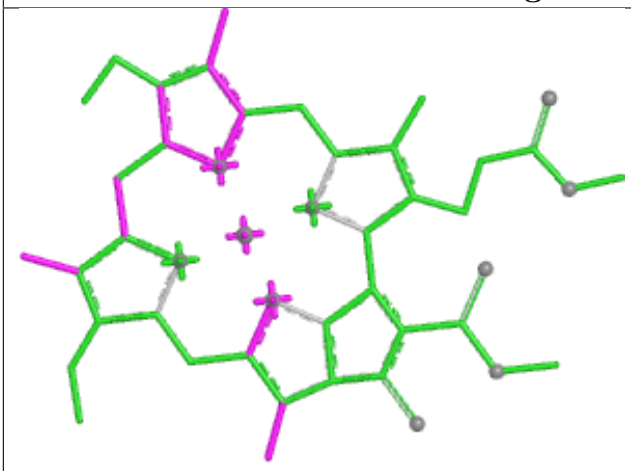
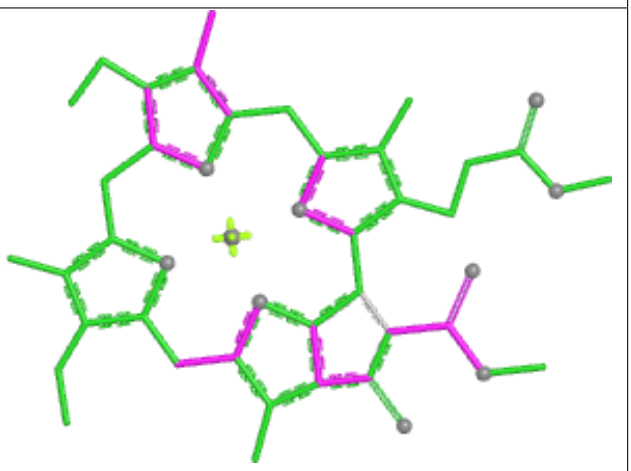


Rings

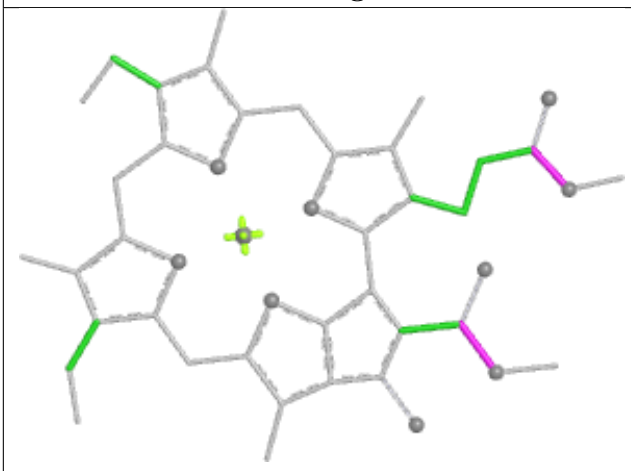
Ligand CLA B 842



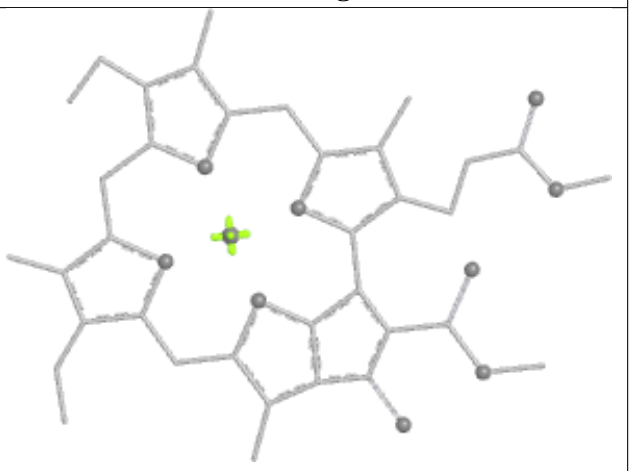
Bond lengths



Bond angles

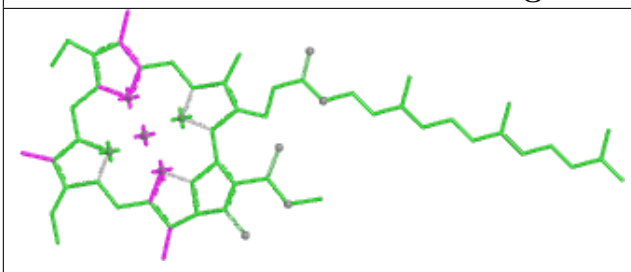


Torsions

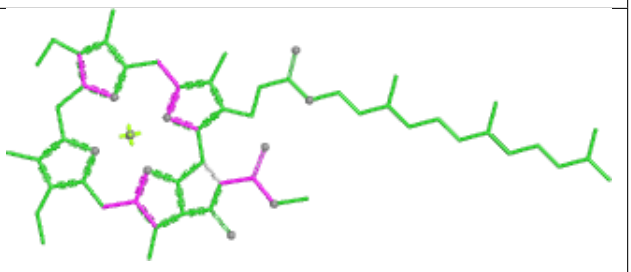


Rings

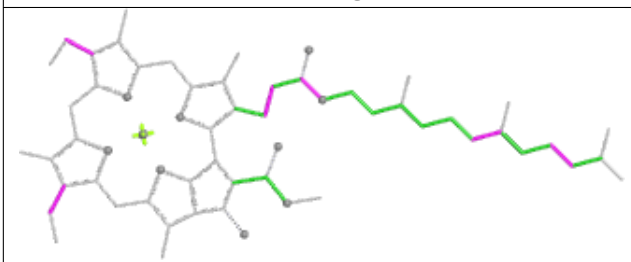
Ligand CLA B 810



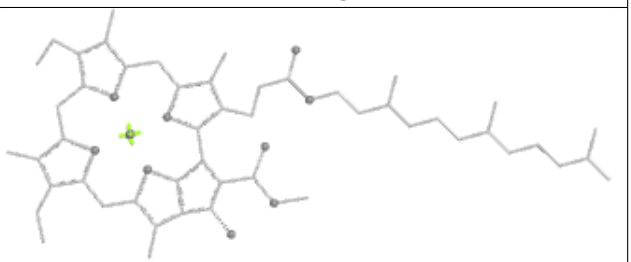
Bond lengths



Bond angles

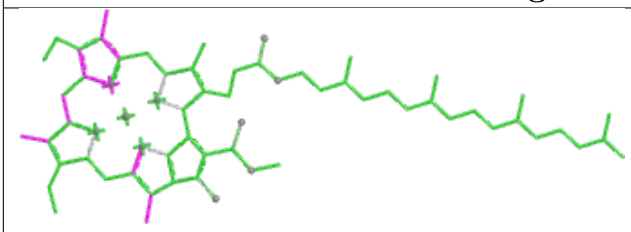


Torsions

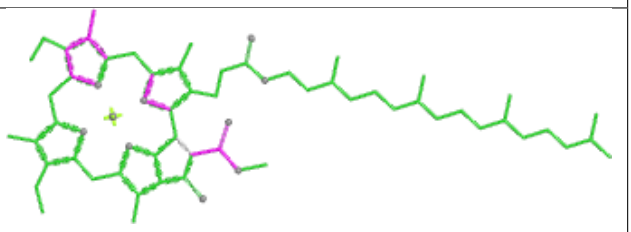


Rings

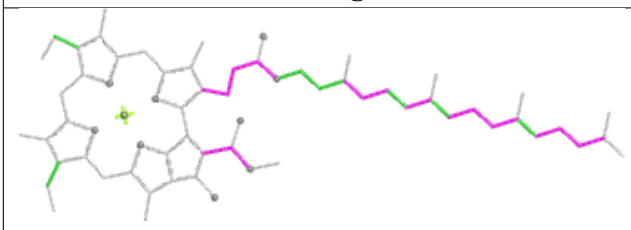
Ligand CLA 1 809



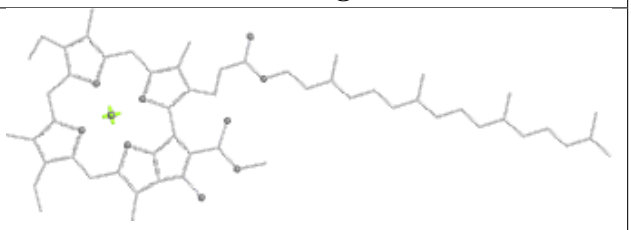
Bond lengths



Bond angles



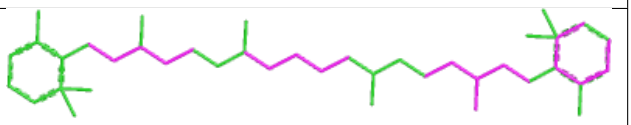
Torsions



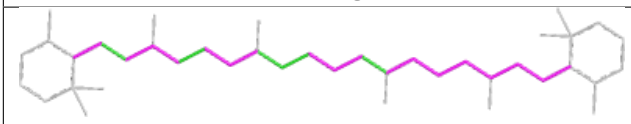
Rings

Ligand BCR 2 850

Bond lengths



Bond angles



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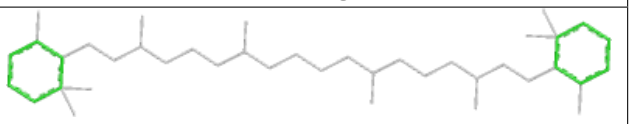
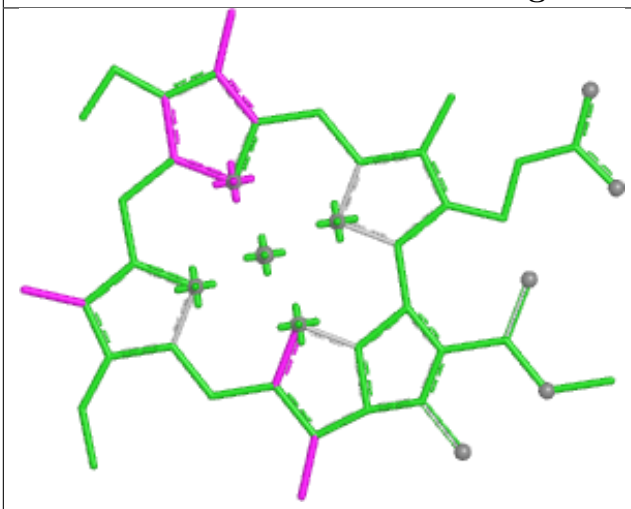


Rings

Ligand CLA 1 816



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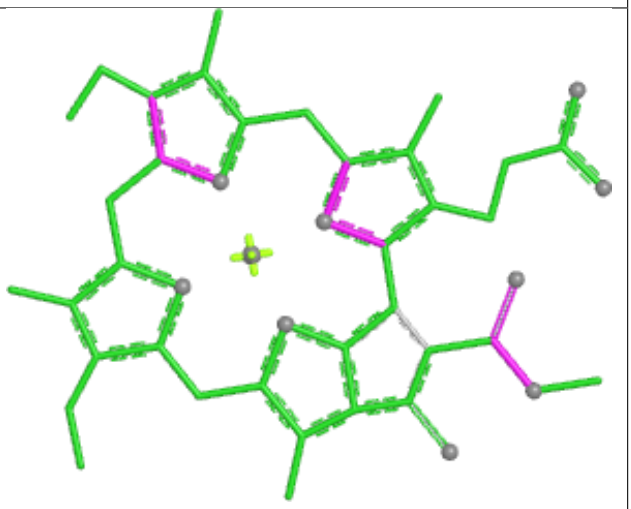
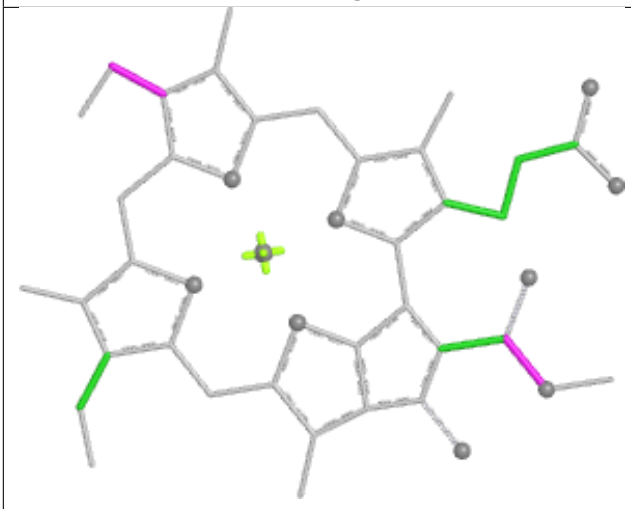


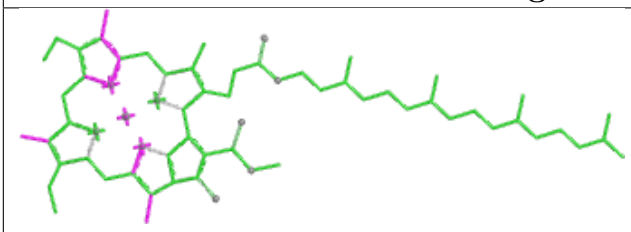
Bond angles



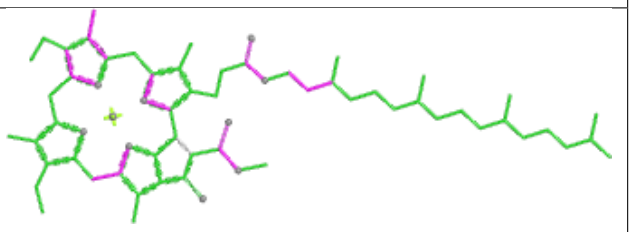
Torsions

Rings

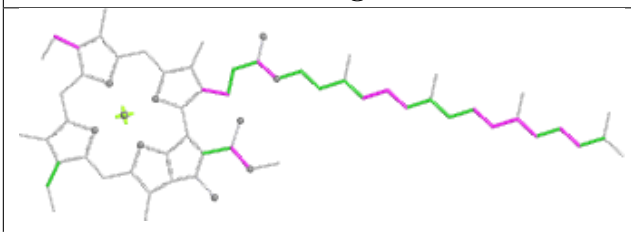
Ligand CLA a 809



Bond lengths



Bond angles



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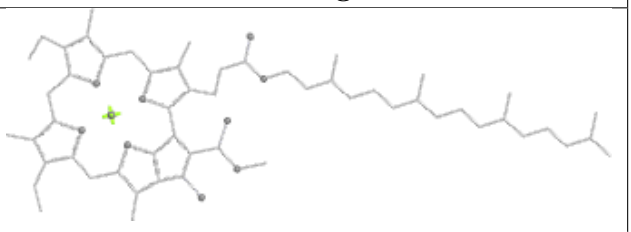
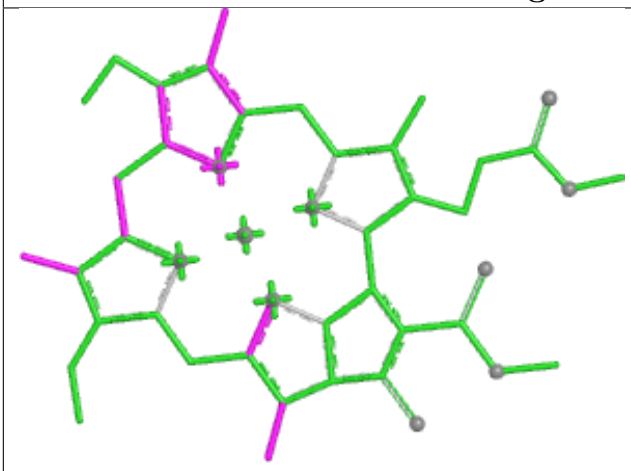


Rings

Ligand CLA 2 816



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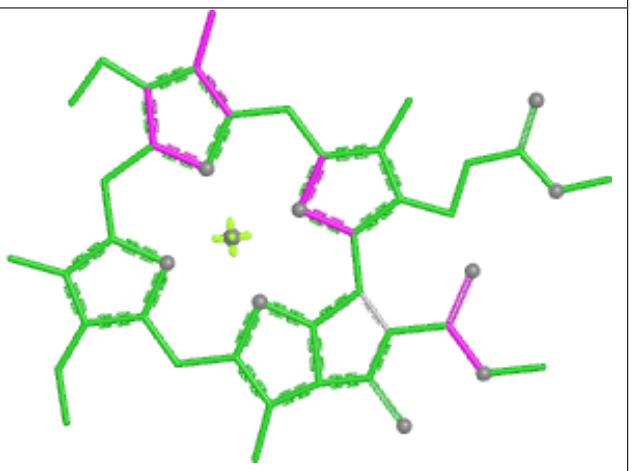
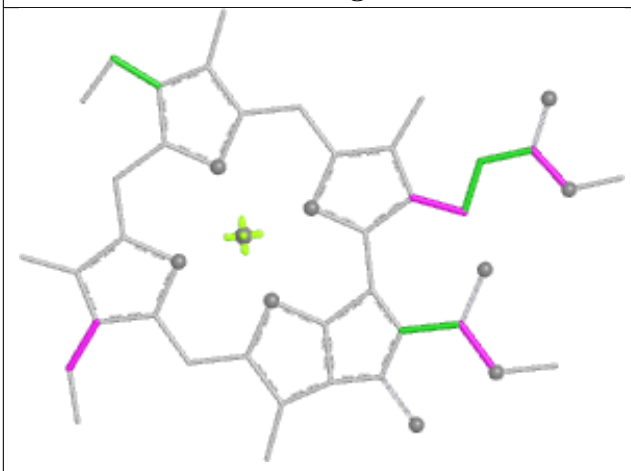
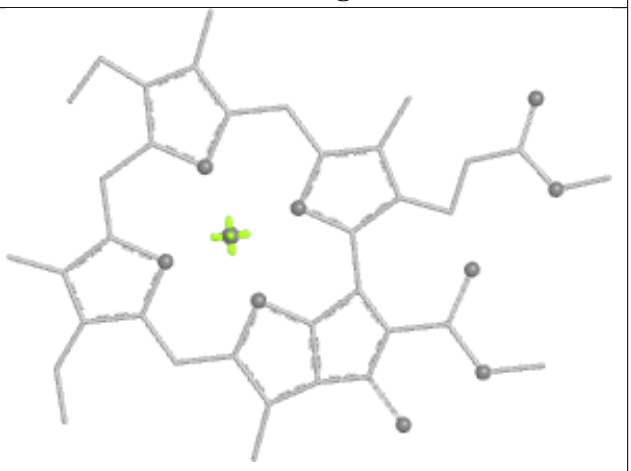


Bond angles

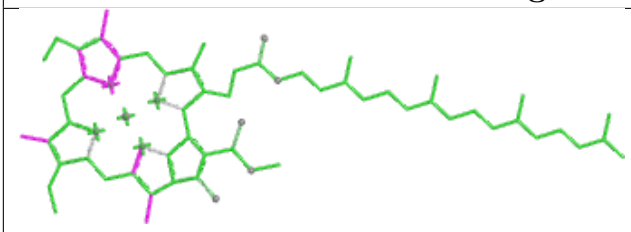


Torsions

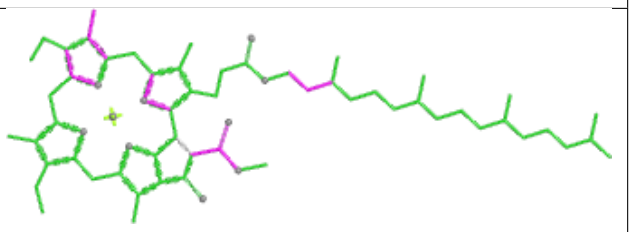


Rings

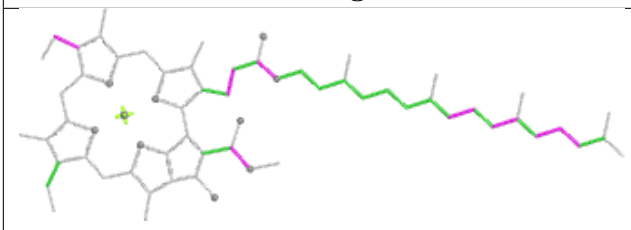
Ligand CLA 1 838



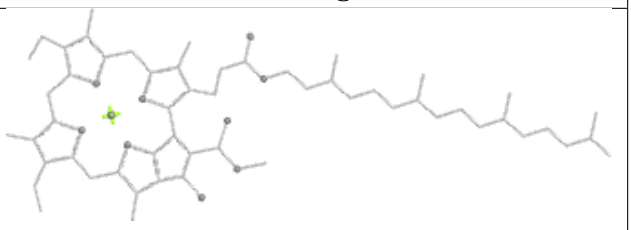
Bond lengths



Bond angles

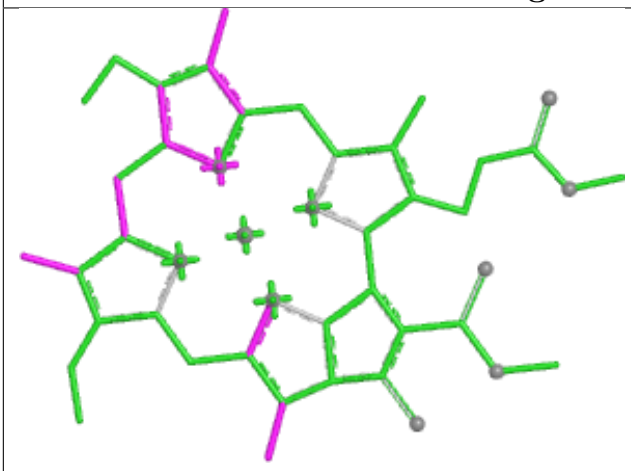


Torsions

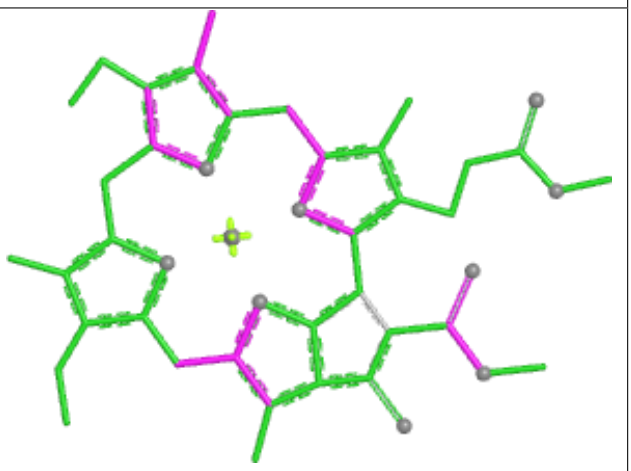


Rings

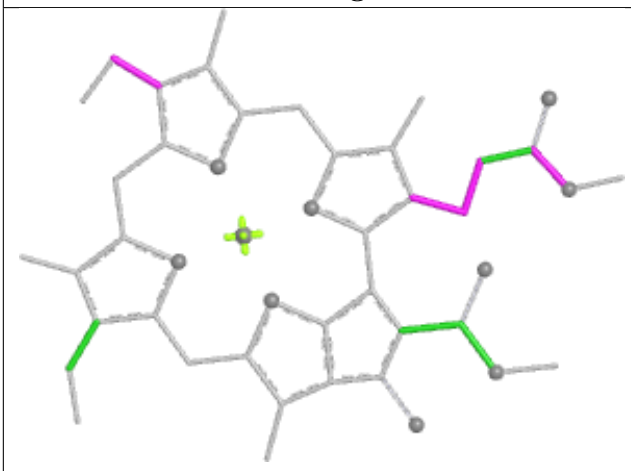
Ligand CLA 2 838



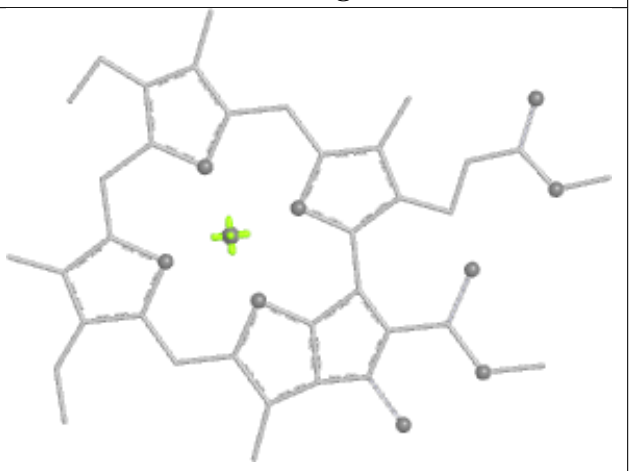
Bond lengths



Bond angles

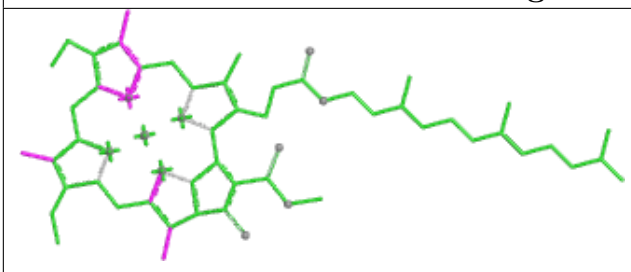


Torsions

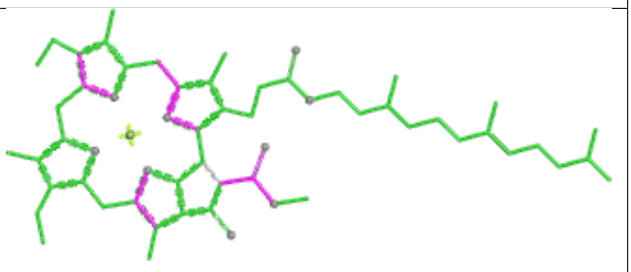


Rings

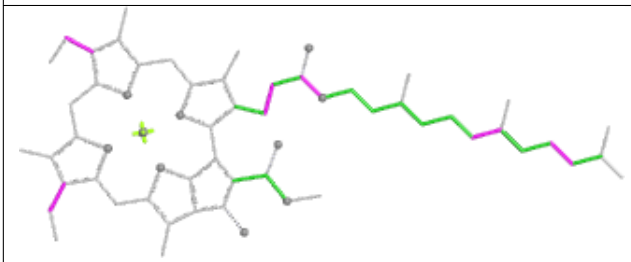
Ligand CLA b 810



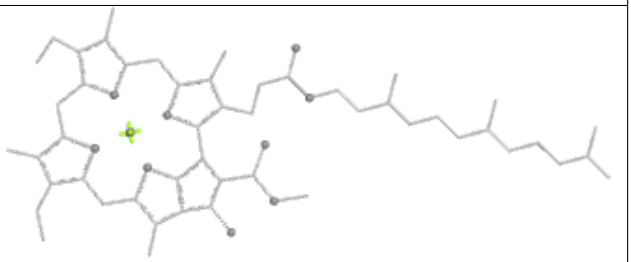
Bond lengths



Bond angles

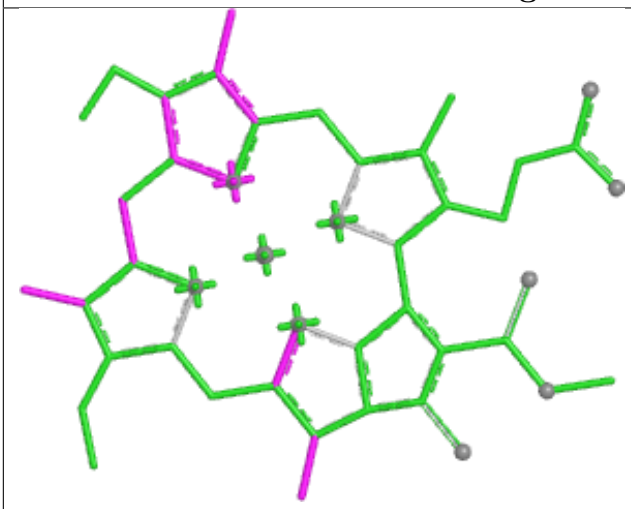


Torsions

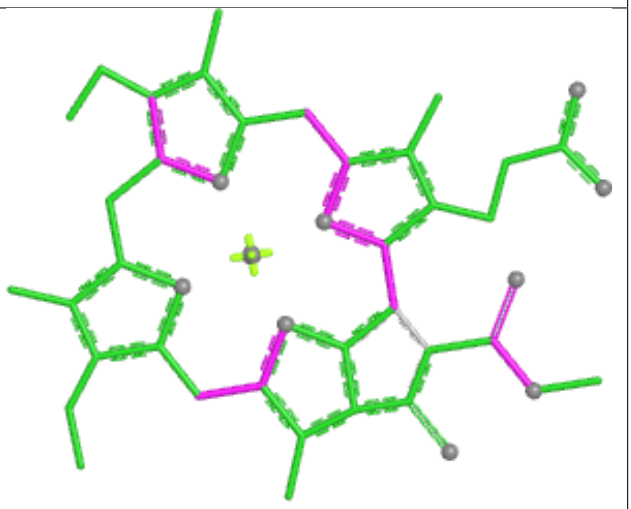


Rings

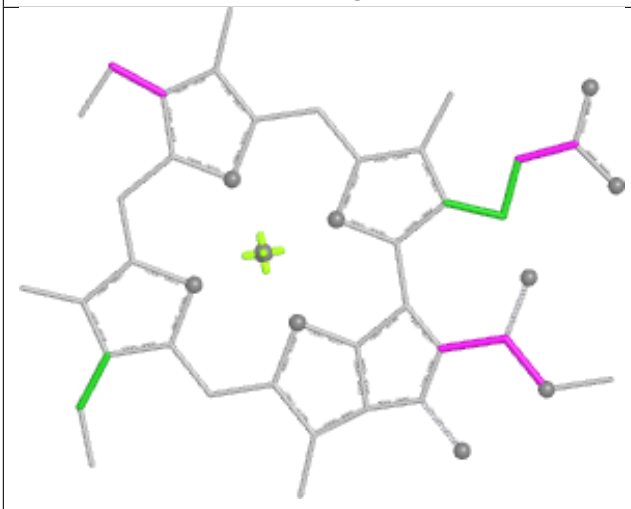
Ligand CLA 8 4002



Bond lengths



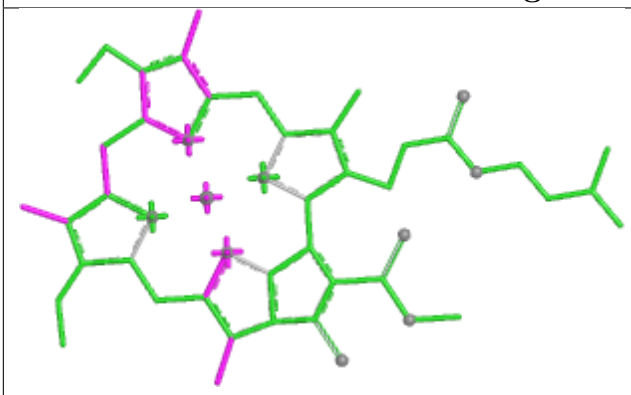
Bond angles



Torsions

Rings

Ligand CLA A 806



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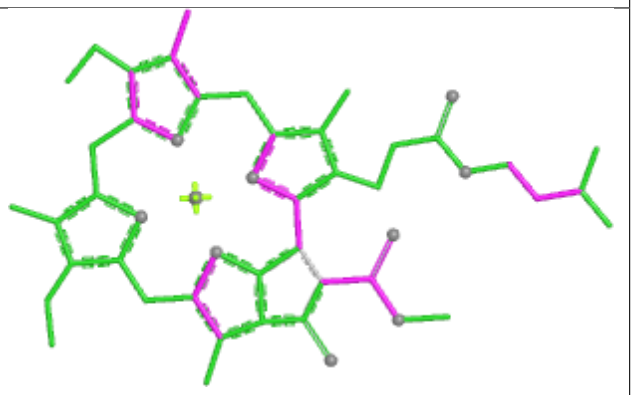
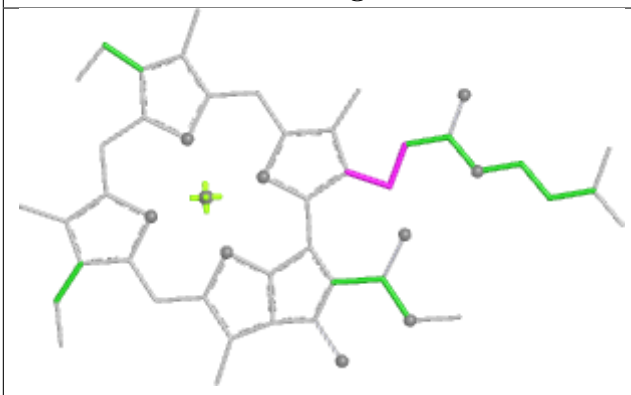
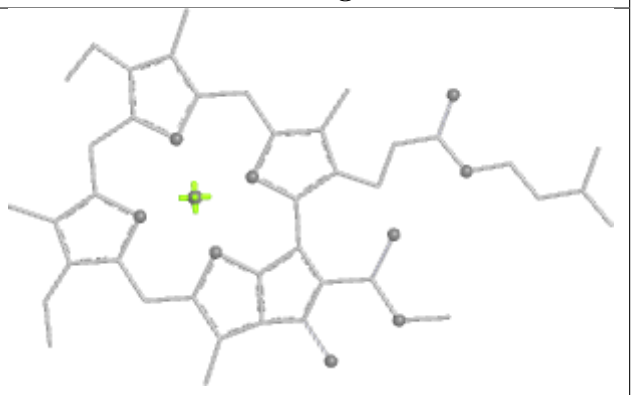


Bond angles

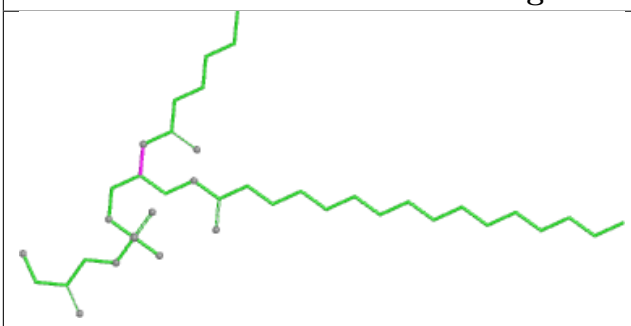


Torsions



Rings

Ligand LHG 2 852



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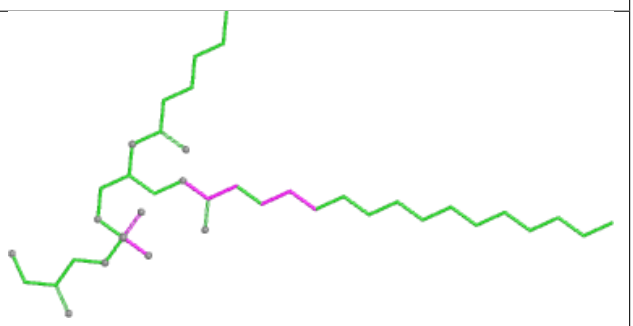
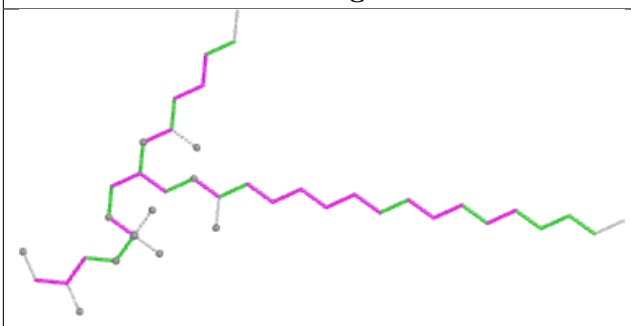


Bond angles



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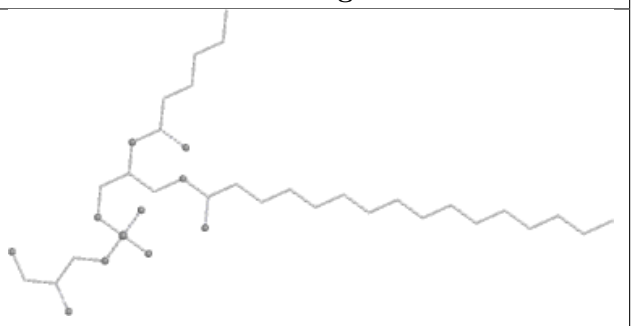
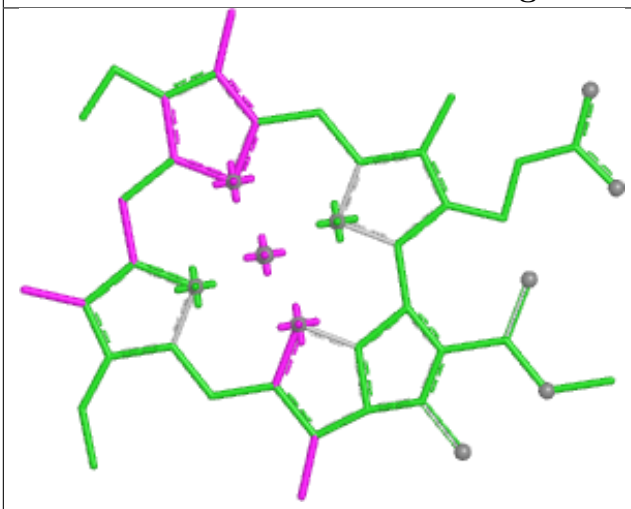


Rings

Ligand CLA 6 4404



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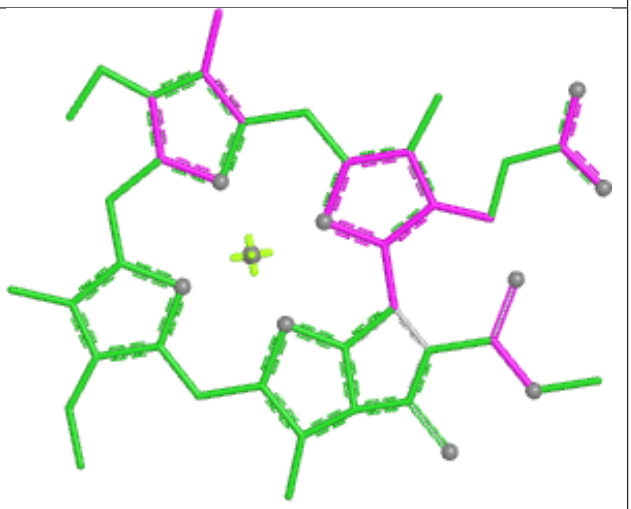

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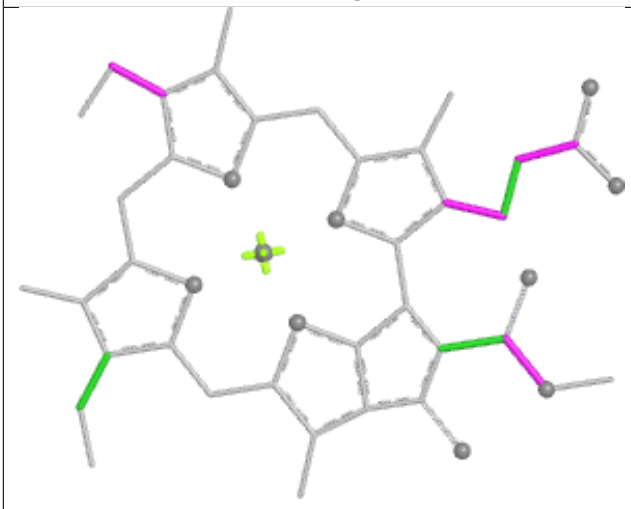
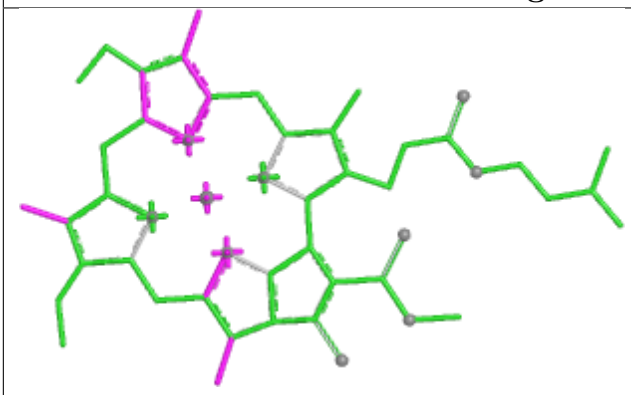


Torsions

Rings

Ligand CLA b 827



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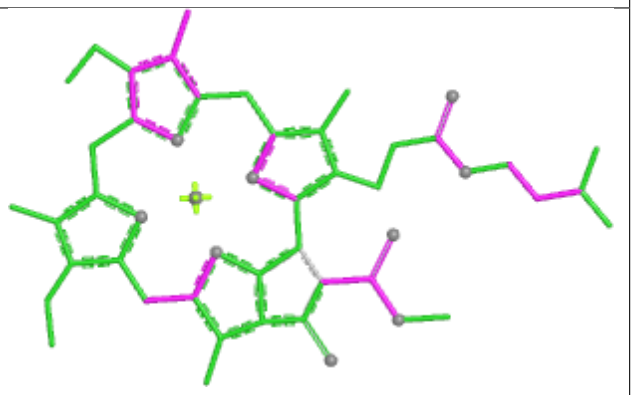

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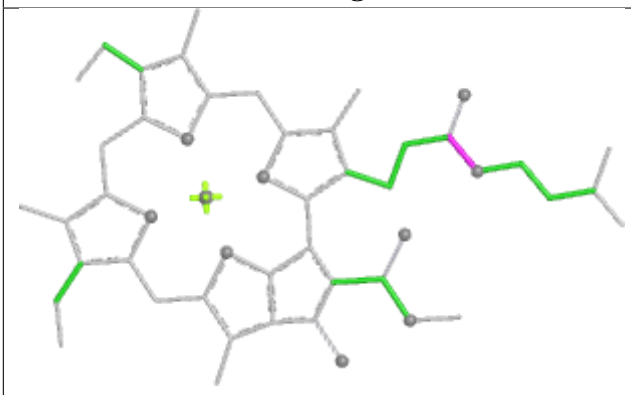

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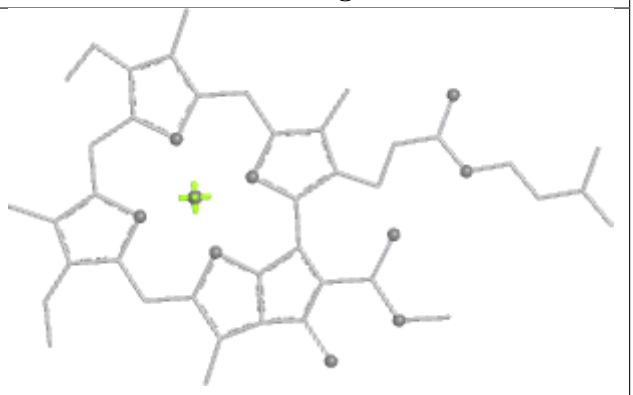
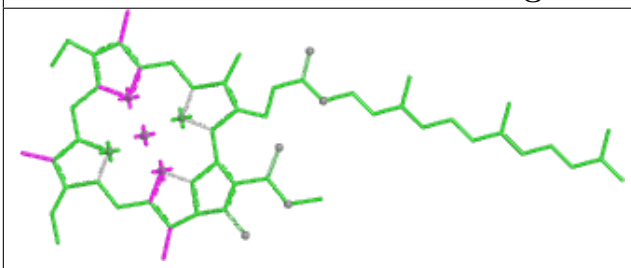


Rings

Ligand CLA B 832



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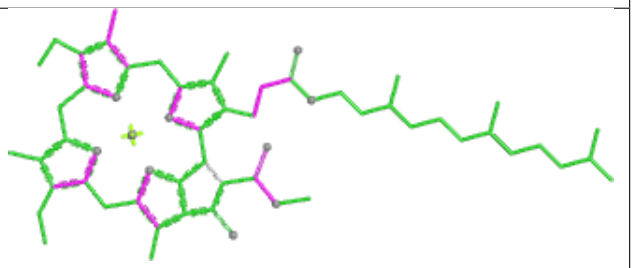
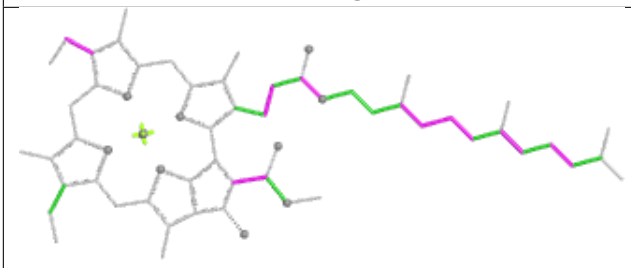


Bond angles



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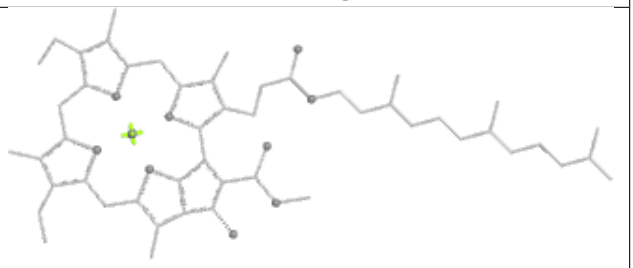
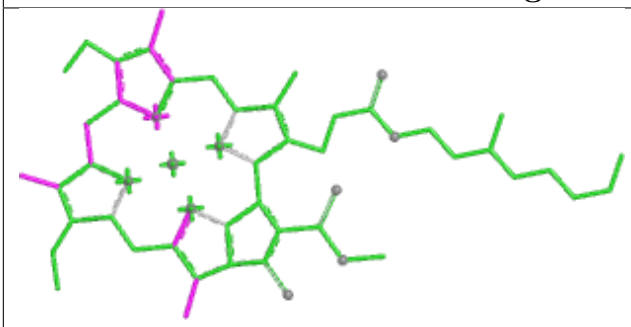


Rings

Ligand CLA B 807



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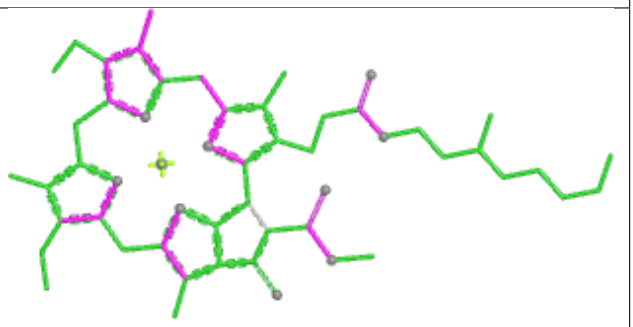
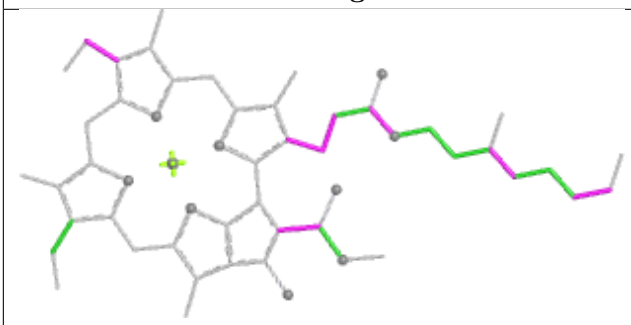
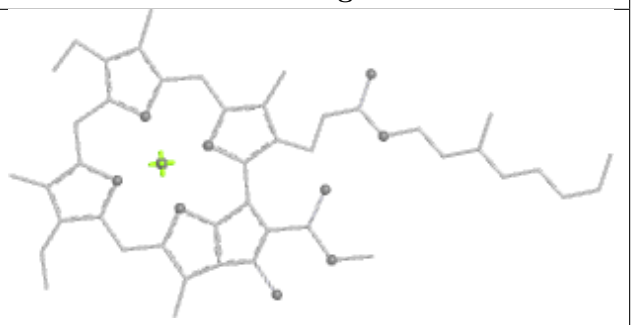


Bond angles

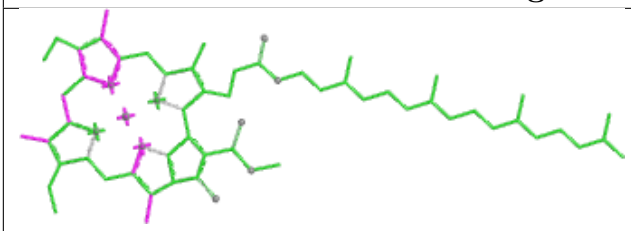


Torsions



Rings

Ligand CLA b 809



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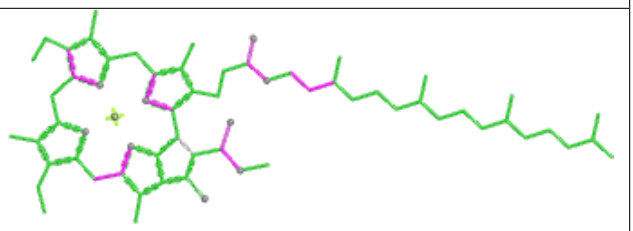
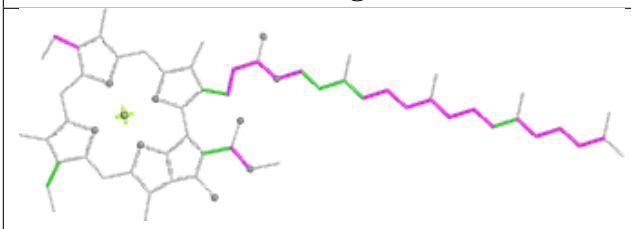
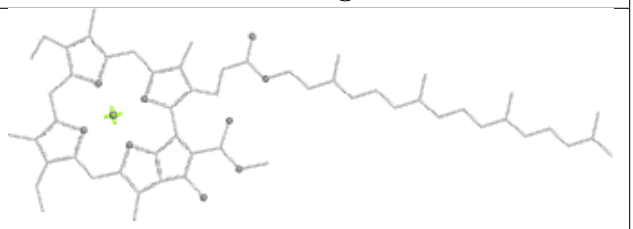


Bond angles

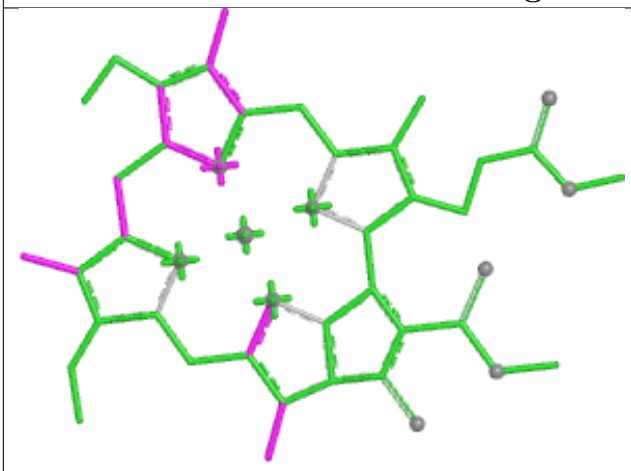


Torsions



Rings

Ligand CLA B 839



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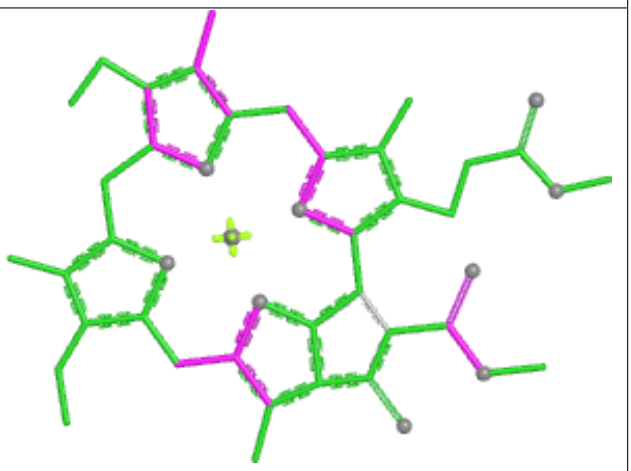

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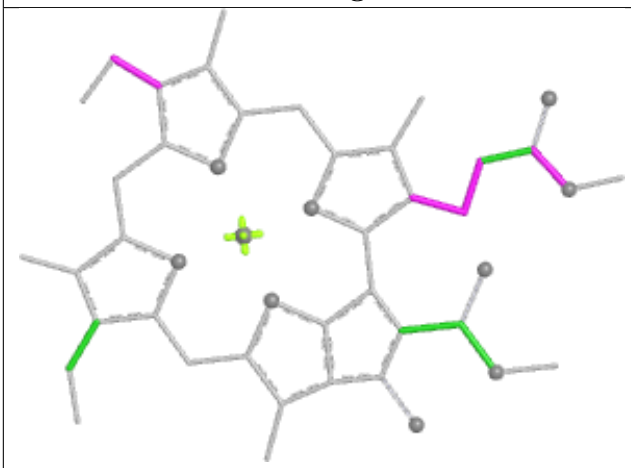

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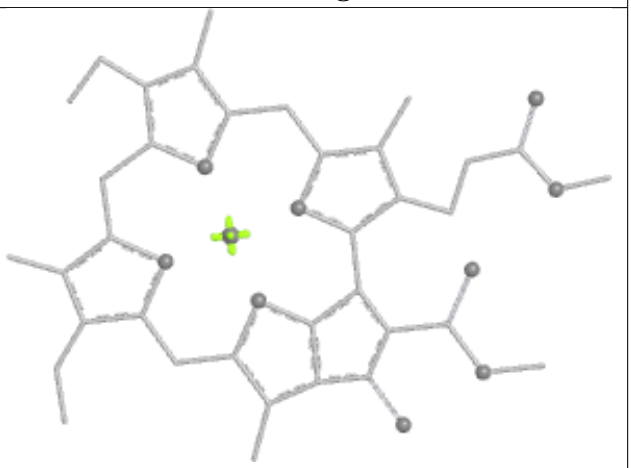
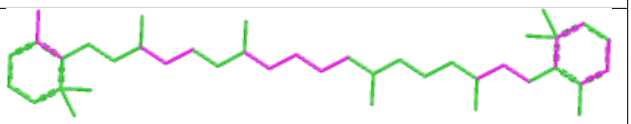


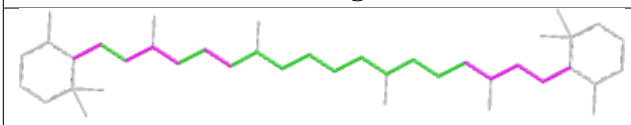
Rings

Ligand BCR 8 4001

Bond lengths



Bond angles



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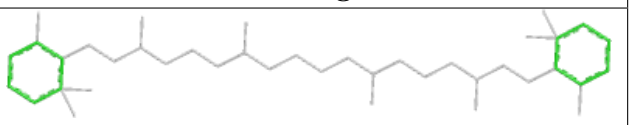
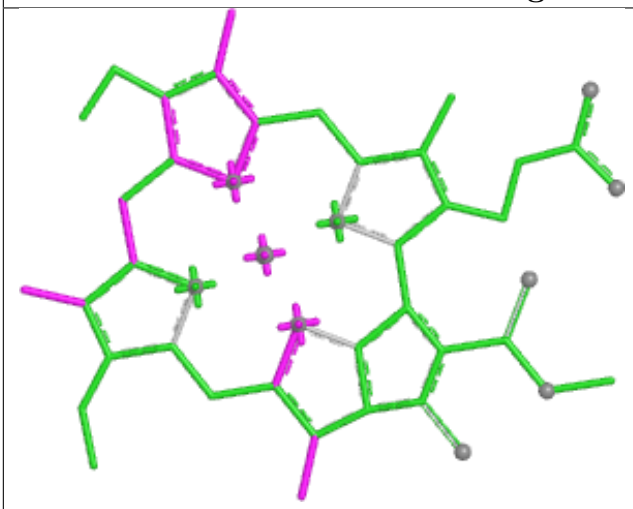


Rings

Ligand CLA b 832



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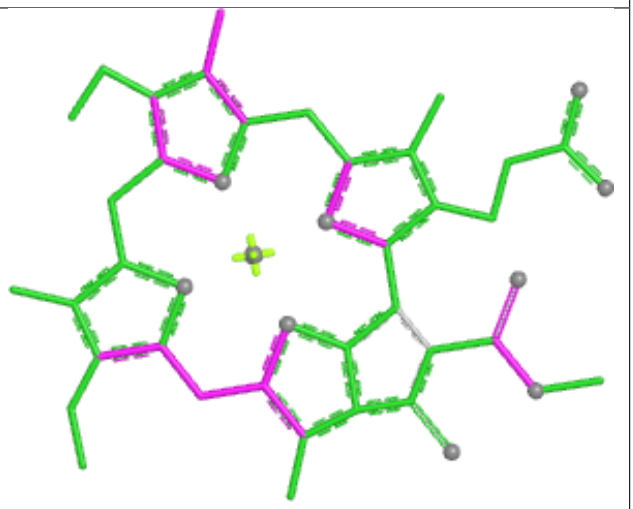

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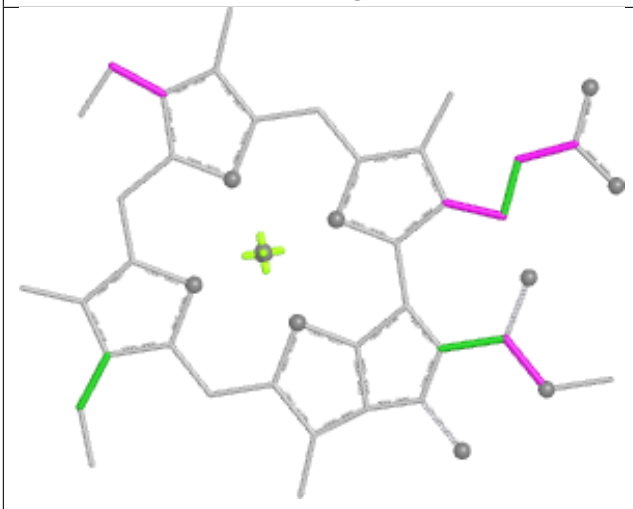
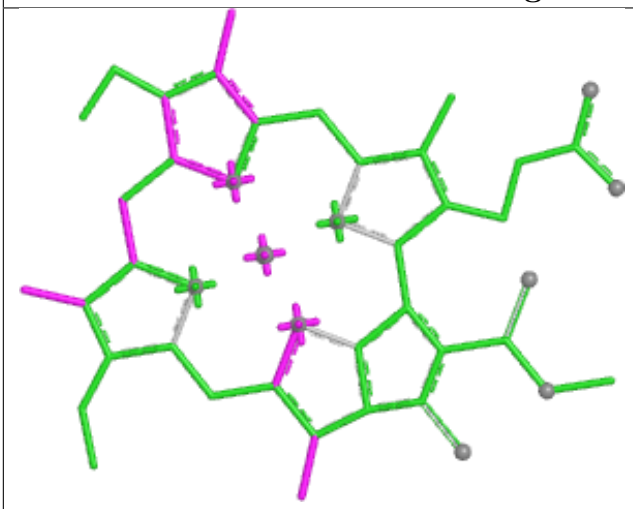


Torsions

Rings

Ligand CLA B 837



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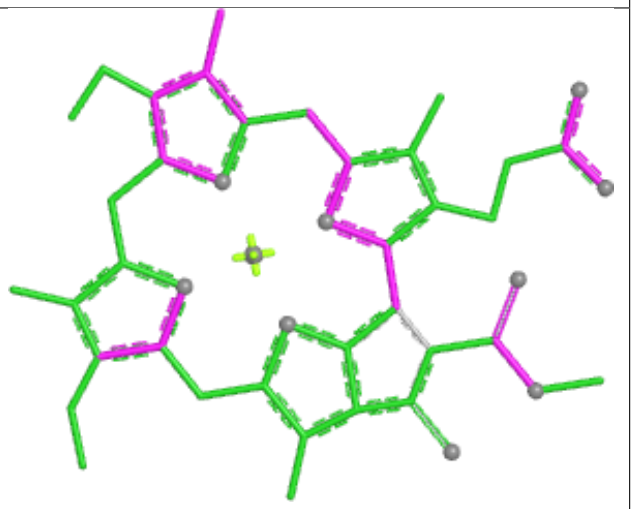
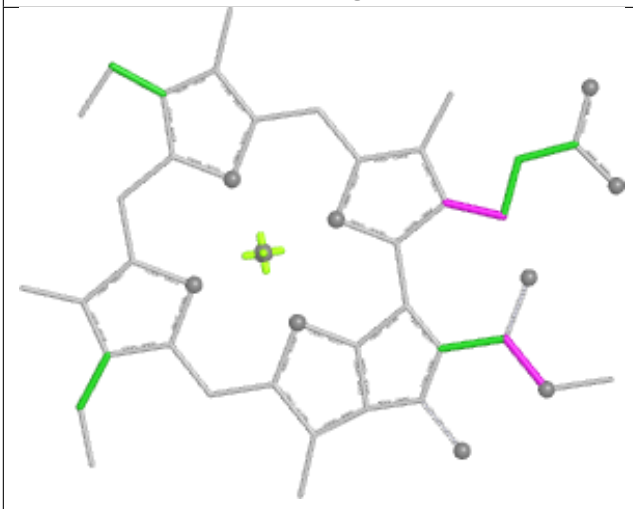
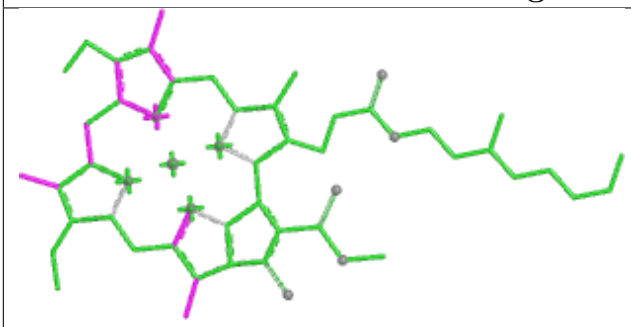
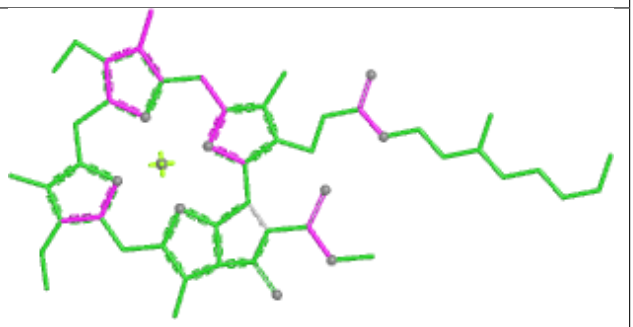
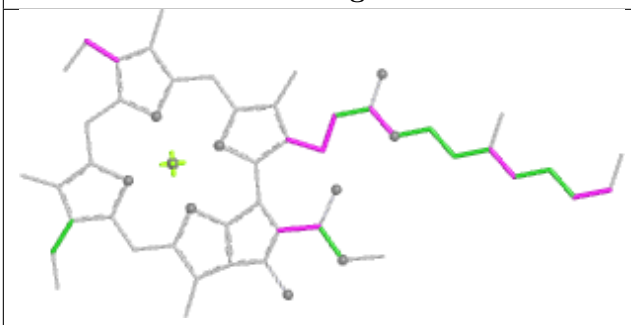
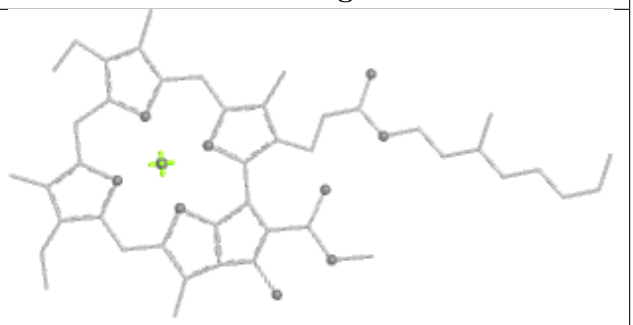


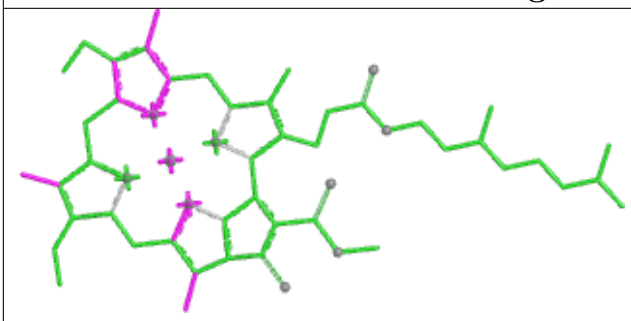
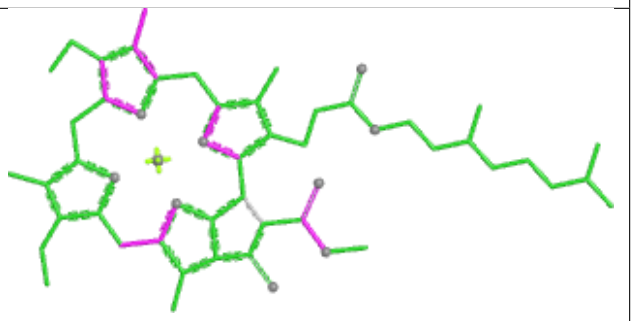
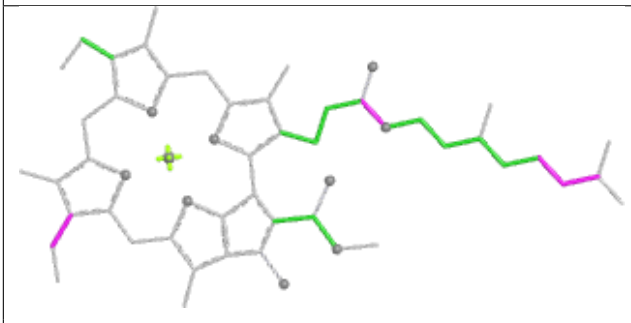
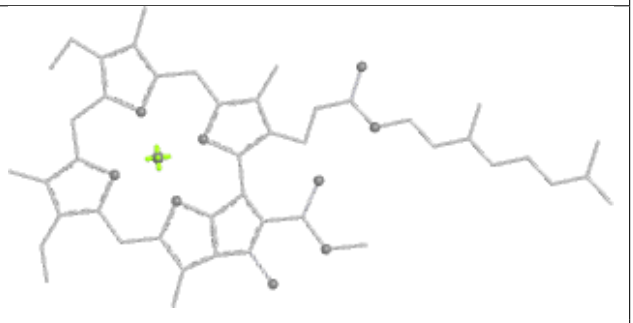
Bond angles



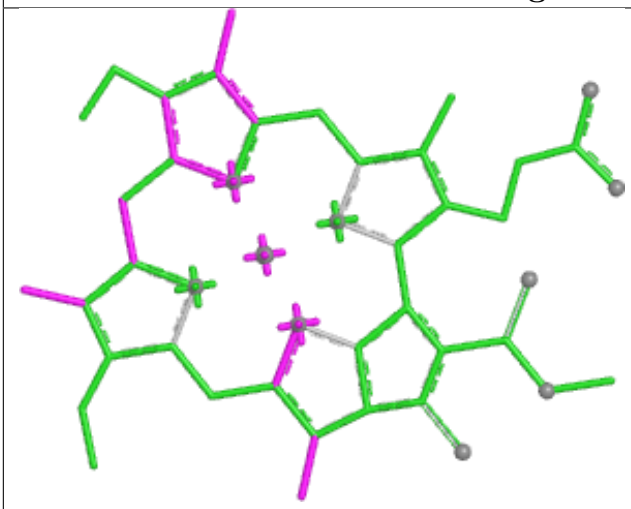
Torsions

Rings

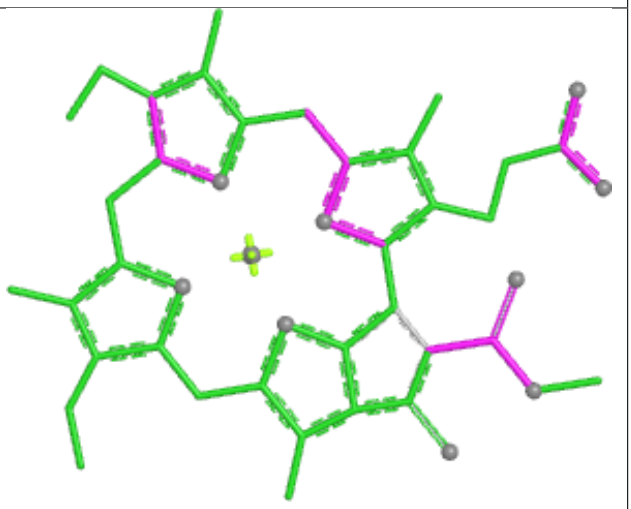
Ligand CLA b 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

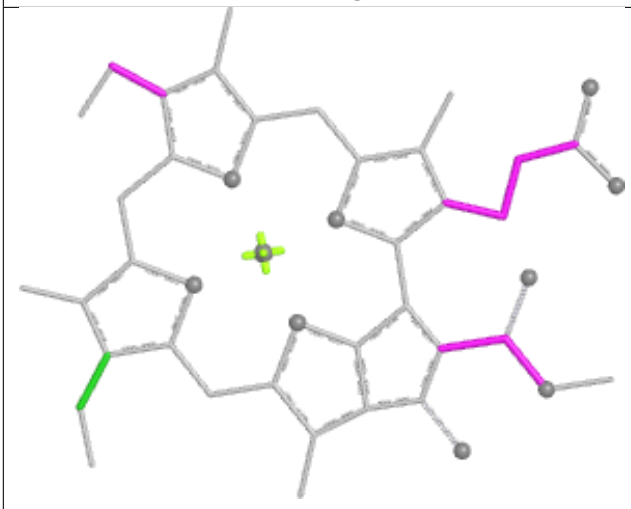
Ligand CLA 2 814



Bond lengths



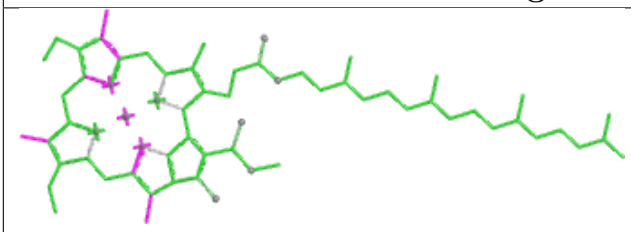
Bond angles



Torsions

Rings

Ligand CLA b 811



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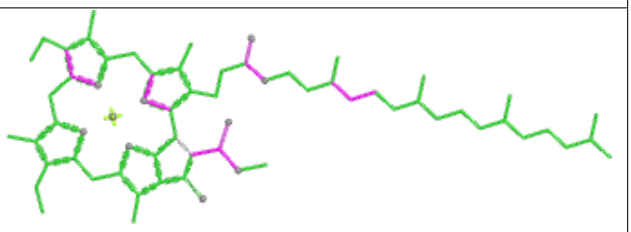
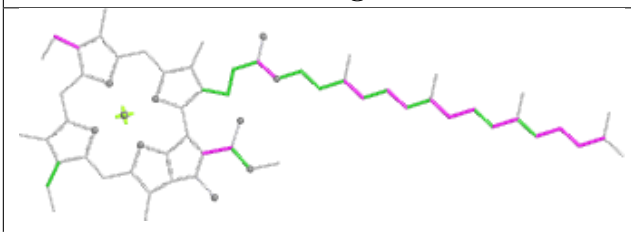
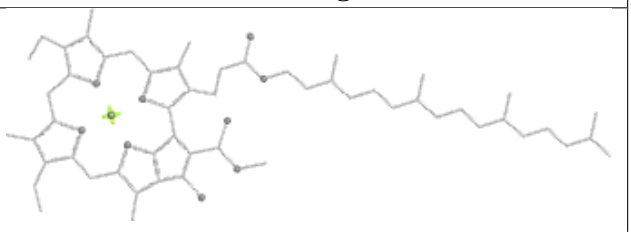


Bond angles

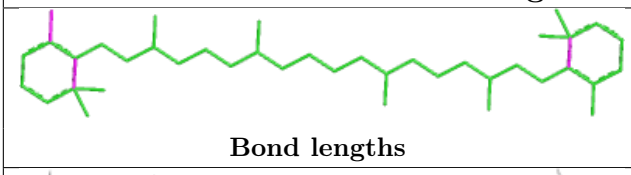


Torsions



Rings

Ligand BCR a 849



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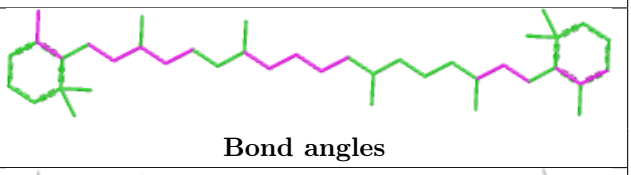
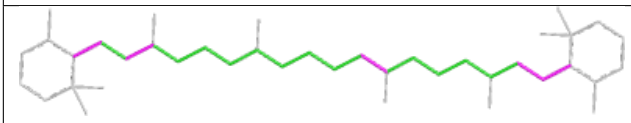


Bond angles



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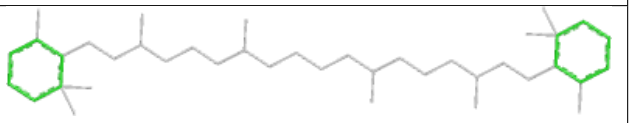
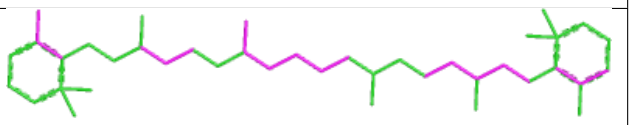


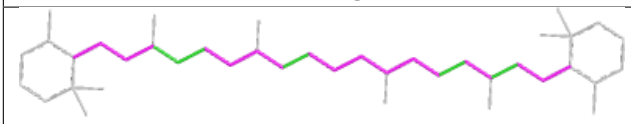
Rings

Ligand BCR a 850

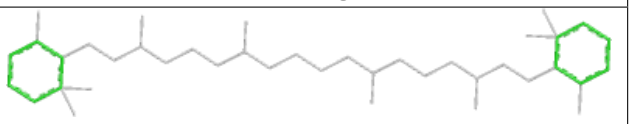
Bond lengths



Bond angles

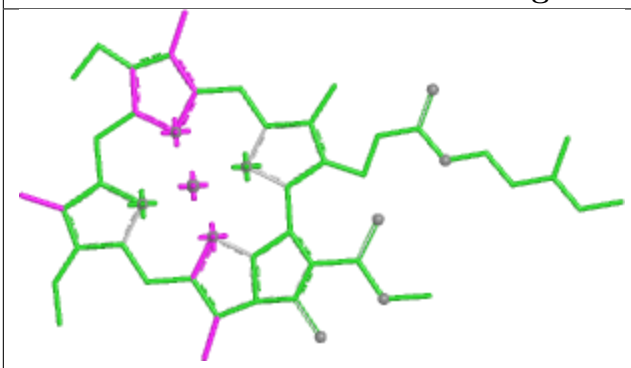


Torsions



Rings

Ligand CLA f 201



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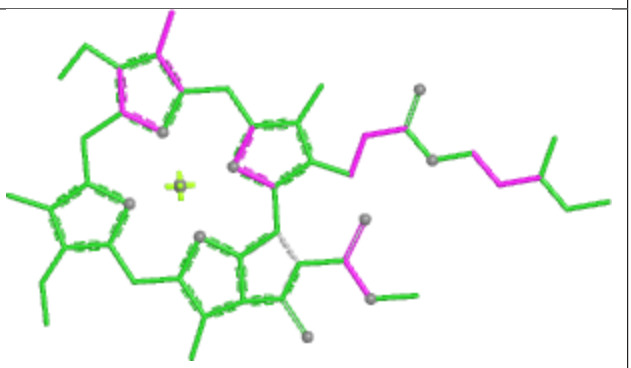
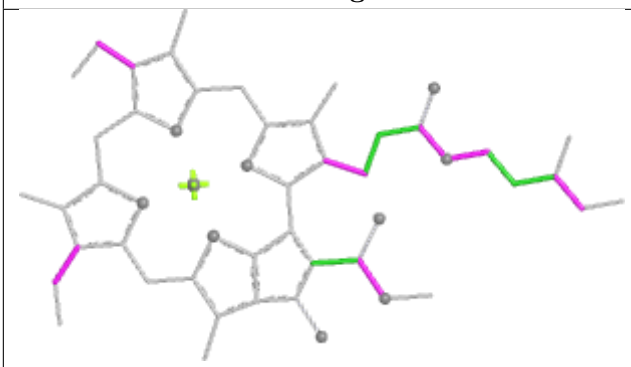
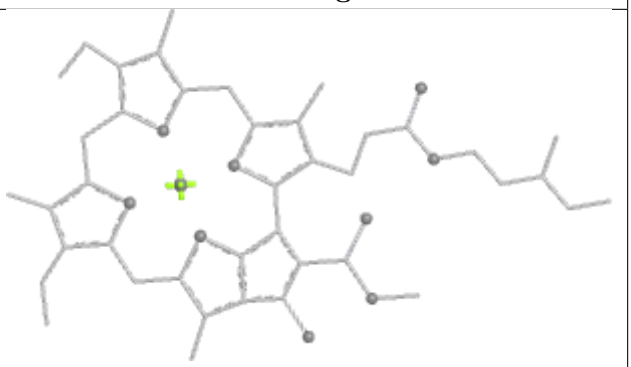


Bond angles

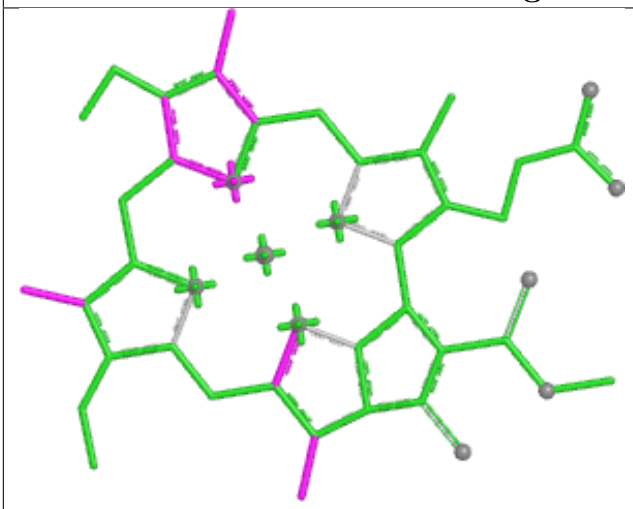


Torsions



Rings

Ligand CLA A 812



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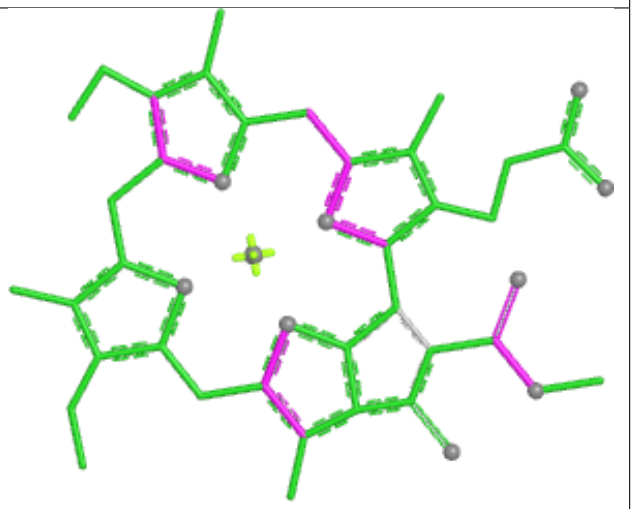
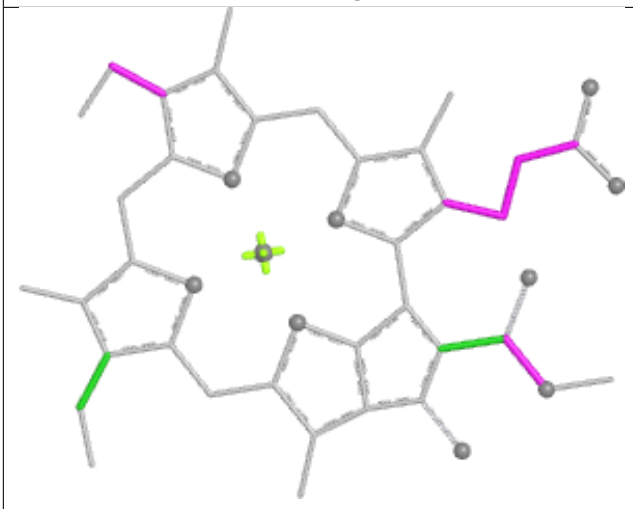


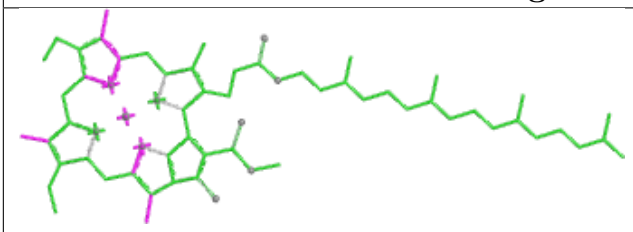
Bond angles



Torsions

Rings

Ligand CLA 1 807



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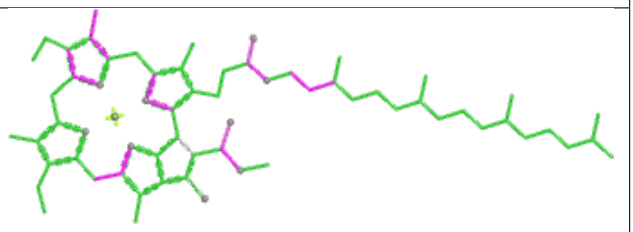
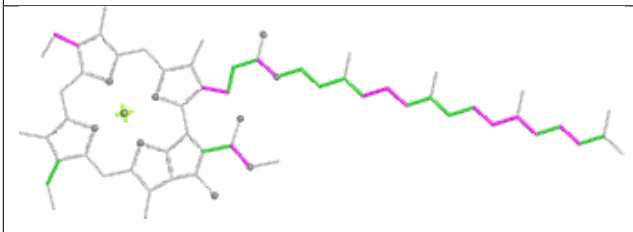
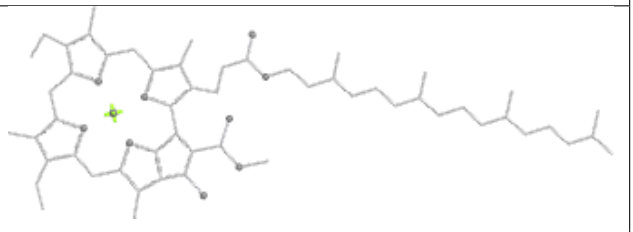


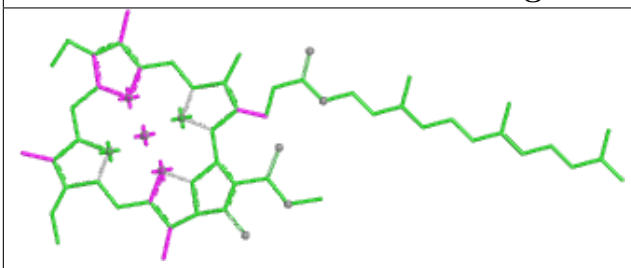
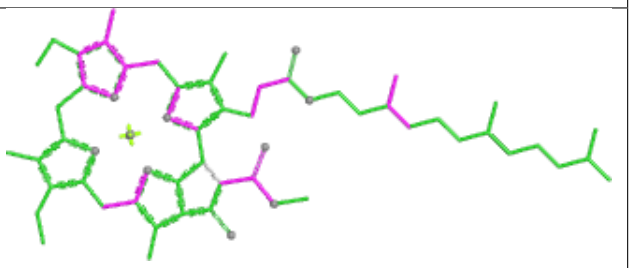
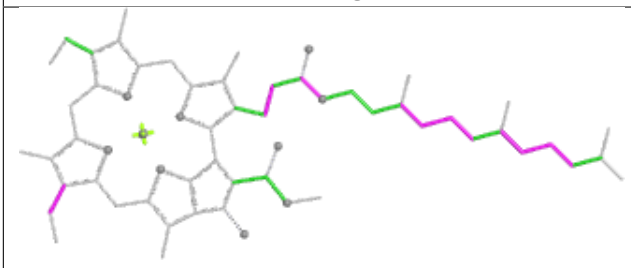
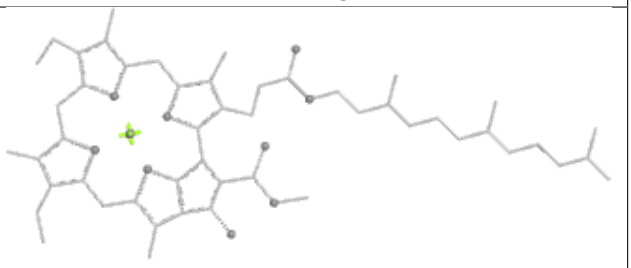
Bond angles

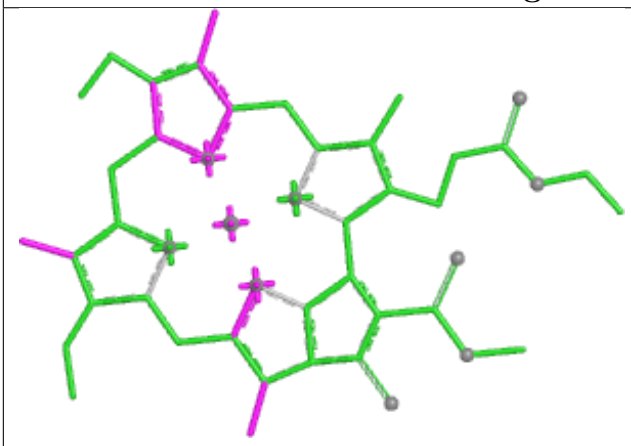
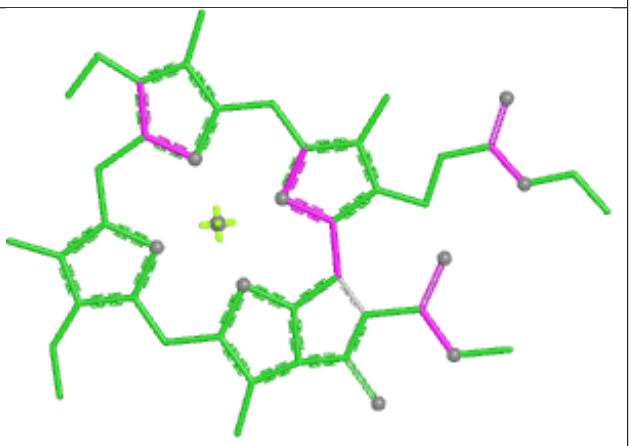
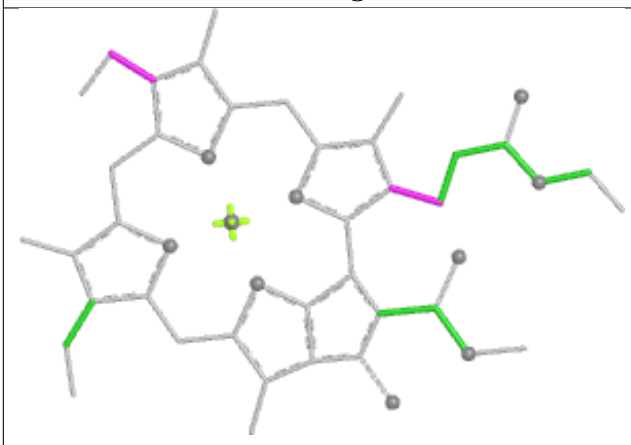
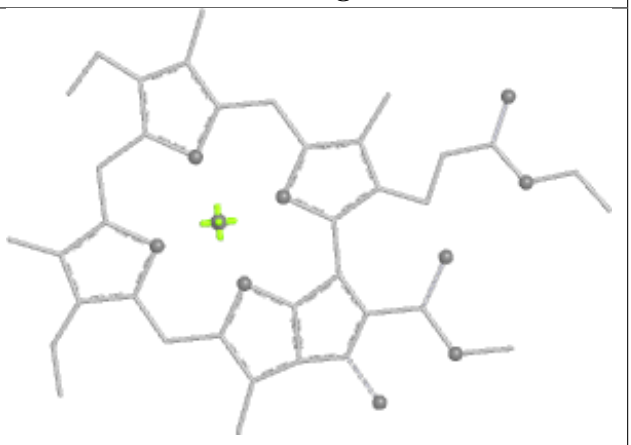


Torsions

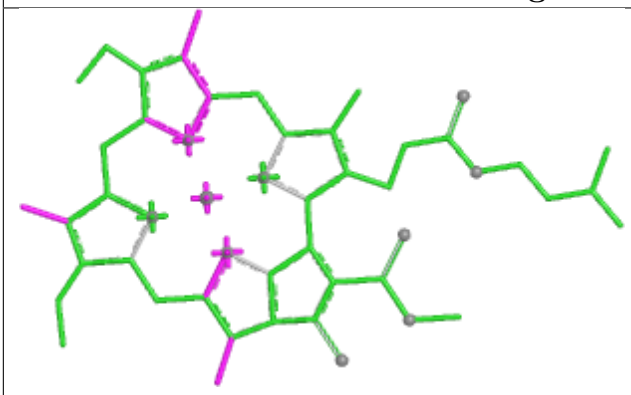


Rings

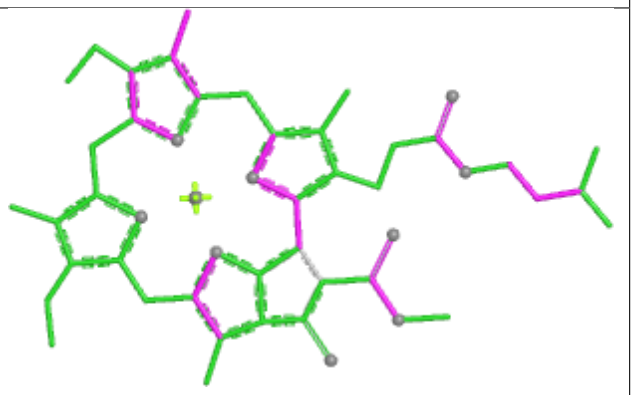
Ligand CLA B 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

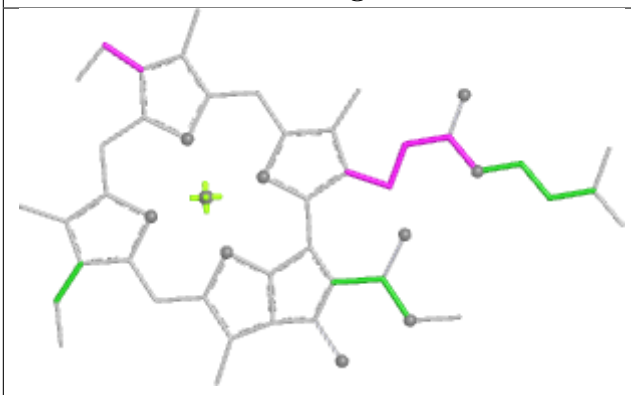
Ligand CLA 1 810



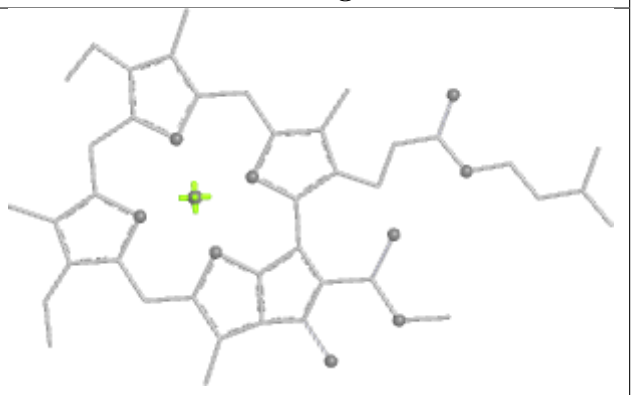
Bond lengths



Bond angles

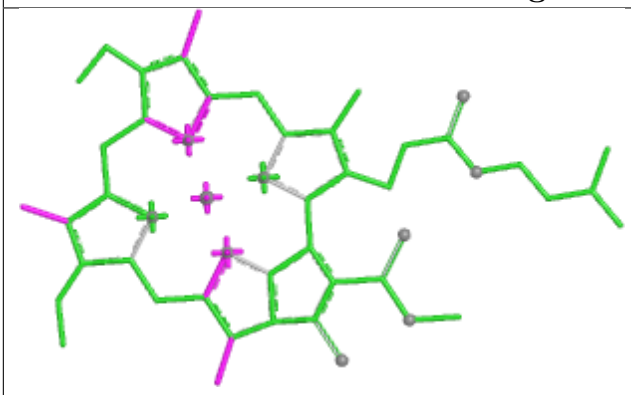


Torsions



Rings

Ligand CLA 1 832



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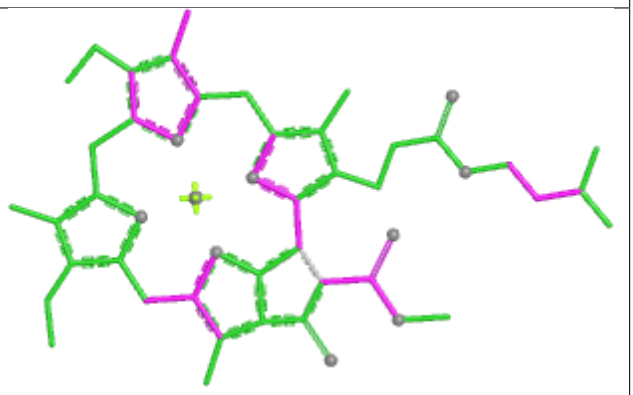

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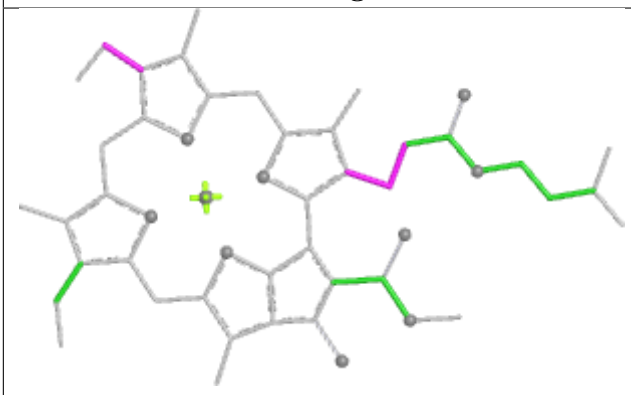

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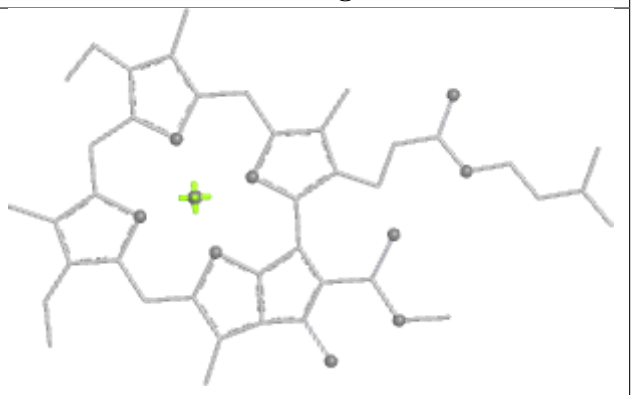
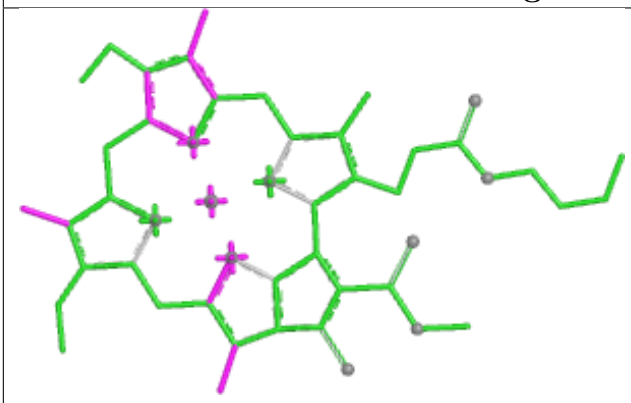


Rings

Ligand CLA A 824



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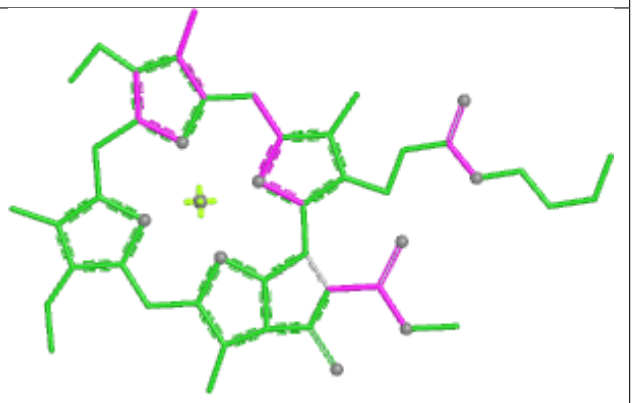
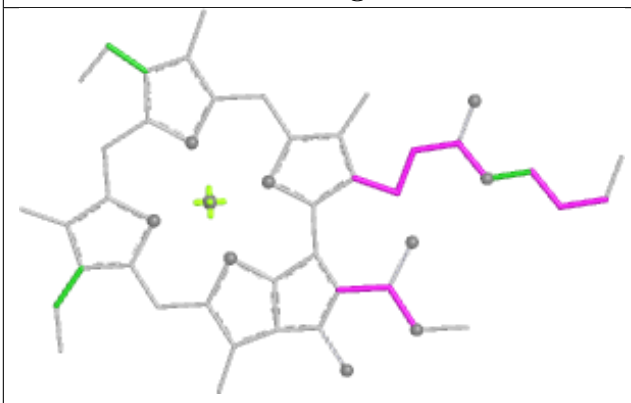


Bond angles



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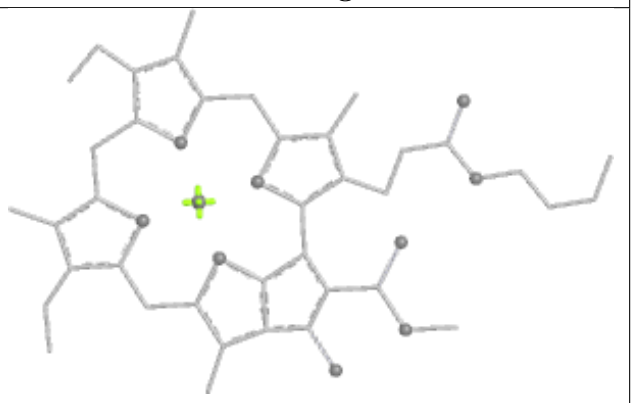
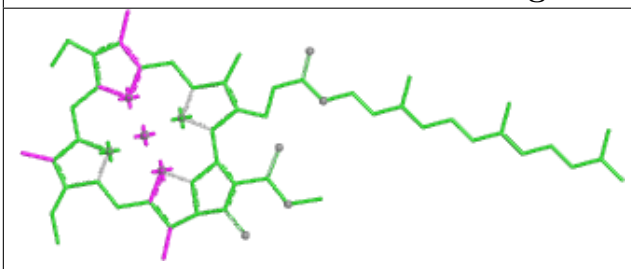


Rings

Ligand CLA 2 820



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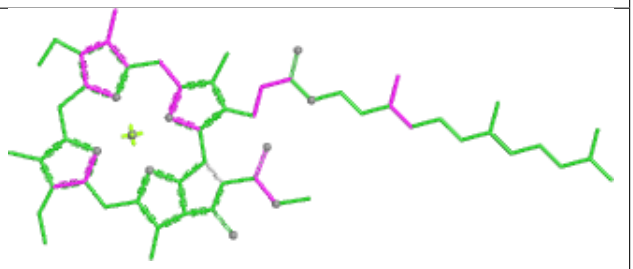
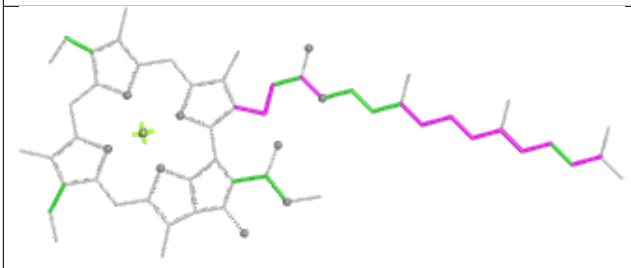
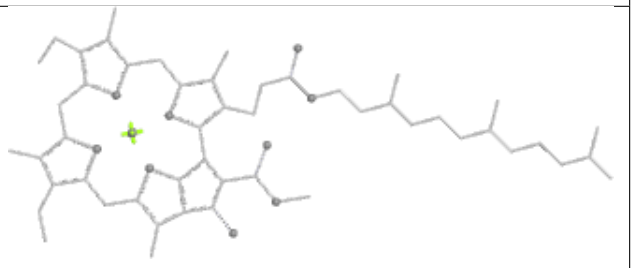


Bond angles

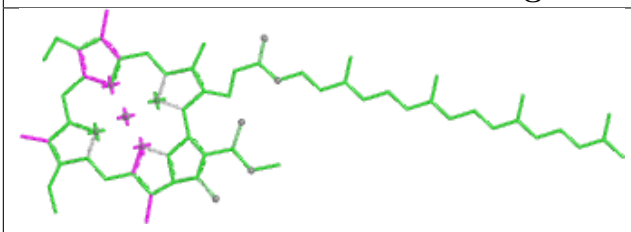


Torsions



Rings

Ligand CLA B 816



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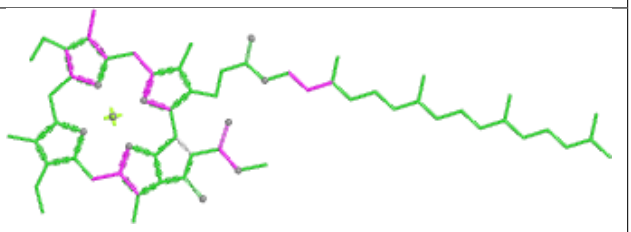
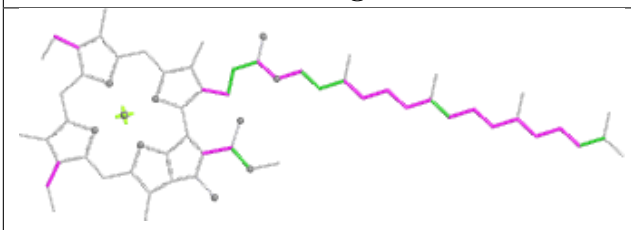
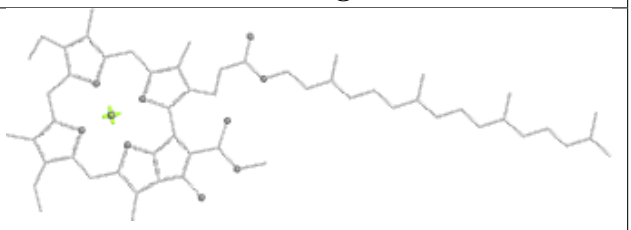


Bond angles



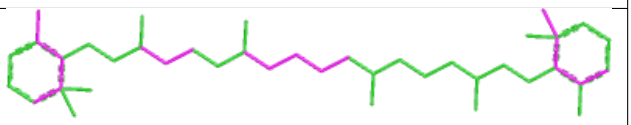
Torsions



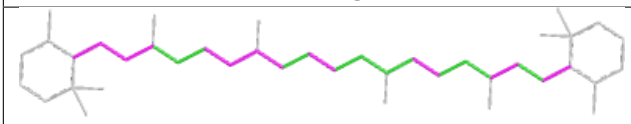
Rings

Ligand BCR F 206

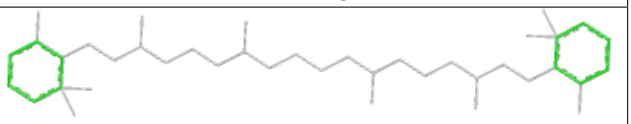
Bond lengths



Bond angles

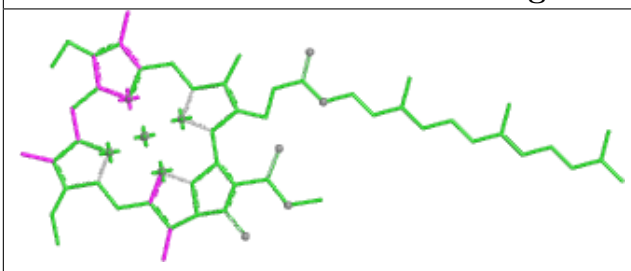


Torsions

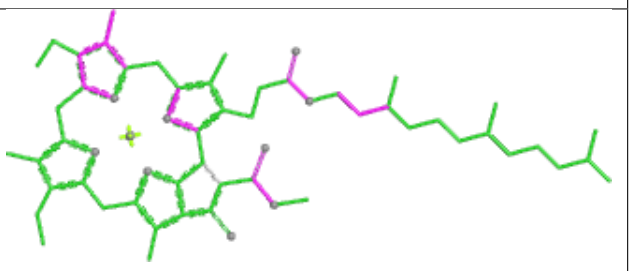


Rings

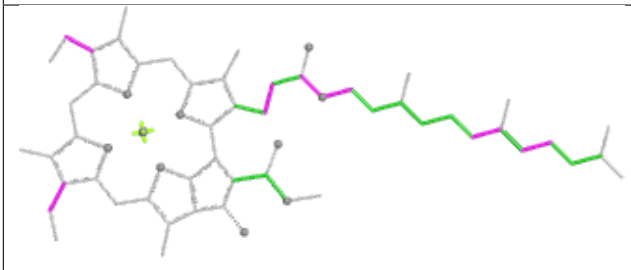
Ligand CLA a 823



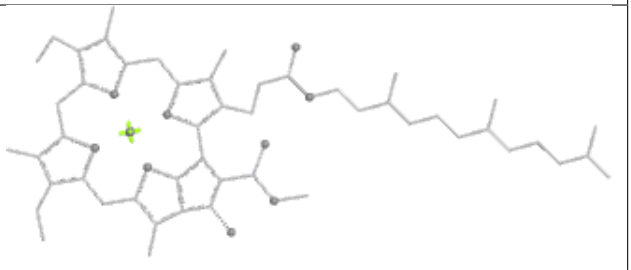
Bond lengths



Bond angles

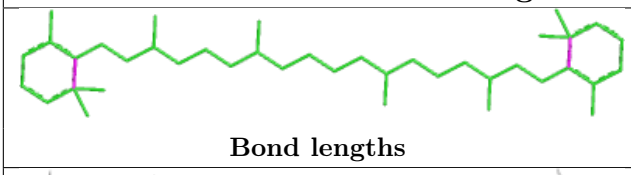


Torsions

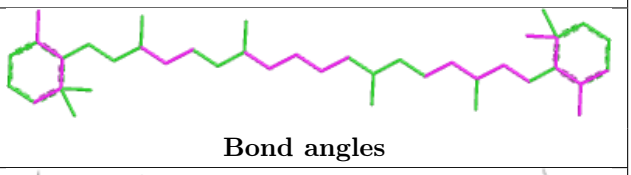


Rings

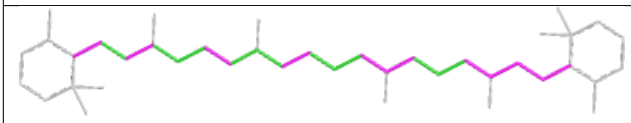
Ligand BCR L 1504



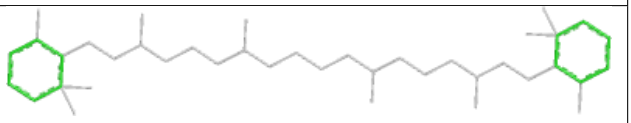
Bond lengths



Bond angles

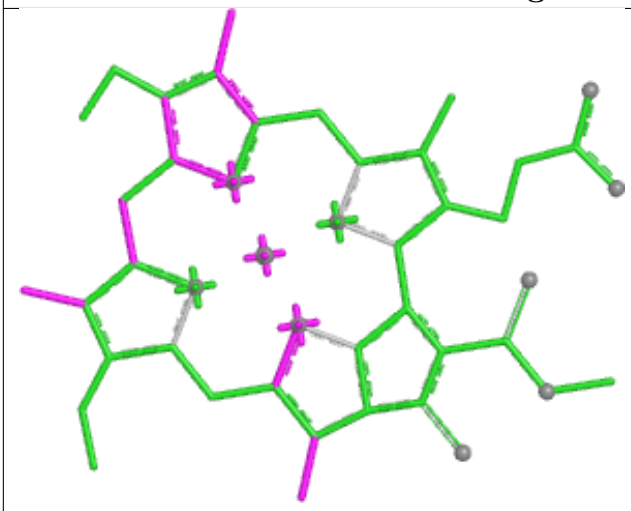


Torsions



Rings

Ligand CLA b 837



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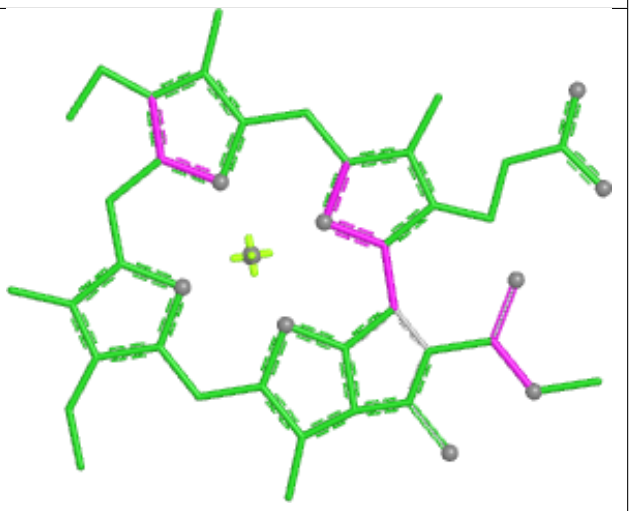
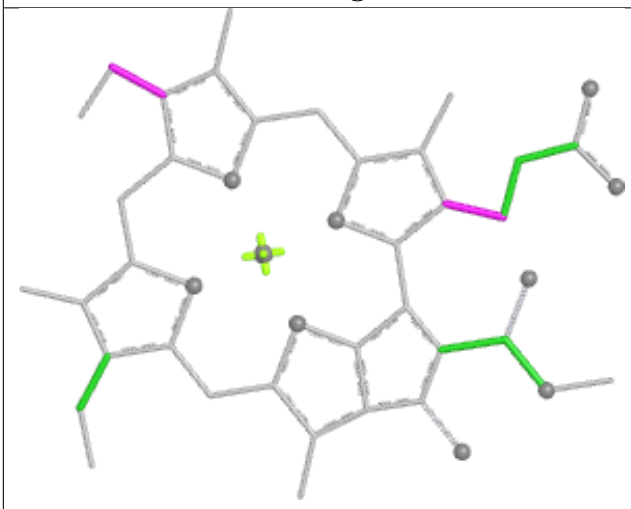


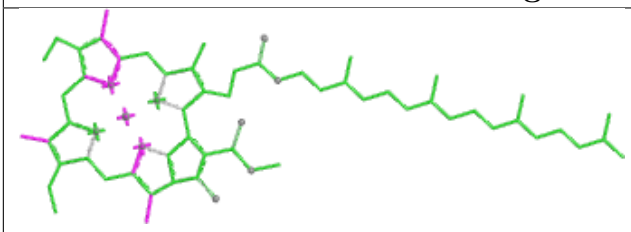
Bond angles



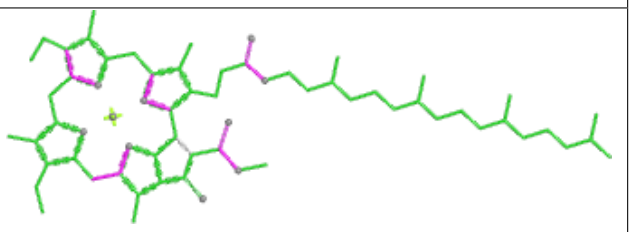
Torsions

Rings

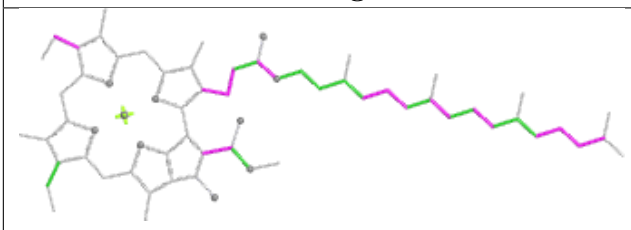
Ligand CLA A 807



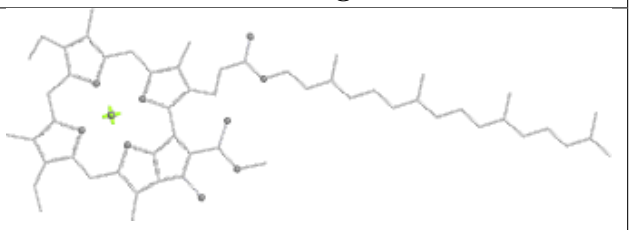
Bond lengths



Bond angles

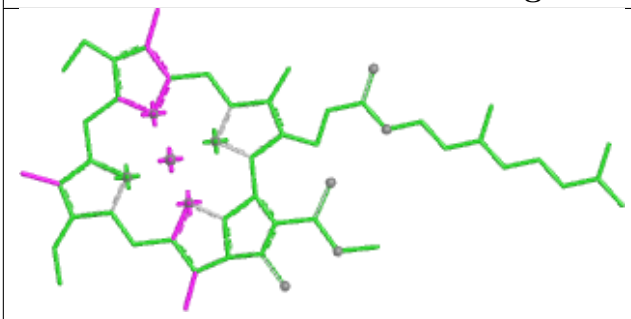


Torsions



Rings

Ligand CLA B 820



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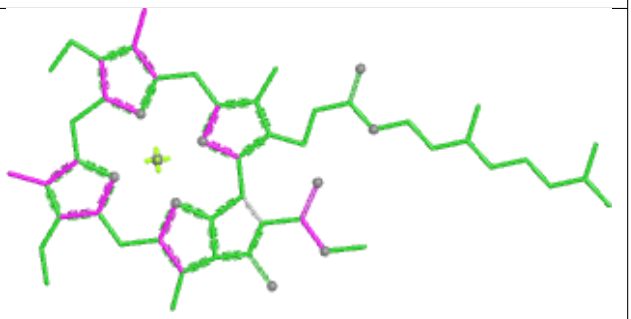
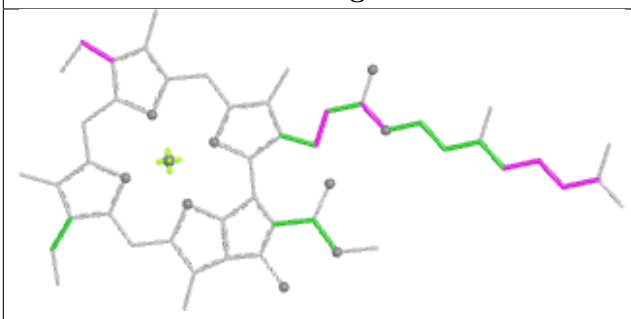
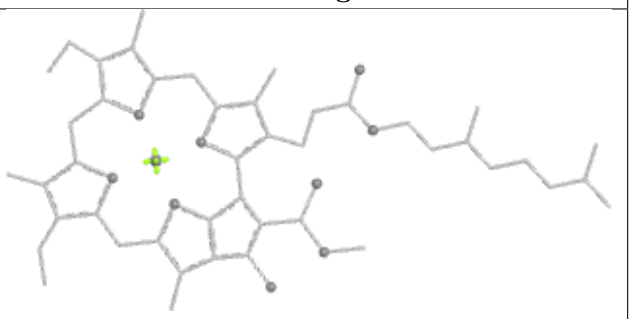


Bond angles

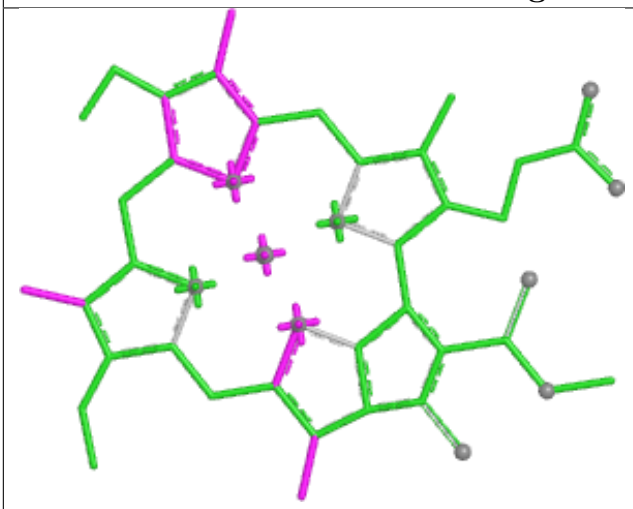


Torsions

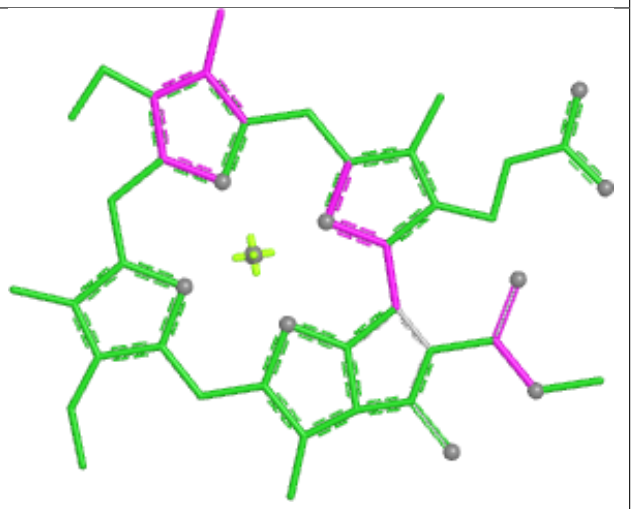


Rings

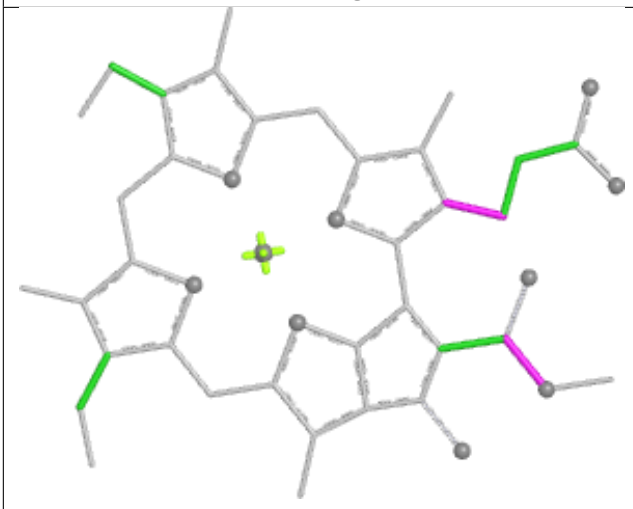
Ligand CLA a 817



Bond lengths

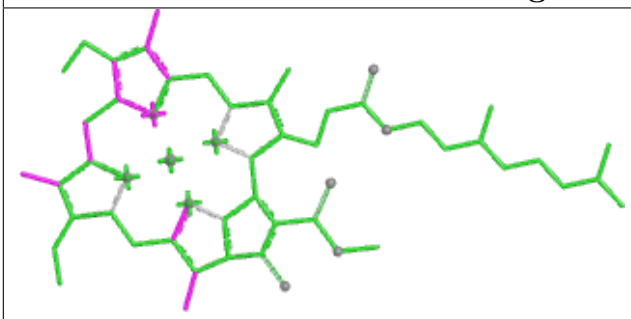
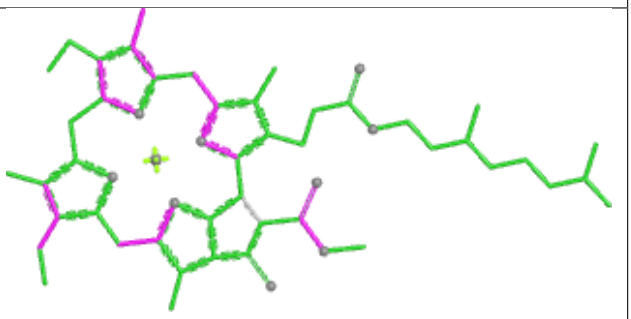
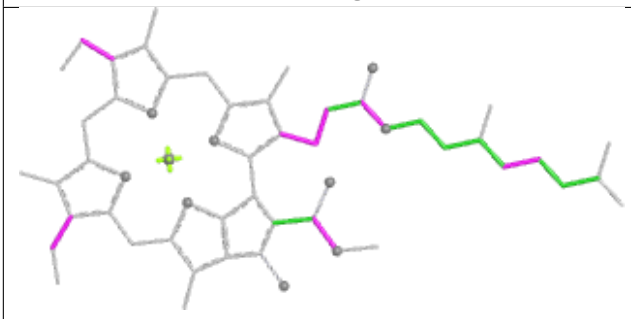
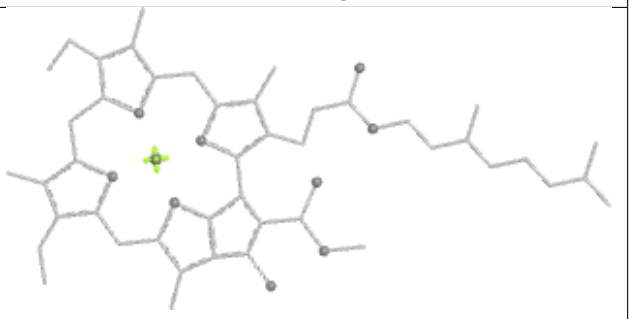


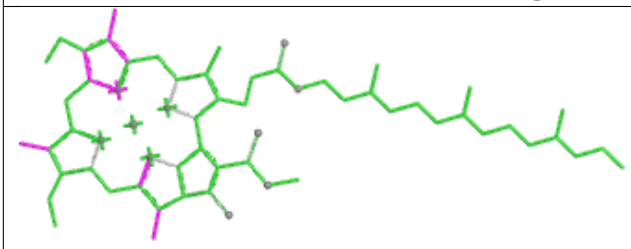
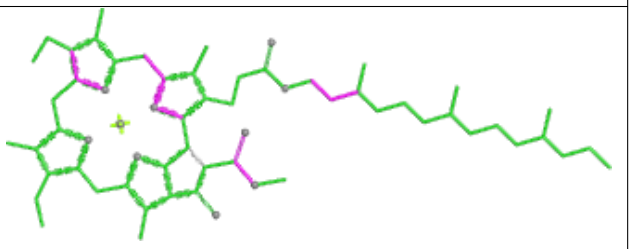
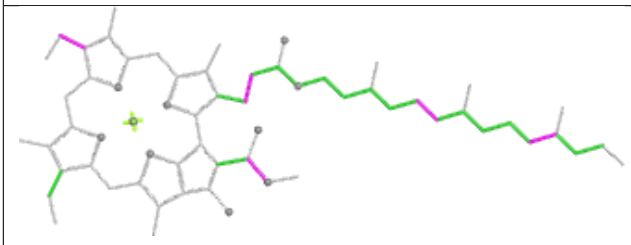
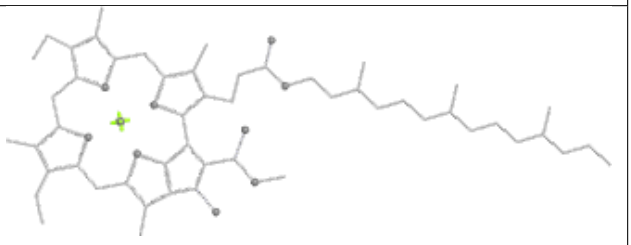
Bond angles



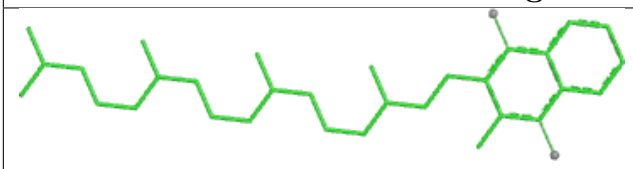
Torsions

Rings

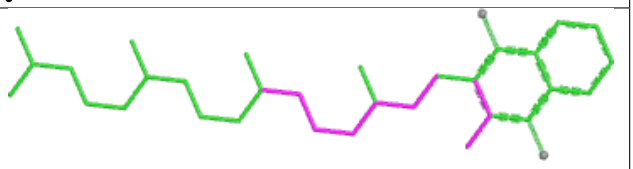
Ligand CLA 1 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

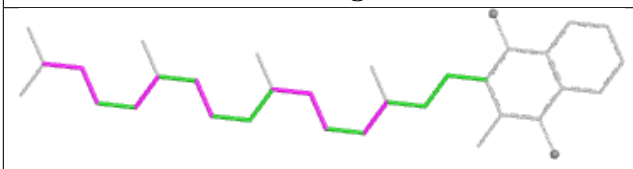
Ligand PQN 2 845



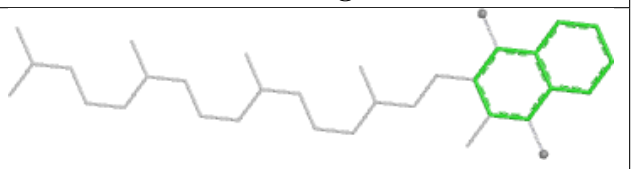
Bond lengths



Bond angles



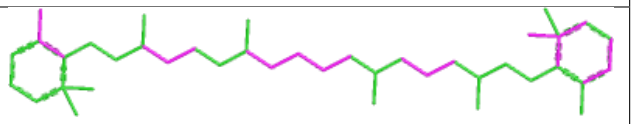
Torsions



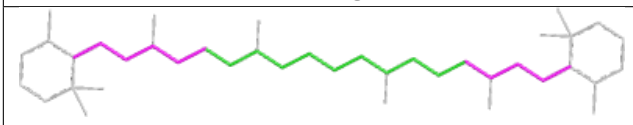
Rings

Ligand BCR L 1505

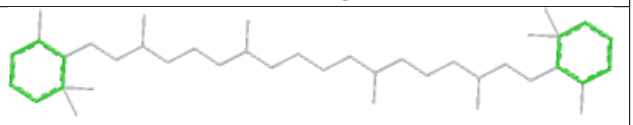
Bond lengths



Bond angles

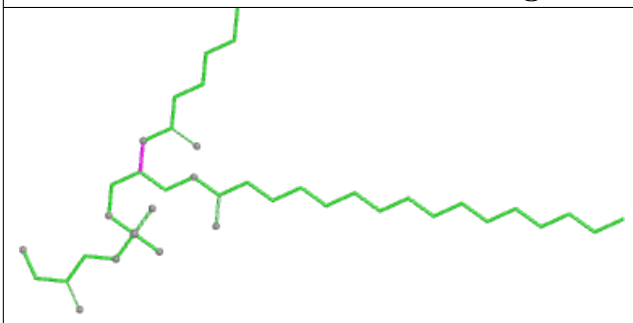


Torsions



Rings

Ligand LHG B 853



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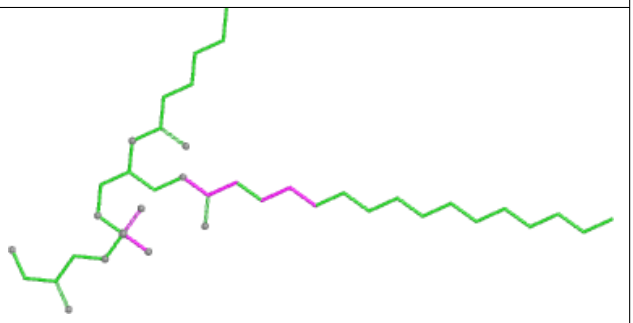
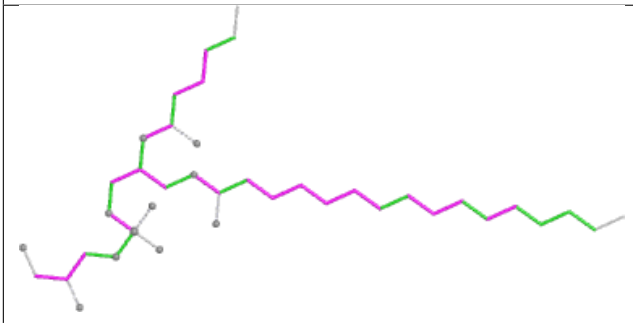
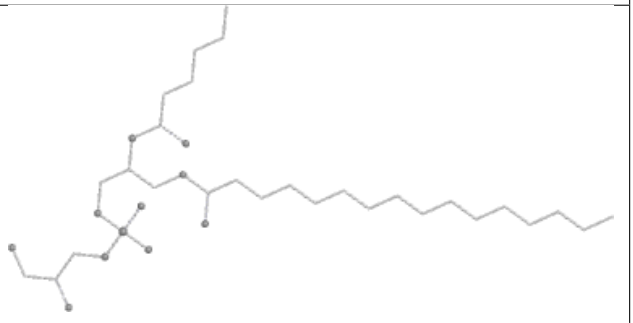


Bond angles

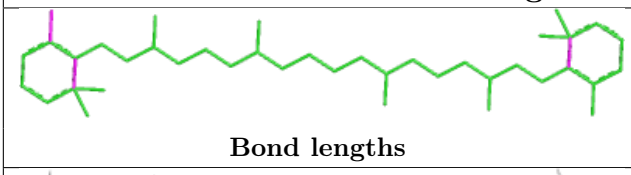


Torsions



Rings

Ligand BCR b 853



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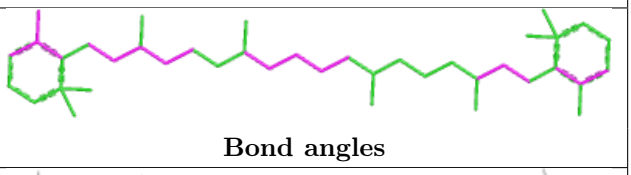
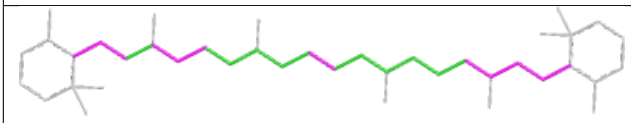
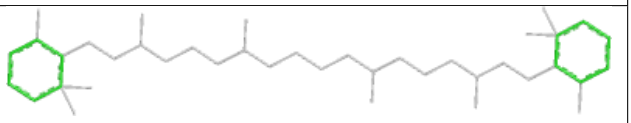


Bond angles

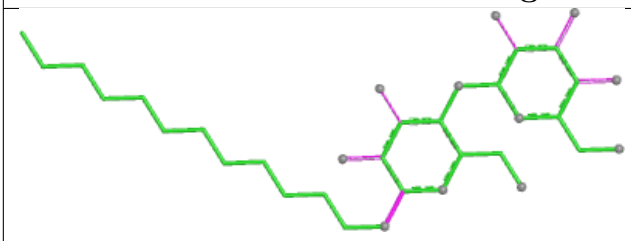


Torsions

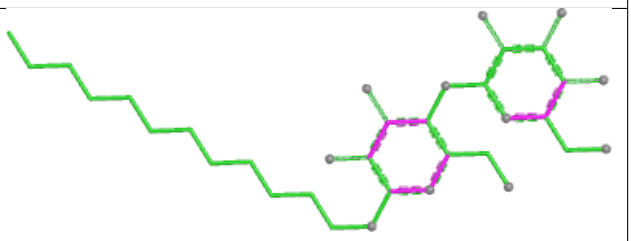


Rings

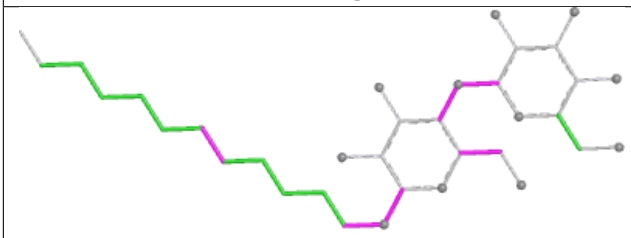
Ligand LMT i 4101



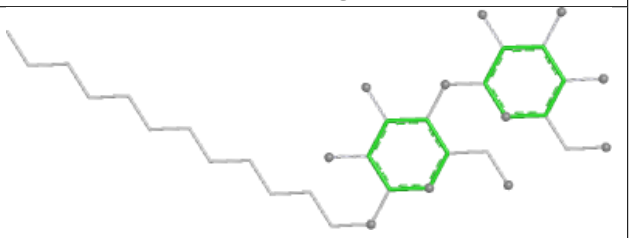
Bond lengths



Bond angles

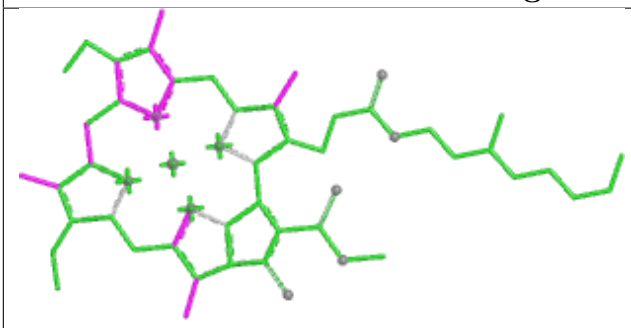


Torsions

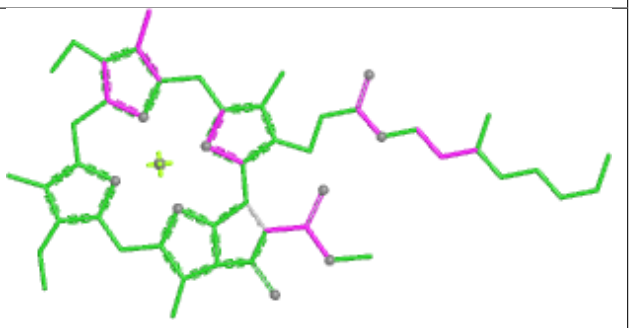


Rings

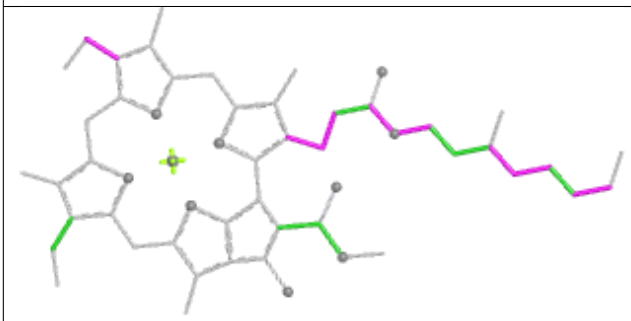
Ligand CLA A 814



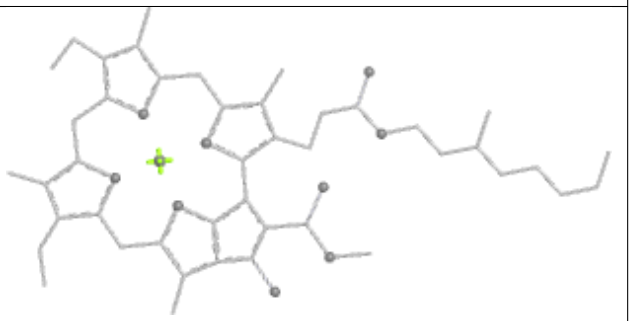
Bond lengths



Bond angles

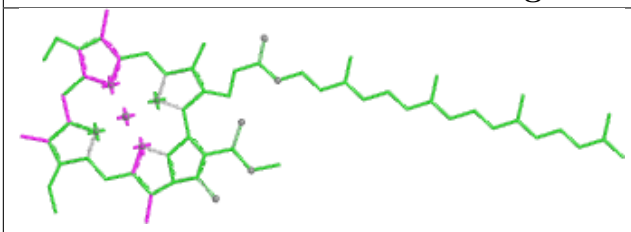


Torsions

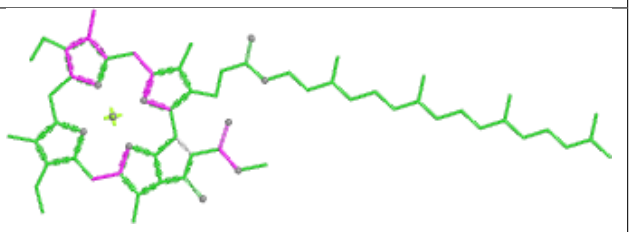


Rings

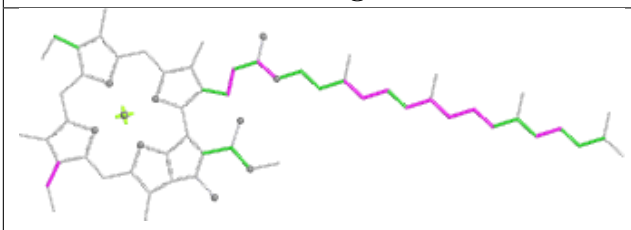
Ligand CLA B 806



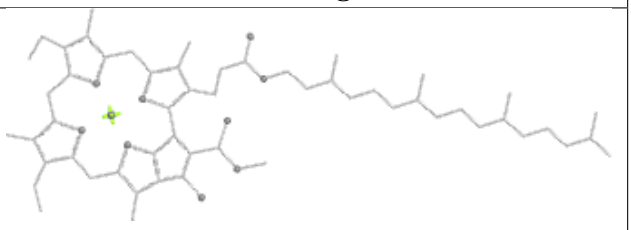
Bond lengths



Bond angles

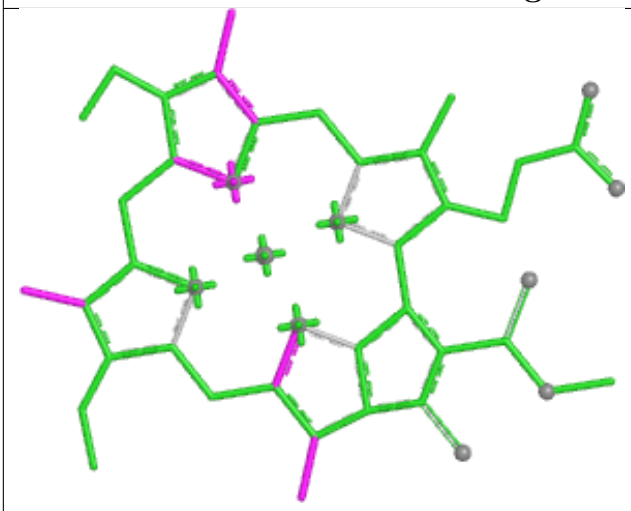


Torsions

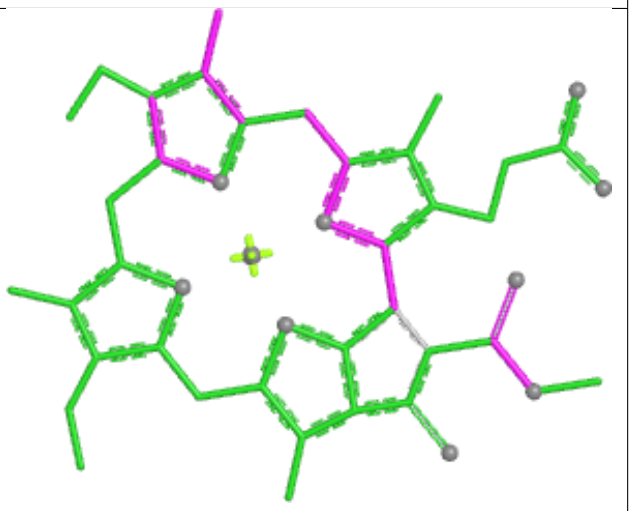


Rings

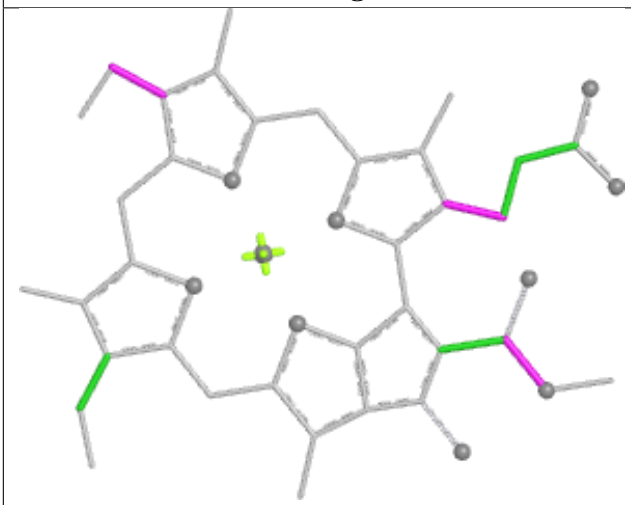
Ligand CLA B 814



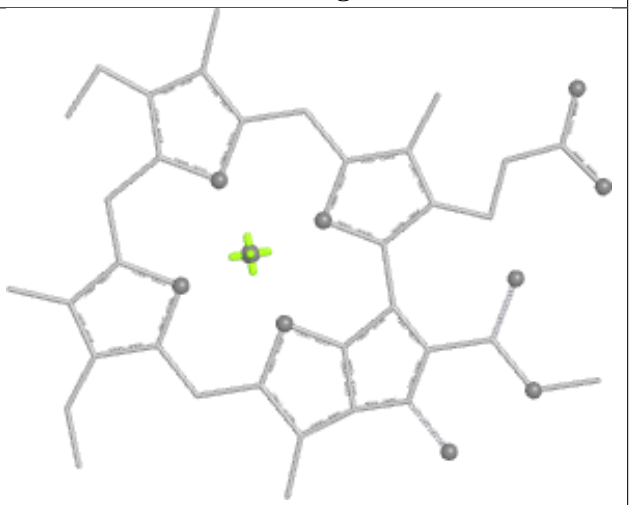
Bond lengths



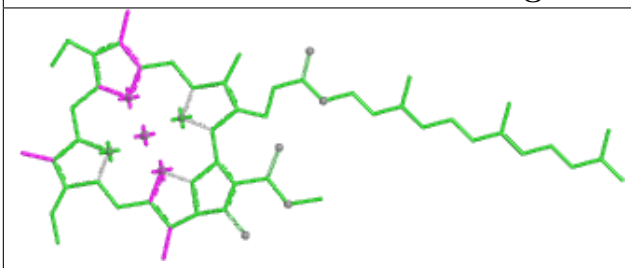
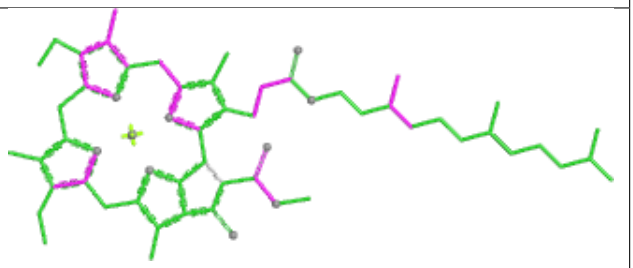
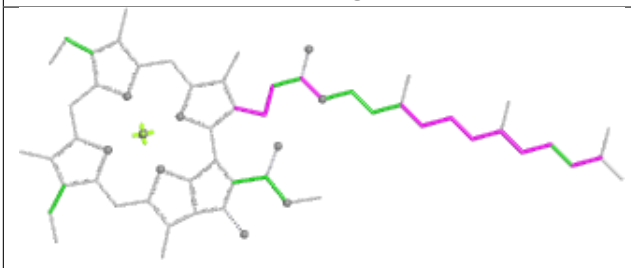
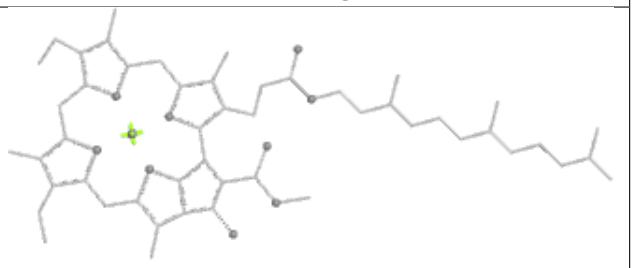
Bond angles

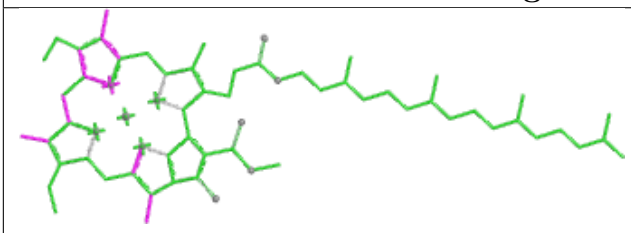
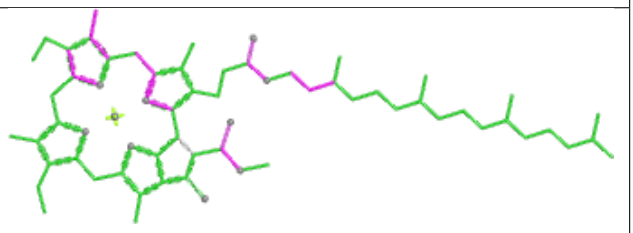
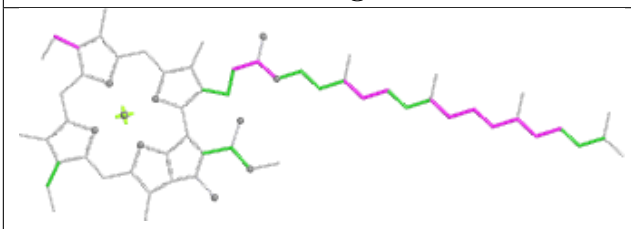
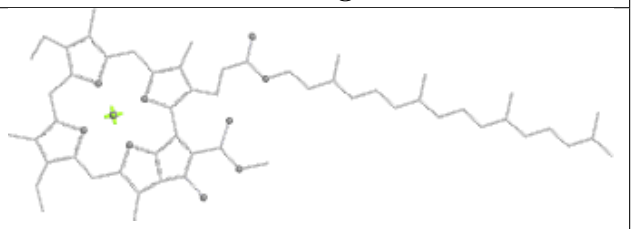


Torsions

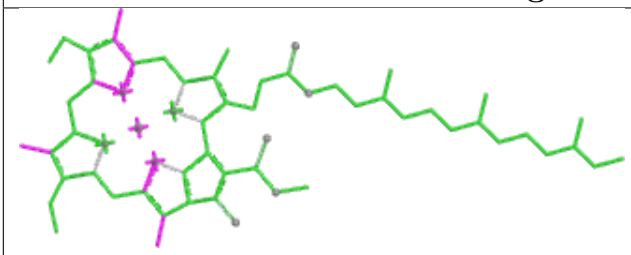


Rings

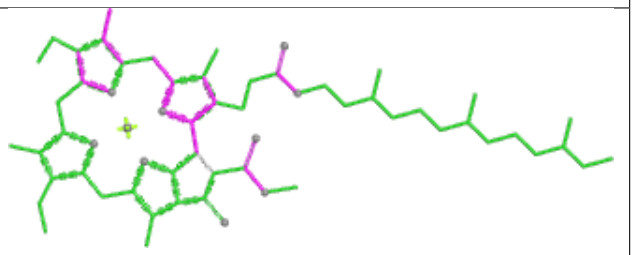
Ligand CLA B 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 4206	
	
Bond lengths	Bond angles
	
Torsions	Rings

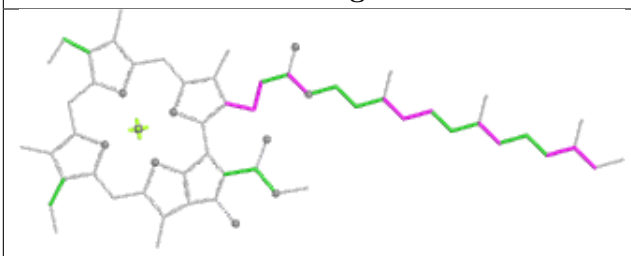
Ligand CLA b 812



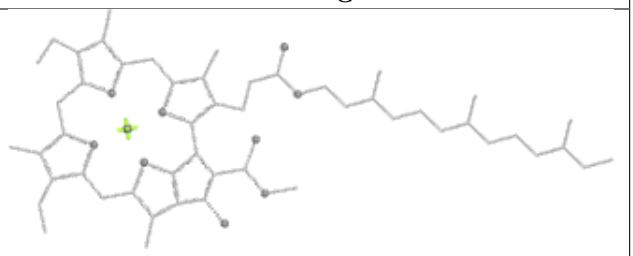
Bond lengths



Bond angles

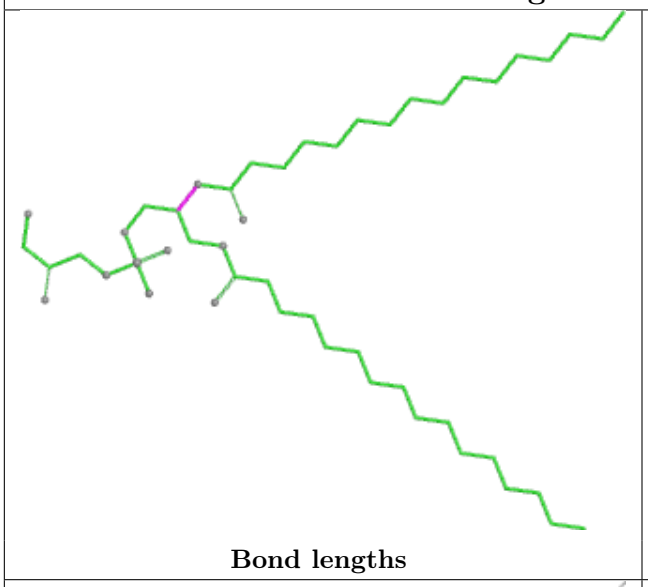


Torsions

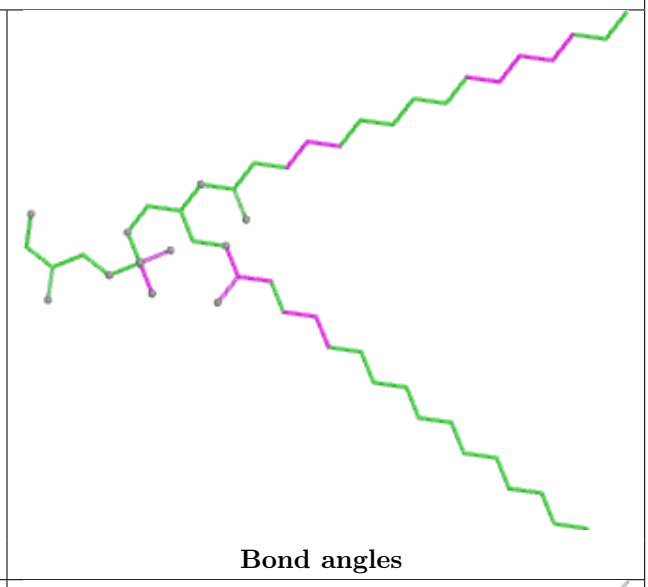


Rings

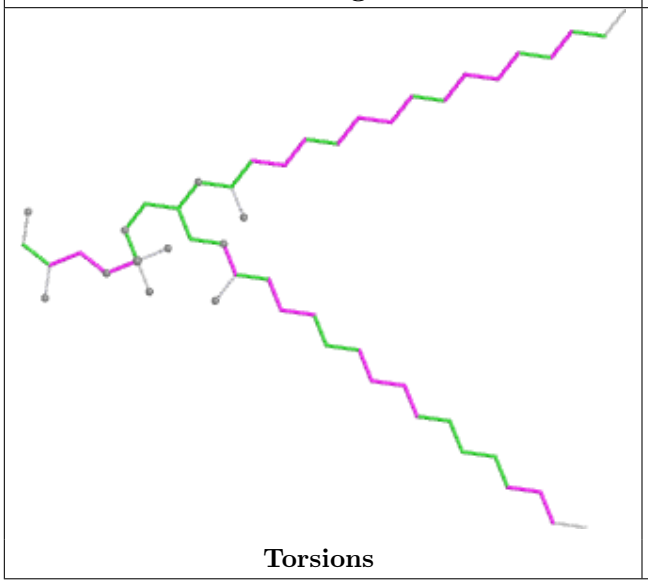
Ligand LHG a 801



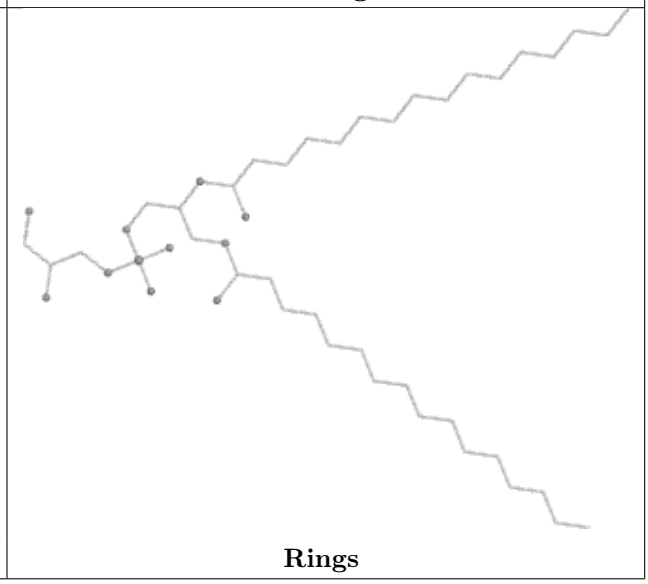
Bond lengths



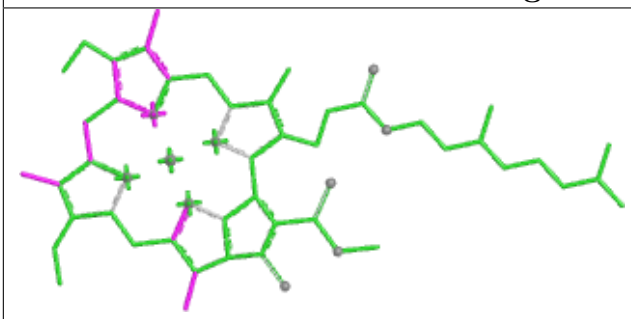
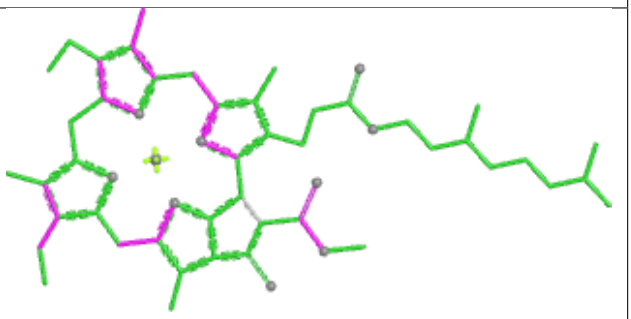
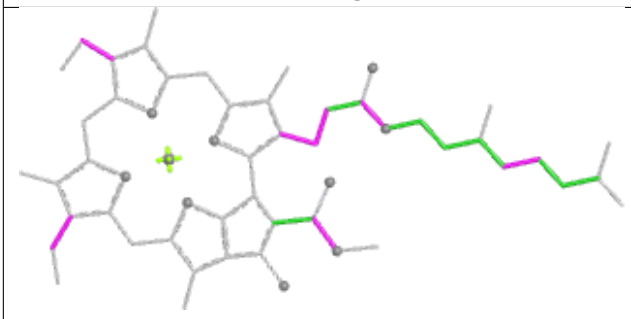
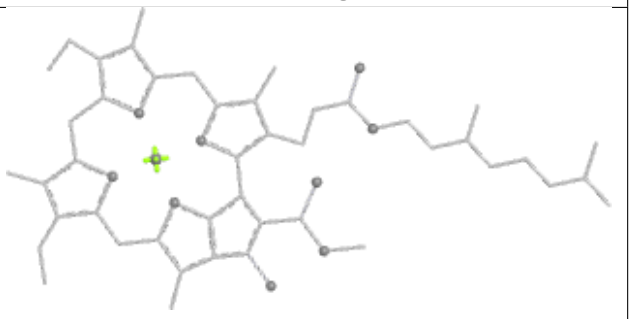
Bond angles

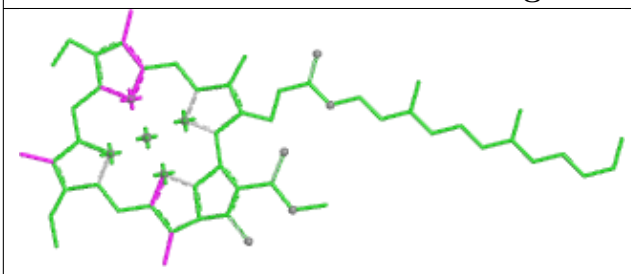
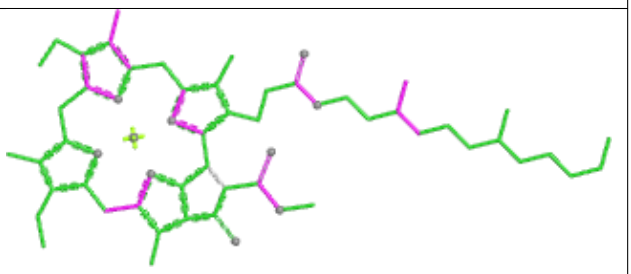
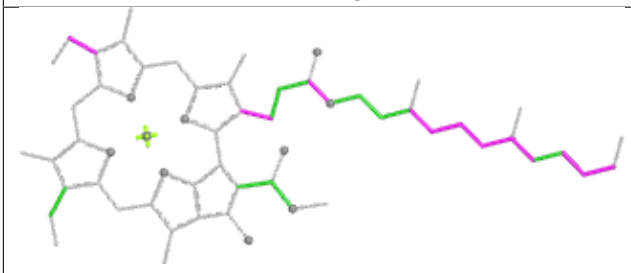
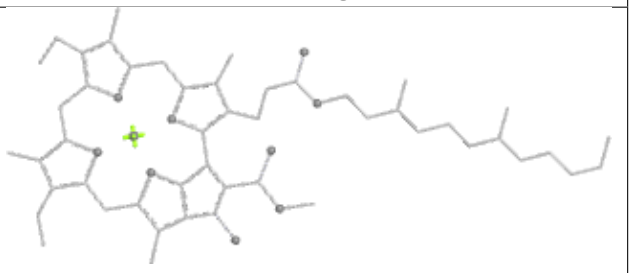


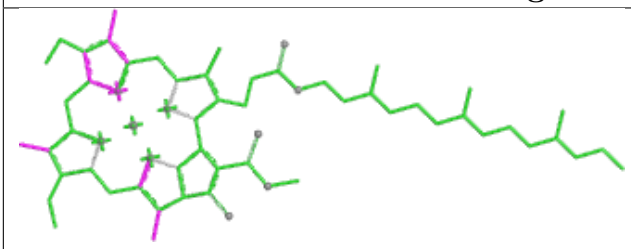
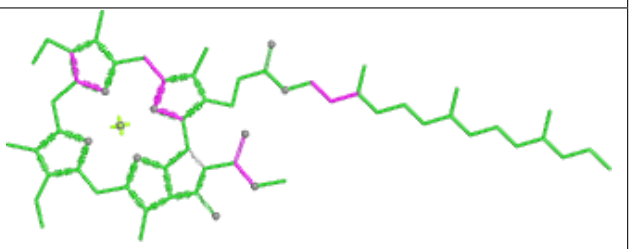
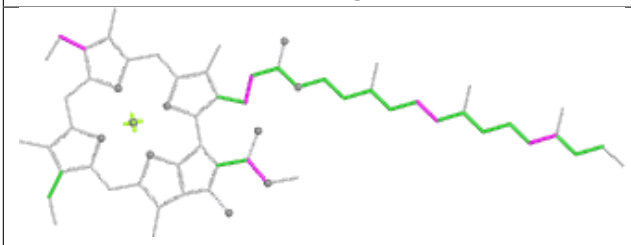
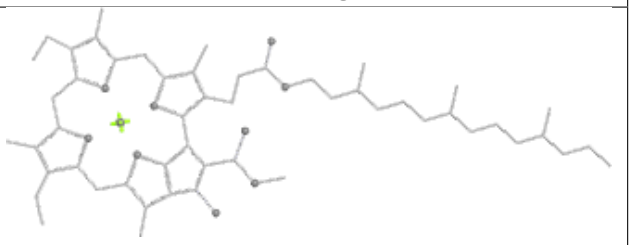
Torsions

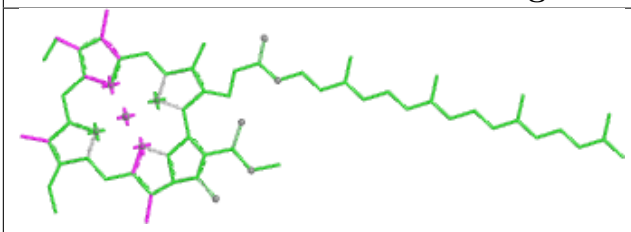
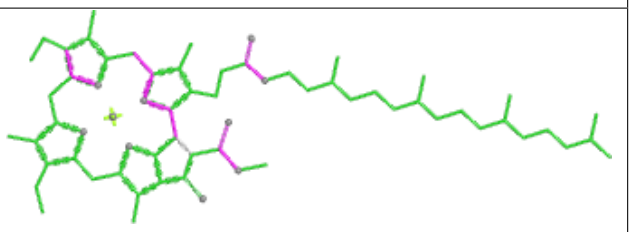
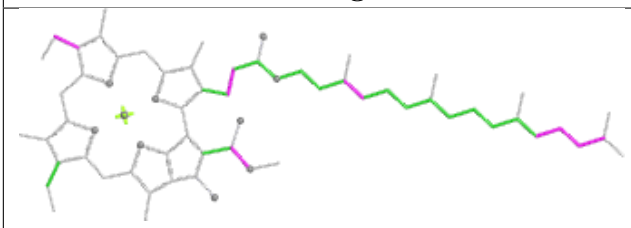
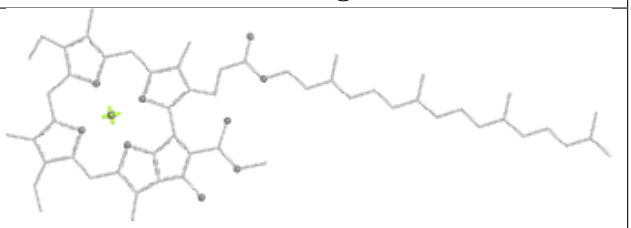


Rings

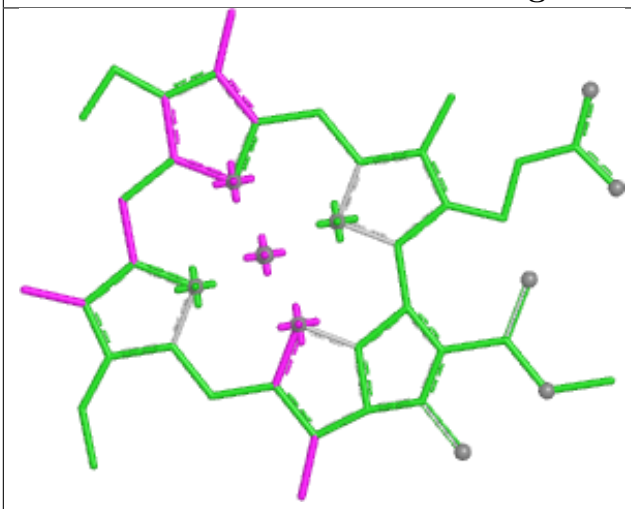
Ligand CLA A 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

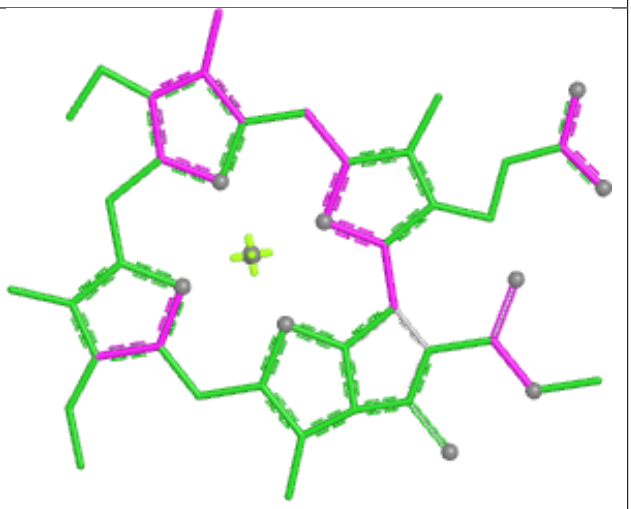
Ligand CLA b 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

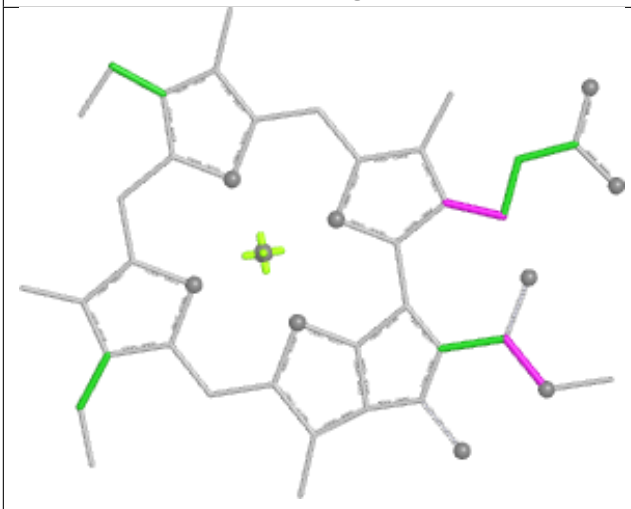
Ligand CLA 2 836



Bond lengths



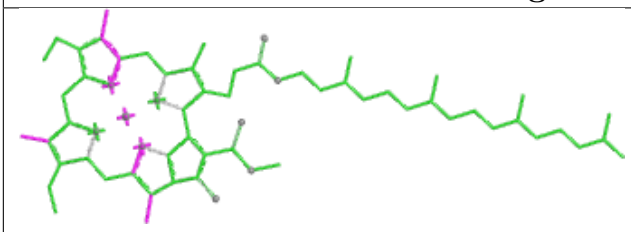
Bond angles



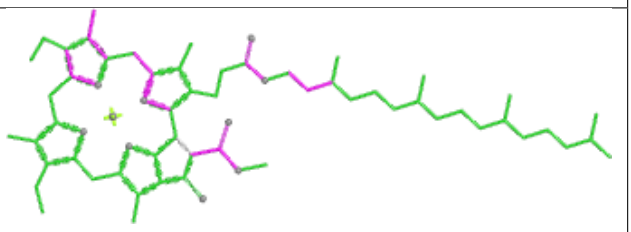
Torsions

Rings

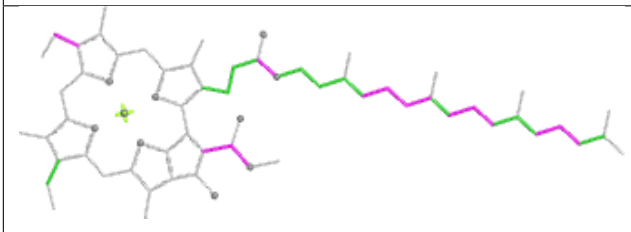
Ligand CLA 1 833



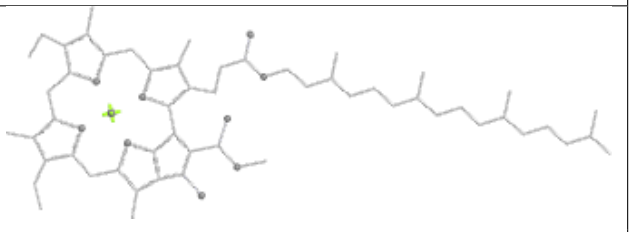
Bond lengths



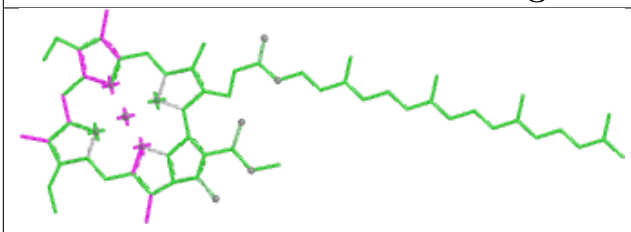
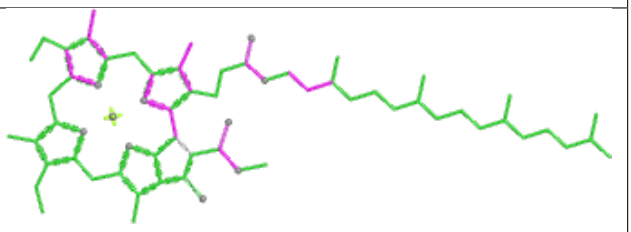
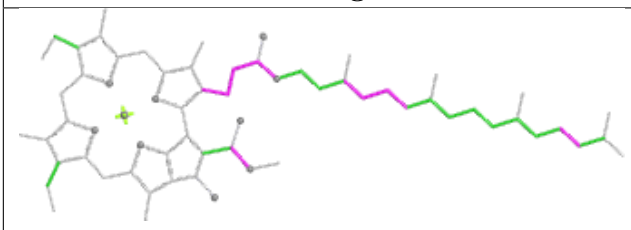
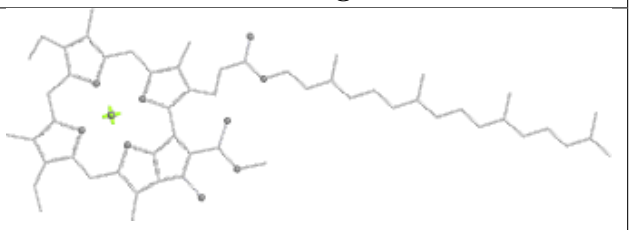
Bond angles

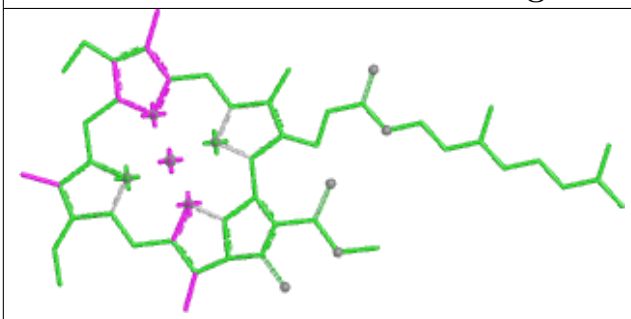
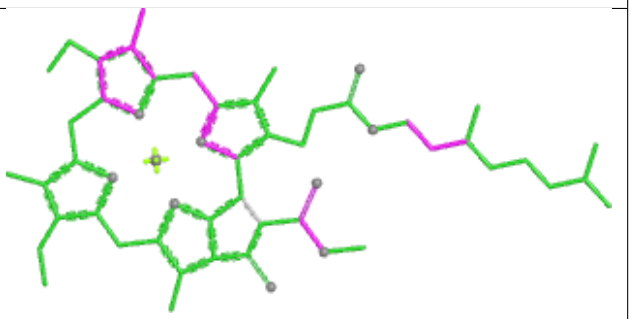
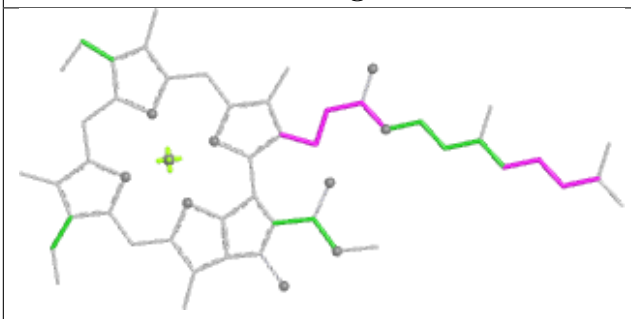
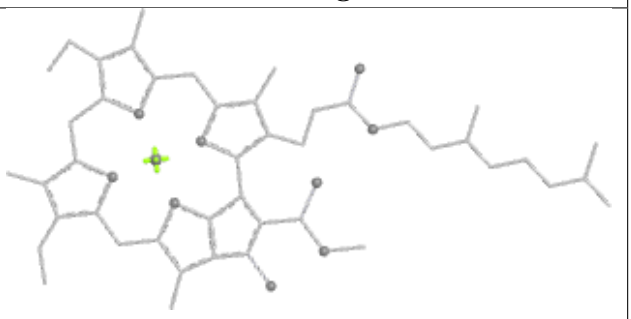


Torsions

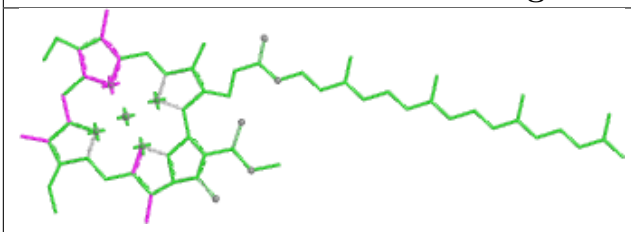


Rings

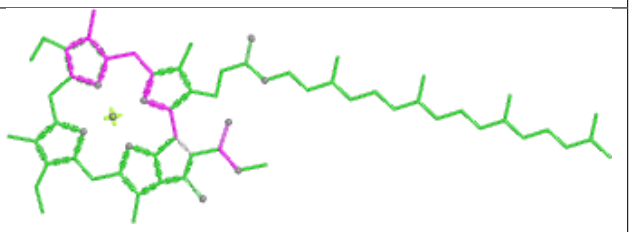
Ligand CLA a 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

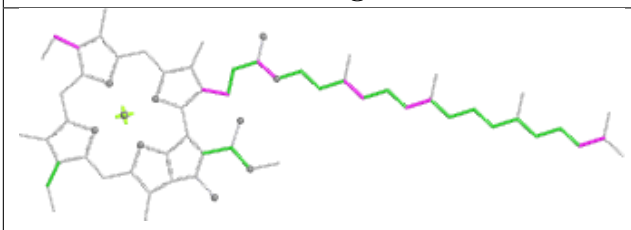
Ligand CLA b 801



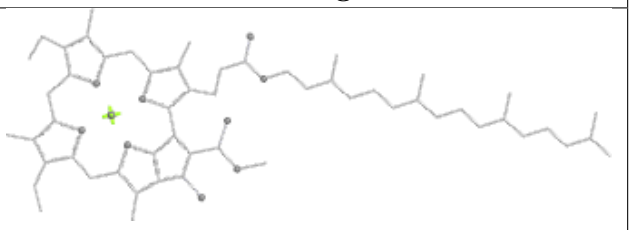
Bond lengths



Bond angles

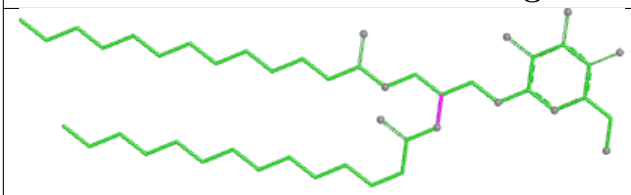


Torsions

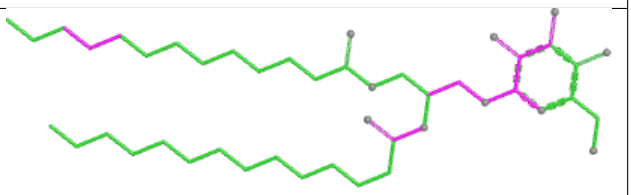


Rings

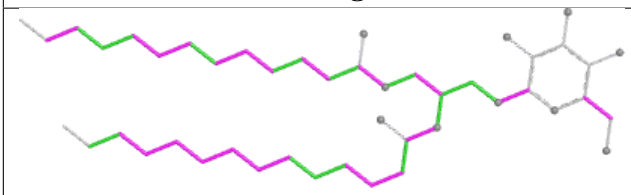
Ligand LMG 0 203



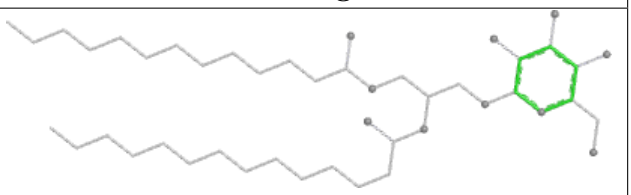
Bond lengths



Bond angles

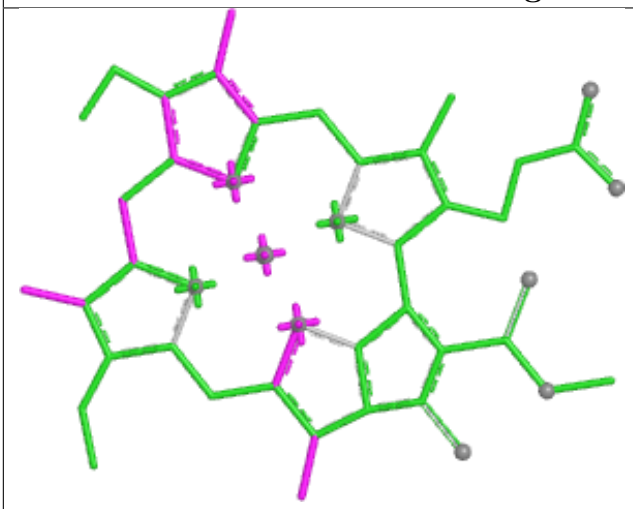


Torsions

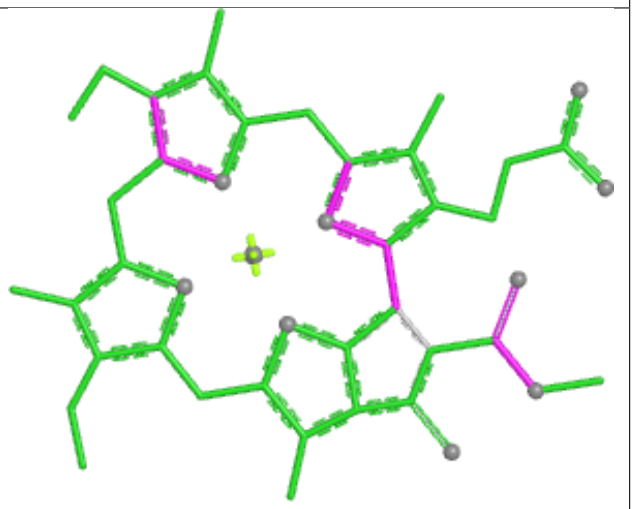


Rings

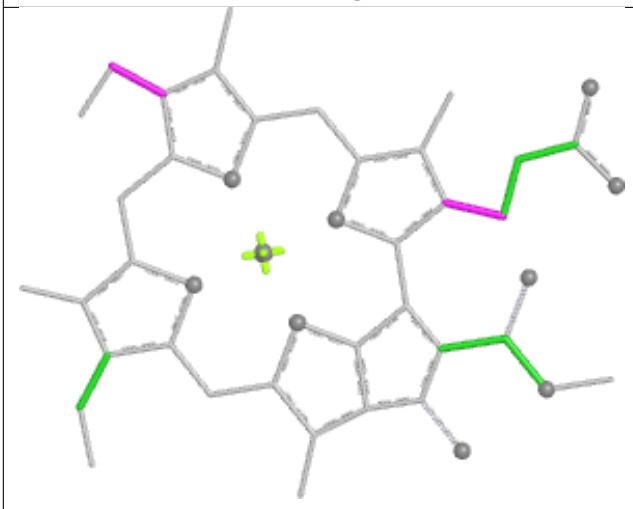
Ligand CLA B 838



Bond lengths



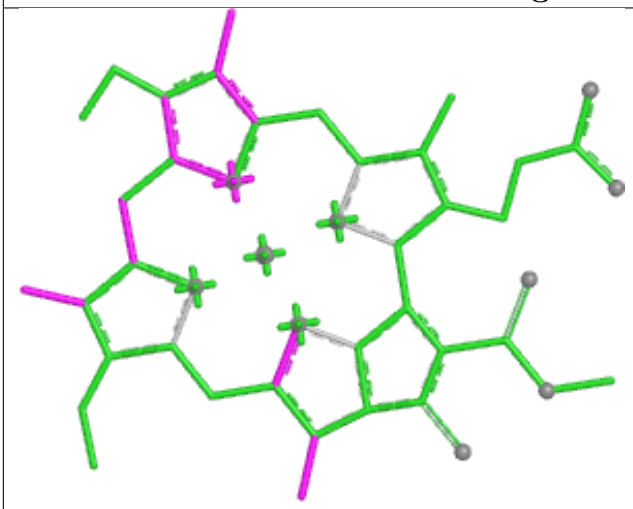
Bond angles



Torsions

Rings

Ligand CLA j 101



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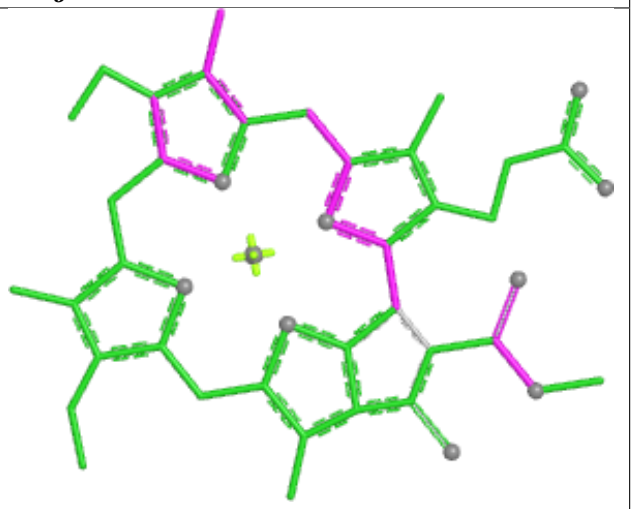
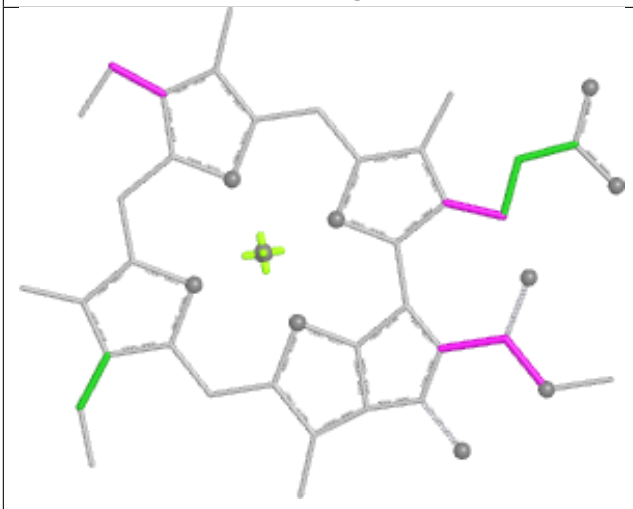


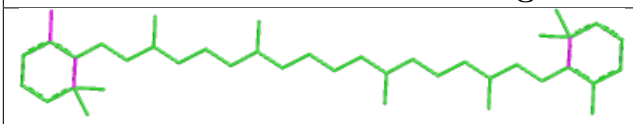
Bond angles



Torsions

Rings

Ligand BCR k 4001



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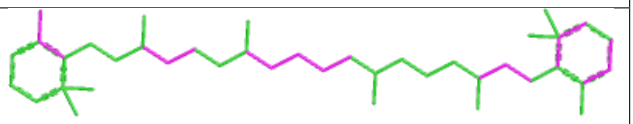
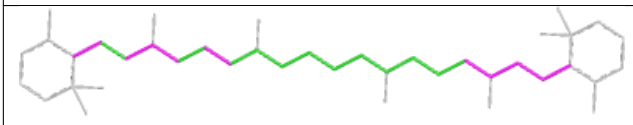
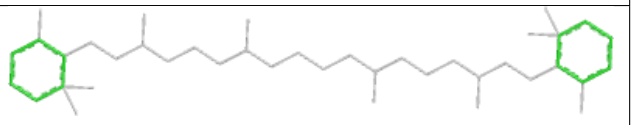


Bond angles

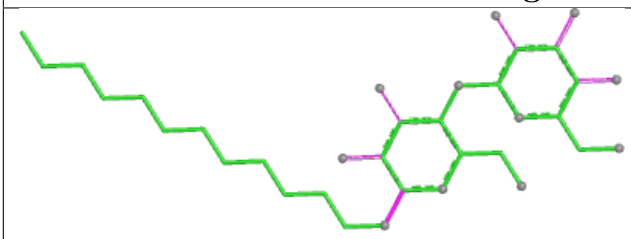


Torsions



Rings

Ligand LMT F 202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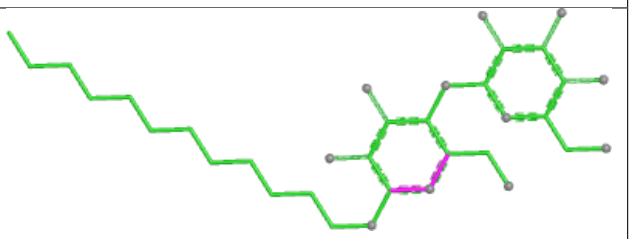
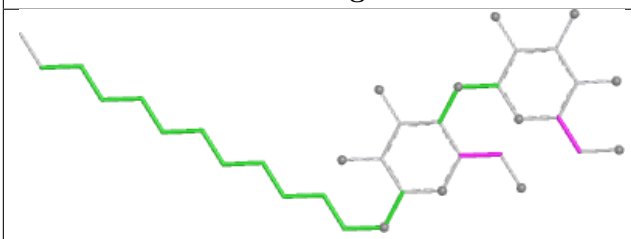

Bond angles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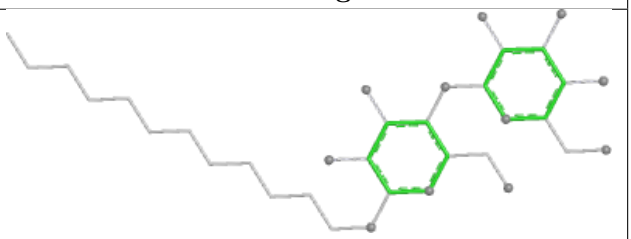
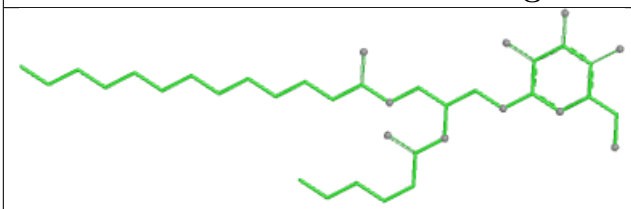

Rings

Ligand LMG 0 201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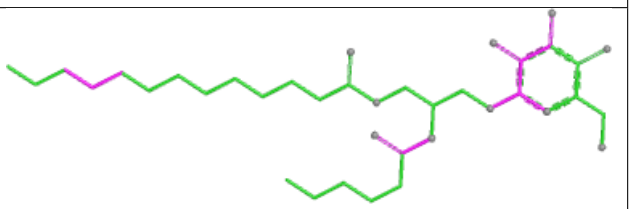
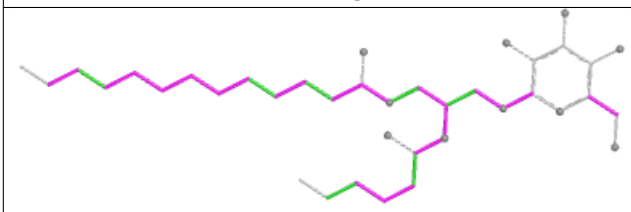

Bond angles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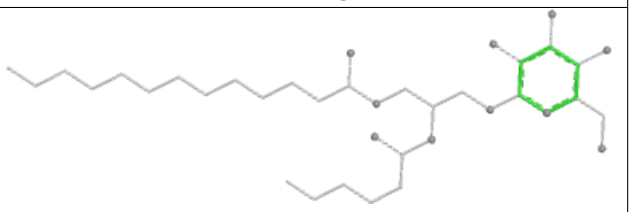
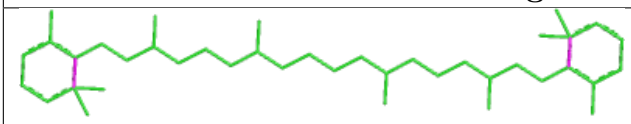

Rings

Ligand BCR 2 847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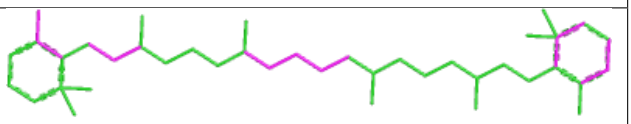
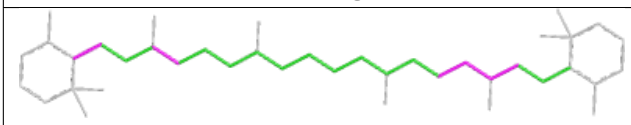

Bond angles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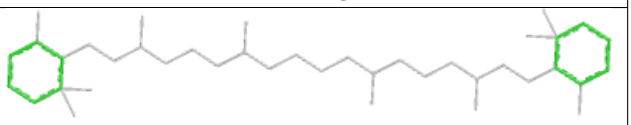
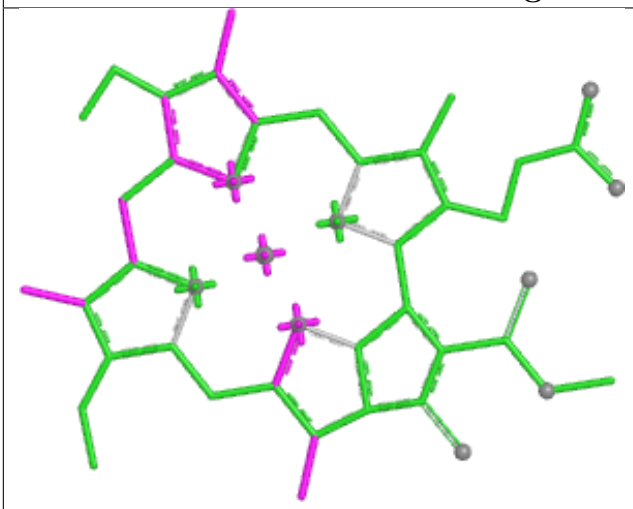

Rings

Ligand CLA B 815



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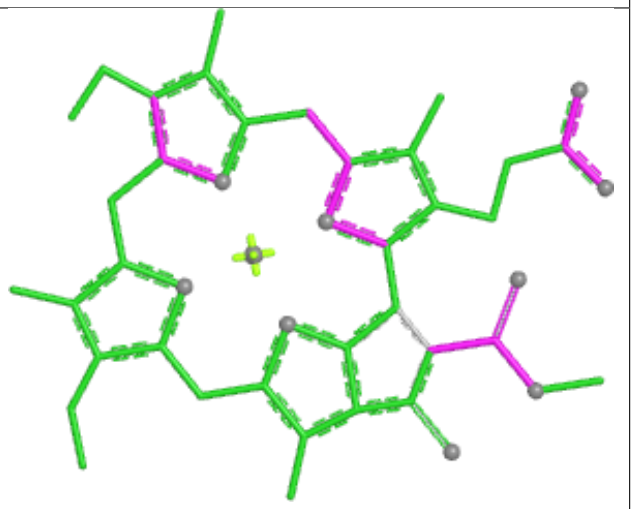
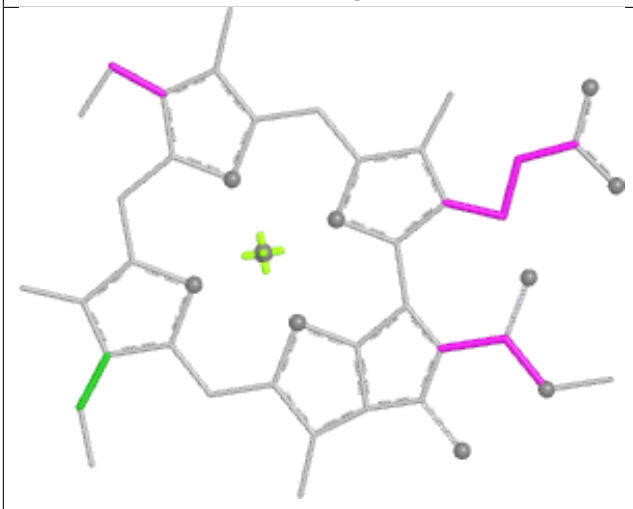


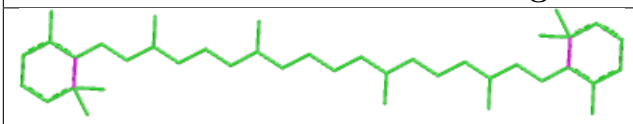
Bond angles



Torsions

Rings

Ligand BCR f 206



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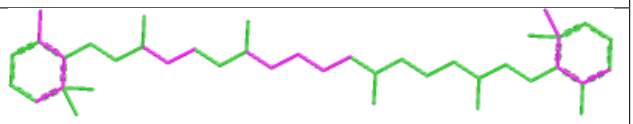
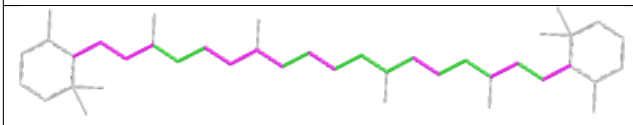
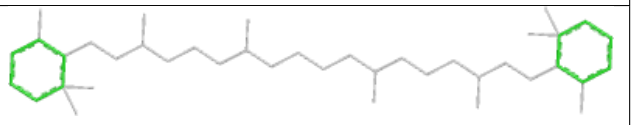


Bond angles

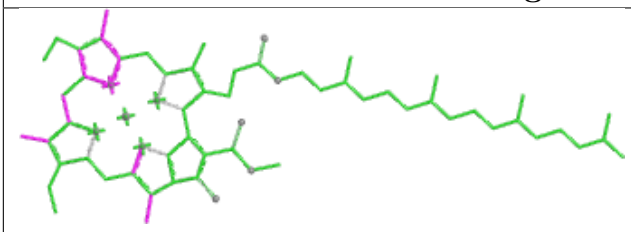


Torsions

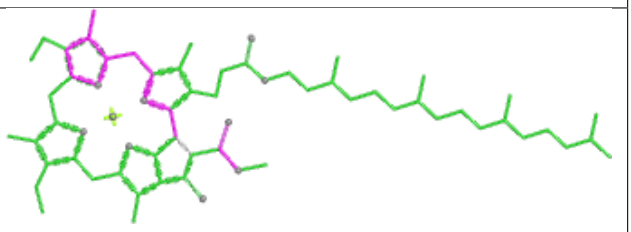


Rings

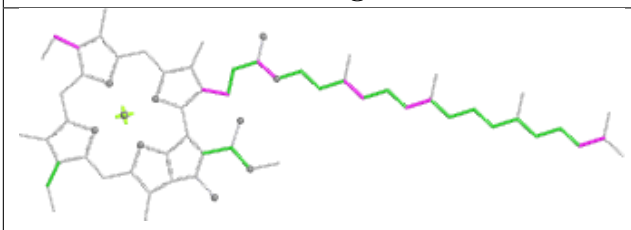
Ligand CLA B 802



Bond lengths



Bond angles



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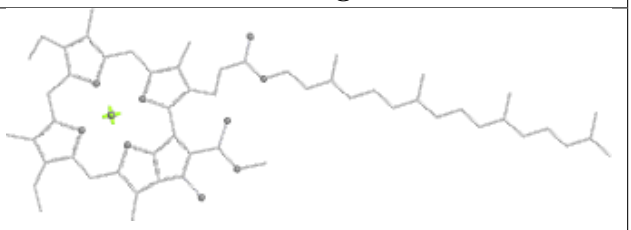
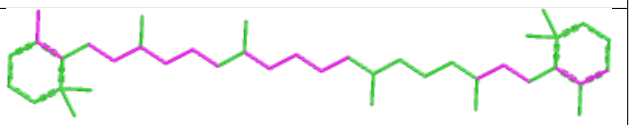


Rings

Ligand BCR 1 847

Bond lengths



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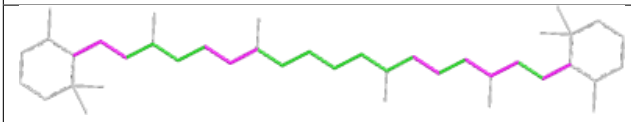

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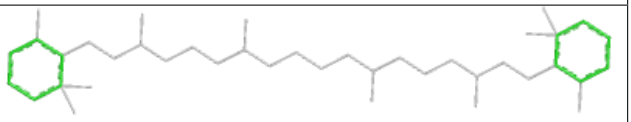
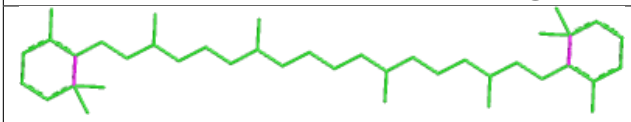


Rings

Ligand BCR a 851



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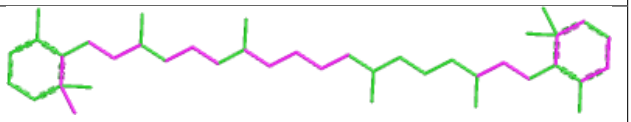
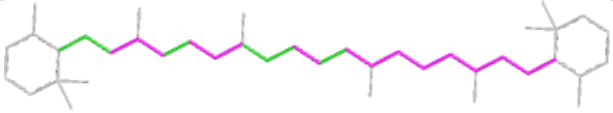


Bond angles



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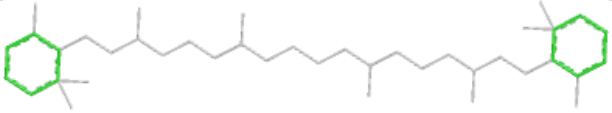
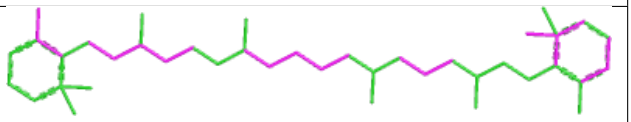


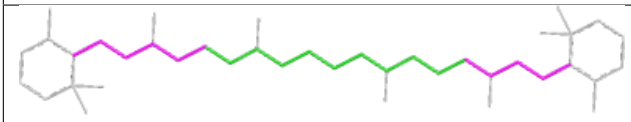
Rings

Ligand BCR 0 204

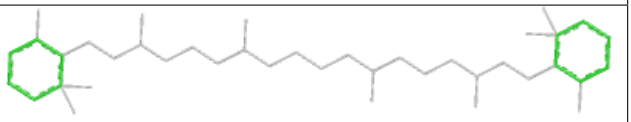
Bond lengths



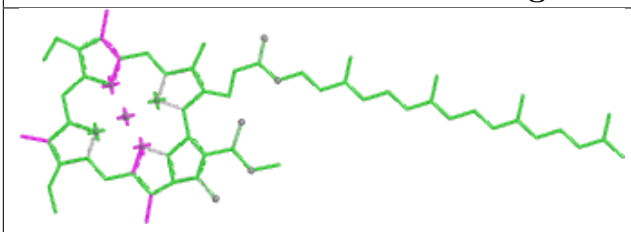
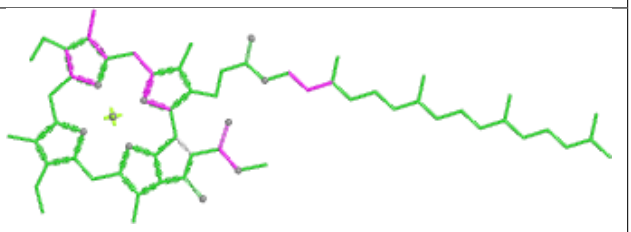
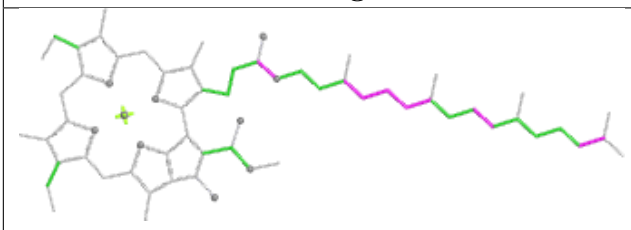
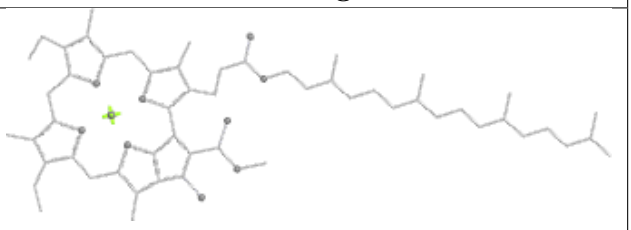
Bond angles

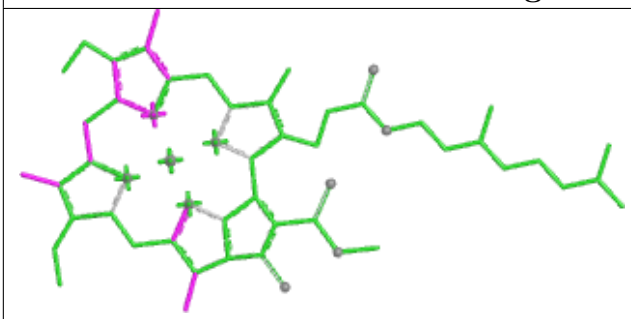
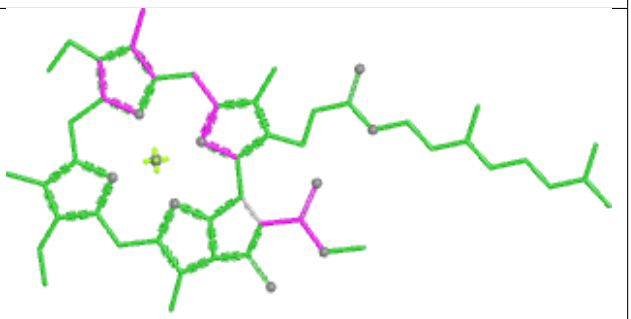
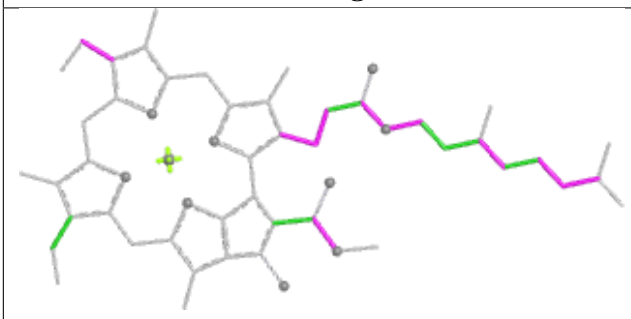
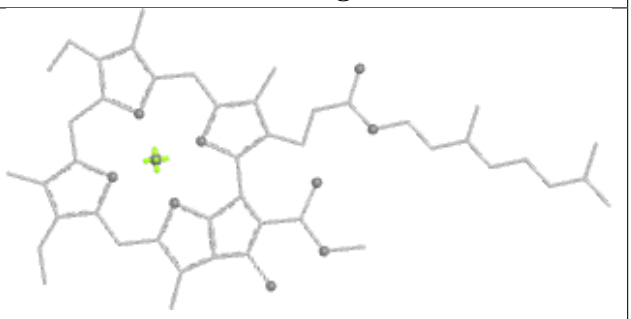


Torsions

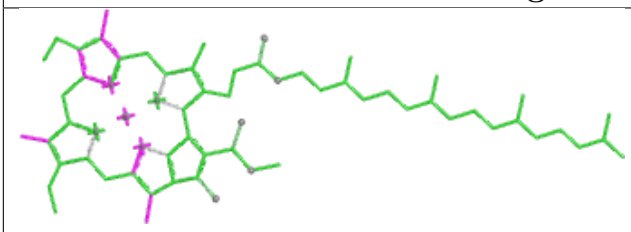


Rings

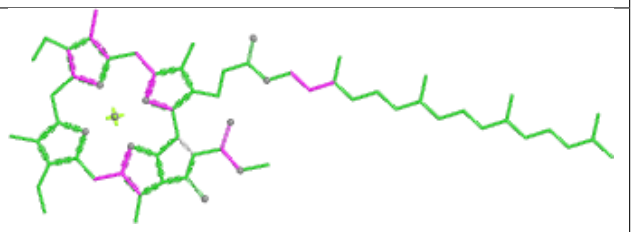
Ligand CLA 1 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

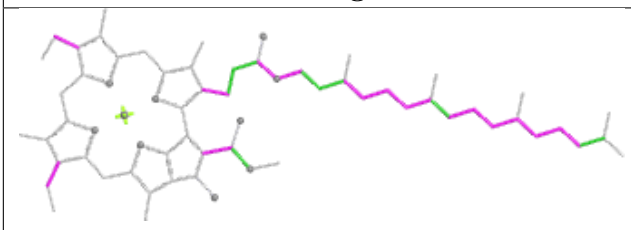
Ligand CLA b 815



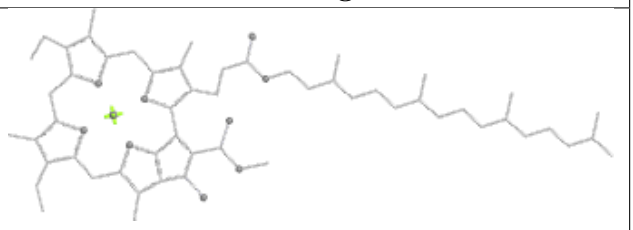
Bond lengths



Bond angles

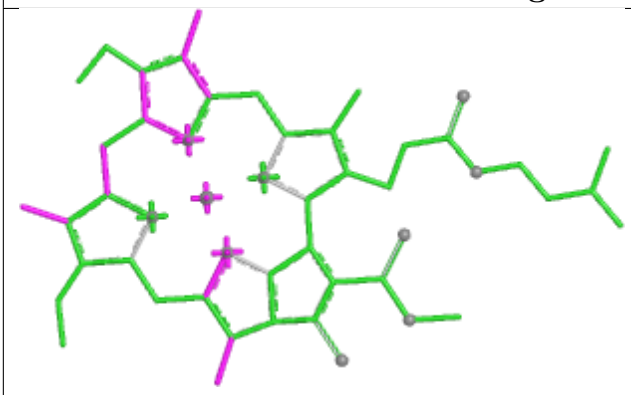


Torsions



Rings

Ligand CLA a 807



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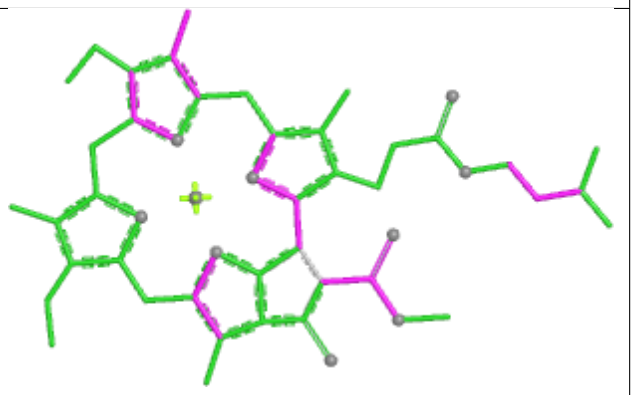
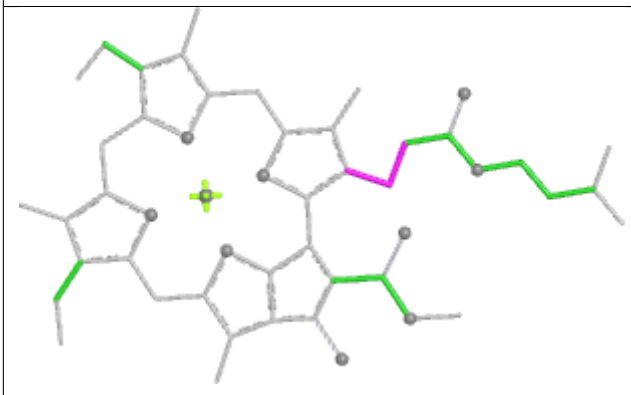
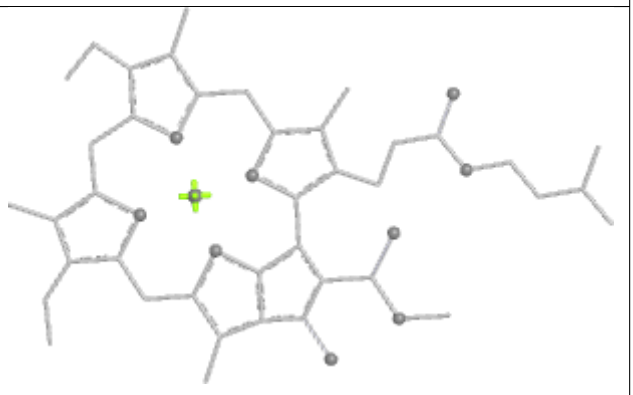


Bond angles

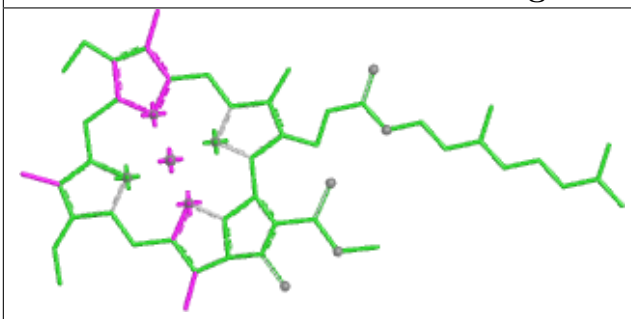


Torsions



Rings

Ligand CLA 2 818



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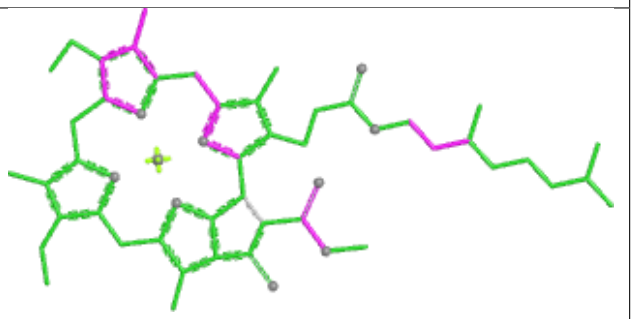
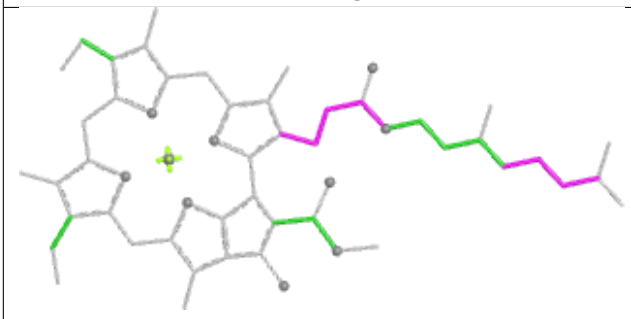


Bond angles



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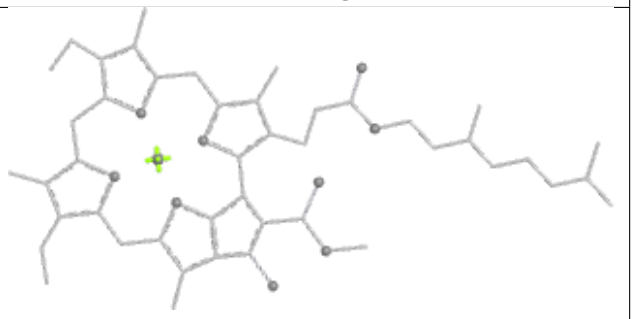
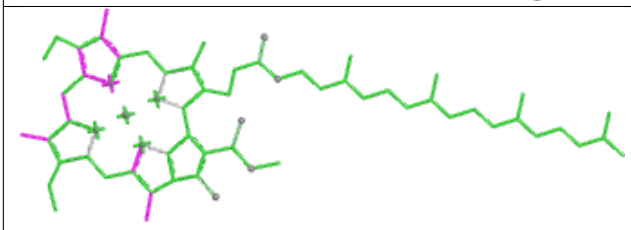


Rings

Ligand CLA 2 828



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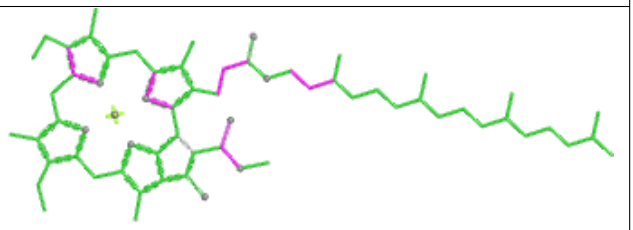
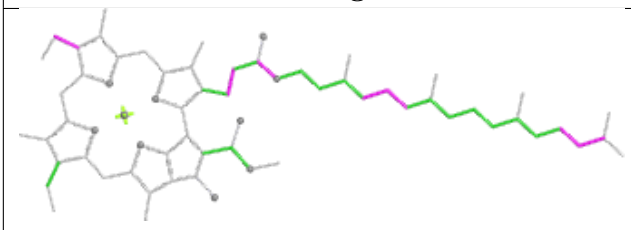


Bond angles



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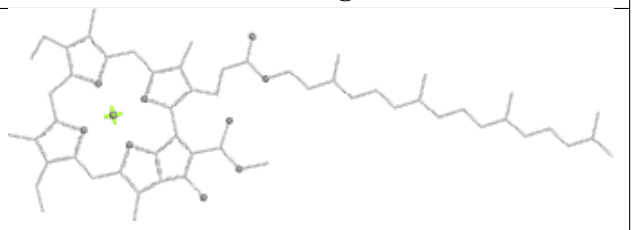
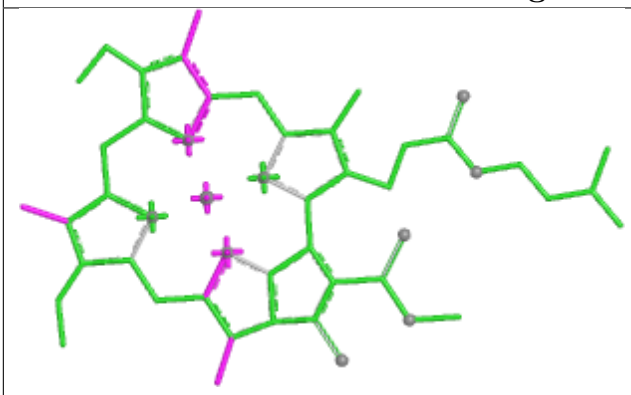


Rings

Ligand CLA 2 839



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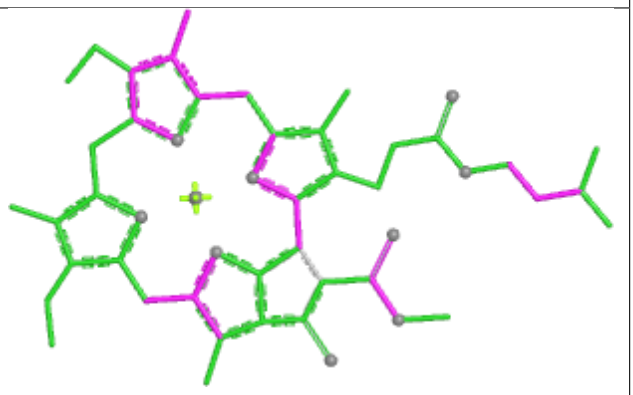
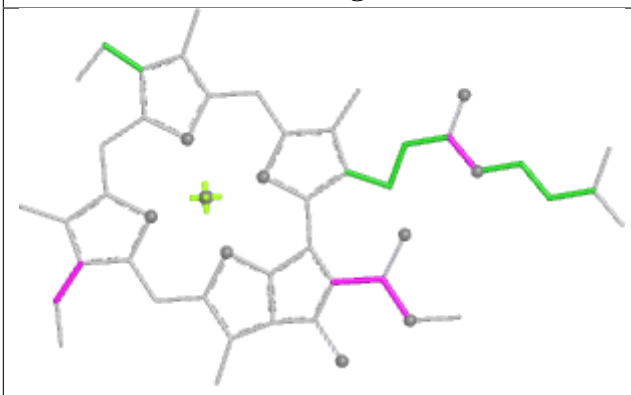


Bond angles



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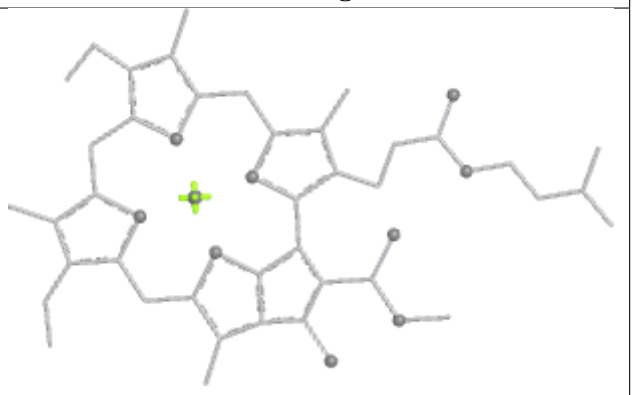
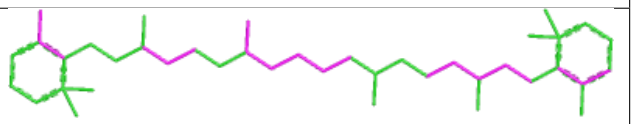


Rings

Ligand BCR A 850

Bond lengths



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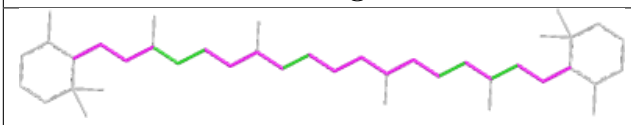

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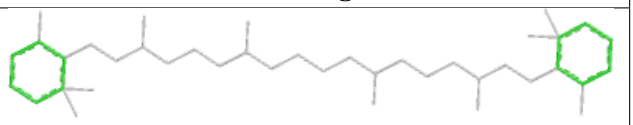
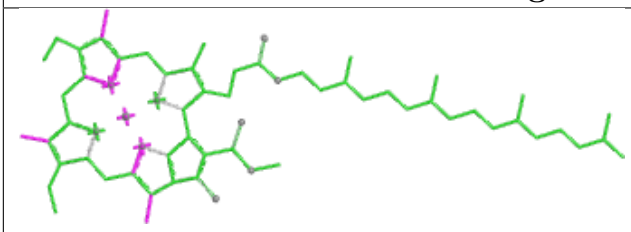


Rings

Ligand CLA 2 830



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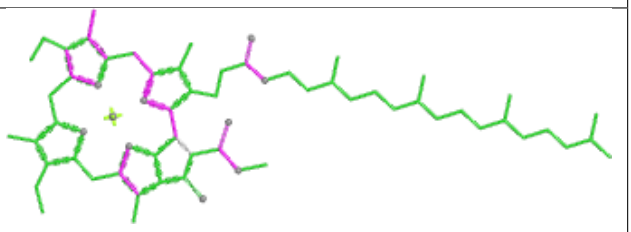
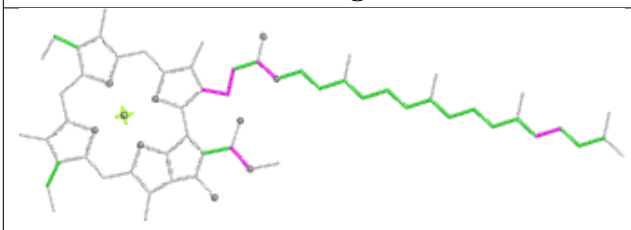


Bond angles



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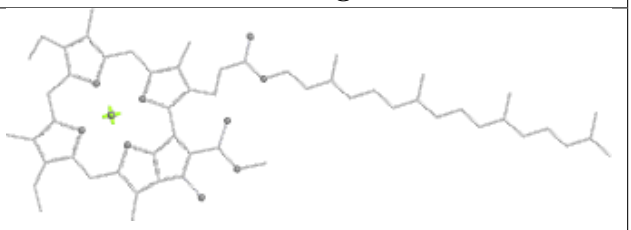
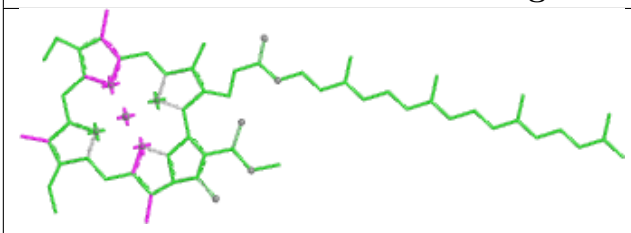


Rings

Ligand CLA a 828



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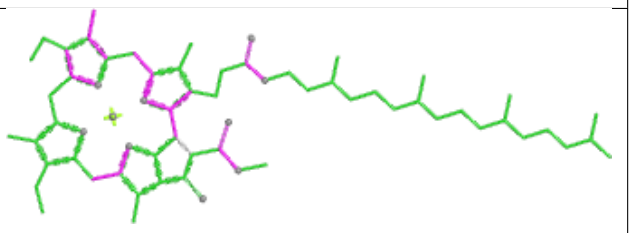

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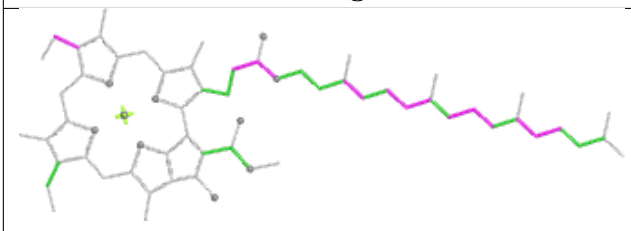

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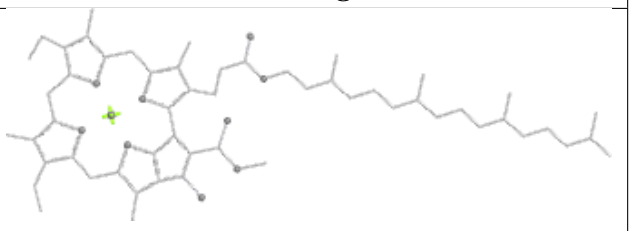
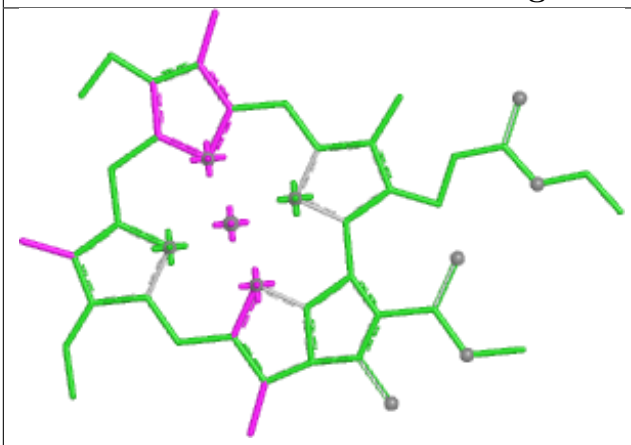


Rings

Ligand CLA 1 839



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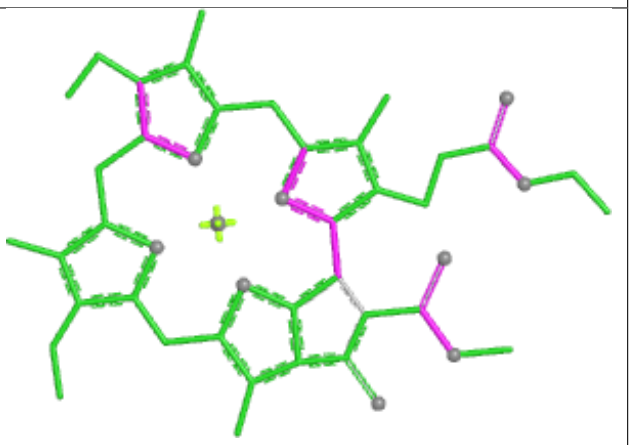
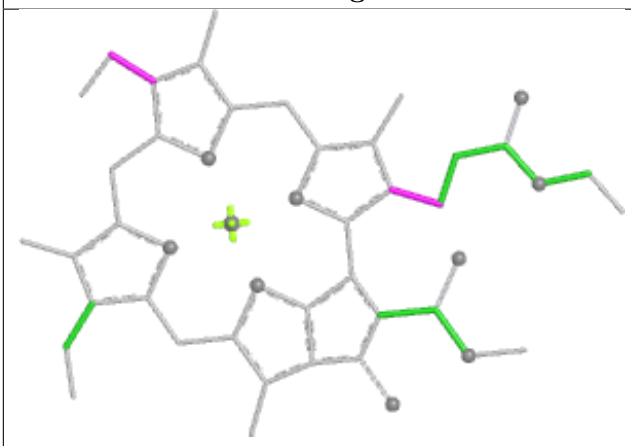


Bond angles



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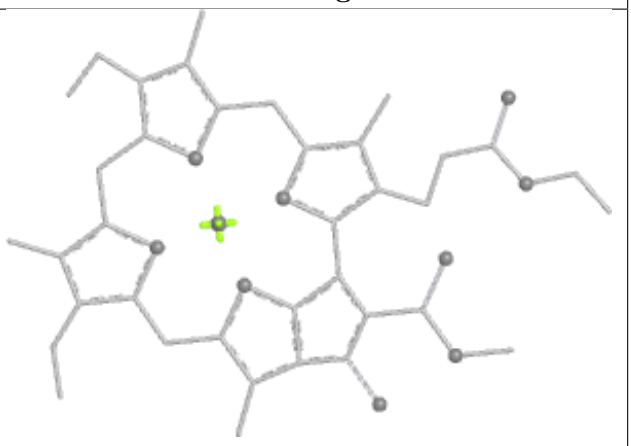
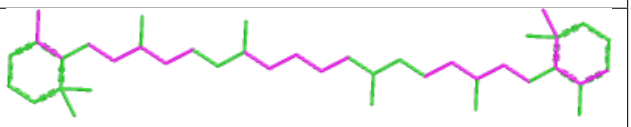


Rings

Ligand BCR B 850

Bond lengths



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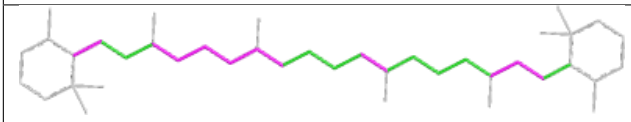

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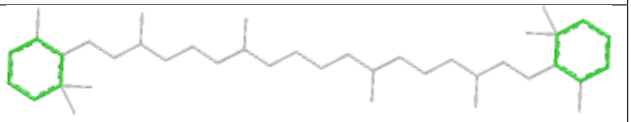
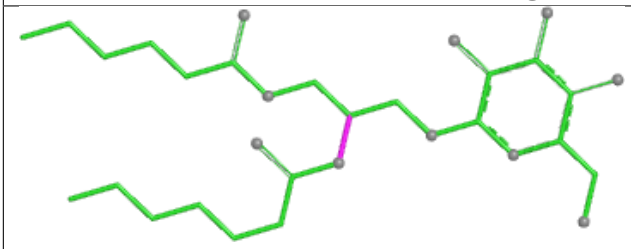


Rings

Ligand LMG 1 852



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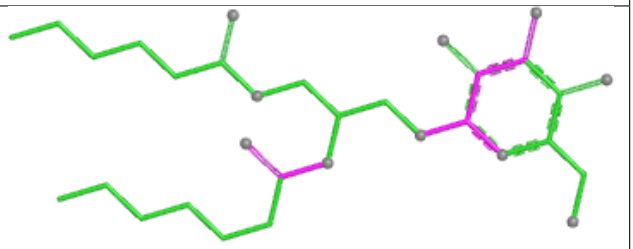
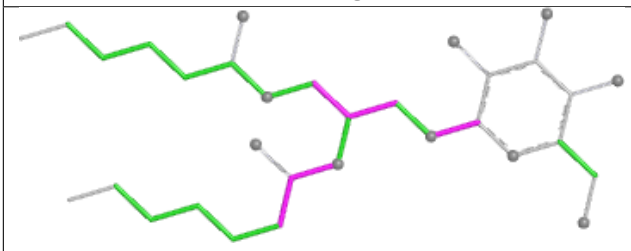


Bond angles



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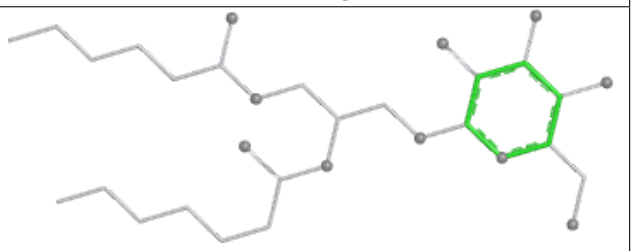
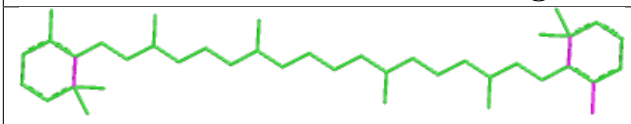


Rings

Ligand BCR f 203



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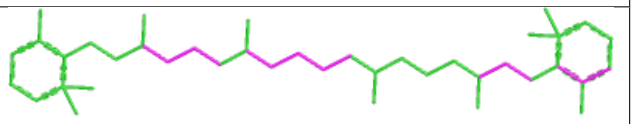
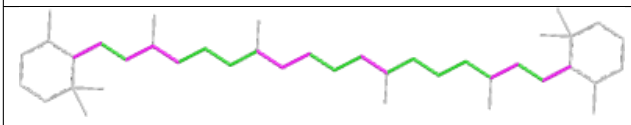
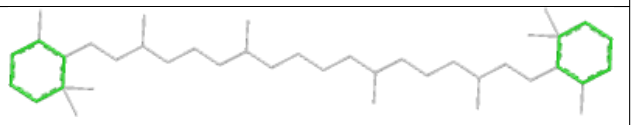


Bond angles

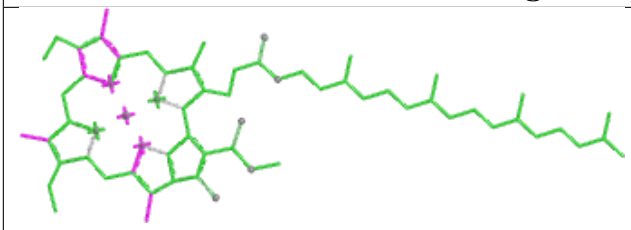


Torsions

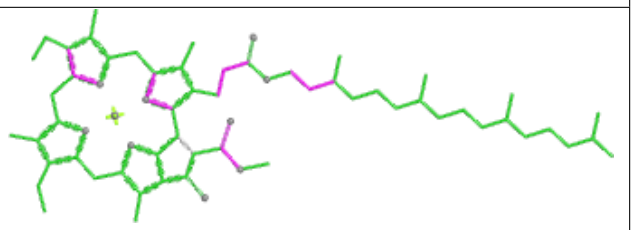


Rings

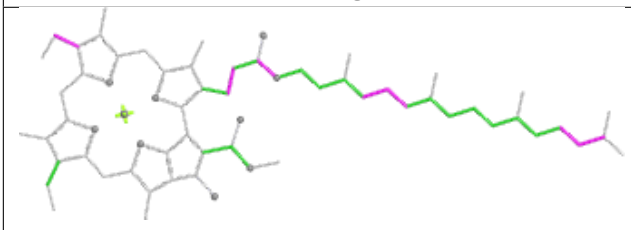
Ligand CLA B 829



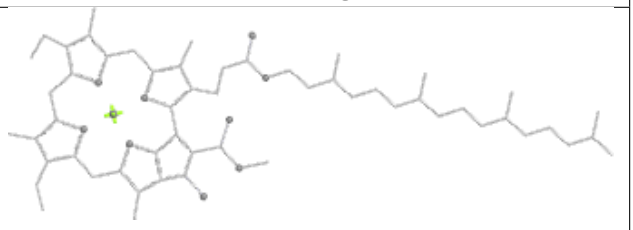
Bond lengths



Bond angles

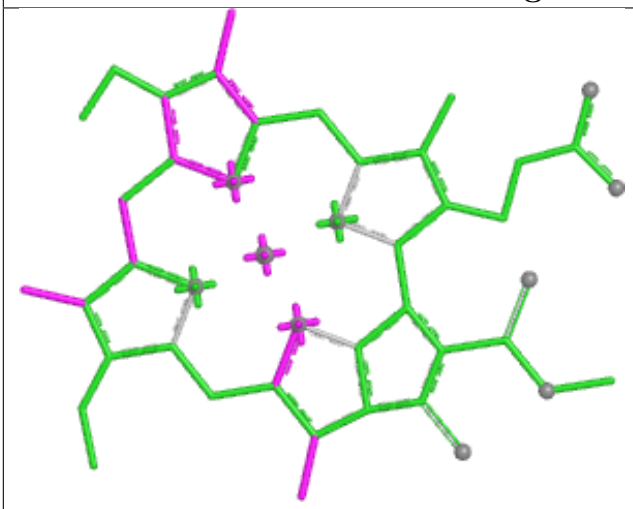


Torsions



Rings

Ligand CLA B 826



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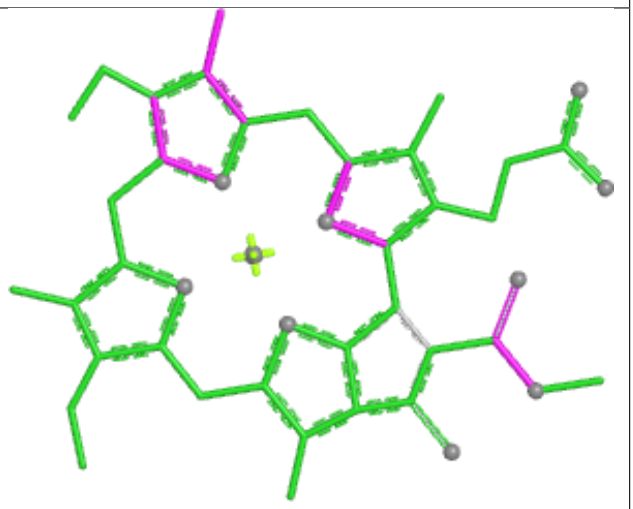
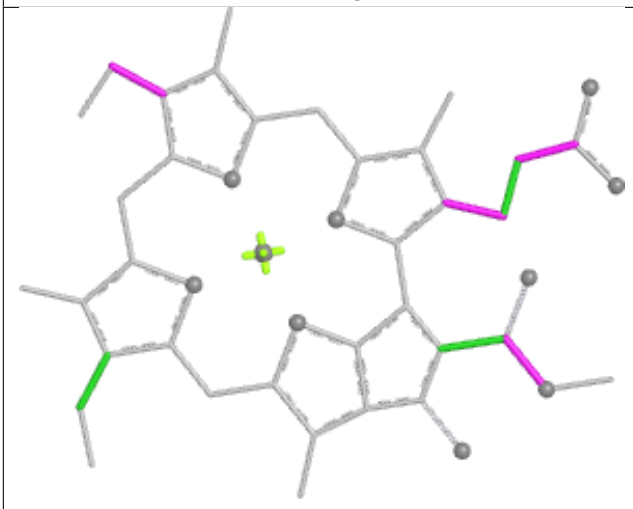


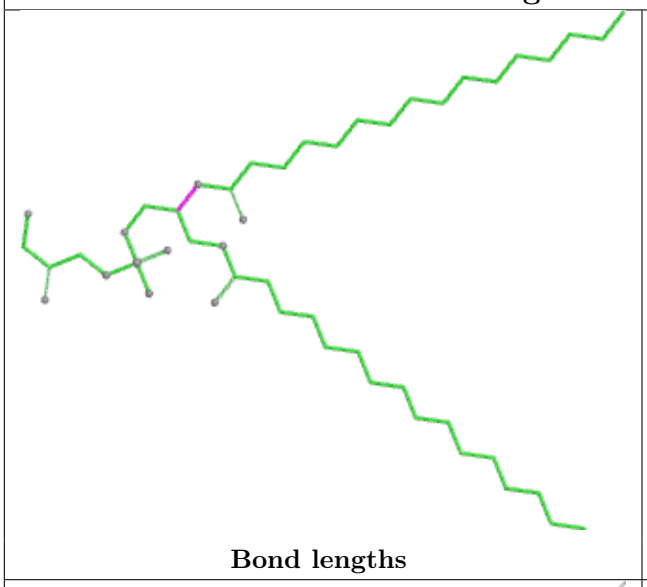
Bond angles



Torsions

Rings

Ligand LHG A 801



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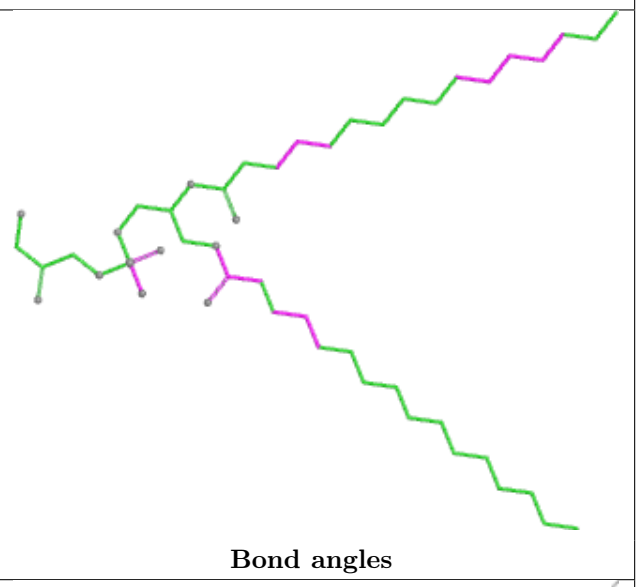
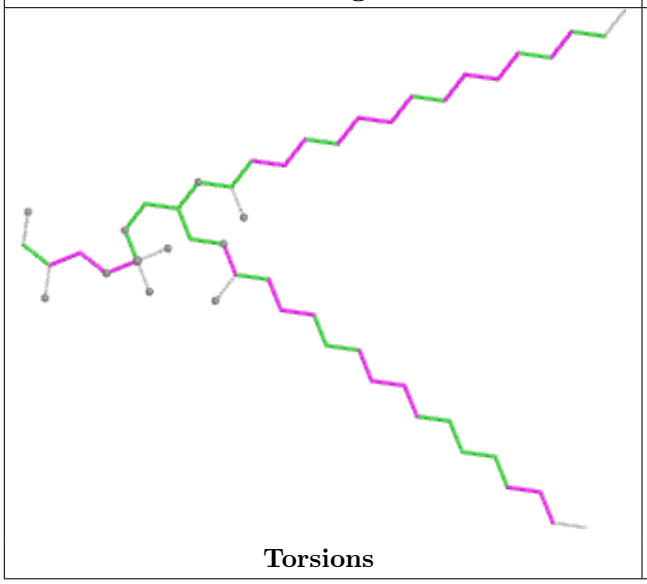
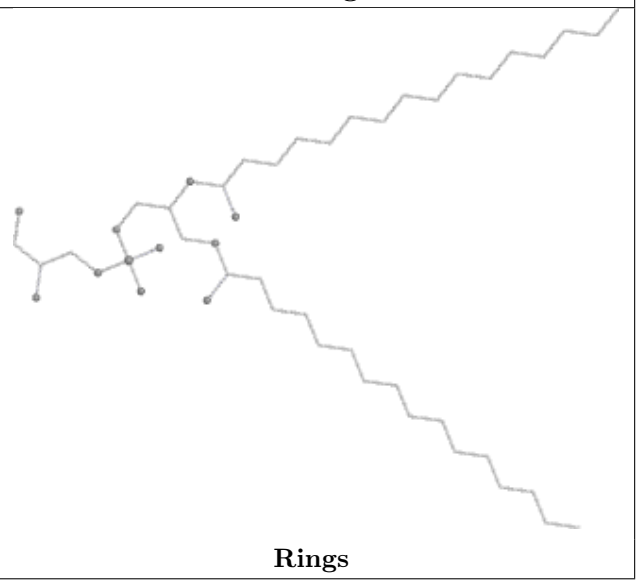


Bond angles

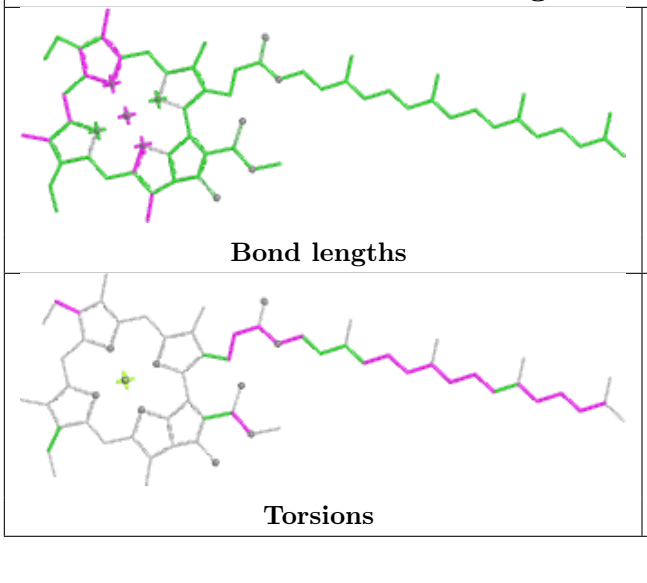


Torsions

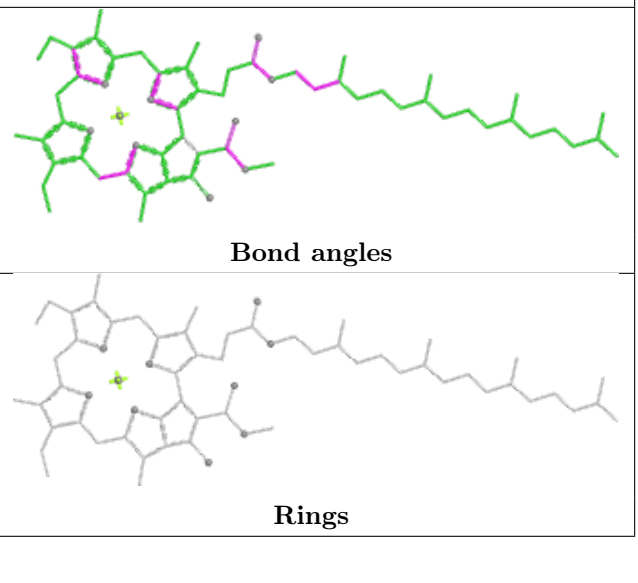


Rings

Ligand CLA 2 808



Bond lengths

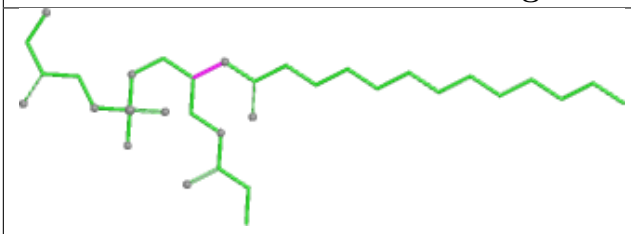


Bond angles

Torsions

Rings

Ligand LHG A 802



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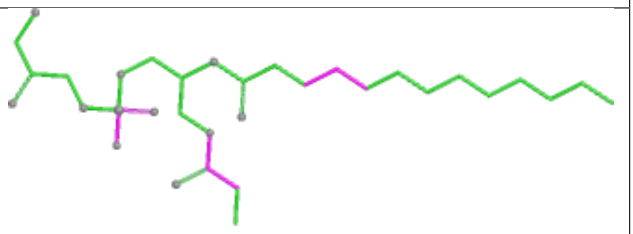
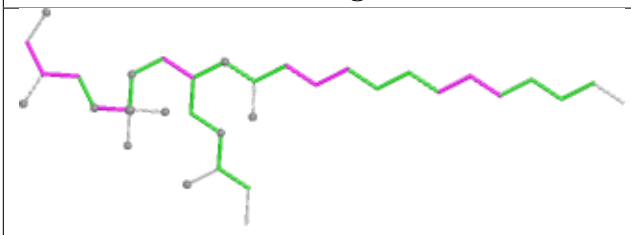
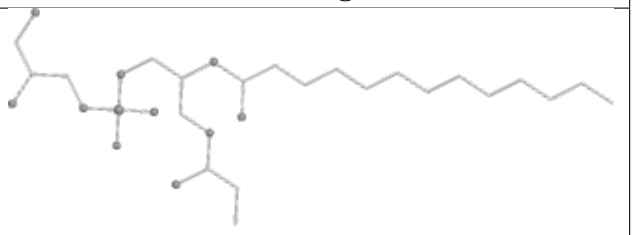


Bond angles

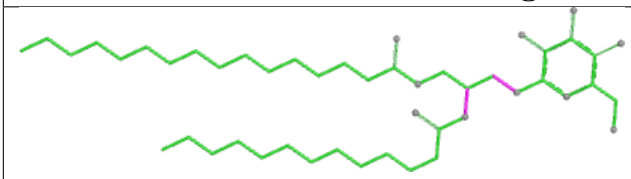


Torsions



Rings

Ligand LMG B 803



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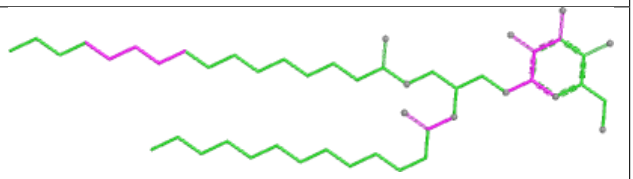
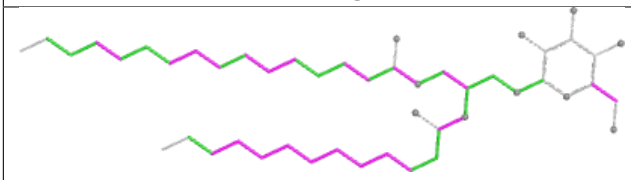


Bond angles



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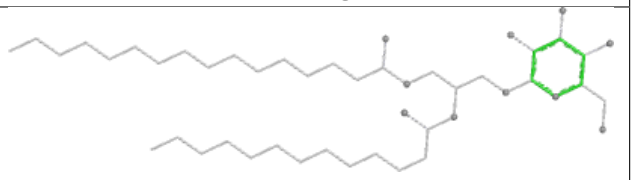
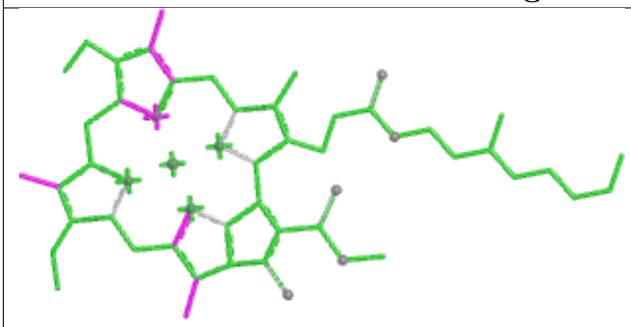


Rings

Ligand CLA A 819



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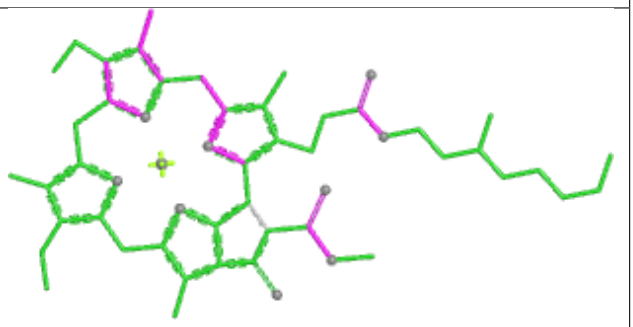
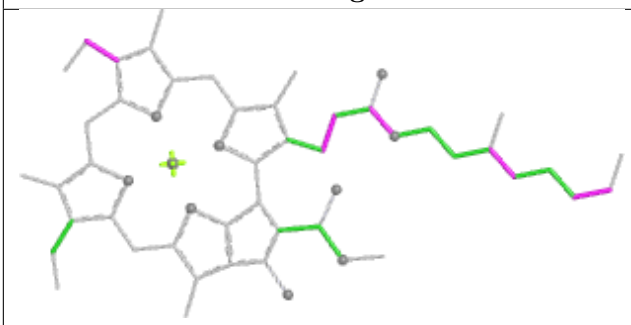
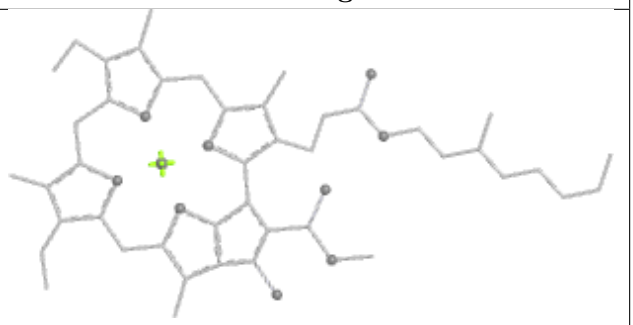


Bond angles

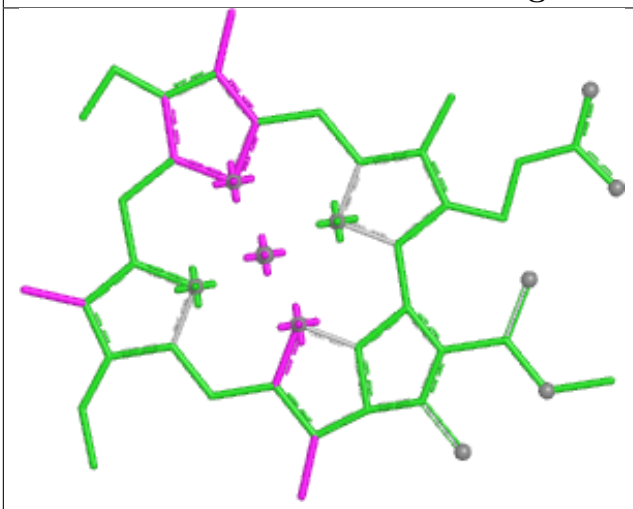


Torsions



Rings

Ligand CLA 1 815



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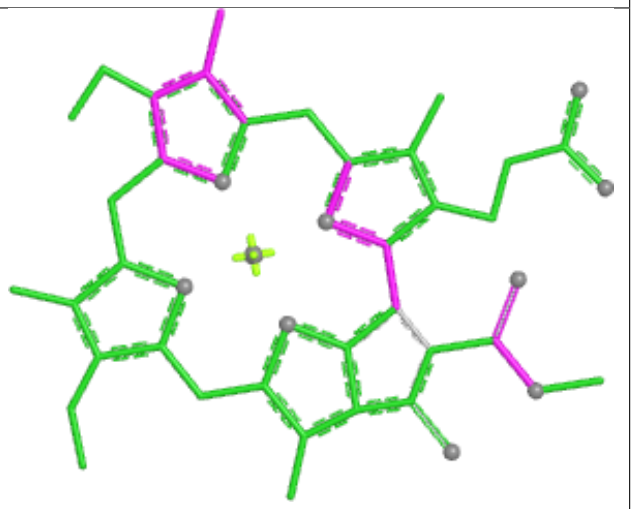
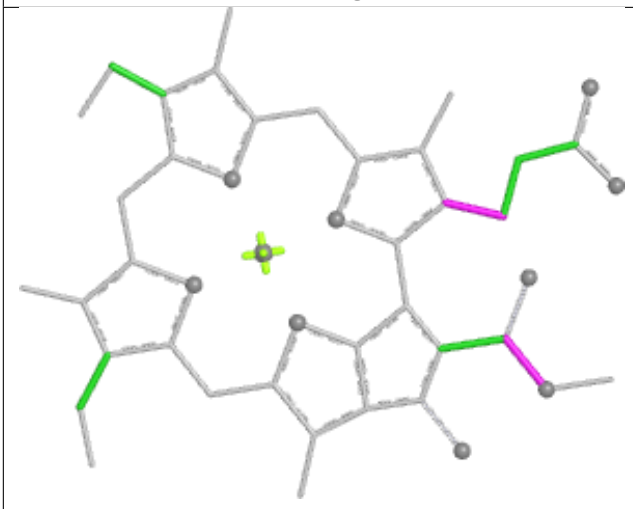


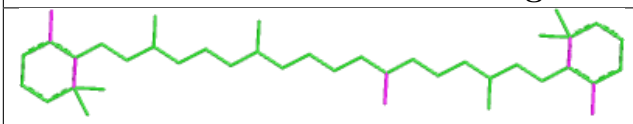
Bond angles



Torsions

Rings

Ligand BCR b 850



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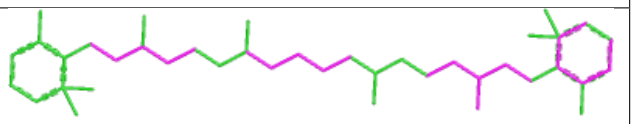
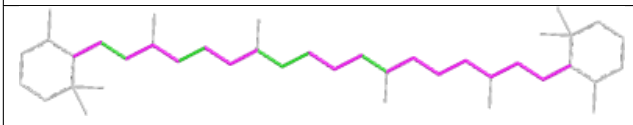


Bond angles



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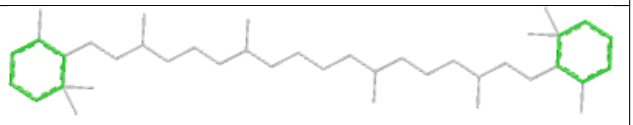
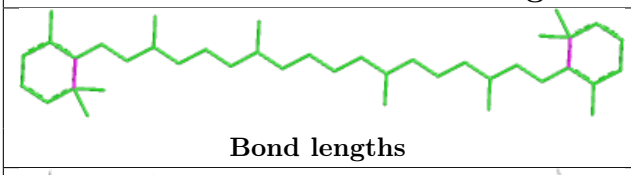


Rings

Ligand BCR 0 210



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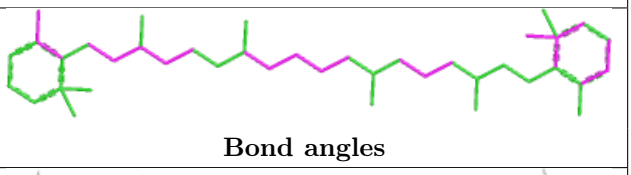
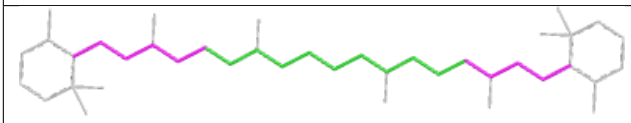


Bond angles



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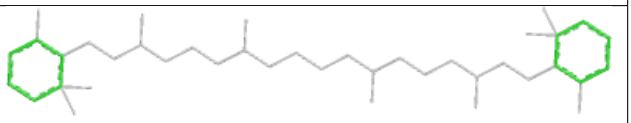
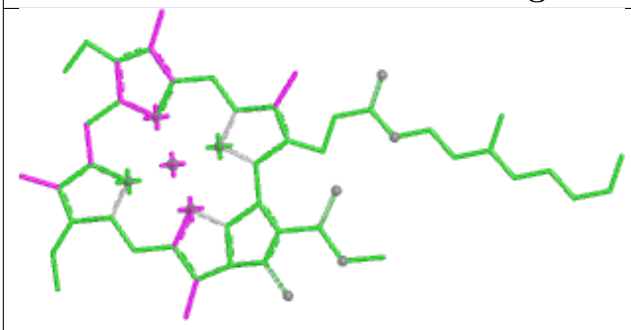


Rings

Ligand CLA a 815



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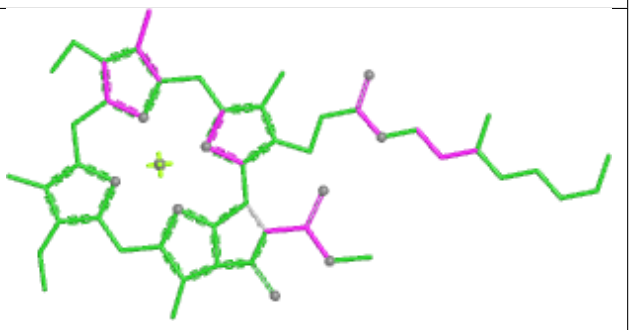
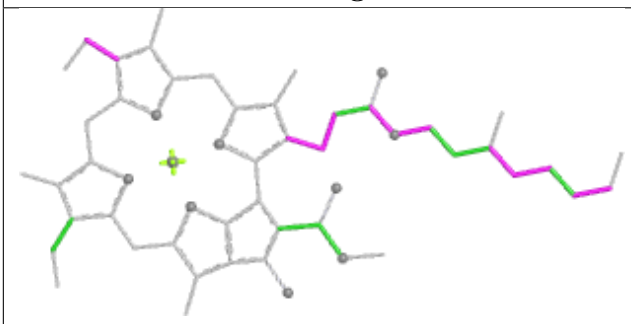


Bond angles



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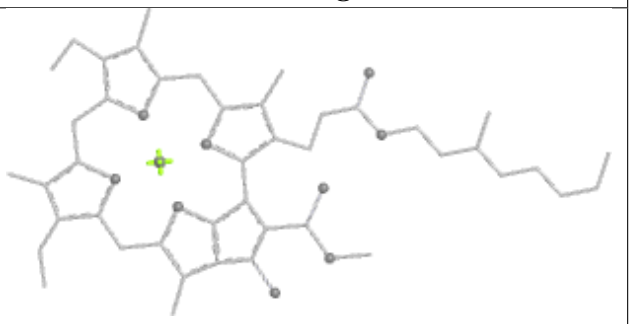
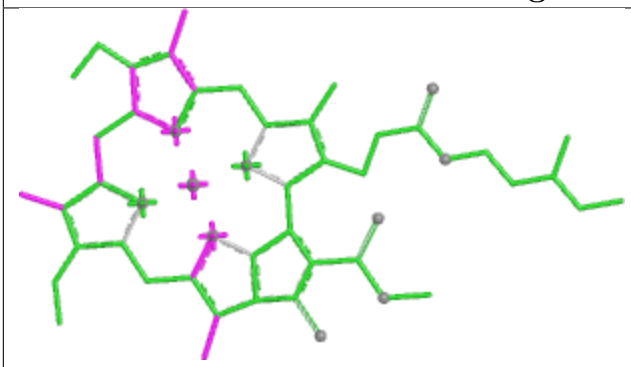


Rings

Ligand CLA a 826



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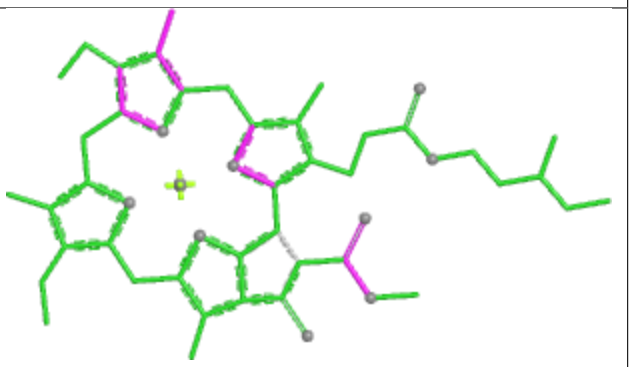
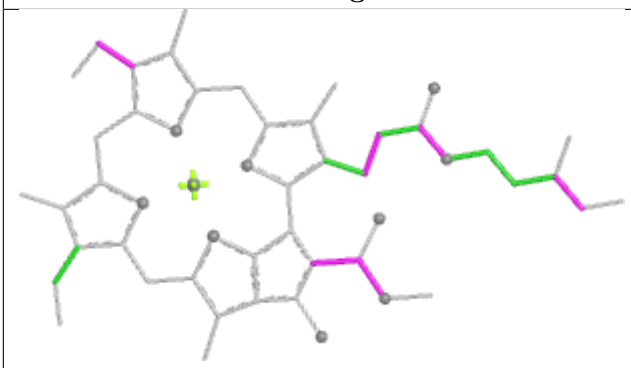
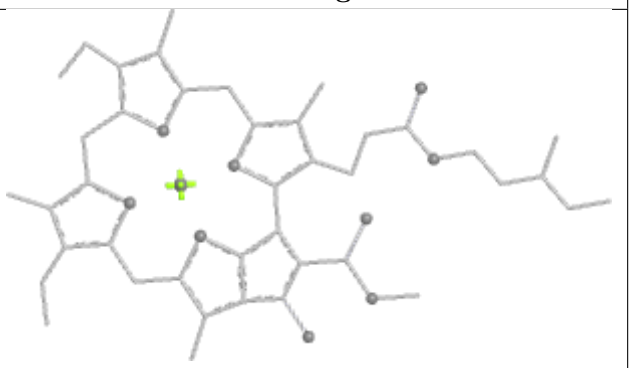


Bond angles

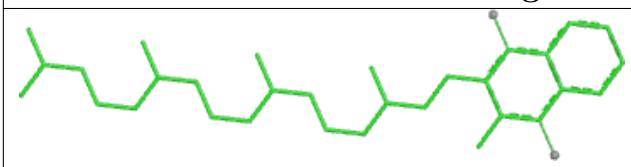


Torsions



Rings

Ligand PQN B 846



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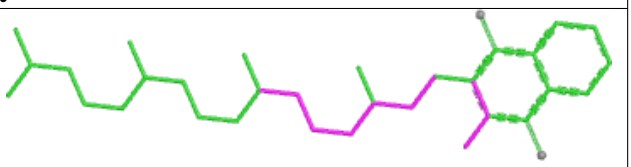

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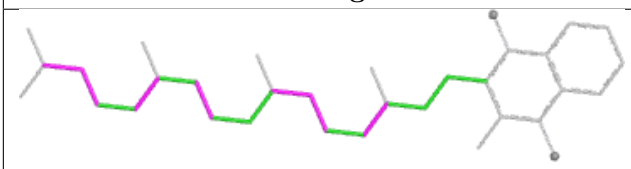

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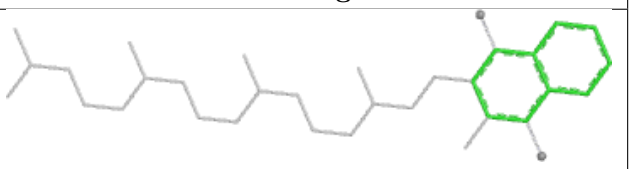
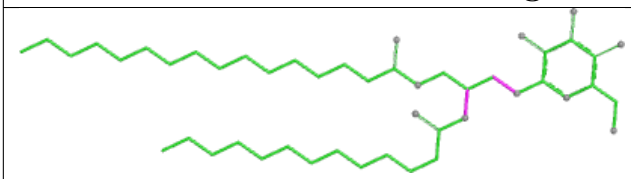


Rings

Ligand LMG 2 802



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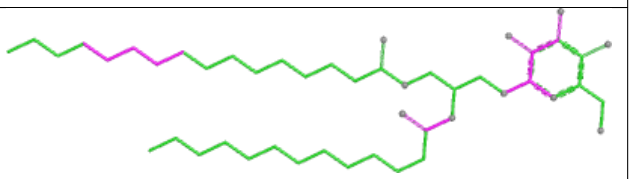
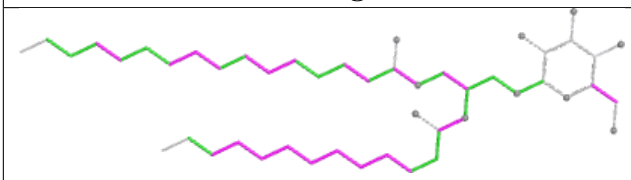


Bond angles



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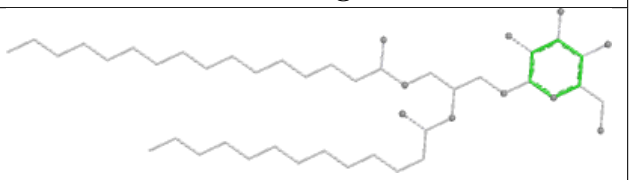
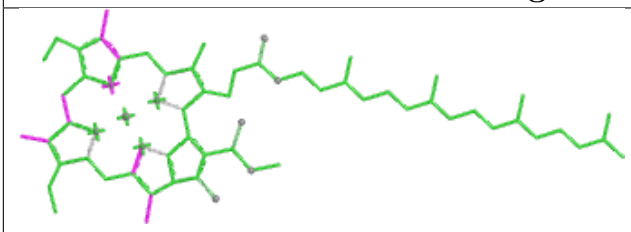


Rings

Ligand CLA a 836



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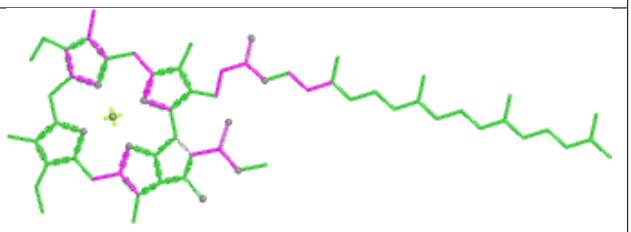
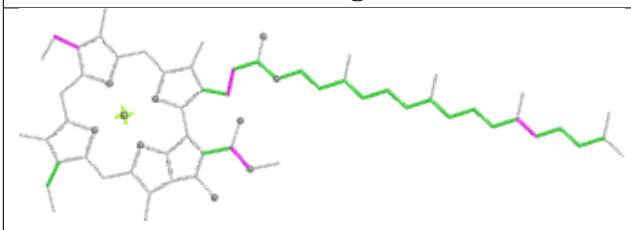


Bond angles



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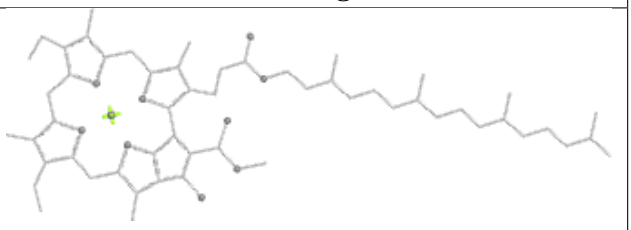
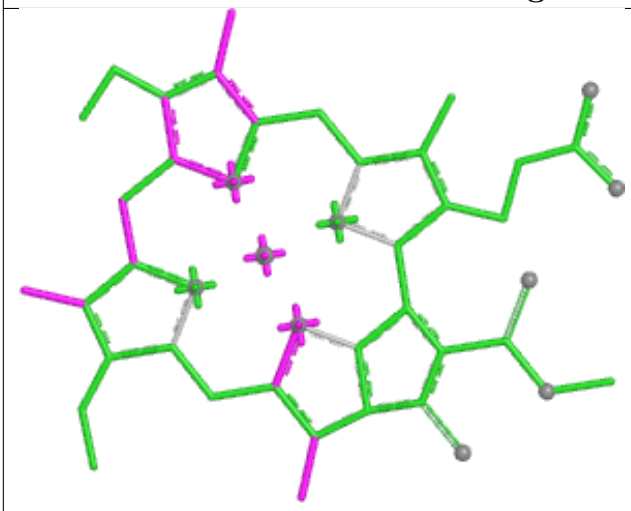


Rings

Ligand CLA b 836



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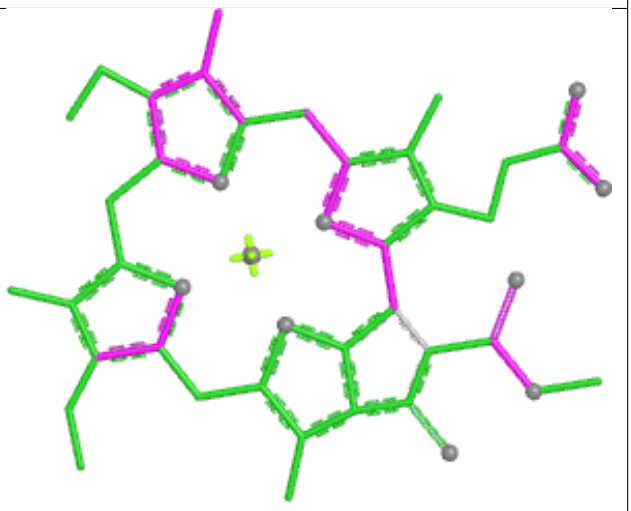
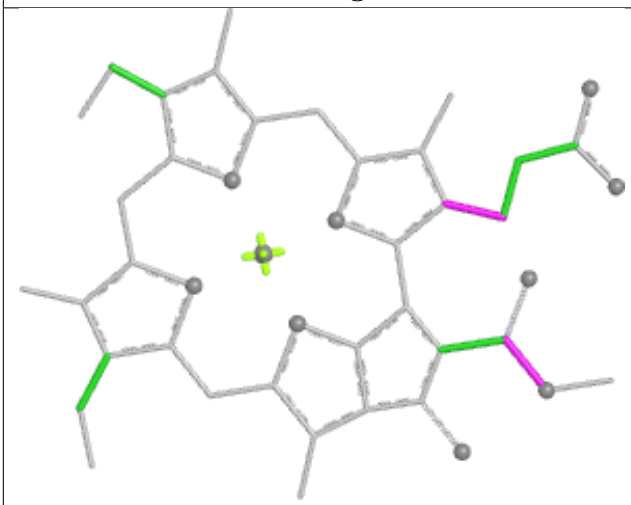
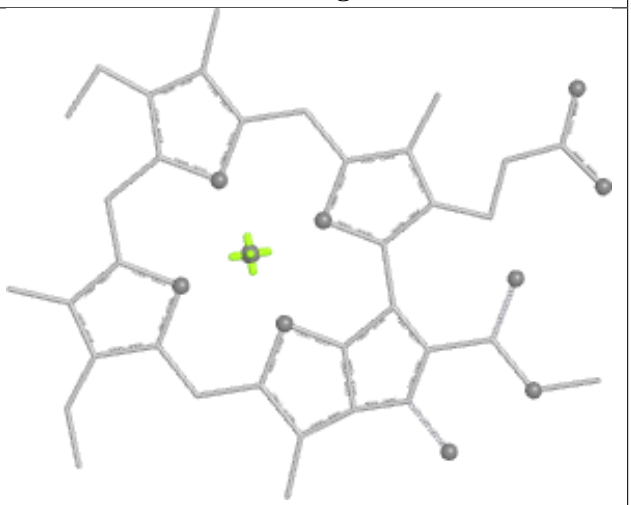


Bond angles

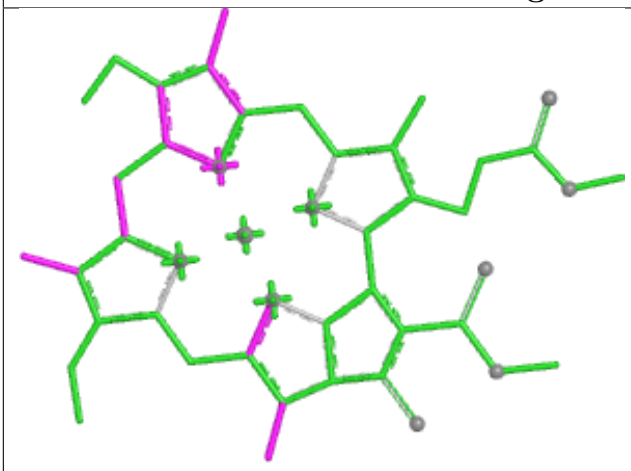


Torsions

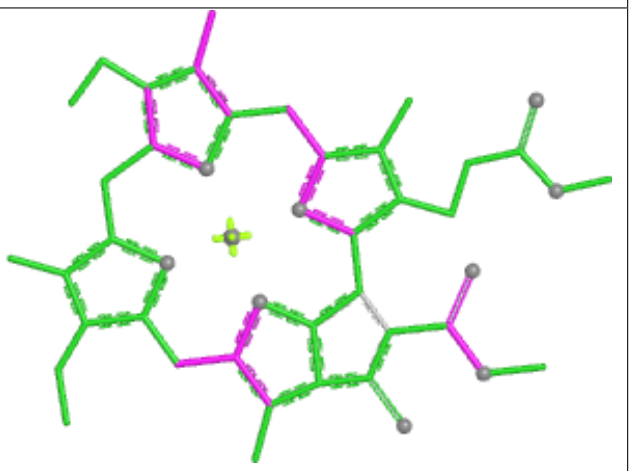


Rings

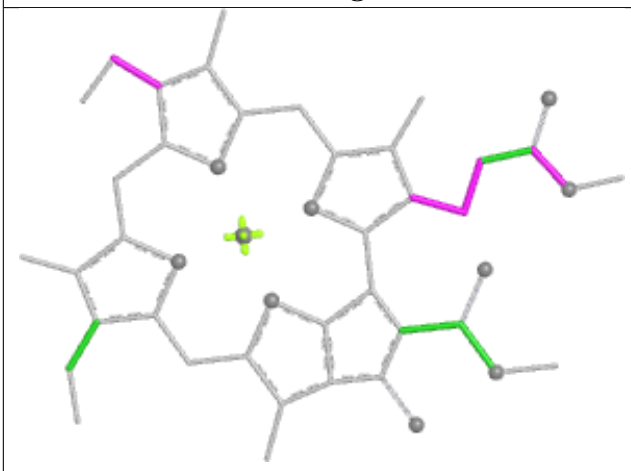
Ligand CLA b 838



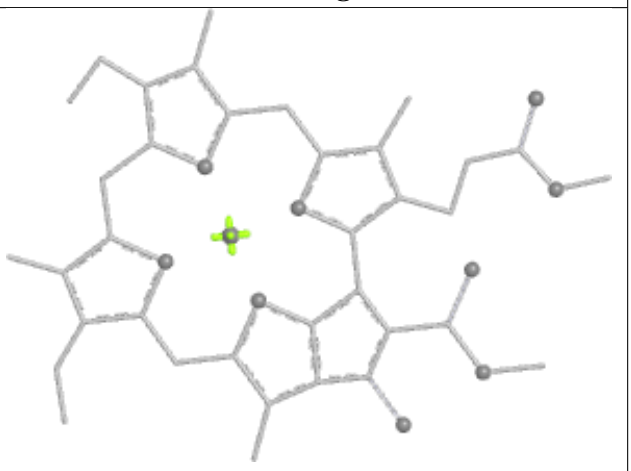
Bond lengths



Bond angles

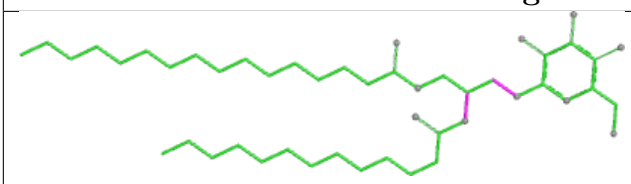


Torsions

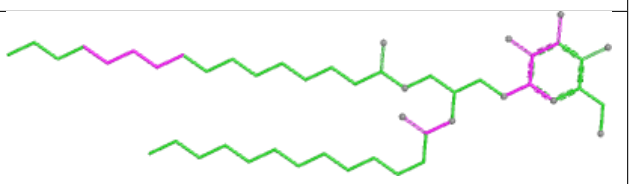


Rings

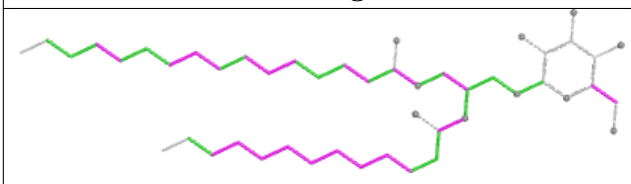
Ligand LMG b 803



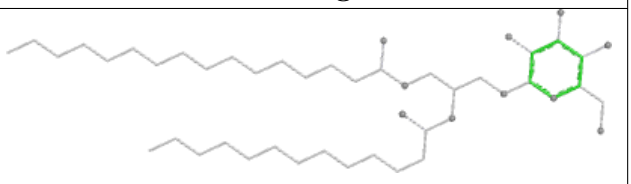
Bond lengths



Bond angles

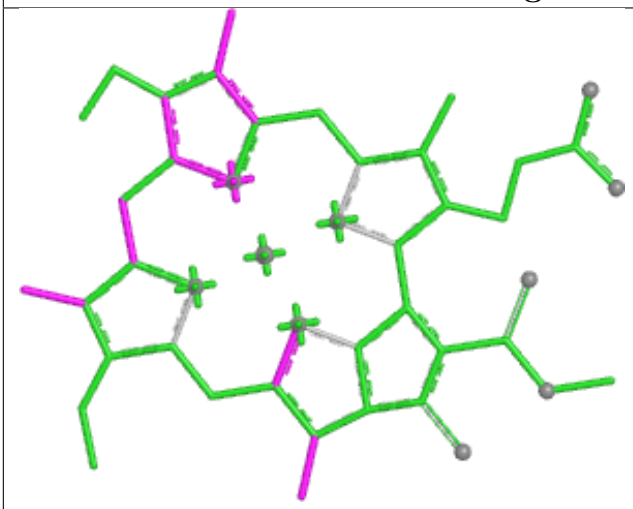


Torsions

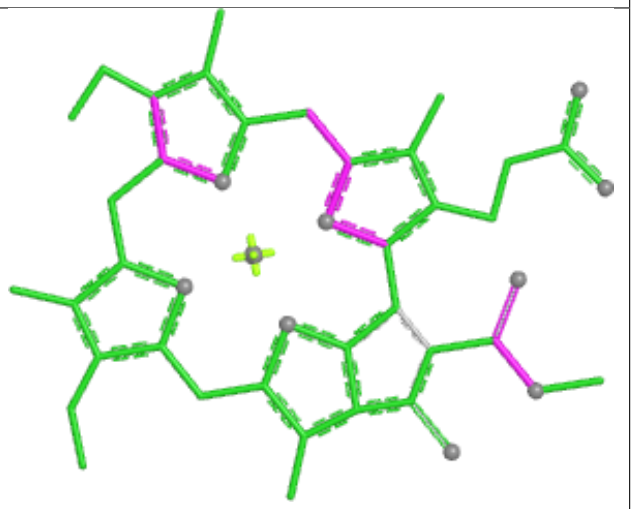


Rings

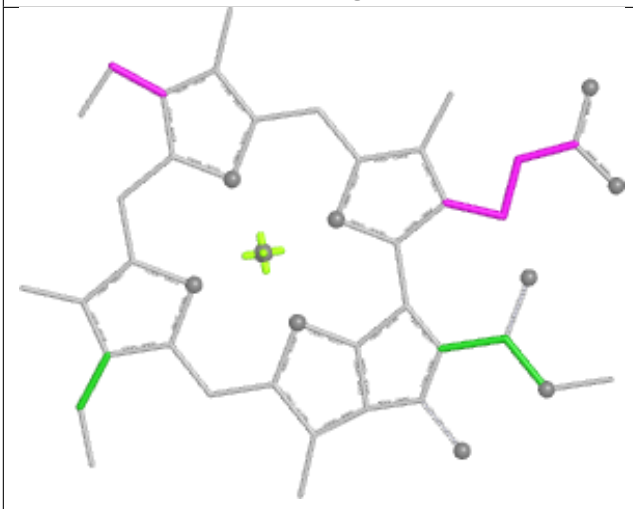
Ligand CLA B 823



Bond lengths



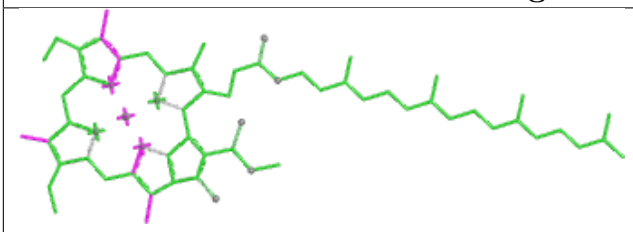
Bond angles



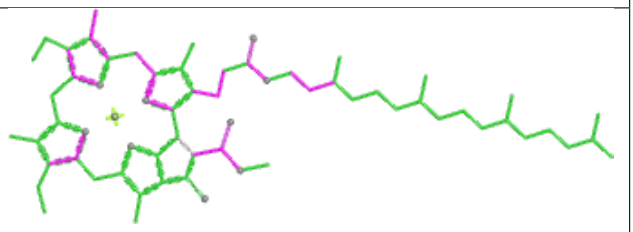
Torsions

Rings

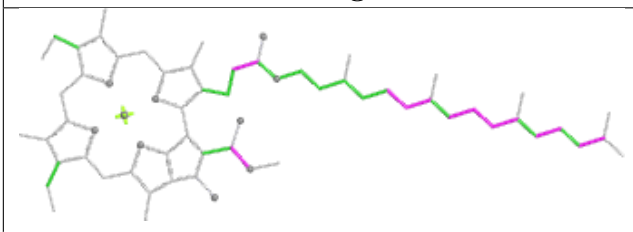
Ligand CLA 2 804



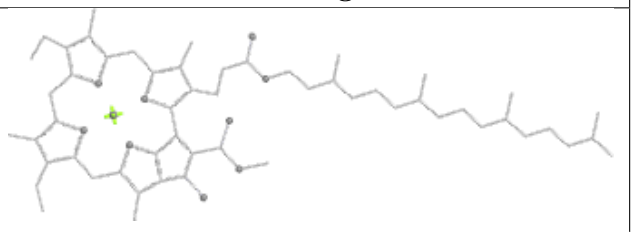
Bond lengths



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.

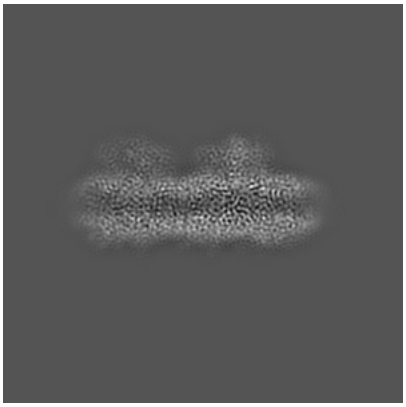
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20963. These allow visual inspection of the internal detail of the map and identification of artifacts.

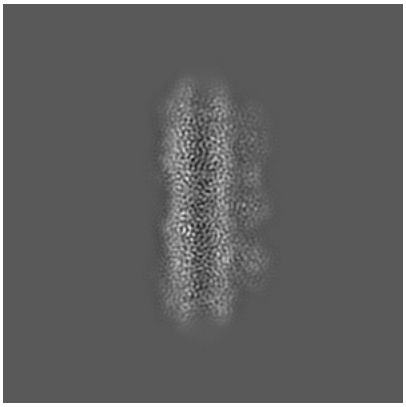
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

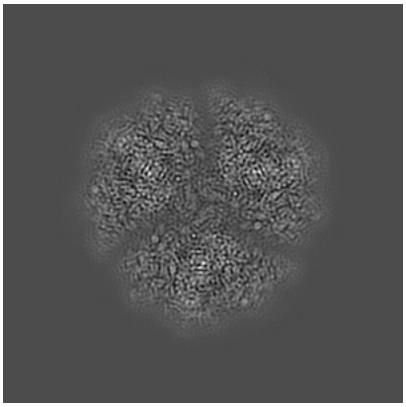
6.1.1 Primary map



X



Y



Z

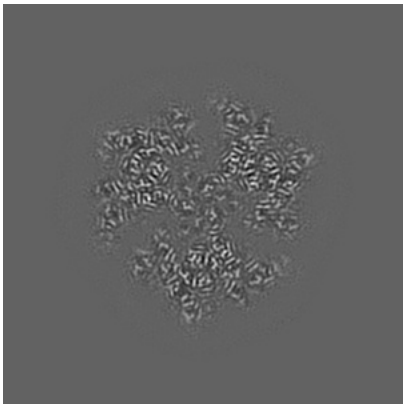
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 155

Y Index: 155



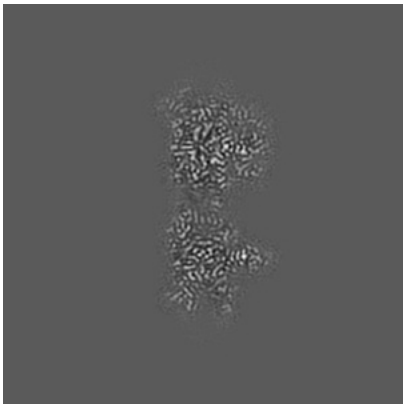
Z Index: 155

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

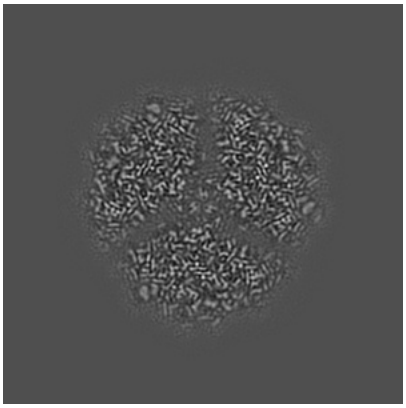
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 113



Y Index: 179

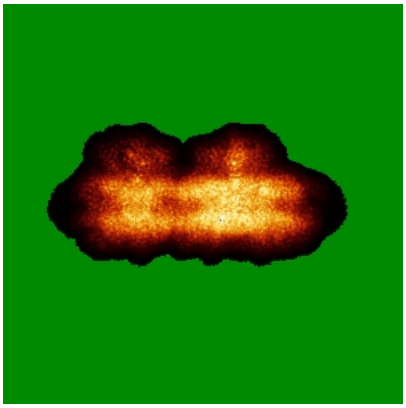


Z Index: 143

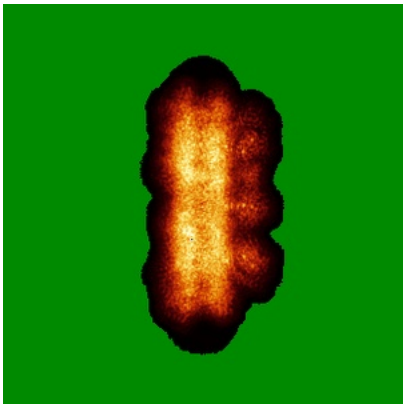
The images above show the largest variance slices of the map in three orthogonal directions.

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

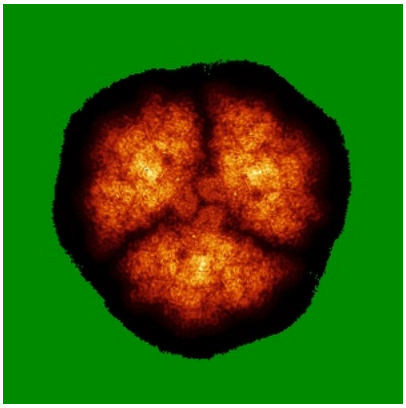
6.4.1 Primary map



X



Y

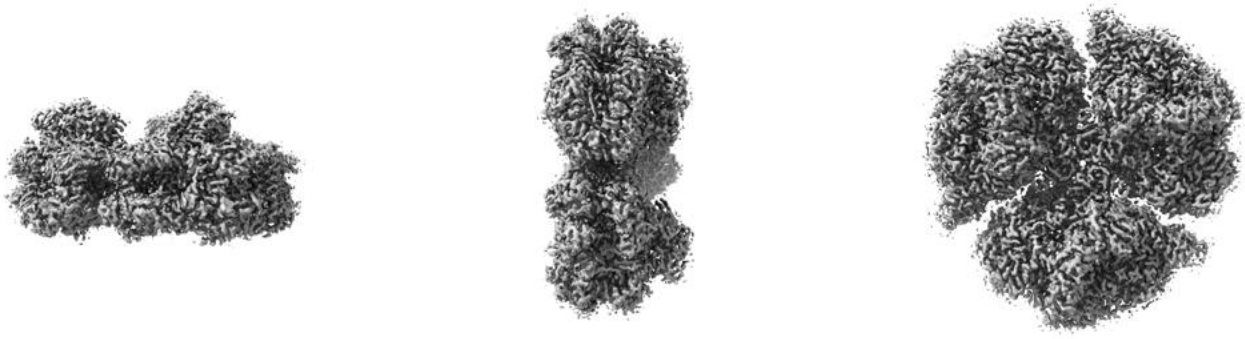


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

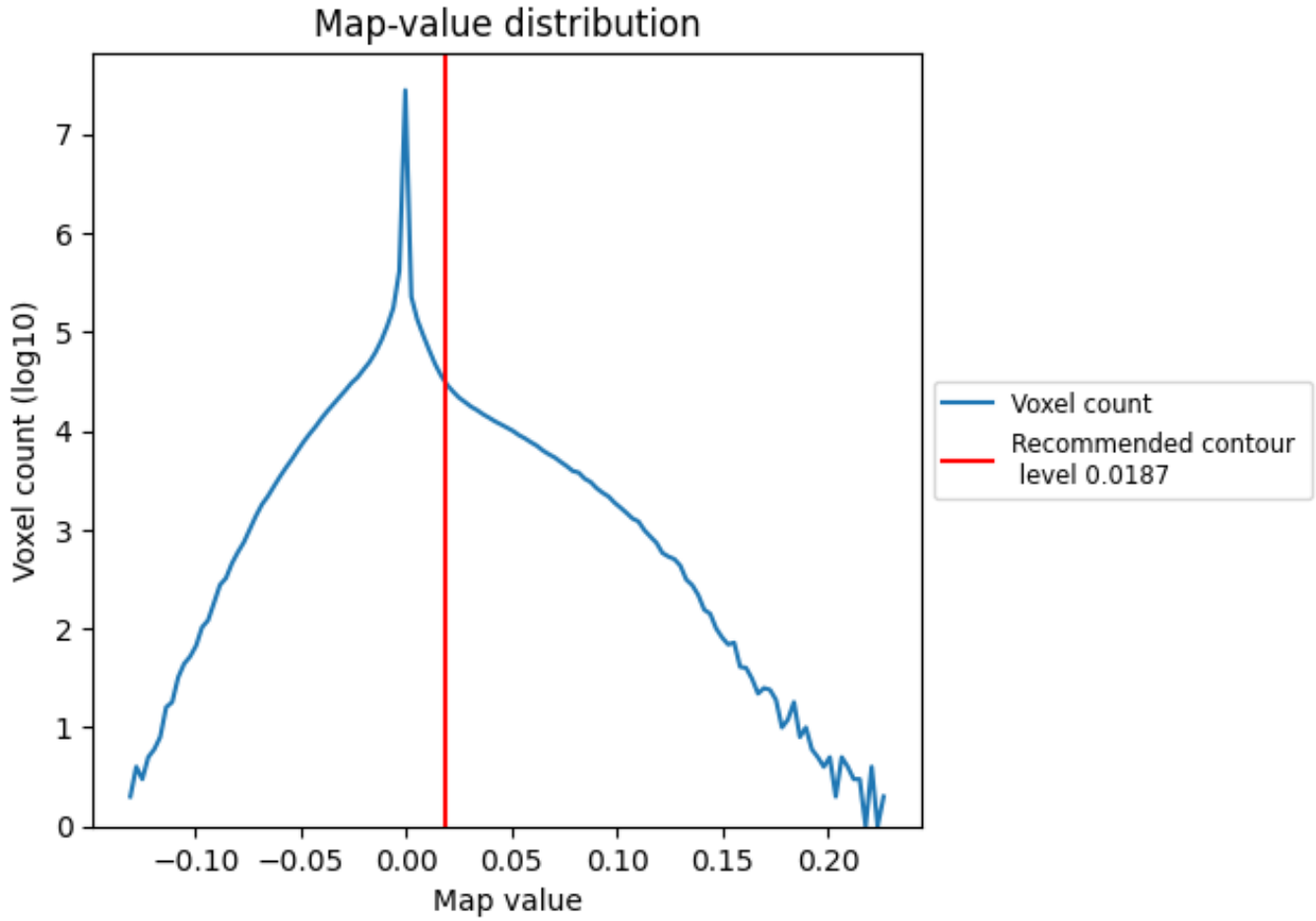
6.6 Mask visualisation (i)

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

7 Map analysis

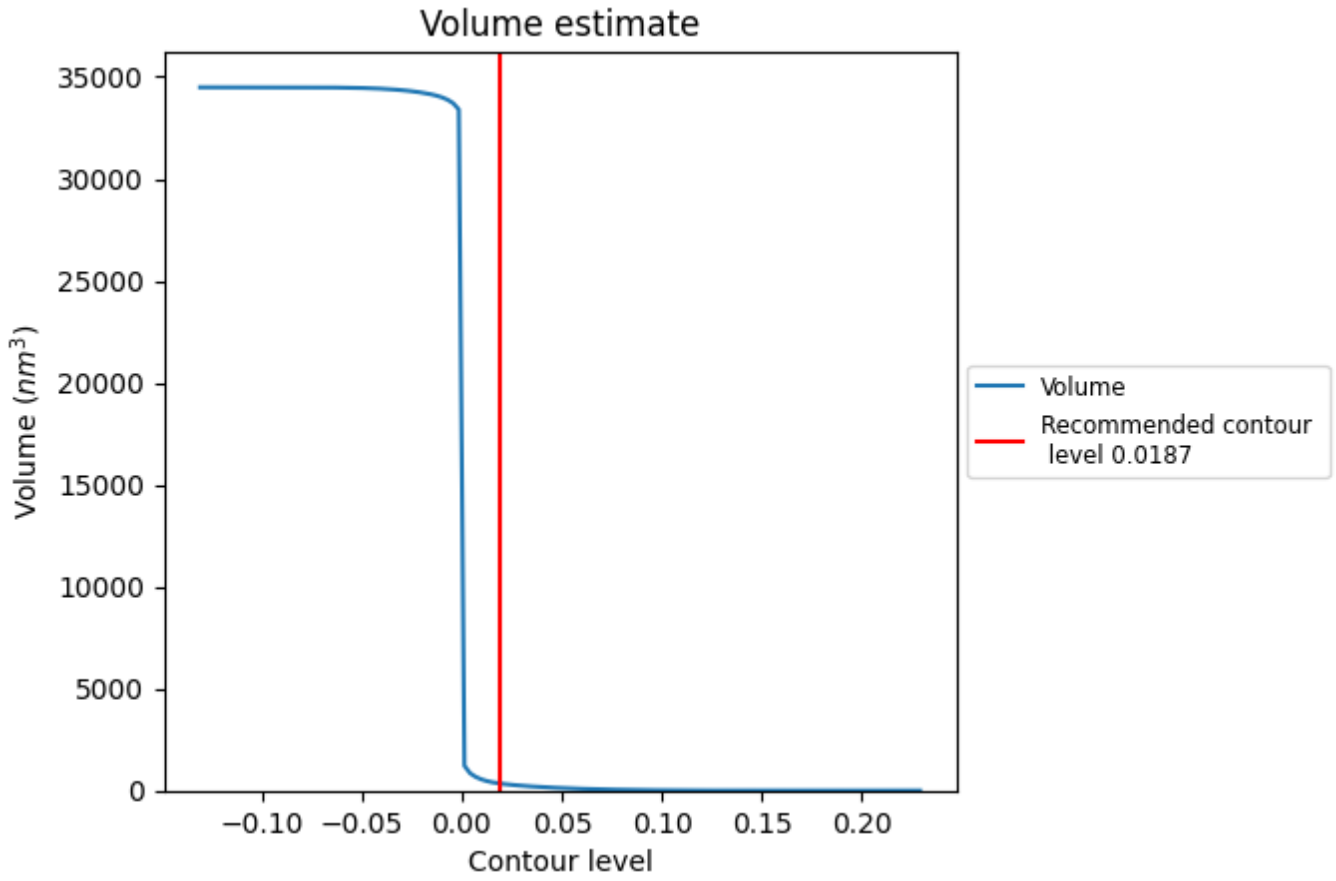
This section contains the results of statistical analysis of the map.

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.

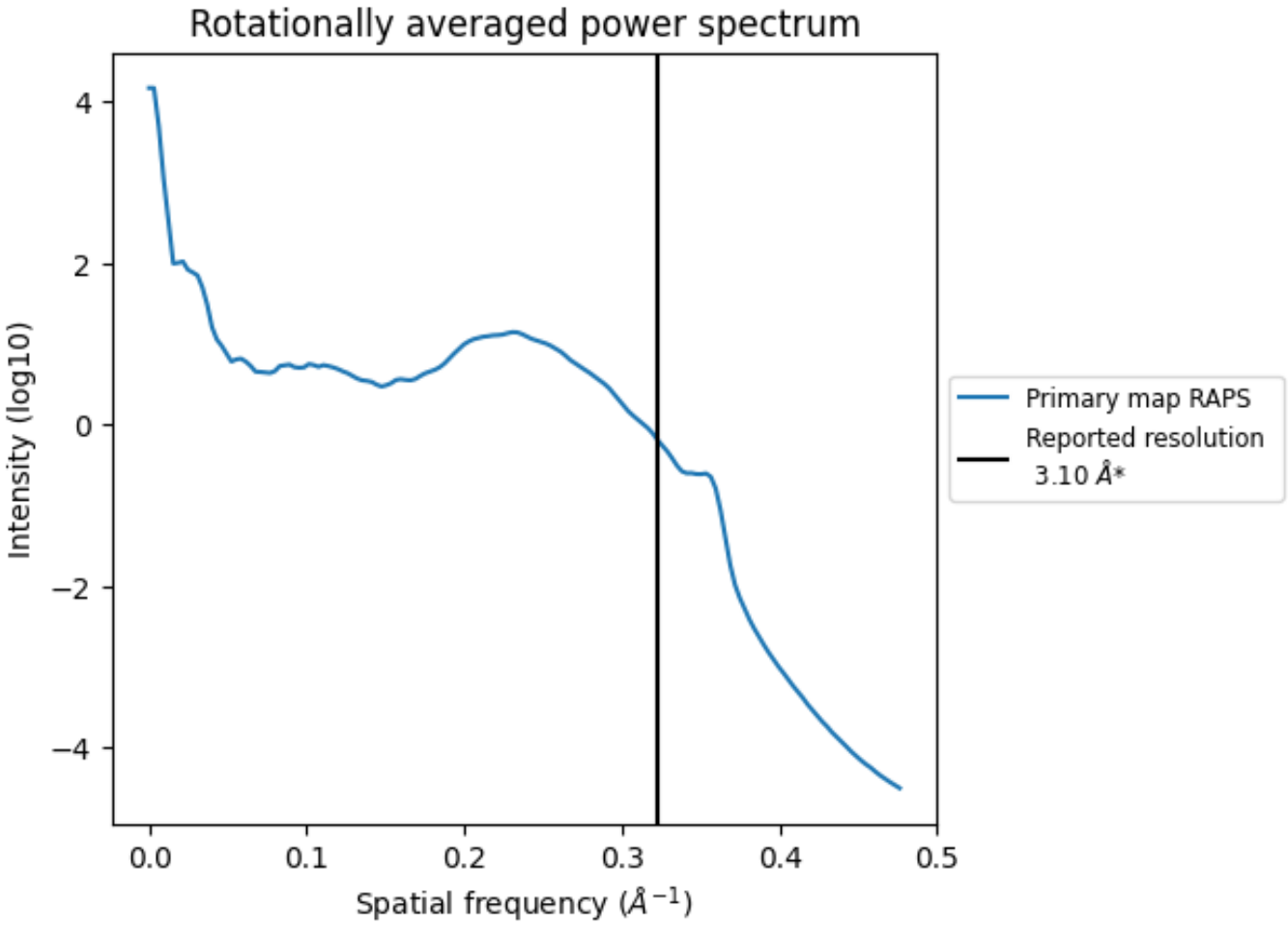
7.2 Volume estimate



The volume at the recommended contour level is 351 nm^3; this corresponds to an approximate mass of 317 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 0.323 Å^{-1}

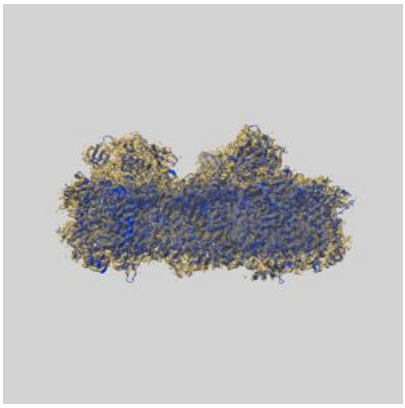
8 Fourier-Shell correlation

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

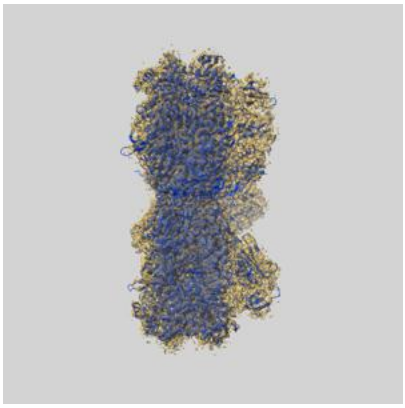
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20963 and PDB model 6UZV. Per-residue inclusion information can be found in section 3 on page 38.

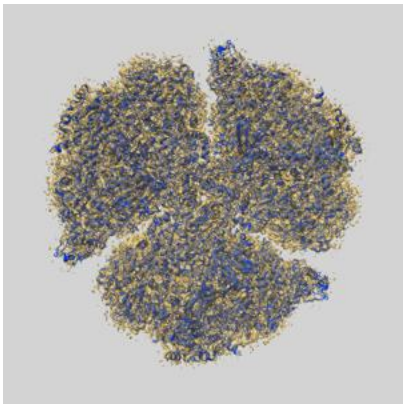
9.1 Map-model overlay



X



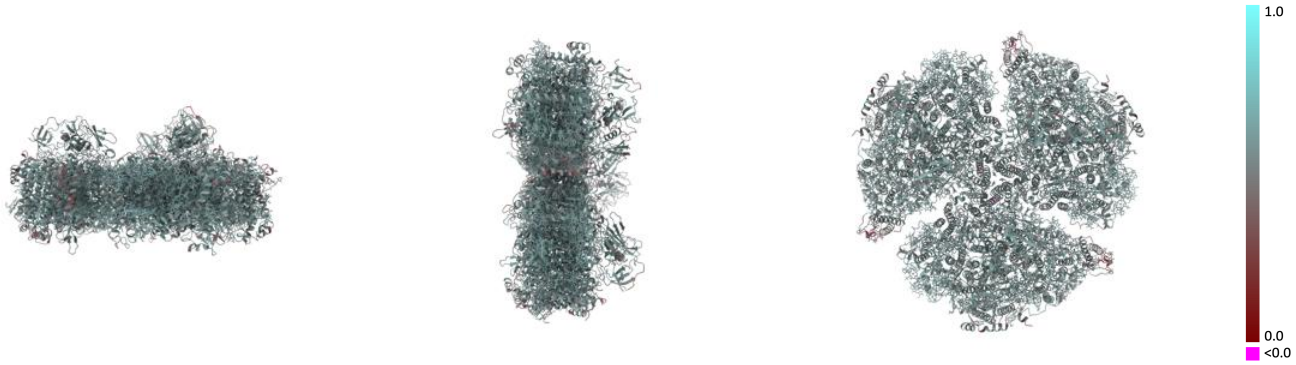
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

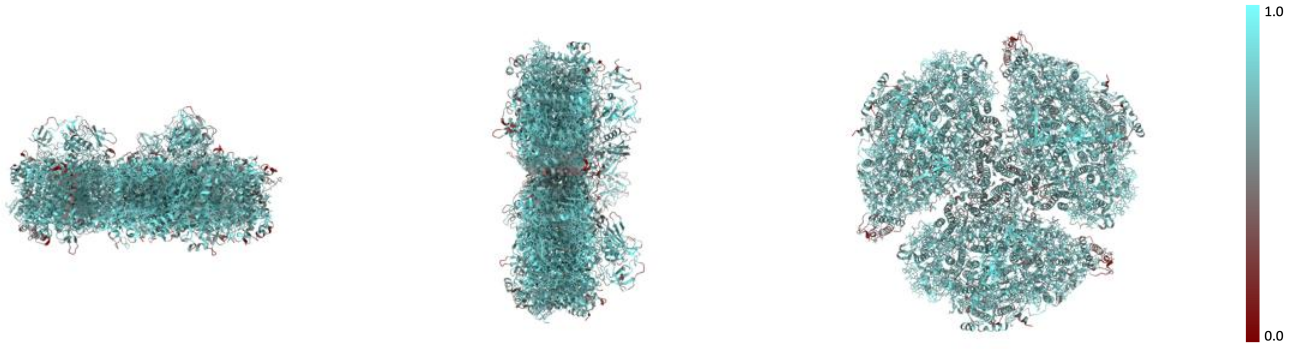
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

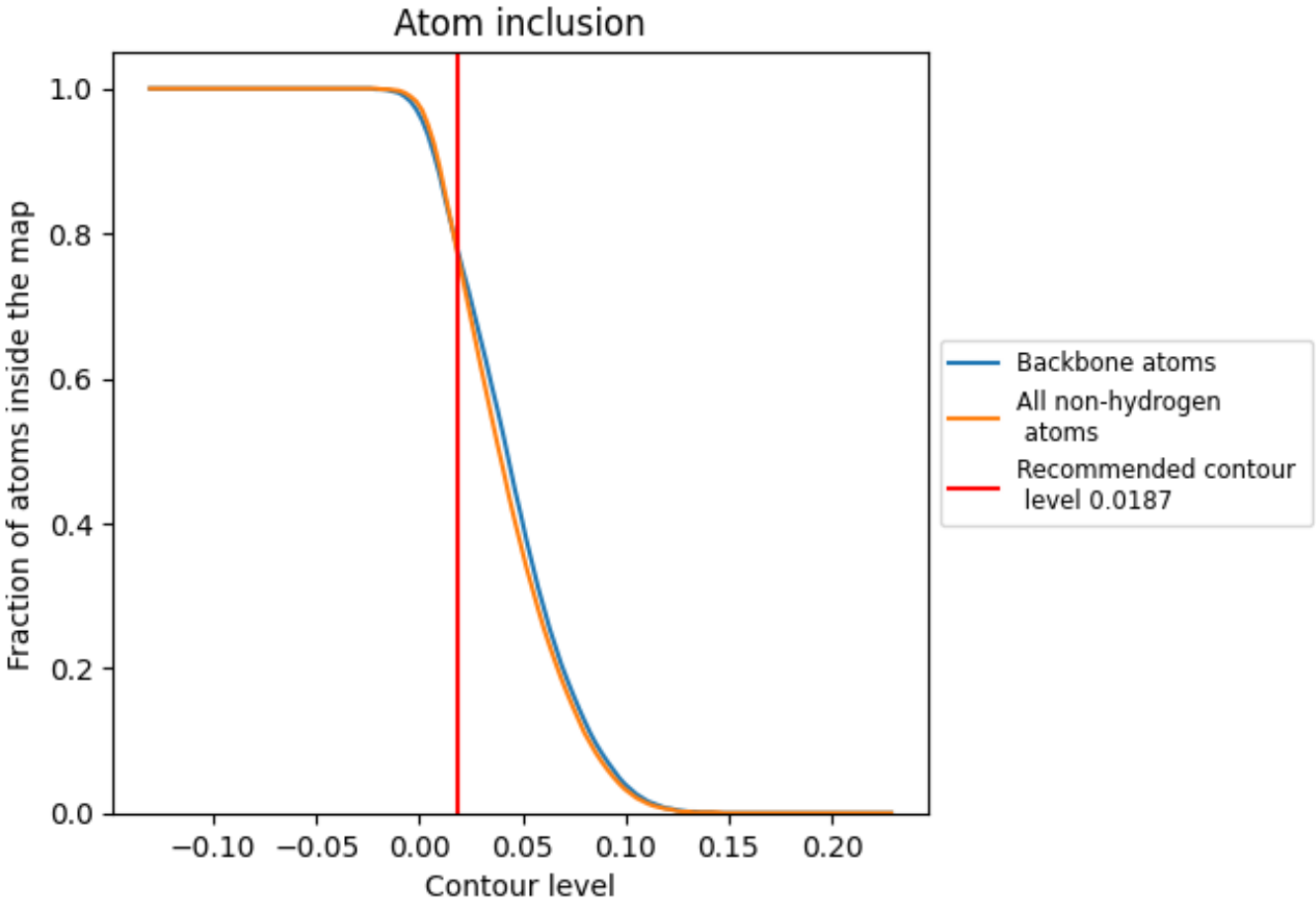
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0187).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.0187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.5660
0	0.7080	0.5640
1	0.8110	0.5790
2	0.8170	0.5800
3	0.8340	0.5710
4	0.6650	0.5280
5	0.6550	0.5010
6	0.6370	0.5200
7	0.6540	0.5280
8	0.5150	0.4620
9	0.6180	0.5450
A	0.8030	0.5800
B	0.8120	0.5820
C	0.8340	0.5710
D	0.6460	0.5280
E	0.6380	0.5110
F	0.6510	0.5260
I	0.7450	0.5690
J	0.6320	0.5210
K	0.5010	0.4640
L	0.7020	0.5600
M	0.6240	0.5470
a	0.8060	0.5790
b	0.8200	0.5820
c	0.8340	0.5710
d	0.6520	0.5240
e	0.6420	0.5020
f	0.6420	0.5220
h	0.7480	0.5690
i	0.7450	0.5670
j	0.6450	0.5260
k	0.4900	0.4500
l	0.7160	0.5640
m	0.6170	0.5450